



Full wwPDB NMR Structure Validation Report ⓘ

Mar 7, 2026 – 02:19 AM UTC

PDB ID : 2LGX / pdb_00002lgx
BMRB ID : 17827
Title : NMR structure for Kindle-2 N-terminus
Authors : Perera, H.D.; Ma, Y.; Yang, J.; Hirbawi, J.; Plow, E.F.; Qin, J.
Deposited on : 2011-08-03

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

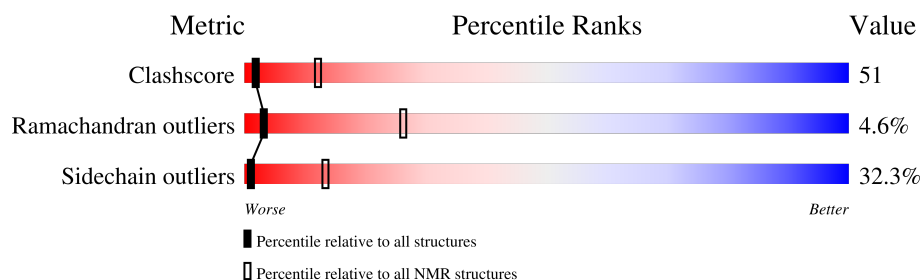
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 78%.

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	112	

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:18-A:51, A:61-A:94 (68)	0.34	9

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1529 atoms, of which 763 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Fermitin family homolog 2.

Mol	Chain	Residues	Atoms						Trace
1	A	94	Total	C	H	N	O	S	0
			1529	493	763	132	137	4	

There are 8 discrepancies between the modelled and reference sequences:

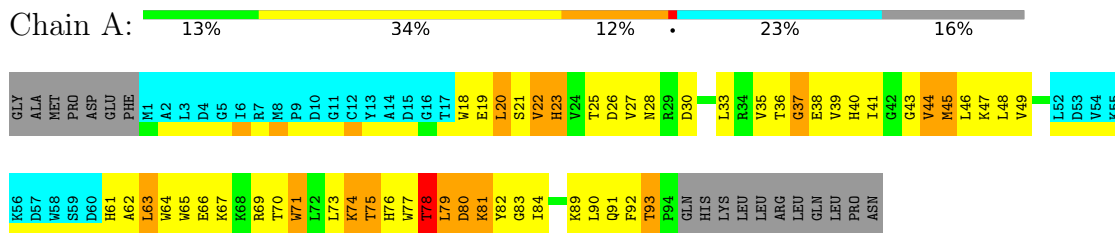
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP Q96AC1
A	-5	ALA	-	expression tag	UNP Q96AC1
A	-4	MET	-	expression tag	UNP Q96AC1
A	-3	PRO	-	expression tag	UNP Q96AC1
A	-2	ASP	-	expression tag	UNP Q96AC1
A	-1	GLU	-	expression tag	UNP Q96AC1
A	0	PHE	-	expression tag	UNP Q96AC1
A	27	VAL	LEU	conflict	UNP Q96AC1

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: Fermitin family homolog 2

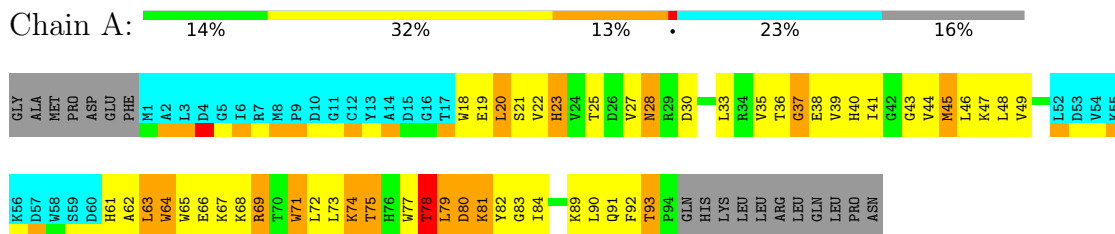


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Fermitin family homolog 2



4.2.2 Score per residue for model 2

- Molecule 1: Fermitin family homolog 2





4.2.3 Score per residue for model 3

- Molecule 1: Fermitin family homolog 2

Chain A: 19% 31% 10% 23% 16%



4.2.4 Score per residue for model 4

- Molecule 1: Fermitin family homolog 2

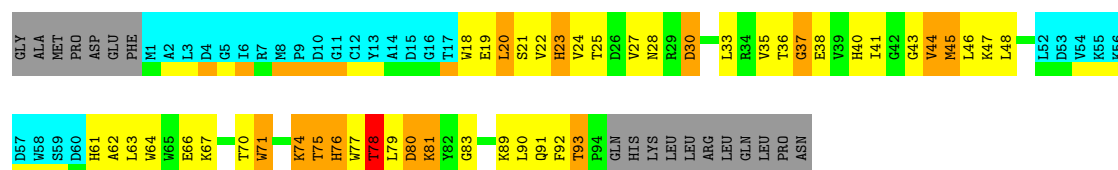
Chain A: 20% 29% 11% 23% 16%



4.2.5 Score per residue for model 5

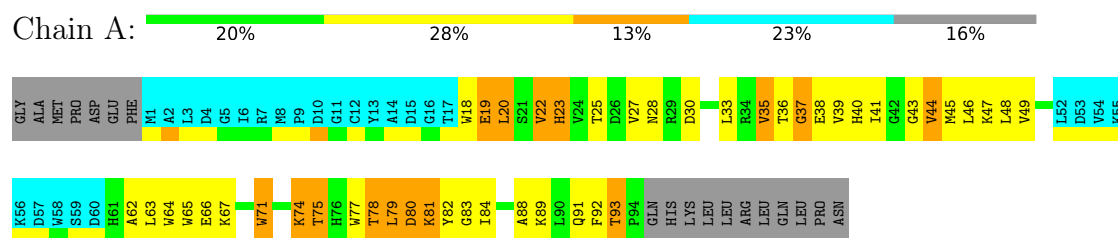
- Molecule 1: Fermitin family homolog 2

Chain A: 20% 29% 12% 23% 16%



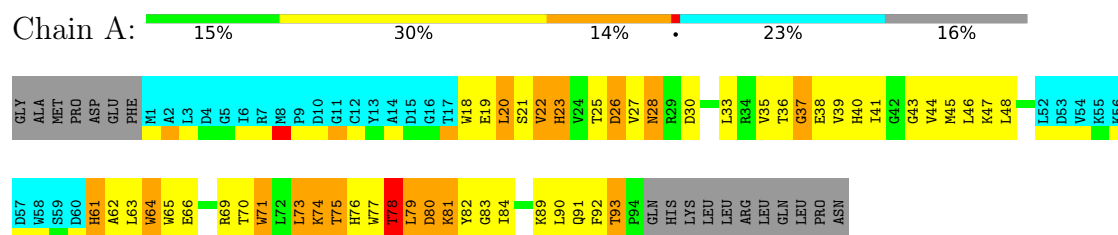
4.2.6 Score per residue for model 6

- Molecule 1: Fermitin family homolog 2



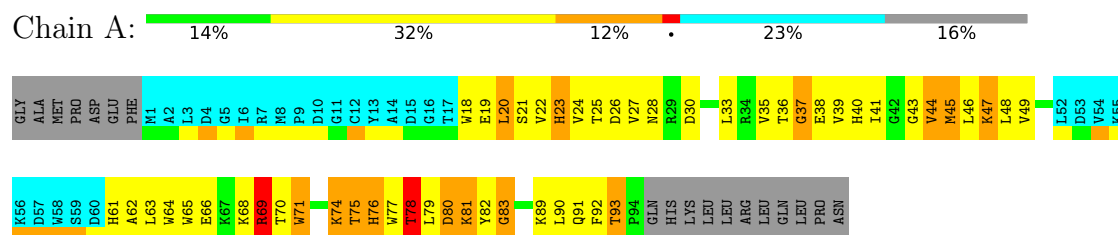
4.2.7 Score per residue for model 7

- Molecule 1: Fermitin family homolog 2



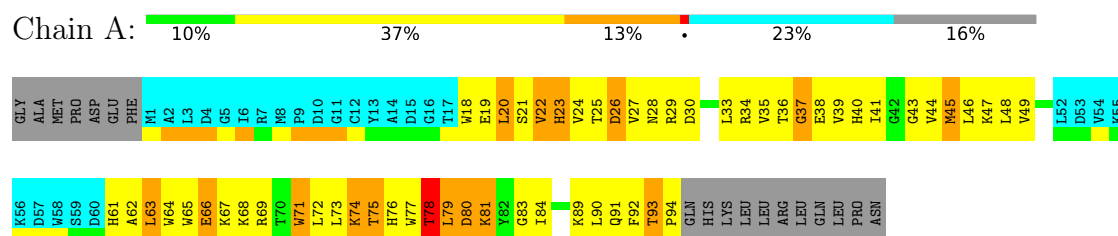
4.2.8 Score per residue for model 8

- Molecule 1: Fermitin family homolog 2



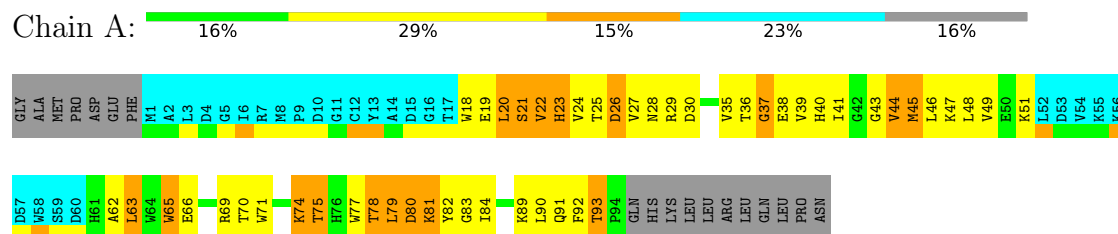
4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Fermitin family homolog 2



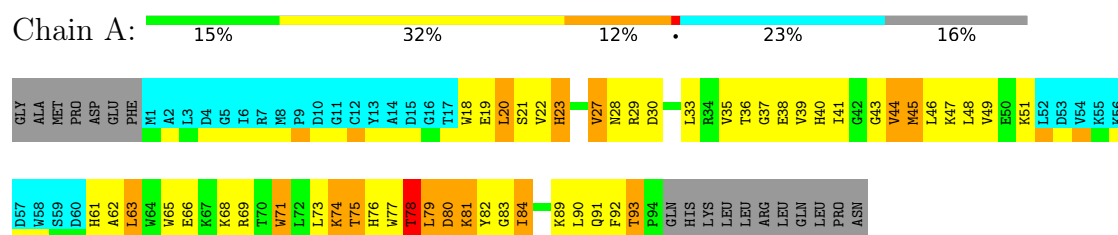
4.2.10 Score per residue for model 10

- Molecule 1: Fermitin family homolog 2



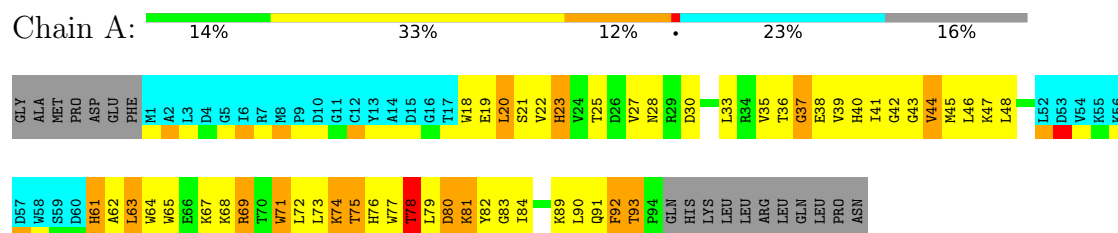
4.2.11 Score per residue for model 11

- Molecule 1: Fermitin family homolog 2



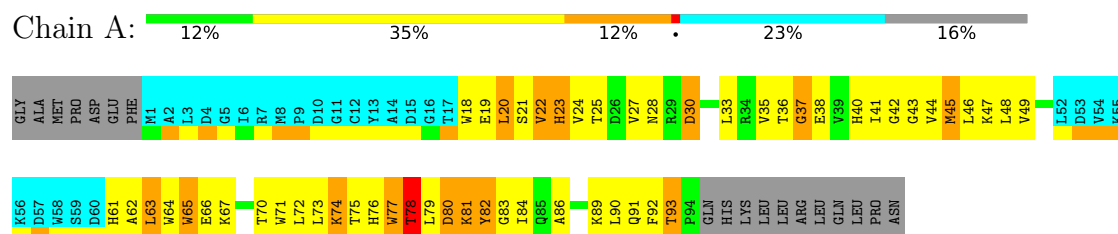
4.2.12 Score per residue for model 12

- Molecule 1: Fermitin family homolog 2



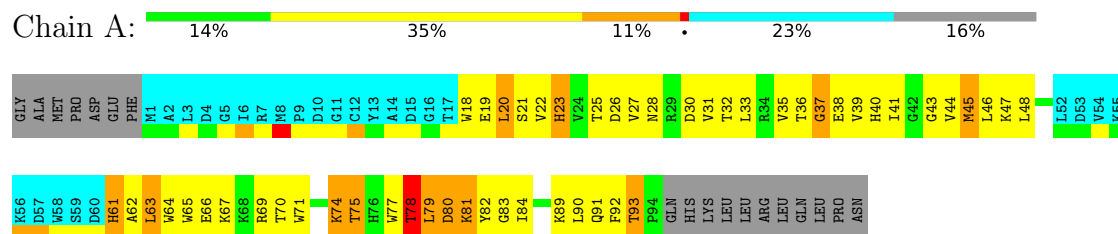
4.2.13 Score per residue for model 13

- Molecule 1: Fermitin family homolog 2



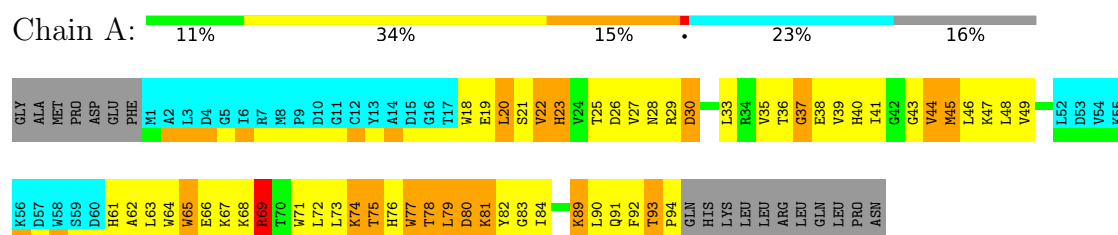
4.2.14 Score per residue for model 14

- Molecule 1: Fermitin family homolog 2



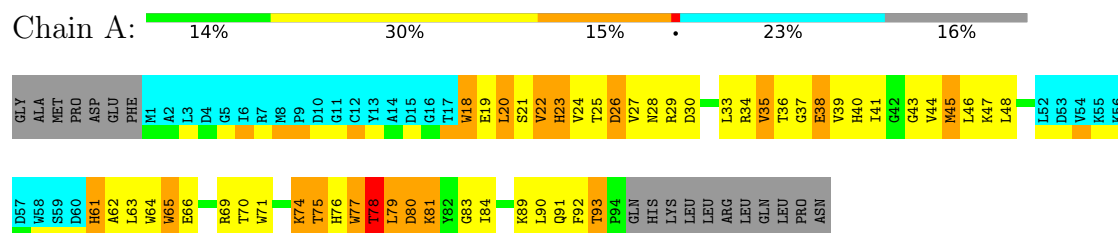
4.2.15 Score per residue for model 15

- Molecule 1: Fermitin family homolog 2



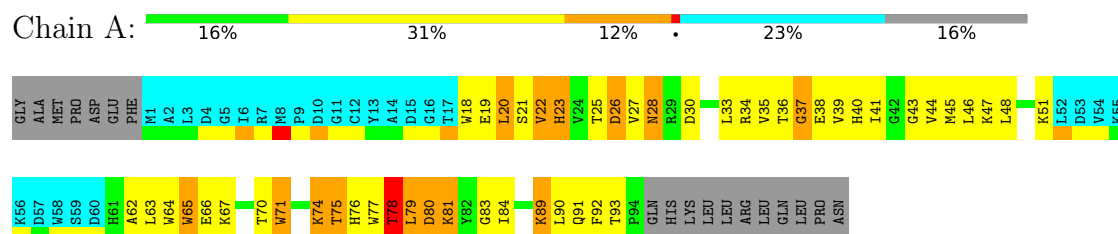
4.2.16 Score per residue for model 16

- Molecule 1: Fermitin family homolog 2



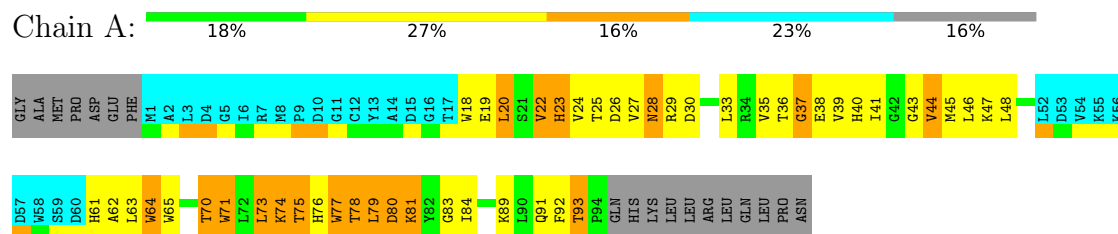
4.2.17 Score per residue for model 17

- Molecule 1: Fermitin family homolog 2



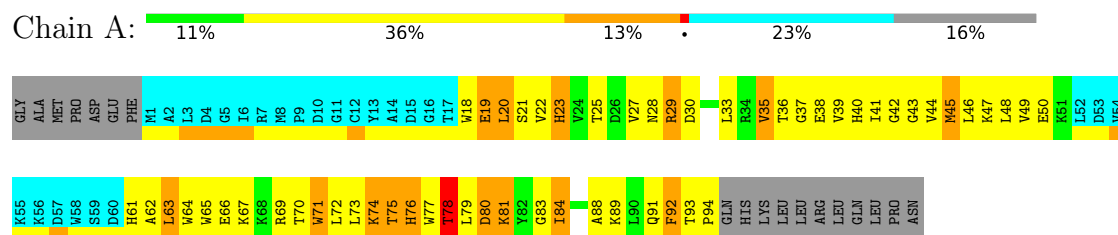
4.2.18 Score per residue for model 18

- Molecule 1: Fermitin family homolog 2



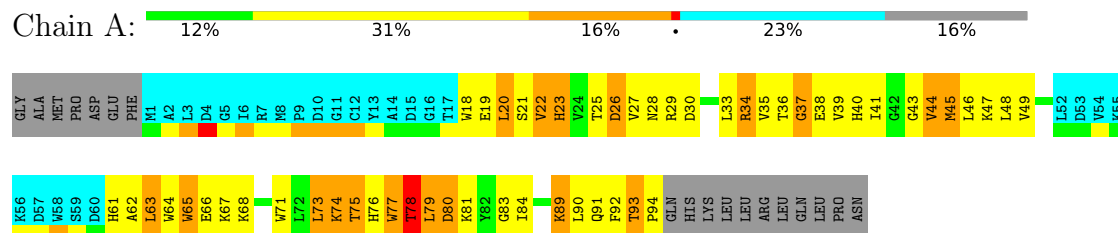
4.2.19 Score per residue for model 19

- Molecule 1: Fermitin family homolog 2



4.2.20 Score per residue for model 20

- Molecule 1: Fermitin family homolog 2



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	
TALOS	geometry optimization	
X-PLOR NIH	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	1088
Number of shifts mapped to atoms	1004
Number of unparsed shifts	0
Number of shifts with mapping errors	84
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.49±0.01	0±0/584 (0.0± 0.0%)	1.27±0.01	0±0/794 (0.0± 0.0%)
All	All	1.49	1/11680 (0.0%)	1.27	3/15880 (0.0%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	92	PHE	C-N	-5.61	1.26	1.33	19	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	42	GLY	N-CA-C	-6.57	107.17	115.31	13	2
1	A	83	GLY	N-CA-C	-5.37	107.12	115.67	8	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	568	578	578	58±6
All	All	11360	11560	11560	1165

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 51.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:HIS:O	1:A:92:PHE:N	0.90	2.05	14	20
1:A:79:LEU:HD22	1:A:79:LEU:H	0.87	1.29	11	4
1:A:41:ILE:HD11	1:A:77:TRP:O	0.83	1.74	6	20
1:A:41:ILE:HD12	1:A:74:LYS:O	0.82	1.75	17	20
1:A:45:MET:O	1:A:49:VAL:HG23	0.81	1.76	9	9
1:A:79:LEU:HD12	1:A:79:LEU:H	0.77	1.39	10	9
1:A:79:LEU:HD12	1:A:79:LEU:N	0.76	1.95	15	9
1:A:63:LEU:HD22	1:A:63:LEU:N	0.74	1.97	3	20
1:A:73:LEU:HD22	1:A:73:LEU:N	0.74	1.98	15	7
1:A:18:TRP:CZ3	1:A:20:LEU:HD23	0.70	2.20	16	18
1:A:18:TRP:CZ2	1:A:37:GLY:N	0.68	2.61	17	20
1:A:71:TRP:CD1	1:A:71:TRP:N	0.66	2.64	17	7
1:A:65:TRP:CD1	1:A:70:THR:H	0.64	2.10	18	1
1:A:70:THR:HG23	1:A:71:TRP:N	0.64	2.07	18	2
1:A:66:GLU:N	1:A:91:GLN:NE2	0.63	2.46	10	7
1:A:71:TRP:N	1:A:71:TRP:CD1	0.63	2.66	18	1
1:A:66:GLU:N	1:A:91:GLN:HE21	0.63	1.92	10	7
1:A:79:LEU:H	1:A:79:LEU:CD2	0.63	2.07	2	6
1:A:71:TRP:H	1:A:71:TRP:CD1	0.62	2.09	19	1
1:A:79:LEU:H	1:A:79:LEU:HD23	0.62	1.54	13	2
1:A:39:VAL:CG1	1:A:79:LEU:HD21	0.62	2.25	17	6
1:A:36:THR:C	1:A:38:GLU:H	0.62	2.03	9	20
1:A:45:MET:SD	1:A:61:HIS:CE1	0.61	2.93	16	1
1:A:65:TRP:NE1	1:A:70:THR:HG22	0.61	2.10	18	1
1:A:19:GLU:O	1:A:20:LEU:HD22	0.61	1.95	4	13
1:A:66:GLU:H	1:A:91:GLN:NE2	0.61	1.93	2	1
1:A:25:THR:HG23	1:A:26:ASP:N	0.61	2.11	16	1
1:A:45:MET:SD	1:A:61:HIS:NE2	0.61	2.74	11	2
1:A:76:HIS:O	1:A:78:THR:N	0.61	2.34	15	4
1:A:62:ALA:N	1:A:93:THR:O	0.60	2.35	19	17
1:A:79:LEU:HD23	1:A:79:LEU:N	0.60	2.11	13	2
1:A:79:LEU:H	1:A:79:LEU:CD1	0.60	2.03	6	9
1:A:79:LEU:N	1:A:79:LEU:HD13	0.60	2.12	2	4
1:A:18:TRP:CH2	1:A:36:THR:C	0.59	2.80	13	19
1:A:36:THR:O	1:A:38:GLU:N	0.59	2.35	7	20
1:A:92:PHE:CD1	1:A:93:THR:N	0.58	2.71	10	3
1:A:80:ASP:O	1:A:83:GLY:N	0.57	2.37	18	20
1:A:73:LEU:N	1:A:73:LEU:CD2	0.57	2.68	15	7
1:A:40:HIS:O	1:A:43:GLY:N	0.56	2.38	6	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:HIS:H	1:A:91:GLN:HA	0.56	1.61	19	20
1:A:62:ALA:O	1:A:93:THR:N	0.56	2.38	19	19
1:A:19:GLU:H	1:A:19:GLU:CD	0.56	2.09	13	4
1:A:63:LEU:N	1:A:63:LEU:CD2	0.56	2.69	14	20
1:A:40:HIS:O	1:A:44:VAL:N	0.56	2.39	1	19
1:A:79:LEU:CD1	1:A:79:LEU:N	0.56	2.69	4	4
1:A:19:GLU:N	1:A:19:GLU:CD	0.56	2.64	2	15
1:A:74:LYS:N	1:A:74:LYS:CE	0.56	2.69	9	17
1:A:19:GLU:CD	1:A:19:GLU:N	0.55	2.64	13	4
1:A:19:GLU:CD	1:A:19:GLU:H	0.55	2.08	11	15
1:A:61:HIS:HD1	1:A:61:HIS:C	0.55	2.09	7	2
1:A:61:HIS:CG	1:A:92:PHE:CZ	0.55	2.93	8	2
1:A:65:TRP:CD1	1:A:65:TRP:O	0.55	2.59	18	2
1:A:66:GLU:N	1:A:91:GLN:OE1	0.55	2.40	11	7
1:A:65:TRP:CZ3	1:A:89:LYS:O	0.55	2.60	2	4
1:A:21:SER:O	1:A:90:LEU:N	0.54	2.40	10	16
1:A:19:GLU:N	1:A:19:GLU:OE1	0.54	2.41	17	12
1:A:65:TRP:O	1:A:69:ARG:N	0.54	2.40	16	7
1:A:61:HIS:CD2	1:A:92:PHE:CZ	0.54	2.95	9	2
1:A:40:HIS:ND1	1:A:75:THR:OG1	0.54	2.39	16	6
1:A:64:TRP:CZ3	1:A:71:TRP:CH2	0.54	2.96	17	2
1:A:25:THR:C	1:A:27:VAL:H	0.54	2.11	9	18
1:A:18:TRP:CH2	1:A:37:GLY:N	0.53	2.76	7	16
1:A:75:THR:O	1:A:77:TRP:N	0.53	2.42	4	9
1:A:40:HIS:CD2	1:A:75:THR:OG1	0.53	2.62	7	5
1:A:64:TRP:O	1:A:91:GLN:NE2	0.53	2.41	18	4
1:A:66:GLU:O	1:A:69:ARG:NH1	0.53	2.41	10	2
1:A:40:HIS:CG	1:A:75:THR:OG1	0.53	2.62	16	18
1:A:35:VAL:HG21	1:A:39:VAL:HG11	0.53	1.80	8	6
1:A:75:THR:HG23	1:A:76:HIS:N	0.53	2.19	13	1
1:A:61:HIS:CD2	1:A:92:PHE:CE2	0.52	2.96	8	1
1:A:65:TRP:CE3	1:A:89:LYS:O	0.52	2.63	20	2
1:A:92:PHE:CD1	1:A:92:PHE:C	0.52	2.88	10	2
1:A:69:ARG:N	1:A:69:ARG:CD	0.52	2.72	4	2
1:A:36:THR:C	1:A:38:GLU:N	0.52	2.68	3	20
1:A:68:LYS:O	1:A:69:ARG:C	0.52	2.52	15	5
1:A:74:LYS:H	1:A:74:LYS:CE	0.52	2.18	10	3
1:A:66:GLU:H	1:A:91:GLN:HE21	0.51	1.46	2	1
1:A:41:ILE:O	1:A:45:MET:SD	0.51	2.68	19	1
1:A:41:ILE:C	1:A:43:GLY:H	0.51	2.14	19	20
1:A:61:HIS:C	1:A:61:HIS:ND1	0.51	2.69	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:ILE:C	1:A:43:GLY:N	0.51	2.68	4	20
1:A:76:HIS:ND1	1:A:76:HIS:O	0.51	2.44	4	2
1:A:41:ILE:CD1	1:A:77:TRP:O	0.51	2.58	8	8
1:A:79:LEU:N	1:A:79:LEU:HD12	0.50	2.21	12	4
1:A:72:LEU:C	1:A:73:LEU:HD22	0.50	2.31	1	6
1:A:71:TRP:CD2	1:A:71:TRP:N	0.50	2.79	8	2
1:A:37:GLY:HA2	1:A:79:LEU:HD13	0.50	1.84	6	8
1:A:74:LYS:CE	1:A:74:LYS:H	0.50	2.20	17	17
1:A:64:TRP:CE3	1:A:91:GLN:OE1	0.50	2.64	14	1
1:A:78:THR:OG1	1:A:81:LYS:CE	0.50	2.60	9	15
1:A:74:LYS:CE	1:A:74:LYS:N	0.50	2.75	10	3
1:A:18:TRP:CH2	1:A:79:LEU:HD11	0.50	2.42	13	2
1:A:30:ASP:N	1:A:30:ASP:OD1	0.49	2.46	5	1
1:A:65:TRP:C	1:A:91:GLN:HE21	0.49	2.15	14	1
1:A:25:THR:O	1:A:27:VAL:N	0.49	2.46	9	3
1:A:66:GLU:O	1:A:67:LYS:C	0.49	2.53	20	7
1:A:66:GLU:O	1:A:69:ARG:CZ	0.49	2.61	19	1
1:A:77:TRP:HE1	1:A:82:TYR:CA	0.49	2.21	13	1
1:A:48:LEU:HD21	1:A:92:PHE:CE2	0.49	2.43	12	2
1:A:79:LEU:N	1:A:79:LEU:CD1	0.49	2.75	7	6
1:A:67:LYS:O	1:A:69:ARG:NH1	0.49	2.46	14	1
1:A:27:VAL:O	1:A:28:ASN:CB	0.48	2.60	11	20
1:A:20:LEU:CD2	1:A:88:ALA:O	0.48	2.61	6	2
1:A:75:THR:CG2	1:A:76:HIS:N	0.48	2.76	13	1
1:A:77:TRP:O	1:A:78:THR:O	0.48	2.31	8	10
1:A:25:THR:OG1	1:A:26:ASP:N	0.48	2.46	9	1
1:A:64:TRP:C	1:A:91:GLN:HE21	0.48	2.15	17	1
1:A:20:LEU:HD23	1:A:21:SER:H	0.48	1.68	19	1
1:A:33:LEU:HD21	1:A:48:LEU:HB2	0.48	1.84	18	18
1:A:64:TRP:O	1:A:91:GLN:CG	0.48	2.61	13	8
1:A:71:TRP:N	1:A:71:TRP:CD2	0.48	2.81	1	1
1:A:18:TRP:O	1:A:35:VAL:O	0.48	2.32	4	19
1:A:75:THR:O	1:A:76:HIS:C	0.47	2.57	18	5
1:A:70:THR:CG2	1:A:71:TRP:N	0.47	2.76	18	1
1:A:42:GLY:O	1:A:46:LEU:CD1	0.47	2.63	19	1
1:A:80:ASP:O	1:A:81:LYS:C	0.47	2.57	18	16
1:A:75:THR:C	1:A:77:TRP:N	0.47	2.72	5	11
1:A:18:TRP:CE3	1:A:35:VAL:O	0.47	2.67	19	1
1:A:46:LEU:O	1:A:47:LYS:C	0.47	2.58	5	20
1:A:25:THR:CG2	1:A:26:ASP:N	0.47	2.77	16	1
1:A:71:TRP:CD1	1:A:71:TRP:H	0.47	2.24	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:HIS:N	1:A:91:GLN:HA	0.46	2.25	15	15
1:A:77:TRP:O	1:A:78:THR:C	0.46	2.58	19	16
1:A:48:LEU:CD2	1:A:92:PHE:CE2	0.46	2.98	1	3
1:A:39:VAL:O	1:A:78:THR:HG22	0.46	2.11	15	2
1:A:45:MET:CB	1:A:61:HIS:NE2	0.46	2.79	11	4
1:A:79:LEU:HD22	1:A:79:LEU:N	0.46	2.10	20	3
1:A:65:TRP:CD1	1:A:67:LYS:H	0.45	2.30	19	5
1:A:27:VAL:CG1	1:A:29:ARG:NE	0.45	2.79	2	5
1:A:18:TRP:HB2	1:A:86:ALA:HB2	0.45	1.87	3	2
1:A:64:TRP:O	1:A:91:GLN:CB	0.45	2.65	18	4
1:A:64:TRP:CH2	1:A:71:TRP:CH2	0.45	3.04	9	3
1:A:78:THR:O	1:A:79:LEU:C	0.45	2.59	6	5
1:A:70:THR:C	1:A:71:TRP:CD1	0.45	2.95	7	1
1:A:22:VAL:CG1	1:A:23:HIS:N	0.45	2.79	18	13
1:A:34:ARG:H	1:A:34:ARG:CD	0.45	2.25	20	1
1:A:79:LEU:N	1:A:79:LEU:CD2	0.45	2.75	13	3
1:A:64:TRP:CD1	1:A:70:THR:O	0.44	2.70	17	2
1:A:65:TRP:CZ2	1:A:84:ILE:CG1	0.44	2.99	19	1
1:A:61:HIS:CD2	1:A:61:HIS:C	0.44	2.95	9	1
1:A:26:ASP:N	1:A:26:ASP:OD1	0.44	2.50	10	3
1:A:26:ASP:O	1:A:26:ASP:CG	0.44	2.60	15	1
1:A:93:THR:OG1	1:A:94:PRO:CD	0.44	2.65	15	1
1:A:76:HIS:CD2	1:A:76:HIS:O	0.44	2.70	5	1
1:A:25:THR:OG1	1:A:93:THR:OG1	0.44	2.35	15	1
1:A:61:HIS:ND1	1:A:61:HIS:C	0.44	2.74	16	2
1:A:66:GLU:CA	1:A:91:GLN:NE2	0.44	2.81	19	2
1:A:25:THR:C	1:A:27:VAL:N	0.44	2.76	8	11
1:A:71:TRP:N	1:A:71:TRP:CE3	0.44	2.86	1	2
1:A:20:LEU:HD21	1:A:88:ALA:O	0.44	2.13	19	1
1:A:40:HIS:C	1:A:43:GLY:H	0.43	2.20	12	8
1:A:93:THR:O	1:A:94:PRO:O	0.43	2.36	9	2
1:A:38:GLU:O	1:A:38:GLU:OE1	0.43	2.36	10	2
1:A:38:GLU:CD	1:A:38:GLU:C	0.43	2.86	8	16
1:A:38:GLU:C	1:A:38:GLU:OE1	0.43	2.62	13	4
1:A:30:ASP:OD1	1:A:30:ASP:N	0.43	2.51	15	1
1:A:45:MET:SD	1:A:61:HIS:CD2	0.43	3.12	11	1
1:A:27:VAL:HG12	1:A:29:ARG:NE	0.43	2.28	2	4
1:A:26:ASP:O	1:A:26:ASP:OD1	0.43	2.36	16	1
1:A:82:TYR:O	1:A:82:TYR:CD1	0.43	2.71	4	1
1:A:71:TRP:HB2	1:A:73:LEU:HD21	0.43	1.91	11	1
1:A:64:TRP:O	1:A:91:GLN:HB2	0.43	2.12	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:TRP:C	1:A:91:GLN:NE2	0.43	2.76	17	1
1:A:39:VAL:HG13	1:A:79:LEU:HD21	0.43	1.91	20	4
1:A:66:GLU:OE1	1:A:66:GLU:C	0.43	2.62	4	1
1:A:31:VAL:HG12	1:A:32:THR:N	0.43	2.29	14	1
1:A:38:GLU:C	1:A:38:GLU:CD	0.43	2.87	13	3
1:A:25:THR:C	1:A:26:ASP:CG	0.42	2.87	17	3
1:A:46:LEU:O	1:A:50:GLU:N	0.42	2.39	19	1
1:A:70:THR:OG1	1:A:71:TRP:CE3	0.42	2.67	8	1
1:A:38:GLU:OE1	1:A:38:GLU:O	0.42	2.37	14	2
1:A:66:GLU:CA	1:A:91:GLN:OE1	0.42	2.67	5	1
1:A:80:ASP:OD1	1:A:80:ASP:C	0.42	2.63	14	1
1:A:46:LEU:C	1:A:48:LEU:N	0.42	2.76	15	9
1:A:19:GLU:CG	1:A:20:LEU:N	0.42	2.81	5	1
1:A:65:TRP:CH2	1:A:84:ILE:HD11	0.42	2.49	11	1
1:A:65:TRP:CZ2	1:A:84:ILE:HD11	0.42	2.50	19	1
1:A:38:GLU:OE1	1:A:38:GLU:C	0.42	2.62	19	2
1:A:74:LYS:H	1:A:74:LYS:HE2	0.42	1.75	14	7
1:A:48:LEU:O	1:A:49:VAL:C	0.42	2.63	9	3
1:A:65:TRP:HD1	1:A:70:THR:H	0.42	1.56	18	1
1:A:65:TRP:C	1:A:91:GLN:NE2	0.42	2.78	14	1
1:A:63:LEU:HD22	1:A:63:LEU:H	0.42	1.74	15	1
1:A:18:TRP:CZ2	1:A:36:THR:C	0.42	2.98	19	1
1:A:79:LEU:CD2	1:A:79:LEU:N	0.41	2.80	11	1
1:A:93:THR:O	1:A:94:PRO:C	0.41	2.63	19	1
1:A:25:THR:HG23	1:A:26:ASP:H	0.41	1.74	16	1
1:A:68:LYS:O	1:A:70:THR:N	0.41	2.54	8	1
1:A:39:VAL:CG1	1:A:79:LEU:HD11	0.41	2.46	9	1
1:A:39:VAL:O	1:A:78:THR:CG2	0.41	2.69	19	1
1:A:34:ARG:H	1:A:34:ARG:HD3	0.41	1.76	20	1
1:A:23:HIS:CE1	1:A:30:ASP:OD1	0.41	2.74	13	1
1:A:40:HIS:O	1:A:41:ILE:C	0.41	2.63	19	1
1:A:73:LEU:HD23	1:A:73:LEU:N	0.40	2.32	7	2
1:A:39:VAL:CG1	1:A:79:LEU:HD22	0.40	2.46	12	1
1:A:73:LEU:N	1:A:73:LEU:HD23	0.40	2.32	20	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	67/112 (60%)	55±1 (83±2%)	9±1 (13±1%)	3±1 (5±1%)	3	26
All	All	1340/2240 (60%)	1107 (83%)	172 (13%)	61 (5%)	3	26

All 8 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	37	GLY	17
1	A	78	THR	16
1	A	76	HIS	12
1	A	26	ASP	5
1	A	35	VAL	4
1	A	77	TRP	4
1	A	69	ARG	2
1	A	18	TRP	1

6.3.2 Protein sidechains ⓘ

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	61/98 (62%)	41±2 (68±4%)	20±2 (32±4%)	1	13
All	All	1220/1960 (62%)	826 (68%)	394 (32%)	1	13

All 39 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	20	LEU	20
1	A	22	VAL	20
1	A	23	HIS	20
1	A	30	ASP	20
1	A	45	MET	20
1	A	74	LYS	20
1	A	78	THR	20
1	A	80	ASP	20

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Mol	Chain	Res	Type	Models (Total)
1	A	81	LYS	20
1	A	89	LYS	20
1	A	75	THR	19
1	A	71	TRP	18
1	A	93	THR	18
1	A	84	ILE	17
1	A	79	LEU	13
1	A	44	VAL	13
1	A	63	LEU	11
1	A	82	TYR	11
1	A	64	TRP	9
1	A	65	TRP	8
1	A	70	THR	8
1	A	24	VAL	8
1	A	28	ASN	5
1	A	61	HIS	5
1	A	69	ARG	4
1	A	26	ASP	4
1	A	34	ARG	4
1	A	68	LYS	3
1	A	73	LEU	3
1	A	29	ARG	3
1	A	19	GLU	2
1	A	47	LYS	1
1	A	66	GLU	1
1	A	21	SER	1
1	A	27	VAL	1
1	A	92	PHE	1
1	A	25	THR	1
1	A	38	GLU	1
1	A	77	TRP	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 76% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1088
Number of shifts mapped to atoms	1004
Number of unparsed shifts	0
Number of shifts with mapping errors	84
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 84 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	96	HIS	HA	4.358	0.03	1
1	A	96	HIS	HB2	2.984	0.03	1
1	A	96	HIS	C	174.808	0.50	1
1	A	96	HIS	CA	56.595	0.50	1
1	A	96	HIS	CB	29.646	0.50	1
1	A	97	LYS	H	7.985	0.03	1
1	A	97	LYS	C	176.22	0.50	1
1	A	97	LYS	CA	56.386	0.50	1
1	A	97	LYS	CB	32.442	0.50	1
1	A	97	LYS	CD	28.488	0.50	1
1	A	97	LYS	CE	41.584	0.50	1
1	A	97	LYS	CG	24.241	0.50	1
1	A	97	LYS	N	120.773	0.25	1
1	A	98	LEU	H	8.062	0.03	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	98	LEU	C	176.953	0.50	1
1	A	98	LEU	CA	55.061	0.50	1
1	A	98	LEU	CB	43.761	0.50	1
1	A	98	LEU	N	122.256	0.25	1
1	A	99	LEU	H	8.013	0.03	1
1	A	99	LEU	HA	4.206	0.03	1
1	A	99	LEU	HB2	1.46	0.03	1
1	A	99	LEU	HB3	1.51	0.03	1
1	A	99	LEU	HD11	0.72	0.03	1
1	A	99	LEU	HD12	0.72	0.03	1
1	A	99	LEU	HD13	0.72	0.03	1
1	A	99	LEU	HG	1.45	0.03	1
1	A	99	LEU	C	176.94	0.50	1
1	A	99	LEU	CA	54.95	0.50	1
1	A	99	LEU	CB	42.04	0.50	1
1	A	99	LEU	CD1	23.47	0.50	1
1	A	99	LEU	CG	26.77	0.50	1
1	A	99	LEU	N	123.01	0.25	1
1	A	100	ARG	H	8.091	0.03	1
1	A	100	ARG	HA	4.205	0.03	1
1	A	100	ARG	HB2	1.65	0.03	1
1	A	100	ARG	HB3	1.723	0.03	1
1	A	100	ARG	HD2	3.065	0.03	1
1	A	100	ARG	C	175.772	0.50	1
1	A	100	ARG	CA	55.62	0.50	1
1	A	100	ARG	CB	30.1	0.50	1
1	A	100	ARG	CD	43.15	0.50	1
1	A	100	ARG	N	121.353	0.25	1
1	A	101	LEU	H	8.032	0.03	1
1	A	101	LEU	HA	4.21	0.03	1
1	A	101	LEU	HB2	1.5	0.03	1
1	A	101	LEU	HB3	1.45	0.03	1
1	A	101	LEU	HD11	0.83	0.03	1
1	A	101	LEU	HD12	0.83	0.03	1
1	A	101	LEU	HD13	0.83	0.03	1
1	A	101	LEU	HD21	0.83	0.03	1
1	A	101	LEU	HD22	0.83	0.03	1
1	A	101	LEU	HD23	0.83	0.03	1
1	A	101	LEU	HG	1.45	0.03	1
1	A	101	LEU	C	176.744	0.50	1
1	A	101	LEU	CA	55.18	0.50	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	101	LEU	CB	42.03	0.50	1
1	A	101	LEU	CD1	23.13	0.50	1
1	A	101	LEU	CD2	24.52	0.50	1
1	A	101	LEU	CG	26.74	0.50	1
1	A	101	LEU	N	122.712	0.25	1
1	A	102	GLN	H	8.21	0.03	1
1	A	102	GLN	HA	4.28	0.03	1
1	A	102	GLN	HB2	1.9	0.03	1
1	A	102	GLN	HB3	2.0	0.03	1
1	A	102	GLN	HG2	2.255	0.03	1
1	A	102	GLN	C	175.167	0.50	1
1	A	102	GLN	CA	55.31	0.50	1
1	A	102	GLN	CB	29.2	0.50	1
1	A	102	GLN	CG	33.46	0.50	1
1	A	102	GLN	N	121.063	0.25	1
1	A	103	LEU	H	8.183	0.03	1
1	A	103	LEU	HA	4.54	0.03	1
1	A	103	LEU	HB2	1.57	0.03	1
1	A	103	LEU	HD11	0.85	0.03	1
1	A	103	LEU	HD12	0.85	0.03	1
1	A	103	LEU	HD13	0.85	0.03	1
1	A	103	LEU	HD21	0.85	0.03	1
1	A	103	LEU	HD22	0.85	0.03	1
1	A	103	LEU	HD23	0.85	0.03	1
1	A	103	LEU	C	174.815	0.50	1
1	A	103	LEU	CA	52.8	0.50	1
1	A	103	LEU	CB	41.55	0.50	1
1	A	103	LEU	CD2	22.86	0.50	1
1	A	103	LEU	N	125.202	0.25	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	93	0.19 ± 0.19	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	91	0.36 ± 0.22	None needed (< 0.5 ppm)
$^{13}\text{C}'$	96	0.13 ± 0.22	None needed (< 0.5 ppm)
^{15}N	95	0.38 ± 0.31	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 78%, i.e. 781 atoms were assigned a chemical shift out of a possible 997. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	325/342 (95%)	132/139 (95%)	127/136 (93%)	66/67 (99%)
Sidechain	444/548 (81%)	291/358 (81%)	151/171 (88%)	2/19 (11%)
Aromatic	12/107 (11%)	7/55 (13%)	0/43 (0%)	5/9 (56%)
Overall	781/997 (78%)	430/552 (78%)	278/350 (79%)	73/95 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 1004 atoms were assigned a chemical shift out of a possible 1321. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	439/473 (93%)	178/193 (92%)	173/188 (92%)	88/92 (96%)
Sidechain	551/720 (77%)	359/469 (77%)	190/227 (84%)	2/24 (8%)
Aromatic	14/128 (11%)	8/65 (12%)	0/53 (0%)	6/10 (60%)
Overall	1004/1321 (76%)	545/727 (75%)	363/468 (78%)	96/126 (76%)

7.1.4 Statistically unusual chemical shifts [i](#)

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

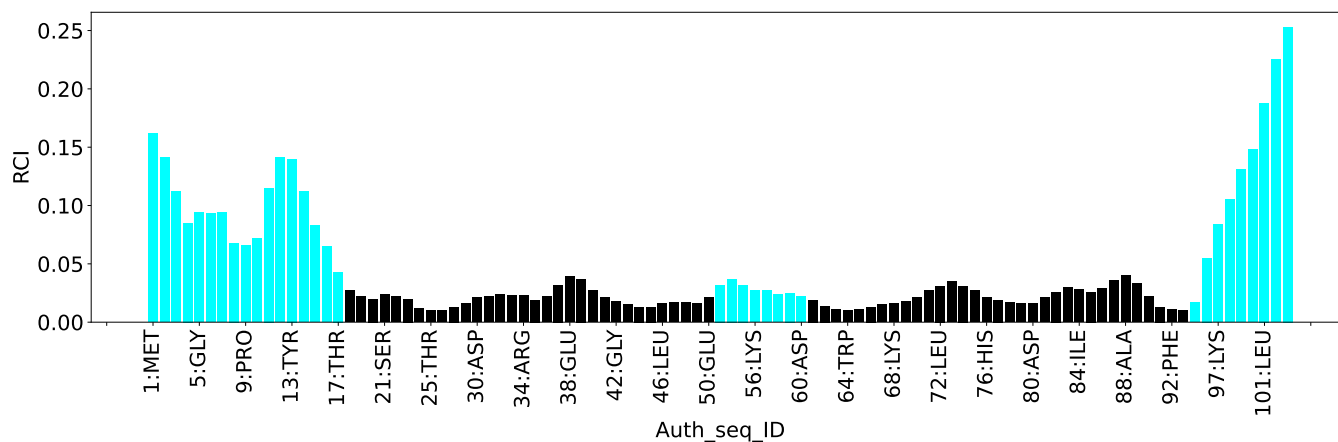
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	74	LYS	HD3	0.10	0.54 – 2.65	-7.1
1	A	41	ILE	CG2	9.20	10.93 – 24.12	-6.3
1	A	35	VAL	HG21	-0.87	-0.58 – 2.19	-6.0
1	A	35	VAL	HG22	-0.87	-0.58 – 2.19	-6.0
1	A	35	VAL	HG23	-0.87	-0.58 – 2.19	-6.0
1	A	68	LYS	HG2	-0.12	0.13 – 2.61	-6.0
1	A	68	LYS	HG3	-0.05	0.04 – 2.67	-5.3
1	A	74	LYS	HD2	0.57	0.58 – 2.64	-5.0

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication

of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



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	1459
Intra-residue ($ i-j =0$)	447
Sequential ($ i-j =1$)	436
Medium range ($ i-j >1$ and $ i-j <5$)	224
Long range ($ i-j \geq 5$)	327
Inter-chain	0
Hydrogen bond restraints	25
Disulfide bond restraints	0
Total dihedral-angle restraints	108
Number of unmapped restraints	0
Number of restraints per residue	14.0
Number of long range restraints per residue ¹	3.0

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)	150.1	0.2
0.2-0.5 (Medium)	61.0	0.49
>0.5 (Large)	1.9	0.89

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)	14.8	9.19
10.0-20.0 (Medium)	0.1	11.3
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

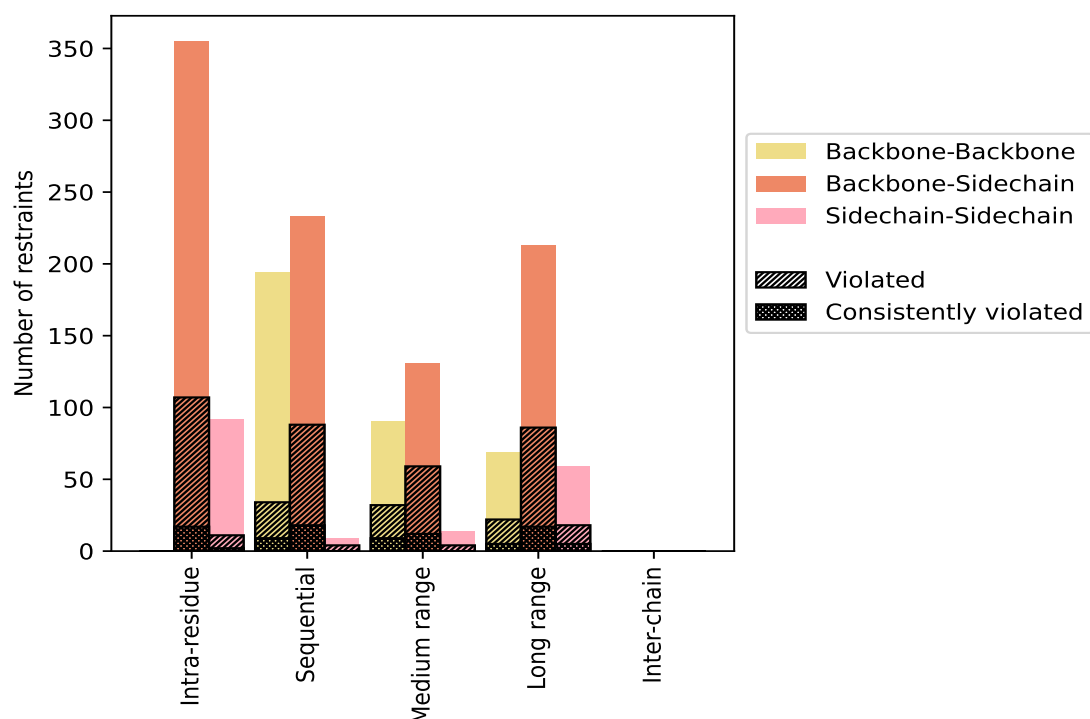
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	447	30.6	118	26.4	8.1	19	4.3	1.3
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	355	24.3	107	30.1	7.3	17	4.8	1.2
Sidechain-Sidechain	92	6.3	11	12.0	0.8	2	2.2	0.1
Sequential ($i-j =1$)	436	29.9	126	28.9	8.6	27	6.2	1.9
Backbone-Backbone	194	13.3	34	17.5	2.3	9	4.6	0.6
Backbone-Sidechain	233	16.0	88	37.8	6.0	18	7.7	1.2
Sidechain-Sidechain	9	0.6	4	44.4	0.3	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	224	15.4	92	41.1	6.3	20	8.9	1.4
Backbone-Backbone	90	6.2	32	35.6	2.2	9	10.0	0.6
Backbone-Sidechain	120	8.2	56	46.7	3.8	11	9.2	0.8
Sidechain-Sidechain	14	1.0	4	28.6	0.3	0	0.0	0.0
Long range ($i-j \geq 5$)	327	22.4	121	37.0	8.3	27	8.3	1.9
Backbone-Backbone	69	4.7	22	31.9	1.5	5	7.2	0.3
Backbone-Sidechain	199	13.6	81	40.7	5.6	17	8.5	1.2
Sidechain-Sidechain	59	4.0	18	30.5	1.2	5	8.5	0.3
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	25	1.7	8	32.0	0.5	1	4.0	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1459	100.0	465	31.9	31.9	94	6.4	6.4
Backbone-Backbone	353	24.2	88	24.9	6.0	23	6.5	1.6
Backbone-Sidechain	932	63.9	340	36.5	23.3	64	6.9	4.4
Sidechain-Sidechain	174	11.9	37	21.3	2.5	7	4.0	0.5

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	43	60	44	62	0	209	0.18	0.61	0.06	0.17
2	49	61	43	65	0	218	0.18	0.58	0.06	0.17
3	47	56	40	68	0	211	0.18	0.61	0.07	0.17
4	48	54	49	59	0	210	0.18	0.78	0.07	0.18
5	46	63	43	67	0	219	0.18	0.48	0.06	0.18
6	46	64	44	71	0	225	0.18	0.56	0.07	0.17
7	41	63	49	72	0	225	0.18	0.82	0.07	0.16
8	48	60	45	72	0	225	0.18	0.57	0.06	0.17
9	44	64	45	64	0	217	0.18	0.77	0.07	0.17
10	45	59	51	70	0	225	0.18	0.57	0.07	0.17

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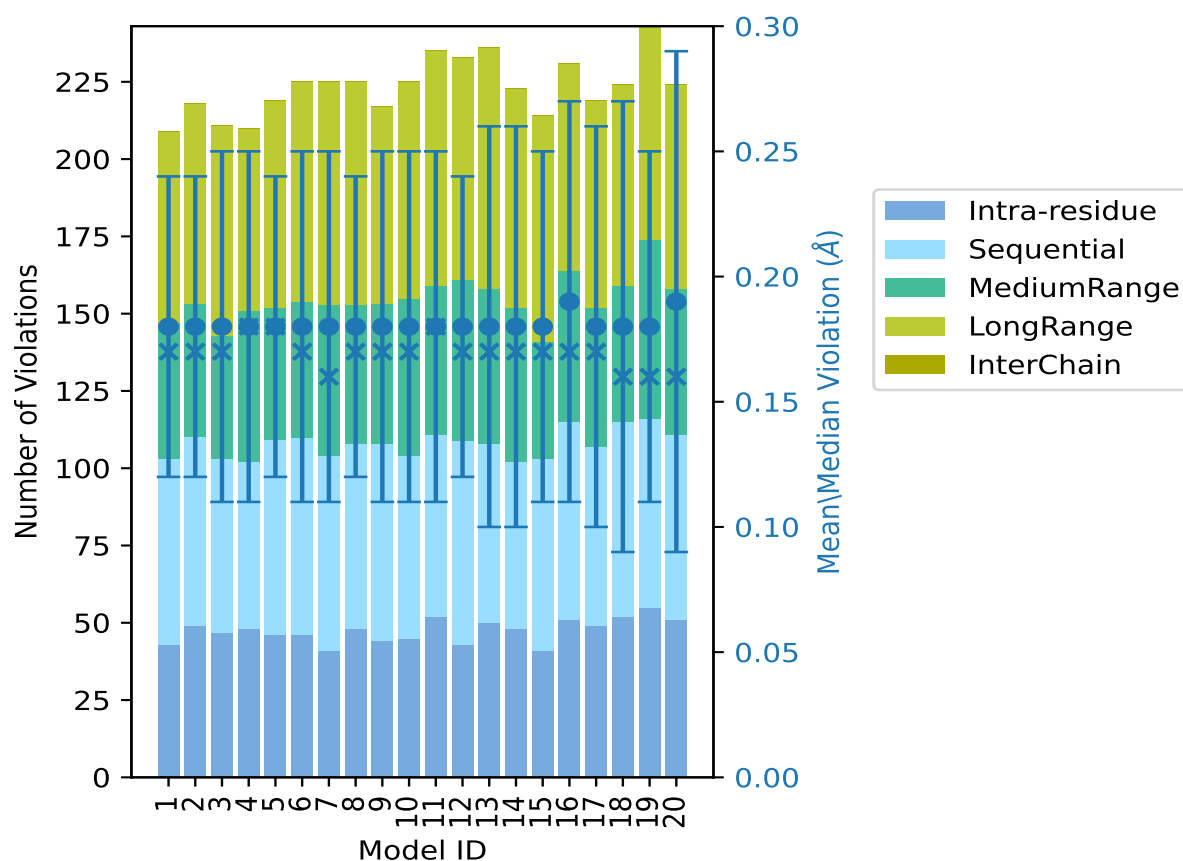
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	52	59	48	76	0	235	0.18	0.61	0.07	0.18
12	43	66	52	72	0	233	0.18	0.41	0.06	0.17
13	50	58	50	78	0	236	0.18	0.78	0.08	0.17
14	48	54	50	71	0	223	0.18	0.85	0.08	0.17
15	41	62	38	73	0	214	0.18	0.59	0.07	0.17
16	51	64	49	67	0	231	0.19	0.77	0.08	0.17
17	49	58	45	67	0	219	0.18	0.65	0.08	0.17
18	52	63	44	65	0	224	0.18	0.77	0.09	0.16
19	55	61	58	69	0	243	0.18	0.56	0.07	0.16
20	51	60	47	66	0	224	0.19	0.89	0.1	0.16

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

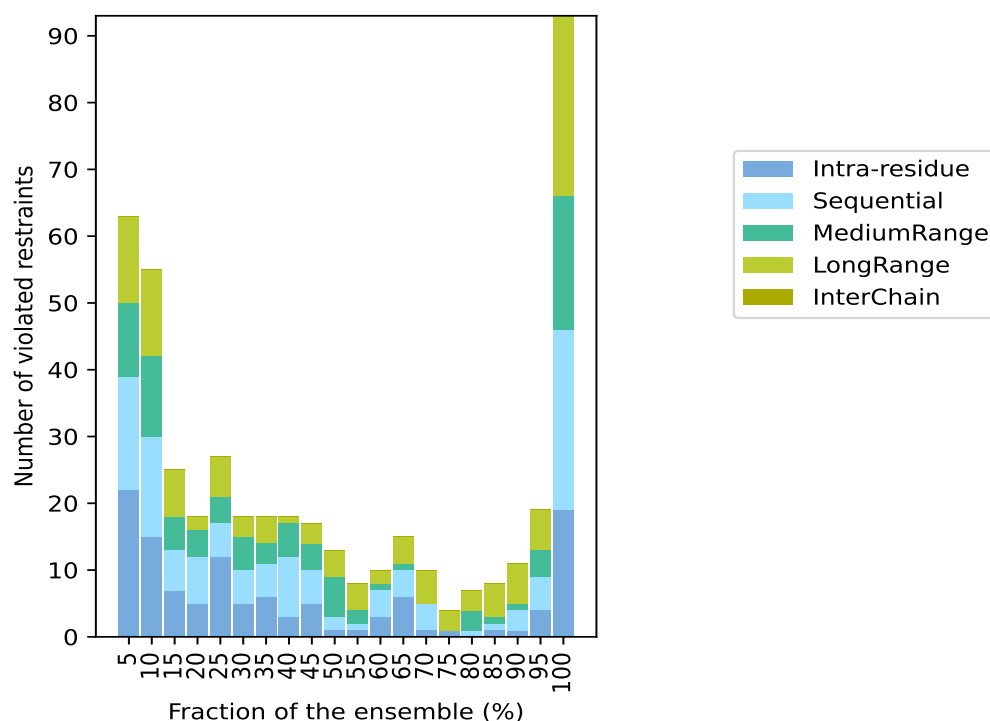
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 977(IR:329, SQ:310, MR:132, LR:206, IC:0) restraints are 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	%
22	17	11	13	0	63	1	5.0
15	15	12	13	0	55	2	10.0
7	6	5	7	0	25	3	15.0
5	7	4	2	0	18	4	20.0
12	5	4	6	0	27	5	25.0
5	5	5	3	0	18	6	30.0
6	5	3	4	0	18	7	35.0
3	9	5	1	0	18	8	40.0
5	5	4	3	0	17	9	45.0
1	2	6	4	0	13	10	50.0
1	1	2	4	0	8	11	55.0
3	4	1	2	0	10	12	60.0
6	4	1	4	0	15	13	65.0
1	4	0	5	0	10	14	70.0
1	0	0	3	0	4	15	75.0
0	1	3	3	0	7	16	80.0
1	1	1	5	0	8	17	85.0
1	3	1	6	0	11	18	90.0
4	5	4	6	0	19	19	95.0
19	27	20	27	0	93	20	100.0

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

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

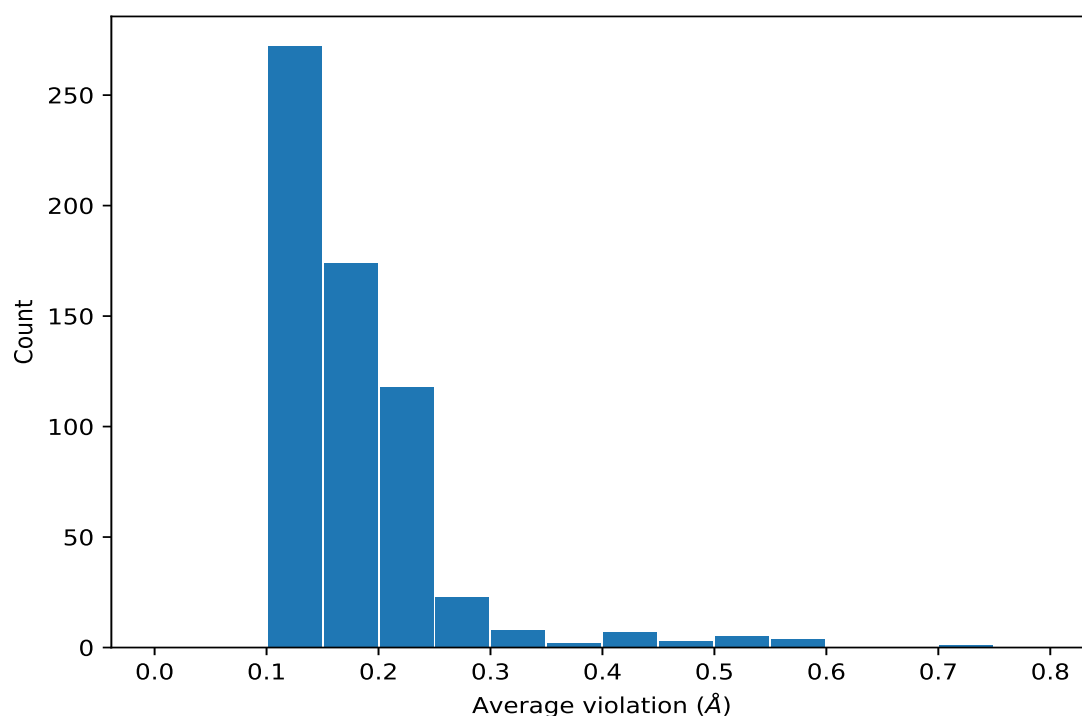
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(2,5)	1:31:A:VAL:O	1:22:A:VAL:N	20	0.29	0.01	0.28
(1,1033)	1:67:A:LYS:HA	1:67:A:LYS:HD3	20	0.27	0.05	0.26
(2,15)	1:64:A:TRP:O	1:92:A:PHE:H	20	0.26	0.03	0.26
(1,1159)	1:77:A:TRP:HB3	1:78:A:THR:H	20	0.26	0.03	0.26
(2,18)	1:23:A:HIS:O	1:93:A:THR:N	20	0.26	0.02	0.25
(1,1111)	1:74:A:LYS:HA	1:74:A:LYS:HD2	20	0.25	0.01	0.25
(1,340)	1:23:A:HIS:H	1:91:A:GLN:HA	20	0.25	0.02	0.25
(1,1328)	1:87:A:ASP:HA	1:88:A:ALA:H	20	0.25	0.01	0.25
(1,508)	1:33:A:LEU:HD21	1:48:A:LEU:H	20	0.25	0.02	0.25
(1,508)	1:33:A:LEU:HD22	1:48:A:LEU:H	20	0.25	0.02	0.25
(1,508)	1:33:A:LEU:HD23	1:48:A:LEU:H	20	0.25	0.02	0.25
(1,297)	1:22:A:VAL:H	1:31:A:VAL:H	20	0.24	0.02	0.24
(1,1076)	1:71:A:TRP:H	1:71:A:TRP:HB3	20	0.24	0.1	0.3
(1,784)	1:47:A:LYS:HG3	1:48:A:LEU:H	20	0.24	0.01	0.24
(1,266)	1:21:A:SER:H	1:22:A:VAL:H	20	0.24	0.02	0.24
(1,1162)	1:77:A:TRP:H	1:81:A:LYS:HE3	20	0.23	0.06	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,184)	1:18:A:TRP:HE1	1:80:A:ASP:HB3	20	0.23	0.05	0.22
(1,523)	1:34:A:ARG:HB3	1:35:A:VAL:H	20	0.23	0.04	0.24
(1,436)	1:28:A:ASN:HB2	1:29:A:ARG:H	20	0.23	0.02	0.22
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD11	20	0.23	0.02	0.22
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD12	20	0.23	0.02	0.22
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD13	20	0.23	0.02	0.22
(1,1341)	1:89:A:LYS:HE3	1:89:A:LYS:HB3	20	0.22	0.01	0.23
(1,433)	1:28:A:ASN:H	1:28:A:ASN:HB3	20	0.22	0.02	0.23
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG11	20	0.22	0.03	0.22
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG12	20	0.22	0.03	0.22
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG13	20	0.22	0.03	0.22
(2,4)	1:33:A:LEU:O	1:20:A:LEU:N	20	0.22	0.03	0.22
(1,1377)	1:91:A:GLN:H	1:91:A:GLN:HB3	20	0.22	0.01	0.22
(3,21)	1:80:A:ASP:O	1:84:A:ILE:H	20	0.21	0.05	0.2
(1,269)	1:21:A:SER:HA	1:23:A:HIS:H	20	0.21	0.01	0.21
(1,1072)	1:70:A:THR:H	1:71:A:TRP:H	20	0.21	0.04	0.2
(1,765)	1:46:A:LEU:H	1:49:A:VAL:H	20	0.21	0.01	0.21
(1,483)	1:32:A:THR:H	1:34:A:ARG:H	20	0.21	0.06	0.2
(1,1177)	1:78:A:THR:H	1:81:A:LYS:H	20	0.21	0.05	0.21
(1,760)	1:46:A:LEU:H	1:48:A:LEU:H	20	0.21	0.03	0.2
(1,992)	1:64:A:TRP:H	1:93:A:THR:HG1	20	0.21	0.03	0.21
(1,1123)	1:74:A:LYS:H	1:74:A:LYS:HD2	20	0.21	0.02	0.2
(1,434)	1:28:A:ASN:HA	1:29:A:ARG:H	20	0.21	0.02	0.2
(1,974)	1:63:A:LEU:HA	1:92:A:PHE:H	20	0.2	0.03	0.2
(1,203)	1:19:A:GLU:HB3	1:20:A:LEU:H	20	0.2	0.02	0.21
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG21	20	0.2	0.04	0.2
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG22	20	0.2	0.04	0.2
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG23	20	0.2	0.04	0.2
(1,200)	1:19:A:GLU:H	1:20:A:LEU:H	20	0.2	0.02	0.2
(1,1246)	1:81:A:LYS:HE3	1:82:A:TYR:H	20	0.2	0.11	0.16
(1,352)	1:23:A:HIS:HB3	1:91:A:GLN:HB2	20	0.2	0.02	0.2
(1,276)	1:21:A:SER:H	1:32:A:THR:HG21	20	0.2	0.02	0.2
(1,276)	1:21:A:SER:H	1:32:A:THR:HG22	20	0.2	0.02	0.2
(1,276)	1:21:A:SER:H	1:32:A:THR:HG23	20	0.2	0.02	0.2
(2,7)	1:29:A:ARG:O	1:24:A:VAL:N	20	0.2	0.01	0.2
(1,511)	1:33:A:LEU:HD21	1:48:A:LEU:HB3	20	0.2	0.05	0.19
(1,511)	1:33:A:LEU:HD22	1:48:A:LEU:HB3	20	0.2	0.05	0.19
(1,511)	1:33:A:LEU:HD23	1:48:A:LEU:HB3	20	0.2	0.05	0.19
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG21	20	0.2	0.06	0.17
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG22	20	0.2	0.06	0.17
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG23	20	0.2	0.06	0.17
(1,1160)	1:77:A:TRP:HB2	1:78:A:THR:H	20	0.19	0.04	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,926)	1:61:A:HIS:H	1:62:A:ALA:H	20	0.19	0.02	0.2
(1,532)	1:35:A:VAL:H	1:35:A:VAL:HB	20	0.19	0.01	0.19
(1,1081)	1:71:A:TRP:HB2	1:72:A:LEU:H	20	0.19	0.05	0.2
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG21	20	0.19	0.01	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG22	20	0.19	0.01	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG23	20	0.19	0.01	0.19
(1,1141)	1:74:A:LYS:HE3	1:78:A:THR:H	20	0.19	0.04	0.18
(2,17)	1:21:A:SER:O	1:91:A:GLN:H	20	0.19	0.02	0.19
(1,978)	1:63:A:LEU:HA	1:93:A:THR:H	20	0.19	0.04	0.18
(1,552)	1:36:A:THR:HB	1:38:A:GLU:H	20	0.19	0.04	0.18
(1,249)	1:20:A:LEU:HB2	1:34:A:ARG:H	20	0.19	0.05	0.19
(1,432)	1:28:A:ASN:H	1:28:A:ASN:HB2	20	0.19	0.03	0.19
(1,437)	1:28:A:ASN:HB3	1:29:A:ARG:H	20	0.18	0.02	0.18
(1,950)	1:63:A:LEU:H	1:63:A:LEU:HG	20	0.18	0.04	0.19
(1,467)	1:31:A:VAL:H	1:32:A:THR:H	20	0.18	0.01	0.18
(1,782)	1:47:A:LYS:HB2	1:48:A:LEU:H	20	0.18	0.02	0.19
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG21	20	0.18	0.05	0.18
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG22	20	0.18	0.05	0.18
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG23	20	0.18	0.05	0.18
(1,1148)	1:75:A:THR:HG21	1:77:A:TRP:H	20	0.18	0.08	0.16
(1,1148)	1:75:A:THR:HG22	1:77:A:TRP:H	20	0.18	0.08	0.16
(1,1148)	1:75:A:THR:HG23	1:77:A:TRP:H	20	0.18	0.08	0.16
(1,294)	1:22:A:VAL:HG11	1:29:A:ARG:H	20	0.18	0.02	0.18
(1,294)	1:22:A:VAL:HG12	1:29:A:ARG:H	20	0.18	0.02	0.18
(1,294)	1:22:A:VAL:HG13	1:29:A:ARG:H	20	0.18	0.02	0.18
(1,694)	1:43:A:GLY:H	1:45:A:MET:H	20	0.18	0.03	0.17
(1,329)	1:23:A:HIS:HB2	1:24:A:VAL:HA	20	0.18	0.02	0.18
(1,1128)	1:74:A:LYS:HE3	1:74:A:LYS:HB3	20	0.18	0.02	0.18
(1,766)	1:46:A:LEU:HA	1:50:A:GLU:H	20	0.18	0.04	0.18
(1,1218)	1:80:A:ASP:HB2	1:82:A:TYR:H	20	0.18	0.04	0.17
(1,737)	1:45:A:MET:HB3	1:48:A:LEU:H	20	0.18	0.03	0.18
(2,13)	1:92:A:PHE:O	1:64:A:TRP:N	20	0.18	0.03	0.18
(1,659)	1:41:A:ILE:HD11	1:44:A:VAL:H	20	0.17	0.02	0.17
(1,659)	1:41:A:ILE:HD12	1:44:A:VAL:H	20	0.17	0.02	0.17
(1,659)	1:41:A:ILE:HD13	1:44:A:VAL:H	20	0.17	0.02	0.17
(1,844)	1:50:A:GLU:H	1:50:A:GLU:HG2	20	0.17	0.02	0.17
(2,19)	1:23:A:HIS:O	1:93:A:THR:H	20	0.17	0.02	0.18
(1,1108)	1:73:A:LEU:HA	1:74:A:LYS:H	20	0.17	0.02	0.18
(1,580)	1:38:A:GLU:HB3	1:39:A:VAL:H	20	0.17	0.03	0.18
(1,350)	1:23:A:HIS:HB2	1:91:A:GLN:HG3	20	0.17	0.03	0.17
(1,683)	1:42:A:GLY:H	1:74:A:LYS:HE3	20	0.17	0.04	0.16
(1,426)	1:27:A:VAL:H	1:28:A:ASN:HB2	20	0.17	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,773)	1:47:A:LYS:H	1:47:A:LYS:HD3	20	0.17	0.03	0.16
(1,692)	1:43:A:GLY:H	1:44:A:VAL:HB	20	0.16	0.02	0.16
(1,972)	1:63:A:LEU:HD11	1:91:A:GLN:H	20	0.16	0.02	0.16
(1,972)	1:63:A:LEU:HD12	1:91:A:GLN:H	20	0.16	0.02	0.16
(1,972)	1:63:A:LEU:HD13	1:91:A:GLN:H	20	0.16	0.02	0.16
(1,377)	1:24:A:VAL:HA	1:30:A:ASP:HA	20	0.16	0.03	0.16
(1,275)	1:21:A:SER:H	1:32:A:THR:HB	20	0.16	0.01	0.16
(1,663)	1:41:A:ILE:HG21	1:72:A:LEU:HG	20	0.16	0.03	0.16
(1,663)	1:41:A:ILE:HG22	1:72:A:LEU:HG	20	0.16	0.03	0.16
(1,663)	1:41:A:ILE:HG23	1:72:A:LEU:HG	20	0.16	0.03	0.16
(1,482)	1:32:A:THR:HA	1:34:A:ARG:H	20	0.16	0.02	0.16
(1,1134)	1:74:A:LYS:HG2	1:75:A:THR:H	20	0.16	0.02	0.16
(1,813)	1:48:A:LEU:H	1:51:A:LYS:H	20	0.15	0.02	0.15
(1,1113)	1:74:A:LYS:HA	1:74:A:LYS:HE3	20	0.15	0.01	0.15
(1,812)	1:48:A:LEU:HA	1:51:A:LYS:HB3	20	0.15	0.02	0.15
(1,1215)	1:80:A:ASP:HB2	1:81:A:LYS:H	20	0.15	0.02	0.15
(1,858)	1:51:A:LYS:H	1:51:A:LYS:HD3	20	0.15	0.01	0.15
(1,312)	1:22:A:VAL:HG21	1:90:A:LEU:H	20	0.14	0.03	0.14
(1,312)	1:22:A:VAL:HG22	1:90:A:LEU:H	20	0.14	0.03	0.14
(1,312)	1:22:A:VAL:HG23	1:90:A:LEU:H	20	0.14	0.03	0.14
(1,1193)	1:79:A:LEU:HA	1:80:A:ASP:H	20	0.13	0.01	0.13
(1,841)	1:50:A:GLU:HA	1:50:A:GLU:HG3	20	0.13	0.02	0.14
(1,473)	1:32:A:THR:HB	1:32:A:THR:H	20	0.13	0.01	0.13
(1,852)	1:51:A:LYS:HA	1:51:A:LYS:HD3	20	0.12	0.01	0.12
(1,175)	1:18:A:TRP:H	1:35:A:VAL:HA	19	0.24	0.03	0.25
(1,95)	1:8:A:MET:HA	1:10:A:ASP:H	19	0.24	0.07	0.28
(1,206)	1:19:A:GLU:H	1:20:A:LEU:HB2	19	0.23	0.03	0.24
(1,818)	1:48:A:LEU:HD21	1:52:A:LEU:H	19	0.23	0.05	0.22
(1,818)	1:48:A:LEU:HD22	1:52:A:LEU:H	19	0.23	0.05	0.22
(1,818)	1:48:A:LEU:HD23	1:52:A:LEU:H	19	0.23	0.05	0.22
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD21	19	0.22	0.04	0.22
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD22	19	0.22	0.04	0.22
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD23	19	0.22	0.04	0.22
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD11	19	0.21	0.04	0.21
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD12	19	0.21	0.04	0.21
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD13	19	0.21	0.04	0.21
(1,387)	1:24:A:VAL:HG11	1:62:A:ALA:H	19	0.2	0.03	0.2
(1,387)	1:24:A:VAL:HG12	1:62:A:ALA:H	19	0.2	0.03	0.2
(1,387)	1:24:A:VAL:HG13	1:62:A:ALA:H	19	0.2	0.03	0.2
(1,195)	1:19:A:GLU:H	1:19:A:GLU:HG2	19	0.2	0.02	0.19
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG11	19	0.2	0.05	0.2
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG12	19	0.2	0.05	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG13	19	0.2	0.05	0.2
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG11	19	0.19	0.05	0.2
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG12	19	0.19	0.05	0.2
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG13	19	0.19	0.05	0.2
(1,1216)	1:80:A:ASP:H	1:81:A:LYS:HD2	19	0.19	0.06	0.17
(1,764)	1:46:A:LEU:HA	1:49:A:VAL:H	19	0.18	0.02	0.18
(1,484)	1:32:A:THR:HA	1:51:A:LYS:HD3	19	0.18	0.02	0.18
(1,1105)	1:73:A:LEU:H	1:73:A:LEU:HB3	19	0.18	0.03	0.17
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD21	19	0.16	0.03	0.16
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD22	19	0.16	0.03	0.16
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD23	19	0.16	0.03	0.16
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD21	19	0.16	0.03	0.16
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD22	19	0.16	0.03	0.16
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD23	19	0.16	0.03	0.16
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD21	19	0.16	0.03	0.16
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD22	19	0.16	0.03	0.16
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD23	19	0.16	0.03	0.16
(1,127)	1:11:A:GLY:HA2	1:12:A:CYS:H	19	0.16	0.03	0.15
(1,323)	1:23:A:HIS:HB2	1:24:A:VAL:H	19	0.15	0.02	0.15
(3,13)	1:92:A:PHE:O	1:64:A:TRP:H	19	0.14	0.01	0.13
(1,1329)	1:87:A:ASP:HB3	1:88:A:ALA:H	19	0.12	0.02	0.12
(1,1225)	1:81:A:LYS:HA	1:81:A:LYS:HG2	19	0.12	0.01	0.12
(1,431)	1:27:A:VAL:H	1:93:A:THR:HB	18	0.19	0.06	0.17
(1,244)	1:20:A:LEU:HD21	1:33:A:LEU:HA	18	0.18	0.04	0.18
(1,244)	1:20:A:LEU:HD22	1:33:A:LEU:HA	18	0.18	0.04	0.18
(1,244)	1:20:A:LEU:HD23	1:33:A:LEU:HA	18	0.18	0.04	0.18
(1,166)	1:17:A:THR:HG21	1:18:A:TRP:H	18	0.18	0.05	0.17
(1,166)	1:17:A:THR:HG22	1:18:A:TRP:H	18	0.18	0.05	0.17
(1,166)	1:17:A:THR:HG23	1:18:A:TRP:H	18	0.18	0.05	0.17
(1,331)	1:23:A:HIS:H	1:30:A:ASP:HB3	18	0.17	0.02	0.17
(1,177)	1:18:A:TRP:HE1	1:36:A:THR:HB	18	0.17	0.03	0.17
(1,1153)	1:76:A:HIS:HB3	1:77:A:TRP:H	18	0.16	0.03	0.17
(1,234)	1:20:A:LEU:HB3	1:21:A:SER:H	18	0.16	0.01	0.16
(2,21)	1:39:A:VAL:O	1:43:A:GLY:N	18	0.16	0.03	0.17
(1,976)	1:63:A:LEU:HG	1:93:A:THR:H	18	0.16	0.04	0.16
(1,251)	1:20:A:LEU:HG	1:35:A:VAL:H	18	0.16	0.03	0.16
(1,640)	1:41:A:ILE:H	1:41:A:ILE:HG12	18	0.14	0.02	0.14
(2,24)	1:45:A:MET:O	1:49:A:VAL:N	18	0.12	0.01	0.12
(1,1235)	1:81:A:LYS:HE3	1:81:A:LYS:HG3	17	0.2	0.03	0.2
(1,588)	1:38:A:GLU:HA	1:80:A:ASP:H	17	0.2	0.07	0.2
(1,112)	1:9:A:PRO:HG3	1:10:A:ASP:H	17	0.18	0.03	0.17
(1,684)	1:42:A:GLY:HA3	1:75:A:THR:HB	17	0.17	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD21	17	0.16	0.04	0.18
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD22	17	0.16	0.04	0.18
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD23	17	0.16	0.04	0.18
(1,1161)	1:77:A:TRP:H	1:81:A:LYS:HD3	17	0.16	0.03	0.16
(1,242)	1:20:A:LEU:HB3	1:33:A:LEU:H	17	0.15	0.05	0.13
(1,968)	1:63:A:LEU:HG	1:90:A:LEU:HA	17	0.14	0.02	0.14
(3,16)	1:42:A:GLY:O	1:46:A:LEU:H	17	0.13	0.02	0.13
(1,1404)	1:92:A:PHE:HB2	1:93:A:THR:HB	16	0.21	0.02	0.2
(1,453)	1:29:A:ARG:HB2	1:31:A:VAL:HA	16	0.2	0.05	0.19
(1,610)	1:39:A:VAL:HG21	1:80:A:ASP:H	16	0.18	0.06	0.16
(1,610)	1:39:A:VAL:HG22	1:80:A:ASP:H	16	0.18	0.06	0.16
(1,610)	1:39:A:VAL:HG23	1:80:A:ASP:H	16	0.18	0.06	0.16
(1,719)	1:44:A:VAL:HG11	1:90:A:LEU:H	16	0.18	0.03	0.17
(1,719)	1:44:A:VAL:HG12	1:90:A:LEU:H	16	0.18	0.03	0.17
(1,719)	1:44:A:VAL:HG13	1:90:A:LEU:H	16	0.18	0.03	0.17
(1,1138)	1:74:A:LYS:HD3	1:77:A:TRP:H	16	0.16	0.02	0.16
(1,554)	1:36:A:THR:H	1:38:A:GLU:HB3	16	0.14	0.01	0.14
(1,392)	1:24:A:VAL:HB	1:92:A:PHE:H	16	0.12	0.02	0.12
(1,838)	1:49:A:VAL:HG21	1:58:A:TRP:H	15	0.22	0.08	0.23
(1,838)	1:49:A:VAL:HG22	1:58:A:TRP:H	15	0.22	0.08	0.23
(1,838)	1:49:A:VAL:HG23	1:58:A:TRP:H	15	0.22	0.08	0.23
(1,981)	1:64:A:TRP:H	1:64:A:TRP:HB3	15	0.15	0.04	0.15
(1,527)	1:34:A:ARG:H	1:51:A:LYS:HD3	15	0.14	0.02	0.13
(1,299)	1:22:A:VAL:H	1:32:A:THR:HB	15	0.13	0.02	0.13
(1,945)	1:62:A:ALA:HB1	1:93:A:THR:HA	14	0.18	0.07	0.16
(1,945)	1:62:A:ALA:HB2	1:93:A:THR:HA	14	0.18	0.07	0.16
(1,945)	1:62:A:ALA:HB3	1:93:A:THR:HA	14	0.18	0.07	0.16
(1,1197)	1:79:A:LEU:HB3	1:80:A:ASP:H	14	0.17	0.04	0.16
(1,414)	1:25:A:THR:H	1:93:A:THR:HG21	14	0.16	0.08	0.14
(1,414)	1:25:A:THR:H	1:93:A:THR:HG22	14	0.16	0.08	0.14
(1,414)	1:25:A:THR:H	1:93:A:THR:HG23	14	0.16	0.08	0.14
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD21	14	0.14	0.03	0.14
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD22	14	0.14	0.03	0.14
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD23	14	0.14	0.03	0.14
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG21	14	0.14	0.02	0.14
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG22	14	0.14	0.02	0.14
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG23	14	0.14	0.02	0.14
(1,1038)	1:67:A:LYS:H	1:67:A:LYS:HG3	14	0.14	0.02	0.13
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB1	14	0.13	0.02	0.14
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB2	14	0.13	0.02	0.14
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB3	14	0.13	0.02	0.14
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB1	14	0.13	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB2	14	0.13	0.02	0.14
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB3	14	0.13	0.02	0.14
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB1	14	0.13	0.02	0.14
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB2	14	0.13	0.02	0.14
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB3	14	0.13	0.02	0.14
(1,383)	1:24:A:VAL:HA	1:31:A:VAL:H	14	0.13	0.02	0.12
(1,561)	1:37:A:GLY:H	1:38:A:GLU:HG3	14	0.12	0.02	0.12
(1,959)	1:63:A:LEU:H	1:64:A:TRP:H	14	0.12	0.02	0.12
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD21	13	0.27	0.06	0.27
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD22	13	0.27	0.06	0.27
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD23	13	0.27	0.06	0.27
(1,34)	1:3:A:LEU:HD21	1:4:A:ASP:H	13	0.21	0.06	0.23
(1,34)	1:3:A:LEU:HD22	1:4:A:ASP:H	13	0.21	0.06	0.23
(1,34)	1:3:A:LEU:HD23	1:4:A:ASP:H	13	0.21	0.06	0.23
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD21	13	0.2	0.04	0.19
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD22	13	0.2	0.04	0.19
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD23	13	0.2	0.04	0.19
(1,1053)	1:67:A:LYS:H	1:88:A:ALA:HA	13	0.19	0.09	0.15
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD11	13	0.19	0.03	0.21
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD12	13	0.19	0.03	0.21
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD13	13	0.19	0.03	0.21
(1,904)	1:58:A:TRP:H	1:58:A:TRP:HB3	13	0.18	0.07	0.14
(1,16)	1:2:A:ALA:H	1:3:A:LEU:HB3	13	0.17	0.05	0.16
(1,1381)	1:91:A:GLN:H	1:91:A:GLN:HG2	13	0.14	0.03	0.14
(1,499)	1:33:A:LEU:HD21	1:34:A:ARG:H	13	0.14	0.03	0.13
(1,499)	1:33:A:LEU:HD22	1:34:A:ARG:H	13	0.14	0.03	0.13
(1,499)	1:33:A:LEU:HD23	1:34:A:ARG:H	13	0.14	0.03	0.13
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD11	13	0.13	0.03	0.13
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD12	13	0.13	0.03	0.13
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD13	13	0.13	0.03	0.13
(1,602)	1:39:A:VAL:HG21	1:43:A:GLY:H	13	0.13	0.01	0.12
(1,602)	1:39:A:VAL:HG22	1:43:A:GLY:H	13	0.13	0.01	0.12
(1,602)	1:39:A:VAL:HG23	1:43:A:GLY:H	13	0.13	0.01	0.12
(1,250)	1:20:A:LEU:H	1:35:A:VAL:H	13	0.12	0.02	0.11
(1,1121)	1:74:A:LYS:H	1:74:A:LYS:HG3	13	0.12	0.01	0.12
(1,1294)	1:85:A:GLN:H	1:85:A:GLN:HG3	13	0.12	0.01	0.12
(1,480)	1:32:A:THR:HG21	1:33:A:LEU:H	13	0.11	0.01	0.11
(1,480)	1:32:A:THR:HG22	1:33:A:LEU:H	13	0.11	0.01	0.11
(1,480)	1:32:A:THR:HG23	1:33:A:LEU:H	13	0.11	0.01	0.11
(1,39)	1:4:A:ASP:H	1:4:A:ASP:HB3	12	0.28	0.11	0.32
(1,67)	1:6:A:ILE:H	1:10:A:ASP:H	12	0.19	0.06	0.2
(1,82)	1:7:A:ARG:HB2	1:8:A:MET:H	12	0.19	0.02	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1169)	1:78:A:THR:HB	1:79:A:LEU:H	12	0.19	0.03	0.2
(1,85)	1:7:A:ARG:HD3	1:8:A:MET:H	12	0.18	0.06	0.16
(1,821)	1:48:A:LEU:HD21	1:63:A:LEU:H	12	0.14	0.02	0.14
(1,821)	1:48:A:LEU:HD22	1:63:A:LEU:H	12	0.14	0.02	0.14
(1,821)	1:48:A:LEU:HD23	1:63:A:LEU:H	12	0.14	0.02	0.14
(1,1196)	1:79:A:LEU:HD21	1:80:A:ASP:H	12	0.13	0.02	0.13
(1,1196)	1:79:A:LEU:HD22	1:80:A:ASP:H	12	0.13	0.02	0.13
(1,1196)	1:79:A:LEU:HD23	1:80:A:ASP:H	12	0.13	0.02	0.13
(1,988)	1:64:A:TRP:H	1:92:A:PHE:HB3	12	0.13	0.01	0.12
(1,1129)	1:74:A:LYS:HE2	1:74:A:LYS:HB3	12	0.12	0.01	0.11
(1,1)	1:1:A:MET:HA	1:1:A:MET:HG3	12	0.11	0.01	0.11
(1,94)	1:8:A:MET:H	1:10:A:ASP:HA	11	0.22	0.07	0.23
(1,78)	1:7:A:ARG:HD3	1:7:A:ARG:HB3	11	0.21	0.07	0.26
(1,671)	1:41:A:ILE:HD11	1:75:A:THR:HA	11	0.19	0.06	0.18
(1,671)	1:41:A:ILE:HD12	1:75:A:THR:HA	11	0.19	0.06	0.18
(1,671)	1:41:A:ILE:HD13	1:75:A:THR:HA	11	0.19	0.06	0.18
(1,1176)	1:78:A:THR:H	1:81:A:LYS:HA	11	0.14	0.02	0.13
(1,611)	1:39:A:VAL:HG11	1:78:A:THR:H	11	0.14	0.03	0.13
(1,611)	1:39:A:VAL:HG12	1:78:A:THR:H	11	0.14	0.03	0.13
(1,611)	1:39:A:VAL:HG13	1:78:A:THR:H	11	0.14	0.03	0.13
(1,204)	1:19:A:GLU:HG2	1:20:A:LEU:H	11	0.13	0.02	0.13
(1,280)	1:21:A:SER:HB3	1:90:A:LEU:H	11	0.13	0.02	0.13
(2,3)	1:20:A:LEU:O	1:33:A:LEU:N	11	0.11	0.02	0.1
(1,100)	1:8:A:MET:H	1:12:A:CYS:HA	10	0.38	0.32	0.16
(1,1205)	1:79:A:LEU:HD11	1:83:A:GLY:H	10	0.24	0.04	0.24
(1,1205)	1:79:A:LEU:HD12	1:83:A:GLY:H	10	0.24	0.04	0.24
(1,1205)	1:79:A:LEU:HD13	1:83:A:GLY:H	10	0.24	0.04	0.24
(1,371)	1:24:A:VAL:HG11	1:29:A:ARG:H	10	0.19	0.06	0.18
(1,371)	1:24:A:VAL:HG12	1:29:A:ARG:H	10	0.19	0.06	0.18
(1,371)	1:24:A:VAL:HG13	1:29:A:ARG:H	10	0.19	0.06	0.18
(1,1049)	1:67:A:LYS:HB3	1:69:A:ARG:HA	10	0.18	0.05	0.2
(1,628)	1:40:A:HIS:H	1:44:A:VAL:HB	10	0.17	0.05	0.18
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG21	10	0.17	0.07	0.15
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG22	10	0.17	0.07	0.15
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG23	10	0.17	0.07	0.15
(1,946)	1:62:A:ALA:H	1:94:A:PRO:HA	10	0.16	0.04	0.15
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG21	10	0.14	0.03	0.12
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG22	10	0.14	0.03	0.12
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG23	10	0.14	0.03	0.12
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD11	10	0.14	0.02	0.14
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD12	10	0.14	0.02	0.14
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD13	10	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,25)	1:77:A:TRP:O	1:81:A:LYS:N	10	0.13	0.02	0.14
(1,1112)	1:74:A:LYS:HA	1:74:A:LYS:HE2	10	0.13	0.02	0.13
(1,1313)	1:85:A:GLN:HB3	1:87:A:ASP:H	10	0.11	0.01	0.11
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB1	10	0.11	0.0	0.11
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB2	10	0.11	0.0	0.11
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB3	10	0.11	0.0	0.11
(1,20)	1:2:A:ALA:HB1	1:4:A:ASP:H	9	0.26	0.21	0.16
(1,20)	1:2:A:ALA:HB2	1:4:A:ASP:H	9	0.26	0.21	0.16
(1,20)	1:2:A:ALA:HB3	1:4:A:ASP:H	9	0.26	0.21	0.16
(1,42)	1:4:A:ASP:H	1:5:A:GLY:HA3	9	0.21	0.08	0.22
(1,430)	1:27:A:VAL:HG21	1:92:A:PHE:H	9	0.18	0.05	0.17
(1,430)	1:27:A:VAL:HG22	1:92:A:PHE:H	9	0.18	0.05	0.17
(1,430)	1:27:A:VAL:HG23	1:92:A:PHE:H	9	0.18	0.05	0.17
(1,676)	1:41:A:ILE:HG13	1:78:A:THR:H	9	0.16	0.05	0.13
(1,147)	1:15:A:ASP:H	1:15:A:ASP:HB2	9	0.16	0.05	0.15
(1,1164)	1:78:A:THR:HG21	1:78:A:THR:H	9	0.16	0.02	0.16
(1,1164)	1:78:A:THR:HG22	1:78:A:THR:H	9	0.16	0.02	0.16
(1,1164)	1:78:A:THR:HG23	1:78:A:THR:H	9	0.16	0.02	0.16
(1,890)	1:56:A:LYS:HA	1:57:A:ASP:HB2	9	0.15	0.03	0.16
(1,1061)	1:69:A:ARG:HD3	1:70:A:THR:HB	9	0.15	0.02	0.14
(1,1382)	1:91:A:GLN:HG2	1:91:A:GLN:HE21	9	0.14	0.02	0.13
(1,997)	1:65:A:TRP:HB3	1:66:A:GLU:H	9	0.14	0.02	0.15
(1,102)	1:8:A:MET:HB3	1:12:A:CYS:H	9	0.14	0.02	0.13
(1,443)	1:29:A:ARG:HB2	1:29:A:ARG:H	9	0.14	0.03	0.12
(1,960)	1:67:A:LYS:HG2	1:69:A:ARG:H	9	0.13	0.01	0.12
(1,1051)	1:67:A:LYS:HG2	1:69:A:ARG:H	9	0.13	0.01	0.12
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG21	9	0.13	0.04	0.11
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG22	9	0.13	0.04	0.11
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG23	9	0.13	0.04	0.11
(1,176)	1:18:A:TRP:H	1:36:A:THR:H	9	0.12	0.02	0.11
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD21	9	0.11	0.01	0.11
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD22	9	0.11	0.01	0.11
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD23	9	0.11	0.01	0.11
(1,1199)	1:79:A:LEU:HG	1:81:A:LYS:H	8	0.51	0.09	0.5
(1,153)	1:15:A:ASP:H	1:17:A:THR:H	8	0.24	0.14	0.18
(1,36)	1:3:A:LEU:HB3	1:4:A:ASP:H	8	0.24	0.08	0.22
(1,86)	1:7:A:ARG:HA	1:10:A:ASP:H	8	0.19	0.04	0.18
(1,87)	1:7:A:ARG:HG3	1:10:A:ASP:H	8	0.19	0.08	0.16
(1,148)	1:15:A:ASP:HA	1:16:A:GLY:H	8	0.19	0.04	0.2
(1,49)	1:5:A:GLY:HA3	1:6:A:ILE:HB	8	0.19	0.06	0.18
(1,1063)	1:69:A:ARG:H	1:70:A:THR:H	8	0.19	0.07	0.17
(1,1407)	1:92:A:PHE:HB2	1:93:A:THR:H	8	0.18	0.06	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,66)	1:6:A:ILE:HB	1:8:A:MET:H	8	0.16	0.06	0.12
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG21	8	0.14	0.02	0.14
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG22	8	0.14	0.02	0.14
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG23	8	0.14	0.02	0.14
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG21	8	0.14	0.02	0.14
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG22	8	0.14	0.02	0.14
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG23	8	0.14	0.02	0.14
(1,40)	1:4:A:ASP:HA	1:5:A:GLY:H	8	0.13	0.02	0.12
(1,1036)	1:67:A:LYS:HE3	1:67:A:LYS:H	8	0.13	0.02	0.14
(1,924)	1:61:A:HIS:H	1:61:A:HIS:HB2	8	0.11	0.01	0.11
(1,1097)	1:72:A:LEU:HD21	1:73:A:LEU:H	8	0.11	0.02	0.11
(1,1097)	1:72:A:LEU:HD22	1:73:A:LEU:H	8	0.11	0.02	0.11
(1,1097)	1:72:A:LEU:HD23	1:73:A:LEU:H	8	0.11	0.02	0.11
(1,1397)	1:91:A:GLN:HB2	1:92:A:PHE:HA	8	0.11	0.01	0.11
(1,799)	1:48:A:LEU:HA	1:49:A:VAL:H	8	0.1	0.0	0.1
(1,68)	1:6:A:ILE:HA	1:10:A:ASP:H	7	0.34	0.09	0.36
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD11	7	0.31	0.12	0.34
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD12	7	0.31	0.12	0.34
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD13	7	0.31	0.12	0.34
(1,90)	1:8:A:MET:H	1:8:A:MET:HG3	7	0.21	0.03	0.22
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD11	7	0.2	0.08	0.15
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD12	7	0.2	0.08	0.15
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD13	7	0.2	0.08	0.15
(1,1408)	1:92:A:PHE:HB3	1:93:A:THR:H	7	0.2	0.08	0.14
(1,903)	1:57:A:ASP:HB2	1:61:A:HIS:H	7	0.19	0.08	0.16
(1,1380)	1:91:A:GLN:H	1:91:A:GLN:HE22	7	0.18	0.04	0.19
(1,19)	1:2:A:ALA:HB1	1:3:A:LEU:H	7	0.17	0.03	0.17
(1,19)	1:2:A:ALA:HB2	1:3:A:LEU:H	7	0.17	0.03	0.17
(1,19)	1:2:A:ALA:HB3	1:3:A:LEU:H	7	0.17	0.03	0.17
(1,142)	1:14:A:ALA:HA	1:15:A:ASP:H	7	0.17	0.05	0.17
(1,169)	1:18:A:TRP:H	1:18:A:TRP:HD1	7	0.16	0.03	0.15
(1,884)	1:56:A:LYS:HE3	1:56:A:LYS:HB3	7	0.13	0.02	0.12
(1,985)	1:64:A:TRP:H	1:90:A:LEU:HA	7	0.13	0.01	0.12
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG21	7	0.13	0.02	0.13
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG22	7	0.13	0.02	0.13
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG23	7	0.13	0.02	0.13
(1,293)	1:22:A:VAL:HG21	1:24:A:VAL:H	7	0.12	0.02	0.11
(1,293)	1:22:A:VAL:HG22	1:24:A:VAL:H	7	0.12	0.02	0.11
(1,293)	1:22:A:VAL:HG23	1:24:A:VAL:H	7	0.12	0.02	0.11
(1,339)	1:23:A:HIS:H	1:90:A:LEU:H	7	0.12	0.01	0.11
(1,889)	1:56:A:LYS:HA	1:57:A:ASP:HB3	7	0.11	0.01	0.11
(1,617)	1:40:A:HIS:HB3	1:41:A:ILE:H	7	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,514)	1:33:A:LEU:HD21	1:50:A:GLU:H	7	0.11	0.01	0.1
(1,514)	1:33:A:LEU:HD22	1:50:A:GLU:H	7	0.11	0.01	0.1
(1,514)	1:33:A:LEU:HD23	1:50:A:GLU:H	7	0.11	0.01	0.1
(1,1020)	1:66:A:GLU:H	1:66:A:GLU:HB3	6	0.6	0.01	0.59
(1,162)	1:17:A:THR:HB	1:18:A:TRP:H	6	0.39	0.04	0.38
(1,103)	1:8:A:MET:HG3	1:12:A:CYS:HB3	6	0.18	0.1	0.15
(1,906)	1:58:A:TRP:H	1:59:A:SER:H	6	0.18	0.08	0.16
(1,1187)	1:79:A:LEU:H	1:79:A:LEU:HD21	6	0.18	0.02	0.17
(1,1187)	1:79:A:LEU:H	1:79:A:LEU:HD22	6	0.18	0.02	0.17
(1,1187)	1:79:A:LEU:H	1:79:A:LEU:HD23	6	0.18	0.02	0.17
(1,1140)	1:74:A:LYS:HA	1:77:A:TRP:H	6	0.17	0.05	0.18
(1,930)	1:61:A:HIS:HB2	1:63:A:LEU:H	6	0.14	0.02	0.15
(1,212)	1:19:A:GLU:HB2	1:33:A:LEU:H	6	0.13	0.02	0.12
(1,805)	1:48:A:LEU:HG	1:49:A:VAL:H	6	0.12	0.02	0.12
(1,942)	1:62:A:ALA:HB1	1:92:A:PHE:HA	6	0.12	0.02	0.12
(1,942)	1:62:A:ALA:HB2	1:92:A:PHE:HA	6	0.12	0.02	0.12
(1,942)	1:62:A:ALA:HB3	1:92:A:PHE:HA	6	0.12	0.02	0.12
(1,395)	1:25:A:THR:HB	1:25:A:THR:H	6	0.12	0.02	0.11
(1,712)	1:44:A:VAL:H	1:46:A:LEU:HG	6	0.12	0.01	0.11
(1,505)	1:33:A:LEU:HD21	1:47:A:LYS:H	6	0.12	0.01	0.11
(1,505)	1:33:A:LEU:HD22	1:47:A:LYS:H	6	0.12	0.01	0.11
(1,505)	1:33:A:LEU:HD23	1:47:A:LYS:H	6	0.12	0.01	0.11
(1,723)	1:45:A:MET:H	1:45:A:MET:HB3	6	0.11	0.01	0.12
(1,923)	1:61:A:HIS:H	1:61:A:HIS:HB3	6	0.11	0.01	0.11
(1,232)	1:20:A:LEU:HG	1:21:A:SER:H	6	0.11	0.01	0.11
(1,695)	1:43:A:GLY:HA2	1:46:A:LEU:H	6	0.11	0.01	0.1
(1,422)	1:27:A:VAL:H	1:28:A:ASN:H	6	0.1	0.01	0.1
(1,520)	1:34:A:ARG:HG3	1:34:A:ARG:HA	5	0.74	0.07	0.77
(1,88)	1:8:A:MET:H	1:8:A:MET:HB3	5	0.35	0.07	0.39
(1,910)	1:58:A:TRP:HB3	1:59:A:SER:H	5	0.34	0.11	0.4
(1,28)	1:3:A:LEU:H	1:3:A:LEU:HB2	5	0.34	0.18	0.25
(1,75)	1:7:A:ARG:H	1:7:A:ARG:HB2	5	0.29	0.11	0.3
(1,113)	1:9:A:PRO:HG3	1:12:A:CYS:HB3	5	0.23	0.06	0.19
(1,45)	1:4:A:ASP:HB3	1:6:A:ILE:H	5	0.21	0.08	0.17
(1,56)	1:6:A:ILE:H	1:6:A:ILE:HG12	5	0.19	0.05	0.18
(1,1021)	1:66:A:GLU:H	1:66:A:GLU:HG2	5	0.18	0.01	0.18
(1,372)	1:24:A:VAL:HG21	1:29:A:ARG:H	5	0.16	0.04	0.18
(1,372)	1:24:A:VAL:HG22	1:29:A:ARG:H	5	0.16	0.04	0.18
(1,372)	1:24:A:VAL:HG23	1:29:A:ARG:H	5	0.16	0.04	0.18
(1,409)	1:25:A:THR:H	1:92:A:PHE:HB2	5	0.16	0.03	0.14
(1,516)	1:34:A:ARG:H	1:34:A:ARG:HG3	5	0.16	0.03	0.16
(1,607)	1:39:A:VAL:H	1:79:A:LEU:H	5	0.15	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,43)	1:4:A:ASP:HB3	1:5:A:GLY:H	5	0.15	0.04	0.13
(1,497)	1:33:A:LEU:HB3	1:34:A:ARG:H	5	0.14	0.04	0.12
(1,688)	1:42:A:GLY:H	1:75:A:THR:HG21	5	0.13	0.04	0.12
(1,688)	1:42:A:GLY:H	1:75:A:THR:HG22	5	0.13	0.04	0.12
(1,688)	1:42:A:GLY:H	1:75:A:THR:HG23	5	0.13	0.04	0.12
(1,454)	1:30:A:ASP:H	1:30:A:ASP:HB3	5	0.13	0.03	0.11
(1,1355)	1:90:A:LEU:H	1:90:A:LEU:HD21	5	0.12	0.02	0.12
(1,1355)	1:90:A:LEU:H	1:90:A:LEU:HD22	5	0.12	0.02	0.12
(1,1355)	1:90:A:LEU:H	1:90:A:LEU:HD23	5	0.12	0.02	0.12
(1,487)	1:33:A:LEU:H	1:33:A:LEU:HD11	5	0.12	0.01	0.12
(1,487)	1:33:A:LEU:H	1:33:A:LEU:HD12	5	0.12	0.01	0.12
(1,487)	1:33:A:LEU:H	1:33:A:LEU:HD13	5	0.12	0.01	0.12
(1,503)	1:33:A:LEU:HB2	1:35:A:VAL:HG11	5	0.12	0.01	0.12
(1,503)	1:33:A:LEU:HB2	1:35:A:VAL:HG12	5	0.12	0.01	0.12
(1,503)	1:33:A:LEU:HB2	1:35:A:VAL:HG13	5	0.12	0.01	0.12
(1,599)	1:39:A:VAL:H	1:40:A:HIS:H	5	0.12	0.01	0.12
(1,1157)	1:77:A:TRP:H	1:77:A:TRP:HB3	5	0.12	0.01	0.12
(1,208)	1:19:A:GLU:HG2	1:32:A:THR:HB	5	0.12	0.02	0.11
(2,14)	1:64:A:TRP:O	1:92:A:PHE:N	5	0.12	0.01	0.11
(1,641)	1:41:A:ILE:H	1:41:A:ILE:HD11	5	0.11	0.01	0.11
(1,641)	1:41:A:ILE:H	1:41:A:ILE:HD12	5	0.11	0.01	0.11
(1,641)	1:41:A:ILE:H	1:41:A:ILE:HD13	5	0.11	0.01	0.11
(1,738)	1:45:A:MET:HA	1:48:A:LEU:H	5	0.11	0.01	0.11
(1,1330)	1:87:A:ASP:H	1:88:A:ALA:HA	5	0.11	0.01	0.1
(1,905)	1:58:A:TRP:H	1:58:A:TRP:HB2	4	0.46	0.16	0.53
(1,18)	1:2:A:ALA:HA	1:3:A:LEU:H	4	0.4	0.11	0.44
(1,146)	1:15:A:ASP:H	1:15:A:ASP:HB3	4	0.26	0.07	0.24
(1,515)	1:34:A:ARG:H	1:34:A:ARG:HB3	4	0.24	0.18	0.15
(1,115)	1:9:A:PRO:HA	1:13:A:TYR:H	4	0.24	0.06	0.26
(1,155)	1:16:A:GLY:HA3	1:17:A:THR:H	4	0.2	0.03	0.21
(1,61)	1:6:A:ILE:H	1:7:A:ARG:H	4	0.2	0.06	0.19
(1,673)	1:41:A:ILE:H	1:77:A:TRP:H	4	0.2	0.05	0.2
(1,156)	1:16:A:GLY:HA2	1:17:A:THR:H	4	0.16	0.04	0.15
(1,878)	1:56:A:LYS:H	1:56:A:LYS:HD3	4	0.15	0.04	0.15
(1,746)	1:45:A:MET:HG3	1:63:A:LEU:HD21	4	0.15	0.04	0.13
(1,746)	1:45:A:MET:HG3	1:63:A:LEU:HD22	4	0.15	0.04	0.13
(1,746)	1:45:A:MET:HG3	1:63:A:LEU:HD23	4	0.15	0.04	0.13
(1,62)	1:6:A:ILE:HG21	1:7:A:ARG:H	4	0.13	0.02	0.13
(1,62)	1:6:A:ILE:HG22	1:7:A:ARG:H	4	0.13	0.02	0.13
(1,62)	1:6:A:ILE:HG23	1:7:A:ARG:H	4	0.13	0.02	0.13
(1,1132)	1:74:A:LYS:HG3	1:75:A:THR:H	4	0.12	0.03	0.12
(1,1289)	1:84:A:ILE:HA	1:88:A:ALA:HB1	4	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1289)	1:84:A:ILE:HA	1:88:A:ALA:HB2	4	0.12	0.01	0.12
(1,1289)	1:84:A:ILE:HA	1:88:A:ALA:HB3	4	0.12	0.01	0.12
(1,1171)	1:78:A:THR:HB	1:80:A:ASP:H	4	0.12	0.0	0.12
(1,731)	1:45:A:MET:H	1:46:A:LEU:HG	4	0.11	0.0	0.11
(1,1376)	1:91:A:GLN:HA	1:91:A:GLN:HE22	4	0.11	0.0	0.11
(1,717)	1:44:A:VAL:HB	1:47:A:LYS:H	4	0.11	0.0	0.11
(1,994)	1:65:A:TRP:H	1:65:A:TRP:HB2	3	0.49	0.25	0.65
(1,74)	1:7:A:ARG:H	1:7:A:ARG:HB3	3	0.48	0.16	0.59
(1,870)	1:52:A:LEU:HG	1:52:A:LEU:HA	3	0.41	0.02	0.42
(1,1203)	1:79:A:LEU:HB3	1:83:A:GLY:H	3	0.26	0.05	0.24
(1,145)	1:14:A:ALA:HB1	1:16:A:GLY:H	3	0.24	0.09	0.2
(1,145)	1:14:A:ALA:HB2	1:16:A:GLY:H	3	0.24	0.09	0.2
(1,145)	1:14:A:ALA:HB3	1:16:A:GLY:H	3	0.24	0.09	0.2
(1,1402)	1:92:A:PHE:H	1:92:A:PHE:HB2	3	0.23	0.05	0.24
(1,17)	1:2:A:ALA:H	1:3:A:LEU:HA	3	0.22	0.03	0.22
(1,47)	1:5:A:GLY:H	1:6:A:ILE:H	3	0.2	0.02	0.2
(1,572)	1:37:A:GLY:H	1:80:A:ASP:H	3	0.18	0.04	0.17
(1,1019)	1:66:A:GLU:H	1:66:A:GLU:HG3	3	0.18	0.0	0.18
(1,1208)	1:79:A:LEU:HA	1:84:A:ILE:H	3	0.15	0.03	0.17
(1,128)	1:11:A:GLY:H	1:12:A:CYS:H	3	0.15	0.01	0.15
(1,369)	1:24:A:VAL:H	1:29:A:ARG:HG3	3	0.15	0.02	0.15
(1,548)	1:36:A:THR:HG21	1:37:A:GLY:H	3	0.14	0.04	0.12
(1,548)	1:36:A:THR:HG22	1:37:A:GLY:H	3	0.14	0.04	0.12
(1,548)	1:36:A:THR:HG23	1:37:A:GLY:H	3	0.14	0.04	0.12
(1,1064)	1:69:A:ARG:HB2	1:70:A:THR:H	3	0.13	0.02	0.13
(1,962)	1:63:A:LEU:HD21	1:72:A:LEU:H	3	0.12	0.01	0.12
(1,962)	1:63:A:LEU:HD22	1:72:A:LEU:H	3	0.12	0.01	0.12
(1,962)	1:63:A:LEU:HD23	1:72:A:LEU:H	3	0.12	0.01	0.12
(1,1066)	1:70:A:THR:HB	1:70:A:THR:H	3	0.12	0.01	0.12
(1,1323)	1:86:A:ALA:HB1	1:88:A:ALA:H	3	0.12	0.02	0.11
(1,1323)	1:86:A:ALA:HB2	1:88:A:ALA:H	3	0.12	0.02	0.11
(1,1323)	1:86:A:ALA:HB3	1:88:A:ALA:H	3	0.12	0.02	0.11
(1,940)	1:62:A:ALA:HB1	1:92:A:PHE:H	3	0.12	0.01	0.11
(1,940)	1:62:A:ALA:HB2	1:92:A:PHE:H	3	0.12	0.01	0.11
(1,940)	1:62:A:ALA:HB3	1:92:A:PHE:H	3	0.12	0.01	0.11
(1,1074)	1:70:A:THR:HG21	1:72:A:LEU:H	3	0.12	0.01	0.11
(1,1074)	1:70:A:THR:HG22	1:72:A:LEU:H	3	0.12	0.01	0.11
(1,1074)	1:70:A:THR:HG23	1:72:A:LEU:H	3	0.12	0.01	0.11
(1,189)	1:18:A:TRP:HD1	1:85:A:GLN:HB3	3	0.11	0.0	0.11
(1,427)	1:27:A:VAL:H	1:29:A:ARG:H	3	0.11	0.0	0.11
(1,899)	1:57:A:ASP:HB2	1:58:A:TRP:H	3	0.11	0.0	0.11
(1,135)	1:13:A:TYR:H	1:13:A:TYR:HB3	3	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,14)	1:91:A:GLN:O	1:23:A:HIS:H	3	0.11	0.01	0.11
(1,270)	1:21:A:SER:HB3	1:32:A:THR:HA	3	0.1	0.0	0.1
(1,235)	1:20:A:LEU:HD11	1:21:A:SER:H	2	0.56	0.0	0.56
(1,235)	1:20:A:LEU:HD12	1:21:A:SER:H	2	0.56	0.0	0.56
(1,235)	1:20:A:LEU:HD13	1:21:A:SER:H	2	0.56	0.0	0.56
(1,37)	1:3:A:LEU:HB2	1:4:A:ASP:H	2	0.53	0.07	0.53
(1,260)	1:20:A:LEU:HD11	1:88:A:ALA:H	2	0.52	0.05	0.52
(1,260)	1:20:A:LEU:HD12	1:88:A:ALA:H	2	0.52	0.05	0.52
(1,260)	1:20:A:LEU:HD13	1:88:A:ALA:H	2	0.52	0.05	0.52
(1,1185)	1:79:A:LEU:HA	1:79:A:LEU:HD11	2	0.44	0.01	0.44
(1,1185)	1:79:A:LEU:HA	1:79:A:LEU:HD12	2	0.44	0.01	0.44
(1,1185)	1:79:A:LEU:HA	1:79:A:LEU:HD13	2	0.44	0.01	0.44
(1,57)	1:6:A:ILE:H	1:6:A:ILE:HB	2	0.44	0.03	0.44
(1,1005)	1:65:A:TRP:HB3	1:70:A:THR:H	2	0.43	0.08	0.43
(1,46)	1:4:A:ASP:H	1:6:A:ILE:HB	2	0.31	0.04	0.31
(1,149)	1:15:A:ASP:H	1:16:A:GLY:HA2	2	0.3	0.01	0.3
(1,27)	1:3:A:LEU:H	1:3:A:LEU:HB3	2	0.27	0.0	0.27
(1,908)	1:58:A:TRP:HB2	1:59:A:SER:H	2	0.22	0.1	0.22
(1,911)	1:58:A:TRP:HB3	1:61:A:HIS:H	2	0.21	0.05	0.21
(1,1178)	1:78:A:THR:HG21	1:81:A:LYS:H	2	0.21	0.01	0.21
(1,1178)	1:78:A:THR:HG22	1:81:A:LYS:H	2	0.21	0.01	0.21
(1,1178)	1:78:A:THR:HG23	1:81:A:LYS:H	2	0.21	0.01	0.21
(1,24)	1:3:A:LEU:H	1:3:A:LEU:HD21	2	0.21	0.09	0.21
(1,24)	1:3:A:LEU:H	1:3:A:LEU:HD22	2	0.21	0.09	0.21
(1,24)	1:3:A:LEU:H	1:3:A:LEU:HD23	2	0.21	0.09	0.21
(1,44)	1:4:A:ASP:HA	1:6:A:ILE:H	2	0.2	0.03	0.2
(1,59)	1:6:A:ILE:H	1:6:A:ILE:HD11	2	0.2	0.02	0.2
(1,59)	1:6:A:ILE:H	1:6:A:ILE:HD12	2	0.2	0.02	0.2
(1,59)	1:6:A:ILE:H	1:6:A:ILE:HD13	2	0.2	0.02	0.2
(1,370)	1:24:A:VAL:H	1:29:A:ARG:H	2	0.2	0.06	0.2
(1,921)	1:60:A:ASP:HB3	1:61:A:HIS:H	2	0.2	0.04	0.2
(1,378)	1:24:A:VAL:HA	1:30:A:ASP:HB3	2	0.18	0.02	0.18
(1,869)	1:52:A:LEU:H	1:52:A:LEU:HD21	2	0.18	0.04	0.18
(1,869)	1:52:A:LEU:H	1:52:A:LEU:HD22	2	0.18	0.04	0.18
(1,869)	1:52:A:LEU:H	1:52:A:LEU:HD23	2	0.18	0.04	0.18
(1,84)	1:7:A:ARG:H	1:8:A:MET:H	2	0.16	0.01	0.16
(1,110)	1:9:A:PRO:HB2	1:10:A:ASP:H	2	0.16	0.06	0.16
(1,33)	1:3:A:LEU:H	1:4:A:ASP:HB3	2	0.16	0.05	0.16
(1,402)	1:25:A:THR:HA	1:29:A:ARG:H	2	0.16	0.05	0.16
(1,58)	1:6:A:ILE:H	1:6:A:ILE:HG21	2	0.15	0.0	0.15
(1,58)	1:6:A:ILE:H	1:6:A:ILE:HG22	2	0.15	0.0	0.15
(1,58)	1:6:A:ILE:H	1:6:A:ILE:HG23	2	0.15	0.0	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,65)	1:6:A:ILE:HA	1:7:A:ARG:H	2	0.14	0.0	0.14
(1,983)	1:64:A:TRP:HB2	1:65:A:TRP:H	2	0.14	0.02	0.14
(1,89)	1:8:A:MET:H	1:8:A:MET:HG2	2	0.14	0.01	0.14
(1,627)	1:40:A:HIS:HB3	1:43:A:GLY:H	2	0.14	0.04	0.14
(1,941)	1:62:A:ALA:H	1:92:A:PHE:HA	2	0.14	0.01	0.14
(1,961)	1:63:A:LEU:H	1:70:A:THR:HG21	2	0.14	0.01	0.14
(1,961)	1:63:A:LEU:H	1:70:A:THR:HG22	2	0.14	0.01	0.14
(1,961)	1:63:A:LEU:H	1:70:A:THR:HG23	2	0.14	0.01	0.14
(1,1018)	1:65:A:TRP:HB2	1:91:A:GLN:HG3	2	0.14	0.01	0.14
(1,140)	1:13:A:TYR:HB3	1:15:A:ASP:H	2	0.12	0.02	0.12
(1,236)	1:20:A:LEU:HD21	1:21:A:SER:H	2	0.12	0.01	0.12
(1,236)	1:20:A:LEU:HD22	1:21:A:SER:H	2	0.12	0.01	0.12
(1,236)	1:20:A:LEU:HD23	1:21:A:SER:H	2	0.12	0.01	0.12
(1,1003)	1:65:A:TRP:H	1:70:A:THR:H	2	0.12	0.01	0.12
(1,1035)	1:67:A:LYS:HE3	1:67:A:LYS:HG3	2	0.12	0.02	0.12
(1,390)	1:24:A:VAL:HG21	1:91:A:GLN:H	2	0.12	0.01	0.12
(1,390)	1:24:A:VAL:HG22	1:91:A:GLN:H	2	0.12	0.01	0.12
(1,390)	1:24:A:VAL:HG23	1:91:A:GLN:H	2	0.12	0.01	0.12
(1,999)	1:65:A:TRP:HA	1:67:A:LYS:H	2	0.12	0.01	0.12
(1,1078)	1:71:A:TRP:H	1:72:A:LEU:HD11	2	0.12	0.0	0.12
(1,1078)	1:71:A:TRP:H	1:72:A:LEU:HD12	2	0.12	0.0	0.12
(1,1078)	1:71:A:TRP:H	1:72:A:LEU:HD13	2	0.12	0.0	0.12
(1,259)	1:20:A:LEU:HD21	1:88:A:ALA:H	2	0.12	0.02	0.12
(1,259)	1:20:A:LEU:HD22	1:88:A:ALA:H	2	0.12	0.02	0.12
(1,259)	1:20:A:LEU:HD23	1:88:A:ALA:H	2	0.12	0.02	0.12
(1,794)	1:48:A:LEU:H	1:48:A:LEU:HD11	2	0.12	0.02	0.12
(1,794)	1:48:A:LEU:H	1:48:A:LEU:HD12	2	0.12	0.02	0.12
(1,794)	1:48:A:LEU:H	1:48:A:LEU:HD13	2	0.12	0.02	0.12
(1,1202)	1:79:A:LEU:HA	1:82:A:TYR:H	2	0.12	0.02	0.12
(1,79)	1:7:A:ARG:HD3	1:7:A:ARG:HB2	2	0.12	0.0	0.12
(1,96)	1:8:A:MET:HG3	1:10:A:ASP:H	2	0.12	0.0	0.12
(1,306)	1:22:A:VAL:HB	1:48:A:LEU:HD21	2	0.12	0.0	0.12
(1,306)	1:22:A:VAL:HB	1:48:A:LEU:HD22	2	0.12	0.0	0.12
(1,306)	1:22:A:VAL:HB	1:48:A:LEU:HD23	2	0.12	0.0	0.12
(1,741)	1:45:A:MET:H	1:48:A:LEU:HD11	2	0.12	0.0	0.12
(1,741)	1:45:A:MET:H	1:48:A:LEU:HD12	2	0.12	0.0	0.12
(1,741)	1:45:A:MET:H	1:48:A:LEU:HD13	2	0.12	0.0	0.12
(1,1211)	1:80:A:ASP:H	1:80:A:ASP:HB2	2	0.12	0.0	0.12
(1,386)	1:24:A:VAL:HG21	1:31:A:VAL:HB	2	0.11	0.0	0.11
(1,386)	1:24:A:VAL:HG22	1:31:A:VAL:HB	2	0.11	0.0	0.11
(1,386)	1:24:A:VAL:HG23	1:31:A:VAL:HB	2	0.11	0.0	0.11
(1,563)	1:37:A:GLY:HA3	1:38:A:GLU:H	2	0.11	0.01	0.11

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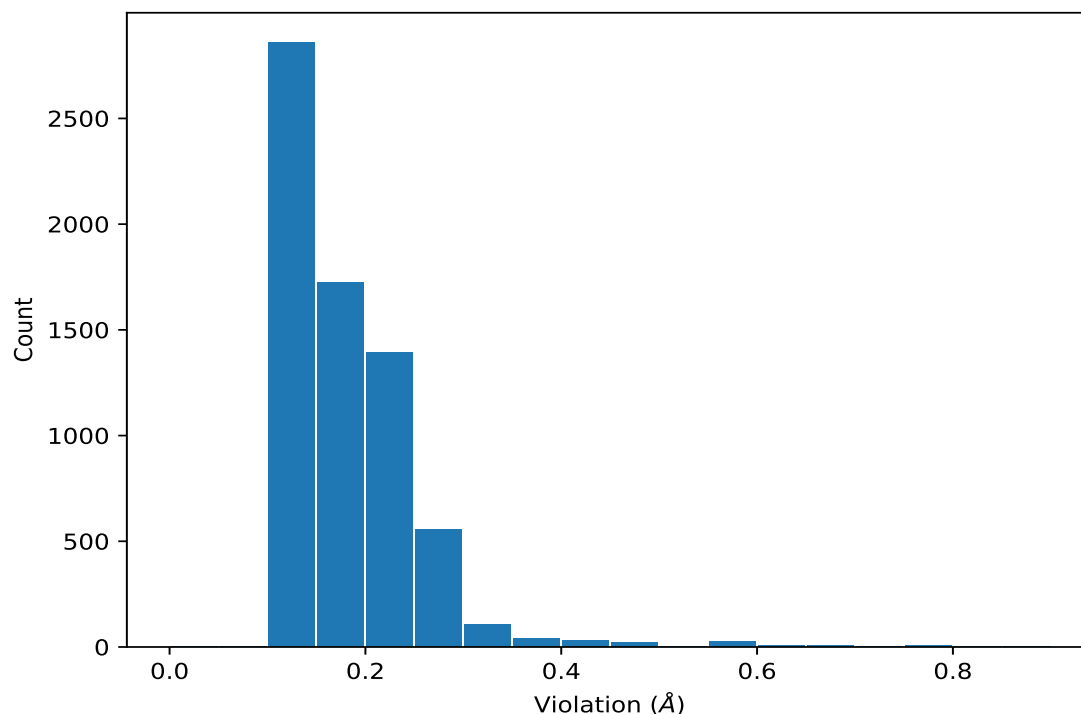
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1052)	1:67:A:LYS:H	1:72:A:LEU:HD11	2	0.11	0.01	0.11
(1,1052)	1:67:A:LYS:H	1:72:A:LEU:HD12	2	0.11	0.01	0.11
(1,1052)	1:67:A:LYS:H	1:72:A:LEU:HD13	2	0.11	0.01	0.11
(1,1120)	1:74:A:LYS:H	1:74:A:LYS:HG2	2	0.11	0.01	0.11
(1,1144)	1:75:A:THR:H	1:75:A:THR:HG21	2	0.11	0.01	0.11
(1,1144)	1:75:A:THR:H	1:75:A:THR:HG22	2	0.11	0.01	0.11
(1,1144)	1:75:A:THR:H	1:75:A:THR:HG23	2	0.11	0.01	0.11
(1,837)	1:49:A:VAL:HA	1:52:A:LEU:H	2	0.11	0.0	0.11
(1,1119)	1:74:A:LYS:H	1:74:A:LYS:HE2	2	0.11	0.0	0.11
(1,464)	1:31:A:VAL:HA	1:32:A:THR:HB	2	0.1	0.0	0.1
(1,584)	1:38:A:GLU:H	1:39:A:VAL:HG11	2	0.1	0.0	0.1
(1,584)	1:38:A:GLU:H	1:39:A:VAL:HG12	2	0.1	0.0	0.1
(1,584)	1:38:A:GLU:H	1:39:A:VAL:HG13	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



9.5.2 Table : All distance violations

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,519)	1:34:A:ARG:HD3	1:34:A:ARG:HA	20	0.89
(1,100)	1:8:A:MET:H	1:12:A:CYS:HA	14	0.85
(1,100)	1:8:A:MET:H	1:12:A:CYS:HA	7	0.82
(1,520)	1:34:A:ARG:HG3	1:34:A:ARG:HA	13	0.78
(1,100)	1:8:A:MET:H	1:12:A:CYS:HA	4	0.78
(1,520)	1:34:A:ARG:HG3	1:34:A:ARG:HA	9	0.77
(1,520)	1:34:A:ARG:HG3	1:34:A:ARG:HA	16	0.77
(1,520)	1:34:A:ARG:HG3	1:34:A:ARG:HA	18	0.77
(1,994)	1:65:A:TRP:H	1:65:A:TRP:HB2	18	0.68
(1,994)	1:65:A:TRP:H	1:65:A:TRP:HB2	13	0.65
(1,100)	1:8:A:MET:H	1:12:A:CYS:HA	17	0.65
(1,20)	1:2:A:ALA:HB1	1:4:A:ASP:H	14	0.65
(1,20)	1:2:A:ALA:HB2	1:4:A:ASP:H	14	0.65
(1,20)	1:2:A:ALA:HB3	1:4:A:ASP:H	14	0.65
(1,20)	1:2:A:ALA:HB1	1:4:A:ASP:H	16	0.64
(1,20)	1:2:A:ALA:HB2	1:4:A:ASP:H	16	0.64
(1,20)	1:2:A:ALA:HB3	1:4:A:ASP:H	16	0.64
(1,1199)	1:79:A:LEU:HG	1:81:A:LYS:H	11	0.61
(1,1199)	1:79:A:LEU:HG	1:81:A:LYS:H	16	0.61
(1,1020)	1:66:A:GLU:H	1:66:A:GLU:HB3	1	0.61
(1,1020)	1:66:A:GLU:H	1:66:A:GLU:HB3	3	0.61
(1,428)	1:27:A:VAL:HG11	1:29:A:ARG:H	11	0.6
(1,428)	1:27:A:VAL:HG12	1:29:A:ARG:H	11	0.6
(1,428)	1:27:A:VAL:HG13	1:29:A:ARG:H	11	0.6
(1,74)	1:7:A:ARG:H	1:7:A:ARG:HB3	17	0.6
(1,37)	1:3:A:LEU:HB2	1:4:A:ASP:H	14	0.6
(1,1199)	1:79:A:LEU:HG	1:81:A:LYS:H	20	0.59
(1,1020)	1:66:A:GLU:H	1:66:A:GLU:HB3	15	0.59
(1,1020)	1:66:A:GLU:H	1:66:A:GLU:HB3	17	0.59
(1,1020)	1:66:A:GLU:H	1:66:A:GLU:HB3	18	0.59
(1,520)	1:34:A:ARG:HG3	1:34:A:ARG:HA	20	0.59
(1,74)	1:7:A:ARG:H	1:7:A:ARG:HB3	20	0.59
(1,1199)	1:79:A:LEU:HG	1:81:A:LYS:H	2	0.58
(1,1020)	1:66:A:GLU:H	1:66:A:GLU:HB3	20	0.58
(1,905)	1:58:A:TRP:H	1:58:A:TRP:HB2	15	0.58
(1,905)	1:58:A:TRP:H	1:58:A:TRP:HB2	8	0.57
(1,28)	1:3:A:LEU:H	1:3:A:LEU:HB2	10	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,260)	1:20:A:LEU:HD11	1:88:A:ALA:H	6	0.56
(1,260)	1:20:A:LEU:HD12	1:88:A:ALA:H	6	0.56
(1,260)	1:20:A:LEU:HD13	1:88:A:ALA:H	6	0.56
(1,235)	1:20:A:LEU:HD11	1:21:A:SER:H	6	0.56
(1,235)	1:20:A:LEU:HD12	1:21:A:SER:H	6	0.56
(1,235)	1:20:A:LEU:HD13	1:21:A:SER:H	6	0.56
(1,235)	1:20:A:LEU:HD11	1:21:A:SER:H	19	0.56
(1,235)	1:20:A:LEU:HD12	1:21:A:SER:H	19	0.56
(1,235)	1:20:A:LEU:HD13	1:21:A:SER:H	19	0.56
(1,515)	1:34:A:ARG:H	1:34:A:ARG:HB3	20	0.54
(1,28)	1:3:A:LEU:H	1:3:A:LEU:HB2	3	0.54
(1,1005)	1:65:A:TRP:HB3	1:70:A:THR:H	18	0.51
(1,905)	1:58:A:TRP:H	1:58:A:TRP:HB2	20	0.49
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD11	19	0.49
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD12	19	0.49
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD13	19	0.49
(1,68)	1:6:A:ILE:HA	1:10:A:ASP:H	5	0.48
(1,18)	1:2:A:ALA:HA	1:3:A:LEU:H	20	0.48
(1,260)	1:20:A:LEU:HD11	1:88:A:ALA:H	19	0.47
(1,260)	1:20:A:LEU:HD12	1:88:A:ALA:H	19	0.47
(1,260)	1:20:A:LEU:HD13	1:88:A:ALA:H	19	0.47
(1,153)	1:15:A:ASP:H	1:17:A:THR:H	17	0.47
(1,57)	1:6:A:ILE:H	1:6:A:ILE:HB	11	0.47
(1,18)	1:2:A:ALA:HA	1:3:A:LEU:H	18	0.47
(1,1246)	1:81:A:LYS:HE3	1:82:A:TYR:H	18	0.46
(1,162)	1:17:A:THR:HB	1:18:A:TRP:H	7	0.46
(1,37)	1:3:A:LEU:HB2	1:4:A:ASP:H	16	0.46
(1,1246)	1:81:A:LYS:HE3	1:82:A:TYR:H	20	0.45
(1,1185)	1:79:A:LEU:HA	1:79:A:LEU:HD11	13	0.45
(1,1185)	1:79:A:LEU:HA	1:79:A:LEU:HD12	13	0.45
(1,1185)	1:79:A:LEU:HA	1:79:A:LEU:HD13	13	0.45
(1,910)	1:58:A:TRP:HB3	1:59:A:SER:H	10	0.45
(1,1185)	1:79:A:LEU:HA	1:79:A:LEU:HD11	19	0.44
(1,1185)	1:79:A:LEU:HA	1:79:A:LEU:HD12	19	0.44
(1,1185)	1:79:A:LEU:HA	1:79:A:LEU:HD13	19	0.44
(1,721)	1:45:A:MET:HA	1:45:A:MET:HG3	19	0.44
(1,414)	1:25:A:THR:H	1:93:A:THR:HG21	15	0.44
(1,414)	1:25:A:THR:H	1:93:A:THR:HG22	15	0.44
(1,414)	1:25:A:THR:H	1:93:A:THR:HG23	15	0.44
(1,1199)	1:79:A:LEU:HG	1:81:A:LYS:H	3	0.43
(1,870)	1:52:A:LEU:HG	1:52:A:LEU:HA	18	0.43
(1,153)	1:15:A:ASP:H	1:17:A:THR:H	10	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1199)	1:79:A:LEU:HG	1:81:A:LYS:H	4	0.42
(1,910)	1:58:A:TRP:HB3	1:59:A:SER:H	8	0.42
(1,870)	1:52:A:LEU:HG	1:52:A:LEU:HA	16	0.42
(1,588)	1:38:A:GLU:HA	1:80:A:ASP:H	8	0.42
(1,75)	1:7:A:ARG:H	1:7:A:ARG:HB2	5	0.42
(1,68)	1:6:A:ILE:HA	1:10:A:ASP:H	9	0.42
(1,18)	1:2:A:ALA:HA	1:3:A:LEU:H	15	0.42
(1,1246)	1:81:A:LYS:HE3	1:82:A:TYR:H	15	0.41
(1,1199)	1:79:A:LEU:HG	1:81:A:LYS:H	5	0.41
(1,1199)	1:79:A:LEU:HG	1:81:A:LYS:H	12	0.41
(1,483)	1:32:A:THR:H	1:34:A:ARG:H	19	0.41
(1,57)	1:6:A:ILE:H	1:6:A:ILE:HB	16	0.41
(1,1148)	1:75:A:THR:HG21	1:77:A:TRP:H	15	0.4
(1,1148)	1:75:A:THR:HG22	1:77:A:TRP:H	15	0.4
(1,1148)	1:75:A:THR:HG23	1:77:A:TRP:H	15	0.4
(1,910)	1:58:A:TRP:HB3	1:59:A:SER:H	20	0.4
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD11	6	0.4
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD12	6	0.4
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD13	6	0.4
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD21	9	0.4
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD22	9	0.4
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD23	9	0.4
(1,162)	1:17:A:THR:HB	1:18:A:TRP:H	16	0.4
(1,1148)	1:75:A:THR:HG21	1:77:A:TRP:H	18	0.39
(1,1148)	1:75:A:THR:HG22	1:77:A:TRP:H	18	0.39
(1,1148)	1:75:A:THR:HG23	1:77:A:TRP:H	18	0.39
(1,870)	1:52:A:LEU:HG	1:52:A:LEU:HA	12	0.39
(1,839)	1:49:A:VAL:HG21	1:58:A:TRP:HB2	11	0.39
(1,839)	1:49:A:VAL:HG22	1:58:A:TRP:HB2	11	0.39
(1,839)	1:49:A:VAL:HG23	1:58:A:TRP:HB2	11	0.39
(1,162)	1:17:A:THR:HB	1:18:A:TRP:H	17	0.39
(1,88)	1:8:A:MET:H	1:8:A:MET:HB3	4	0.39
(1,88)	1:8:A:MET:H	1:8:A:MET:HB3	7	0.39
(1,88)	1:8:A:MET:H	1:8:A:MET:HB3	17	0.39
(1,39)	1:4:A:ASP:H	1:4:A:ASP:HB3	3	0.39
(1,39)	1:4:A:ASP:H	1:4:A:ASP:HB3	9	0.39
(1,1053)	1:67:A:LYS:H	1:88:A:ALA:HA	2	0.38
(1,162)	1:17:A:THR:HB	1:18:A:TRP:H	5	0.38
(1,103)	1:8:A:MET:HG3	1:12:A:CYS:HB3	5	0.38
(1,39)	1:4:A:ASP:H	1:4:A:ASP:HB3	2	0.38
(1,39)	1:4:A:ASP:H	1:4:A:ASP:HB3	13	0.38
(1,39)	1:4:A:ASP:H	1:4:A:ASP:HB3	20	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,146)	1:15:A:ASP:H	1:15:A:ASP:HB3	10	0.37
(1,145)	1:14:A:ALA:HB1	1:16:A:GLY:H	19	0.37
(1,145)	1:14:A:ALA:HB2	1:16:A:GLY:H	19	0.37
(1,145)	1:14:A:ALA:HB3	1:16:A:GLY:H	19	0.37
(1,88)	1:8:A:MET:H	1:8:A:MET:HB3	14	0.37
(1,87)	1:7:A:ARG:HG3	1:10:A:ASP:H	12	0.37
(1,68)	1:6:A:ILE:HA	1:10:A:ASP:H	12	0.37
(1,39)	1:4:A:ASP:H	1:4:A:ASP:HB3	18	0.37
(1,1216)	1:80:A:ASP:H	1:81:A:LYS:HD2	18	0.36
(1,1162)	1:77:A:TRP:H	1:81:A:LYS:HE3	15	0.36
(1,1033)	1:67:A:LYS:HA	1:67:A:LYS:HD3	12	0.36
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD11	14	0.36
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD12	14	0.36
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD13	14	0.36
(1,818)	1:48:A:LEU:HD21	1:52:A:LEU:H	18	0.36
(1,818)	1:48:A:LEU:HD22	1:52:A:LEU:H	18	0.36
(1,818)	1:48:A:LEU:HD23	1:52:A:LEU:H	18	0.36
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD21	14	0.36
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD22	14	0.36
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD23	14	0.36
(1,162)	1:17:A:THR:HB	1:18:A:TRP:H	3	0.36
(1,75)	1:7:A:ARG:H	1:7:A:ARG:HB2	12	0.36
(1,68)	1:6:A:ILE:HA	1:10:A:ASP:H	7	0.36
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD11	19	0.35
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD12	19	0.35
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD13	19	0.35
(1,1053)	1:67:A:LYS:H	1:88:A:ALA:HA	6	0.35
(1,945)	1:62:A:ALA:HB1	1:93:A:THR:HA	8	0.35
(1,945)	1:62:A:ALA:HB2	1:93:A:THR:HA	8	0.35
(1,945)	1:62:A:ALA:HB3	1:93:A:THR:HA	8	0.35
(1,904)	1:58:A:TRP:H	1:58:A:TRP:HB3	2	0.35
(1,903)	1:57:A:ASP:HB2	1:61:A:HIS:H	10	0.35
(1,838)	1:49:A:VAL:HG21	1:58:A:TRP:H	7	0.35
(1,838)	1:49:A:VAL:HG22	1:58:A:TRP:H	7	0.35
(1,838)	1:49:A:VAL:HG23	1:58:A:TRP:H	7	0.35
(1,724)	1:45:A:MET:H	1:45:A:MET:HG3	19	0.35
(1,249)	1:20:A:LEU:HB2	1:34:A:ARG:H	6	0.35
(1,162)	1:17:A:THR:HB	1:18:A:TRP:H	1	0.35
(1,36)	1:3:A:LEU:HB3	1:4:A:ASP:H	3	0.35
(2,15)	1:64:A:TRP:O	1:92:A:PHE:H	10	0.34
(1,1076)	1:71:A:TRP:H	1:71:A:TRP:HB3	1	0.34
(1,1076)	1:71:A:TRP:H	1:71:A:TRP:HB3	4	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1076)	1:71:A:TRP:H	1:71:A:TRP:HB3	18	0.34
(1,1072)	1:70:A:THR:H	1:71:A:TRP:H	11	0.34
(1,1063)	1:69:A:ARG:H	1:70:A:THR:H	13	0.34
(1,1005)	1:65:A:TRP:HB3	1:70:A:THR:H	13	0.34
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD11	12	0.34
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD12	12	0.34
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD13	12	0.34
(1,838)	1:49:A:VAL:HG21	1:58:A:TRP:H	2	0.34
(1,838)	1:49:A:VAL:HG22	1:58:A:TRP:H	2	0.34
(1,838)	1:49:A:VAL:HG23	1:58:A:TRP:H	2	0.34
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG21	8	0.34
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG22	8	0.34
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG23	8	0.34
(1,153)	1:15:A:ASP:H	1:17:A:THR:H	14	0.34
(1,46)	1:4:A:ASP:H	1:6:A:ILE:HB	4	0.34
(1,45)	1:4:A:ASP:HB3	1:6:A:ILE:H	9	0.34
(1,36)	1:3:A:LEU:HB3	1:4:A:ASP:H	13	0.34
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG21	8	0.33
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG22	8	0.33
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG23	8	0.33
(1,1162)	1:77:A:TRP:H	1:81:A:LYS:HE3	18	0.33
(1,1141)	1:74:A:LYS:HE3	1:78:A:THR:H	13	0.33
(1,1076)	1:71:A:TRP:H	1:71:A:TRP:HB3	3	0.33
(1,1076)	1:71:A:TRP:H	1:71:A:TRP:HB3	6	0.33
(1,1076)	1:71:A:TRP:H	1:71:A:TRP:HB3	9	0.33
(1,1076)	1:71:A:TRP:H	1:71:A:TRP:HB3	12	0.33
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD11	16	0.33
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD12	16	0.33
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD13	16	0.33
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG21	9	0.33
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG22	9	0.33
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG23	9	0.33
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD21	7	0.33
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD22	7	0.33
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD23	7	0.33
(1,184)	1:18:A:TRP:HE1	1:80:A:ASP:HB3	6	0.33
(1,113)	1:9:A:PRO:HG3	1:12:A:CYS:HB3	4	0.33
(1,85)	1:7:A:ARG:HD3	1:8:A:MET:H	12	0.33
(2,15)	1:64:A:TRP:O	1:92:A:PHE:H	16	0.32
(2,5)	1:31:A:VAL:O	1:22:A:VAL:N	14	0.32
(1,1216)	1:80:A:ASP:H	1:81:A:LYS:HD2	15	0.32
(1,1203)	1:79:A:LEU:HB3	1:83:A:GLY:H	8	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:75:A:THR:HG21	1:77:A:TRP:H	20	0.32
(1,1148)	1:75:A:THR:HG22	1:77:A:TRP:H	20	0.32
(1,1148)	1:75:A:THR:HG23	1:77:A:TRP:H	20	0.32
(1,1076)	1:71:A:TRP:H	1:71:A:TRP:HB3	8	0.32
(1,1076)	1:71:A:TRP:H	1:71:A:TRP:HB3	17	0.32
(1,1033)	1:67:A:LYS:HA	1:67:A:LYS:HD3	4	0.32
(1,1033)	1:67:A:LYS:HA	1:67:A:LYS:HD3	7	0.32
(1,945)	1:62:A:ALA:HB1	1:93:A:THR:HA	9	0.32
(1,945)	1:62:A:ALA:HB2	1:93:A:THR:HA	9	0.32
(1,945)	1:62:A:ALA:HB3	1:93:A:THR:HA	9	0.32
(1,908)	1:58:A:TRP:HB2	1:59:A:SER:H	5	0.32
(1,838)	1:49:A:VAL:HG21	1:58:A:TRP:H	14	0.32
(1,838)	1:49:A:VAL:HG22	1:58:A:TRP:H	14	0.32
(1,838)	1:49:A:VAL:HG23	1:58:A:TRP:H	14	0.32
(1,671)	1:41:A:ILE:HD11	1:75:A:THR:HA	13	0.32
(1,671)	1:41:A:ILE:HD12	1:75:A:THR:HA	13	0.32
(1,671)	1:41:A:ILE:HD13	1:75:A:THR:HA	13	0.32
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG11	16	0.32
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG12	16	0.32
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG13	16	0.32
(1,242)	1:20:A:LEU:HB3	1:33:A:LEU:H	19	0.32
(1,95)	1:8:A:MET:HA	1:10:A:ASP:H	9	0.32
(1,95)	1:8:A:MET:HA	1:10:A:ASP:H	20	0.32
(1,94)	1:8:A:MET:H	1:10:A:ASP:HA	1	0.32
(1,42)	1:4:A:ASP:H	1:5:A:GLY:HA3	2	0.32
(1,36)	1:3:A:LEU:HB3	1:4:A:ASP:H	10	0.32
(3,21)	1:80:A:ASP:O	1:84:A:ILE:H	4	0.31
(3,21)	1:80:A:ASP:O	1:84:A:ILE:H	12	0.31
(2,5)	1:31:A:VAL:O	1:22:A:VAL:N	9	0.31
(1,1408)	1:92:A:PHE:HB3	1:93:A:THR:H	3	0.31
(1,1159)	1:77:A:TRP:HB3	1:78:A:THR:H	16	0.31
(1,1033)	1:67:A:LYS:HA	1:67:A:LYS:HD3	10	0.31
(1,910)	1:58:A:TRP:HB3	1:59:A:SER:H	15	0.31
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG21	16	0.31
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG22	16	0.31
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG23	16	0.31
(1,511)	1:33:A:LEU:HD21	1:48:A:LEU:HB3	10	0.31
(1,511)	1:33:A:LEU:HD22	1:48:A:LEU:HB3	10	0.31
(1,511)	1:33:A:LEU:HD23	1:48:A:LEU:HB3	10	0.31
(1,453)	1:29:A:ARG:HB2	1:31:A:VAL:HA	19	0.31
(1,431)	1:27:A:VAL:H	1:93:A:THR:HB	12	0.31
(1,419)	1:27:A:VAL:H	1:27:A:VAL:HB	11	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,297)	1:22:A:VAL:H	1:31:A:VAL:H	14	0.31
(1,95)	1:8:A:MET:HA	1:10:A:ASP:H	6	0.31
(1,95)	1:8:A:MET:HA	1:10:A:ASP:H	8	0.31
(1,94)	1:8:A:MET:H	1:10:A:ASP:HA	12	0.31
(1,78)	1:7:A:ARG:HD3	1:7:A:ARG:HB3	5	0.31
(2,5)	1:31:A:VAL:O	1:22:A:VAL:N	8	0.3
(2,5)	1:31:A:VAL:O	1:22:A:VAL:N	17	0.3
(2,5)	1:31:A:VAL:O	1:22:A:VAL:N	20	0.3
(1,1408)	1:92:A:PHE:HB3	1:93:A:THR:H	10	0.3
(1,1205)	1:79:A:LEU:HD11	1:83:A:GLY:H	4	0.3
(1,1205)	1:79:A:LEU:HD12	1:83:A:GLY:H	4	0.3
(1,1205)	1:79:A:LEU:HD13	1:83:A:GLY:H	4	0.3
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD11	13	0.3
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD12	13	0.3
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD13	13	0.3
(1,1162)	1:77:A:TRP:H	1:81:A:LYS:HE3	6	0.3
(1,1159)	1:77:A:TRP:HB3	1:78:A:THR:H	4	0.3
(1,1159)	1:77:A:TRP:HB3	1:78:A:THR:H	12	0.3
(1,1159)	1:77:A:TRP:HB3	1:78:A:THR:H	13	0.3
(1,1076)	1:71:A:TRP:H	1:71:A:TRP:HB3	7	0.3
(1,1033)	1:67:A:LYS:HA	1:67:A:LYS:HD3	1	0.3
(1,1033)	1:67:A:LYS:HA	1:67:A:LYS:HD3	3	0.3
(1,1033)	1:67:A:LYS:HA	1:67:A:LYS:HD3	9	0.3
(1,1033)	1:67:A:LYS:HA	1:67:A:LYS:HD3	17	0.3
(1,766)	1:46:A:LEU:HA	1:50:A:GLU:H	19	0.3
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD21	9	0.3
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD22	9	0.3
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD23	9	0.3
(1,371)	1:24:A:VAL:HG11	1:29:A:ARG:H	3	0.3
(1,371)	1:24:A:VAL:HG12	1:29:A:ARG:H	3	0.3
(1,371)	1:24:A:VAL:HG13	1:29:A:ARG:H	3	0.3
(1,340)	1:23:A:HIS:H	1:91:A:GLN:HA	15	0.3
(1,266)	1:21:A:SER:H	1:22:A:VAL:H	6	0.3
(1,266)	1:21:A:SER:H	1:22:A:VAL:H	19	0.3
(1,175)	1:18:A:TRP:H	1:35:A:VAL:HA	3	0.3
(1,149)	1:15:A:ASP:H	1:16:A:GLY:HA2	2	0.3
(1,95)	1:8:A:MET:HA	1:10:A:ASP:H	2	0.3
(1,75)	1:7:A:ARG:H	1:7:A:ARG:HB2	3	0.3
(1,61)	1:6:A:ILE:H	1:7:A:ARG:H	12	0.3
(1,42)	1:4:A:ASP:H	1:5:A:GLY:HA3	15	0.3
(1,24)	1:3:A:LEU:H	1:3:A:LEU:HD21	2	0.3
(1,24)	1:3:A:LEU:H	1:3:A:LEU:HD22	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:3:A:LEU:H	1:3:A:LEU:HD23	2	0.3
(2,18)	1:23:A:HIS:O	1:93:A:THR:N	13	0.29
(2,5)	1:31:A:VAL:O	1:22:A:VAL:N	10	0.29
(2,5)	1:31:A:VAL:O	1:22:A:VAL:N	11	0.29
(2,5)	1:31:A:VAL:O	1:22:A:VAL:N	13	0.29
(2,5)	1:31:A:VAL:O	1:22:A:VAL:N	16	0.29
(1,1402)	1:92:A:PHE:H	1:92:A:PHE:HB2	10	0.29
(1,1328)	1:87:A:ASP:HA	1:88:A:ALA:H	6	0.29
(1,1159)	1:77:A:TRP:HB3	1:78:A:THR:H	5	0.29
(1,1076)	1:71:A:TRP:H	1:71:A:TRP:HB3	15	0.29
(1,906)	1:58:A:TRP:H	1:59:A:SER:H	15	0.29
(1,838)	1:49:A:VAL:HG21	1:58:A:TRP:H	16	0.29
(1,838)	1:49:A:VAL:HG22	1:58:A:TRP:H	16	0.29
(1,838)	1:49:A:VAL:HG23	1:58:A:TRP:H	16	0.29
(1,818)	1:48:A:LEU:HD21	1:52:A:LEU:H	16	0.29
(1,818)	1:48:A:LEU:HD22	1:52:A:LEU:H	16	0.29
(1,818)	1:48:A:LEU:HD23	1:52:A:LEU:H	16	0.29
(1,818)	1:48:A:LEU:HD21	1:52:A:LEU:H	19	0.29
(1,818)	1:48:A:LEU:HD22	1:52:A:LEU:H	19	0.29
(1,818)	1:48:A:LEU:HD23	1:52:A:LEU:H	19	0.29
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG21	7	0.29
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG22	7	0.29
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG23	7	0.29
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG21	12	0.29
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG22	12	0.29
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG23	12	0.29
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD21	20	0.29
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD22	20	0.29
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD23	20	0.29
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD21	17	0.29
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD22	17	0.29
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD23	17	0.29
(1,453)	1:29:A:ARG:HB2	1:31:A:VAL:HA	11	0.29
(1,431)	1:27:A:VAL:H	1:93:A:THR:HB	15	0.29
(1,340)	1:23:A:HIS:H	1:91:A:GLN:HA	19	0.29
(1,184)	1:18:A:TRP:HE1	1:80:A:ASP:HB3	10	0.29
(1,149)	1:15:A:ASP:H	1:16:A:GLY:HA2	10	0.29
(1,137)	1:13:A:TYR:HA	1:14:A:ALA:H	19	0.29
(1,115)	1:9:A:PRO:HA	1:13:A:TYR:H	14	0.29
(1,95)	1:8:A:MET:HA	1:10:A:ASP:H	5	0.29
(1,95)	1:8:A:MET:HA	1:10:A:ASP:H	11	0.29
(1,95)	1:8:A:MET:HA	1:10:A:ASP:H	15	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,68)	1:6:A:ILE:HA	1:10:A:ASP:H	4	0.29
(3,21)	1:80:A:ASP:O	1:84:A:ILE:H	5	0.28
(2,18)	1:23:A:HIS:O	1:93:A:THR:N	3	0.28
(2,18)	1:23:A:HIS:O	1:93:A:THR:N	14	0.28
(2,15)	1:64:A:TRP:O	1:92:A:PHE:H	6	0.28
(2,15)	1:64:A:TRP:O	1:92:A:PHE:H	8	0.28
(2,5)	1:31:A:VAL:O	1:22:A:VAL:N	2	0.28
(2,5)	1:31:A:VAL:O	1:22:A:VAL:N	3	0.28
(2,5)	1:31:A:VAL:O	1:22:A:VAL:N	4	0.28
(2,5)	1:31:A:VAL:O	1:22:A:VAL:N	5	0.28
(2,5)	1:31:A:VAL:O	1:22:A:VAL:N	6	0.28
(2,5)	1:31:A:VAL:O	1:22:A:VAL:N	12	0.28
(2,5)	1:31:A:VAL:O	1:22:A:VAL:N	15	0.28
(2,5)	1:31:A:VAL:O	1:22:A:VAL:N	18	0.28
(2,4)	1:33:A:LEU:O	1:20:A:LEU:N	20	0.28
(1,1218)	1:80:A:ASP:HB2	1:82:A:TYR:H	20	0.28
(1,1205)	1:79:A:LEU:HD11	1:83:A:GLY:H	3	0.28
(1,1205)	1:79:A:LEU:HD12	1:83:A:GLY:H	3	0.28
(1,1205)	1:79:A:LEU:HD13	1:83:A:GLY:H	3	0.28
(1,1205)	1:79:A:LEU:HD11	1:83:A:GLY:H	5	0.28
(1,1205)	1:79:A:LEU:HD12	1:83:A:GLY:H	5	0.28
(1,1205)	1:79:A:LEU:HD13	1:83:A:GLY:H	5	0.28
(1,1205)	1:79:A:LEU:HD11	1:83:A:GLY:H	12	0.28
(1,1205)	1:79:A:LEU:HD12	1:83:A:GLY:H	12	0.28
(1,1205)	1:79:A:LEU:HD13	1:83:A:GLY:H	12	0.28
(1,1177)	1:78:A:THR:H	1:81:A:LYS:H	4	0.28
(1,1162)	1:77:A:TRP:H	1:81:A:LYS:HE3	10	0.28
(1,1160)	1:77:A:TRP:HB2	1:78:A:THR:H	16	0.28
(1,1033)	1:67:A:LYS:HA	1:67:A:LYS:HD3	8	0.28
(1,1033)	1:67:A:LYS:HA	1:67:A:LYS:HD3	19	0.28
(1,818)	1:48:A:LEU:HD21	1:52:A:LEU:H	17	0.28
(1,818)	1:48:A:LEU:HD22	1:52:A:LEU:H	17	0.28
(1,818)	1:48:A:LEU:HD23	1:52:A:LEU:H	17	0.28
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG21	5	0.28
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG22	5	0.28
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG23	5	0.28
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG21	11	0.28
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG22	11	0.28
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG23	11	0.28
(1,773)	1:47:A:LYS:H	1:47:A:LYS:HD3	17	0.28
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD21	7	0.28
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD22	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD23	7	0.28
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG11	20	0.28
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG12	20	0.28
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG13	20	0.28
(1,610)	1:39:A:VAL:HG21	1:80:A:ASP:H	11	0.28
(1,610)	1:39:A:VAL:HG22	1:80:A:ASP:H	11	0.28
(1,610)	1:39:A:VAL:HG23	1:80:A:ASP:H	11	0.28
(1,610)	1:39:A:VAL:HG21	1:80:A:ASP:H	16	0.28
(1,610)	1:39:A:VAL:HG22	1:80:A:ASP:H	16	0.28
(1,610)	1:39:A:VAL:HG23	1:80:A:ASP:H	16	0.28
(1,610)	1:39:A:VAL:HG21	1:80:A:ASP:H	20	0.28
(1,610)	1:39:A:VAL:HG22	1:80:A:ASP:H	20	0.28
(1,610)	1:39:A:VAL:HG23	1:80:A:ASP:H	20	0.28
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD21	1	0.28
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD22	1	0.28
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD23	1	0.28
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD21	10	0.28
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD22	10	0.28
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD23	10	0.28
(1,483)	1:32:A:THR:H	1:34:A:ARG:H	15	0.28
(1,184)	1:18:A:TRP:HE1	1:80:A:ASP:HB3	1	0.28
(1,184)	1:18:A:TRP:HE1	1:80:A:ASP:HB3	9	0.28
(1,184)	1:18:A:TRP:HE1	1:80:A:ASP:HB3	14	0.28
(1,115)	1:9:A:PRO:HA	1:13:A:TYR:H	7	0.28
(1,95)	1:8:A:MET:HA	1:10:A:ASP:H	3	0.28
(1,95)	1:8:A:MET:HA	1:10:A:ASP:H	18	0.28
(1,94)	1:8:A:MET:H	1:10:A:ASP:HA	10	0.28
(1,75)	1:7:A:ARG:H	1:7:A:ARG:HB2	9	0.28
(1,66)	1:6:A:ILE:HB	1:8:A:MET:H	17	0.28
(1,49)	1:5:A:GLY:HA3	1:6:A:ILE:HB	14	0.28
(1,42)	1:4:A:ASP:H	1:5:A:GLY:HA3	8	0.28
(1,39)	1:4:A:ASP:H	1:4:A:ASP:HB3	8	0.28
(1,34)	1:3:A:LEU:HD21	1:4:A:ASP:H	12	0.28
(1,34)	1:3:A:LEU:HD22	1:4:A:ASP:H	12	0.28
(1,34)	1:3:A:LEU:HD23	1:4:A:ASP:H	12	0.28
(3,21)	1:80:A:ASP:O	1:84:A:ILE:H	3	0.27
(2,18)	1:23:A:HIS:O	1:93:A:THR:N	5	0.27
(2,18)	1:23:A:HIS:O	1:93:A:THR:N	11	0.27
(2,18)	1:23:A:HIS:O	1:93:A:THR:N	12	0.27
(2,18)	1:23:A:HIS:O	1:93:A:THR:N	18	0.27
(2,15)	1:64:A:TRP:O	1:92:A:PHE:H	3	0.27
(2,15)	1:64:A:TRP:O	1:92:A:PHE:H	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,15)	1:64:A:TRP:O	1:92:A:PHE:H	12	0.27
(2,15)	1:64:A:TRP:O	1:92:A:PHE:H	19	0.27
(2,5)	1:31:A:VAL:O	1:22:A:VAL:N	1	0.27
(2,5)	1:31:A:VAL:O	1:22:A:VAL:N	7	0.27
(2,5)	1:31:A:VAL:O	1:22:A:VAL:N	19	0.27
(1,1404)	1:92:A:PHE:HB2	1:93:A:THR:HB	14	0.27
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG21	13	0.27
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG22	13	0.27
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG23	13	0.27
(1,1246)	1:81:A:LYS:HE3	1:82:A:TYR:H	13	0.27
(1,1177)	1:78:A:THR:H	1:81:A:LYS:H	3	0.27
(1,1177)	1:78:A:THR:H	1:81:A:LYS:H	12	0.27
(1,1162)	1:77:A:TRP:H	1:81:A:LYS:HE3	20	0.27
(1,1111)	1:74:A:LYS:HA	1:74:A:LYS:HD2	5	0.27
(1,1111)	1:74:A:LYS:HA	1:74:A:LYS:HD2	7	0.27
(1,1111)	1:74:A:LYS:HA	1:74:A:LYS:HD2	10	0.27
(1,1111)	1:74:A:LYS:HA	1:74:A:LYS:HD2	11	0.27
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD11	18	0.27
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD12	18	0.27
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD13	18	0.27
(1,1049)	1:67:A:LYS:HB3	1:69:A:ARG:HA	19	0.27
(1,978)	1:63:A:LEU:HA	1:93:A:THR:H	12	0.27
(1,974)	1:63:A:LEU:HA	1:92:A:PHE:H	18	0.27
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD11	2	0.27
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD12	2	0.27
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD13	2	0.27
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD11	7	0.27
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD12	7	0.27
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD13	7	0.27
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD11	14	0.27
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD12	14	0.27
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD13	14	0.27
(1,904)	1:58:A:TRP:H	1:58:A:TRP:HB3	11	0.27
(1,903)	1:57:A:ASP:HB2	1:61:A:HIS:H	8	0.27
(1,784)	1:47:A:LYS:HG3	1:48:A:LEU:H	8	0.27
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD21	12	0.27
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD22	12	0.27
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD23	12	0.27
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG21	14	0.27
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG22	14	0.27
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG23	14	0.27
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG11	11	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG12	11	0.27
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG13	11	0.27
(1,610)	1:39:A:VAL:HG21	1:80:A:ASP:H	2	0.27
(1,610)	1:39:A:VAL:HG22	1:80:A:ASP:H	2	0.27
(1,610)	1:39:A:VAL:HG23	1:80:A:ASP:H	2	0.27
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD21	12	0.27
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD22	12	0.27
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD23	12	0.27
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD21	18	0.27
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD22	18	0.27
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD23	18	0.27
(1,552)	1:36:A:THR:HB	1:38:A:GLU:H	8	0.27
(1,523)	1:34:A:ARG:HB3	1:35:A:VAL:H	5	0.27
(1,523)	1:34:A:ARG:HB3	1:35:A:VAL:H	10	0.27
(1,523)	1:34:A:ARG:HB3	1:35:A:VAL:H	14	0.27
(1,508)	1:33:A:LEU:HD21	1:48:A:LEU:H	7	0.27
(1,508)	1:33:A:LEU:HD22	1:48:A:LEU:H	7	0.27
(1,508)	1:33:A:LEU:HD23	1:48:A:LEU:H	7	0.27
(1,508)	1:33:A:LEU:HD21	1:48:A:LEU:H	13	0.27
(1,508)	1:33:A:LEU:HD22	1:48:A:LEU:H	13	0.27
(1,508)	1:33:A:LEU:HD23	1:48:A:LEU:H	13	0.27
(1,508)	1:33:A:LEU:HD21	1:48:A:LEU:H	14	0.27
(1,508)	1:33:A:LEU:HD22	1:48:A:LEU:H	14	0.27
(1,508)	1:33:A:LEU:HD23	1:48:A:LEU:H	14	0.27
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG11	14	0.27
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG12	14	0.27
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG13	14	0.27
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG11	16	0.27
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG12	16	0.27
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG13	16	0.27
(1,444)	1:29:A:ARG:H	1:29:A:ARG:HG2	11	0.27
(1,436)	1:28:A:ASN:HB2	1:29:A:ARG:H	11	0.27
(1,430)	1:27:A:VAL:HG21	1:92:A:PHE:H	15	0.27
(1,430)	1:27:A:VAL:HG22	1:92:A:PHE:H	15	0.27
(1,430)	1:27:A:VAL:HG23	1:92:A:PHE:H	15	0.27
(1,371)	1:24:A:VAL:HG11	1:29:A:ARG:H	5	0.27
(1,371)	1:24:A:VAL:HG12	1:29:A:ARG:H	5	0.27
(1,371)	1:24:A:VAL:HG13	1:29:A:ARG:H	5	0.27
(1,340)	1:23:A:HIS:H	1:91:A:GLN:HA	2	0.27
(1,340)	1:23:A:HIS:H	1:91:A:GLN:HA	4	0.27
(1,340)	1:23:A:HIS:H	1:91:A:GLN:HA	18	0.27
(1,297)	1:22:A:VAL:H	1:31:A:VAL:H	18	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,206)	1:19:A:GLU:H	1:20:A:LEU:HB2	10	0.27
(1,184)	1:18:A:TRP:HE1	1:80:A:ASP:HB3	7	0.27
(1,175)	1:18:A:TRP:H	1:35:A:VAL:HA	14	0.27
(1,175)	1:18:A:TRP:H	1:35:A:VAL:HA	18	0.27
(1,166)	1:17:A:THR:HG21	1:18:A:TRP:H	4	0.27
(1,166)	1:17:A:THR:HG22	1:18:A:TRP:H	4	0.27
(1,166)	1:17:A:THR:HG23	1:18:A:TRP:H	4	0.27
(1,147)	1:15:A:ASP:H	1:15:A:ASP:HB2	19	0.27
(1,146)	1:15:A:ASP:H	1:15:A:ASP:HB3	2	0.27
(1,113)	1:9:A:PRO:HG3	1:12:A:CYS:HB3	17	0.27
(1,85)	1:7:A:ARG:HD3	1:8:A:MET:H	9	0.27
(1,78)	1:7:A:ARG:HD3	1:7:A:ARG:HB3	19	0.27
(1,68)	1:6:A:ILE:HA	1:10:A:ASP:H	3	0.27
(1,67)	1:6:A:ILE:H	1:10:A:ASP:H	12	0.27
(1,56)	1:6:A:ILE:H	1:6:A:ILE:HG12	16	0.27
(1,46)	1:4:A:ASP:H	1:6:A:ILE:HB	1	0.27
(1,39)	1:4:A:ASP:H	1:4:A:ASP:HB3	15	0.27
(1,27)	1:3:A:LEU:H	1:3:A:LEU:HB3	1	0.27
(1,27)	1:3:A:LEU:H	1:3:A:LEU:HB3	19	0.27
(3,21)	1:80:A:ASP:O	1:84:A:ILE:H	11	0.26
(2,15)	1:64:A:TRP:O	1:92:A:PHE:H	5	0.26
(2,15)	1:64:A:TRP:O	1:92:A:PHE:H	7	0.26
(2,15)	1:64:A:TRP:O	1:92:A:PHE:H	11	0.26
(2,15)	1:64:A:TRP:O	1:92:A:PHE:H	13	0.26
(2,4)	1:33:A:LEU:O	1:20:A:LEU:N	8	0.26
(1,1328)	1:87:A:ASP:HA	1:88:A:ALA:H	11	0.26
(1,1216)	1:80:A:ASP:H	1:81:A:LYS:HD2	6	0.26
(1,1177)	1:78:A:THR:H	1:81:A:LYS:H	5	0.26
(1,1160)	1:77:A:TRP:HB2	1:78:A:THR:H	4	0.26
(1,1159)	1:77:A:TRP:HB3	1:78:A:THR:H	2	0.26
(1,1159)	1:77:A:TRP:HB3	1:78:A:THR:H	3	0.26
(1,1159)	1:77:A:TRP:HB3	1:78:A:THR:H	10	0.26
(1,1159)	1:77:A:TRP:HB3	1:78:A:THR:H	11	0.26
(1,1159)	1:77:A:TRP:HB3	1:78:A:THR:H	14	0.26
(1,1111)	1:74:A:LYS:HA	1:74:A:LYS:HD2	2	0.26
(1,1111)	1:74:A:LYS:HA	1:74:A:LYS:HD2	6	0.26
(1,1111)	1:74:A:LYS:HA	1:74:A:LYS:HD2	16	0.26
(1,1111)	1:74:A:LYS:HA	1:74:A:LYS:HD2	17	0.26
(1,1081)	1:71:A:TRP:HB2	1:72:A:LEU:H	16	0.26
(1,1072)	1:70:A:THR:H	1:71:A:TRP:H	2	0.26
(1,1072)	1:70:A:THR:H	1:71:A:TRP:H	19	0.26
(1,911)	1:58:A:TRP:HB3	1:61:A:HIS:H	12	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:50:A:GLU:H	1:50:A:GLU:HG2	19	0.26
(1,838)	1:49:A:VAL:HG21	1:58:A:TRP:H	12	0.26
(1,838)	1:49:A:VAL:HG22	1:58:A:TRP:H	12	0.26
(1,838)	1:49:A:VAL:HG23	1:58:A:TRP:H	12	0.26
(1,784)	1:47:A:LYS:HG3	1:48:A:LEU:H	18	0.26
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD21	2	0.26
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD22	2	0.26
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD23	2	0.26
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD21	8	0.26
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD22	8	0.26
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD23	8	0.26
(1,676)	1:41:A:ILE:HG13	1:78:A:THR:H	13	0.26
(1,673)	1:41:A:ILE:H	1:77:A:TRP:H	18	0.26
(1,588)	1:38:A:GLU:HA	1:80:A:ASP:H	13	0.26
(1,523)	1:34:A:ARG:HB3	1:35:A:VAL:H	1	0.26
(1,523)	1:34:A:ARG:HB3	1:35:A:VAL:H	3	0.26
(1,523)	1:34:A:ARG:HB3	1:35:A:VAL:H	7	0.26
(1,511)	1:33:A:LEU:HD21	1:48:A:LEU:HB3	3	0.26
(1,511)	1:33:A:LEU:HD22	1:48:A:LEU:HB3	3	0.26
(1,511)	1:33:A:LEU:HD23	1:48:A:LEU:HB3	3	0.26
(1,508)	1:33:A:LEU:HD21	1:48:A:LEU:H	5	0.26
(1,508)	1:33:A:LEU:HD22	1:48:A:LEU:H	5	0.26
(1,508)	1:33:A:LEU:HD23	1:48:A:LEU:H	5	0.26
(1,508)	1:33:A:LEU:HD21	1:48:A:LEU:H	10	0.26
(1,508)	1:33:A:LEU:HD22	1:48:A:LEU:H	10	0.26
(1,508)	1:33:A:LEU:HD23	1:48:A:LEU:H	10	0.26
(1,508)	1:33:A:LEU:HD21	1:48:A:LEU:H	11	0.26
(1,508)	1:33:A:LEU:HD22	1:48:A:LEU:H	11	0.26
(1,508)	1:33:A:LEU:HD23	1:48:A:LEU:H	11	0.26
(1,508)	1:33:A:LEU:HD21	1:48:A:LEU:H	17	0.26
(1,508)	1:33:A:LEU:HD22	1:48:A:LEU:H	17	0.26
(1,508)	1:33:A:LEU:HD23	1:48:A:LEU:H	17	0.26
(1,508)	1:33:A:LEU:HD21	1:48:A:LEU:H	18	0.26
(1,508)	1:33:A:LEU:HD22	1:48:A:LEU:H	18	0.26
(1,508)	1:33:A:LEU:HD23	1:48:A:LEU:H	18	0.26
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG11	6	0.26
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG12	6	0.26
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG13	6	0.26
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG11	12	0.26
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG12	12	0.26
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG13	12	0.26
(1,453)	1:29:A:ARG:HB2	1:31:A:VAL:HA	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:29:A:ARG:HB2	1:31:A:VAL:HA	20	0.26
(1,430)	1:27:A:VAL:HG21	1:92:A:PHE:H	14	0.26
(1,430)	1:27:A:VAL:HG22	1:92:A:PHE:H	14	0.26
(1,430)	1:27:A:VAL:HG23	1:92:A:PHE:H	14	0.26
(1,387)	1:24:A:VAL:HG11	1:62:A:ALA:H	12	0.26
(1,387)	1:24:A:VAL:HG12	1:62:A:ALA:H	12	0.26
(1,387)	1:24:A:VAL:HG13	1:62:A:ALA:H	12	0.26
(1,370)	1:24:A:VAL:H	1:29:A:ARG:H	11	0.26
(1,340)	1:23:A:HIS:H	1:91:A:GLN:HA	6	0.26
(1,340)	1:23:A:HIS:H	1:91:A:GLN:HA	7	0.26
(1,340)	1:23:A:HIS:H	1:91:A:GLN:HA	9	0.26
(1,340)	1:23:A:HIS:H	1:91:A:GLN:HA	16	0.26
(1,297)	1:22:A:VAL:H	1:31:A:VAL:H	6	0.26
(1,297)	1:22:A:VAL:H	1:31:A:VAL:H	8	0.26
(1,297)	1:22:A:VAL:H	1:31:A:VAL:H	13	0.26
(1,297)	1:22:A:VAL:H	1:31:A:VAL:H	16	0.26
(1,206)	1:19:A:GLU:H	1:20:A:LEU:HB2	2	0.26
(1,206)	1:19:A:GLU:H	1:20:A:LEU:HB2	3	0.26
(1,203)	1:19:A:GLU:HB3	1:20:A:LEU:H	5	0.26
(1,200)	1:19:A:GLU:H	1:20:A:LEU:H	6	0.26
(1,195)	1:19:A:GLU:H	1:19:A:GLU:HG2	6	0.26
(1,184)	1:18:A:TRP:HE1	1:80:A:ASP:HB3	15	0.26
(1,175)	1:18:A:TRP:H	1:35:A:VAL:HA	1	0.26
(1,175)	1:18:A:TRP:H	1:35:A:VAL:HA	2	0.26
(1,175)	1:18:A:TRP:H	1:35:A:VAL:HA	4	0.26
(1,175)	1:18:A:TRP:H	1:35:A:VAL:HA	5	0.26
(1,175)	1:18:A:TRP:H	1:35:A:VAL:HA	7	0.26
(1,175)	1:18:A:TRP:H	1:35:A:VAL:HA	16	0.26
(1,166)	1:17:A:THR:HG21	1:18:A:TRP:H	8	0.26
(1,166)	1:17:A:THR:HG22	1:18:A:TRP:H	8	0.26
(1,166)	1:17:A:THR:HG23	1:18:A:TRP:H	8	0.26
(1,112)	1:9:A:PRO:HG3	1:10:A:ASP:H	9	0.26
(1,94)	1:8:A:MET:H	1:10:A:ASP:HA	13	0.26
(1,86)	1:7:A:ARG:HA	1:10:A:ASP:H	16	0.26
(1,78)	1:7:A:ARG:HD3	1:7:A:ARG:HB3	1	0.26
(1,78)	1:7:A:ARG:HD3	1:7:A:ARG:HB3	11	0.26
(1,78)	1:7:A:ARG:HD3	1:7:A:ARG:HB3	13	0.26
(1,78)	1:7:A:ARG:HD3	1:7:A:ARG:HB3	16	0.26
(1,67)	1:6:A:ILE:H	1:10:A:ASP:H	20	0.26
(1,49)	1:5:A:GLY:HA3	1:6:A:ILE:HB	3	0.26
(1,42)	1:4:A:ASP:H	1:5:A:GLY:HA3	9	0.26
(1,34)	1:3:A:LEU:HD21	1:4:A:ASP:H	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:3:A:LEU:HD22	1:4:A:ASP:H	5	0.26
(1,34)	1:3:A:LEU:HD23	1:4:A:ASP:H	5	0.26
(3,21)	1:80:A:ASP:O	1:84:A:ILE:H	16	0.25
(2,18)	1:23:A:HIS:O	1:93:A:THR:N	2	0.25
(2,18)	1:23:A:HIS:O	1:93:A:THR:N	4	0.25
(2,18)	1:23:A:HIS:O	1:93:A:THR:N	7	0.25
(2,18)	1:23:A:HIS:O	1:93:A:THR:N	8	0.25
(2,18)	1:23:A:HIS:O	1:93:A:THR:N	16	0.25
(2,18)	1:23:A:HIS:O	1:93:A:THR:N	17	0.25
(2,18)	1:23:A:HIS:O	1:93:A:THR:N	20	0.25
(2,17)	1:21:A:SER:O	1:91:A:GLN:H	6	0.25
(2,15)	1:64:A:TRP:O	1:92:A:PHE:H	1	0.25
(2,15)	1:64:A:TRP:O	1:92:A:PHE:H	2	0.25
(2,4)	1:33:A:LEU:O	1:20:A:LEU:N	13	0.25
(1,1408)	1:92:A:PHE:HB3	1:93:A:THR:H	8	0.25
(1,1407)	1:92:A:PHE:HB2	1:93:A:THR:H	1	0.25
(1,1407)	1:92:A:PHE:HB2	1:93:A:THR:H	15	0.25
(1,1407)	1:92:A:PHE:HB2	1:93:A:THR:H	19	0.25
(1,1328)	1:87:A:ASP:HA	1:88:A:ALA:H	2	0.25
(1,1328)	1:87:A:ASP:HA	1:88:A:ALA:H	4	0.25
(1,1328)	1:87:A:ASP:HA	1:88:A:ALA:H	5	0.25
(1,1328)	1:87:A:ASP:HA	1:88:A:ALA:H	7	0.25
(1,1328)	1:87:A:ASP:HA	1:88:A:ALA:H	8	0.25
(1,1328)	1:87:A:ASP:HA	1:88:A:ALA:H	9	0.25
(1,1328)	1:87:A:ASP:HA	1:88:A:ALA:H	10	0.25
(1,1328)	1:87:A:ASP:HA	1:88:A:ALA:H	12	0.25
(1,1328)	1:87:A:ASP:HA	1:88:A:ALA:H	15	0.25
(1,1328)	1:87:A:ASP:HA	1:88:A:ALA:H	18	0.25
(1,1328)	1:87:A:ASP:HA	1:88:A:ALA:H	19	0.25
(1,1197)	1:79:A:LEU:HB3	1:80:A:ASP:H	13	0.25
(1,1177)	1:78:A:THR:H	1:81:A:LYS:H	2	0.25
(1,1162)	1:77:A:TRP:H	1:81:A:LYS:HE3	1	0.25
(1,1162)	1:77:A:TRP:H	1:81:A:LYS:HE3	7	0.25
(1,1162)	1:77:A:TRP:H	1:81:A:LYS:HE3	9	0.25
(1,1162)	1:77:A:TRP:H	1:81:A:LYS:HE3	14	0.25
(1,1162)	1:77:A:TRP:H	1:81:A:LYS:HE3	17	0.25
(1,1160)	1:77:A:TRP:HB2	1:78:A:THR:H	5	0.25
(1,1160)	1:77:A:TRP:HB2	1:78:A:THR:H	12	0.25
(1,1159)	1:77:A:TRP:HB3	1:78:A:THR:H	6	0.25
(1,1159)	1:77:A:TRP:HB3	1:78:A:THR:H	7	0.25
(1,1159)	1:77:A:TRP:HB3	1:78:A:THR:H	9	0.25
(1,1159)	1:77:A:TRP:HB3	1:78:A:THR:H	17	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1123)	1:74:A:LYS:H	1:74:A:LYS:HD2	7	0.25
(1,1111)	1:74:A:LYS:HA	1:74:A:LYS:HD2	1	0.25
(1,1111)	1:74:A:LYS:HA	1:74:A:LYS:HD2	3	0.25
(1,1111)	1:74:A:LYS:HA	1:74:A:LYS:HD2	4	0.25
(1,1111)	1:74:A:LYS:HA	1:74:A:LYS:HD2	8	0.25
(1,1111)	1:74:A:LYS:HA	1:74:A:LYS:HD2	9	0.25
(1,1111)	1:74:A:LYS:HA	1:74:A:LYS:HD2	12	0.25
(1,1111)	1:74:A:LYS:HA	1:74:A:LYS:HD2	14	0.25
(1,1111)	1:74:A:LYS:HA	1:74:A:LYS:HD2	19	0.25
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD11	8	0.25
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD12	8	0.25
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD13	8	0.25
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD11	13	0.25
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD12	13	0.25
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD13	13	0.25
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD11	16	0.25
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD12	16	0.25
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD13	16	0.25
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD11	17	0.25
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD12	17	0.25
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD13	17	0.25
(1,1081)	1:71:A:TRP:HB2	1:72:A:LEU:H	3	0.25
(1,1081)	1:71:A:TRP:HB2	1:72:A:LEU:H	10	0.25
(1,1063)	1:69:A:ARG:H	1:70:A:THR:H	12	0.25
(1,1053)	1:67:A:LYS:H	1:88:A:ALA:HA	10	0.25
(1,1033)	1:67:A:LYS:HA	1:67:A:LYS:HD3	2	0.25
(1,1033)	1:67:A:LYS:HA	1:67:A:LYS:HD3	6	0.25
(1,1033)	1:67:A:LYS:HA	1:67:A:LYS:HD3	15	0.25
(1,992)	1:64:A:TRP:H	1:93:A:THR:HG1	10	0.25
(1,978)	1:63:A:LEU:HA	1:93:A:THR:H	9	0.25
(1,976)	1:63:A:LEU:HG	1:93:A:THR:H	12	0.25
(1,974)	1:63:A:LEU:HA	1:92:A:PHE:H	5	0.25
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD11	11	0.25
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD12	11	0.25
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD13	11	0.25
(1,950)	1:63:A:LEU:H	1:63:A:LEU:HG	7	0.25
(1,946)	1:62:A:ALA:H	1:94:A:PRO:HA	19	0.25
(1,945)	1:62:A:ALA:HB1	1:93:A:THR:HA	12	0.25
(1,945)	1:62:A:ALA:HB2	1:93:A:THR:HA	12	0.25
(1,945)	1:62:A:ALA:HB3	1:93:A:THR:HA	12	0.25
(1,906)	1:58:A:TRP:H	1:59:A:SER:H	19	0.25
(1,838)	1:49:A:VAL:HG21	1:58:A:TRP:H	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,838)	1:49:A:VAL:HG22	1:58:A:TRP:H	10	0.25
(1,838)	1:49:A:VAL:HG23	1:58:A:TRP:H	10	0.25
(1,818)	1:48:A:LEU:HD21	1:52:A:LEU:H	9	0.25
(1,818)	1:48:A:LEU:HD22	1:52:A:LEU:H	9	0.25
(1,818)	1:48:A:LEU:HD23	1:52:A:LEU:H	9	0.25
(1,818)	1:48:A:LEU:HD21	1:52:A:LEU:H	14	0.25
(1,818)	1:48:A:LEU:HD22	1:52:A:LEU:H	14	0.25
(1,818)	1:48:A:LEU:HD23	1:52:A:LEU:H	14	0.25
(1,818)	1:48:A:LEU:HD21	1:52:A:LEU:H	20	0.25
(1,818)	1:48:A:LEU:HD22	1:52:A:LEU:H	20	0.25
(1,818)	1:48:A:LEU:HD23	1:52:A:LEU:H	20	0.25
(1,784)	1:47:A:LYS:HG3	1:48:A:LEU:H	10	0.25
(1,784)	1:47:A:LYS:HG3	1:48:A:LEU:H	11	0.25
(1,784)	1:47:A:LYS:HG3	1:48:A:LEU:H	12	0.25
(1,784)	1:47:A:LYS:HG3	1:48:A:LEU:H	14	0.25
(1,784)	1:47:A:LYS:HG3	1:48:A:LEU:H	19	0.25
(1,764)	1:46:A:LEU:HA	1:49:A:VAL:H	3	0.25
(1,760)	1:46:A:LEU:H	1:48:A:LEU:H	14	0.25
(1,760)	1:46:A:LEU:H	1:48:A:LEU:H	17	0.25
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD21	5	0.25
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD22	5	0.25
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD23	5	0.25
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD21	11	0.25
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD22	11	0.25
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD23	11	0.25
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG21	7	0.25
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG22	7	0.25
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG23	7	0.25
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG11	7	0.25
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG12	7	0.25
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG13	7	0.25
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG11	19	0.25
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG12	19	0.25
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG13	19	0.25
(1,694)	1:43:A:GLY:H	1:45:A:MET:H	12	0.25
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD21	15	0.25
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD22	15	0.25
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD23	15	0.25
(1,523)	1:34:A:ARG:HB3	1:35:A:VAL:H	6	0.25
(1,523)	1:34:A:ARG:HB3	1:35:A:VAL:H	11	0.25
(1,523)	1:34:A:ARG:HB3	1:35:A:VAL:H	15	0.25
(1,511)	1:33:A:LEU:HD21	1:48:A:LEU:HB3	20	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:33:A:LEU:HD22	1:48:A:LEU:HB3	20	0.25
(1,511)	1:33:A:LEU:HD23	1:48:A:LEU:HB3	20	0.25
(1,508)	1:33:A:LEU:HD21	1:48:A:LEU:H	6	0.25
(1,508)	1:33:A:LEU:HD22	1:48:A:LEU:H	6	0.25
(1,508)	1:33:A:LEU:HD23	1:48:A:LEU:H	6	0.25
(1,508)	1:33:A:LEU:HD21	1:48:A:LEU:H	16	0.25
(1,508)	1:33:A:LEU:HD22	1:48:A:LEU:H	16	0.25
(1,508)	1:33:A:LEU:HD23	1:48:A:LEU:H	16	0.25
(1,508)	1:33:A:LEU:HD21	1:48:A:LEU:H	20	0.25
(1,508)	1:33:A:LEU:HD22	1:48:A:LEU:H	20	0.25
(1,508)	1:33:A:LEU:HD23	1:48:A:LEU:H	20	0.25
(1,483)	1:32:A:THR:H	1:34:A:ARG:H	5	0.25
(1,453)	1:29:A:ARG:HB2	1:31:A:VAL:HA	17	0.25
(1,436)	1:28:A:ASN:HB2	1:29:A:ARG:H	6	0.25
(1,436)	1:28:A:ASN:HB2	1:29:A:ARG:H	7	0.25
(1,434)	1:28:A:ASN:HA	1:29:A:ARG:H	11	0.25
(1,387)	1:24:A:VAL:HG11	1:62:A:ALA:H	14	0.25
(1,387)	1:24:A:VAL:HG12	1:62:A:ALA:H	14	0.25
(1,387)	1:24:A:VAL:HG13	1:62:A:ALA:H	14	0.25
(1,371)	1:24:A:VAL:HG11	1:29:A:ARG:H	10	0.25
(1,371)	1:24:A:VAL:HG12	1:29:A:ARG:H	10	0.25
(1,371)	1:24:A:VAL:HG13	1:29:A:ARG:H	10	0.25
(1,350)	1:23:A:HIS:HB2	1:91:A:GLN:HG3	10	0.25
(1,340)	1:23:A:HIS:H	1:91:A:GLN:HA	11	0.25
(1,340)	1:23:A:HIS:H	1:91:A:GLN:HA	17	0.25
(1,340)	1:23:A:HIS:H	1:91:A:GLN:HA	20	0.25
(1,297)	1:22:A:VAL:H	1:31:A:VAL:H	5	0.25
(1,297)	1:22:A:VAL:H	1:31:A:VAL:H	20	0.25
(1,266)	1:21:A:SER:H	1:22:A:VAL:H	12	0.25
(1,244)	1:20:A:LEU:HD21	1:33:A:LEU:HA	8	0.25
(1,244)	1:20:A:LEU:HD22	1:33:A:LEU:HA	8	0.25
(1,244)	1:20:A:LEU:HD23	1:33:A:LEU:HA	8	0.25
(1,206)	1:19:A:GLU:H	1:20:A:LEU:HB2	9	0.25
(1,206)	1:19:A:GLU:H	1:20:A:LEU:HB2	11	0.25
(1,206)	1:19:A:GLU:H	1:20:A:LEU:HB2	15	0.25
(1,206)	1:19:A:GLU:H	1:20:A:LEU:HB2	20	0.25
(1,184)	1:18:A:TRP:HE1	1:80:A:ASP:HB3	18	0.25
(1,177)	1:18:A:TRP:HE1	1:36:A:THR:HB	8	0.25
(1,175)	1:18:A:TRP:H	1:35:A:VAL:HA	20	0.25
(1,166)	1:17:A:THR:HG21	1:18:A:TRP:H	6	0.25
(1,166)	1:17:A:THR:HG22	1:18:A:TRP:H	6	0.25
(1,166)	1:17:A:THR:HG23	1:18:A:TRP:H	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:8:A:MET:H	1:10:A:ASP:HA	19	0.25
(1,86)	1:7:A:ARG:HA	1:10:A:ASP:H	19	0.25
(1,74)	1:7:A:ARG:H	1:7:A:ARG:HB3	14	0.25
(1,67)	1:6:A:ILE:H	1:10:A:ASP:H	19	0.25
(1,45)	1:4:A:ASP:HB3	1:6:A:ILE:H	3	0.25
(1,34)	1:3:A:LEU:HD21	1:4:A:ASP:H	4	0.25
(1,34)	1:3:A:LEU:HD22	1:4:A:ASP:H	4	0.25
(1,34)	1:3:A:LEU:HD23	1:4:A:ASP:H	4	0.25
(1,34)	1:3:A:LEU:HD21	1:4:A:ASP:H	11	0.25
(1,34)	1:3:A:LEU:HD22	1:4:A:ASP:H	11	0.25
(1,34)	1:3:A:LEU:HD23	1:4:A:ASP:H	11	0.25
(1,28)	1:3:A:LEU:H	1:3:A:LEU:HB2	19	0.25
(1,17)	1:2:A:ALA:H	1:3:A:LEU:HA	15	0.25
(3,21)	1:80:A:ASP:O	1:84:A:ILE:H	13	0.24
(2,18)	1:23:A:HIS:O	1:93:A:THR:N	1	0.24
(2,18)	1:23:A:HIS:O	1:93:A:THR:N	6	0.24
(2,18)	1:23:A:HIS:O	1:93:A:THR:N	10	0.24
(2,18)	1:23:A:HIS:O	1:93:A:THR:N	15	0.24
(2,15)	1:64:A:TRP:O	1:92:A:PHE:H	14	0.24
(2,15)	1:64:A:TRP:O	1:92:A:PHE:H	17	0.24
(2,15)	1:64:A:TRP:O	1:92:A:PHE:H	20	0.24
(2,4)	1:33:A:LEU:O	1:20:A:LEU:N	7	0.24
(1,1402)	1:92:A:PHE:H	1:92:A:PHE:HB2	3	0.24
(1,1328)	1:87:A:ASP:HA	1:88:A:ALA:H	1	0.24
(1,1328)	1:87:A:ASP:HA	1:88:A:ALA:H	3	0.24
(1,1328)	1:87:A:ASP:HA	1:88:A:ALA:H	14	0.24
(1,1328)	1:87:A:ASP:HA	1:88:A:ALA:H	17	0.24
(1,1328)	1:87:A:ASP:HA	1:88:A:ALA:H	20	0.24
(1,1218)	1:80:A:ASP:HB2	1:82:A:TYR:H	18	0.24
(1,1216)	1:80:A:ASP:H	1:81:A:LYS:HD2	20	0.24
(1,1205)	1:79:A:LEU:HD11	1:83:A:GLY:H	13	0.24
(1,1205)	1:79:A:LEU:HD12	1:83:A:GLY:H	13	0.24
(1,1205)	1:79:A:LEU:HD13	1:83:A:GLY:H	13	0.24
(1,1203)	1:79:A:LEU:HB3	1:83:A:GLY:H	13	0.24
(1,1177)	1:78:A:THR:H	1:81:A:LYS:H	13	0.24
(1,1177)	1:78:A:THR:H	1:81:A:LYS:H	16	0.24
(1,1177)	1:78:A:THR:H	1:81:A:LYS:H	19	0.24
(1,1161)	1:77:A:TRP:H	1:81:A:LYS:HD3	13	0.24
(1,1159)	1:77:A:TRP:HB3	1:78:A:THR:H	1	0.24
(1,1159)	1:77:A:TRP:HB3	1:78:A:THR:H	15	0.24
(1,1140)	1:74:A:LYS:HA	1:77:A:TRP:H	15	0.24
(1,1123)	1:74:A:LYS:H	1:74:A:LYS:HD2	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1111)	1:74:A:LYS:HA	1:74:A:LYS:HD2	13	0.24
(1,1111)	1:74:A:LYS:HA	1:74:A:LYS:HD2	15	0.24
(1,1111)	1:74:A:LYS:HA	1:74:A:LYS:HD2	18	0.24
(1,1111)	1:74:A:LYS:HA	1:74:A:LYS:HD2	20	0.24
(1,1105)	1:73:A:LEU:H	1:73:A:LEU:HB3	2	0.24
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD11	6	0.24
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD12	6	0.24
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD13	6	0.24
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD11	10	0.24
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD12	10	0.24
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD13	10	0.24
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD11	19	0.24
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD12	19	0.24
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD13	19	0.24
(1,1072)	1:70:A:THR:H	1:71:A:TRP:H	16	0.24
(1,1033)	1:67:A:LYS:HA	1:67:A:LYS:HD3	5	0.24
(1,1033)	1:67:A:LYS:HA	1:67:A:LYS:HD3	16	0.24
(1,1033)	1:67:A:LYS:HA	1:67:A:LYS:HD3	20	0.24
(1,992)	1:64:A:TRP:H	1:93:A:THR:HG1	8	0.24
(1,992)	1:64:A:TRP:H	1:93:A:THR:HG1	19	0.24
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD11	6	0.24
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD12	6	0.24
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD13	6	0.24
(1,950)	1:63:A:LEU:H	1:63:A:LEU:HG	2	0.24
(1,926)	1:61:A:HIS:H	1:62:A:ALA:H	10	0.24
(1,921)	1:60:A:ASP:HB3	1:61:A:HIS:H	5	0.24
(1,784)	1:47:A:LYS:HG3	1:48:A:LEU:H	1	0.24
(1,784)	1:47:A:LYS:HG3	1:48:A:LEU:H	3	0.24
(1,784)	1:47:A:LYS:HG3	1:48:A:LEU:H	4	0.24
(1,784)	1:47:A:LYS:HG3	1:48:A:LEU:H	6	0.24
(1,784)	1:47:A:LYS:HG3	1:48:A:LEU:H	13	0.24
(1,784)	1:47:A:LYS:HG3	1:48:A:LEU:H	17	0.24
(1,784)	1:47:A:LYS:HG3	1:48:A:LEU:H	20	0.24
(1,766)	1:46:A:LEU:HA	1:50:A:GLU:H	9	0.24
(1,760)	1:46:A:LEU:H	1:48:A:LEU:H	7	0.24
(1,760)	1:46:A:LEU:H	1:48:A:LEU:H	8	0.24
(1,760)	1:46:A:LEU:H	1:48:A:LEU:H	10	0.24
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG21	16	0.24
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG22	16	0.24
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG23	16	0.24
(1,719)	1:44:A:VAL:HG11	1:90:A:LEU:H	3	0.24
(1,719)	1:44:A:VAL:HG12	1:90:A:LEU:H	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,719)	1:44:A:VAL:HG13	1:90:A:LEU:H	3	0.24
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG11	1	0.24
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG12	1	0.24
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG13	1	0.24
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG11	9	0.24
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG12	9	0.24
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG13	9	0.24
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG11	14	0.24
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG12	14	0.24
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG13	14	0.24
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG11	17	0.24
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG12	17	0.24
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG13	17	0.24
(1,694)	1:43:A:GLY:H	1:45:A:MET:H	20	0.24
(1,683)	1:42:A:GLY:H	1:74:A:LYS:HE3	9	0.24
(1,683)	1:42:A:GLY:H	1:74:A:LYS:HE3	17	0.24
(1,673)	1:41:A:ILE:H	1:77:A:TRP:H	15	0.24
(1,628)	1:40:A:HIS:H	1:44:A:VAL:HB	19	0.24
(1,588)	1:38:A:GLU:HA	1:80:A:ASP:H	16	0.24
(1,588)	1:38:A:GLU:HA	1:80:A:ASP:H	20	0.24
(1,572)	1:37:A:GLY:H	1:80:A:ASP:H	19	0.24
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD21	1	0.24
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD22	1	0.24
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD23	1	0.24
(1,552)	1:36:A:THR:HB	1:38:A:GLU:H	11	0.24
(1,523)	1:34:A:ARG:HB3	1:35:A:VAL:H	8	0.24
(1,523)	1:34:A:ARG:HB3	1:35:A:VAL:H	19	0.24
(1,511)	1:33:A:LEU:HD21	1:48:A:LEU:HB3	2	0.24
(1,511)	1:33:A:LEU:HD22	1:48:A:LEU:HB3	2	0.24
(1,511)	1:33:A:LEU:HD23	1:48:A:LEU:HB3	2	0.24
(1,508)	1:33:A:LEU:HD21	1:48:A:LEU:H	2	0.24
(1,508)	1:33:A:LEU:HD22	1:48:A:LEU:H	2	0.24
(1,508)	1:33:A:LEU:HD23	1:48:A:LEU:H	2	0.24
(1,508)	1:33:A:LEU:HD21	1:48:A:LEU:H	3	0.24
(1,508)	1:33:A:LEU:HD22	1:48:A:LEU:H	3	0.24
(1,508)	1:33:A:LEU:HD23	1:48:A:LEU:H	3	0.24
(1,508)	1:33:A:LEU:HD21	1:48:A:LEU:H	4	0.24
(1,508)	1:33:A:LEU:HD22	1:48:A:LEU:H	4	0.24
(1,508)	1:33:A:LEU:HD23	1:48:A:LEU:H	4	0.24
(1,508)	1:33:A:LEU:HD21	1:48:A:LEU:H	8	0.24
(1,508)	1:33:A:LEU:HD22	1:48:A:LEU:H	8	0.24
(1,508)	1:33:A:LEU:HD23	1:48:A:LEU:H	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG11	2	0.24
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG12	2	0.24
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG13	2	0.24
(1,453)	1:29:A:ARG:HB2	1:31:A:VAL:HA	2	0.24
(1,436)	1:28:A:ASN:HB2	1:29:A:ARG:H	1	0.24
(1,436)	1:28:A:ASN:HB2	1:29:A:ARG:H	9	0.24
(1,434)	1:28:A:ASN:HA	1:29:A:ARG:H	12	0.24
(1,433)	1:28:A:ASN:H	1:28:A:ASN:HB3	3	0.24
(1,433)	1:28:A:ASN:H	1:28:A:ASN:HB3	5	0.24
(1,433)	1:28:A:ASN:H	1:28:A:ASN:HB3	13	0.24
(1,433)	1:28:A:ASN:H	1:28:A:ASN:HB3	16	0.24
(1,432)	1:28:A:ASN:H	1:28:A:ASN:HB2	11	0.24
(1,431)	1:27:A:VAL:H	1:93:A:THR:HB	7	0.24
(1,387)	1:24:A:VAL:HG11	1:62:A:ALA:H	1	0.24
(1,387)	1:24:A:VAL:HG12	1:62:A:ALA:H	1	0.24
(1,387)	1:24:A:VAL:HG13	1:62:A:ALA:H	1	0.24
(1,352)	1:23:A:HIS:HB3	1:91:A:GLN:HB2	16	0.24
(1,340)	1:23:A:HIS:H	1:91:A:GLN:HA	1	0.24
(1,340)	1:23:A:HIS:H	1:91:A:GLN:HA	5	0.24
(1,340)	1:23:A:HIS:H	1:91:A:GLN:HA	8	0.24
(1,340)	1:23:A:HIS:H	1:91:A:GLN:HA	10	0.24
(1,340)	1:23:A:HIS:H	1:91:A:GLN:HA	12	0.24
(1,340)	1:23:A:HIS:H	1:91:A:GLN:HA	13	0.24
(1,297)	1:22:A:VAL:H	1:31:A:VAL:H	2	0.24
(1,297)	1:22:A:VAL:H	1:31:A:VAL:H	3	0.24
(1,297)	1:22:A:VAL:H	1:31:A:VAL:H	9	0.24
(1,297)	1:22:A:VAL:H	1:31:A:VAL:H	10	0.24
(1,297)	1:22:A:VAL:H	1:31:A:VAL:H	11	0.24
(1,297)	1:22:A:VAL:H	1:31:A:VAL:H	15	0.24
(1,297)	1:22:A:VAL:H	1:31:A:VAL:H	17	0.24
(1,276)	1:21:A:SER:H	1:32:A:THR:HG21	6	0.24
(1,276)	1:21:A:SER:H	1:32:A:THR:HG22	6	0.24
(1,276)	1:21:A:SER:H	1:32:A:THR:HG23	6	0.24
(1,266)	1:21:A:SER:H	1:22:A:VAL:H	1	0.24
(1,266)	1:21:A:SER:H	1:22:A:VAL:H	4	0.24
(1,266)	1:21:A:SER:H	1:22:A:VAL:H	8	0.24
(1,266)	1:21:A:SER:H	1:22:A:VAL:H	9	0.24
(1,266)	1:21:A:SER:H	1:22:A:VAL:H	11	0.24
(1,266)	1:21:A:SER:H	1:22:A:VAL:H	15	0.24
(1,266)	1:21:A:SER:H	1:22:A:VAL:H	18	0.24
(1,206)	1:19:A:GLU:H	1:20:A:LEU:HB2	1	0.24
(1,206)	1:19:A:GLU:H	1:20:A:LEU:HB2	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,206)	1:19:A:GLU:H	1:20:A:LEU:HB2	13	0.24
(1,206)	1:19:A:GLU:H	1:20:A:LEU:HB2	14	0.24
(1,206)	1:19:A:GLU:H	1:20:A:LEU:HB2	16	0.24
(1,206)	1:19:A:GLU:H	1:20:A:LEU:HB2	18	0.24
(1,200)	1:19:A:GLU:H	1:20:A:LEU:H	19	0.24
(1,195)	1:19:A:GLU:H	1:19:A:GLU:HG2	17	0.24
(1,175)	1:18:A:TRP:H	1:35:A:VAL:HA	9	0.24
(1,175)	1:18:A:TRP:H	1:35:A:VAL:HA	10	0.24
(1,175)	1:18:A:TRP:H	1:35:A:VAL:HA	13	0.24
(1,175)	1:18:A:TRP:H	1:35:A:VAL:HA	17	0.24
(1,155)	1:16:A:GLY:HA3	1:17:A:THR:H	8	0.24
(1,148)	1:15:A:ASP:HA	1:16:A:GLY:H	14	0.24
(1,148)	1:15:A:ASP:HA	1:16:A:GLY:H	17	0.24
(1,115)	1:9:A:PRO:HA	1:13:A:TYR:H	17	0.24
(1,90)	1:8:A:MET:H	1:8:A:MET:HG3	8	0.24
(1,90)	1:8:A:MET:H	1:8:A:MET:HG3	18	0.24
(1,87)	1:7:A:ARG:HG3	1:10:A:ASP:H	20	0.24
(1,44)	1:4:A:ASP:HA	1:6:A:ILE:H	12	0.24
(1,34)	1:3:A:LEU:HD21	1:4:A:ASP:H	6	0.24
(1,34)	1:3:A:LEU:HD22	1:4:A:ASP:H	6	0.24
(1,34)	1:3:A:LEU:HD23	1:4:A:ASP:H	6	0.24
(1,34)	1:3:A:LEU:HD21	1:4:A:ASP:H	17	0.24
(1,34)	1:3:A:LEU:HD22	1:4:A:ASP:H	17	0.24
(1,34)	1:3:A:LEU:HD23	1:4:A:ASP:H	17	0.24
(1,20)	1:2:A:ALA:HB1	1:4:A:ASP:H	13	0.24
(1,20)	1:2:A:ALA:HB2	1:4:A:ASP:H	13	0.24
(1,20)	1:2:A:ALA:HB3	1:4:A:ASP:H	13	0.24
(1,16)	1:2:A:ALA:H	1:3:A:LEU:HB3	9	0.24
(3,21)	1:80:A:ASP:O	1:84:A:ILE:H	2	0.23
(2,18)	1:23:A:HIS:O	1:93:A:THR:N	9	0.23
(2,18)	1:23:A:HIS:O	1:93:A:THR:N	19	0.23
(2,15)	1:64:A:TRP:O	1:92:A:PHE:H	4	0.23
(2,15)	1:64:A:TRP:O	1:92:A:PHE:H	15	0.23
(2,15)	1:64:A:TRP:O	1:92:A:PHE:H	18	0.23
(2,4)	1:33:A:LEU:O	1:20:A:LEU:N	2	0.23
(2,4)	1:33:A:LEU:O	1:20:A:LEU:N	9	0.23
(2,4)	1:33:A:LEU:O	1:20:A:LEU:N	12	0.23
(2,4)	1:33:A:LEU:O	1:20:A:LEU:N	16	0.23
(2,4)	1:33:A:LEU:O	1:20:A:LEU:N	18	0.23
(1,1404)	1:92:A:PHE:HB2	1:93:A:THR:HB	7	0.23
(1,1380)	1:91:A:GLN:H	1:91:A:GLN:HE22	15	0.23
(1,1377)	1:91:A:GLN:H	1:91:A:GLN:HB3	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1377)	1:91:A:GLN:H	1:91:A:GLN:HB3	18	0.23
(1,1377)	1:91:A:GLN:H	1:91:A:GLN:HB3	19	0.23
(1,1341)	1:89:A:LYS:HE3	1:89:A:LYS:HB3	3	0.23
(1,1341)	1:89:A:LYS:HE3	1:89:A:LYS:HB3	4	0.23
(1,1341)	1:89:A:LYS:HE3	1:89:A:LYS:HB3	5	0.23
(1,1341)	1:89:A:LYS:HE3	1:89:A:LYS:HB3	7	0.23
(1,1341)	1:89:A:LYS:HE3	1:89:A:LYS:HB3	8	0.23
(1,1341)	1:89:A:LYS:HE3	1:89:A:LYS:HB3	11	0.23
(1,1341)	1:89:A:LYS:HE3	1:89:A:LYS:HB3	13	0.23
(1,1341)	1:89:A:LYS:HE3	1:89:A:LYS:HB3	14	0.23
(1,1341)	1:89:A:LYS:HE3	1:89:A:LYS:HB3	15	0.23
(1,1341)	1:89:A:LYS:HE3	1:89:A:LYS:HB3	17	0.23
(1,1341)	1:89:A:LYS:HE3	1:89:A:LYS:HB3	18	0.23
(1,1328)	1:87:A:ASP:HA	1:88:A:ALA:H	13	0.23
(1,1328)	1:87:A:ASP:HA	1:88:A:ALA:H	16	0.23
(1,1235)	1:81:A:LYS:HE3	1:81:A:LYS:HG3	19	0.23
(1,1205)	1:79:A:LEU:HD11	1:83:A:GLY:H	19	0.23
(1,1205)	1:79:A:LEU:HD12	1:83:A:GLY:H	19	0.23
(1,1205)	1:79:A:LEU:HD13	1:83:A:GLY:H	19	0.23
(1,1141)	1:74:A:LYS:HE3	1:78:A:THR:H	15	0.23
(1,1141)	1:74:A:LYS:HE3	1:78:A:THR:H	18	0.23
(1,1123)	1:74:A:LYS:H	1:74:A:LYS:HD2	19	0.23
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD11	11	0.23
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD12	11	0.23
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD13	11	0.23
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD11	3	0.23
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD12	3	0.23
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD13	3	0.23
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD11	5	0.23
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD12	5	0.23
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD13	5	0.23
(1,1081)	1:71:A:TRP:HB2	1:72:A:LEU:H	1	0.23
(1,1081)	1:71:A:TRP:HB2	1:72:A:LEU:H	18	0.23
(1,1072)	1:70:A:THR:H	1:71:A:TRP:H	7	0.23
(1,1053)	1:67:A:LYS:H	1:88:A:ALA:HA	17	0.23
(1,1049)	1:67:A:LYS:HB3	1:69:A:ARG:HA	11	0.23
(1,1033)	1:67:A:LYS:HA	1:67:A:LYS:HD3	14	0.23
(1,992)	1:64:A:TRP:H	1:93:A:THR:HG1	6	0.23
(1,992)	1:64:A:TRP:H	1:93:A:THR:HG1	11	0.23
(1,992)	1:64:A:TRP:H	1:93:A:THR:HG1	16	0.23
(1,981)	1:64:A:TRP:H	1:64:A:TRP:HB3	5	0.23
(1,981)	1:64:A:TRP:H	1:64:A:TRP:HB3	18	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,978)	1:63:A:LEU:HA	1:93:A:THR:H	7	0.23
(1,974)	1:63:A:LEU:HA	1:92:A:PHE:H	2	0.23
(1,950)	1:63:A:LEU:H	1:63:A:LEU:HG	14	0.23
(1,926)	1:61:A:HIS:H	1:62:A:ALA:H	14	0.23
(1,895)	1:57:A:ASP:H	1:57:A:ASP:HB2	2	0.23
(1,838)	1:49:A:VAL:HG21	1:58:A:TRP:H	5	0.23
(1,838)	1:49:A:VAL:HG22	1:58:A:TRP:H	5	0.23
(1,838)	1:49:A:VAL:HG23	1:58:A:TRP:H	5	0.23
(1,838)	1:49:A:VAL:HG21	1:58:A:TRP:H	6	0.23
(1,838)	1:49:A:VAL:HG22	1:58:A:TRP:H	6	0.23
(1,838)	1:49:A:VAL:HG23	1:58:A:TRP:H	6	0.23
(1,818)	1:48:A:LEU:HD21	1:52:A:LEU:H	3	0.23
(1,818)	1:48:A:LEU:HD22	1:52:A:LEU:H	3	0.23
(1,818)	1:48:A:LEU:HD23	1:52:A:LEU:H	3	0.23
(1,818)	1:48:A:LEU:HD21	1:52:A:LEU:H	4	0.23
(1,818)	1:48:A:LEU:HD22	1:52:A:LEU:H	4	0.23
(1,818)	1:48:A:LEU:HD23	1:52:A:LEU:H	4	0.23
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG21	14	0.23
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG22	14	0.23
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG23	14	0.23
(1,784)	1:47:A:LYS:HG3	1:48:A:LEU:H	2	0.23
(1,784)	1:47:A:LYS:HG3	1:48:A:LEU:H	5	0.23
(1,784)	1:47:A:LYS:HG3	1:48:A:LEU:H	7	0.23
(1,784)	1:47:A:LYS:HG3	1:48:A:LEU:H	16	0.23
(1,765)	1:46:A:LEU:H	1:49:A:VAL:H	14	0.23
(1,765)	1:46:A:LEU:H	1:49:A:VAL:H	16	0.23
(1,760)	1:46:A:LEU:H	1:48:A:LEU:H	5	0.23
(1,760)	1:46:A:LEU:H	1:48:A:LEU:H	6	0.23
(1,760)	1:46:A:LEU:H	1:48:A:LEU:H	11	0.23
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD21	3	0.23
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD22	3	0.23
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD23	3	0.23
(1,737)	1:45:A:MET:HB3	1:48:A:LEU:H	9	0.23
(1,719)	1:44:A:VAL:HG11	1:90:A:LEU:H	6	0.23
(1,719)	1:44:A:VAL:HG12	1:90:A:LEU:H	6	0.23
(1,719)	1:44:A:VAL:HG13	1:90:A:LEU:H	6	0.23
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG11	13	0.23
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG12	13	0.23
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG13	13	0.23
(1,684)	1:42:A:GLY:HA3	1:75:A:THR:HB	1	0.23
(1,684)	1:42:A:GLY:HA3	1:75:A:THR:HB	6	0.23
(1,684)	1:42:A:GLY:HA3	1:75:A:THR:HB	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,684)	1:42:A:GLY:HA3	1:75:A:THR:HB	17	0.23
(1,683)	1:42:A:GLY:H	1:74:A:LYS:HE3	14	0.23
(1,671)	1:41:A:ILE:HD11	1:75:A:THR:HA	18	0.23
(1,671)	1:41:A:ILE:HD12	1:75:A:THR:HA	18	0.23
(1,671)	1:41:A:ILE:HD13	1:75:A:THR:HA	18	0.23
(1,671)	1:41:A:ILE:HD11	1:75:A:THR:HA	20	0.23
(1,671)	1:41:A:ILE:HD12	1:75:A:THR:HA	20	0.23
(1,671)	1:41:A:ILE:HD13	1:75:A:THR:HA	20	0.23
(1,663)	1:41:A:ILE:HG21	1:72:A:LEU:HG	7	0.23
(1,663)	1:41:A:ILE:HG22	1:72:A:LEU:HG	7	0.23
(1,663)	1:41:A:ILE:HG23	1:72:A:LEU:HG	7	0.23
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG11	3	0.23
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG12	3	0.23
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG13	3	0.23
(1,588)	1:38:A:GLU:HA	1:80:A:ASP:H	7	0.23
(1,588)	1:38:A:GLU:HA	1:80:A:ASP:H	14	0.23
(1,552)	1:36:A:THR:HB	1:38:A:GLU:H	17	0.23
(1,552)	1:36:A:THR:HB	1:38:A:GLU:H	18	0.23
(1,523)	1:34:A:ARG:HB3	1:35:A:VAL:H	2	0.23
(1,523)	1:34:A:ARG:HB3	1:35:A:VAL:H	4	0.23
(1,523)	1:34:A:ARG:HB3	1:35:A:VAL:H	12	0.23
(1,511)	1:33:A:LEU:HD21	1:48:A:LEU:HB3	13	0.23
(1,511)	1:33:A:LEU:HD22	1:48:A:LEU:HB3	13	0.23
(1,511)	1:33:A:LEU:HD23	1:48:A:LEU:HB3	13	0.23
(1,511)	1:33:A:LEU:HD21	1:48:A:LEU:HB3	16	0.23
(1,511)	1:33:A:LEU:HD22	1:48:A:LEU:HB3	16	0.23
(1,511)	1:33:A:LEU:HD23	1:48:A:LEU:HB3	16	0.23
(1,508)	1:33:A:LEU:HD21	1:48:A:LEU:H	1	0.23
(1,508)	1:33:A:LEU:HD22	1:48:A:LEU:H	1	0.23
(1,508)	1:33:A:LEU:HD23	1:48:A:LEU:H	1	0.23
(1,508)	1:33:A:LEU:HD21	1:48:A:LEU:H	9	0.23
(1,508)	1:33:A:LEU:HD22	1:48:A:LEU:H	9	0.23
(1,508)	1:33:A:LEU:HD23	1:48:A:LEU:H	9	0.23
(1,508)	1:33:A:LEU:HD21	1:48:A:LEU:H	19	0.23
(1,508)	1:33:A:LEU:HD22	1:48:A:LEU:H	19	0.23
(1,508)	1:33:A:LEU:HD23	1:48:A:LEU:H	19	0.23
(1,484)	1:32:A:THR:HA	1:51:A:LYS:HD3	5	0.23
(1,484)	1:32:A:THR:HA	1:51:A:LYS:HD3	6	0.23
(1,483)	1:32:A:THR:H	1:34:A:ARG:H	6	0.23
(1,483)	1:32:A:THR:H	1:34:A:ARG:H	8	0.23
(1,483)	1:32:A:THR:H	1:34:A:ARG:H	14	0.23
(1,482)	1:32:A:THR:HA	1:34:A:ARG:H	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG11	5	0.23
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG12	5	0.23
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG13	5	0.23
(1,436)	1:28:A:ASN:HB2	1:29:A:ARG:H	12	0.23
(1,436)	1:28:A:ASN:HB2	1:29:A:ARG:H	13	0.23
(1,436)	1:28:A:ASN:HB2	1:29:A:ARG:H	14	0.23
(1,436)	1:28:A:ASN:HB2	1:29:A:ARG:H	18	0.23
(1,433)	1:28:A:ASN:H	1:28:A:ASN:HB3	8	0.23
(1,433)	1:28:A:ASN:H	1:28:A:ASN:HB3	9	0.23
(1,433)	1:28:A:ASN:H	1:28:A:ASN:HB3	10	0.23
(1,433)	1:28:A:ASN:H	1:28:A:ASN:HB3	11	0.23
(1,433)	1:28:A:ASN:H	1:28:A:ASN:HB3	14	0.23
(1,433)	1:28:A:ASN:H	1:28:A:ASN:HB3	15	0.23
(1,433)	1:28:A:ASN:H	1:28:A:ASN:HB3	18	0.23
(1,432)	1:28:A:ASN:H	1:28:A:ASN:HB2	13	0.23
(1,432)	1:28:A:ASN:H	1:28:A:ASN:HB2	16	0.23
(1,431)	1:27:A:VAL:H	1:93:A:THR:HB	1	0.23
(1,431)	1:27:A:VAL:H	1:93:A:THR:HB	2	0.23
(1,431)	1:27:A:VAL:H	1:93:A:THR:HB	11	0.23
(1,387)	1:24:A:VAL:HG11	1:62:A:ALA:H	3	0.23
(1,387)	1:24:A:VAL:HG12	1:62:A:ALA:H	3	0.23
(1,387)	1:24:A:VAL:HG13	1:62:A:ALA:H	3	0.23
(1,387)	1:24:A:VAL:HG11	1:62:A:ALA:H	8	0.23
(1,387)	1:24:A:VAL:HG12	1:62:A:ALA:H	8	0.23
(1,387)	1:24:A:VAL:HG13	1:62:A:ALA:H	8	0.23
(1,387)	1:24:A:VAL:HG11	1:62:A:ALA:H	17	0.23
(1,387)	1:24:A:VAL:HG12	1:62:A:ALA:H	17	0.23
(1,387)	1:24:A:VAL:HG13	1:62:A:ALA:H	17	0.23
(1,352)	1:23:A:HIS:HB3	1:91:A:GLN:HB2	20	0.23
(1,340)	1:23:A:HIS:H	1:91:A:GLN:HA	3	0.23
(1,297)	1:22:A:VAL:H	1:31:A:VAL:H	4	0.23
(1,276)	1:21:A:SER:H	1:32:A:THR:HG21	20	0.23
(1,276)	1:21:A:SER:H	1:32:A:THR:HG22	20	0.23
(1,276)	1:21:A:SER:H	1:32:A:THR:HG23	20	0.23
(1,269)	1:21:A:SER:HA	1:23:A:HIS:H	6	0.23
(1,269)	1:21:A:SER:HA	1:23:A:HIS:H	8	0.23
(1,269)	1:21:A:SER:HA	1:23:A:HIS:H	12	0.23
(1,269)	1:21:A:SER:HA	1:23:A:HIS:H	19	0.23
(1,266)	1:21:A:SER:H	1:22:A:VAL:H	2	0.23
(1,266)	1:21:A:SER:H	1:22:A:VAL:H	7	0.23
(1,266)	1:21:A:SER:H	1:22:A:VAL:H	14	0.23
(1,244)	1:20:A:LEU:HD21	1:33:A:LEU:HA	16	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,244)	1:20:A:LEU:HD22	1:33:A:LEU:HA	16	0.23
(1,244)	1:20:A:LEU:HD23	1:33:A:LEU:HA	16	0.23
(1,206)	1:19:A:GLU:H	1:20:A:LEU:HB2	12	0.23
(1,206)	1:19:A:GLU:H	1:20:A:LEU:HB2	17	0.23
(1,184)	1:18:A:TRP:HE1	1:80:A:ASP:HB3	17	0.23
(1,184)	1:18:A:TRP:HE1	1:80:A:ASP:HB3	19	0.23
(1,175)	1:18:A:TRP:H	1:35:A:VAL:HA	8	0.23
(1,175)	1:18:A:TRP:H	1:35:A:VAL:HA	15	0.23
(1,166)	1:17:A:THR:HG21	1:18:A:TRP:H	19	0.23
(1,166)	1:17:A:THR:HG22	1:18:A:TRP:H	19	0.23
(1,166)	1:17:A:THR:HG23	1:18:A:TRP:H	19	0.23
(1,142)	1:14:A:ALA:HA	1:15:A:ASP:H	6	0.23
(1,142)	1:14:A:ALA:HA	1:15:A:ASP:H	14	0.23
(1,142)	1:14:A:ALA:HA	1:15:A:ASP:H	17	0.23
(1,94)	1:8:A:MET:H	1:10:A:ASP:HA	8	0.23
(1,67)	1:6:A:ILE:H	1:10:A:ASP:H	1	0.23
(1,66)	1:6:A:ILE:HB	1:8:A:MET:H	16	0.23
(1,56)	1:6:A:ILE:H	1:6:A:ILE:HG12	11	0.23
(1,36)	1:3:A:LEU:HB3	1:4:A:ASP:H	8	0.23
(1,34)	1:3:A:LEU:HD21	1:4:A:ASP:H	13	0.23
(1,34)	1:3:A:LEU:HD22	1:4:A:ASP:H	13	0.23
(1,34)	1:3:A:LEU:HD23	1:4:A:ASP:H	13	0.23
(1,19)	1:2:A:ALA:HB1	1:3:A:LEU:H	1	0.23
(1,19)	1:2:A:ALA:HB2	1:3:A:LEU:H	1	0.23
(1,19)	1:2:A:ALA:HB3	1:3:A:LEU:H	1	0.23
(2,21)	1:39:A:VAL:O	1:43:A:GLY:N	20	0.22
(2,17)	1:21:A:SER:O	1:91:A:GLN:H	19	0.22
(2,13)	1:92:A:PHE:O	1:64:A:TRP:N	20	0.22
(2,7)	1:29:A:ARG:O	1:24:A:VAL:N	11	0.22
(2,7)	1:29:A:ARG:O	1:24:A:VAL:N	15	0.22
(2,4)	1:33:A:LEU:O	1:20:A:LEU:N	10	0.22
(1,1404)	1:92:A:PHE:HB2	1:93:A:THR:HB	3	0.22
(1,1404)	1:92:A:PHE:HB2	1:93:A:THR:HB	8	0.22
(1,1380)	1:91:A:GLN:H	1:91:A:GLN:HE22	6	0.22
(1,1377)	1:91:A:GLN:H	1:91:A:GLN:HB3	2	0.22
(1,1377)	1:91:A:GLN:H	1:91:A:GLN:HB3	7	0.22
(1,1377)	1:91:A:GLN:H	1:91:A:GLN:HB3	8	0.22
(1,1377)	1:91:A:GLN:H	1:91:A:GLN:HB3	12	0.22
(1,1377)	1:91:A:GLN:H	1:91:A:GLN:HB3	13	0.22
(1,1377)	1:91:A:GLN:H	1:91:A:GLN:HB3	16	0.22
(1,1377)	1:91:A:GLN:H	1:91:A:GLN:HB3	17	0.22
(1,1341)	1:89:A:LYS:HE3	1:89:A:LYS:HB3	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1341)	1:89:A:LYS:HE3	1:89:A:LYS:HB3	2	0.22
(1,1341)	1:89:A:LYS:HE3	1:89:A:LYS:HB3	6	0.22
(1,1341)	1:89:A:LYS:HE3	1:89:A:LYS:HB3	9	0.22
(1,1341)	1:89:A:LYS:HE3	1:89:A:LYS:HB3	10	0.22
(1,1341)	1:89:A:LYS:HE3	1:89:A:LYS:HB3	12	0.22
(1,1341)	1:89:A:LYS:HE3	1:89:A:LYS:HB3	16	0.22
(1,1341)	1:89:A:LYS:HE3	1:89:A:LYS:HB3	20	0.22
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG21	3	0.22
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG22	3	0.22
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG23	3	0.22
(1,1235)	1:81:A:LYS:HE3	1:81:A:LYS:HG3	3	0.22
(1,1235)	1:81:A:LYS:HE3	1:81:A:LYS:HG3	5	0.22
(1,1205)	1:79:A:LEU:HD11	1:83:A:GLY:H	11	0.22
(1,1205)	1:79:A:LEU:HD12	1:83:A:GLY:H	11	0.22
(1,1205)	1:79:A:LEU:HD13	1:83:A:GLY:H	11	0.22
(1,1178)	1:78:A:THR:HG21	1:81:A:LYS:H	15	0.22
(1,1178)	1:78:A:THR:HG22	1:81:A:LYS:H	15	0.22
(1,1178)	1:78:A:THR:HG23	1:81:A:LYS:H	15	0.22
(1,1177)	1:78:A:THR:H	1:81:A:LYS:H	11	0.22
(1,1177)	1:78:A:THR:H	1:81:A:LYS:H	20	0.22
(1,1169)	1:78:A:THR:HB	1:79:A:LEU:H	6	0.22
(1,1169)	1:78:A:THR:HB	1:79:A:LEU:H	7	0.22
(1,1169)	1:78:A:THR:HB	1:79:A:LEU:H	10	0.22
(1,1169)	1:78:A:THR:HB	1:79:A:LEU:H	17	0.22
(1,1162)	1:77:A:TRP:H	1:81:A:LYS:HE3	3	0.22
(1,1162)	1:77:A:TRP:H	1:81:A:LYS:HE3	19	0.22
(1,1160)	1:77:A:TRP:HB2	1:78:A:THR:H	13	0.22
(1,1159)	1:77:A:TRP:HB3	1:78:A:THR:H	19	0.22
(1,1141)	1:74:A:LYS:HE3	1:78:A:THR:H	8	0.22
(1,1134)	1:74:A:LYS:HG2	1:75:A:THR:H	13	0.22
(1,1123)	1:74:A:LYS:H	1:74:A:LYS:HD2	2	0.22
(1,1123)	1:74:A:LYS:H	1:74:A:LYS:HD2	5	0.22
(1,1123)	1:74:A:LYS:H	1:74:A:LYS:HD2	11	0.22
(1,1110)	1:73:A:LEU:HB3	1:74:A:LYS:H	7	0.22
(1,1105)	1:73:A:LEU:H	1:73:A:LEU:HB3	1	0.22
(1,1105)	1:73:A:LEU:H	1:73:A:LEU:HB3	9	0.22
(1,1105)	1:73:A:LEU:H	1:73:A:LEU:HB3	19	0.22
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD11	4	0.22
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD12	4	0.22
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD13	4	0.22
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD11	7	0.22
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD12	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD13	7	0.22
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD11	9	0.22
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD12	9	0.22
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD13	9	0.22
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD11	12	0.22
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD12	12	0.22
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD13	12	0.22
(1,1081)	1:71:A:TRP:HB2	1:72:A:LEU:H	4	0.22
(1,1081)	1:71:A:TRP:HB2	1:72:A:LEU:H	5	0.22
(1,1081)	1:71:A:TRP:HB2	1:72:A:LEU:H	6	0.22
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD21	6	0.22
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD22	6	0.22
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD23	6	0.22
(1,1053)	1:67:A:LYS:H	1:88:A:ALA:HA	16	0.22
(1,1033)	1:67:A:LYS:HA	1:67:A:LYS:HD3	11	0.22
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD21	17	0.22
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD22	17	0.22
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD23	17	0.22
(1,992)	1:64:A:TRP:H	1:93:A:THR:HG1	12	0.22
(1,992)	1:64:A:TRP:H	1:93:A:THR:HG1	17	0.22
(1,981)	1:64:A:TRP:H	1:64:A:TRP:HB3	1	0.22
(1,978)	1:63:A:LEU:HA	1:93:A:THR:H	2	0.22
(1,974)	1:63:A:LEU:HA	1:92:A:PHE:H	4	0.22
(1,974)	1:63:A:LEU:HA	1:92:A:PHE:H	7	0.22
(1,974)	1:63:A:LEU:HA	1:92:A:PHE:H	13	0.22
(1,974)	1:63:A:LEU:HA	1:92:A:PHE:H	15	0.22
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD11	1	0.22
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD12	1	0.22
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD13	1	0.22
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD11	3	0.22
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD12	3	0.22
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD13	3	0.22
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD11	12	0.22
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD12	12	0.22
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD13	12	0.22
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD11	16	0.22
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD12	16	0.22
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD13	16	0.22
(1,904)	1:58:A:TRP:H	1:58:A:TRP:HB3	7	0.22
(1,890)	1:56:A:LYS:HA	1:57:A:ASP:HB2	10	0.22
(1,869)	1:52:A:LEU:H	1:52:A:LEU:HD21	19	0.22
(1,869)	1:52:A:LEU:H	1:52:A:LEU:HD22	19	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,869)	1:52:A:LEU:H	1:52:A:LEU:HD23	19	0.22
(1,862)	1:51:A:LYS:HB3	1:52:A:LEU:H	19	0.22
(1,818)	1:48:A:LEU:HD21	1:52:A:LEU:H	5	0.22
(1,818)	1:48:A:LEU:HD22	1:52:A:LEU:H	5	0.22
(1,818)	1:48:A:LEU:HD23	1:52:A:LEU:H	5	0.22
(1,784)	1:47:A:LYS:HG3	1:48:A:LEU:H	15	0.22
(1,782)	1:47:A:LYS:HB2	1:48:A:LEU:H	3	0.22
(1,765)	1:46:A:LEU:H	1:49:A:VAL:H	1	0.22
(1,765)	1:46:A:LEU:H	1:49:A:VAL:H	3	0.22
(1,765)	1:46:A:LEU:H	1:49:A:VAL:H	4	0.22
(1,765)	1:46:A:LEU:H	1:49:A:VAL:H	7	0.22
(1,765)	1:46:A:LEU:H	1:49:A:VAL:H	10	0.22
(1,765)	1:46:A:LEU:H	1:49:A:VAL:H	20	0.22
(1,764)	1:46:A:LEU:HA	1:49:A:VAL:H	11	0.22
(1,760)	1:46:A:LEU:H	1:48:A:LEU:H	3	0.22
(1,746)	1:45:A:MET:HG3	1:63:A:LEU:HD21	19	0.22
(1,746)	1:45:A:MET:HG3	1:63:A:LEU:HD22	19	0.22
(1,746)	1:45:A:MET:HG3	1:63:A:LEU:HD23	19	0.22
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD21	16	0.22
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD22	16	0.22
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD23	16	0.22
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD21	17	0.22
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD22	17	0.22
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD23	17	0.22
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG21	1	0.22
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG22	1	0.22
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG23	1	0.22
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG21	8	0.22
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG22	8	0.22
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG23	8	0.22
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG21	13	0.22
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG22	13	0.22
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG23	13	0.22
(1,737)	1:45:A:MET:HB3	1:48:A:LEU:H	12	0.22
(1,719)	1:44:A:VAL:HG11	1:90:A:LEU:H	5	0.22
(1,719)	1:44:A:VAL:HG12	1:90:A:LEU:H	5	0.22
(1,719)	1:44:A:VAL:HG13	1:90:A:LEU:H	5	0.22
(1,683)	1:42:A:GLY:H	1:74:A:LYS:HE3	13	0.22
(1,676)	1:41:A:ILE:HG13	1:78:A:THR:H	18	0.22
(1,659)	1:41:A:ILE:HD11	1:44:A:VAL:H	16	0.22
(1,659)	1:41:A:ILE:HD12	1:44:A:VAL:H	16	0.22
(1,659)	1:41:A:ILE:HD13	1:44:A:VAL:H	16	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG11	4	0.22
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG12	4	0.22
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG13	4	0.22
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG11	5	0.22
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG12	5	0.22
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG13	5	0.22
(1,628)	1:40:A:HIS:H	1:44:A:VAL:HB	1	0.22
(1,628)	1:40:A:HIS:H	1:44:A:VAL:HB	17	0.22
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD21	15	0.22
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD22	15	0.22
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD23	15	0.22
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD21	17	0.22
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD22	17	0.22
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD23	17	0.22
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG21	1	0.22
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG22	1	0.22
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG23	1	0.22
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG21	15	0.22
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG22	15	0.22
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG23	15	0.22
(1,552)	1:36:A:THR:HB	1:38:A:GLU:H	1	0.22
(1,552)	1:36:A:THR:HB	1:38:A:GLU:H	7	0.22
(1,511)	1:33:A:LEU:HD21	1:48:A:LEU:HB3	7	0.22
(1,511)	1:33:A:LEU:HD22	1:48:A:LEU:HB3	7	0.22
(1,511)	1:33:A:LEU:HD23	1:48:A:LEU:HB3	7	0.22
(1,508)	1:33:A:LEU:HD21	1:48:A:LEU:H	12	0.22
(1,508)	1:33:A:LEU:HD22	1:48:A:LEU:H	12	0.22
(1,508)	1:33:A:LEU:HD23	1:48:A:LEU:H	12	0.22
(1,508)	1:33:A:LEU:HD21	1:48:A:LEU:H	15	0.22
(1,508)	1:33:A:LEU:HD22	1:48:A:LEU:H	15	0.22
(1,508)	1:33:A:LEU:HD23	1:48:A:LEU:H	15	0.22
(1,497)	1:33:A:LEU:HB3	1:34:A:ARG:H	20	0.22
(1,483)	1:32:A:THR:H	1:34:A:ARG:H	3	0.22
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG11	1	0.22
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG12	1	0.22
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG13	1	0.22
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG11	4	0.22
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG12	4	0.22
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG13	4	0.22
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG11	18	0.22
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG12	18	0.22
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG13	18	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG11	19	0.22
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG12	19	0.22
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG13	19	0.22
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG11	20	0.22
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG12	20	0.22
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG13	20	0.22
(1,436)	1:28:A:ASN:HB2	1:29:A:ARG:H	2	0.22
(1,436)	1:28:A:ASN:HB2	1:29:A:ARG:H	5	0.22
(1,436)	1:28:A:ASN:HB2	1:29:A:ARG:H	8	0.22
(1,436)	1:28:A:ASN:HB2	1:29:A:ARG:H	15	0.22
(1,436)	1:28:A:ASN:HB2	1:29:A:ARG:H	16	0.22
(1,436)	1:28:A:ASN:HB2	1:29:A:ARG:H	17	0.22
(1,436)	1:28:A:ASN:HB2	1:29:A:ARG:H	19	0.22
(1,436)	1:28:A:ASN:HB2	1:29:A:ARG:H	20	0.22
(1,434)	1:28:A:ASN:HA	1:29:A:ARG:H	1	0.22
(1,434)	1:28:A:ASN:HA	1:29:A:ARG:H	2	0.22
(1,434)	1:28:A:ASN:HA	1:29:A:ARG:H	4	0.22
(1,434)	1:28:A:ASN:HA	1:29:A:ARG:H	5	0.22
(1,433)	1:28:A:ASN:H	1:28:A:ASN:HB3	12	0.22
(1,433)	1:28:A:ASN:H	1:28:A:ASN:HB3	20	0.22
(1,432)	1:28:A:ASN:H	1:28:A:ASN:HB2	5	0.22
(1,426)	1:27:A:VAL:H	1:28:A:ASN:HB2	11	0.22
(1,387)	1:24:A:VAL:HG11	1:62:A:ALA:H	5	0.22
(1,387)	1:24:A:VAL:HG12	1:62:A:ALA:H	5	0.22
(1,387)	1:24:A:VAL:HG13	1:62:A:ALA:H	5	0.22
(1,377)	1:24:A:VAL:HA	1:30:A:ASP:HA	5	0.22
(1,352)	1:23:A:HIS:HB3	1:91:A:GLN:HB2	6	0.22
(1,352)	1:23:A:HIS:HB3	1:91:A:GLN:HB2	15	0.22
(1,350)	1:23:A:HIS:HB2	1:91:A:GLN:HG3	16	0.22
(1,331)	1:23:A:HIS:H	1:30:A:ASP:HB3	20	0.22
(1,297)	1:22:A:VAL:H	1:31:A:VAL:H	7	0.22
(1,276)	1:21:A:SER:H	1:32:A:THR:HG21	2	0.22
(1,276)	1:21:A:SER:H	1:32:A:THR:HG22	2	0.22
(1,276)	1:21:A:SER:H	1:32:A:THR:HG23	2	0.22
(1,276)	1:21:A:SER:H	1:32:A:THR:HG21	10	0.22
(1,276)	1:21:A:SER:H	1:32:A:THR:HG22	10	0.22
(1,276)	1:21:A:SER:H	1:32:A:THR:HG23	10	0.22
(1,269)	1:21:A:SER:HA	1:23:A:HIS:H	1	0.22
(1,269)	1:21:A:SER:HA	1:23:A:HIS:H	17	0.22
(1,269)	1:21:A:SER:HA	1:23:A:HIS:H	18	0.22
(1,266)	1:21:A:SER:H	1:22:A:VAL:H	3	0.22
(1,266)	1:21:A:SER:H	1:22:A:VAL:H	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,266)	1:21:A:SER:H	1:22:A:VAL:H	10	0.22
(1,266)	1:21:A:SER:H	1:22:A:VAL:H	13	0.22
(1,266)	1:21:A:SER:H	1:22:A:VAL:H	17	0.22
(1,266)	1:21:A:SER:H	1:22:A:VAL:H	20	0.22
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG21	14	0.22
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG22	14	0.22
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG23	14	0.22
(1,251)	1:20:A:LEU:HG	1:35:A:VAL:H	5	0.22
(1,249)	1:20:A:LEU:HB2	1:34:A:ARG:H	19	0.22
(1,244)	1:20:A:LEU:HD21	1:33:A:LEU:HA	2	0.22
(1,244)	1:20:A:LEU:HD22	1:33:A:LEU:HA	2	0.22
(1,244)	1:20:A:LEU:HD23	1:33:A:LEU:HA	2	0.22
(1,244)	1:20:A:LEU:HD21	1:33:A:LEU:HA	9	0.22
(1,244)	1:20:A:LEU:HD22	1:33:A:LEU:HA	9	0.22
(1,244)	1:20:A:LEU:HD23	1:33:A:LEU:HA	9	0.22
(1,244)	1:20:A:LEU:HD21	1:33:A:LEU:HA	10	0.22
(1,244)	1:20:A:LEU:HD22	1:33:A:LEU:HA	10	0.22
(1,244)	1:20:A:LEU:HD23	1:33:A:LEU:HA	10	0.22
(1,244)	1:20:A:LEU:HD21	1:33:A:LEU:HA	11	0.22
(1,244)	1:20:A:LEU:HD22	1:33:A:LEU:HA	11	0.22
(1,244)	1:20:A:LEU:HD23	1:33:A:LEU:HA	11	0.22
(1,244)	1:20:A:LEU:HD21	1:33:A:LEU:HA	15	0.22
(1,244)	1:20:A:LEU:HD22	1:33:A:LEU:HA	15	0.22
(1,244)	1:20:A:LEU:HD23	1:33:A:LEU:HA	15	0.22
(1,242)	1:20:A:LEU:HB3	1:33:A:LEU:H	6	0.22
(1,206)	1:19:A:GLU:H	1:20:A:LEU:HB2	4	0.22
(1,206)	1:19:A:GLU:H	1:20:A:LEU:HB2	7	0.22
(1,203)	1:19:A:GLU:HB3	1:20:A:LEU:H	11	0.22
(1,203)	1:19:A:GLU:HB3	1:20:A:LEU:H	16	0.22
(1,203)	1:19:A:GLU:HB3	1:20:A:LEU:H	17	0.22
(1,203)	1:19:A:GLU:HB3	1:20:A:LEU:H	20	0.22
(1,195)	1:19:A:GLU:H	1:19:A:GLU:HG2	11	0.22
(1,195)	1:19:A:GLU:H	1:19:A:GLU:HG2	13	0.22
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG21	13	0.22
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG22	13	0.22
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG23	13	0.22
(1,184)	1:18:A:TRP:HE1	1:80:A:ASP:HB3	5	0.22
(1,177)	1:18:A:TRP:HE1	1:36:A:THR:HB	15	0.22
(1,175)	1:18:A:TRP:H	1:35:A:VAL:HA	11	0.22
(1,166)	1:17:A:THR:HG21	1:18:A:TRP:H	18	0.22
(1,166)	1:17:A:THR:HG22	1:18:A:TRP:H	18	0.22
(1,166)	1:17:A:THR:HG23	1:18:A:TRP:H	18	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,156)	1:16:A:GLY:HA2	1:17:A:THR:H	4	0.22
(1,155)	1:16:A:GLY:HA3	1:17:A:THR:H	5	0.22
(1,112)	1:9:A:PRO:HG3	1:10:A:ASP:H	20	0.22
(1,110)	1:9:A:PRO:HB2	1:10:A:ASP:H	12	0.22
(1,95)	1:8:A:MET:HA	1:10:A:ASP:H	12	0.22
(1,94)	1:8:A:MET:H	1:10:A:ASP:HA	16	0.22
(1,90)	1:8:A:MET:H	1:8:A:MET:HG3	11	0.22
(1,90)	1:8:A:MET:H	1:8:A:MET:HG3	15	0.22
(1,67)	1:6:A:ILE:H	1:10:A:ASP:H	10	0.22
(1,59)	1:6:A:ILE:H	1:6:A:ILE:HD11	11	0.22
(1,59)	1:6:A:ILE:H	1:6:A:ILE:HD12	11	0.22
(1,59)	1:6:A:ILE:H	1:6:A:ILE:HD13	11	0.22
(1,47)	1:5:A:GLY:H	1:6:A:ILE:H	19	0.22
(1,42)	1:4:A:ASP:H	1:5:A:GLY:HA3	3	0.22
(1,34)	1:3:A:LEU:HD21	1:4:A:ASP:H	7	0.22
(1,34)	1:3:A:LEU:HD22	1:4:A:ASP:H	7	0.22
(1,34)	1:3:A:LEU:HD23	1:4:A:ASP:H	7	0.22
(1,34)	1:3:A:LEU:HD21	1:4:A:ASP:H	8	0.22
(1,34)	1:3:A:LEU:HD22	1:4:A:ASP:H	8	0.22
(1,34)	1:3:A:LEU:HD23	1:4:A:ASP:H	8	0.22
(1,17)	1:2:A:ALA:H	1:3:A:LEU:HA	20	0.22
(1,16)	1:2:A:ALA:H	1:3:A:LEU:HB3	6	0.22
(1,16)	1:2:A:ALA:H	1:3:A:LEU:HB3	10	0.22
(1,16)	1:2:A:ALA:H	1:3:A:LEU:HB3	12	0.22
(3,21)	1:80:A:ASP:O	1:84:A:ILE:H	18	0.21
(2,21)	1:39:A:VAL:O	1:43:A:GLY:N	12	0.21
(2,17)	1:21:A:SER:O	1:91:A:GLN:H	11	0.21
(2,13)	1:92:A:PHE:O	1:64:A:TRP:N	13	0.21
(2,13)	1:92:A:PHE:O	1:64:A:TRP:N	15	0.21
(2,7)	1:29:A:ARG:O	1:24:A:VAL:N	8	0.21
(2,7)	1:29:A:ARG:O	1:24:A:VAL:N	9	0.21
(2,7)	1:29:A:ARG:O	1:24:A:VAL:N	10	0.21
(2,7)	1:29:A:ARG:O	1:24:A:VAL:N	14	0.21
(2,7)	1:29:A:ARG:O	1:24:A:VAL:N	16	0.21
(2,4)	1:33:A:LEU:O	1:20:A:LEU:N	11	0.21
(1,1404)	1:92:A:PHE:HB2	1:93:A:THR:HB	2	0.21
(1,1404)	1:92:A:PHE:HB2	1:93:A:THR:HB	6	0.21
(1,1404)	1:92:A:PHE:HB2	1:93:A:THR:HB	9	0.21
(1,1404)	1:92:A:PHE:HB2	1:93:A:THR:HB	10	0.21
(1,1377)	1:91:A:GLN:H	1:91:A:GLN:HB3	1	0.21
(1,1377)	1:91:A:GLN:H	1:91:A:GLN:HB3	3	0.21
(1,1377)	1:91:A:GLN:H	1:91:A:GLN:HB3	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1377)	1:91:A:GLN:H	1:91:A:GLN:HB3	5	0.21
(1,1377)	1:91:A:GLN:H	1:91:A:GLN:HB3	6	0.21
(1,1377)	1:91:A:GLN:H	1:91:A:GLN:HB3	9	0.21
(1,1377)	1:91:A:GLN:H	1:91:A:GLN:HB3	10	0.21
(1,1377)	1:91:A:GLN:H	1:91:A:GLN:HB3	11	0.21
(1,1377)	1:91:A:GLN:H	1:91:A:GLN:HB3	15	0.21
(1,1377)	1:91:A:GLN:H	1:91:A:GLN:HB3	20	0.21
(1,1341)	1:89:A:LYS:HE3	1:89:A:LYS:HB3	19	0.21
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG21	4	0.21
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG22	4	0.21
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG23	4	0.21
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG21	14	0.21
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG22	14	0.21
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG23	14	0.21
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG21	20	0.21
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG22	20	0.21
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG23	20	0.21
(1,1235)	1:81:A:LYS:HE3	1:81:A:LYS:HG3	2	0.21
(1,1235)	1:81:A:LYS:HE3	1:81:A:LYS:HG3	9	0.21
(1,1235)	1:81:A:LYS:HE3	1:81:A:LYS:HG3	17	0.21
(1,1218)	1:80:A:ASP:HB2	1:82:A:TYR:H	4	0.21
(1,1218)	1:80:A:ASP:HB2	1:82:A:TYR:H	5	0.21
(1,1205)	1:79:A:LEU:HD11	1:83:A:GLY:H	2	0.21
(1,1205)	1:79:A:LEU:HD12	1:83:A:GLY:H	2	0.21
(1,1205)	1:79:A:LEU:HD13	1:83:A:GLY:H	2	0.21
(1,1205)	1:79:A:LEU:HD11	1:83:A:GLY:H	20	0.21
(1,1205)	1:79:A:LEU:HD12	1:83:A:GLY:H	20	0.21
(1,1205)	1:79:A:LEU:HD13	1:83:A:GLY:H	20	0.21
(1,1203)	1:79:A:LEU:HB3	1:83:A:GLY:H	19	0.21
(1,1197)	1:79:A:LEU:HB3	1:80:A:ASP:H	18	0.21
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD11	8	0.21
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD12	8	0.21
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD13	8	0.21
(1,1187)	1:79:A:LEU:H	1:79:A:LEU:HD21	13	0.21
(1,1187)	1:79:A:LEU:H	1:79:A:LEU:HD22	13	0.21
(1,1187)	1:79:A:LEU:H	1:79:A:LEU:HD23	13	0.21
(1,1169)	1:78:A:THR:HB	1:79:A:LEU:H	14	0.21
(1,1160)	1:77:A:TRP:HB2	1:78:A:THR:H	8	0.21
(1,1159)	1:77:A:TRP:HB3	1:78:A:THR:H	18	0.21
(1,1159)	1:77:A:TRP:HB3	1:78:A:THR:H	20	0.21
(1,1153)	1:76:A:HIS:HB3	1:77:A:TRP:H	12	0.21
(1,1140)	1:74:A:LYS:HA	1:77:A:TRP:H	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1140)	1:74:A:LYS:HA	1:77:A:TRP:H	20	0.21
(1,1128)	1:74:A:LYS:HE3	1:74:A:LYS:HB3	13	0.21
(1,1128)	1:74:A:LYS:HE3	1:74:A:LYS:HB3	15	0.21
(1,1123)	1:74:A:LYS:H	1:74:A:LYS:HD2	6	0.21
(1,1123)	1:74:A:LYS:H	1:74:A:LYS:HD2	10	0.21
(1,1123)	1:74:A:LYS:H	1:74:A:LYS:HD2	15	0.21
(1,1123)	1:74:A:LYS:H	1:74:A:LYS:HD2	18	0.21
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD11	5	0.21
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD12	5	0.21
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD13	5	0.21
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD11	8	0.21
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD12	8	0.21
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD13	8	0.21
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD11	10	0.21
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD12	10	0.21
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD13	10	0.21
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD11	14	0.21
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD12	14	0.21
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD13	14	0.21
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD11	16	0.21
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD12	16	0.21
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD13	16	0.21
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD11	17	0.21
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD12	17	0.21
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD13	17	0.21
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD11	1	0.21
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD12	1	0.21
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD13	1	0.21
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD11	15	0.21
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD12	15	0.21
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD13	15	0.21
(1,1081)	1:71:A:TRP:HB2	1:72:A:LEU:H	12	0.21
(1,1081)	1:71:A:TRP:HB2	1:72:A:LEU:H	15	0.21
(1,1072)	1:70:A:THR:H	1:71:A:TRP:H	1	0.21
(1,1072)	1:70:A:THR:H	1:71:A:TRP:H	10	0.21
(1,1072)	1:70:A:THR:H	1:71:A:TRP:H	12	0.21
(1,1072)	1:70:A:THR:H	1:71:A:TRP:H	14	0.21
(1,1072)	1:70:A:THR:H	1:71:A:TRP:H	20	0.21
(1,1063)	1:69:A:ARG:H	1:70:A:THR:H	5	0.21
(1,1053)	1:67:A:LYS:H	1:88:A:ALA:HA	20	0.21
(1,1049)	1:67:A:LYS:HB3	1:69:A:ARG:HA	16	0.21
(1,992)	1:64:A:TRP:H	1:93:A:THR:HG1	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,992)	1:64:A:TRP:H	1:93:A:THR:HG1	5	0.21
(1,992)	1:64:A:TRP:H	1:93:A:THR:HG1	7	0.21
(1,992)	1:64:A:TRP:H	1:93:A:THR:HG1	9	0.21
(1,992)	1:64:A:TRP:H	1:93:A:THR:HG1	13	0.21
(1,992)	1:64:A:TRP:H	1:93:A:THR:HG1	18	0.21
(1,978)	1:63:A:LEU:HA	1:93:A:THR:H	6	0.21
(1,978)	1:63:A:LEU:HA	1:93:A:THR:H	14	0.21
(1,974)	1:63:A:LEU:HA	1:92:A:PHE:H	10	0.21
(1,974)	1:63:A:LEU:HA	1:92:A:PHE:H	16	0.21
(1,972)	1:63:A:LEU:HD11	1:91:A:GLN:H	12	0.21
(1,972)	1:63:A:LEU:HD12	1:91:A:GLN:H	12	0.21
(1,972)	1:63:A:LEU:HD13	1:91:A:GLN:H	12	0.21
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD11	5	0.21
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD12	5	0.21
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD13	5	0.21
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD11	8	0.21
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD12	8	0.21
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD13	8	0.21
(1,950)	1:63:A:LEU:H	1:63:A:LEU:HG	8	0.21
(1,950)	1:63:A:LEU:H	1:63:A:LEU:HG	20	0.21
(1,946)	1:62:A:ALA:H	1:94:A:PRO:HA	5	0.21
(1,926)	1:61:A:HIS:H	1:62:A:ALA:H	3	0.21
(1,926)	1:61:A:HIS:H	1:62:A:ALA:H	12	0.21
(1,926)	1:61:A:HIS:H	1:62:A:ALA:H	16	0.21
(1,906)	1:58:A:TRP:H	1:59:A:SER:H	5	0.21
(1,903)	1:57:A:ASP:HB2	1:61:A:HIS:H	11	0.21
(1,878)	1:56:A:LYS:H	1:56:A:LYS:HD3	9	0.21
(1,838)	1:49:A:VAL:HG21	1:58:A:TRP:H	9	0.21
(1,838)	1:49:A:VAL:HG22	1:58:A:TRP:H	9	0.21
(1,838)	1:49:A:VAL:HG23	1:58:A:TRP:H	9	0.21
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD21	3	0.21
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD22	3	0.21
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD23	3	0.21
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD21	3	0.21
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD22	3	0.21
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD23	3	0.21
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD21	3	0.21
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD22	3	0.21
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD23	3	0.21
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD21	20	0.21
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD22	20	0.21
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD23	20	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD21	20	0.21
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD22	20	0.21
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD23	20	0.21
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD21	20	0.21
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD22	20	0.21
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD23	20	0.21
(1,818)	1:48:A:LEU:HD21	1:52:A:LEU:H	6	0.21
(1,818)	1:48:A:LEU:HD22	1:52:A:LEU:H	6	0.21
(1,818)	1:48:A:LEU:HD23	1:52:A:LEU:H	6	0.21
(1,818)	1:48:A:LEU:HD21	1:52:A:LEU:H	10	0.21
(1,818)	1:48:A:LEU:HD22	1:52:A:LEU:H	10	0.21
(1,818)	1:48:A:LEU:HD23	1:52:A:LEU:H	10	0.21
(1,818)	1:48:A:LEU:HD21	1:52:A:LEU:H	12	0.21
(1,818)	1:48:A:LEU:HD22	1:52:A:LEU:H	12	0.21
(1,818)	1:48:A:LEU:HD23	1:52:A:LEU:H	12	0.21
(1,784)	1:47:A:LYS:HG3	1:48:A:LEU:H	9	0.21
(1,765)	1:46:A:LEU:H	1:49:A:VAL:H	5	0.21
(1,765)	1:46:A:LEU:H	1:49:A:VAL:H	6	0.21
(1,765)	1:46:A:LEU:H	1:49:A:VAL:H	8	0.21
(1,765)	1:46:A:LEU:H	1:49:A:VAL:H	11	0.21
(1,765)	1:46:A:LEU:H	1:49:A:VAL:H	15	0.21
(1,765)	1:46:A:LEU:H	1:49:A:VAL:H	17	0.21
(1,765)	1:46:A:LEU:H	1:49:A:VAL:H	19	0.21
(1,764)	1:46:A:LEU:HA	1:49:A:VAL:H	10	0.21
(1,760)	1:46:A:LEU:H	1:48:A:LEU:H	18	0.21
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD21	18	0.21
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD22	18	0.21
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD23	18	0.21
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG21	12	0.21
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG22	12	0.21
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG23	12	0.21
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG21	17	0.21
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG22	17	0.21
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG23	17	0.21
(1,737)	1:45:A:MET:HB3	1:48:A:LEU:H	13	0.21
(1,692)	1:43:A:GLY:H	1:44:A:VAL:HB	3	0.21
(1,684)	1:42:A:GLY:HA3	1:75:A:THR:HB	9	0.21
(1,676)	1:41:A:ILE:HG13	1:78:A:THR:H	20	0.21
(1,671)	1:41:A:ILE:HD11	1:75:A:THR:HA	15	0.21
(1,671)	1:41:A:ILE:HD12	1:75:A:THR:HA	15	0.21
(1,671)	1:41:A:ILE:HD13	1:75:A:THR:HA	15	0.21
(1,671)	1:41:A:ILE:HD11	1:75:A:THR:HA	19	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,671)	1:41:A:ILE:HD12	1:75:A:THR:HA	19	0.21
(1,671)	1:41:A:ILE:HD13	1:75:A:THR:HA	19	0.21
(1,659)	1:41:A:ILE:HD11	1:44:A:VAL:H	5	0.21
(1,659)	1:41:A:ILE:HD12	1:44:A:VAL:H	5	0.21
(1,659)	1:41:A:ILE:HD13	1:44:A:VAL:H	5	0.21
(1,659)	1:41:A:ILE:HD11	1:44:A:VAL:H	8	0.21
(1,659)	1:41:A:ILE:HD12	1:44:A:VAL:H	8	0.21
(1,659)	1:41:A:ILE:HD13	1:44:A:VAL:H	8	0.21
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG11	2	0.21
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG12	2	0.21
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG13	2	0.21
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG11	6	0.21
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG12	6	0.21
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG13	6	0.21
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG11	8	0.21
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG12	8	0.21
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG13	8	0.21
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD21	3	0.21
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD22	3	0.21
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD23	3	0.21
(1,588)	1:38:A:GLU:HA	1:80:A:ASP:H	2	0.21
(1,588)	1:38:A:GLU:HA	1:80:A:ASP:H	11	0.21
(1,580)	1:38:A:GLU:HB3	1:39:A:VAL:H	4	0.21
(1,580)	1:38:A:GLU:HB3	1:39:A:VAL:H	18	0.21
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG21	10	0.21
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG22	10	0.21
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG23	10	0.21
(1,532)	1:35:A:VAL:H	1:35:A:VAL:HB	20	0.21
(1,523)	1:34:A:ARG:HB3	1:35:A:VAL:H	20	0.21
(1,511)	1:33:A:LEU:HD21	1:48:A:LEU:HB3	11	0.21
(1,511)	1:33:A:LEU:HD22	1:48:A:LEU:HB3	11	0.21
(1,511)	1:33:A:LEU:HD23	1:48:A:LEU:HB3	11	0.21
(1,483)	1:32:A:THR:H	1:34:A:ARG:H	10	0.21
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG11	7	0.21
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG12	7	0.21
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG13	7	0.21
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG11	17	0.21
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG12	17	0.21
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG13	17	0.21
(1,443)	1:29:A:ARG:HB2	1:29:A:ARG:H	11	0.21
(1,437)	1:28:A:ASN:HB3	1:29:A:ARG:H	7	0.21
(1,437)	1:28:A:ASN:HB3	1:29:A:ARG:H	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,437)	1:28:A:ASN:HB3	1:29:A:ARG:H	14	0.21
(1,436)	1:28:A:ASN:HB2	1:29:A:ARG:H	3	0.21
(1,436)	1:28:A:ASN:HB2	1:29:A:ARG:H	4	0.21
(1,436)	1:28:A:ASN:HB2	1:29:A:ARG:H	10	0.21
(1,434)	1:28:A:ASN:HA	1:29:A:ARG:H	3	0.21
(1,434)	1:28:A:ASN:HA	1:29:A:ARG:H	10	0.21
(1,434)	1:28:A:ASN:HA	1:29:A:ARG:H	19	0.21
(1,434)	1:28:A:ASN:HA	1:29:A:ARG:H	20	0.21
(1,433)	1:28:A:ASN:H	1:28:A:ASN:HB3	1	0.21
(1,433)	1:28:A:ASN:H	1:28:A:ASN:HB3	17	0.21
(1,433)	1:28:A:ASN:H	1:28:A:ASN:HB3	19	0.21
(1,432)	1:28:A:ASN:H	1:28:A:ASN:HB2	3	0.21
(1,432)	1:28:A:ASN:H	1:28:A:ASN:HB2	10	0.21
(1,432)	1:28:A:ASN:H	1:28:A:ASN:HB2	18	0.21
(1,431)	1:27:A:VAL:H	1:93:A:THR:HB	6	0.21
(1,426)	1:27:A:VAL:H	1:28:A:ASN:HB2	2	0.21
(1,426)	1:27:A:VAL:H	1:28:A:ASN:HB2	12	0.21
(1,409)	1:25:A:THR:H	1:92:A:PHE:HB2	3	0.21
(1,387)	1:24:A:VAL:HG11	1:62:A:ALA:H	4	0.21
(1,387)	1:24:A:VAL:HG12	1:62:A:ALA:H	4	0.21
(1,387)	1:24:A:VAL:HG13	1:62:A:ALA:H	4	0.21
(1,387)	1:24:A:VAL:HG11	1:62:A:ALA:H	18	0.21
(1,387)	1:24:A:VAL:HG12	1:62:A:ALA:H	18	0.21
(1,387)	1:24:A:VAL:HG13	1:62:A:ALA:H	18	0.21
(1,378)	1:24:A:VAL:HA	1:30:A:ASP:HB3	13	0.21
(1,377)	1:24:A:VAL:HA	1:30:A:ASP:HA	14	0.21
(1,372)	1:24:A:VAL:HG21	1:29:A:ARG:H	1	0.21
(1,372)	1:24:A:VAL:HG22	1:29:A:ARG:H	1	0.21
(1,372)	1:24:A:VAL:HG23	1:29:A:ARG:H	1	0.21
(1,352)	1:23:A:HIS:HB3	1:91:A:GLN:HB2	4	0.21
(1,352)	1:23:A:HIS:HB3	1:91:A:GLN:HB2	7	0.21
(1,352)	1:23:A:HIS:HB3	1:91:A:GLN:HB2	9	0.21
(1,329)	1:23:A:HIS:HB2	1:24:A:VAL:HA	1	0.21
(1,297)	1:22:A:VAL:H	1:31:A:VAL:H	1	0.21
(1,297)	1:22:A:VAL:H	1:31:A:VAL:H	12	0.21
(1,297)	1:22:A:VAL:H	1:31:A:VAL:H	19	0.21
(1,294)	1:22:A:VAL:HG11	1:29:A:ARG:H	2	0.21
(1,294)	1:22:A:VAL:HG12	1:29:A:ARG:H	2	0.21
(1,294)	1:22:A:VAL:HG13	1:29:A:ARG:H	2	0.21
(1,294)	1:22:A:VAL:HG11	1:29:A:ARG:H	11	0.21
(1,294)	1:22:A:VAL:HG12	1:29:A:ARG:H	11	0.21
(1,294)	1:22:A:VAL:HG13	1:29:A:ARG:H	11	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,276)	1:21:A:SER:H	1:32:A:THR:HG21	16	0.21
(1,276)	1:21:A:SER:H	1:32:A:THR:HG22	16	0.21
(1,276)	1:21:A:SER:H	1:32:A:THR:HG23	16	0.21
(1,269)	1:21:A:SER:HA	1:23:A:HIS:H	3	0.21
(1,269)	1:21:A:SER:HA	1:23:A:HIS:H	4	0.21
(1,269)	1:21:A:SER:HA	1:23:A:HIS:H	7	0.21
(1,269)	1:21:A:SER:HA	1:23:A:HIS:H	9	0.21
(1,269)	1:21:A:SER:HA	1:23:A:HIS:H	10	0.21
(1,269)	1:21:A:SER:HA	1:23:A:HIS:H	13	0.21
(1,269)	1:21:A:SER:HA	1:23:A:HIS:H	15	0.21
(1,269)	1:21:A:SER:HA	1:23:A:HIS:H	20	0.21
(1,266)	1:21:A:SER:H	1:22:A:VAL:H	16	0.21
(1,249)	1:20:A:LEU:HB2	1:34:A:ARG:H	16	0.21
(1,244)	1:20:A:LEU:HD21	1:33:A:LEU:HA	18	0.21
(1,244)	1:20:A:LEU:HD22	1:33:A:LEU:HA	18	0.21
(1,244)	1:20:A:LEU:HD23	1:33:A:LEU:HA	18	0.21
(1,203)	1:19:A:GLU:HB3	1:20:A:LEU:H	1	0.21
(1,203)	1:19:A:GLU:HB3	1:20:A:LEU:H	2	0.21
(1,203)	1:19:A:GLU:HB3	1:20:A:LEU:H	6	0.21
(1,203)	1:19:A:GLU:HB3	1:20:A:LEU:H	8	0.21
(1,203)	1:19:A:GLU:HB3	1:20:A:LEU:H	10	0.21
(1,203)	1:19:A:GLU:HB3	1:20:A:LEU:H	15	0.21
(1,203)	1:19:A:GLU:HB3	1:20:A:LEU:H	19	0.21
(1,200)	1:19:A:GLU:H	1:20:A:LEU:H	9	0.21
(1,200)	1:19:A:GLU:H	1:20:A:LEU:H	11	0.21
(1,200)	1:19:A:GLU:H	1:20:A:LEU:H	13	0.21
(1,200)	1:19:A:GLU:H	1:20:A:LEU:H	17	0.21
(1,195)	1:19:A:GLU:H	1:19:A:GLU:HG2	1	0.21
(1,195)	1:19:A:GLU:H	1:19:A:GLU:HG2	8	0.21
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG21	19	0.21
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG22	19	0.21
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG23	19	0.21
(1,184)	1:18:A:TRP:HE1	1:80:A:ASP:HB3	2	0.21
(1,184)	1:18:A:TRP:HE1	1:80:A:ASP:HB3	13	0.21
(1,184)	1:18:A:TRP:HE1	1:80:A:ASP:HB3	20	0.21
(1,153)	1:15:A:ASP:H	1:17:A:THR:H	11	0.21
(1,148)	1:15:A:ASP:HA	1:16:A:GLY:H	3	0.21
(1,146)	1:15:A:ASP:H	1:15:A:ASP:HB3	9	0.21
(1,127)	1:11:A:GLY:HA2	1:12:A:CYS:H	4	0.21
(1,127)	1:11:A:GLY:HA2	1:12:A:CYS:H	14	0.21
(1,112)	1:9:A:PRO:HG3	1:10:A:ASP:H	19	0.21
(1,95)	1:8:A:MET:HA	1:10:A:ASP:H	13	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:8:A:MET:H	1:10:A:ASP:HA	3	0.21
(1,90)	1:8:A:MET:H	1:8:A:MET:HG3	2	0.21
(1,87)	1:7:A:ARG:HG3	1:10:A:ASP:H	9	0.21
(1,86)	1:7:A:ARG:HA	1:10:A:ASP:H	15	0.21
(1,85)	1:7:A:ARG:HD3	1:8:A:MET:H	3	0.21
(1,82)	1:7:A:ARG:HB2	1:8:A:MET:H	8	0.21
(1,82)	1:7:A:ARG:HB2	1:8:A:MET:H	16	0.21
(1,82)	1:7:A:ARG:HB2	1:8:A:MET:H	19	0.21
(1,68)	1:6:A:ILE:HA	1:10:A:ASP:H	14	0.21
(1,67)	1:6:A:ILE:H	1:10:A:ASP:H	6	0.21
(1,49)	1:5:A:GLY:HA3	1:6:A:ILE:HB	9	0.21
(1,28)	1:3:A:LEU:H	1:3:A:LEU:HB2	1	0.21
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD11	2	0.21
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD12	2	0.21
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD13	2	0.21
(1,19)	1:2:A:ALA:HB1	1:3:A:LEU:H	12	0.21
(1,19)	1:2:A:ALA:HB2	1:3:A:LEU:H	12	0.21
(1,19)	1:2:A:ALA:HB3	1:3:A:LEU:H	12	0.21
(1,18)	1:2:A:ALA:HA	1:3:A:LEU:H	14	0.21
(1,16)	1:2:A:ALA:H	1:3:A:LEU:HB3	7	0.21
(3,21)	1:80:A:ASP:O	1:84:A:ILE:H	20	0.2
(2,19)	1:23:A:HIS:O	1:93:A:THR:H	13	0.2
(2,19)	1:23:A:HIS:O	1:93:A:THR:H	18	0.2
(2,17)	1:21:A:SER:O	1:91:A:GLN:H	2	0.2
(2,17)	1:21:A:SER:O	1:91:A:GLN:H	16	0.2
(2,7)	1:29:A:ARG:O	1:24:A:VAL:N	3	0.2
(2,7)	1:29:A:ARG:O	1:24:A:VAL:N	5	0.2
(2,7)	1:29:A:ARG:O	1:24:A:VAL:N	13	0.2
(2,7)	1:29:A:ARG:O	1:24:A:VAL:N	18	0.2
(2,4)	1:33:A:LEU:O	1:20:A:LEU:N	3	0.2
(2,4)	1:33:A:LEU:O	1:20:A:LEU:N	4	0.2
(2,4)	1:33:A:LEU:O	1:20:A:LEU:N	5	0.2
(2,4)	1:33:A:LEU:O	1:20:A:LEU:N	6	0.2
(2,4)	1:33:A:LEU:O	1:20:A:LEU:N	15	0.2
(2,4)	1:33:A:LEU:O	1:20:A:LEU:N	17	0.2
(1,1407)	1:92:A:PHE:HB2	1:93:A:THR:H	12	0.2
(1,1404)	1:92:A:PHE:HB2	1:93:A:THR:HB	5	0.2
(1,1404)	1:92:A:PHE:HB2	1:93:A:THR:HB	13	0.2
(1,1404)	1:92:A:PHE:HB2	1:93:A:THR:HB	18	0.2
(1,1404)	1:92:A:PHE:HB2	1:93:A:THR:HB	20	0.2
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG21	19	0.2
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG22	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG23	19	0.2
(1,1246)	1:81:A:LYS:HE3	1:82:A:TYR:H	4	0.2
(1,1235)	1:81:A:LYS:HE3	1:81:A:LYS:HG3	1	0.2
(1,1235)	1:81:A:LYS:HE3	1:81:A:LYS:HG3	4	0.2
(1,1235)	1:81:A:LYS:HE3	1:81:A:LYS:HG3	6	0.2
(1,1235)	1:81:A:LYS:HE3	1:81:A:LYS:HG3	8	0.2
(1,1235)	1:81:A:LYS:HE3	1:81:A:LYS:HG3	11	0.2
(1,1235)	1:81:A:LYS:HE3	1:81:A:LYS:HG3	12	0.2
(1,1218)	1:80:A:ASP:HB2	1:82:A:TYR:H	3	0.2
(1,1218)	1:80:A:ASP:HB2	1:82:A:TYR:H	11	0.2
(1,1218)	1:80:A:ASP:HB2	1:82:A:TYR:H	12	0.2
(1,1216)	1:80:A:ASP:H	1:81:A:LYS:HD2	1	0.2
(1,1197)	1:79:A:LEU:HB3	1:80:A:ASP:H	15	0.2
(1,1197)	1:79:A:LEU:HB3	1:80:A:ASP:H	19	0.2
(1,1178)	1:78:A:THR:HG21	1:81:A:LYS:H	18	0.2
(1,1178)	1:78:A:THR:HG22	1:81:A:LYS:H	18	0.2
(1,1178)	1:78:A:THR:HG23	1:81:A:LYS:H	18	0.2
(1,1177)	1:78:A:THR:H	1:81:A:LYS:H	6	0.2
(1,1177)	1:78:A:THR:H	1:81:A:LYS:H	8	0.2
(1,1177)	1:78:A:THR:H	1:81:A:LYS:H	14	0.2
(1,1169)	1:78:A:THR:HB	1:79:A:LEU:H	1	0.2
(1,1162)	1:77:A:TRP:H	1:81:A:LYS:HE3	2	0.2
(1,1162)	1:77:A:TRP:H	1:81:A:LYS:HE3	5	0.2
(1,1162)	1:77:A:TRP:H	1:81:A:LYS:HE3	8	0.2
(1,1161)	1:77:A:TRP:H	1:81:A:LYS:HD3	8	0.2
(1,1160)	1:77:A:TRP:HB2	1:78:A:THR:H	2	0.2
(1,1159)	1:77:A:TRP:HB3	1:78:A:THR:H	8	0.2
(1,1141)	1:74:A:LYS:HE3	1:78:A:THR:H	3	0.2
(1,1141)	1:74:A:LYS:HE3	1:78:A:THR:H	5	0.2
(1,1141)	1:74:A:LYS:HE3	1:78:A:THR:H	11	0.2
(1,1141)	1:74:A:LYS:HE3	1:78:A:THR:H	19	0.2
(1,1128)	1:74:A:LYS:HE3	1:74:A:LYS:HB3	18	0.2
(1,1128)	1:74:A:LYS:HE3	1:74:A:LYS:HB3	19	0.2
(1,1128)	1:74:A:LYS:HE3	1:74:A:LYS:HB3	20	0.2
(1,1123)	1:74:A:LYS:H	1:74:A:LYS:HD2	3	0.2
(1,1123)	1:74:A:LYS:H	1:74:A:LYS:HD2	8	0.2
(1,1123)	1:74:A:LYS:H	1:74:A:LYS:HD2	16	0.2
(1,1108)	1:73:A:LEU:HA	1:74:A:LYS:H	11	0.2
(1,1105)	1:73:A:LEU:H	1:73:A:LEU:HB3	12	0.2
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD11	4	0.2
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD12	4	0.2
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD13	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD11	6	0.2
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD12	6	0.2
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD13	6	0.2
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD11	2	0.2
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD12	2	0.2
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD13	2	0.2
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD11	11	0.2
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD12	11	0.2
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD13	11	0.2
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD11	14	0.2
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD12	14	0.2
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD13	14	0.2
(1,1081)	1:71:A:TRP:HB2	1:72:A:LEU:H	11	0.2
(1,1081)	1:71:A:TRP:HB2	1:72:A:LEU:H	14	0.2
(1,1076)	1:71:A:TRP:H	1:71:A:TRP:HB3	2	0.2
(1,1072)	1:70:A:THR:H	1:71:A:TRP:H	5	0.2
(1,1072)	1:70:A:THR:H	1:71:A:TRP:H	6	0.2
(1,1072)	1:70:A:THR:H	1:71:A:TRP:H	17	0.2
(1,1061)	1:69:A:ARG:HD3	1:70:A:THR:HB	18	0.2
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD21	2	0.2
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD22	2	0.2
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD23	2	0.2
(1,1049)	1:67:A:LYS:HB3	1:69:A:ARG:HA	4	0.2
(1,1049)	1:67:A:LYS:HB3	1:69:A:ARG:HA	14	0.2
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD21	10	0.2
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD22	10	0.2
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD23	10	0.2
(1,992)	1:64:A:TRP:H	1:93:A:THR:HG1	3	0.2
(1,978)	1:63:A:LEU:HA	1:93:A:THR:H	4	0.2
(1,978)	1:63:A:LEU:HA	1:93:A:THR:H	8	0.2
(1,974)	1:63:A:LEU:HA	1:92:A:PHE:H	3	0.2
(1,974)	1:63:A:LEU:HA	1:92:A:PHE:H	6	0.2
(1,974)	1:63:A:LEU:HA	1:92:A:PHE:H	12	0.2
(1,974)	1:63:A:LEU:HA	1:92:A:PHE:H	19	0.2
(1,972)	1:63:A:LEU:HD11	1:91:A:GLN:H	1	0.2
(1,972)	1:63:A:LEU:HD12	1:91:A:GLN:H	1	0.2
(1,972)	1:63:A:LEU:HD13	1:91:A:GLN:H	1	0.2
(1,972)	1:63:A:LEU:HD11	1:91:A:GLN:H	9	0.2
(1,972)	1:63:A:LEU:HD12	1:91:A:GLN:H	9	0.2
(1,972)	1:63:A:LEU:HD13	1:91:A:GLN:H	9	0.2
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD11	4	0.2
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD12	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD13	4	0.2
(1,950)	1:63:A:LEU:H	1:63:A:LEU:HG	9	0.2
(1,950)	1:63:A:LEU:H	1:63:A:LEU:HG	11	0.2
(1,950)	1:63:A:LEU:H	1:63:A:LEU:HG	16	0.2
(1,926)	1:61:A:HIS:H	1:62:A:ALA:H	2	0.2
(1,926)	1:61:A:HIS:H	1:62:A:ALA:H	5	0.2
(1,926)	1:61:A:HIS:H	1:62:A:ALA:H	7	0.2
(1,926)	1:61:A:HIS:H	1:62:A:ALA:H	8	0.2
(1,926)	1:61:A:HIS:H	1:62:A:ALA:H	11	0.2
(1,844)	1:50:A:GLU:H	1:50:A:GLU:HG2	1	0.2
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD21	17	0.2
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD22	17	0.2
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD23	17	0.2
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD21	17	0.2
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD22	17	0.2
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD23	17	0.2
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD21	17	0.2
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD22	17	0.2
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD23	17	0.2
(1,818)	1:48:A:LEU:HD21	1:52:A:LEU:H	15	0.2
(1,818)	1:48:A:LEU:HD22	1:52:A:LEU:H	15	0.2
(1,818)	1:48:A:LEU:HD23	1:52:A:LEU:H	15	0.2
(1,782)	1:47:A:LYS:HB2	1:48:A:LEU:H	5	0.2
(1,782)	1:47:A:LYS:HB2	1:48:A:LEU:H	10	0.2
(1,782)	1:47:A:LYS:HB2	1:48:A:LEU:H	11	0.2
(1,782)	1:47:A:LYS:HB2	1:48:A:LEU:H	12	0.2
(1,782)	1:47:A:LYS:HB2	1:48:A:LEU:H	15	0.2
(1,782)	1:47:A:LYS:HB2	1:48:A:LEU:H	16	0.2
(1,782)	1:47:A:LYS:HB2	1:48:A:LEU:H	20	0.2
(1,766)	1:46:A:LEU:HA	1:50:A:GLU:H	18	0.2
(1,765)	1:46:A:LEU:H	1:49:A:VAL:H	13	0.2
(1,765)	1:46:A:LEU:H	1:49:A:VAL:H	18	0.2
(1,764)	1:46:A:LEU:HA	1:49:A:VAL:H	12	0.2
(1,764)	1:46:A:LEU:HA	1:49:A:VAL:H	20	0.2
(1,760)	1:46:A:LEU:H	1:48:A:LEU:H	16	0.2
(1,760)	1:46:A:LEU:H	1:48:A:LEU:H	19	0.2
(1,760)	1:46:A:LEU:H	1:48:A:LEU:H	20	0.2
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD21	14	0.2
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD22	14	0.2
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD23	14	0.2
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG21	4	0.2
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG22	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG23	4	0.2
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG21	5	0.2
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG22	5	0.2
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG23	5	0.2
(1,737)	1:45:A:MET:HB3	1:48:A:LEU:H	1	0.2
(1,737)	1:45:A:MET:HB3	1:48:A:LEU:H	2	0.2
(1,737)	1:45:A:MET:HB3	1:48:A:LEU:H	4	0.2
(1,737)	1:45:A:MET:HB3	1:48:A:LEU:H	15	0.2
(1,719)	1:44:A:VAL:HG11	1:90:A:LEU:H	11	0.2
(1,719)	1:44:A:VAL:HG12	1:90:A:LEU:H	11	0.2
(1,719)	1:44:A:VAL:HG13	1:90:A:LEU:H	11	0.2
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG11	2	0.2
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG12	2	0.2
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG13	2	0.2
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG11	10	0.2
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG12	10	0.2
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG13	10	0.2
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG11	12	0.2
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG12	12	0.2
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG13	12	0.2
(1,694)	1:43:A:GLY:H	1:45:A:MET:H	2	0.2
(1,694)	1:43:A:GLY:H	1:45:A:MET:H	11	0.2
(1,694)	1:43:A:GLY:H	1:45:A:MET:H	16	0.2
(1,692)	1:43:A:GLY:H	1:44:A:VAL:HB	16	0.2
(1,688)	1:42:A:GLY:H	1:75:A:THR:HG21	13	0.2
(1,688)	1:42:A:GLY:H	1:75:A:THR:HG22	13	0.2
(1,688)	1:42:A:GLY:H	1:75:A:THR:HG23	13	0.2
(1,684)	1:42:A:GLY:HA3	1:75:A:THR:HB	14	0.2
(1,659)	1:41:A:ILE:HD11	1:44:A:VAL:H	12	0.2
(1,659)	1:41:A:ILE:HD12	1:44:A:VAL:H	12	0.2
(1,659)	1:41:A:ILE:HD13	1:44:A:VAL:H	12	0.2
(1,659)	1:41:A:ILE:HD11	1:44:A:VAL:H	20	0.2
(1,659)	1:41:A:ILE:HD12	1:44:A:VAL:H	20	0.2
(1,659)	1:41:A:ILE:HD13	1:44:A:VAL:H	20	0.2
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG11	10	0.2
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG12	10	0.2
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG13	10	0.2
(1,628)	1:40:A:HIS:H	1:44:A:VAL:HB	9	0.2
(1,610)	1:39:A:VAL:HG21	1:80:A:ASP:H	10	0.2
(1,610)	1:39:A:VAL:HG22	1:80:A:ASP:H	10	0.2
(1,610)	1:39:A:VAL:HG23	1:80:A:ASP:H	10	0.2
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD21	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD22	6	0.2
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD23	6	0.2
(1,588)	1:38:A:GLU:HA	1:80:A:ASP:H	17	0.2
(1,580)	1:38:A:GLU:HB3	1:39:A:VAL:H	1	0.2
(1,580)	1:38:A:GLU:HB3	1:39:A:VAL:H	9	0.2
(1,580)	1:38:A:GLU:HB3	1:39:A:VAL:H	10	0.2
(1,580)	1:38:A:GLU:HB3	1:39:A:VAL:H	14	0.2
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD21	18	0.2
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD22	18	0.2
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD23	18	0.2
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG21	9	0.2
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG22	9	0.2
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG23	9	0.2
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG21	14	0.2
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG22	14	0.2
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG23	14	0.2
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG21	17	0.2
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG22	17	0.2
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG23	17	0.2
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG21	18	0.2
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG22	18	0.2
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG23	18	0.2
(1,552)	1:36:A:THR:HB	1:38:A:GLU:H	4	0.2
(1,552)	1:36:A:THR:HB	1:38:A:GLU:H	13	0.2
(1,552)	1:36:A:THR:HB	1:38:A:GLU:H	14	0.2
(1,532)	1:35:A:VAL:H	1:35:A:VAL:HB	3	0.2
(1,532)	1:35:A:VAL:H	1:35:A:VAL:HB	5	0.2
(1,532)	1:35:A:VAL:H	1:35:A:VAL:HB	6	0.2
(1,532)	1:35:A:VAL:H	1:35:A:VAL:HB	8	0.2
(1,532)	1:35:A:VAL:H	1:35:A:VAL:HB	11	0.2
(1,532)	1:35:A:VAL:H	1:35:A:VAL:HB	16	0.2
(1,532)	1:35:A:VAL:H	1:35:A:VAL:HB	18	0.2
(1,532)	1:35:A:VAL:H	1:35:A:VAL:HB	19	0.2
(1,518)	1:34:A:ARG:HD3	1:34:A:ARG:HB3	10	0.2
(1,516)	1:34:A:ARG:H	1:34:A:ARG:HG3	16	0.2
(1,484)	1:32:A:THR:HA	1:51:A:LYS:HD3	4	0.2
(1,484)	1:32:A:THR:HA	1:51:A:LYS:HD3	7	0.2
(1,484)	1:32:A:THR:HA	1:51:A:LYS:HD3	11	0.2
(1,484)	1:32:A:THR:HA	1:51:A:LYS:HD3	19	0.2
(1,483)	1:32:A:THR:H	1:34:A:ARG:H	4	0.2
(1,483)	1:32:A:THR:H	1:34:A:ARG:H	11	0.2
(1,483)	1:32:A:THR:H	1:34:A:ARG:H	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,467)	1:31:A:VAL:H	1:32:A:THR:H	14	0.2
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG11	3	0.2
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG12	3	0.2
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG13	3	0.2
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG11	8	0.2
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG12	8	0.2
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG13	8	0.2
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG11	9	0.2
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG12	9	0.2
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG13	9	0.2
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG11	15	0.2
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG12	15	0.2
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG13	15	0.2
(1,453)	1:29:A:ARG:HB2	1:31:A:VAL:HA	1	0.2
(1,453)	1:29:A:ARG:HB2	1:31:A:VAL:HA	16	0.2
(1,437)	1:28:A:ASN:HB3	1:29:A:ARG:H	6	0.2
(1,437)	1:28:A:ASN:HB3	1:29:A:ARG:H	11	0.2
(1,437)	1:28:A:ASN:HB3	1:29:A:ARG:H	13	0.2
(1,437)	1:28:A:ASN:HB3	1:29:A:ARG:H	18	0.2
(1,434)	1:28:A:ASN:HA	1:29:A:ARG:H	6	0.2
(1,434)	1:28:A:ASN:HA	1:29:A:ARG:H	13	0.2
(1,434)	1:28:A:ASN:HA	1:29:A:ARG:H	15	0.2
(1,434)	1:28:A:ASN:HA	1:29:A:ARG:H	17	0.2
(1,433)	1:28:A:ASN:H	1:28:A:ASN:HB3	4	0.2
(1,433)	1:28:A:ASN:H	1:28:A:ASN:HB3	6	0.2
(1,433)	1:28:A:ASN:H	1:28:A:ASN:HB3	7	0.2
(1,432)	1:28:A:ASN:H	1:28:A:ASN:HB2	9	0.2
(1,432)	1:28:A:ASN:H	1:28:A:ASN:HB2	14	0.2
(1,430)	1:27:A:VAL:HG21	1:92:A:PHE:H	13	0.2
(1,430)	1:27:A:VAL:HG22	1:92:A:PHE:H	13	0.2
(1,430)	1:27:A:VAL:HG23	1:92:A:PHE:H	13	0.2
(1,426)	1:27:A:VAL:H	1:28:A:ASN:HB2	7	0.2
(1,414)	1:25:A:THR:H	1:93:A:THR:HG21	11	0.2
(1,414)	1:25:A:THR:H	1:93:A:THR:HG22	11	0.2
(1,414)	1:25:A:THR:H	1:93:A:THR:HG23	11	0.2
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG21	16	0.2
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG22	16	0.2
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG23	16	0.2
(1,402)	1:25:A:THR:HA	1:29:A:ARG:H	11	0.2
(1,387)	1:24:A:VAL:HG11	1:62:A:ALA:H	2	0.2
(1,387)	1:24:A:VAL:HG12	1:62:A:ALA:H	2	0.2
(1,387)	1:24:A:VAL:HG13	1:62:A:ALA:H	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:24:A:VAL:HG11	1:62:A:ALA:H	7	0.2
(1,387)	1:24:A:VAL:HG12	1:62:A:ALA:H	7	0.2
(1,387)	1:24:A:VAL:HG13	1:62:A:ALA:H	7	0.2
(1,387)	1:24:A:VAL:HG11	1:62:A:ALA:H	11	0.2
(1,387)	1:24:A:VAL:HG12	1:62:A:ALA:H	11	0.2
(1,387)	1:24:A:VAL:HG13	1:62:A:ALA:H	11	0.2
(1,371)	1:24:A:VAL:HG11	1:29:A:ARG:H	12	0.2
(1,371)	1:24:A:VAL:HG12	1:29:A:ARG:H	12	0.2
(1,371)	1:24:A:VAL:HG13	1:29:A:ARG:H	12	0.2
(1,371)	1:24:A:VAL:HG11	1:29:A:ARG:H	13	0.2
(1,371)	1:24:A:VAL:HG12	1:29:A:ARG:H	13	0.2
(1,371)	1:24:A:VAL:HG13	1:29:A:ARG:H	13	0.2
(1,352)	1:23:A:HIS:HB3	1:91:A:GLN:HB2	2	0.2
(1,352)	1:23:A:HIS:HB3	1:91:A:GLN:HB2	3	0.2
(1,352)	1:23:A:HIS:HB3	1:91:A:GLN:HB2	8	0.2
(1,340)	1:23:A:HIS:H	1:91:A:GLN:HA	14	0.2
(1,329)	1:23:A:HIS:HB2	1:24:A:VAL:HA	17	0.2
(1,329)	1:23:A:HIS:HB2	1:24:A:VAL:HA	18	0.2
(1,329)	1:23:A:HIS:HB2	1:24:A:VAL:HA	19	0.2
(1,312)	1:22:A:VAL:HG21	1:90:A:LEU:H	14	0.2
(1,312)	1:22:A:VAL:HG22	1:90:A:LEU:H	14	0.2
(1,312)	1:22:A:VAL:HG23	1:90:A:LEU:H	14	0.2
(1,312)	1:22:A:VAL:HG21	1:90:A:LEU:H	19	0.2
(1,312)	1:22:A:VAL:HG22	1:90:A:LEU:H	19	0.2
(1,312)	1:22:A:VAL:HG23	1:90:A:LEU:H	19	0.2
(1,299)	1:22:A:VAL:H	1:32:A:THR:HB	6	0.2
(1,294)	1:22:A:VAL:HG11	1:29:A:ARG:H	1	0.2
(1,294)	1:22:A:VAL:HG12	1:29:A:ARG:H	1	0.2
(1,294)	1:22:A:VAL:HG13	1:29:A:ARG:H	1	0.2
(1,294)	1:22:A:VAL:HG11	1:29:A:ARG:H	9	0.2
(1,294)	1:22:A:VAL:HG12	1:29:A:ARG:H	9	0.2
(1,294)	1:22:A:VAL:HG13	1:29:A:ARG:H	9	0.2
(1,294)	1:22:A:VAL:HG11	1:29:A:ARG:H	13	0.2
(1,294)	1:22:A:VAL:HG12	1:29:A:ARG:H	13	0.2
(1,294)	1:22:A:VAL:HG13	1:29:A:ARG:H	13	0.2
(1,276)	1:21:A:SER:H	1:32:A:THR:HG21	1	0.2
(1,276)	1:21:A:SER:H	1:32:A:THR:HG22	1	0.2
(1,276)	1:21:A:SER:H	1:32:A:THR:HG23	1	0.2
(1,276)	1:21:A:SER:H	1:32:A:THR:HG21	3	0.2
(1,276)	1:21:A:SER:H	1:32:A:THR:HG22	3	0.2
(1,276)	1:21:A:SER:H	1:32:A:THR:HG23	3	0.2
(1,276)	1:21:A:SER:H	1:32:A:THR:HG21	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,276)	1:21:A:SER:H	1:32:A:THR:HG22	4	0.2
(1,276)	1:21:A:SER:H	1:32:A:THR:HG23	4	0.2
(1,276)	1:21:A:SER:H	1:32:A:THR:HG21	7	0.2
(1,276)	1:21:A:SER:H	1:32:A:THR:HG22	7	0.2
(1,276)	1:21:A:SER:H	1:32:A:THR:HG23	7	0.2
(1,276)	1:21:A:SER:H	1:32:A:THR:HG21	9	0.2
(1,276)	1:21:A:SER:H	1:32:A:THR:HG22	9	0.2
(1,276)	1:21:A:SER:H	1:32:A:THR:HG23	9	0.2
(1,269)	1:21:A:SER:HA	1:23:A:HIS:H	2	0.2
(1,269)	1:21:A:SER:HA	1:23:A:HIS:H	5	0.2
(1,269)	1:21:A:SER:HA	1:23:A:HIS:H	11	0.2
(1,269)	1:21:A:SER:HA	1:23:A:HIS:H	16	0.2
(1,251)	1:20:A:LEU:HG	1:35:A:VAL:H	4	0.2
(1,251)	1:20:A:LEU:HG	1:35:A:VAL:H	15	0.2
(1,249)	1:20:A:LEU:HB2	1:34:A:ARG:H	8	0.2
(1,249)	1:20:A:LEU:HB2	1:34:A:ARG:H	9	0.2
(1,249)	1:20:A:LEU:HB2	1:34:A:ARG:H	18	0.2
(1,203)	1:19:A:GLU:HB3	1:20:A:LEU:H	9	0.2
(1,203)	1:19:A:GLU:HB3	1:20:A:LEU:H	13	0.2
(1,203)	1:19:A:GLU:HB3	1:20:A:LEU:H	18	0.2
(1,200)	1:19:A:GLU:H	1:20:A:LEU:H	1	0.2
(1,200)	1:19:A:GLU:H	1:20:A:LEU:H	2	0.2
(1,200)	1:19:A:GLU:H	1:20:A:LEU:H	3	0.2
(1,200)	1:19:A:GLU:H	1:20:A:LEU:H	10	0.2
(1,200)	1:19:A:GLU:H	1:20:A:LEU:H	12	0.2
(1,200)	1:19:A:GLU:H	1:20:A:LEU:H	14	0.2
(1,200)	1:19:A:GLU:H	1:20:A:LEU:H	15	0.2
(1,200)	1:19:A:GLU:H	1:20:A:LEU:H	16	0.2
(1,200)	1:19:A:GLU:H	1:20:A:LEU:H	18	0.2
(1,200)	1:19:A:GLU:H	1:20:A:LEU:H	20	0.2
(1,195)	1:19:A:GLU:H	1:19:A:GLU:HG2	9	0.2
(1,195)	1:19:A:GLU:H	1:19:A:GLU:HG2	15	0.2
(1,195)	1:19:A:GLU:H	1:19:A:GLU:HG2	18	0.2
(1,184)	1:18:A:TRP:HE1	1:80:A:ASP:HB3	3	0.2
(1,184)	1:18:A:TRP:HE1	1:80:A:ASP:HB3	12	0.2
(1,177)	1:18:A:TRP:HE1	1:36:A:THR:HB	10	0.2
(1,177)	1:18:A:TRP:HE1	1:36:A:THR:HB	16	0.2
(1,177)	1:18:A:TRP:HE1	1:36:A:THR:HB	18	0.2
(1,175)	1:18:A:TRP:H	1:35:A:VAL:HA	12	0.2
(1,169)	1:18:A:TRP:H	1:18:A:TRP:HD1	11	0.2
(1,169)	1:18:A:TRP:H	1:18:A:TRP:HD1	16	0.2
(1,155)	1:16:A:GLY:HA3	1:17:A:THR:H	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,148)	1:15:A:ASP:HA	1:16:A:GLY:H	11	0.2
(1,146)	1:15:A:ASP:H	1:15:A:ASP:HB3	12	0.2
(1,145)	1:14:A:ALA:HB1	1:16:A:GLY:H	4	0.2
(1,145)	1:14:A:ALA:HB2	1:16:A:GLY:H	4	0.2
(1,145)	1:14:A:ALA:HB3	1:16:A:GLY:H	4	0.2
(1,112)	1:9:A:PRO:HG3	1:10:A:ASP:H	10	0.2
(1,112)	1:9:A:PRO:HG3	1:10:A:ASP:H	12	0.2
(1,112)	1:9:A:PRO:HG3	1:10:A:ASP:H	13	0.2
(1,103)	1:8:A:MET:HG3	1:12:A:CYS:HB3	13	0.2
(1,95)	1:8:A:MET:HA	1:10:A:ASP:H	19	0.2
(1,90)	1:8:A:MET:H	1:8:A:MET:HG3	6	0.2
(1,88)	1:8:A:MET:H	1:8:A:MET:HB3	5	0.2
(1,82)	1:7:A:ARG:HB2	1:8:A:MET:H	1	0.2
(1,82)	1:7:A:ARG:HB2	1:8:A:MET:H	11	0.2
(1,82)	1:7:A:ARG:HB2	1:8:A:MET:H	13	0.2
(1,61)	1:6:A:ILE:H	1:7:A:ARG:H	3	0.2
(1,49)	1:5:A:GLY:HA3	1:6:A:ILE:HB	5	0.2
(1,47)	1:5:A:GLY:H	1:6:A:ILE:H	5	0.2
(1,43)	1:4:A:ASP:HB3	1:5:A:GLY:H	15	0.2
(1,36)	1:3:A:LEU:HB3	1:4:A:ASP:H	7	0.2
(1,33)	1:3:A:LEU:H	1:4:A:ASP:HB3	1	0.2
(1,16)	1:2:A:ALA:H	1:3:A:LEU:HB3	4	0.2
(3,21)	1:80:A:ASP:O	1:84:A:ILE:H	7	0.19
(3,21)	1:80:A:ASP:O	1:84:A:ILE:H	14	0.19
(2,25)	1:77:A:TRP:O	1:81:A:LYS:N	13	0.19
(2,21)	1:39:A:VAL:O	1:43:A:GLY:N	18	0.19
(2,19)	1:23:A:HIS:O	1:93:A:THR:H	9	0.19
(2,19)	1:23:A:HIS:O	1:93:A:THR:H	12	0.19
(2,19)	1:23:A:HIS:O	1:93:A:THR:H	15	0.19
(2,17)	1:21:A:SER:O	1:91:A:GLN:H	1	0.19
(2,17)	1:21:A:SER:O	1:91:A:GLN:H	4	0.19
(2,17)	1:21:A:SER:O	1:91:A:GLN:H	5	0.19
(2,17)	1:21:A:SER:O	1:91:A:GLN:H	7	0.19
(2,17)	1:21:A:SER:O	1:91:A:GLN:H	13	0.19
(2,17)	1:21:A:SER:O	1:91:A:GLN:H	14	0.19
(2,17)	1:21:A:SER:O	1:91:A:GLN:H	15	0.19
(2,13)	1:92:A:PHE:O	1:64:A:TRP:N	3	0.19
(2,13)	1:92:A:PHE:O	1:64:A:TRP:N	5	0.19
(2,13)	1:92:A:PHE:O	1:64:A:TRP:N	11	0.19
(2,13)	1:92:A:PHE:O	1:64:A:TRP:N	17	0.19
(2,13)	1:92:A:PHE:O	1:64:A:TRP:N	18	0.19
(2,7)	1:29:A:ARG:O	1:24:A:VAL:N	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:29:A:ARG:O	1:24:A:VAL:N	12	0.19
(2,7)	1:29:A:ARG:O	1:24:A:VAL:N	17	0.19
(2,7)	1:29:A:ARG:O	1:24:A:VAL:N	19	0.19
(2,4)	1:33:A:LEU:O	1:20:A:LEU:N	1	0.19
(2,4)	1:33:A:LEU:O	1:20:A:LEU:N	14	0.19
(1,1404)	1:92:A:PHE:HB2	1:93:A:THR:HB	4	0.19
(1,1404)	1:92:A:PHE:HB2	1:93:A:THR:HB	16	0.19
(1,1382)	1:91:A:GLN:HG2	1:91:A:GLN:HE21	17	0.19
(1,1381)	1:91:A:GLN:H	1:91:A:GLN:HG2	18	0.19
(1,1380)	1:91:A:GLN:H	1:91:A:GLN:HE22	1	0.19
(1,1380)	1:91:A:GLN:H	1:91:A:GLN:HE22	4	0.19
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG21	5	0.19
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG22	5	0.19
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG23	5	0.19
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG21	9	0.19
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG22	9	0.19
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG23	9	0.19
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG21	12	0.19
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG22	12	0.19
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG23	12	0.19
(1,1235)	1:81:A:LYS:HE3	1:81:A:LYS:HG3	7	0.19
(1,1235)	1:81:A:LYS:HE3	1:81:A:LYS:HG3	14	0.19
(1,1235)	1:81:A:LYS:HE3	1:81:A:LYS:HG3	16	0.19
(1,1216)	1:80:A:ASP:H	1:81:A:LYS:HD2	9	0.19
(1,1205)	1:79:A:LEU:HD11	1:83:A:GLY:H	16	0.19
(1,1205)	1:79:A:LEU:HD12	1:83:A:GLY:H	16	0.19
(1,1205)	1:79:A:LEU:HD13	1:83:A:GLY:H	16	0.19
(1,1197)	1:79:A:LEU:HB3	1:80:A:ASP:H	8	0.19
(1,1187)	1:79:A:LEU:H	1:79:A:LEU:HD21	20	0.19
(1,1187)	1:79:A:LEU:H	1:79:A:LEU:HD22	20	0.19
(1,1187)	1:79:A:LEU:H	1:79:A:LEU:HD23	20	0.19
(1,1177)	1:78:A:THR:H	1:81:A:LYS:H	1	0.19
(1,1176)	1:78:A:THR:H	1:81:A:LYS:HA	15	0.19
(1,1169)	1:78:A:THR:HB	1:79:A:LEU:H	9	0.19
(1,1169)	1:78:A:THR:HB	1:79:A:LEU:H	19	0.19
(1,1164)	1:78:A:THR:HG21	1:78:A:THR:H	4	0.19
(1,1164)	1:78:A:THR:HG22	1:78:A:THR:H	4	0.19
(1,1164)	1:78:A:THR:HG23	1:78:A:THR:H	4	0.19
(1,1162)	1:77:A:TRP:H	1:81:A:LYS:HE3	4	0.19
(1,1162)	1:77:A:TRP:H	1:81:A:LYS:HE3	12	0.19
(1,1161)	1:77:A:TRP:H	1:81:A:LYS:HD3	2	0.19
(1,1161)	1:77:A:TRP:H	1:81:A:LYS:HD3	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1161)	1:77:A:TRP:H	1:81:A:LYS:HD3	19	0.19
(1,1160)	1:77:A:TRP:HB2	1:78:A:THR:H	3	0.19
(1,1160)	1:77:A:TRP:HB2	1:78:A:THR:H	11	0.19
(1,1153)	1:76:A:HIS:HB3	1:77:A:TRP:H	5	0.19
(1,1153)	1:76:A:HIS:HB3	1:77:A:TRP:H	10	0.19
(1,1141)	1:74:A:LYS:HE3	1:78:A:THR:H	1	0.19
(1,1141)	1:74:A:LYS:HE3	1:78:A:THR:H	2	0.19
(1,1128)	1:74:A:LYS:HE3	1:74:A:LYS:HB3	3	0.19
(1,1128)	1:74:A:LYS:HE3	1:74:A:LYS:HB3	8	0.19
(1,1128)	1:74:A:LYS:HE3	1:74:A:LYS:HB3	9	0.19
(1,1128)	1:74:A:LYS:HE3	1:74:A:LYS:HB3	12	0.19
(1,1128)	1:74:A:LYS:HE3	1:74:A:LYS:HB3	14	0.19
(1,1123)	1:74:A:LYS:H	1:74:A:LYS:HD2	1	0.19
(1,1123)	1:74:A:LYS:H	1:74:A:LYS:HD2	4	0.19
(1,1123)	1:74:A:LYS:H	1:74:A:LYS:HD2	9	0.19
(1,1123)	1:74:A:LYS:H	1:74:A:LYS:HD2	12	0.19
(1,1123)	1:74:A:LYS:H	1:74:A:LYS:HD2	17	0.19
(1,1108)	1:73:A:LEU:HA	1:74:A:LYS:H	5	0.19
(1,1108)	1:73:A:LEU:HA	1:74:A:LYS:H	6	0.19
(1,1108)	1:73:A:LEU:HA	1:74:A:LYS:H	7	0.19
(1,1108)	1:73:A:LEU:HA	1:74:A:LYS:H	10	0.19
(1,1108)	1:73:A:LEU:HA	1:74:A:LYS:H	13	0.19
(1,1108)	1:73:A:LEU:HA	1:74:A:LYS:H	18	0.19
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD11	3	0.19
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD12	3	0.19
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD13	3	0.19
(1,1072)	1:70:A:THR:H	1:71:A:TRP:H	8	0.19
(1,1072)	1:70:A:THR:H	1:71:A:TRP:H	15	0.19
(1,1063)	1:69:A:ARG:H	1:70:A:THR:H	15	0.19
(1,1049)	1:67:A:LYS:HB3	1:69:A:ARG:HA	9	0.19
(1,1021)	1:66:A:GLU:H	1:66:A:GLU:HG2	5	0.19
(1,1021)	1:66:A:GLU:H	1:66:A:GLU:HG2	19	0.19
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD21	3	0.19
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD22	3	0.19
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD23	3	0.19
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD21	4	0.19
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD22	4	0.19
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD23	4	0.19
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD21	6	0.19
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD22	6	0.19
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD23	6	0.19
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD21	18	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD22	18	0.19
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD23	18	0.19
(1,992)	1:64:A:TRP:H	1:93:A:THR:HG1	2	0.19
(1,992)	1:64:A:TRP:H	1:93:A:THR:HG1	20	0.19
(1,978)	1:63:A:LEU:HA	1:93:A:THR:H	17	0.19
(1,978)	1:63:A:LEU:HA	1:93:A:THR:H	18	0.19
(1,976)	1:63:A:LEU:HG	1:93:A:THR:H	6	0.19
(1,976)	1:63:A:LEU:HG	1:93:A:THR:H	15	0.19
(1,974)	1:63:A:LEU:HA	1:92:A:PHE:H	1	0.19
(1,974)	1:63:A:LEU:HA	1:92:A:PHE:H	11	0.19
(1,974)	1:63:A:LEU:HA	1:92:A:PHE:H	17	0.19
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD11	17	0.19
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD12	17	0.19
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD13	17	0.19
(1,950)	1:63:A:LEU:H	1:63:A:LEU:HG	3	0.19
(1,950)	1:63:A:LEU:H	1:63:A:LEU:HG	5	0.19
(1,950)	1:63:A:LEU:H	1:63:A:LEU:HG	13	0.19
(1,950)	1:63:A:LEU:H	1:63:A:LEU:HG	18	0.19
(1,926)	1:61:A:HIS:H	1:62:A:ALA:H	4	0.19
(1,926)	1:61:A:HIS:H	1:62:A:ALA:H	6	0.19
(1,926)	1:61:A:HIS:H	1:62:A:ALA:H	15	0.19
(1,905)	1:58:A:TRP:H	1:58:A:TRP:HB2	10	0.19
(1,904)	1:58:A:TRP:H	1:58:A:TRP:HB3	12	0.19
(1,844)	1:50:A:GLU:H	1:50:A:GLU:HG2	16	0.19
(1,838)	1:49:A:VAL:HG21	1:58:A:TRP:H	11	0.19
(1,838)	1:49:A:VAL:HG22	1:58:A:TRP:H	11	0.19
(1,838)	1:49:A:VAL:HG23	1:58:A:TRP:H	11	0.19
(1,838)	1:49:A:VAL:HG21	1:58:A:TRP:H	13	0.19
(1,838)	1:49:A:VAL:HG22	1:58:A:TRP:H	13	0.19
(1,838)	1:49:A:VAL:HG23	1:58:A:TRP:H	13	0.19
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD21	2	0.19
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD22	2	0.19
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD23	2	0.19
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD21	2	0.19
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD22	2	0.19
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD23	2	0.19
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD21	2	0.19
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD22	2	0.19
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD23	2	0.19
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD21	8	0.19
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD22	8	0.19
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD23	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD21	8	0.19
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD22	8	0.19
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD23	8	0.19
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD21	8	0.19
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD22	8	0.19
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD23	8	0.19
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD21	16	0.19
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD22	16	0.19
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD23	16	0.19
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD21	16	0.19
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD22	16	0.19
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD23	16	0.19
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD21	16	0.19
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD22	16	0.19
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD23	16	0.19
(1,818)	1:48:A:LEU:HD21	1:52:A:LEU:H	1	0.19
(1,818)	1:48:A:LEU:HD22	1:52:A:LEU:H	1	0.19
(1,818)	1:48:A:LEU:HD23	1:52:A:LEU:H	1	0.19
(1,813)	1:48:A:LEU:H	1:51:A:LYS:H	12	0.19
(1,782)	1:47:A:LYS:HB2	1:48:A:LEU:H	2	0.19
(1,782)	1:47:A:LYS:HB2	1:48:A:LEU:H	7	0.19
(1,782)	1:47:A:LYS:HB2	1:48:A:LEU:H	18	0.19
(1,766)	1:46:A:LEU:HA	1:50:A:GLU:H	1	0.19
(1,766)	1:46:A:LEU:HA	1:50:A:GLU:H	4	0.19
(1,765)	1:46:A:LEU:H	1:49:A:VAL:H	2	0.19
(1,765)	1:46:A:LEU:H	1:49:A:VAL:H	9	0.19
(1,764)	1:46:A:LEU:HA	1:49:A:VAL:H	4	0.19
(1,764)	1:46:A:LEU:HA	1:49:A:VAL:H	5	0.19
(1,764)	1:46:A:LEU:HA	1:49:A:VAL:H	6	0.19
(1,764)	1:46:A:LEU:HA	1:49:A:VAL:H	16	0.19
(1,760)	1:46:A:LEU:H	1:48:A:LEU:H	1	0.19
(1,760)	1:46:A:LEU:H	1:48:A:LEU:H	4	0.19
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD21	9	0.19
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD22	9	0.19
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD23	9	0.19
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG21	11	0.19
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG22	11	0.19
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG23	11	0.19
(1,737)	1:45:A:MET:HB3	1:48:A:LEU:H	16	0.19
(1,737)	1:45:A:MET:HB3	1:48:A:LEU:H	18	0.19
(1,737)	1:45:A:MET:HB3	1:48:A:LEU:H	19	0.19
(1,719)	1:44:A:VAL:HG11	1:90:A:LEU:H	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,719)	1:44:A:VAL:HG12	1:90:A:LEU:H	4	0.19
(1,719)	1:44:A:VAL:HG13	1:90:A:LEU:H	4	0.19
(1,719)	1:44:A:VAL:HG11	1:90:A:LEU:H	20	0.19
(1,719)	1:44:A:VAL:HG12	1:90:A:LEU:H	20	0.19
(1,719)	1:44:A:VAL:HG13	1:90:A:LEU:H	20	0.19
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG11	6	0.19
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG12	6	0.19
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG13	6	0.19
(1,694)	1:43:A:GLY:H	1:45:A:MET:H	3	0.19
(1,692)	1:43:A:GLY:H	1:44:A:VAL:HB	5	0.19
(1,685)	1:42:A:GLY:H	1:75:A:THR:HB	13	0.19
(1,684)	1:42:A:GLY:HA3	1:75:A:THR:HB	7	0.19
(1,683)	1:42:A:GLY:H	1:74:A:LYS:HE3	1	0.19
(1,683)	1:42:A:GLY:H	1:74:A:LYS:HE3	10	0.19
(1,683)	1:42:A:GLY:H	1:74:A:LYS:HE3	15	0.19
(1,663)	1:41:A:ILE:HG21	1:72:A:LEU:HG	1	0.19
(1,663)	1:41:A:ILE:HG22	1:72:A:LEU:HG	1	0.19
(1,663)	1:41:A:ILE:HG23	1:72:A:LEU:HG	1	0.19
(1,663)	1:41:A:ILE:HG21	1:72:A:LEU:HG	2	0.19
(1,663)	1:41:A:ILE:HG22	1:72:A:LEU:HG	2	0.19
(1,663)	1:41:A:ILE:HG23	1:72:A:LEU:HG	2	0.19
(1,663)	1:41:A:ILE:HG21	1:72:A:LEU:HG	6	0.19
(1,663)	1:41:A:ILE:HG22	1:72:A:LEU:HG	6	0.19
(1,663)	1:41:A:ILE:HG23	1:72:A:LEU:HG	6	0.19
(1,659)	1:41:A:ILE:HD11	1:44:A:VAL:H	3	0.19
(1,659)	1:41:A:ILE:HD12	1:44:A:VAL:H	3	0.19
(1,659)	1:41:A:ILE:HD13	1:44:A:VAL:H	3	0.19
(1,659)	1:41:A:ILE:HD11	1:44:A:VAL:H	4	0.19
(1,659)	1:41:A:ILE:HD12	1:44:A:VAL:H	4	0.19
(1,659)	1:41:A:ILE:HD13	1:44:A:VAL:H	4	0.19
(1,659)	1:41:A:ILE:HD11	1:44:A:VAL:H	11	0.19
(1,659)	1:41:A:ILE:HD12	1:44:A:VAL:H	11	0.19
(1,659)	1:41:A:ILE:HD13	1:44:A:VAL:H	11	0.19
(1,640)	1:41:A:ILE:H	1:41:A:ILE:HG12	20	0.19
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG11	12	0.19
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG12	12	0.19
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG13	12	0.19
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG11	18	0.19
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG12	18	0.19
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG13	18	0.19
(1,628)	1:40:A:HIS:H	1:44:A:VAL:HB	7	0.19
(1,611)	1:39:A:VAL:HG11	1:78:A:THR:H	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,611)	1:39:A:VAL:HG12	1:78:A:THR:H	11	0.19
(1,611)	1:39:A:VAL:HG13	1:78:A:THR:H	11	0.19
(1,610)	1:39:A:VAL:HG21	1:80:A:ASP:H	18	0.19
(1,610)	1:39:A:VAL:HG22	1:80:A:ASP:H	18	0.19
(1,610)	1:39:A:VAL:HG23	1:80:A:ASP:H	18	0.19
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD21	4	0.19
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD22	4	0.19
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD23	4	0.19
(1,580)	1:38:A:GLU:HB3	1:39:A:VAL:H	5	0.19
(1,580)	1:38:A:GLU:HB3	1:39:A:VAL:H	7	0.19
(1,580)	1:38:A:GLU:HB3	1:39:A:VAL:H	15	0.19
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD21	10	0.19
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD22	10	0.19
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD23	10	0.19
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD21	14	0.19
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD22	14	0.19
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD23	14	0.19
(1,561)	1:37:A:GLY:H	1:38:A:GLU:HG3	11	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG21	2	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG22	2	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG23	2	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG21	7	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG22	7	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG23	7	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG21	8	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG22	8	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG23	8	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG21	13	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG22	13	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG23	13	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG21	16	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG22	16	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG23	16	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG21	19	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG22	19	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG23	19	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG21	20	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG22	20	0.19
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG23	20	0.19
(1,552)	1:36:A:THR:HB	1:38:A:GLU:H	16	0.19
(1,548)	1:36:A:THR:HG21	1:37:A:GLY:H	11	0.19
(1,548)	1:36:A:THR:HG22	1:37:A:GLY:H	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,548)	1:36:A:THR:HG23	1:37:A:GLY:H	11	0.19
(1,532)	1:35:A:VAL:H	1:35:A:VAL:HB	1	0.19
(1,532)	1:35:A:VAL:H	1:35:A:VAL:HB	2	0.19
(1,532)	1:35:A:VAL:H	1:35:A:VAL:HB	4	0.19
(1,532)	1:35:A:VAL:H	1:35:A:VAL:HB	9	0.19
(1,532)	1:35:A:VAL:H	1:35:A:VAL:HB	10	0.19
(1,532)	1:35:A:VAL:H	1:35:A:VAL:HB	13	0.19
(1,532)	1:35:A:VAL:H	1:35:A:VAL:HB	14	0.19
(1,532)	1:35:A:VAL:H	1:35:A:VAL:HB	15	0.19
(1,532)	1:35:A:VAL:H	1:35:A:VAL:HB	17	0.19
(1,527)	1:34:A:ARG:H	1:51:A:LYS:HD3	16	0.19
(1,523)	1:34:A:ARG:HB3	1:35:A:VAL:H	16	0.19
(1,523)	1:34:A:ARG:HB3	1:35:A:VAL:H	17	0.19
(1,511)	1:33:A:LEU:HD21	1:48:A:LEU:HB3	5	0.19
(1,511)	1:33:A:LEU:HD22	1:48:A:LEU:HB3	5	0.19
(1,511)	1:33:A:LEU:HD23	1:48:A:LEU:HB3	5	0.19
(1,511)	1:33:A:LEU:HD21	1:48:A:LEU:HB3	12	0.19
(1,511)	1:33:A:LEU:HD22	1:48:A:LEU:HB3	12	0.19
(1,511)	1:33:A:LEU:HD23	1:48:A:LEU:HB3	12	0.19
(1,511)	1:33:A:LEU:HD21	1:48:A:LEU:HB3	17	0.19
(1,511)	1:33:A:LEU:HD22	1:48:A:LEU:HB3	17	0.19
(1,511)	1:33:A:LEU:HD23	1:48:A:LEU:HB3	17	0.19
(1,483)	1:32:A:THR:H	1:34:A:ARG:H	1	0.19
(1,482)	1:32:A:THR:HA	1:34:A:ARG:H	15	0.19
(1,467)	1:31:A:VAL:H	1:32:A:THR:H	2	0.19
(1,467)	1:31:A:VAL:H	1:32:A:THR:H	5	0.19
(1,467)	1:31:A:VAL:H	1:32:A:THR:H	8	0.19
(1,467)	1:31:A:VAL:H	1:32:A:THR:H	10	0.19
(1,467)	1:31:A:VAL:H	1:32:A:THR:H	20	0.19
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG11	13	0.19
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG12	13	0.19
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG13	13	0.19
(1,437)	1:28:A:ASN:HB3	1:29:A:ARG:H	1	0.19
(1,437)	1:28:A:ASN:HB3	1:29:A:ARG:H	15	0.19
(1,434)	1:28:A:ASN:HA	1:29:A:ARG:H	7	0.19
(1,434)	1:28:A:ASN:HA	1:29:A:ARG:H	8	0.19
(1,434)	1:28:A:ASN:HA	1:29:A:ARG:H	16	0.19
(1,433)	1:28:A:ASN:H	1:28:A:ASN:HB3	2	0.19
(1,432)	1:28:A:ASN:H	1:28:A:ASN:HB2	8	0.19
(1,432)	1:28:A:ASN:H	1:28:A:ASN:HB2	15	0.19
(1,426)	1:27:A:VAL:H	1:28:A:ASN:HB2	1	0.19
(1,372)	1:24:A:VAL:HG21	1:29:A:ARG:H	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,372)	1:24:A:VAL:HG22	1:29:A:ARG:H	7	0.19
(1,372)	1:24:A:VAL:HG23	1:29:A:ARG:H	7	0.19
(1,352)	1:23:A:HIS:HB3	1:91:A:GLN:HB2	5	0.19
(1,352)	1:23:A:HIS:HB3	1:91:A:GLN:HB2	10	0.19
(1,352)	1:23:A:HIS:HB3	1:91:A:GLN:HB2	13	0.19
(1,352)	1:23:A:HIS:HB3	1:91:A:GLN:HB2	17	0.19
(1,350)	1:23:A:HIS:HB2	1:91:A:GLN:HG3	14	0.19
(1,331)	1:23:A:HIS:H	1:30:A:ASP:HB3	2	0.19
(1,331)	1:23:A:HIS:H	1:30:A:ASP:HB3	4	0.19
(1,331)	1:23:A:HIS:H	1:30:A:ASP:HB3	9	0.19
(1,331)	1:23:A:HIS:H	1:30:A:ASP:HB3	17	0.19
(1,331)	1:23:A:HIS:H	1:30:A:ASP:HB3	19	0.19
(1,329)	1:23:A:HIS:HB2	1:24:A:VAL:HA	2	0.19
(1,329)	1:23:A:HIS:HB2	1:24:A:VAL:HA	4	0.19
(1,329)	1:23:A:HIS:HB2	1:24:A:VAL:HA	8	0.19
(1,329)	1:23:A:HIS:HB2	1:24:A:VAL:HA	9	0.19
(1,329)	1:23:A:HIS:HB2	1:24:A:VAL:HA	10	0.19
(1,294)	1:22:A:VAL:HG11	1:29:A:ARG:H	5	0.19
(1,294)	1:22:A:VAL:HG12	1:29:A:ARG:H	5	0.19
(1,294)	1:22:A:VAL:HG13	1:29:A:ARG:H	5	0.19
(1,294)	1:22:A:VAL:HG11	1:29:A:ARG:H	19	0.19
(1,294)	1:22:A:VAL:HG12	1:29:A:ARG:H	19	0.19
(1,294)	1:22:A:VAL:HG13	1:29:A:ARG:H	19	0.19
(1,276)	1:21:A:SER:H	1:32:A:THR:HG21	11	0.19
(1,276)	1:21:A:SER:H	1:32:A:THR:HG22	11	0.19
(1,276)	1:21:A:SER:H	1:32:A:THR:HG23	11	0.19
(1,276)	1:21:A:SER:H	1:32:A:THR:HG21	13	0.19
(1,276)	1:21:A:SER:H	1:32:A:THR:HG22	13	0.19
(1,276)	1:21:A:SER:H	1:32:A:THR:HG23	13	0.19
(1,276)	1:21:A:SER:H	1:32:A:THR:HG21	17	0.19
(1,276)	1:21:A:SER:H	1:32:A:THR:HG22	17	0.19
(1,276)	1:21:A:SER:H	1:32:A:THR:HG23	17	0.19
(1,276)	1:21:A:SER:H	1:32:A:THR:HG21	18	0.19
(1,276)	1:21:A:SER:H	1:32:A:THR:HG22	18	0.19
(1,276)	1:21:A:SER:H	1:32:A:THR:HG23	18	0.19
(1,275)	1:21:A:SER:H	1:32:A:THR:HB	2	0.19
(1,269)	1:21:A:SER:HA	1:23:A:HIS:H	14	0.19
(1,251)	1:20:A:LEU:HG	1:35:A:VAL:H	1	0.19
(1,249)	1:20:A:LEU:HB2	1:34:A:ARG:H	1	0.19
(1,249)	1:20:A:LEU:HB2	1:34:A:ARG:H	2	0.19
(1,249)	1:20:A:LEU:HB2	1:34:A:ARG:H	5	0.19
(1,249)	1:20:A:LEU:HB2	1:34:A:ARG:H	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,249)	1:20:A:LEU:HB2	1:34:A:ARG:H	20	0.19
(1,206)	1:19:A:GLU:H	1:20:A:LEU:HB2	8	0.19
(1,203)	1:19:A:GLU:HB3	1:20:A:LEU:H	3	0.19
(1,203)	1:19:A:GLU:HB3	1:20:A:LEU:H	4	0.19
(1,200)	1:19:A:GLU:H	1:20:A:LEU:H	4	0.19
(1,200)	1:19:A:GLU:H	1:20:A:LEU:H	8	0.19
(1,195)	1:19:A:GLU:H	1:19:A:GLU:HG2	4	0.19
(1,195)	1:19:A:GLU:H	1:19:A:GLU:HG2	10	0.19
(1,195)	1:19:A:GLU:H	1:19:A:GLU:HG2	12	0.19
(1,195)	1:19:A:GLU:H	1:19:A:GLU:HG2	19	0.19
(1,184)	1:18:A:TRP:HE1	1:80:A:ASP:HB3	4	0.19
(1,177)	1:18:A:TRP:HE1	1:36:A:THR:HB	2	0.19
(1,166)	1:17:A:THR:HG21	1:18:A:TRP:H	2	0.19
(1,166)	1:17:A:THR:HG22	1:18:A:TRP:H	2	0.19
(1,166)	1:17:A:THR:HG23	1:18:A:TRP:H	2	0.19
(1,166)	1:17:A:THR:HG21	1:18:A:TRP:H	14	0.19
(1,166)	1:17:A:THR:HG22	1:18:A:TRP:H	14	0.19
(1,166)	1:17:A:THR:HG23	1:18:A:TRP:H	14	0.19
(1,148)	1:15:A:ASP:HA	1:16:A:GLY:H	9	0.19
(1,147)	1:15:A:ASP:H	1:15:A:ASP:HB2	10	0.19
(1,127)	1:11:A:GLY:HA2	1:12:A:CYS:H	5	0.19
(1,113)	1:9:A:PRO:HG3	1:12:A:CYS:HB3	5	0.19
(1,113)	1:9:A:PRO:HG3	1:12:A:CYS:HB3	14	0.19
(1,112)	1:9:A:PRO:HG3	1:10:A:ASP:H	1	0.19
(1,95)	1:8:A:MET:HA	1:10:A:ASP:H	1	0.19
(1,95)	1:8:A:MET:HA	1:10:A:ASP:H	10	0.19
(1,85)	1:7:A:ARG:HD3	1:8:A:MET:H	6	0.19
(1,82)	1:7:A:ARG:HB2	1:8:A:MET:H	6	0.19
(1,78)	1:7:A:ARG:HD3	1:7:A:ARG:HB3	10	0.19
(1,67)	1:6:A:ILE:H	1:10:A:ASP:H	13	0.19
(1,66)	1:6:A:ILE:HB	1:8:A:MET:H	11	0.19
(1,59)	1:6:A:ILE:H	1:6:A:ILE:HD11	16	0.19
(1,59)	1:6:A:ILE:H	1:6:A:ILE:HD12	16	0.19
(1,59)	1:6:A:ILE:H	1:6:A:ILE:HD13	16	0.19
(1,39)	1:4:A:ASP:H	1:4:A:ASP:HB3	19	0.19
(1,34)	1:3:A:LEU:HD21	1:4:A:ASP:H	9	0.19
(1,34)	1:3:A:LEU:HD22	1:4:A:ASP:H	9	0.19
(1,34)	1:3:A:LEU:HD23	1:4:A:ASP:H	9	0.19
(3,21)	1:80:A:ASP:O	1:84:A:ILE:H	1	0.18
(3,21)	1:80:A:ASP:O	1:84:A:ILE:H	9	0.18
(3,21)	1:80:A:ASP:O	1:84:A:ILE:H	10	0.18
(3,21)	1:80:A:ASP:O	1:84:A:ILE:H	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:80:A:ASP:O	1:84:A:ILE:H	17	0.18
(2,21)	1:39:A:VAL:O	1:43:A:GLY:N	4	0.18
(2,21)	1:39:A:VAL:O	1:43:A:GLY:N	11	0.18
(2,21)	1:39:A:VAL:O	1:43:A:GLY:N	15	0.18
(2,21)	1:39:A:VAL:O	1:43:A:GLY:N	16	0.18
(2,19)	1:23:A:HIS:O	1:93:A:THR:H	2	0.18
(2,19)	1:23:A:HIS:O	1:93:A:THR:H	4	0.18
(2,19)	1:23:A:HIS:O	1:93:A:THR:H	5	0.18
(2,19)	1:23:A:HIS:O	1:93:A:THR:H	16	0.18
(2,19)	1:23:A:HIS:O	1:93:A:THR:H	17	0.18
(2,19)	1:23:A:HIS:O	1:93:A:THR:H	20	0.18
(2,17)	1:21:A:SER:O	1:91:A:GLN:H	9	0.18
(2,17)	1:21:A:SER:O	1:91:A:GLN:H	10	0.18
(2,17)	1:21:A:SER:O	1:91:A:GLN:H	18	0.18
(2,17)	1:21:A:SER:O	1:91:A:GLN:H	20	0.18
(2,13)	1:92:A:PHE:O	1:64:A:TRP:N	4	0.18
(2,13)	1:92:A:PHE:O	1:64:A:TRP:N	8	0.18
(2,13)	1:92:A:PHE:O	1:64:A:TRP:N	14	0.18
(2,7)	1:29:A:ARG:O	1:24:A:VAL:N	1	0.18
(2,7)	1:29:A:ARG:O	1:24:A:VAL:N	2	0.18
(2,7)	1:29:A:ARG:O	1:24:A:VAL:N	7	0.18
(2,7)	1:29:A:ARG:O	1:24:A:VAL:N	20	0.18
(1,1404)	1:92:A:PHE:HB2	1:93:A:THR:HB	11	0.18
(1,1404)	1:92:A:PHE:HB2	1:93:A:THR:HB	17	0.18
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG21	4	0.18
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG22	4	0.18
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG23	4	0.18
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG21	11	0.18
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG22	11	0.18
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG23	11	0.18
(1,1246)	1:81:A:LYS:HE3	1:82:A:TYR:H	14	0.18
(1,1235)	1:81:A:LYS:HE3	1:81:A:LYS:HG3	10	0.18
(1,1218)	1:80:A:ASP:HB2	1:82:A:TYR:H	2	0.18
(1,1218)	1:80:A:ASP:HB2	1:82:A:TYR:H	16	0.18
(1,1216)	1:80:A:ASP:H	1:81:A:LYS:HD2	10	0.18
(1,1216)	1:80:A:ASP:H	1:81:A:LYS:HD2	13	0.18
(1,1216)	1:80:A:ASP:H	1:81:A:LYS:HD2	14	0.18
(1,1215)	1:80:A:ASP:HB2	1:81:A:LYS:H	2	0.18
(1,1208)	1:79:A:LEU:HA	1:84:A:ILE:H	13	0.18
(1,1177)	1:78:A:THR:H	1:81:A:LYS:H	7	0.18
(1,1177)	1:78:A:THR:H	1:81:A:LYS:H	9	0.18
(1,1164)	1:78:A:THR:HG21	1:78:A:THR:H	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1164)	1:78:A:THR:HG22	1:78:A:THR:H	12	0.18
(1,1164)	1:78:A:THR:HG23	1:78:A:THR:H	12	0.18
(1,1162)	1:77:A:TRP:H	1:81:A:LYS:HE3	11	0.18
(1,1160)	1:77:A:TRP:HB2	1:78:A:THR:H	9	0.18
(1,1160)	1:77:A:TRP:HB2	1:78:A:THR:H	14	0.18
(1,1160)	1:77:A:TRP:HB2	1:78:A:THR:H	15	0.18
(1,1160)	1:77:A:TRP:HB2	1:78:A:THR:H	17	0.18
(1,1160)	1:77:A:TRP:HB2	1:78:A:THR:H	19	0.18
(1,1153)	1:76:A:HIS:HB3	1:77:A:TRP:H	4	0.18
(1,1153)	1:76:A:HIS:HB3	1:77:A:TRP:H	7	0.18
(1,1153)	1:76:A:HIS:HB3	1:77:A:TRP:H	11	0.18
(1,1153)	1:76:A:HIS:HB3	1:77:A:TRP:H	16	0.18
(1,1148)	1:75:A:THR:HG21	1:77:A:TRP:H	13	0.18
(1,1148)	1:75:A:THR:HG22	1:77:A:TRP:H	13	0.18
(1,1148)	1:75:A:THR:HG23	1:77:A:TRP:H	13	0.18
(1,1141)	1:74:A:LYS:HE3	1:78:A:THR:H	4	0.18
(1,1141)	1:74:A:LYS:HE3	1:78:A:THR:H	12	0.18
(1,1138)	1:74:A:LYS:HD3	1:77:A:TRP:H	1	0.18
(1,1138)	1:74:A:LYS:HD3	1:77:A:TRP:H	5	0.18
(1,1138)	1:74:A:LYS:HD3	1:77:A:TRP:H	8	0.18
(1,1138)	1:74:A:LYS:HD3	1:77:A:TRP:H	19	0.18
(1,1134)	1:74:A:LYS:HG2	1:75:A:THR:H	15	0.18
(1,1134)	1:74:A:LYS:HG2	1:75:A:THR:H	18	0.18
(1,1128)	1:74:A:LYS:HE3	1:74:A:LYS:HB3	1	0.18
(1,1128)	1:74:A:LYS:HE3	1:74:A:LYS:HB3	2	0.18
(1,1128)	1:74:A:LYS:HE3	1:74:A:LYS:HB3	4	0.18
(1,1123)	1:74:A:LYS:H	1:74:A:LYS:HD2	14	0.18
(1,1123)	1:74:A:LYS:H	1:74:A:LYS:HD2	20	0.18
(1,1108)	1:73:A:LEU:HA	1:74:A:LYS:H	8	0.18
(1,1108)	1:73:A:LEU:HA	1:74:A:LYS:H	16	0.18
(1,1108)	1:73:A:LEU:HA	1:74:A:LYS:H	17	0.18
(1,1105)	1:73:A:LEU:H	1:73:A:LEU:HB3	11	0.18
(1,1105)	1:73:A:LEU:H	1:73:A:LEU:HB3	14	0.18
(1,1105)	1:73:A:LEU:H	1:73:A:LEU:HB3	15	0.18
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD11	7	0.18
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD12	7	0.18
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD13	7	0.18
(1,1072)	1:70:A:THR:H	1:71:A:TRP:H	3	0.18
(1,1072)	1:70:A:THR:H	1:71:A:TRP:H	9	0.18
(1,1033)	1:67:A:LYS:HA	1:67:A:LYS:HD3	13	0.18
(1,1021)	1:66:A:GLU:H	1:66:A:GLU:HG2	9	0.18
(1,1019)	1:66:A:GLU:H	1:66:A:GLU:HG3	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1019)	1:66:A:GLU:H	1:66:A:GLU:HG3	17	0.18
(1,1019)	1:66:A:GLU:H	1:66:A:GLU:HG3	18	0.18
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD21	5	0.18
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD22	5	0.18
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD23	5	0.18
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD21	11	0.18
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD22	11	0.18
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD23	11	0.18
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD21	16	0.18
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD22	16	0.18
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD23	16	0.18
(1,997)	1:65:A:TRP:HB3	1:66:A:GLU:H	13	0.18
(1,992)	1:64:A:TRP:H	1:93:A:THR:HG1	4	0.18
(1,981)	1:64:A:TRP:H	1:64:A:TRP:HB3	12	0.18
(1,978)	1:63:A:LEU:HA	1:93:A:THR:H	5	0.18
(1,978)	1:63:A:LEU:HA	1:93:A:THR:H	11	0.18
(1,976)	1:63:A:LEU:HG	1:93:A:THR:H	9	0.18
(1,976)	1:63:A:LEU:HG	1:93:A:THR:H	18	0.18
(1,974)	1:63:A:LEU:HA	1:92:A:PHE:H	14	0.18
(1,972)	1:63:A:LEU:HD11	1:91:A:GLN:H	4	0.18
(1,972)	1:63:A:LEU:HD12	1:91:A:GLN:H	4	0.18
(1,972)	1:63:A:LEU:HD13	1:91:A:GLN:H	4	0.18
(1,972)	1:63:A:LEU:HD11	1:91:A:GLN:H	7	0.18
(1,972)	1:63:A:LEU:HD12	1:91:A:GLN:H	7	0.18
(1,972)	1:63:A:LEU:HD13	1:91:A:GLN:H	7	0.18
(1,972)	1:63:A:LEU:HD11	1:91:A:GLN:H	8	0.18
(1,972)	1:63:A:LEU:HD12	1:91:A:GLN:H	8	0.18
(1,972)	1:63:A:LEU:HD13	1:91:A:GLN:H	8	0.18
(1,972)	1:63:A:LEU:HD11	1:91:A:GLN:H	19	0.18
(1,972)	1:63:A:LEU:HD12	1:91:A:GLN:H	19	0.18
(1,972)	1:63:A:LEU:HD13	1:91:A:GLN:H	19	0.18
(1,968)	1:63:A:LEU:HG	1:90:A:LEU:HA	19	0.18
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD11	9	0.18
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD12	9	0.18
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD13	9	0.18
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD11	10	0.18
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD12	10	0.18
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD13	10	0.18
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD11	19	0.18
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD12	19	0.18
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD13	19	0.18
(1,946)	1:62:A:ALA:H	1:94:A:PRO:HA	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,926)	1:61:A:HIS:H	1:62:A:ALA:H	1	0.18
(1,926)	1:61:A:HIS:H	1:62:A:ALA:H	9	0.18
(1,926)	1:61:A:HIS:H	1:62:A:ALA:H	13	0.18
(1,926)	1:61:A:HIS:H	1:62:A:ALA:H	20	0.18
(1,884)	1:56:A:LYS:HE3	1:56:A:LYS:HB3	4	0.18
(1,866)	1:52:A:LEU:HA	1:52:A:LEU:HD21	12	0.18
(1,866)	1:52:A:LEU:HA	1:52:A:LEU:HD22	12	0.18
(1,866)	1:52:A:LEU:HA	1:52:A:LEU:HD23	12	0.18
(1,844)	1:50:A:GLU:H	1:50:A:GLU:HG2	4	0.18
(1,844)	1:50:A:GLU:H	1:50:A:GLU:HG2	6	0.18
(1,844)	1:50:A:GLU:H	1:50:A:GLU:HG2	14	0.18
(1,844)	1:50:A:GLU:H	1:50:A:GLU:HG2	18	0.18
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD21	9	0.18
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD22	9	0.18
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD23	9	0.18
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD21	9	0.18
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD22	9	0.18
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD23	9	0.18
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD21	9	0.18
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD22	9	0.18
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD23	9	0.18
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD21	11	0.18
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD22	11	0.18
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD23	11	0.18
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD21	11	0.18
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD22	11	0.18
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD23	11	0.18
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD21	11	0.18
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD22	11	0.18
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD23	11	0.18
(1,818)	1:48:A:LEU:HD21	1:52:A:LEU:H	8	0.18
(1,818)	1:48:A:LEU:HD22	1:52:A:LEU:H	8	0.18
(1,818)	1:48:A:LEU:HD23	1:52:A:LEU:H	8	0.18
(1,818)	1:48:A:LEU:HD21	1:52:A:LEU:H	11	0.18
(1,818)	1:48:A:LEU:HD22	1:52:A:LEU:H	11	0.18
(1,818)	1:48:A:LEU:HD23	1:52:A:LEU:H	11	0.18
(1,818)	1:48:A:LEU:HD21	1:52:A:LEU:H	13	0.18
(1,818)	1:48:A:LEU:HD22	1:52:A:LEU:H	13	0.18
(1,818)	1:48:A:LEU:HD23	1:52:A:LEU:H	13	0.18
(1,813)	1:48:A:LEU:H	1:51:A:LYS:H	2	0.18
(1,812)	1:48:A:LEU:HA	1:51:A:LYS:HB3	9	0.18
(1,812)	1:48:A:LEU:HA	1:51:A:LYS:HB3	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG21	2	0.18
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG22	2	0.18
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG23	2	0.18
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG21	3	0.18
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG22	3	0.18
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG23	3	0.18
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG21	6	0.18
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG22	6	0.18
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG23	6	0.18
(1,782)	1:47:A:LYS:HB2	1:48:A:LEU:H	4	0.18
(1,773)	1:47:A:LYS:H	1:47:A:LYS:HD3	5	0.18
(1,773)	1:47:A:LYS:H	1:47:A:LYS:HD3	15	0.18
(1,766)	1:46:A:LEU:HA	1:50:A:GLU:H	2	0.18
(1,766)	1:46:A:LEU:HA	1:50:A:GLU:H	6	0.18
(1,766)	1:46:A:LEU:HA	1:50:A:GLU:H	8	0.18
(1,766)	1:46:A:LEU:HA	1:50:A:GLU:H	11	0.18
(1,766)	1:46:A:LEU:HA	1:50:A:GLU:H	12	0.18
(1,766)	1:46:A:LEU:HA	1:50:A:GLU:H	15	0.18
(1,764)	1:46:A:LEU:HA	1:49:A:VAL:H	7	0.18
(1,764)	1:46:A:LEU:HA	1:49:A:VAL:H	17	0.18
(1,764)	1:46:A:LEU:HA	1:49:A:VAL:H	18	0.18
(1,760)	1:46:A:LEU:H	1:48:A:LEU:H	12	0.18
(1,760)	1:46:A:LEU:H	1:48:A:LEU:H	13	0.18
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD21	13	0.18
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD22	13	0.18
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD23	13	0.18
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG21	6	0.18
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG22	6	0.18
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG23	6	0.18
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG21	15	0.18
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG22	15	0.18
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG23	15	0.18
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG21	19	0.18
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG22	19	0.18
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG23	19	0.18
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG21	20	0.18
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG22	20	0.18
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG23	20	0.18
(1,737)	1:45:A:MET:HB3	1:48:A:LEU:H	6	0.18
(1,719)	1:44:A:VAL:HG11	1:90:A:LEU:H	16	0.18
(1,719)	1:44:A:VAL:HG12	1:90:A:LEU:H	16	0.18
(1,719)	1:44:A:VAL:HG13	1:90:A:LEU:H	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG11	8	0.18
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG12	8	0.18
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG13	8	0.18
(1,694)	1:43:A:GLY:H	1:45:A:MET:H	4	0.18
(1,694)	1:43:A:GLY:H	1:45:A:MET:H	19	0.18
(1,692)	1:43:A:GLY:H	1:44:A:VAL:HB	4	0.18
(1,684)	1:42:A:GLY:HA3	1:75:A:THR:HB	12	0.18
(1,683)	1:42:A:GLY:H	1:74:A:LYS:HE3	12	0.18
(1,683)	1:42:A:GLY:H	1:74:A:LYS:HE3	16	0.18
(1,671)	1:41:A:ILE:HD11	1:75:A:THR:HA	8	0.18
(1,671)	1:41:A:ILE:HD12	1:75:A:THR:HA	8	0.18
(1,671)	1:41:A:ILE:HD13	1:75:A:THR:HA	8	0.18
(1,663)	1:41:A:ILE:HG21	1:72:A:LEU:HG	9	0.18
(1,663)	1:41:A:ILE:HG22	1:72:A:LEU:HG	9	0.18
(1,663)	1:41:A:ILE:HG23	1:72:A:LEU:HG	9	0.18
(1,659)	1:41:A:ILE:HD11	1:44:A:VAL:H	2	0.18
(1,659)	1:41:A:ILE:HD12	1:44:A:VAL:H	2	0.18
(1,659)	1:41:A:ILE:HD13	1:44:A:VAL:H	2	0.18
(1,640)	1:41:A:ILE:H	1:41:A:ILE:HG12	13	0.18
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG11	15	0.18
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG12	15	0.18
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG13	15	0.18
(1,628)	1:40:A:HIS:H	1:44:A:VAL:HB	14	0.18
(1,610)	1:39:A:VAL:HG21	1:80:A:ASP:H	6	0.18
(1,610)	1:39:A:VAL:HG22	1:80:A:ASP:H	6	0.18
(1,610)	1:39:A:VAL:HG23	1:80:A:ASP:H	6	0.18
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD21	5	0.18
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD22	5	0.18
(1,606)	1:39:A:VAL:H	1:79:A:LEU:HD23	5	0.18
(1,580)	1:38:A:GLU:HB3	1:39:A:VAL:H	3	0.18
(1,580)	1:38:A:GLU:HB3	1:39:A:VAL:H	6	0.18
(1,580)	1:38:A:GLU:HB3	1:39:A:VAL:H	17	0.18
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD21	3	0.18
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD22	3	0.18
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD23	3	0.18
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD21	6	0.18
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD22	6	0.18
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD23	6	0.18
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG21	3	0.18
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG22	3	0.18
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG23	3	0.18
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG21	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG22	4	0.18
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG23	4	0.18
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG21	5	0.18
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG22	5	0.18
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG23	5	0.18
(1,552)	1:36:A:THR:HB	1:38:A:GLU:H	10	0.18
(1,532)	1:35:A:VAL:H	1:35:A:VAL:HB	7	0.18
(1,527)	1:34:A:ARG:H	1:51:A:LYS:HD3	7	0.18
(1,499)	1:33:A:LEU:HD21	1:34:A:ARG:H	1	0.18
(1,499)	1:33:A:LEU:HD22	1:34:A:ARG:H	1	0.18
(1,499)	1:33:A:LEU:HD23	1:34:A:ARG:H	1	0.18
(1,499)	1:33:A:LEU:HD21	1:34:A:ARG:H	12	0.18
(1,499)	1:33:A:LEU:HD22	1:34:A:ARG:H	12	0.18
(1,499)	1:33:A:LEU:HD23	1:34:A:ARG:H	12	0.18
(1,484)	1:32:A:THR:HA	1:51:A:LYS:HD3	1	0.18
(1,484)	1:32:A:THR:HA	1:51:A:LYS:HD3	2	0.18
(1,484)	1:32:A:THR:HA	1:51:A:LYS:HD3	14	0.18
(1,484)	1:32:A:THR:HA	1:51:A:LYS:HD3	17	0.18
(1,483)	1:32:A:THR:H	1:34:A:ARG:H	2	0.18
(1,483)	1:32:A:THR:H	1:34:A:ARG:H	17	0.18
(1,482)	1:32:A:THR:HA	1:34:A:ARG:H	6	0.18
(1,482)	1:32:A:THR:HA	1:34:A:ARG:H	14	0.18
(1,467)	1:31:A:VAL:H	1:32:A:THR:H	1	0.18
(1,467)	1:31:A:VAL:H	1:32:A:THR:H	3	0.18
(1,467)	1:31:A:VAL:H	1:32:A:THR:H	4	0.18
(1,467)	1:31:A:VAL:H	1:32:A:THR:H	6	0.18
(1,467)	1:31:A:VAL:H	1:32:A:THR:H	7	0.18
(1,467)	1:31:A:VAL:H	1:32:A:THR:H	9	0.18
(1,467)	1:31:A:VAL:H	1:32:A:THR:H	11	0.18
(1,467)	1:31:A:VAL:H	1:32:A:THR:H	12	0.18
(1,467)	1:31:A:VAL:H	1:32:A:THR:H	13	0.18
(1,467)	1:31:A:VAL:H	1:32:A:THR:H	15	0.18
(1,467)	1:31:A:VAL:H	1:32:A:THR:H	16	0.18
(1,467)	1:31:A:VAL:H	1:32:A:THR:H	17	0.18
(1,467)	1:31:A:VAL:H	1:32:A:THR:H	19	0.18
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG11	10	0.18
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG12	10	0.18
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG13	10	0.18
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG11	11	0.18
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG12	11	0.18
(1,459)	1:30:A:ASP:HA	1:31:A:VAL:HG13	11	0.18
(1,453)	1:29:A:ARG:HB2	1:31:A:VAL:HA	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:29:A:ARG:HB2	1:31:A:VAL:HA	18	0.18
(1,437)	1:28:A:ASN:HB3	1:29:A:ARG:H	5	0.18
(1,437)	1:28:A:ASN:HB3	1:29:A:ARG:H	8	0.18
(1,437)	1:28:A:ASN:HB3	1:29:A:ARG:H	16	0.18
(1,437)	1:28:A:ASN:HB3	1:29:A:ARG:H	20	0.18
(1,434)	1:28:A:ASN:HA	1:29:A:ARG:H	9	0.18
(1,434)	1:28:A:ASN:HA	1:29:A:ARG:H	18	0.18
(1,430)	1:27:A:VAL:HG21	1:92:A:PHE:H	5	0.18
(1,430)	1:27:A:VAL:HG22	1:92:A:PHE:H	5	0.18
(1,430)	1:27:A:VAL:HG23	1:92:A:PHE:H	5	0.18
(1,426)	1:27:A:VAL:H	1:28:A:ASN:HB2	4	0.18
(1,426)	1:27:A:VAL:H	1:28:A:ASN:HB2	6	0.18
(1,426)	1:27:A:VAL:H	1:28:A:ASN:HB2	15	0.18
(1,426)	1:27:A:VAL:H	1:28:A:ASN:HB2	17	0.18
(1,387)	1:24:A:VAL:HG11	1:62:A:ALA:H	6	0.18
(1,387)	1:24:A:VAL:HG12	1:62:A:ALA:H	6	0.18
(1,387)	1:24:A:VAL:HG13	1:62:A:ALA:H	6	0.18
(1,387)	1:24:A:VAL:HG11	1:62:A:ALA:H	9	0.18
(1,387)	1:24:A:VAL:HG12	1:62:A:ALA:H	9	0.18
(1,387)	1:24:A:VAL:HG13	1:62:A:ALA:H	9	0.18
(1,387)	1:24:A:VAL:HG11	1:62:A:ALA:H	10	0.18
(1,387)	1:24:A:VAL:HG12	1:62:A:ALA:H	10	0.18
(1,387)	1:24:A:VAL:HG13	1:62:A:ALA:H	10	0.18
(1,383)	1:24:A:VAL:HA	1:31:A:VAL:H	5	0.18
(1,377)	1:24:A:VAL:HA	1:30:A:ASP:HA	3	0.18
(1,377)	1:24:A:VAL:HA	1:30:A:ASP:HA	8	0.18
(1,377)	1:24:A:VAL:HA	1:30:A:ASP:HA	10	0.18
(1,377)	1:24:A:VAL:HA	1:30:A:ASP:HA	11	0.18
(1,377)	1:24:A:VAL:HA	1:30:A:ASP:HA	16	0.18
(1,372)	1:24:A:VAL:HG21	1:29:A:ARG:H	6	0.18
(1,372)	1:24:A:VAL:HG22	1:29:A:ARG:H	6	0.18
(1,372)	1:24:A:VAL:HG23	1:29:A:ARG:H	6	0.18
(1,352)	1:23:A:HIS:HB3	1:91:A:GLN:HB2	1	0.18
(1,352)	1:23:A:HIS:HB3	1:91:A:GLN:HB2	11	0.18
(1,352)	1:23:A:HIS:HB3	1:91:A:GLN:HB2	19	0.18
(1,350)	1:23:A:HIS:HB2	1:91:A:GLN:HG3	7	0.18
(1,350)	1:23:A:HIS:HB2	1:91:A:GLN:HG3	8	0.18
(1,350)	1:23:A:HIS:HB2	1:91:A:GLN:HG3	9	0.18
(1,350)	1:23:A:HIS:HB2	1:91:A:GLN:HG3	11	0.18
(1,350)	1:23:A:HIS:HB2	1:91:A:GLN:HG3	19	0.18
(1,331)	1:23:A:HIS:H	1:30:A:ASP:HB3	8	0.18
(1,331)	1:23:A:HIS:H	1:30:A:ASP:HB3	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,329)	1:23:A:HIS:HB2	1:24:A:VAL:HA	3	0.18
(1,329)	1:23:A:HIS:HB2	1:24:A:VAL:HA	5	0.18
(1,329)	1:23:A:HIS:HB2	1:24:A:VAL:HA	11	0.18
(1,329)	1:23:A:HIS:HB2	1:24:A:VAL:HA	12	0.18
(1,329)	1:23:A:HIS:HB2	1:24:A:VAL:HA	13	0.18
(1,329)	1:23:A:HIS:HB2	1:24:A:VAL:HA	20	0.18
(1,323)	1:23:A:HIS:HB2	1:24:A:VAL:H	12	0.18
(1,294)	1:22:A:VAL:HG11	1:29:A:ARG:H	4	0.18
(1,294)	1:22:A:VAL:HG12	1:29:A:ARG:H	4	0.18
(1,294)	1:22:A:VAL:HG13	1:29:A:ARG:H	4	0.18
(1,294)	1:22:A:VAL:HG11	1:29:A:ARG:H	6	0.18
(1,294)	1:22:A:VAL:HG12	1:29:A:ARG:H	6	0.18
(1,294)	1:22:A:VAL:HG13	1:29:A:ARG:H	6	0.18
(1,294)	1:22:A:VAL:HG11	1:29:A:ARG:H	7	0.18
(1,294)	1:22:A:VAL:HG12	1:29:A:ARG:H	7	0.18
(1,294)	1:22:A:VAL:HG13	1:29:A:ARG:H	7	0.18
(1,294)	1:22:A:VAL:HG11	1:29:A:ARG:H	15	0.18
(1,294)	1:22:A:VAL:HG12	1:29:A:ARG:H	15	0.18
(1,294)	1:22:A:VAL:HG13	1:29:A:ARG:H	15	0.18
(1,294)	1:22:A:VAL:HG11	1:29:A:ARG:H	16	0.18
(1,294)	1:22:A:VAL:HG12	1:29:A:ARG:H	16	0.18
(1,294)	1:22:A:VAL:HG13	1:29:A:ARG:H	16	0.18
(1,294)	1:22:A:VAL:HG11	1:29:A:ARG:H	18	0.18
(1,294)	1:22:A:VAL:HG12	1:29:A:ARG:H	18	0.18
(1,294)	1:22:A:VAL:HG13	1:29:A:ARG:H	18	0.18
(1,276)	1:21:A:SER:H	1:32:A:THR:HG21	5	0.18
(1,276)	1:21:A:SER:H	1:32:A:THR:HG22	5	0.18
(1,276)	1:21:A:SER:H	1:32:A:THR:HG23	5	0.18
(1,276)	1:21:A:SER:H	1:32:A:THR:HG21	8	0.18
(1,276)	1:21:A:SER:H	1:32:A:THR:HG22	8	0.18
(1,276)	1:21:A:SER:H	1:32:A:THR:HG23	8	0.18
(1,276)	1:21:A:SER:H	1:32:A:THR:HG21	12	0.18
(1,276)	1:21:A:SER:H	1:32:A:THR:HG22	12	0.18
(1,276)	1:21:A:SER:H	1:32:A:THR:HG23	12	0.18
(1,276)	1:21:A:SER:H	1:32:A:THR:HG21	14	0.18
(1,276)	1:21:A:SER:H	1:32:A:THR:HG22	14	0.18
(1,276)	1:21:A:SER:H	1:32:A:THR:HG23	14	0.18
(1,276)	1:21:A:SER:H	1:32:A:THR:HG21	19	0.18
(1,276)	1:21:A:SER:H	1:32:A:THR:HG22	19	0.18
(1,276)	1:21:A:SER:H	1:32:A:THR:HG23	19	0.18
(1,275)	1:21:A:SER:H	1:32:A:THR:HB	20	0.18
(1,249)	1:20:A:LEU:HB2	1:34:A:ARG:H	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,249)	1:20:A:LEU:HB2	1:34:A:ARG:H	11	0.18
(1,244)	1:20:A:LEU:HD21	1:33:A:LEU:HA	1	0.18
(1,244)	1:20:A:LEU:HD22	1:33:A:LEU:HA	1	0.18
(1,244)	1:20:A:LEU:HD23	1:33:A:LEU:HA	1	0.18
(1,244)	1:20:A:LEU:HD21	1:33:A:LEU:HA	17	0.18
(1,244)	1:20:A:LEU:HD22	1:33:A:LEU:HA	17	0.18
(1,244)	1:20:A:LEU:HD23	1:33:A:LEU:HA	17	0.18
(1,244)	1:20:A:LEU:HD21	1:33:A:LEU:HA	20	0.18
(1,244)	1:20:A:LEU:HD22	1:33:A:LEU:HA	20	0.18
(1,244)	1:20:A:LEU:HD23	1:33:A:LEU:HA	20	0.18
(1,234)	1:20:A:LEU:HB3	1:21:A:SER:H	2	0.18
(1,234)	1:20:A:LEU:HB3	1:21:A:SER:H	8	0.18
(1,234)	1:20:A:LEU:HB3	1:21:A:SER:H	10	0.18
(1,212)	1:19:A:GLU:HB2	1:33:A:LEU:H	6	0.18
(1,200)	1:19:A:GLU:H	1:20:A:LEU:H	7	0.18
(1,195)	1:19:A:GLU:H	1:19:A:GLU:HG2	2	0.18
(1,195)	1:19:A:GLU:H	1:19:A:GLU:HG2	20	0.18
(1,177)	1:18:A:TRP:HE1	1:36:A:THR:HB	1	0.18
(1,177)	1:18:A:TRP:HE1	1:36:A:THR:HB	13	0.18
(1,177)	1:18:A:TRP:HE1	1:36:A:THR:HB	20	0.18
(1,166)	1:17:A:THR:HG21	1:18:A:TRP:H	9	0.18
(1,166)	1:17:A:THR:HG22	1:18:A:TRP:H	9	0.18
(1,166)	1:17:A:THR:HG23	1:18:A:TRP:H	9	0.18
(1,148)	1:15:A:ASP:HA	1:16:A:GLY:H	12	0.18
(1,147)	1:15:A:ASP:H	1:15:A:ASP:HB2	4	0.18
(1,127)	1:11:A:GLY:HA2	1:12:A:CYS:H	7	0.18
(1,127)	1:11:A:GLY:HA2	1:12:A:CYS:H	12	0.18
(1,112)	1:9:A:PRO:HG3	1:10:A:ASP:H	5	0.18
(1,100)	1:8:A:MET:H	1:12:A:CYS:HA	12	0.18
(1,86)	1:7:A:ARG:HA	1:10:A:ASP:H	13	0.18
(1,85)	1:7:A:ARG:HD3	1:8:A:MET:H	15	0.18
(1,82)	1:7:A:ARG:HB2	1:8:A:MET:H	2	0.18
(1,82)	1:7:A:ARG:HB2	1:8:A:MET:H	12	0.18
(1,61)	1:6:A:ILE:H	1:7:A:ARG:H	5	0.18
(1,56)	1:6:A:ILE:H	1:6:A:ILE:HG12	17	0.18
(1,43)	1:4:A:ASP:HB3	1:5:A:GLY:H	2	0.18
(1,36)	1:3:A:LEU:HB3	1:4:A:ASP:H	17	0.18
(1,17)	1:2:A:ALA:H	1:3:A:LEU:HA	18	0.18
(3,21)	1:80:A:ASP:O	1:84:A:ILE:H	8	0.17
(2,21)	1:39:A:VAL:O	1:43:A:GLY:N	2	0.17
(2,21)	1:39:A:VAL:O	1:43:A:GLY:N	5	0.17
(2,21)	1:39:A:VAL:O	1:43:A:GLY:N	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,19)	1:23:A:HIS:O	1:93:A:THR:H	1	0.17
(2,19)	1:23:A:HIS:O	1:93:A:THR:H	3	0.17
(2,19)	1:23:A:HIS:O	1:93:A:THR:H	7	0.17
(2,19)	1:23:A:HIS:O	1:93:A:THR:H	8	0.17
(2,19)	1:23:A:HIS:O	1:93:A:THR:H	11	0.17
(2,19)	1:23:A:HIS:O	1:93:A:THR:H	19	0.17
(2,17)	1:21:A:SER:O	1:91:A:GLN:H	8	0.17
(2,17)	1:21:A:SER:O	1:91:A:GLN:H	12	0.17
(2,17)	1:21:A:SER:O	1:91:A:GLN:H	17	0.17
(2,13)	1:92:A:PHE:O	1:64:A:TRP:N	2	0.17
(2,7)	1:29:A:ARG:O	1:24:A:VAL:N	6	0.17
(2,4)	1:33:A:LEU:O	1:20:A:LEU:N	19	0.17
(2,3)	1:20:A:LEU:O	1:33:A:LEU:N	19	0.17
(1,1402)	1:92:A:PHE:H	1:92:A:PHE:HB2	8	0.17
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD11	10	0.17
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD12	10	0.17
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD13	10	0.17
(1,1329)	1:87:A:ASP:HB3	1:88:A:ALA:H	19	0.17
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG21	12	0.17
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG22	12	0.17
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG23	12	0.17
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG21	14	0.17
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG22	14	0.17
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG23	14	0.17
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG21	15	0.17
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG22	15	0.17
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG23	15	0.17
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG21	15	0.17
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG22	15	0.17
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG23	15	0.17
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG21	16	0.17
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG22	16	0.17
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG23	16	0.17
(1,1246)	1:81:A:LYS:HE3	1:82:A:TYR:H	11	0.17
(1,1246)	1:81:A:LYS:HE3	1:82:A:TYR:H	16	0.17
(1,1218)	1:80:A:ASP:HB2	1:82:A:TYR:H	1	0.17
(1,1218)	1:80:A:ASP:HB2	1:82:A:TYR:H	15	0.17
(1,1216)	1:80:A:ASP:H	1:81:A:LYS:HD2	7	0.17
(1,1216)	1:80:A:ASP:H	1:81:A:LYS:HD2	17	0.17
(1,1215)	1:80:A:ASP:HB2	1:81:A:LYS:H	4	0.17
(1,1215)	1:80:A:ASP:HB2	1:81:A:LYS:H	5	0.17
(1,1215)	1:80:A:ASP:HB2	1:81:A:LYS:H	16	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1215)	1:80:A:ASP:HB2	1:81:A:LYS:H	20	0.17
(1,1208)	1:79:A:LEU:HA	1:84:A:ILE:H	8	0.17
(1,1187)	1:79:A:LEU:H	1:79:A:LEU:HD21	11	0.17
(1,1187)	1:79:A:LEU:H	1:79:A:LEU:HD22	11	0.17
(1,1187)	1:79:A:LEU:H	1:79:A:LEU:HD23	11	0.17
(1,1187)	1:79:A:LEU:H	1:79:A:LEU:HD21	19	0.17
(1,1187)	1:79:A:LEU:H	1:79:A:LEU:HD22	19	0.17
(1,1187)	1:79:A:LEU:H	1:79:A:LEU:HD23	19	0.17
(1,1177)	1:78:A:THR:H	1:81:A:LYS:H	17	0.17
(1,1176)	1:78:A:THR:H	1:81:A:LYS:HA	13	0.17
(1,1164)	1:78:A:THR:HG21	1:78:A:THR:H	5	0.17
(1,1164)	1:78:A:THR:HG22	1:78:A:THR:H	5	0.17
(1,1164)	1:78:A:THR:HG23	1:78:A:THR:H	5	0.17
(1,1162)	1:77:A:TRP:H	1:81:A:LYS:HE3	16	0.17
(1,1161)	1:77:A:TRP:H	1:81:A:LYS:HD3	4	0.17
(1,1161)	1:77:A:TRP:H	1:81:A:LYS:HD3	5	0.17
(1,1161)	1:77:A:TRP:H	1:81:A:LYS:HD3	6	0.17
(1,1160)	1:77:A:TRP:HB2	1:78:A:THR:H	1	0.17
(1,1160)	1:77:A:TRP:HB2	1:78:A:THR:H	6	0.17
(1,1160)	1:77:A:TRP:HB2	1:78:A:THR:H	7	0.17
(1,1160)	1:77:A:TRP:HB2	1:78:A:THR:H	10	0.17
(1,1153)	1:76:A:HIS:HB3	1:77:A:TRP:H	3	0.17
(1,1153)	1:76:A:HIS:HB3	1:77:A:TRP:H	6	0.17
(1,1153)	1:76:A:HIS:HB3	1:77:A:TRP:H	9	0.17
(1,1153)	1:76:A:HIS:HB3	1:77:A:TRP:H	14	0.17
(1,1148)	1:75:A:THR:HG21	1:77:A:TRP:H	1	0.17
(1,1148)	1:75:A:THR:HG22	1:77:A:TRP:H	1	0.17
(1,1148)	1:75:A:THR:HG23	1:77:A:TRP:H	1	0.17
(1,1148)	1:75:A:THR:HG21	1:77:A:TRP:H	8	0.17
(1,1148)	1:75:A:THR:HG22	1:77:A:TRP:H	8	0.17
(1,1148)	1:75:A:THR:HG23	1:77:A:TRP:H	8	0.17
(1,1148)	1:75:A:THR:HG21	1:77:A:TRP:H	10	0.17
(1,1148)	1:75:A:THR:HG22	1:77:A:TRP:H	10	0.17
(1,1148)	1:75:A:THR:HG23	1:77:A:TRP:H	10	0.17
(1,1141)	1:74:A:LYS:HE3	1:78:A:THR:H	9	0.17
(1,1141)	1:74:A:LYS:HE3	1:78:A:THR:H	10	0.17
(1,1141)	1:74:A:LYS:HE3	1:78:A:THR:H	14	0.17
(1,1138)	1:74:A:LYS:HD3	1:77:A:TRP:H	2	0.17
(1,1138)	1:74:A:LYS:HD3	1:77:A:TRP:H	4	0.17
(1,1138)	1:74:A:LYS:HD3	1:77:A:TRP:H	11	0.17
(1,1134)	1:74:A:LYS:HG2	1:75:A:THR:H	1	0.17
(1,1134)	1:74:A:LYS:HG2	1:75:A:THR:H	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1134)	1:74:A:LYS:HG2	1:75:A:THR:H	7	0.17
(1,1134)	1:74:A:LYS:HG2	1:75:A:THR:H	14	0.17
(1,1132)	1:74:A:LYS:HG3	1:75:A:THR:H	13	0.17
(1,1128)	1:74:A:LYS:HE3	1:74:A:LYS:HB3	16	0.17
(1,1128)	1:74:A:LYS:HE3	1:74:A:LYS:HB3	17	0.17
(1,1113)	1:74:A:LYS:HA	1:74:A:LYS:HE3	13	0.17
(1,1113)	1:74:A:LYS:HA	1:74:A:LYS:HE3	19	0.17
(1,1108)	1:73:A:LEU:HA	1:74:A:LYS:H	2	0.17
(1,1108)	1:73:A:LEU:HA	1:74:A:LYS:H	3	0.17
(1,1108)	1:73:A:LEU:HA	1:74:A:LYS:H	4	0.17
(1,1108)	1:73:A:LEU:HA	1:74:A:LYS:H	14	0.17
(1,1108)	1:73:A:LEU:HA	1:74:A:LYS:H	20	0.17
(1,1105)	1:73:A:LEU:H	1:73:A:LEU:HB3	5	0.17
(1,1105)	1:73:A:LEU:H	1:73:A:LEU:HB3	6	0.17
(1,1105)	1:73:A:LEU:H	1:73:A:LEU:HB3	13	0.17
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD11	20	0.17
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD12	20	0.17
(1,1086)	1:72:A:LEU:H	1:72:A:LEU:HD13	20	0.17
(1,1081)	1:71:A:TRP:HB2	1:72:A:LEU:H	8	0.17
(1,1072)	1:70:A:THR:H	1:71:A:TRP:H	4	0.17
(1,1072)	1:70:A:THR:H	1:71:A:TRP:H	13	0.17
(1,1061)	1:69:A:ARG:HD3	1:70:A:THR:HB	17	0.17
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD21	8	0.17
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD22	8	0.17
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD23	8	0.17
(1,981)	1:64:A:TRP:H	1:64:A:TRP:HB3	6	0.17
(1,978)	1:63:A:LEU:HA	1:93:A:THR:H	1	0.17
(1,978)	1:63:A:LEU:HA	1:93:A:THR:H	13	0.17
(1,978)	1:63:A:LEU:HA	1:93:A:THR:H	15	0.17
(1,976)	1:63:A:LEU:HG	1:93:A:THR:H	2	0.17
(1,976)	1:63:A:LEU:HG	1:93:A:THR:H	19	0.17
(1,974)	1:63:A:LEU:HA	1:92:A:PHE:H	9	0.17
(1,974)	1:63:A:LEU:HA	1:92:A:PHE:H	20	0.17
(1,972)	1:63:A:LEU:HD11	1:91:A:GLN:H	14	0.17
(1,972)	1:63:A:LEU:HD12	1:91:A:GLN:H	14	0.17
(1,972)	1:63:A:LEU:HD13	1:91:A:GLN:H	14	0.17
(1,972)	1:63:A:LEU:HD11	1:91:A:GLN:H	15	0.17
(1,972)	1:63:A:LEU:HD12	1:91:A:GLN:H	15	0.17
(1,972)	1:63:A:LEU:HD13	1:91:A:GLN:H	15	0.17
(1,968)	1:63:A:LEU:HG	1:90:A:LEU:HA	2	0.17
(1,968)	1:63:A:LEU:HG	1:90:A:LEU:HA	8	0.17
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD11	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD12	15	0.17
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD13	15	0.17
(1,950)	1:63:A:LEU:H	1:63:A:LEU:HG	17	0.17
(1,945)	1:62:A:ALA:HB1	1:93:A:THR:HA	14	0.17
(1,945)	1:62:A:ALA:HB2	1:93:A:THR:HA	14	0.17
(1,945)	1:62:A:ALA:HB3	1:93:A:THR:HA	14	0.17
(1,945)	1:62:A:ALA:HB1	1:93:A:THR:HA	15	0.17
(1,945)	1:62:A:ALA:HB2	1:93:A:THR:HA	15	0.17
(1,945)	1:62:A:ALA:HB3	1:93:A:THR:HA	15	0.17
(1,926)	1:61:A:HIS:H	1:62:A:ALA:H	17	0.17
(1,926)	1:61:A:HIS:H	1:62:A:ALA:H	18	0.17
(1,904)	1:58:A:TRP:H	1:58:A:TRP:HB3	14	0.17
(1,890)	1:56:A:LYS:HA	1:57:A:ASP:HB2	6	0.17
(1,890)	1:56:A:LYS:HA	1:57:A:ASP:HB2	9	0.17
(1,890)	1:56:A:LYS:HA	1:57:A:ASP:HB2	12	0.17
(1,878)	1:56:A:LYS:H	1:56:A:LYS:HD3	12	0.17
(1,858)	1:51:A:LYS:H	1:51:A:LYS:HD3	7	0.17
(1,844)	1:50:A:GLU:H	1:50:A:GLU:HG2	5	0.17
(1,844)	1:50:A:GLU:H	1:50:A:GLU:HG2	7	0.17
(1,844)	1:50:A:GLU:H	1:50:A:GLU:HG2	8	0.17
(1,844)	1:50:A:GLU:H	1:50:A:GLU:HG2	15	0.17
(1,844)	1:50:A:GLU:H	1:50:A:GLU:HG2	20	0.17
(1,841)	1:50:A:GLU:HA	1:50:A:GLU:HG3	19	0.17
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD21	6	0.17
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD22	6	0.17
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD23	6	0.17
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD21	6	0.17
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD22	6	0.17
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD23	6	0.17
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD21	6	0.17
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD22	6	0.17
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD23	6	0.17
(1,813)	1:48:A:LEU:H	1:51:A:LYS:H	7	0.17
(1,813)	1:48:A:LEU:H	1:51:A:LYS:H	8	0.17
(1,813)	1:48:A:LEU:H	1:51:A:LYS:H	9	0.17
(1,813)	1:48:A:LEU:H	1:51:A:LYS:H	13	0.17
(1,813)	1:48:A:LEU:H	1:51:A:LYS:H	19	0.17
(1,812)	1:48:A:LEU:HA	1:51:A:LYS:HB3	14	0.17
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG21	4	0.17
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG22	4	0.17
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG23	4	0.17
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG21	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG22	8	0.17
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG23	8	0.17
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG21	13	0.17
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG22	13	0.17
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG23	13	0.17
(1,782)	1:47:A:LYS:HB2	1:48:A:LEU:H	6	0.17
(1,782)	1:47:A:LYS:HB2	1:48:A:LEU:H	8	0.17
(1,782)	1:47:A:LYS:HB2	1:48:A:LEU:H	13	0.17
(1,773)	1:47:A:LYS:H	1:47:A:LYS:HD3	2	0.17
(1,773)	1:47:A:LYS:H	1:47:A:LYS:HD3	3	0.17
(1,773)	1:47:A:LYS:H	1:47:A:LYS:HD3	16	0.17
(1,773)	1:47:A:LYS:H	1:47:A:LYS:HD3	20	0.17
(1,766)	1:46:A:LEU:HA	1:50:A:GLU:H	13	0.17
(1,766)	1:46:A:LEU:HA	1:50:A:GLU:H	14	0.17
(1,765)	1:46:A:LEU:H	1:49:A:VAL:H	12	0.17
(1,764)	1:46:A:LEU:HA	1:49:A:VAL:H	8	0.17
(1,764)	1:46:A:LEU:HA	1:49:A:VAL:H	15	0.17
(1,760)	1:46:A:LEU:H	1:48:A:LEU:H	2	0.17
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD21	10	0.17
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD22	10	0.17
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD23	10	0.17
(1,719)	1:44:A:VAL:HG11	1:90:A:LEU:H	2	0.17
(1,719)	1:44:A:VAL:HG12	1:90:A:LEU:H	2	0.17
(1,719)	1:44:A:VAL:HG13	1:90:A:LEU:H	2	0.17
(1,719)	1:44:A:VAL:HG11	1:90:A:LEU:H	8	0.17
(1,719)	1:44:A:VAL:HG12	1:90:A:LEU:H	8	0.17
(1,719)	1:44:A:VAL:HG13	1:90:A:LEU:H	8	0.17
(1,694)	1:43:A:GLY:H	1:45:A:MET:H	6	0.17
(1,694)	1:43:A:GLY:H	1:45:A:MET:H	8	0.17
(1,694)	1:43:A:GLY:H	1:45:A:MET:H	9	0.17
(1,694)	1:43:A:GLY:H	1:45:A:MET:H	13	0.17
(1,694)	1:43:A:GLY:H	1:45:A:MET:H	17	0.17
(1,694)	1:43:A:GLY:H	1:45:A:MET:H	18	0.17
(1,692)	1:43:A:GLY:H	1:44:A:VAL:HB	6	0.17
(1,692)	1:43:A:GLY:H	1:44:A:VAL:HB	10	0.17
(1,692)	1:43:A:GLY:H	1:44:A:VAL:HB	12	0.17
(1,692)	1:43:A:GLY:H	1:44:A:VAL:HB	13	0.17
(1,692)	1:43:A:GLY:H	1:44:A:VAL:HB	17	0.17
(1,692)	1:43:A:GLY:H	1:44:A:VAL:HB	20	0.17
(1,663)	1:41:A:ILE:HG21	1:72:A:LEU:HG	8	0.17
(1,663)	1:41:A:ILE:HG22	1:72:A:LEU:HG	8	0.17
(1,663)	1:41:A:ILE:HG23	1:72:A:LEU:HG	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,663)	1:41:A:ILE:HG21	1:72:A:LEU:HG	11	0.17
(1,663)	1:41:A:ILE:HG22	1:72:A:LEU:HG	11	0.17
(1,663)	1:41:A:ILE:HG23	1:72:A:LEU:HG	11	0.17
(1,659)	1:41:A:ILE:HD11	1:44:A:VAL:H	15	0.17
(1,659)	1:41:A:ILE:HD12	1:44:A:VAL:H	15	0.17
(1,659)	1:41:A:ILE:HD13	1:44:A:VAL:H	15	0.17
(1,659)	1:41:A:ILE:HD11	1:44:A:VAL:H	18	0.17
(1,659)	1:41:A:ILE:HD12	1:44:A:VAL:H	18	0.17
(1,659)	1:41:A:ILE:HD13	1:44:A:VAL:H	18	0.17
(1,627)	1:40:A:HIS:HB3	1:43:A:GLY:H	13	0.17
(1,611)	1:39:A:VAL:HG11	1:78:A:THR:H	2	0.17
(1,611)	1:39:A:VAL:HG12	1:78:A:THR:H	2	0.17
(1,611)	1:39:A:VAL:HG13	1:78:A:THR:H	2	0.17
(1,611)	1:39:A:VAL:HG11	1:78:A:THR:H	8	0.17
(1,611)	1:39:A:VAL:HG12	1:78:A:THR:H	8	0.17
(1,611)	1:39:A:VAL:HG13	1:78:A:THR:H	8	0.17
(1,610)	1:39:A:VAL:HG21	1:80:A:ASP:H	15	0.17
(1,610)	1:39:A:VAL:HG22	1:80:A:ASP:H	15	0.17
(1,610)	1:39:A:VAL:HG23	1:80:A:ASP:H	15	0.17
(1,607)	1:39:A:VAL:H	1:79:A:LEU:H	8	0.17
(1,607)	1:39:A:VAL:H	1:79:A:LEU:H	19	0.17
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG21	14	0.17
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG22	14	0.17
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG23	14	0.17
(1,580)	1:38:A:GLU:HB3	1:39:A:VAL:H	8	0.17
(1,572)	1:37:A:GLY:H	1:80:A:ASP:H	8	0.17
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD21	5	0.17
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD22	5	0.17
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD23	5	0.17
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD21	7	0.17
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD22	7	0.17
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD23	7	0.17
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG21	6	0.17
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG22	6	0.17
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG23	6	0.17
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG21	11	0.17
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG22	11	0.17
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG23	11	0.17
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG21	12	0.17
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG22	12	0.17
(1,558)	1:36:A:THR:H	1:39:A:VAL:HG23	12	0.17
(1,552)	1:36:A:THR:HB	1:38:A:GLU:H	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,552)	1:36:A:THR:HB	1:38:A:GLU:H	9	0.17
(1,532)	1:35:A:VAL:H	1:35:A:VAL:HB	12	0.17
(1,516)	1:34:A:ARG:H	1:34:A:ARG:HG3	9	0.17
(1,511)	1:33:A:LEU:HD21	1:48:A:LEU:HB3	8	0.17
(1,511)	1:33:A:LEU:HD22	1:48:A:LEU:HB3	8	0.17
(1,511)	1:33:A:LEU:HD23	1:48:A:LEU:HB3	8	0.17
(1,511)	1:33:A:LEU:HD21	1:48:A:LEU:HB3	9	0.17
(1,511)	1:33:A:LEU:HD22	1:48:A:LEU:HB3	9	0.17
(1,511)	1:33:A:LEU:HD23	1:48:A:LEU:HB3	9	0.17
(1,511)	1:33:A:LEU:HD21	1:48:A:LEU:HB3	14	0.17
(1,511)	1:33:A:LEU:HD22	1:48:A:LEU:HB3	14	0.17
(1,511)	1:33:A:LEU:HD23	1:48:A:LEU:HB3	14	0.17
(1,499)	1:33:A:LEU:HD21	1:34:A:ARG:H	15	0.17
(1,499)	1:33:A:LEU:HD22	1:34:A:ARG:H	15	0.17
(1,499)	1:33:A:LEU:HD23	1:34:A:ARG:H	15	0.17
(1,484)	1:32:A:THR:HA	1:51:A:LYS:HD3	3	0.17
(1,484)	1:32:A:THR:HA	1:51:A:LYS:HD3	13	0.17
(1,484)	1:32:A:THR:HA	1:51:A:LYS:HD3	15	0.17
(1,484)	1:32:A:THR:HA	1:51:A:LYS:HD3	16	0.17
(1,483)	1:32:A:THR:H	1:34:A:ARG:H	7	0.17
(1,483)	1:32:A:THR:H	1:34:A:ARG:H	9	0.17
(1,483)	1:32:A:THR:H	1:34:A:ARG:H	12	0.17
(1,483)	1:32:A:THR:H	1:34:A:ARG:H	16	0.17
(1,483)	1:32:A:THR:H	1:34:A:ARG:H	18	0.17
(1,482)	1:32:A:THR:HA	1:34:A:ARG:H	11	0.17
(1,467)	1:31:A:VAL:H	1:32:A:THR:H	18	0.17
(1,454)	1:30:A:ASP:H	1:30:A:ASP:HB3	13	0.17
(1,454)	1:30:A:ASP:H	1:30:A:ASP:HB3	18	0.17
(1,437)	1:28:A:ASN:HB3	1:29:A:ARG:H	3	0.17
(1,437)	1:28:A:ASN:HB3	1:29:A:ARG:H	10	0.17
(1,437)	1:28:A:ASN:HB3	1:29:A:ARG:H	12	0.17
(1,437)	1:28:A:ASN:HB3	1:29:A:ARG:H	17	0.17
(1,437)	1:28:A:ASN:HB3	1:29:A:ARG:H	19	0.17
(1,434)	1:28:A:ASN:HA	1:29:A:ARG:H	14	0.17
(1,432)	1:28:A:ASN:H	1:28:A:ASN:HB2	12	0.17
(1,432)	1:28:A:ASN:H	1:28:A:ASN:HB2	20	0.17
(1,431)	1:27:A:VAL:H	1:93:A:THR:HB	3	0.17
(1,431)	1:27:A:VAL:H	1:93:A:THR:HB	4	0.17
(1,431)	1:27:A:VAL:H	1:93:A:THR:HB	5	0.17
(1,431)	1:27:A:VAL:H	1:93:A:THR:HB	19	0.17
(1,430)	1:27:A:VAL:HG21	1:92:A:PHE:H	11	0.17
(1,430)	1:27:A:VAL:HG22	1:92:A:PHE:H	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,430)	1:27:A:VAL:HG23	1:92:A:PHE:H	11	0.17
(1,430)	1:27:A:VAL:HG21	1:92:A:PHE:H	16	0.17
(1,430)	1:27:A:VAL:HG22	1:92:A:PHE:H	16	0.17
(1,430)	1:27:A:VAL:HG23	1:92:A:PHE:H	16	0.17
(1,426)	1:27:A:VAL:H	1:28:A:ASN:HB2	20	0.17
(1,415)	1:25:A:THR:H	1:93:A:THR:HB	12	0.17
(1,414)	1:25:A:THR:H	1:93:A:THR:HG21	16	0.17
(1,414)	1:25:A:THR:H	1:93:A:THR:HG22	16	0.17
(1,414)	1:25:A:THR:H	1:93:A:THR:HG23	16	0.17
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG21	2	0.17
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG22	2	0.17
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG23	2	0.17
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG21	20	0.17
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG22	20	0.17
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG23	20	0.17
(1,409)	1:25:A:THR:H	1:92:A:PHE:HB2	10	0.17
(1,387)	1:24:A:VAL:HG11	1:62:A:ALA:H	20	0.17
(1,387)	1:24:A:VAL:HG12	1:62:A:ALA:H	20	0.17
(1,387)	1:24:A:VAL:HG13	1:62:A:ALA:H	20	0.17
(1,377)	1:24:A:VAL:HA	1:30:A:ASP:HA	6	0.17
(1,377)	1:24:A:VAL:HA	1:30:A:ASP:HA	7	0.17
(1,371)	1:24:A:VAL:HG11	1:29:A:ARG:H	8	0.17
(1,371)	1:24:A:VAL:HG12	1:29:A:ARG:H	8	0.17
(1,371)	1:24:A:VAL:HG13	1:29:A:ARG:H	8	0.17
(1,369)	1:24:A:VAL:H	1:29:A:ARG:HG3	10	0.17
(1,352)	1:23:A:HIS:HB3	1:91:A:GLN:HB2	12	0.17
(1,352)	1:23:A:HIS:HB3	1:91:A:GLN:HB2	14	0.17
(1,352)	1:23:A:HIS:HB3	1:91:A:GLN:HB2	18	0.17
(1,350)	1:23:A:HIS:HB2	1:91:A:GLN:HG3	2	0.17
(1,350)	1:23:A:HIS:HB2	1:91:A:GLN:HG3	5	0.17
(1,350)	1:23:A:HIS:HB2	1:91:A:GLN:HG3	13	0.17
(1,350)	1:23:A:HIS:HB2	1:91:A:GLN:HG3	17	0.17
(1,331)	1:23:A:HIS:H	1:30:A:ASP:HB3	6	0.17
(1,331)	1:23:A:HIS:H	1:30:A:ASP:HB3	7	0.17
(1,331)	1:23:A:HIS:H	1:30:A:ASP:HB3	12	0.17
(1,329)	1:23:A:HIS:HB2	1:24:A:VAL:HA	7	0.17
(1,329)	1:23:A:HIS:HB2	1:24:A:VAL:HA	16	0.17
(1,312)	1:22:A:VAL:HG21	1:90:A:LEU:H	6	0.17
(1,312)	1:22:A:VAL:HG22	1:90:A:LEU:H	6	0.17
(1,312)	1:22:A:VAL:HG23	1:90:A:LEU:H	6	0.17
(1,294)	1:22:A:VAL:HG11	1:29:A:ARG:H	8	0.17
(1,294)	1:22:A:VAL:HG12	1:29:A:ARG:H	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,294)	1:22:A:VAL:HG13	1:29:A:ARG:H	8	0.17
(1,294)	1:22:A:VAL:HG11	1:29:A:ARG:H	17	0.17
(1,294)	1:22:A:VAL:HG12	1:29:A:ARG:H	17	0.17
(1,294)	1:22:A:VAL:HG13	1:29:A:ARG:H	17	0.17
(1,293)	1:22:A:VAL:HG21	1:24:A:VAL:H	14	0.17
(1,293)	1:22:A:VAL:HG22	1:24:A:VAL:H	14	0.17
(1,293)	1:22:A:VAL:HG23	1:24:A:VAL:H	14	0.17
(1,280)	1:21:A:SER:HB3	1:90:A:LEU:H	6	0.17
(1,275)	1:21:A:SER:H	1:32:A:THR:HB	7	0.17
(1,275)	1:21:A:SER:H	1:32:A:THR:HB	9	0.17
(1,275)	1:21:A:SER:H	1:32:A:THR:HB	10	0.17
(1,275)	1:21:A:SER:H	1:32:A:THR:HB	11	0.17
(1,275)	1:21:A:SER:H	1:32:A:THR:HB	13	0.17
(1,275)	1:21:A:SER:H	1:32:A:THR:HB	14	0.17
(1,275)	1:21:A:SER:H	1:32:A:THR:HB	16	0.17
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB1	16	0.17
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB2	16	0.17
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB3	16	0.17
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB1	16	0.17
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB2	16	0.17
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB3	16	0.17
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB1	16	0.17
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB2	16	0.17
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB3	16	0.17
(1,251)	1:20:A:LEU:HG	1:35:A:VAL:H	12	0.17
(1,251)	1:20:A:LEU:HG	1:35:A:VAL:H	14	0.17
(1,251)	1:20:A:LEU:HG	1:35:A:VAL:H	17	0.17
(1,250)	1:20:A:LEU:H	1:35:A:VAL:H	5	0.17
(1,234)	1:20:A:LEU:HB3	1:21:A:SER:H	1	0.17
(1,234)	1:20:A:LEU:HB3	1:21:A:SER:H	9	0.17
(1,234)	1:20:A:LEU:HB3	1:21:A:SER:H	11	0.17
(1,234)	1:20:A:LEU:HB3	1:21:A:SER:H	12	0.17
(1,234)	1:20:A:LEU:HB3	1:21:A:SER:H	20	0.17
(1,203)	1:19:A:GLU:HB3	1:20:A:LEU:H	12	0.17
(1,203)	1:19:A:GLU:HB3	1:20:A:LEU:H	14	0.17
(1,195)	1:19:A:GLU:H	1:19:A:GLU:HG2	3	0.17
(1,195)	1:19:A:GLU:H	1:19:A:GLU:HG2	14	0.17
(1,195)	1:19:A:GLU:H	1:19:A:GLU:HG2	16	0.17
(1,176)	1:18:A:TRP:H	1:36:A:THR:H	8	0.17
(1,169)	1:18:A:TRP:H	1:18:A:TRP:HD1	17	0.17
(1,166)	1:17:A:THR:HG21	1:18:A:TRP:H	10	0.17
(1,166)	1:17:A:THR:HG22	1:18:A:TRP:H	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,166)	1:17:A:THR:HG23	1:18:A:TRP:H	10	0.17
(1,166)	1:17:A:THR:HG21	1:18:A:TRP:H	20	0.17
(1,166)	1:17:A:THR:HG22	1:18:A:TRP:H	20	0.17
(1,166)	1:17:A:THR:HG23	1:18:A:TRP:H	20	0.17
(1,142)	1:14:A:ALA:HA	1:15:A:ASP:H	12	0.17
(1,136)	1:13:A:TYR:H	1:13:A:TYR:HB2	4	0.17
(1,127)	1:11:A:GLY:HA2	1:12:A:CYS:H	15	0.17
(1,127)	1:11:A:GLY:HA2	1:12:A:CYS:H	19	0.17
(1,117)	1:10:A:ASP:H	1:10:A:ASP:HB3	17	0.17
(1,112)	1:9:A:PRO:HG3	1:10:A:ASP:H	6	0.17
(1,103)	1:8:A:MET:HG3	1:12:A:CYS:HB3	10	0.17
(1,102)	1:8:A:MET:HB3	1:12:A:CYS:H	9	0.17
(1,102)	1:8:A:MET:HB3	1:12:A:CYS:H	13	0.17
(1,87)	1:7:A:ARG:HG3	1:10:A:ASP:H	10	0.17
(1,86)	1:7:A:ARG:HA	1:10:A:ASP:H	10	0.17
(1,86)	1:7:A:ARG:HA	1:10:A:ASP:H	18	0.17
(1,85)	1:7:A:ARG:HD3	1:8:A:MET:H	8	0.17
(1,84)	1:7:A:ARG:H	1:8:A:MET:H	12	0.17
(1,62)	1:6:A:ILE:HG21	1:7:A:ARG:H	16	0.17
(1,62)	1:6:A:ILE:HG22	1:7:A:ARG:H	16	0.17
(1,62)	1:6:A:ILE:HG23	1:7:A:ARG:H	16	0.17
(1,47)	1:5:A:GLY:H	1:6:A:ILE:H	1	0.17
(1,45)	1:4:A:ASP:HB3	1:6:A:ILE:H	5	0.17
(1,44)	1:4:A:ASP:HA	1:6:A:ILE:H	14	0.17
(1,20)	1:2:A:ALA:HB1	1:4:A:ASP:H	9	0.17
(1,20)	1:2:A:ALA:HB2	1:4:A:ASP:H	9	0.17
(1,20)	1:2:A:ALA:HB3	1:4:A:ASP:H	9	0.17
(1,19)	1:2:A:ALA:HB1	1:3:A:LEU:H	2	0.17
(1,19)	1:2:A:ALA:HB2	1:3:A:LEU:H	2	0.17
(1,19)	1:2:A:ALA:HB3	1:3:A:LEU:H	2	0.17
(1,19)	1:2:A:ALA:HB1	1:3:A:LEU:H	13	0.17
(1,19)	1:2:A:ALA:HB2	1:3:A:LEU:H	13	0.17
(1,19)	1:2:A:ALA:HB3	1:3:A:LEU:H	13	0.17
(3,16)	1:42:A:GLY:O	1:46:A:LEU:H	12	0.16
(3,13)	1:92:A:PHE:O	1:64:A:TRP:H	13	0.16
(3,13)	1:92:A:PHE:O	1:64:A:TRP:H	15	0.16
(3,13)	1:92:A:PHE:O	1:64:A:TRP:H	20	0.16
(2,21)	1:39:A:VAL:O	1:43:A:GLY:N	3	0.16
(2,17)	1:21:A:SER:O	1:91:A:GLN:H	3	0.16
(2,13)	1:92:A:PHE:O	1:64:A:TRP:N	1	0.16
(2,13)	1:92:A:PHE:O	1:64:A:TRP:N	6	0.16
(2,13)	1:92:A:PHE:O	1:64:A:TRP:N	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,13)	1:92:A:PHE:O	1:64:A:TRP:N	9	0.16
(2,13)	1:92:A:PHE:O	1:64:A:TRP:N	19	0.16
(1,1382)	1:91:A:GLN:HG2	1:91:A:GLN:HE21	10	0.16
(1,1382)	1:91:A:GLN:HG2	1:91:A:GLN:HE21	16	0.16
(1,1381)	1:91:A:GLN:H	1:91:A:GLN:HG2	4	0.16
(1,1381)	1:91:A:GLN:H	1:91:A:GLN:HG2	20	0.16
(1,1355)	1:90:A:LEU:H	1:90:A:LEU:HD21	10	0.16
(1,1355)	1:90:A:LEU:H	1:90:A:LEU:HD22	10	0.16
(1,1355)	1:90:A:LEU:H	1:90:A:LEU:HD23	10	0.16
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD11	8	0.16
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD12	8	0.16
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD13	8	0.16
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD11	16	0.16
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD12	16	0.16
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD13	16	0.16
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG21	5	0.16
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG22	5	0.16
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG23	5	0.16
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG21	3	0.16
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG22	3	0.16
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG23	3	0.16
(1,1246)	1:81:A:LYS:HE3	1:82:A:TYR:H	9	0.16
(1,1246)	1:81:A:LYS:HE3	1:82:A:TYR:H	12	0.16
(1,1218)	1:80:A:ASP:HB2	1:82:A:TYR:H	6	0.16
(1,1218)	1:80:A:ASP:HB2	1:82:A:TYR:H	7	0.16
(1,1218)	1:80:A:ASP:HB2	1:82:A:TYR:H	10	0.16
(1,1218)	1:80:A:ASP:HB2	1:82:A:TYR:H	14	0.16
(1,1218)	1:80:A:ASP:HB2	1:82:A:TYR:H	17	0.16
(1,1216)	1:80:A:ASP:H	1:81:A:LYS:HD2	2	0.16
(1,1216)	1:80:A:ASP:H	1:81:A:LYS:HD2	4	0.16
(1,1215)	1:80:A:ASP:HB2	1:81:A:LYS:H	3	0.16
(1,1215)	1:80:A:ASP:HB2	1:81:A:LYS:H	6	0.16
(1,1215)	1:80:A:ASP:HB2	1:81:A:LYS:H	12	0.16
(1,1215)	1:80:A:ASP:HB2	1:81:A:LYS:H	13	0.16
(1,1197)	1:79:A:LEU:HB3	1:80:A:ASP:H	7	0.16
(1,1197)	1:79:A:LEU:HB3	1:80:A:ASP:H	17	0.16
(1,1193)	1:79:A:LEU:HA	1:80:A:ASP:H	8	0.16
(1,1187)	1:79:A:LEU:H	1:79:A:LEU:HD21	2	0.16
(1,1187)	1:79:A:LEU:H	1:79:A:LEU:HD22	2	0.16
(1,1187)	1:79:A:LEU:H	1:79:A:LEU:HD23	2	0.16
(1,1187)	1:79:A:LEU:H	1:79:A:LEU:HD21	16	0.16
(1,1187)	1:79:A:LEU:H	1:79:A:LEU:HD22	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1187)	1:79:A:LEU:H	1:79:A:LEU:HD23	16	0.16
(1,1176)	1:78:A:THR:H	1:81:A:LYS:HA	18	0.16
(1,1169)	1:78:A:THR:HB	1:79:A:LEU:H	15	0.16
(1,1164)	1:78:A:THR:HG21	1:78:A:THR:H	3	0.16
(1,1164)	1:78:A:THR:HG22	1:78:A:THR:H	3	0.16
(1,1164)	1:78:A:THR:HG23	1:78:A:THR:H	3	0.16
(1,1164)	1:78:A:THR:HG21	1:78:A:THR:H	8	0.16
(1,1164)	1:78:A:THR:HG22	1:78:A:THR:H	8	0.16
(1,1164)	1:78:A:THR:HG23	1:78:A:THR:H	8	0.16
(1,1161)	1:77:A:TRP:H	1:81:A:LYS:HD3	12	0.16
(1,1153)	1:76:A:HIS:HB3	1:77:A:TRP:H	2	0.16
(1,1153)	1:76:A:HIS:HB3	1:77:A:TRP:H	17	0.16
(1,1148)	1:75:A:THR:HG21	1:77:A:TRP:H	9	0.16
(1,1148)	1:75:A:THR:HG22	1:77:A:TRP:H	9	0.16
(1,1148)	1:75:A:THR:HG23	1:77:A:TRP:H	9	0.16
(1,1148)	1:75:A:THR:HG21	1:77:A:TRP:H	14	0.16
(1,1148)	1:75:A:THR:HG22	1:77:A:TRP:H	14	0.16
(1,1148)	1:75:A:THR:HG23	1:77:A:TRP:H	14	0.16
(1,1148)	1:75:A:THR:HG21	1:77:A:TRP:H	17	0.16
(1,1148)	1:75:A:THR:HG22	1:77:A:TRP:H	17	0.16
(1,1148)	1:75:A:THR:HG23	1:77:A:TRP:H	17	0.16
(1,1141)	1:74:A:LYS:HE3	1:78:A:THR:H	6	0.16
(1,1141)	1:74:A:LYS:HE3	1:78:A:THR:H	20	0.16
(1,1138)	1:74:A:LYS:HD3	1:77:A:TRP:H	3	0.16
(1,1138)	1:74:A:LYS:HD3	1:77:A:TRP:H	12	0.16
(1,1138)	1:74:A:LYS:HD3	1:77:A:TRP:H	14	0.16
(1,1134)	1:74:A:LYS:HG2	1:75:A:THR:H	2	0.16
(1,1134)	1:74:A:LYS:HG2	1:75:A:THR:H	9	0.16
(1,1134)	1:74:A:LYS:HG2	1:75:A:THR:H	10	0.16
(1,1134)	1:74:A:LYS:HG2	1:75:A:THR:H	11	0.16
(1,1134)	1:74:A:LYS:HG2	1:75:A:THR:H	19	0.16
(1,1128)	1:74:A:LYS:HE3	1:74:A:LYS:HB3	6	0.16
(1,1113)	1:74:A:LYS:HA	1:74:A:LYS:HE3	2	0.16
(1,1113)	1:74:A:LYS:HA	1:74:A:LYS:HE3	3	0.16
(1,1113)	1:74:A:LYS:HA	1:74:A:LYS:HE3	8	0.16
(1,1113)	1:74:A:LYS:HA	1:74:A:LYS:HE3	12	0.16
(1,1113)	1:74:A:LYS:HA	1:74:A:LYS:HE3	15	0.16
(1,1113)	1:74:A:LYS:HA	1:74:A:LYS:HE3	18	0.16
(1,1112)	1:74:A:LYS:HA	1:74:A:LYS:HE2	7	0.16
(1,1112)	1:74:A:LYS:HA	1:74:A:LYS:HE2	11	0.16
(1,1108)	1:73:A:LEU:HA	1:74:A:LYS:H	1	0.16
(1,1105)	1:73:A:LEU:H	1:73:A:LEU:HB3	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1105)	1:73:A:LEU:H	1:73:A:LEU:HB3	8	0.16
(1,1105)	1:73:A:LEU:H	1:73:A:LEU:HB3	10	0.16
(1,1105)	1:73:A:LEU:H	1:73:A:LEU:HB3	16	0.16
(1,1081)	1:71:A:TRP:HB2	1:72:A:LEU:H	9	0.16
(1,1081)	1:71:A:TRP:HB2	1:72:A:LEU:H	19	0.16
(1,1076)	1:71:A:TRP:H	1:71:A:TRP:HB3	11	0.16
(1,1072)	1:70:A:THR:H	1:71:A:TRP:H	18	0.16
(1,1064)	1:69:A:ARG:HB2	1:70:A:THR:H	13	0.16
(1,1061)	1:69:A:ARG:HD3	1:70:A:THR:HB	5	0.16
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD21	15	0.16
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD22	15	0.16
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD23	15	0.16
(1,1049)	1:67:A:LYS:HB3	1:69:A:ARG:HA	8	0.16
(1,1038)	1:67:A:LYS:H	1:67:A:LYS:HG3	15	0.16
(1,1038)	1:67:A:LYS:H	1:67:A:LYS:HG3	20	0.16
(1,1021)	1:66:A:GLU:H	1:66:A:GLU:HG2	4	0.16
(1,1021)	1:66:A:GLU:H	1:66:A:GLU:HG2	14	0.16
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD21	20	0.16
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD22	20	0.16
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD23	20	0.16
(1,997)	1:65:A:TRP:HB3	1:66:A:GLU:H	6	0.16
(1,997)	1:65:A:TRP:HB3	1:66:A:GLU:H	20	0.16
(1,992)	1:64:A:TRP:H	1:93:A:THR:HG1	14	0.16
(1,988)	1:64:A:TRP:H	1:92:A:PHE:HB3	20	0.16
(1,983)	1:64:A:TRP:HB2	1:65:A:TRP:H	18	0.16
(1,981)	1:64:A:TRP:H	1:64:A:TRP:HB3	7	0.16
(1,978)	1:63:A:LEU:HA	1:93:A:THR:H	10	0.16
(1,978)	1:63:A:LEU:HA	1:93:A:THR:H	19	0.16
(1,976)	1:63:A:LEU:HG	1:93:A:THR:H	1	0.16
(1,976)	1:63:A:LEU:HG	1:93:A:THR:H	5	0.16
(1,976)	1:63:A:LEU:HG	1:93:A:THR:H	7	0.16
(1,974)	1:63:A:LEU:HA	1:92:A:PHE:H	8	0.16
(1,972)	1:63:A:LEU:HD11	1:91:A:GLN:H	2	0.16
(1,972)	1:63:A:LEU:HD12	1:91:A:GLN:H	2	0.16
(1,972)	1:63:A:LEU:HD13	1:91:A:GLN:H	2	0.16
(1,972)	1:63:A:LEU:HD11	1:91:A:GLN:H	6	0.16
(1,972)	1:63:A:LEU:HD12	1:91:A:GLN:H	6	0.16
(1,972)	1:63:A:LEU:HD13	1:91:A:GLN:H	6	0.16
(1,972)	1:63:A:LEU:HD11	1:91:A:GLN:H	11	0.16
(1,972)	1:63:A:LEU:HD12	1:91:A:GLN:H	11	0.16
(1,972)	1:63:A:LEU:HD13	1:91:A:GLN:H	11	0.16
(1,972)	1:63:A:LEU:HD11	1:91:A:GLN:H	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,972)	1:63:A:LEU:HD12	1:91:A:GLN:H	16	0.16
(1,972)	1:63:A:LEU:HD13	1:91:A:GLN:H	16	0.16
(1,968)	1:63:A:LEU:HG	1:90:A:LEU:HA	9	0.16
(1,968)	1:63:A:LEU:HG	1:90:A:LEU:HA	13	0.16
(1,968)	1:63:A:LEU:HG	1:90:A:LEU:HA	17	0.16
(1,959)	1:63:A:LEU:H	1:64:A:TRP:H	19	0.16
(1,950)	1:63:A:LEU:H	1:63:A:LEU:HG	4	0.16
(1,950)	1:63:A:LEU:H	1:63:A:LEU:HG	10	0.16
(1,950)	1:63:A:LEU:H	1:63:A:LEU:HG	12	0.16
(1,946)	1:62:A:ALA:H	1:94:A:PRO:HA	11	0.16
(1,945)	1:62:A:ALA:HB1	1:93:A:THR:HA	1	0.16
(1,945)	1:62:A:ALA:HB2	1:93:A:THR:HA	1	0.16
(1,945)	1:62:A:ALA:HB3	1:93:A:THR:HA	1	0.16
(1,945)	1:62:A:ALA:HB1	1:93:A:THR:HA	17	0.16
(1,945)	1:62:A:ALA:HB2	1:93:A:THR:HA	17	0.16
(1,945)	1:62:A:ALA:HB3	1:93:A:THR:HA	17	0.16
(1,945)	1:62:A:ALA:HB1	1:93:A:THR:HA	19	0.16
(1,945)	1:62:A:ALA:HB2	1:93:A:THR:HA	19	0.16
(1,945)	1:62:A:ALA:HB3	1:93:A:THR:HA	19	0.16
(1,945)	1:62:A:ALA:HB1	1:93:A:THR:HA	20	0.16
(1,945)	1:62:A:ALA:HB2	1:93:A:THR:HA	20	0.16
(1,945)	1:62:A:ALA:HB3	1:93:A:THR:HA	20	0.16
(1,930)	1:61:A:HIS:HB2	1:63:A:LEU:H	20	0.16
(1,911)	1:58:A:TRP:HB3	1:61:A:HIS:H	19	0.16
(1,904)	1:58:A:TRP:H	1:58:A:TRP:HB3	17	0.16
(1,903)	1:57:A:ASP:HB2	1:61:A:HIS:H	2	0.16
(1,903)	1:57:A:ASP:HB2	1:61:A:HIS:H	12	0.16
(1,890)	1:56:A:LYS:HA	1:57:A:ASP:HB2	5	0.16
(1,858)	1:51:A:LYS:H	1:51:A:LYS:HD3	10	0.16
(1,858)	1:51:A:LYS:H	1:51:A:LYS:HD3	16	0.16
(1,858)	1:51:A:LYS:H	1:51:A:LYS:HD3	18	0.16
(1,858)	1:51:A:LYS:H	1:51:A:LYS:HD3	19	0.16
(1,858)	1:51:A:LYS:H	1:51:A:LYS:HD3	20	0.16
(1,844)	1:50:A:GLU:H	1:50:A:GLU:HG2	3	0.16
(1,844)	1:50:A:GLU:H	1:50:A:GLU:HG2	9	0.16
(1,844)	1:50:A:GLU:H	1:50:A:GLU:HG2	10	0.16
(1,844)	1:50:A:GLU:H	1:50:A:GLU:HG2	11	0.16
(1,844)	1:50:A:GLU:H	1:50:A:GLU:HG2	13	0.16
(1,844)	1:50:A:GLU:H	1:50:A:GLU:HG2	17	0.16
(1,841)	1:50:A:GLU:HA	1:50:A:GLU:HG3	17	0.16
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD21	4	0.16
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD22	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD23	4	0.16
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD21	4	0.16
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD22	4	0.16
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD23	4	0.16
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD21	4	0.16
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD22	4	0.16
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD23	4	0.16
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD21	5	0.16
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD22	5	0.16
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD23	5	0.16
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD21	5	0.16
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD22	5	0.16
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD23	5	0.16
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD21	5	0.16
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD22	5	0.16
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD23	5	0.16
(1,821)	1:48:A:LEU:HD21	1:63:A:LEU:H	9	0.16
(1,821)	1:48:A:LEU:HD22	1:63:A:LEU:H	9	0.16
(1,821)	1:48:A:LEU:HD23	1:63:A:LEU:H	9	0.16
(1,821)	1:48:A:LEU:HD21	1:63:A:LEU:H	12	0.16
(1,821)	1:48:A:LEU:HD22	1:63:A:LEU:H	12	0.16
(1,821)	1:48:A:LEU:HD23	1:63:A:LEU:H	12	0.16
(1,821)	1:48:A:LEU:HD21	1:63:A:LEU:H	19	0.16
(1,821)	1:48:A:LEU:HD22	1:63:A:LEU:H	19	0.16
(1,821)	1:48:A:LEU:HD23	1:63:A:LEU:H	19	0.16
(1,820)	1:48:A:LEU:H	1:52:A:LEU:H	18	0.16
(1,818)	1:48:A:LEU:HD21	1:52:A:LEU:H	7	0.16
(1,818)	1:48:A:LEU:HD22	1:52:A:LEU:H	7	0.16
(1,818)	1:48:A:LEU:HD23	1:52:A:LEU:H	7	0.16
(1,813)	1:48:A:LEU:H	1:51:A:LYS:H	1	0.16
(1,813)	1:48:A:LEU:H	1:51:A:LYS:H	11	0.16
(1,812)	1:48:A:LEU:HA	1:51:A:LYS:HB3	1	0.16
(1,812)	1:48:A:LEU:HA	1:51:A:LYS:HB3	6	0.16
(1,812)	1:48:A:LEU:HA	1:51:A:LYS:HB3	13	0.16
(1,812)	1:48:A:LEU:HA	1:51:A:LYS:HB3	19	0.16
(1,805)	1:48:A:LEU:HG	1:49:A:VAL:H	12	0.16
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG21	9	0.16
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG22	9	0.16
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG23	9	0.16
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG21	10	0.16
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG22	10	0.16
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG23	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG21	18	0.16
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG22	18	0.16
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG23	18	0.16
(1,782)	1:47:A:LYS:HB2	1:48:A:LEU:H	1	0.16
(1,782)	1:47:A:LYS:HB2	1:48:A:LEU:H	14	0.16
(1,782)	1:47:A:LYS:HB2	1:48:A:LEU:H	19	0.16
(1,773)	1:47:A:LYS:H	1:47:A:LYS:HD3	4	0.16
(1,773)	1:47:A:LYS:H	1:47:A:LYS:HD3	6	0.16
(1,773)	1:47:A:LYS:H	1:47:A:LYS:HD3	7	0.16
(1,773)	1:47:A:LYS:H	1:47:A:LYS:HD3	9	0.16
(1,773)	1:47:A:LYS:H	1:47:A:LYS:HD3	11	0.16
(1,773)	1:47:A:LYS:H	1:47:A:LYS:HD3	13	0.16
(1,773)	1:47:A:LYS:H	1:47:A:LYS:HD3	19	0.16
(1,766)	1:46:A:LEU:HA	1:50:A:GLU:H	7	0.16
(1,766)	1:46:A:LEU:HA	1:50:A:GLU:H	16	0.16
(1,766)	1:46:A:LEU:HA	1:50:A:GLU:H	17	0.16
(1,764)	1:46:A:LEU:HA	1:49:A:VAL:H	1	0.16
(1,764)	1:46:A:LEU:HA	1:49:A:VAL:H	2	0.16
(1,764)	1:46:A:LEU:HA	1:49:A:VAL:H	13	0.16
(1,764)	1:46:A:LEU:HA	1:49:A:VAL:H	14	0.16
(1,760)	1:46:A:LEU:H	1:48:A:LEU:H	15	0.16
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD21	1	0.16
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD22	1	0.16
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD23	1	0.16
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD21	4	0.16
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD22	4	0.16
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD23	4	0.16
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD21	15	0.16
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD22	15	0.16
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD23	15	0.16
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG21	3	0.16
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG22	3	0.16
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG23	3	0.16
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG21	18	0.16
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG22	18	0.16
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG23	18	0.16
(1,737)	1:45:A:MET:HB3	1:48:A:LEU:H	14	0.16
(1,737)	1:45:A:MET:HB3	1:48:A:LEU:H	17	0.16
(1,737)	1:45:A:MET:HB3	1:48:A:LEU:H	20	0.16
(1,719)	1:44:A:VAL:HG11	1:90:A:LEU:H	12	0.16
(1,719)	1:44:A:VAL:HG12	1:90:A:LEU:H	12	0.16
(1,719)	1:44:A:VAL:HG13	1:90:A:LEU:H	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,719)	1:44:A:VAL:HG11	1:90:A:LEU:H	14	0.16
(1,719)	1:44:A:VAL:HG12	1:90:A:LEU:H	14	0.16
(1,719)	1:44:A:VAL:HG13	1:90:A:LEU:H	14	0.16
(1,719)	1:44:A:VAL:HG11	1:90:A:LEU:H	17	0.16
(1,719)	1:44:A:VAL:HG12	1:90:A:LEU:H	17	0.16
(1,719)	1:44:A:VAL:HG13	1:90:A:LEU:H	17	0.16
(1,719)	1:44:A:VAL:HG11	1:90:A:LEU:H	18	0.16
(1,719)	1:44:A:VAL:HG12	1:90:A:LEU:H	18	0.16
(1,719)	1:44:A:VAL:HG13	1:90:A:LEU:H	18	0.16
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG11	11	0.16
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG12	11	0.16
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG13	11	0.16
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG11	15	0.16
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG12	15	0.16
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG13	15	0.16
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG11	18	0.16
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG12	18	0.16
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG13	18	0.16
(1,694)	1:43:A:GLY:H	1:45:A:MET:H	1	0.16
(1,694)	1:43:A:GLY:H	1:45:A:MET:H	5	0.16
(1,694)	1:43:A:GLY:H	1:45:A:MET:H	10	0.16
(1,694)	1:43:A:GLY:H	1:45:A:MET:H	15	0.16
(1,692)	1:43:A:GLY:H	1:44:A:VAL:HB	7	0.16
(1,692)	1:43:A:GLY:H	1:44:A:VAL:HB	11	0.16
(1,692)	1:43:A:GLY:H	1:44:A:VAL:HB	14	0.16
(1,692)	1:43:A:GLY:H	1:44:A:VAL:HB	19	0.16
(1,684)	1:42:A:GLY:HA3	1:75:A:THR:HB	3	0.16
(1,683)	1:42:A:GLY:H	1:74:A:LYS:HE3	3	0.16
(1,683)	1:42:A:GLY:H	1:74:A:LYS:HE3	6	0.16
(1,683)	1:42:A:GLY:H	1:74:A:LYS:HE3	18	0.16
(1,676)	1:41:A:ILE:HG13	1:78:A:THR:H	15	0.16
(1,673)	1:41:A:ILE:H	1:77:A:TRP:H	20	0.16
(1,671)	1:41:A:ILE:HD11	1:75:A:THR:HA	2	0.16
(1,671)	1:41:A:ILE:HD12	1:75:A:THR:HA	2	0.16
(1,671)	1:41:A:ILE:HD13	1:75:A:THR:HA	2	0.16
(1,663)	1:41:A:ILE:HG21	1:72:A:LEU:HG	5	0.16
(1,663)	1:41:A:ILE:HG22	1:72:A:LEU:HG	5	0.16
(1,663)	1:41:A:ILE:HG23	1:72:A:LEU:HG	5	0.16
(1,663)	1:41:A:ILE:HG21	1:72:A:LEU:HG	12	0.16
(1,663)	1:41:A:ILE:HG22	1:72:A:LEU:HG	12	0.16
(1,663)	1:41:A:ILE:HG23	1:72:A:LEU:HG	12	0.16
(1,663)	1:41:A:ILE:HG21	1:72:A:LEU:HG	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,663)	1:41:A:ILE:HG22	1:72:A:LEU:HG	15	0.16
(1,663)	1:41:A:ILE:HG23	1:72:A:LEU:HG	15	0.16
(1,663)	1:41:A:ILE:HG21	1:72:A:LEU:HG	16	0.16
(1,663)	1:41:A:ILE:HG22	1:72:A:LEU:HG	16	0.16
(1,663)	1:41:A:ILE:HG23	1:72:A:LEU:HG	16	0.16
(1,663)	1:41:A:ILE:HG21	1:72:A:LEU:HG	19	0.16
(1,663)	1:41:A:ILE:HG22	1:72:A:LEU:HG	19	0.16
(1,663)	1:41:A:ILE:HG23	1:72:A:LEU:HG	19	0.16
(1,659)	1:41:A:ILE:HD11	1:44:A:VAL:H	6	0.16
(1,659)	1:41:A:ILE:HD12	1:44:A:VAL:H	6	0.16
(1,659)	1:41:A:ILE:HD13	1:44:A:VAL:H	6	0.16
(1,659)	1:41:A:ILE:HD11	1:44:A:VAL:H	13	0.16
(1,659)	1:41:A:ILE:HD12	1:44:A:VAL:H	13	0.16
(1,659)	1:41:A:ILE:HD13	1:44:A:VAL:H	13	0.16
(1,659)	1:41:A:ILE:HD11	1:44:A:VAL:H	19	0.16
(1,659)	1:41:A:ILE:HD12	1:44:A:VAL:H	19	0.16
(1,659)	1:41:A:ILE:HD13	1:44:A:VAL:H	19	0.16
(1,640)	1:41:A:ILE:H	1:41:A:ILE:HG12	18	0.16
(1,610)	1:39:A:VAL:HG21	1:80:A:ASP:H	9	0.16
(1,610)	1:39:A:VAL:HG22	1:80:A:ASP:H	9	0.16
(1,610)	1:39:A:VAL:HG23	1:80:A:ASP:H	9	0.16
(1,602)	1:39:A:VAL:HG21	1:43:A:GLY:H	12	0.16
(1,602)	1:39:A:VAL:HG22	1:43:A:GLY:H	12	0.16
(1,602)	1:39:A:VAL:HG23	1:43:A:GLY:H	12	0.16
(1,588)	1:38:A:GLU:HA	1:80:A:ASP:H	9	0.16
(1,588)	1:38:A:GLU:HA	1:80:A:ASP:H	12	0.16
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG21	7	0.16
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG22	7	0.16
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG23	7	0.16
(1,580)	1:38:A:GLU:HB3	1:39:A:VAL:H	12	0.16
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD21	4	0.16
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD22	4	0.16
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD23	4	0.16
(1,561)	1:37:A:GLY:H	1:38:A:GLU:HG3	16	0.16
(1,552)	1:36:A:THR:HB	1:38:A:GLU:H	2	0.16
(1,552)	1:36:A:THR:HB	1:38:A:GLU:H	3	0.16
(1,552)	1:36:A:THR:HB	1:38:A:GLU:H	15	0.16
(1,527)	1:34:A:ARG:H	1:51:A:LYS:HD3	19	0.16
(1,523)	1:34:A:ARG:HB3	1:35:A:VAL:H	9	0.16
(1,523)	1:34:A:ARG:HB3	1:35:A:VAL:H	18	0.16
(1,516)	1:34:A:ARG:H	1:34:A:ARG:HG3	18	0.16
(1,515)	1:34:A:ARG:H	1:34:A:ARG:HB3	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:33:A:LEU:HD21	1:48:A:LEU:HB3	1	0.16
(1,511)	1:33:A:LEU:HD22	1:48:A:LEU:HB3	1	0.16
(1,511)	1:33:A:LEU:HD23	1:48:A:LEU:HB3	1	0.16
(1,511)	1:33:A:LEU:HD21	1:48:A:LEU:HB3	4	0.16
(1,511)	1:33:A:LEU:HD22	1:48:A:LEU:HB3	4	0.16
(1,511)	1:33:A:LEU:HD23	1:48:A:LEU:HB3	4	0.16
(1,511)	1:33:A:LEU:HD21	1:48:A:LEU:HB3	6	0.16
(1,511)	1:33:A:LEU:HD22	1:48:A:LEU:HB3	6	0.16
(1,511)	1:33:A:LEU:HD23	1:48:A:LEU:HB3	6	0.16
(1,499)	1:33:A:LEU:HD21	1:34:A:ARG:H	7	0.16
(1,499)	1:33:A:LEU:HD22	1:34:A:ARG:H	7	0.16
(1,499)	1:33:A:LEU:HD23	1:34:A:ARG:H	7	0.16
(1,484)	1:32:A:THR:HA	1:51:A:LYS:HD3	9	0.16
(1,482)	1:32:A:THR:HA	1:34:A:ARG:H	1	0.16
(1,482)	1:32:A:THR:HA	1:34:A:ARG:H	2	0.16
(1,482)	1:32:A:THR:HA	1:34:A:ARG:H	3	0.16
(1,482)	1:32:A:THR:HA	1:34:A:ARG:H	4	0.16
(1,482)	1:32:A:THR:HA	1:34:A:ARG:H	5	0.16
(1,482)	1:32:A:THR:HA	1:34:A:ARG:H	8	0.16
(1,482)	1:32:A:THR:HA	1:34:A:ARG:H	13	0.16
(1,453)	1:29:A:ARG:HB2	1:31:A:VAL:HA	8	0.16
(1,453)	1:29:A:ARG:HB2	1:31:A:VAL:HA	12	0.16
(1,437)	1:28:A:ASN:HB3	1:29:A:ARG:H	2	0.16
(1,432)	1:28:A:ASN:H	1:28:A:ASN:HB2	17	0.16
(1,432)	1:28:A:ASN:H	1:28:A:ASN:HB2	19	0.16
(1,431)	1:27:A:VAL:H	1:93:A:THR:HB	10	0.16
(1,431)	1:27:A:VAL:H	1:93:A:THR:HB	17	0.16
(1,430)	1:27:A:VAL:HG21	1:92:A:PHE:H	3	0.16
(1,430)	1:27:A:VAL:HG22	1:92:A:PHE:H	3	0.16
(1,430)	1:27:A:VAL:HG23	1:92:A:PHE:H	3	0.16
(1,426)	1:27:A:VAL:H	1:28:A:ASN:HB2	8	0.16
(1,426)	1:27:A:VAL:H	1:28:A:ASN:HB2	9	0.16
(1,426)	1:27:A:VAL:H	1:28:A:ASN:HB2	14	0.16
(1,426)	1:27:A:VAL:H	1:28:A:ASN:HB2	18	0.16
(1,426)	1:27:A:VAL:H	1:28:A:ASN:HB2	19	0.16
(1,414)	1:25:A:THR:H	1:93:A:THR:HG21	8	0.16
(1,414)	1:25:A:THR:H	1:93:A:THR:HG22	8	0.16
(1,414)	1:25:A:THR:H	1:93:A:THR:HG23	8	0.16
(1,414)	1:25:A:THR:H	1:93:A:THR:HG21	19	0.16
(1,414)	1:25:A:THR:H	1:93:A:THR:HG22	19	0.16
(1,414)	1:25:A:THR:H	1:93:A:THR:HG23	19	0.16
(1,392)	1:24:A:VAL:HB	1:92:A:PHE:H	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:24:A:VAL:HG11	1:62:A:ALA:H	13	0.16
(1,387)	1:24:A:VAL:HG12	1:62:A:ALA:H	13	0.16
(1,387)	1:24:A:VAL:HG13	1:62:A:ALA:H	13	0.16
(1,387)	1:24:A:VAL:HG11	1:62:A:ALA:H	16	0.16
(1,387)	1:24:A:VAL:HG12	1:62:A:ALA:H	16	0.16
(1,387)	1:24:A:VAL:HG13	1:62:A:ALA:H	16	0.16
(1,387)	1:24:A:VAL:HG11	1:62:A:ALA:H	19	0.16
(1,387)	1:24:A:VAL:HG12	1:62:A:ALA:H	19	0.16
(1,387)	1:24:A:VAL:HG13	1:62:A:ALA:H	19	0.16
(1,383)	1:24:A:VAL:HA	1:31:A:VAL:H	14	0.16
(1,378)	1:24:A:VAL:HA	1:30:A:ASP:HB3	18	0.16
(1,377)	1:24:A:VAL:HA	1:30:A:ASP:HA	2	0.16
(1,377)	1:24:A:VAL:HA	1:30:A:ASP:HA	15	0.16
(1,377)	1:24:A:VAL:HA	1:30:A:ASP:HA	20	0.16
(1,350)	1:23:A:HIS:HB2	1:91:A:GLN:HG3	4	0.16
(1,350)	1:23:A:HIS:HB2	1:91:A:GLN:HG3	6	0.16
(1,350)	1:23:A:HIS:HB2	1:91:A:GLN:HG3	12	0.16
(1,350)	1:23:A:HIS:HB2	1:91:A:GLN:HG3	20	0.16
(1,331)	1:23:A:HIS:H	1:30:A:ASP:HB3	1	0.16
(1,331)	1:23:A:HIS:H	1:30:A:ASP:HB3	3	0.16
(1,331)	1:23:A:HIS:H	1:30:A:ASP:HB3	10	0.16
(1,331)	1:23:A:HIS:H	1:30:A:ASP:HB3	15	0.16
(1,331)	1:23:A:HIS:H	1:30:A:ASP:HB3	16	0.16
(1,323)	1:23:A:HIS:HB2	1:24:A:VAL:H	1	0.16
(1,323)	1:23:A:HIS:HB2	1:24:A:VAL:H	9	0.16
(1,323)	1:23:A:HIS:HB2	1:24:A:VAL:H	10	0.16
(1,323)	1:23:A:HIS:HB2	1:24:A:VAL:H	18	0.16
(1,323)	1:23:A:HIS:HB2	1:24:A:VAL:H	20	0.16
(1,312)	1:22:A:VAL:HG21	1:90:A:LEU:H	1	0.16
(1,312)	1:22:A:VAL:HG22	1:90:A:LEU:H	1	0.16
(1,312)	1:22:A:VAL:HG23	1:90:A:LEU:H	1	0.16
(1,299)	1:22:A:VAL:H	1:32:A:THR:HB	20	0.16
(1,294)	1:22:A:VAL:HG11	1:29:A:ARG:H	14	0.16
(1,294)	1:22:A:VAL:HG12	1:29:A:ARG:H	14	0.16
(1,294)	1:22:A:VAL:HG13	1:29:A:ARG:H	14	0.16
(1,294)	1:22:A:VAL:HG11	1:29:A:ARG:H	20	0.16
(1,294)	1:22:A:VAL:HG12	1:29:A:ARG:H	20	0.16
(1,294)	1:22:A:VAL:HG13	1:29:A:ARG:H	20	0.16
(1,276)	1:21:A:SER:H	1:32:A:THR:HG21	15	0.16
(1,276)	1:21:A:SER:H	1:32:A:THR:HG22	15	0.16
(1,276)	1:21:A:SER:H	1:32:A:THR:HG23	15	0.16
(1,275)	1:21:A:SER:H	1:32:A:THR:HB	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,275)	1:21:A:SER:H	1:32:A:THR:HB	6	0.16
(1,275)	1:21:A:SER:H	1:32:A:THR:HB	17	0.16
(1,275)	1:21:A:SER:H	1:32:A:THR:HB	18	0.16
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG21	11	0.16
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG22	11	0.16
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG23	11	0.16
(1,251)	1:20:A:LEU:HG	1:35:A:VAL:H	16	0.16
(1,251)	1:20:A:LEU:HG	1:35:A:VAL:H	18	0.16
(1,250)	1:20:A:LEU:H	1:35:A:VAL:H	8	0.16
(1,249)	1:20:A:LEU:HB2	1:34:A:ARG:H	7	0.16
(1,249)	1:20:A:LEU:HB2	1:34:A:ARG:H	13	0.16
(1,244)	1:20:A:LEU:HD21	1:33:A:LEU:HA	7	0.16
(1,244)	1:20:A:LEU:HD22	1:33:A:LEU:HA	7	0.16
(1,244)	1:20:A:LEU:HD23	1:33:A:LEU:HA	7	0.16
(1,242)	1:20:A:LEU:HB3	1:33:A:LEU:H	5	0.16
(1,234)	1:20:A:LEU:HB3	1:21:A:SER:H	3	0.16
(1,234)	1:20:A:LEU:HB3	1:21:A:SER:H	5	0.16
(1,234)	1:20:A:LEU:HB3	1:21:A:SER:H	7	0.16
(1,234)	1:20:A:LEU:HB3	1:21:A:SER:H	15	0.16
(1,234)	1:20:A:LEU:HB3	1:21:A:SER:H	16	0.16
(1,234)	1:20:A:LEU:HB3	1:21:A:SER:H	18	0.16
(1,204)	1:19:A:GLU:HG2	1:20:A:LEU:H	16	0.16
(1,203)	1:19:A:GLU:HB3	1:20:A:LEU:H	7	0.16
(1,195)	1:19:A:GLU:H	1:19:A:GLU:HG2	7	0.16
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG21	17	0.16
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG22	17	0.16
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG23	17	0.16
(1,177)	1:18:A:TRP:HE1	1:36:A:THR:HB	3	0.16
(1,177)	1:18:A:TRP:HE1	1:36:A:THR:HB	5	0.16
(1,177)	1:18:A:TRP:HE1	1:36:A:THR:HB	14	0.16
(1,166)	1:17:A:THR:HG21	1:18:A:TRP:H	15	0.16
(1,166)	1:17:A:THR:HG22	1:18:A:TRP:H	15	0.16
(1,166)	1:17:A:THR:HG23	1:18:A:TRP:H	15	0.16
(1,153)	1:15:A:ASP:H	1:17:A:THR:H	12	0.16
(1,147)	1:15:A:ASP:H	1:15:A:ASP:HB2	17	0.16
(1,128)	1:11:A:GLY:H	1:12:A:CYS:H	20	0.16
(1,127)	1:11:A:GLY:HA2	1:12:A:CYS:H	10	0.16
(1,112)	1:9:A:PRO:HG3	1:10:A:ASP:H	8	0.16
(1,112)	1:9:A:PRO:HG3	1:10:A:ASP:H	15	0.16
(1,102)	1:8:A:MET:HB3	1:12:A:CYS:H	10	0.16
(1,86)	1:7:A:ARG:HA	1:10:A:ASP:H	1	0.16
(1,85)	1:7:A:ARG:HD3	1:8:A:MET:H	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,84)	1:7:A:ARG:H	1:8:A:MET:H	17	0.16
(1,82)	1:7:A:ARG:HB2	1:8:A:MET:H	15	0.16
(1,82)	1:7:A:ARG:HB2	1:8:A:MET:H	18	0.16
(1,49)	1:5:A:GLY:HA3	1:6:A:ILE:HB	19	0.16
(1,42)	1:4:A:ASP:H	1:5:A:GLY:HA3	20	0.16
(1,40)	1:4:A:ASP:HA	1:5:A:GLY:H	7	0.16
(1,40)	1:4:A:ASP:HA	1:5:A:GLY:H	11	0.16
(1,36)	1:3:A:LEU:HB3	1:4:A:ASP:H	11	0.16
(1,26)	1:3:A:LEU:H	1:3:A:LEU:HG	2	0.16
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD11	19	0.16
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD12	19	0.16
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD13	19	0.16
(1,20)	1:2:A:ALA:HB1	1:4:A:ASP:H	19	0.16
(1,20)	1:2:A:ALA:HB2	1:4:A:ASP:H	19	0.16
(1,20)	1:2:A:ALA:HB3	1:4:A:ASP:H	19	0.16
(1,19)	1:2:A:ALA:HB1	1:3:A:LEU:H	7	0.16
(1,19)	1:2:A:ALA:HB2	1:3:A:LEU:H	7	0.16
(1,19)	1:2:A:ALA:HB3	1:3:A:LEU:H	7	0.16
(1,19)	1:2:A:ALA:HB1	1:3:A:LEU:H	19	0.16
(1,19)	1:2:A:ALA:HB2	1:3:A:LEU:H	19	0.16
(1,19)	1:2:A:ALA:HB3	1:3:A:LEU:H	19	0.16
(1,16)	1:2:A:ALA:H	1:3:A:LEU:HB3	1	0.16
(3,16)	1:42:A:GLY:O	1:46:A:LEU:H	17	0.15
(3,13)	1:92:A:PHE:O	1:64:A:TRP:H	3	0.15
(3,13)	1:92:A:PHE:O	1:64:A:TRP:H	5	0.15
(3,13)	1:92:A:PHE:O	1:64:A:TRP:H	11	0.15
(2,25)	1:77:A:TRP:O	1:81:A:LYS:N	12	0.15
(2,24)	1:45:A:MET:O	1:49:A:VAL:N	11	0.15
(2,21)	1:39:A:VAL:O	1:43:A:GLY:N	6	0.15
(2,19)	1:23:A:HIS:O	1:93:A:THR:H	6	0.15
(2,19)	1:23:A:HIS:O	1:93:A:THR:H	10	0.15
(2,13)	1:92:A:PHE:O	1:64:A:TRP:N	16	0.15
(2,3)	1:20:A:LEU:O	1:33:A:LEU:N	6	0.15
(1,1382)	1:91:A:GLN:HG2	1:91:A:GLN:HE21	19	0.15
(1,1381)	1:91:A:GLN:H	1:91:A:GLN:HG2	3	0.15
(1,1381)	1:91:A:GLN:H	1:91:A:GLN:HG2	13	0.15
(1,1381)	1:91:A:GLN:H	1:91:A:GLN:HG2	17	0.15
(1,1380)	1:91:A:GLN:H	1:91:A:GLN:HE22	12	0.15
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD11	19	0.15
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD12	19	0.15
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD13	19	0.15
(1,1323)	1:86:A:ALA:HB1	1:88:A:ALA:H	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1323)	1:86:A:ALA:HB2	1:88:A:ALA:H	19	0.15
(1,1323)	1:86:A:ALA:HB3	1:88:A:ALA:H	19	0.15
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG21	3	0.15
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG22	3	0.15
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG23	3	0.15
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG21	4	0.15
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG22	4	0.15
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG23	4	0.15
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG21	7	0.15
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG22	7	0.15
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG23	7	0.15
(1,1246)	1:81:A:LYS:HE3	1:82:A:TYR:H	1	0.15
(1,1246)	1:81:A:LYS:HE3	1:82:A:TYR:H	7	0.15
(1,1218)	1:80:A:ASP:HB2	1:82:A:TYR:H	9	0.15
(1,1215)	1:80:A:ASP:HB2	1:81:A:LYS:H	11	0.15
(1,1197)	1:79:A:LEU:HB3	1:80:A:ASP:H	6	0.15
(1,1197)	1:79:A:LEU:HB3	1:80:A:ASP:H	14	0.15
(1,1196)	1:79:A:LEU:HD21	1:80:A:ASP:H	1	0.15
(1,1196)	1:79:A:LEU:HD22	1:80:A:ASP:H	1	0.15
(1,1196)	1:79:A:LEU:HD23	1:80:A:ASP:H	1	0.15
(1,1196)	1:79:A:LEU:HD21	1:80:A:ASP:H	7	0.15
(1,1196)	1:79:A:LEU:HD22	1:80:A:ASP:H	7	0.15
(1,1196)	1:79:A:LEU:HD23	1:80:A:ASP:H	7	0.15
(1,1196)	1:79:A:LEU:HD21	1:80:A:ASP:H	14	0.15
(1,1196)	1:79:A:LEU:HD22	1:80:A:ASP:H	14	0.15
(1,1196)	1:79:A:LEU:HD23	1:80:A:ASP:H	14	0.15
(1,1196)	1:79:A:LEU:HD21	1:80:A:ASP:H	17	0.15
(1,1196)	1:79:A:LEU:HD22	1:80:A:ASP:H	17	0.15
(1,1196)	1:79:A:LEU:HD23	1:80:A:ASP:H	17	0.15
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD11	10	0.15
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD12	10	0.15
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD13	10	0.15
(1,1177)	1:78:A:THR:H	1:81:A:LYS:H	10	0.15
(1,1176)	1:78:A:THR:H	1:81:A:LYS:HA	6	0.15
(1,1164)	1:78:A:THR:HG21	1:78:A:THR:H	19	0.15
(1,1164)	1:78:A:THR:HG22	1:78:A:THR:H	19	0.15
(1,1164)	1:78:A:THR:HG23	1:78:A:THR:H	19	0.15
(1,1161)	1:77:A:TRP:H	1:81:A:LYS:HD3	11	0.15
(1,1161)	1:77:A:TRP:H	1:81:A:LYS:HD3	16	0.15
(1,1153)	1:76:A:HIS:HB3	1:77:A:TRP:H	19	0.15
(1,1148)	1:75:A:THR:HG21	1:77:A:TRP:H	6	0.15
(1,1148)	1:75:A:THR:HG22	1:77:A:TRP:H	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:75:A:THR:HG23	1:77:A:TRP:H	6	0.15
(1,1141)	1:74:A:LYS:HE3	1:78:A:THR:H	17	0.15
(1,1138)	1:74:A:LYS:HD3	1:77:A:TRP:H	6	0.15
(1,1138)	1:74:A:LYS:HD3	1:77:A:TRP:H	10	0.15
(1,1138)	1:74:A:LYS:HD3	1:77:A:TRP:H	16	0.15
(1,1134)	1:74:A:LYS:HG2	1:75:A:THR:H	3	0.15
(1,1134)	1:74:A:LYS:HG2	1:75:A:THR:H	12	0.15
(1,1134)	1:74:A:LYS:HG2	1:75:A:THR:H	16	0.15
(1,1134)	1:74:A:LYS:HG2	1:75:A:THR:H	17	0.15
(1,1128)	1:74:A:LYS:HE3	1:74:A:LYS:HB3	5	0.15
(1,1121)	1:74:A:LYS:H	1:74:A:LYS:HG3	7	0.15
(1,1113)	1:74:A:LYS:HA	1:74:A:LYS:HE3	4	0.15
(1,1113)	1:74:A:LYS:HA	1:74:A:LYS:HE3	5	0.15
(1,1113)	1:74:A:LYS:HA	1:74:A:LYS:HE3	6	0.15
(1,1113)	1:74:A:LYS:HA	1:74:A:LYS:HE3	11	0.15
(1,1113)	1:74:A:LYS:HA	1:74:A:LYS:HE3	14	0.15
(1,1113)	1:74:A:LYS:HA	1:74:A:LYS:HE3	16	0.15
(1,1112)	1:74:A:LYS:HA	1:74:A:LYS:HE2	10	0.15
(1,1108)	1:73:A:LEU:HA	1:74:A:LYS:H	15	0.15
(1,1105)	1:73:A:LEU:H	1:73:A:LEU:HB3	3	0.15
(1,1105)	1:73:A:LEU:H	1:73:A:LEU:HB3	17	0.15
(1,1097)	1:72:A:LEU:HD21	1:73:A:LEU:H	7	0.15
(1,1097)	1:72:A:LEU:HD22	1:73:A:LEU:H	7	0.15
(1,1097)	1:72:A:LEU:HD23	1:73:A:LEU:H	7	0.15
(1,1076)	1:71:A:TRP:H	1:71:A:TRP:HB3	20	0.15
(1,1063)	1:69:A:ARG:H	1:70:A:THR:H	2	0.15
(1,1061)	1:69:A:ARG:HD3	1:70:A:THR:HB	2	0.15
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD21	8	0.15
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD22	8	0.15
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD23	8	0.15
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD21	11	0.15
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD22	11	0.15
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD23	11	0.15
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD21	17	0.15
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD22	17	0.15
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD23	17	0.15
(1,1053)	1:67:A:LYS:H	1:88:A:ALA:HA	7	0.15
(1,1051)	1:67:A:LYS:HG2	1:69:A:ARG:H	1	0.15
(1,1051)	1:67:A:LYS:HG2	1:69:A:ARG:H	17	0.15
(1,1038)	1:67:A:LYS:H	1:67:A:LYS:HG3	4	0.15
(1,1038)	1:67:A:LYS:H	1:67:A:LYS:HG3	13	0.15
(1,1038)	1:67:A:LYS:H	1:67:A:LYS:HG3	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1036)	1:67:A:LYS:HE3	1:67:A:LYS:H	13	0.15
(1,1036)	1:67:A:LYS:HE3	1:67:A:LYS:H	20	0.15
(1,1033)	1:67:A:LYS:HA	1:67:A:LYS:HD3	18	0.15
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG21	13	0.15
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG22	13	0.15
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG23	13	0.15
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG21	15	0.15
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG22	15	0.15
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG23	15	0.15
(1,997)	1:65:A:TRP:HB3	1:66:A:GLU:H	2	0.15
(1,997)	1:65:A:TRP:HB3	1:66:A:GLU:H	17	0.15
(1,988)	1:64:A:TRP:H	1:92:A:PHE:HB3	4	0.15
(1,985)	1:64:A:TRP:H	1:90:A:LEU:HA	15	0.15
(1,981)	1:64:A:TRP:H	1:64:A:TRP:HB3	3	0.15
(1,981)	1:64:A:TRP:H	1:64:A:TRP:HB3	4	0.15
(1,981)	1:64:A:TRP:H	1:64:A:TRP:HB3	10	0.15
(1,978)	1:63:A:LEU:HA	1:93:A:THR:H	20	0.15
(1,976)	1:63:A:LEU:HG	1:93:A:THR:H	4	0.15
(1,972)	1:63:A:LEU:HD11	1:91:A:GLN:H	13	0.15
(1,972)	1:63:A:LEU:HD12	1:91:A:GLN:H	13	0.15
(1,972)	1:63:A:LEU:HD13	1:91:A:GLN:H	13	0.15
(1,972)	1:63:A:LEU:HD11	1:91:A:GLN:H	17	0.15
(1,972)	1:63:A:LEU:HD12	1:91:A:GLN:H	17	0.15
(1,972)	1:63:A:LEU:HD13	1:91:A:GLN:H	17	0.15
(1,972)	1:63:A:LEU:HD11	1:91:A:GLN:H	20	0.15
(1,972)	1:63:A:LEU:HD12	1:91:A:GLN:H	20	0.15
(1,972)	1:63:A:LEU:HD13	1:91:A:GLN:H	20	0.15
(1,968)	1:63:A:LEU:HG	1:90:A:LEU:HA	1	0.15
(1,968)	1:63:A:LEU:HG	1:90:A:LEU:HA	6	0.15
(1,960)	1:67:A:LYS:HG2	1:69:A:ARG:H	1	0.15
(1,960)	1:67:A:LYS:HG2	1:69:A:ARG:H	17	0.15
(1,959)	1:63:A:LEU:H	1:64:A:TRP:H	16	0.15
(1,950)	1:63:A:LEU:H	1:63:A:LEU:HG	1	0.15
(1,950)	1:63:A:LEU:H	1:63:A:LEU:HG	6	0.15
(1,946)	1:62:A:ALA:H	1:94:A:PRO:HA	13	0.15
(1,946)	1:62:A:ALA:H	1:94:A:PRO:HA	14	0.15
(1,946)	1:62:A:ALA:H	1:94:A:PRO:HA	16	0.15
(1,942)	1:62:A:ALA:HB1	1:92:A:PHE:HA	19	0.15
(1,942)	1:62:A:ALA:HB2	1:92:A:PHE:HA	19	0.15
(1,942)	1:62:A:ALA:HB3	1:92:A:PHE:HA	19	0.15
(1,930)	1:61:A:HIS:HB2	1:63:A:LEU:H	10	0.15
(1,930)	1:61:A:HIS:HB2	1:63:A:LEU:H	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,930)	1:61:A:HIS:HB2	1:63:A:LEU:H	17	0.15
(1,926)	1:61:A:HIS:H	1:62:A:ALA:H	19	0.15
(1,921)	1:60:A:ASP:HB3	1:61:A:HIS:H	16	0.15
(1,890)	1:56:A:LYS:HA	1:57:A:ASP:HB2	7	0.15
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD11	9	0.15
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD12	9	0.15
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD13	9	0.15
(1,858)	1:51:A:LYS:H	1:51:A:LYS:HD3	5	0.15
(1,858)	1:51:A:LYS:H	1:51:A:LYS:HD3	9	0.15
(1,858)	1:51:A:LYS:H	1:51:A:LYS:HD3	12	0.15
(1,858)	1:51:A:LYS:H	1:51:A:LYS:HD3	13	0.15
(1,844)	1:50:A:GLU:H	1:50:A:GLU:HG2	2	0.15
(1,844)	1:50:A:GLU:H	1:50:A:GLU:HG2	12	0.15
(1,841)	1:50:A:GLU:HA	1:50:A:GLU:HG3	5	0.15
(1,841)	1:50:A:GLU:HA	1:50:A:GLU:HG3	12	0.15
(1,841)	1:50:A:GLU:HA	1:50:A:GLU:HG3	18	0.15
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD21	10	0.15
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD22	10	0.15
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD23	10	0.15
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD21	10	0.15
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD22	10	0.15
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD23	10	0.15
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD21	10	0.15
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD22	10	0.15
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD23	10	0.15
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD21	13	0.15
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD22	13	0.15
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD23	13	0.15
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD21	13	0.15
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD22	13	0.15
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD23	13	0.15
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD21	13	0.15
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD22	13	0.15
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD23	13	0.15
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD21	15	0.15
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD22	15	0.15
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD23	15	0.15
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD21	15	0.15
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD22	15	0.15
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD23	15	0.15
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD21	15	0.15
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD22	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD23	15	0.15
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD21	18	0.15
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD22	18	0.15
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD23	18	0.15
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD21	18	0.15
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD22	18	0.15
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD23	18	0.15
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD21	18	0.15
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD22	18	0.15
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD23	18	0.15
(1,821)	1:48:A:LEU:HD21	1:63:A:LEU:H	8	0.15
(1,821)	1:48:A:LEU:HD22	1:63:A:LEU:H	8	0.15
(1,821)	1:48:A:LEU:HD23	1:63:A:LEU:H	8	0.15
(1,813)	1:48:A:LEU:H	1:51:A:LYS:H	14	0.15
(1,813)	1:48:A:LEU:H	1:51:A:LYS:H	17	0.15
(1,812)	1:48:A:LEU:HA	1:51:A:LYS:HB3	2	0.15
(1,812)	1:48:A:LEU:HA	1:51:A:LYS:HB3	8	0.15
(1,812)	1:48:A:LEU:HA	1:51:A:LYS:HB3	15	0.15
(1,812)	1:48:A:LEU:HA	1:51:A:LYS:HB3	18	0.15
(1,805)	1:48:A:LEU:HG	1:49:A:VAL:H	11	0.15
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG21	1	0.15
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG22	1	0.15
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG23	1	0.15
(1,782)	1:47:A:LYS:HB2	1:48:A:LEU:H	9	0.15
(1,782)	1:47:A:LYS:HB2	1:48:A:LEU:H	17	0.15
(1,773)	1:47:A:LYS:H	1:47:A:LYS:HD3	10	0.15
(1,773)	1:47:A:LYS:H	1:47:A:LYS:HD3	12	0.15
(1,773)	1:47:A:LYS:H	1:47:A:LYS:HD3	14	0.15
(1,773)	1:47:A:LYS:H	1:47:A:LYS:HD3	18	0.15
(1,766)	1:46:A:LEU:HA	1:50:A:GLU:H	20	0.15
(1,760)	1:46:A:LEU:H	1:48:A:LEU:H	9	0.15
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD21	6	0.15
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD22	6	0.15
(1,745)	1:45:A:MET:H	1:63:A:LEU:HD23	6	0.15
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG21	2	0.15
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG22	2	0.15
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG23	2	0.15
(1,737)	1:45:A:MET:HB3	1:48:A:LEU:H	3	0.15
(1,719)	1:44:A:VAL:HG11	1:90:A:LEU:H	10	0.15
(1,719)	1:44:A:VAL:HG12	1:90:A:LEU:H	10	0.15
(1,719)	1:44:A:VAL:HG13	1:90:A:LEU:H	10	0.15
(1,694)	1:43:A:GLY:H	1:45:A:MET:H	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,692)	1:43:A:GLY:H	1:44:A:VAL:HB	1	0.15
(1,692)	1:43:A:GLY:H	1:44:A:VAL:HB	2	0.15
(1,692)	1:43:A:GLY:H	1:44:A:VAL:HB	9	0.15
(1,684)	1:42:A:GLY:HA3	1:75:A:THR:HB	4	0.15
(1,684)	1:42:A:GLY:HA3	1:75:A:THR:HB	11	0.15
(1,684)	1:42:A:GLY:HA3	1:75:A:THR:HB	16	0.15
(1,683)	1:42:A:GLY:H	1:74:A:LYS:HE3	4	0.15
(1,683)	1:42:A:GLY:H	1:74:A:LYS:HE3	20	0.15
(1,671)	1:41:A:ILE:HD11	1:75:A:THR:HA	5	0.15
(1,671)	1:41:A:ILE:HD12	1:75:A:THR:HA	5	0.15
(1,671)	1:41:A:ILE:HD13	1:75:A:THR:HA	5	0.15
(1,663)	1:41:A:ILE:HG21	1:72:A:LEU:HG	4	0.15
(1,663)	1:41:A:ILE:HG22	1:72:A:LEU:HG	4	0.15
(1,663)	1:41:A:ILE:HG23	1:72:A:LEU:HG	4	0.15
(1,663)	1:41:A:ILE:HG21	1:72:A:LEU:HG	10	0.15
(1,663)	1:41:A:ILE:HG22	1:72:A:LEU:HG	10	0.15
(1,663)	1:41:A:ILE:HG23	1:72:A:LEU:HG	10	0.15
(1,663)	1:41:A:ILE:HG21	1:72:A:LEU:HG	14	0.15
(1,663)	1:41:A:ILE:HG22	1:72:A:LEU:HG	14	0.15
(1,663)	1:41:A:ILE:HG23	1:72:A:LEU:HG	14	0.15
(1,663)	1:41:A:ILE:HG21	1:72:A:LEU:HG	17	0.15
(1,663)	1:41:A:ILE:HG22	1:72:A:LEU:HG	17	0.15
(1,663)	1:41:A:ILE:HG23	1:72:A:LEU:HG	17	0.15
(1,659)	1:41:A:ILE:HD11	1:44:A:VAL:H	1	0.15
(1,659)	1:41:A:ILE:HD12	1:44:A:VAL:H	1	0.15
(1,659)	1:41:A:ILE:HD13	1:44:A:VAL:H	1	0.15
(1,659)	1:41:A:ILE:HD11	1:44:A:VAL:H	7	0.15
(1,659)	1:41:A:ILE:HD12	1:44:A:VAL:H	7	0.15
(1,659)	1:41:A:ILE:HD13	1:44:A:VAL:H	7	0.15
(1,659)	1:41:A:ILE:HD11	1:44:A:VAL:H	10	0.15
(1,659)	1:41:A:ILE:HD12	1:44:A:VAL:H	10	0.15
(1,659)	1:41:A:ILE:HD13	1:44:A:VAL:H	10	0.15
(1,659)	1:41:A:ILE:HD11	1:44:A:VAL:H	14	0.15
(1,659)	1:41:A:ILE:HD12	1:44:A:VAL:H	14	0.15
(1,659)	1:41:A:ILE:HD13	1:44:A:VAL:H	14	0.15
(1,640)	1:41:A:ILE:H	1:41:A:ILE:HG12	12	0.15
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG11	14	0.15
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG12	14	0.15
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG13	14	0.15
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG11	17	0.15
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG12	17	0.15
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG13	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,610)	1:39:A:VAL:HG21	1:80:A:ASP:H	1	0.15
(1,610)	1:39:A:VAL:HG22	1:80:A:ASP:H	1	0.15
(1,610)	1:39:A:VAL:HG23	1:80:A:ASP:H	1	0.15
(1,588)	1:38:A:GLU:HA	1:80:A:ASP:H	15	0.15
(1,580)	1:38:A:GLU:HB3	1:39:A:VAL:H	20	0.15
(1,554)	1:36:A:THR:H	1:38:A:GLU:HB3	8	0.15
(1,554)	1:36:A:THR:H	1:38:A:GLU:HB3	11	0.15
(1,554)	1:36:A:THR:H	1:38:A:GLU:HB3	15	0.15
(1,554)	1:36:A:THR:H	1:38:A:GLU:HB3	16	0.15
(1,552)	1:36:A:THR:HB	1:38:A:GLU:H	12	0.15
(1,552)	1:36:A:THR:HB	1:38:A:GLU:H	20	0.15
(1,527)	1:34:A:ARG:H	1:51:A:LYS:HD3	8	0.15
(1,527)	1:34:A:ARG:H	1:51:A:LYS:HD3	11	0.15
(1,523)	1:34:A:ARG:HB3	1:35:A:VAL:H	13	0.15
(1,516)	1:34:A:ARG:H	1:34:A:ARG:HG3	13	0.15
(1,511)	1:33:A:LEU:HD21	1:48:A:LEU:HB3	15	0.15
(1,511)	1:33:A:LEU:HD22	1:48:A:LEU:HB3	15	0.15
(1,511)	1:33:A:LEU:HD23	1:48:A:LEU:HB3	15	0.15
(1,484)	1:32:A:THR:HA	1:51:A:LYS:HD3	8	0.15
(1,484)	1:32:A:THR:HA	1:51:A:LYS:HD3	10	0.15
(1,484)	1:32:A:THR:HA	1:51:A:LYS:HD3	12	0.15
(1,482)	1:32:A:THR:HA	1:34:A:ARG:H	9	0.15
(1,482)	1:32:A:THR:HA	1:34:A:ARG:H	10	0.15
(1,482)	1:32:A:THR:HA	1:34:A:ARG:H	12	0.15
(1,482)	1:32:A:THR:HA	1:34:A:ARG:H	17	0.15
(1,482)	1:32:A:THR:HA	1:34:A:ARG:H	18	0.15
(1,473)	1:32:A:THR:HB	1:32:A:THR:H	2	0.15
(1,473)	1:32:A:THR:HB	1:32:A:THR:H	7	0.15
(1,453)	1:29:A:ARG:HB2	1:31:A:VAL:HA	6	0.15
(1,453)	1:29:A:ARG:HB2	1:31:A:VAL:HA	15	0.15
(1,443)	1:29:A:ARG:HB2	1:29:A:ARG:H	7	0.15
(1,437)	1:28:A:ASN:HB3	1:29:A:ARG:H	4	0.15
(1,432)	1:28:A:ASN:H	1:28:A:ASN:HB2	1	0.15
(1,432)	1:28:A:ASN:H	1:28:A:ASN:HB2	4	0.15
(1,432)	1:28:A:ASN:H	1:28:A:ASN:HB2	6	0.15
(1,431)	1:27:A:VAL:H	1:93:A:THR:HB	13	0.15
(1,430)	1:27:A:VAL:HG21	1:92:A:PHE:H	18	0.15
(1,430)	1:27:A:VAL:HG22	1:92:A:PHE:H	18	0.15
(1,430)	1:27:A:VAL:HG23	1:92:A:PHE:H	18	0.15
(1,414)	1:25:A:THR:H	1:93:A:THR:HG21	10	0.15
(1,414)	1:25:A:THR:H	1:93:A:THR:HG22	10	0.15
(1,414)	1:25:A:THR:H	1:93:A:THR:HG23	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG21	11	0.15
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG22	11	0.15
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG23	11	0.15
(1,392)	1:24:A:VAL:HB	1:92:A:PHE:H	10	0.15
(1,383)	1:24:A:VAL:HA	1:31:A:VAL:H	11	0.15
(1,377)	1:24:A:VAL:HA	1:30:A:ASP:HA	9	0.15
(1,377)	1:24:A:VAL:HA	1:30:A:ASP:HA	12	0.15
(1,377)	1:24:A:VAL:HA	1:30:A:ASP:HA	18	0.15
(1,371)	1:24:A:VAL:HG11	1:29:A:ARG:H	1	0.15
(1,371)	1:24:A:VAL:HG12	1:29:A:ARG:H	1	0.15
(1,371)	1:24:A:VAL:HG13	1:29:A:ARG:H	1	0.15
(1,369)	1:24:A:VAL:H	1:29:A:ARG:HG3	18	0.15
(1,350)	1:23:A:HIS:HB2	1:91:A:GLN:HG3	1	0.15
(1,331)	1:23:A:HIS:H	1:30:A:ASP:HB3	5	0.15
(1,331)	1:23:A:HIS:H	1:30:A:ASP:HB3	11	0.15
(1,329)	1:23:A:HIS:HB2	1:24:A:VAL:HA	15	0.15
(1,323)	1:23:A:HIS:HB2	1:24:A:VAL:H	4	0.15
(1,323)	1:23:A:HIS:HB2	1:24:A:VAL:H	8	0.15
(1,323)	1:23:A:HIS:HB2	1:24:A:VAL:H	13	0.15
(1,323)	1:23:A:HIS:HB2	1:24:A:VAL:H	15	0.15
(1,323)	1:23:A:HIS:HB2	1:24:A:VAL:H	16	0.15
(1,323)	1:23:A:HIS:HB2	1:24:A:VAL:H	17	0.15
(1,323)	1:23:A:HIS:HB2	1:24:A:VAL:H	19	0.15
(1,312)	1:22:A:VAL:HG21	1:90:A:LEU:H	3	0.15
(1,312)	1:22:A:VAL:HG22	1:90:A:LEU:H	3	0.15
(1,312)	1:22:A:VAL:HG23	1:90:A:LEU:H	3	0.15
(1,312)	1:22:A:VAL:HG21	1:90:A:LEU:H	4	0.15
(1,312)	1:22:A:VAL:HG22	1:90:A:LEU:H	4	0.15
(1,312)	1:22:A:VAL:HG23	1:90:A:LEU:H	4	0.15
(1,312)	1:22:A:VAL:HG21	1:90:A:LEU:H	9	0.15
(1,312)	1:22:A:VAL:HG22	1:90:A:LEU:H	9	0.15
(1,312)	1:22:A:VAL:HG23	1:90:A:LEU:H	9	0.15
(1,312)	1:22:A:VAL:HG21	1:90:A:LEU:H	12	0.15
(1,312)	1:22:A:VAL:HG22	1:90:A:LEU:H	12	0.15
(1,312)	1:22:A:VAL:HG23	1:90:A:LEU:H	12	0.15
(1,312)	1:22:A:VAL:HG21	1:90:A:LEU:H	15	0.15
(1,312)	1:22:A:VAL:HG22	1:90:A:LEU:H	15	0.15
(1,312)	1:22:A:VAL:HG23	1:90:A:LEU:H	15	0.15
(1,299)	1:22:A:VAL:H	1:32:A:THR:HB	5	0.15
(1,299)	1:22:A:VAL:H	1:32:A:THR:HB	19	0.15
(1,294)	1:22:A:VAL:HG11	1:29:A:ARG:H	3	0.15
(1,294)	1:22:A:VAL:HG12	1:29:A:ARG:H	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,294)	1:22:A:VAL:HG13	1:29:A:ARG:H	3	0.15
(1,294)	1:22:A:VAL:HG11	1:29:A:ARG:H	12	0.15
(1,294)	1:22:A:VAL:HG12	1:29:A:ARG:H	12	0.15
(1,294)	1:22:A:VAL:HG13	1:29:A:ARG:H	12	0.15
(1,275)	1:21:A:SER:H	1:32:A:THR:HB	3	0.15
(1,275)	1:21:A:SER:H	1:32:A:THR:HB	4	0.15
(1,275)	1:21:A:SER:H	1:32:A:THR:HB	5	0.15
(1,275)	1:21:A:SER:H	1:32:A:THR:HB	12	0.15
(1,275)	1:21:A:SER:H	1:32:A:THR:HB	15	0.15
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB1	5	0.15
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB2	5	0.15
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB3	5	0.15
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB1	5	0.15
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB2	5	0.15
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB3	5	0.15
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB1	5	0.15
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB2	5	0.15
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB3	5	0.15
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB1	7	0.15
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB2	7	0.15
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB3	7	0.15
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB1	7	0.15
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB2	7	0.15
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB3	7	0.15
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB1	7	0.15
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB2	7	0.15
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB3	7	0.15
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB1	20	0.15
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB2	20	0.15
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB3	20	0.15
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB1	20	0.15
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB2	20	0.15
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB3	20	0.15
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB1	20	0.15
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB2	20	0.15
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB3	20	0.15
(1,251)	1:20:A:LEU:HG	1:35:A:VAL:H	8	0.15
(1,250)	1:20:A:LEU:H	1:35:A:VAL:H	13	0.15
(1,249)	1:20:A:LEU:HB2	1:34:A:ARG:H	3	0.15
(1,249)	1:20:A:LEU:HB2	1:34:A:ARG:H	12	0.15
(1,244)	1:20:A:LEU:HD21	1:33:A:LEU:HA	13	0.15
(1,244)	1:20:A:LEU:HD22	1:33:A:LEU:HA	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,244)	1:20:A:LEU:HD23	1:33:A:LEU:HA	13	0.15
(1,244)	1:20:A:LEU:HD21	1:33:A:LEU:HA	14	0.15
(1,244)	1:20:A:LEU:HD22	1:33:A:LEU:HA	14	0.15
(1,244)	1:20:A:LEU:HD23	1:33:A:LEU:HA	14	0.15
(1,242)	1:20:A:LEU:HB3	1:33:A:LEU:H	4	0.15
(1,242)	1:20:A:LEU:HB3	1:33:A:LEU:H	12	0.15
(1,242)	1:20:A:LEU:HB3	1:33:A:LEU:H	14	0.15
(1,242)	1:20:A:LEU:HB3	1:33:A:LEU:H	15	0.15
(1,234)	1:20:A:LEU:HB3	1:21:A:SER:H	13	0.15
(1,234)	1:20:A:LEU:HB3	1:21:A:SER:H	14	0.15
(1,234)	1:20:A:LEU:HB3	1:21:A:SER:H	17	0.15
(1,200)	1:19:A:GLU:H	1:20:A:LEU:H	5	0.15
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG21	15	0.15
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG22	15	0.15
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG23	15	0.15
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG21	18	0.15
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG22	18	0.15
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG23	18	0.15
(1,184)	1:18:A:TRP:HE1	1:80:A:ASP:HB3	8	0.15
(1,184)	1:18:A:TRP:HE1	1:80:A:ASP:HB3	16	0.15
(1,177)	1:18:A:TRP:HE1	1:36:A:THR:HB	7	0.15
(1,177)	1:18:A:TRP:HE1	1:36:A:THR:HB	9	0.15
(1,177)	1:18:A:TRP:HE1	1:36:A:THR:HB	11	0.15
(1,177)	1:18:A:TRP:HE1	1:36:A:THR:HB	17	0.15
(1,175)	1:18:A:TRP:H	1:35:A:VAL:HA	6	0.15
(1,169)	1:18:A:TRP:H	1:18:A:TRP:HD1	8	0.15
(1,166)	1:17:A:THR:HG21	1:18:A:TRP:H	13	0.15
(1,166)	1:17:A:THR:HG22	1:18:A:TRP:H	13	0.15
(1,166)	1:17:A:THR:HG23	1:18:A:TRP:H	13	0.15
(1,156)	1:16:A:GLY:HA2	1:17:A:THR:H	20	0.15
(1,155)	1:16:A:GLY:HA3	1:17:A:THR:H	13	0.15
(1,147)	1:15:A:ASP:H	1:15:A:ASP:HB2	2	0.15
(1,145)	1:14:A:ALA:HB1	1:16:A:GLY:H	16	0.15
(1,145)	1:14:A:ALA:HB2	1:16:A:GLY:H	16	0.15
(1,145)	1:14:A:ALA:HB3	1:16:A:GLY:H	16	0.15
(1,128)	1:11:A:GLY:H	1:12:A:CYS:H	9	0.15
(1,127)	1:11:A:GLY:HA2	1:12:A:CYS:H	1	0.15
(1,127)	1:11:A:GLY:HA2	1:12:A:CYS:H	3	0.15
(1,127)	1:11:A:GLY:HA2	1:12:A:CYS:H	13	0.15
(1,127)	1:11:A:GLY:HA2	1:12:A:CYS:H	16	0.15
(1,127)	1:11:A:GLY:HA2	1:12:A:CYS:H	20	0.15
(1,113)	1:9:A:PRO:HG3	1:12:A:CYS:HB3	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,112)	1:9:A:PRO:HG3	1:10:A:ASP:H	2	0.15
(1,112)	1:9:A:PRO:HG3	1:10:A:ASP:H	16	0.15
(1,112)	1:9:A:PRO:HG3	1:10:A:ASP:H	18	0.15
(1,95)	1:8:A:MET:HA	1:10:A:ASP:H	7	0.15
(1,95)	1:8:A:MET:HA	1:10:A:ASP:H	16	0.15
(1,94)	1:8:A:MET:H	1:10:A:ASP:HA	2	0.15
(1,83)	1:7:A:ARG:HB3	1:8:A:MET:H	20	0.15
(1,67)	1:6:A:ILE:H	1:10:A:ASP:H	15	0.15
(1,58)	1:6:A:ILE:H	1:6:A:ILE:HG21	16	0.15
(1,58)	1:6:A:ILE:H	1:6:A:ILE:HG22	16	0.15
(1,58)	1:6:A:ILE:H	1:6:A:ILE:HG23	16	0.15
(1,56)	1:6:A:ILE:H	1:6:A:ILE:HG12	1	0.15
(1,45)	1:4:A:ASP:HB3	1:6:A:ILE:H	20	0.15
(1,40)	1:4:A:ASP:HA	1:5:A:GLY:H	12	0.15
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD11	1	0.15
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD12	1	0.15
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD13	1	0.15
(1,16)	1:2:A:ALA:H	1:3:A:LEU:HB3	5	0.15
(1,16)	1:2:A:ALA:H	1:3:A:LEU:HB3	15	0.15
(3,21)	1:80:A:ASP:O	1:84:A:ILE:H	6	0.14
(3,21)	1:80:A:ASP:O	1:84:A:ILE:H	19	0.14
(3,16)	1:42:A:GLY:O	1:46:A:LEU:H	1	0.14
(3,16)	1:42:A:GLY:O	1:46:A:LEU:H	6	0.14
(3,16)	1:42:A:GLY:O	1:46:A:LEU:H	7	0.14
(3,13)	1:92:A:PHE:O	1:64:A:TRP:H	14	0.14
(3,13)	1:92:A:PHE:O	1:64:A:TRP:H	17	0.14
(3,13)	1:92:A:PHE:O	1:64:A:TRP:H	18	0.14
(2,25)	1:77:A:TRP:O	1:81:A:LYS:N	4	0.14
(2,25)	1:77:A:TRP:O	1:81:A:LYS:N	8	0.14
(2,25)	1:77:A:TRP:O	1:81:A:LYS:N	19	0.14
(2,24)	1:45:A:MET:O	1:49:A:VAL:N	10	0.14
(2,24)	1:45:A:MET:O	1:49:A:VAL:N	19	0.14
(2,21)	1:39:A:VAL:O	1:43:A:GLY:N	14	0.14
(2,14)	1:64:A:TRP:O	1:92:A:PHE:N	16	0.14
(2,13)	1:92:A:PHE:O	1:64:A:TRP:N	10	0.14
(1,1408)	1:92:A:PHE:HB3	1:93:A:THR:H	14	0.14
(1,1407)	1:92:A:PHE:HB2	1:93:A:THR:H	4	0.14
(1,1407)	1:92:A:PHE:HB2	1:93:A:THR:H	9	0.14
(1,1381)	1:91:A:GLN:H	1:91:A:GLN:HG2	1	0.14
(1,1380)	1:91:A:GLN:H	1:91:A:GLN:HE22	5	0.14
(1,1355)	1:90:A:LEU:H	1:90:A:LEU:HD21	16	0.14
(1,1355)	1:90:A:LEU:H	1:90:A:LEU:HD22	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1355)	1:90:A:LEU:H	1:90:A:LEU:HD23	16	0.14
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD11	20	0.14
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD12	20	0.14
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD13	20	0.14
(1,1329)	1:87:A:ASP:HB3	1:88:A:ALA:H	6	0.14
(1,1329)	1:87:A:ASP:HB3	1:88:A:ALA:H	14	0.14
(1,1329)	1:87:A:ASP:HB3	1:88:A:ALA:H	16	0.14
(1,1313)	1:85:A:GLN:HB3	1:87:A:ASP:H	14	0.14
(1,1289)	1:84:A:ILE:HA	1:88:A:ALA:HB1	2	0.14
(1,1289)	1:84:A:ILE:HA	1:88:A:ALA:HB2	2	0.14
(1,1289)	1:84:A:ILE:HA	1:88:A:ALA:HB3	2	0.14
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG21	8	0.14
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG22	8	0.14
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG23	8	0.14
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG21	5	0.14
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG22	5	0.14
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG23	5	0.14
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG21	9	0.14
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG22	9	0.14
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG23	9	0.14
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG21	1	0.14
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG22	1	0.14
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG23	1	0.14
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG21	7	0.14
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG22	7	0.14
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG23	7	0.14
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG21	17	0.14
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG22	17	0.14
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG23	17	0.14
(1,1246)	1:81:A:LYS:HE3	1:82:A:TYR:H	2	0.14
(1,1246)	1:81:A:LYS:HE3	1:82:A:TYR:H	5	0.14
(1,1246)	1:81:A:LYS:HE3	1:82:A:TYR:H	6	0.14
(1,1246)	1:81:A:LYS:HE3	1:82:A:TYR:H	8	0.14
(1,1246)	1:81:A:LYS:HE3	1:82:A:TYR:H	10	0.14
(1,1229)	1:81:A:LYS:H	1:81:A:LYS:HG2	20	0.14
(1,1216)	1:80:A:ASP:H	1:81:A:LYS:HD2	5	0.14
(1,1216)	1:80:A:ASP:H	1:81:A:LYS:HD2	11	0.14
(1,1216)	1:80:A:ASP:H	1:81:A:LYS:HD2	12	0.14
(1,1216)	1:80:A:ASP:H	1:81:A:LYS:HD2	16	0.14
(1,1216)	1:80:A:ASP:H	1:81:A:LYS:HD2	19	0.14
(1,1215)	1:80:A:ASP:HB2	1:81:A:LYS:H	1	0.14
(1,1215)	1:80:A:ASP:HB2	1:81:A:LYS:H	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1215)	1:80:A:ASP:HB2	1:81:A:LYS:H	19	0.14
(1,1197)	1:79:A:LEU:HB3	1:80:A:ASP:H	1	0.14
(1,1197)	1:79:A:LEU:HB3	1:80:A:ASP:H	20	0.14
(1,1196)	1:79:A:LEU:HD21	1:80:A:ASP:H	12	0.14
(1,1196)	1:79:A:LEU:HD22	1:80:A:ASP:H	12	0.14
(1,1196)	1:79:A:LEU:HD23	1:80:A:ASP:H	12	0.14
(1,1193)	1:79:A:LEU:HA	1:80:A:ASP:H	6	0.14
(1,1193)	1:79:A:LEU:HA	1:80:A:ASP:H	7	0.14
(1,1193)	1:79:A:LEU:HA	1:80:A:ASP:H	9	0.14
(1,1193)	1:79:A:LEU:HA	1:80:A:ASP:H	14	0.14
(1,1193)	1:79:A:LEU:HA	1:80:A:ASP:H	15	0.14
(1,1193)	1:79:A:LEU:HA	1:80:A:ASP:H	17	0.14
(1,1193)	1:79:A:LEU:HA	1:80:A:ASP:H	19	0.14
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD11	6	0.14
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD12	6	0.14
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD13	6	0.14
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD11	15	0.14
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD12	15	0.14
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD13	15	0.14
(1,1176)	1:78:A:THR:H	1:81:A:LYS:HA	20	0.14
(1,1169)	1:78:A:THR:HB	1:79:A:LEU:H	13	0.14
(1,1164)	1:78:A:THR:HG21	1:78:A:THR:H	16	0.14
(1,1164)	1:78:A:THR:HG22	1:78:A:THR:H	16	0.14
(1,1164)	1:78:A:THR:HG23	1:78:A:THR:H	16	0.14
(1,1160)	1:77:A:TRP:HB2	1:78:A:THR:H	20	0.14
(1,1153)	1:76:A:HIS:HB3	1:77:A:TRP:H	1	0.14
(1,1148)	1:75:A:THR:HG21	1:77:A:TRP:H	2	0.14
(1,1148)	1:75:A:THR:HG22	1:77:A:TRP:H	2	0.14
(1,1148)	1:75:A:THR:HG23	1:77:A:TRP:H	2	0.14
(1,1148)	1:75:A:THR:HG21	1:77:A:TRP:H	7	0.14
(1,1148)	1:75:A:THR:HG22	1:77:A:TRP:H	7	0.14
(1,1148)	1:75:A:THR:HG23	1:77:A:TRP:H	7	0.14
(1,1148)	1:75:A:THR:HG21	1:77:A:TRP:H	11	0.14
(1,1148)	1:75:A:THR:HG22	1:77:A:TRP:H	11	0.14
(1,1148)	1:75:A:THR:HG23	1:77:A:TRP:H	11	0.14
(1,1148)	1:75:A:THR:HG21	1:77:A:TRP:H	12	0.14
(1,1148)	1:75:A:THR:HG22	1:77:A:TRP:H	12	0.14
(1,1148)	1:75:A:THR:HG23	1:77:A:TRP:H	12	0.14
(1,1141)	1:74:A:LYS:HE3	1:78:A:THR:H	7	0.14
(1,1141)	1:74:A:LYS:HE3	1:78:A:THR:H	16	0.14
(1,1140)	1:74:A:LYS:HA	1:77:A:TRP:H	13	0.14
(1,1138)	1:74:A:LYS:HD3	1:77:A:TRP:H	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1138)	1:74:A:LYS:HD3	1:77:A:TRP:H	9	0.14
(1,1134)	1:74:A:LYS:HG2	1:75:A:THR:H	5	0.14
(1,1129)	1:74:A:LYS:HE2	1:74:A:LYS:HB3	20	0.14
(1,1128)	1:74:A:LYS:HE3	1:74:A:LYS:HB3	7	0.14
(1,1128)	1:74:A:LYS:HE3	1:74:A:LYS:HB3	10	0.14
(1,1121)	1:74:A:LYS:H	1:74:A:LYS:HG3	13	0.14
(1,1113)	1:74:A:LYS:HA	1:74:A:LYS:HE3	1	0.14
(1,1113)	1:74:A:LYS:HA	1:74:A:LYS:HE3	9	0.14
(1,1113)	1:74:A:LYS:HA	1:74:A:LYS:HE3	10	0.14
(1,1113)	1:74:A:LYS:HA	1:74:A:LYS:HE3	17	0.14
(1,1113)	1:74:A:LYS:HA	1:74:A:LYS:HE3	20	0.14
(1,1112)	1:74:A:LYS:HA	1:74:A:LYS:HE2	6	0.14
(1,1108)	1:73:A:LEU:HA	1:74:A:LYS:H	9	0.14
(1,1108)	1:73:A:LEU:HA	1:74:A:LYS:H	12	0.14
(1,1108)	1:73:A:LEU:HA	1:74:A:LYS:H	19	0.14
(1,1081)	1:71:A:TRP:HB2	1:72:A:LEU:H	13	0.14
(1,1081)	1:71:A:TRP:HB2	1:72:A:LEU:H	17	0.14
(1,1061)	1:69:A:ARG:HD3	1:70:A:THR:HB	14	0.14
(1,1061)	1:69:A:ARG:HD3	1:70:A:THR:HB	16	0.14
(1,1061)	1:69:A:ARG:HD3	1:70:A:THR:HB	19	0.14
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD21	19	0.14
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD22	19	0.14
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD23	19	0.14
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD21	20	0.14
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD22	20	0.14
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD23	20	0.14
(1,1053)	1:67:A:LYS:H	1:88:A:ALA:HA	4	0.14
(1,1051)	1:67:A:LYS:HG2	1:69:A:ARG:H	12	0.14
(1,1051)	1:67:A:LYS:HG2	1:69:A:ARG:H	19	0.14
(1,1038)	1:67:A:LYS:H	1:67:A:LYS:HG3	2	0.14
(1,1036)	1:67:A:LYS:HE3	1:67:A:LYS:H	2	0.14
(1,1036)	1:67:A:LYS:HE3	1:67:A:LYS:H	18	0.14
(1,1035)	1:67:A:LYS:HE3	1:67:A:LYS:HG3	17	0.14
(1,1018)	1:65:A:TRP:HB2	1:91:A:GLN:HG3	16	0.14
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD21	14	0.14
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD22	14	0.14
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD23	14	0.14
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG21	16	0.14
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG22	16	0.14
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG23	16	0.14
(1,988)	1:64:A:TRP:H	1:92:A:PHE:HB3	15	0.14
(1,988)	1:64:A:TRP:H	1:92:A:PHE:HB3	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,985)	1:64:A:TRP:H	1:90:A:LEU:HA	16	0.14
(1,981)	1:64:A:TRP:H	1:64:A:TRP:HB3	19	0.14
(1,978)	1:63:A:LEU:HA	1:93:A:THR:H	16	0.14
(1,976)	1:63:A:LEU:HG	1:93:A:THR:H	14	0.14
(1,976)	1:63:A:LEU:HG	1:93:A:THR:H	16	0.14
(1,976)	1:63:A:LEU:HG	1:93:A:THR:H	17	0.14
(1,972)	1:63:A:LEU:HD11	1:91:A:GLN:H	18	0.14
(1,972)	1:63:A:LEU:HD12	1:91:A:GLN:H	18	0.14
(1,972)	1:63:A:LEU:HD13	1:91:A:GLN:H	18	0.14
(1,968)	1:63:A:LEU:HG	1:90:A:LEU:HA	10	0.14
(1,962)	1:63:A:LEU:HD21	1:72:A:LEU:H	8	0.14
(1,962)	1:63:A:LEU:HD22	1:72:A:LEU:H	8	0.14
(1,962)	1:63:A:LEU:HD23	1:72:A:LEU:H	8	0.14
(1,961)	1:63:A:LEU:H	1:70:A:THR:HG21	14	0.14
(1,961)	1:63:A:LEU:H	1:70:A:THR:HG22	14	0.14
(1,961)	1:63:A:LEU:H	1:70:A:THR:HG23	14	0.14
(1,960)	1:67:A:LYS:HG2	1:69:A:ARG:H	12	0.14
(1,960)	1:67:A:LYS:HG2	1:69:A:ARG:H	19	0.14
(1,959)	1:63:A:LEU:H	1:64:A:TRP:H	1	0.14
(1,959)	1:63:A:LEU:H	1:64:A:TRP:H	15	0.14
(1,946)	1:62:A:ALA:H	1:94:A:PRO:HA	2	0.14
(1,945)	1:62:A:ALA:HB1	1:93:A:THR:HA	7	0.14
(1,945)	1:62:A:ALA:HB2	1:93:A:THR:HA	7	0.14
(1,945)	1:62:A:ALA:HB3	1:93:A:THR:HA	7	0.14
(1,944)	1:62:A:ALA:H	1:93:A:THR:HG21	11	0.14
(1,944)	1:62:A:ALA:H	1:93:A:THR:HG22	11	0.14
(1,944)	1:62:A:ALA:H	1:93:A:THR:HG23	11	0.14
(1,941)	1:62:A:ALA:H	1:92:A:PHE:HA	8	0.14
(1,924)	1:61:A:HIS:H	1:61:A:HIS:HB2	8	0.14
(1,910)	1:58:A:TRP:HB3	1:59:A:SER:H	19	0.14
(1,904)	1:58:A:TRP:H	1:58:A:TRP:HB3	1	0.14
(1,904)	1:58:A:TRP:H	1:58:A:TRP:HB3	4	0.14
(1,904)	1:58:A:TRP:H	1:58:A:TRP:HB3	16	0.14
(1,884)	1:56:A:LYS:HE3	1:56:A:LYS:HB3	1	0.14
(1,873)	1:56:A:LYS:HA	1:56:A:LYS:HD3	20	0.14
(1,858)	1:51:A:LYS:H	1:51:A:LYS:HD3	2	0.14
(1,858)	1:51:A:LYS:H	1:51:A:LYS:HD3	3	0.14
(1,858)	1:51:A:LYS:H	1:51:A:LYS:HD3	8	0.14
(1,858)	1:51:A:LYS:H	1:51:A:LYS:HD3	14	0.14
(1,858)	1:51:A:LYS:H	1:51:A:LYS:HD3	17	0.14
(1,841)	1:50:A:GLU:HA	1:50:A:GLU:HG3	2	0.14
(1,841)	1:50:A:GLU:HA	1:50:A:GLU:HG3	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,841)	1:50:A:GLU:HA	1:50:A:GLU:HG3	6	0.14
(1,841)	1:50:A:GLU:HA	1:50:A:GLU:HG3	11	0.14
(1,841)	1:50:A:GLU:HA	1:50:A:GLU:HG3	13	0.14
(1,841)	1:50:A:GLU:HA	1:50:A:GLU:HG3	15	0.14
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD21	14	0.14
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD22	14	0.14
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD23	14	0.14
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD21	14	0.14
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD22	14	0.14
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD23	14	0.14
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD21	14	0.14
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD22	14	0.14
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD23	14	0.14
(1,821)	1:48:A:LEU:HD21	1:63:A:LEU:H	4	0.14
(1,821)	1:48:A:LEU:HD22	1:63:A:LEU:H	4	0.14
(1,821)	1:48:A:LEU:HD23	1:63:A:LEU:H	4	0.14
(1,821)	1:48:A:LEU:HD21	1:63:A:LEU:H	13	0.14
(1,821)	1:48:A:LEU:HD22	1:63:A:LEU:H	13	0.14
(1,821)	1:48:A:LEU:HD23	1:63:A:LEU:H	13	0.14
(1,821)	1:48:A:LEU:HD21	1:63:A:LEU:H	15	0.14
(1,821)	1:48:A:LEU:HD22	1:63:A:LEU:H	15	0.14
(1,821)	1:48:A:LEU:HD23	1:63:A:LEU:H	15	0.14
(1,821)	1:48:A:LEU:HD21	1:63:A:LEU:H	18	0.14
(1,821)	1:48:A:LEU:HD22	1:63:A:LEU:H	18	0.14
(1,821)	1:48:A:LEU:HD23	1:63:A:LEU:H	18	0.14
(1,813)	1:48:A:LEU:H	1:51:A:LYS:H	6	0.14
(1,813)	1:48:A:LEU:H	1:51:A:LYS:H	10	0.14
(1,813)	1:48:A:LEU:H	1:51:A:LYS:H	15	0.14
(1,813)	1:48:A:LEU:H	1:51:A:LYS:H	18	0.14
(1,813)	1:48:A:LEU:H	1:51:A:LYS:H	20	0.14
(1,812)	1:48:A:LEU:HA	1:51:A:LYS:HB3	7	0.14
(1,812)	1:48:A:LEU:HA	1:51:A:LYS:HB3	11	0.14
(1,812)	1:48:A:LEU:HA	1:51:A:LYS:HB3	16	0.14
(1,812)	1:48:A:LEU:HA	1:51:A:LYS:HB3	17	0.14
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG21	15	0.14
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG22	15	0.14
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG23	15	0.14
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG21	17	0.14
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG22	17	0.14
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG23	17	0.14
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG21	20	0.14
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG22	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG23	20	0.14
(1,773)	1:47:A:LYS:H	1:47:A:LYS:HD3	1	0.14
(1,773)	1:47:A:LYS:H	1:47:A:LYS:HD3	8	0.14
(1,766)	1:46:A:LEU:HA	1:50:A:GLU:H	3	0.14
(1,766)	1:46:A:LEU:HA	1:50:A:GLU:H	5	0.14
(1,764)	1:46:A:LEU:HA	1:49:A:VAL:H	19	0.14
(1,746)	1:45:A:MET:HG3	1:63:A:LEU:HD21	9	0.14
(1,746)	1:45:A:MET:HG3	1:63:A:LEU:HD22	9	0.14
(1,746)	1:45:A:MET:HG3	1:63:A:LEU:HD23	9	0.14
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG21	10	0.14
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG22	10	0.14
(1,742)	1:45:A:MET:HA	1:49:A:VAL:HG23	10	0.14
(1,739)	1:45:A:MET:HG3	1:48:A:LEU:H	19	0.14
(1,737)	1:45:A:MET:HB3	1:48:A:LEU:H	5	0.14
(1,737)	1:45:A:MET:HB3	1:48:A:LEU:H	7	0.14
(1,737)	1:45:A:MET:HB3	1:48:A:LEU:H	8	0.14
(1,737)	1:45:A:MET:HB3	1:48:A:LEU:H	10	0.14
(1,737)	1:45:A:MET:HB3	1:48:A:LEU:H	11	0.14
(1,728)	1:45:A:MET:HG3	1:46:A:LEU:H	19	0.14
(1,719)	1:44:A:VAL:HG11	1:90:A:LEU:H	7	0.14
(1,719)	1:44:A:VAL:HG12	1:90:A:LEU:H	7	0.14
(1,719)	1:44:A:VAL:HG13	1:90:A:LEU:H	7	0.14
(1,712)	1:44:A:VAL:H	1:46:A:LEU:HG	19	0.14
(1,692)	1:43:A:GLY:H	1:44:A:VAL:HB	8	0.14
(1,692)	1:43:A:GLY:H	1:44:A:VAL:HB	18	0.14
(1,684)	1:42:A:GLY:HA3	1:75:A:THR:HB	5	0.14
(1,683)	1:42:A:GLY:H	1:74:A:LYS:HE3	7	0.14
(1,673)	1:41:A:ILE:H	1:77:A:TRP:H	13	0.14
(1,663)	1:41:A:ILE:HG21	1:72:A:LEU:HG	3	0.14
(1,663)	1:41:A:ILE:HG22	1:72:A:LEU:HG	3	0.14
(1,663)	1:41:A:ILE:HG23	1:72:A:LEU:HG	3	0.14
(1,663)	1:41:A:ILE:HG21	1:72:A:LEU:HG	18	0.14
(1,663)	1:41:A:ILE:HG22	1:72:A:LEU:HG	18	0.14
(1,663)	1:41:A:ILE:HG23	1:72:A:LEU:HG	18	0.14
(1,659)	1:41:A:ILE:HD11	1:44:A:VAL:H	9	0.14
(1,659)	1:41:A:ILE:HD12	1:44:A:VAL:H	9	0.14
(1,659)	1:41:A:ILE:HD13	1:44:A:VAL:H	9	0.14
(1,659)	1:41:A:ILE:HD11	1:44:A:VAL:H	17	0.14
(1,659)	1:41:A:ILE:HD12	1:44:A:VAL:H	17	0.14
(1,659)	1:41:A:ILE:HD13	1:44:A:VAL:H	17	0.14
(1,640)	1:41:A:ILE:H	1:41:A:ILE:HG12	2	0.14
(1,640)	1:41:A:ILE:H	1:41:A:ILE:HG12	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,640)	1:41:A:ILE:H	1:41:A:ILE:HG12	4	0.14
(1,640)	1:41:A:ILE:H	1:41:A:ILE:HG12	5	0.14
(1,640)	1:41:A:ILE:H	1:41:A:ILE:HG12	7	0.14
(1,640)	1:41:A:ILE:H	1:41:A:ILE:HG12	11	0.14
(1,640)	1:41:A:ILE:H	1:41:A:ILE:HG12	16	0.14
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG11	19	0.14
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG12	19	0.14
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG13	19	0.14
(1,628)	1:40:A:HIS:H	1:44:A:VAL:HB	13	0.14
(1,611)	1:39:A:VAL:HG11	1:78:A:THR:H	6	0.14
(1,611)	1:39:A:VAL:HG12	1:78:A:THR:H	6	0.14
(1,611)	1:39:A:VAL:HG13	1:78:A:THR:H	6	0.14
(1,611)	1:39:A:VAL:HG11	1:78:A:THR:H	10	0.14
(1,611)	1:39:A:VAL:HG12	1:78:A:THR:H	10	0.14
(1,611)	1:39:A:VAL:HG13	1:78:A:THR:H	10	0.14
(1,610)	1:39:A:VAL:HG21	1:80:A:ASP:H	3	0.14
(1,610)	1:39:A:VAL:HG22	1:80:A:ASP:H	3	0.14
(1,610)	1:39:A:VAL:HG23	1:80:A:ASP:H	3	0.14
(1,607)	1:39:A:VAL:H	1:79:A:LEU:H	2	0.14
(1,602)	1:39:A:VAL:HG21	1:43:A:GLY:H	13	0.14
(1,602)	1:39:A:VAL:HG22	1:43:A:GLY:H	13	0.14
(1,602)	1:39:A:VAL:HG23	1:43:A:GLY:H	13	0.14
(1,602)	1:39:A:VAL:HG21	1:43:A:GLY:H	17	0.14
(1,602)	1:39:A:VAL:HG22	1:43:A:GLY:H	17	0.14
(1,602)	1:39:A:VAL:HG23	1:43:A:GLY:H	17	0.14
(1,599)	1:39:A:VAL:H	1:40:A:HIS:H	6	0.14
(1,588)	1:38:A:GLU:HA	1:80:A:ASP:H	1	0.14
(1,588)	1:38:A:GLU:HA	1:80:A:ASP:H	10	0.14
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG21	15	0.14
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG22	15	0.14
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG23	15	0.14
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG21	18	0.14
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG22	18	0.14
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG23	18	0.14
(1,580)	1:38:A:GLU:HB3	1:39:A:VAL:H	2	0.14
(1,580)	1:38:A:GLU:HB3	1:39:A:VAL:H	16	0.14
(1,572)	1:37:A:GLY:H	1:80:A:ASP:H	13	0.14
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD21	12	0.14
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD22	12	0.14
(1,571)	1:37:A:GLY:H	1:79:A:LEU:HD23	12	0.14
(1,554)	1:36:A:THR:H	1:38:A:GLU:HB3	7	0.14
(1,554)	1:36:A:THR:H	1:38:A:GLU:HB3	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,554)	1:36:A:THR:H	1:38:A:GLU:HB3	10	0.14
(1,554)	1:36:A:THR:H	1:38:A:GLU:HB3	14	0.14
(1,554)	1:36:A:THR:H	1:38:A:GLU:HB3	17	0.14
(1,554)	1:36:A:THR:H	1:38:A:GLU:HB3	20	0.14
(1,527)	1:34:A:ARG:H	1:51:A:LYS:HD3	5	0.14
(1,527)	1:34:A:ARG:H	1:51:A:LYS:HD3	10	0.14
(1,515)	1:34:A:ARG:H	1:34:A:ARG:HB3	18	0.14
(1,511)	1:33:A:LEU:HD21	1:48:A:LEU:HB3	18	0.14
(1,511)	1:33:A:LEU:HD22	1:48:A:LEU:HB3	18	0.14
(1,511)	1:33:A:LEU:HD23	1:48:A:LEU:HB3	18	0.14
(1,505)	1:33:A:LEU:HD21	1:47:A:LYS:H	14	0.14
(1,505)	1:33:A:LEU:HD22	1:47:A:LYS:H	14	0.14
(1,505)	1:33:A:LEU:HD23	1:47:A:LYS:H	14	0.14
(1,503)	1:33:A:LEU:HB2	1:35:A:VAL:HG11	16	0.14
(1,503)	1:33:A:LEU:HB2	1:35:A:VAL:HG12	16	0.14
(1,503)	1:33:A:LEU:HB2	1:35:A:VAL:HG13	16	0.14
(1,499)	1:33:A:LEU:HD21	1:34:A:ARG:H	8	0.14
(1,499)	1:33:A:LEU:HD22	1:34:A:ARG:H	8	0.14
(1,499)	1:33:A:LEU:HD23	1:34:A:ARG:H	8	0.14
(1,487)	1:33:A:LEU:H	1:33:A:LEU:HD11	6	0.14
(1,487)	1:33:A:LEU:H	1:33:A:LEU:HD12	6	0.14
(1,487)	1:33:A:LEU:H	1:33:A:LEU:HD13	6	0.14
(1,484)	1:32:A:THR:HA	1:51:A:LYS:HD3	18	0.14
(1,482)	1:32:A:THR:HA	1:34:A:ARG:H	7	0.14
(1,482)	1:32:A:THR:HA	1:34:A:ARG:H	16	0.14
(1,473)	1:32:A:THR:HB	1:32:A:THR:H	1	0.14
(1,473)	1:32:A:THR:HB	1:32:A:THR:H	4	0.14
(1,473)	1:32:A:THR:HB	1:32:A:THR:H	9	0.14
(1,473)	1:32:A:THR:HB	1:32:A:THR:H	12	0.14
(1,453)	1:29:A:ARG:HB2	1:31:A:VAL:HA	7	0.14
(1,453)	1:29:A:ARG:HB2	1:31:A:VAL:HA	10	0.14
(1,443)	1:29:A:ARG:HB2	1:29:A:ARG:H	1	0.14
(1,443)	1:29:A:ARG:HB2	1:29:A:ARG:H	6	0.14
(1,432)	1:28:A:ASN:H	1:28:A:ASN:HB2	2	0.14
(1,432)	1:28:A:ASN:H	1:28:A:ASN:HB2	7	0.14
(1,431)	1:27:A:VAL:H	1:93:A:THR:HB	20	0.14
(1,426)	1:27:A:VAL:H	1:28:A:ASN:HB2	16	0.14
(1,414)	1:25:A:THR:H	1:93:A:THR:HG21	18	0.14
(1,414)	1:25:A:THR:H	1:93:A:THR:HG22	18	0.14
(1,414)	1:25:A:THR:H	1:93:A:THR:HG23	18	0.14
(1,409)	1:25:A:THR:H	1:92:A:PHE:HB2	8	0.14
(1,409)	1:25:A:THR:H	1:92:A:PHE:HB2	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,409)	1:25:A:THR:H	1:92:A:PHE:HB2	14	0.14
(1,395)	1:25:A:THR:HB	1:25:A:THR:H	3	0.14
(1,395)	1:25:A:THR:HB	1:25:A:THR:H	15	0.14
(1,383)	1:24:A:VAL:HA	1:31:A:VAL:H	15	0.14
(1,377)	1:24:A:VAL:HA	1:30:A:ASP:HA	4	0.14
(1,377)	1:24:A:VAL:HA	1:30:A:ASP:HA	17	0.14
(1,350)	1:23:A:HIS:HB2	1:91:A:GLN:HG3	3	0.14
(1,350)	1:23:A:HIS:HB2	1:91:A:GLN:HG3	18	0.14
(1,329)	1:23:A:HIS:HB2	1:24:A:VAL:HA	6	0.14
(1,323)	1:23:A:HIS:HB2	1:24:A:VAL:H	2	0.14
(1,323)	1:23:A:HIS:HB2	1:24:A:VAL:H	3	0.14
(1,323)	1:23:A:HIS:HB2	1:24:A:VAL:H	5	0.14
(1,323)	1:23:A:HIS:HB2	1:24:A:VAL:H	7	0.14
(1,312)	1:22:A:VAL:HG21	1:90:A:LEU:H	2	0.14
(1,312)	1:22:A:VAL:HG22	1:90:A:LEU:H	2	0.14
(1,312)	1:22:A:VAL:HG23	1:90:A:LEU:H	2	0.14
(1,312)	1:22:A:VAL:HG21	1:90:A:LEU:H	7	0.14
(1,312)	1:22:A:VAL:HG22	1:90:A:LEU:H	7	0.14
(1,312)	1:22:A:VAL:HG23	1:90:A:LEU:H	7	0.14
(1,312)	1:22:A:VAL:HG21	1:90:A:LEU:H	11	0.14
(1,312)	1:22:A:VAL:HG22	1:90:A:LEU:H	11	0.14
(1,312)	1:22:A:VAL:HG23	1:90:A:LEU:H	11	0.14
(1,294)	1:22:A:VAL:HG11	1:29:A:ARG:H	10	0.14
(1,294)	1:22:A:VAL:HG12	1:29:A:ARG:H	10	0.14
(1,294)	1:22:A:VAL:HG13	1:29:A:ARG:H	10	0.14
(1,293)	1:22:A:VAL:HG21	1:24:A:VAL:H	2	0.14
(1,293)	1:22:A:VAL:HG22	1:24:A:VAL:H	2	0.14
(1,293)	1:22:A:VAL:HG23	1:24:A:VAL:H	2	0.14
(1,280)	1:21:A:SER:HB3	1:90:A:LEU:H	10	0.14
(1,280)	1:21:A:SER:HB3	1:90:A:LEU:H	16	0.14
(1,280)	1:21:A:SER:HB3	1:90:A:LEU:H	19	0.14
(1,275)	1:21:A:SER:H	1:32:A:THR:HB	8	0.14
(1,275)	1:21:A:SER:H	1:32:A:THR:HB	19	0.14
(1,261)	1:20:A:LEU:HD11	1:90:A:LEU:HA	6	0.14
(1,261)	1:20:A:LEU:HD12	1:90:A:LEU:HA	6	0.14
(1,261)	1:20:A:LEU:HD13	1:90:A:LEU:HA	6	0.14
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB1	2	0.14
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB2	2	0.14
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB3	2	0.14
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB1	2	0.14
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB2	2	0.14
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB3	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB1	2	0.14
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB2	2	0.14
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB3	2	0.14
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB1	3	0.14
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB2	3	0.14
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB3	3	0.14
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB1	3	0.14
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB2	3	0.14
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB3	3	0.14
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB1	3	0.14
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB2	3	0.14
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB3	3	0.14
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB1	11	0.14
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB2	11	0.14
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB3	11	0.14
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB1	11	0.14
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB2	11	0.14
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB3	11	0.14
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB1	11	0.14
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB2	11	0.14
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB3	11	0.14
(1,251)	1:20:A:LEU:HG	1:35:A:VAL:H	2	0.14
(1,250)	1:20:A:LEU:H	1:35:A:VAL:H	3	0.14
(1,249)	1:20:A:LEU:HB2	1:34:A:ARG:H	4	0.14
(1,249)	1:20:A:LEU:HB2	1:34:A:ARG:H	14	0.14
(1,244)	1:20:A:LEU:HD21	1:33:A:LEU:HA	3	0.14
(1,244)	1:20:A:LEU:HD22	1:33:A:LEU:HA	3	0.14
(1,244)	1:20:A:LEU:HD23	1:33:A:LEU:HA	3	0.14
(1,244)	1:20:A:LEU:HD21	1:33:A:LEU:HA	12	0.14
(1,244)	1:20:A:LEU:HD22	1:33:A:LEU:HA	12	0.14
(1,244)	1:20:A:LEU:HD23	1:33:A:LEU:HA	12	0.14
(1,242)	1:20:A:LEU:HB3	1:33:A:LEU:H	3	0.14
(1,234)	1:20:A:LEU:HB3	1:21:A:SER:H	4	0.14
(1,208)	1:19:A:GLU:HG2	1:32:A:THR:HB	5	0.14
(1,206)	1:19:A:GLU:H	1:20:A:LEU:HB2	6	0.14
(1,204)	1:19:A:GLU:HG2	1:20:A:LEU:H	2	0.14
(1,204)	1:19:A:GLU:HG2	1:20:A:LEU:H	5	0.14
(1,204)	1:19:A:GLU:HG2	1:20:A:LEU:H	10	0.14
(1,204)	1:19:A:GLU:HG2	1:20:A:LEU:H	11	0.14
(1,184)	1:18:A:TRP:HE1	1:80:A:ASP:HB3	11	0.14
(1,177)	1:18:A:TRP:HE1	1:36:A:THR:HB	4	0.14
(1,169)	1:18:A:TRP:H	1:18:A:TRP:HD1	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,166)	1:17:A:THR:HG21	1:18:A:TRP:H	11	0.14
(1,166)	1:17:A:THR:HG22	1:18:A:TRP:H	11	0.14
(1,166)	1:17:A:THR:HG23	1:18:A:TRP:H	11	0.14
(1,166)	1:17:A:THR:HG21	1:18:A:TRP:H	12	0.14
(1,166)	1:17:A:THR:HG22	1:18:A:TRP:H	12	0.14
(1,166)	1:17:A:THR:HG23	1:18:A:TRP:H	12	0.14
(1,166)	1:17:A:THR:HG21	1:18:A:TRP:H	16	0.14
(1,166)	1:17:A:THR:HG22	1:18:A:TRP:H	16	0.14
(1,166)	1:17:A:THR:HG23	1:18:A:TRP:H	16	0.14
(1,156)	1:16:A:GLY:HA2	1:17:A:THR:H	10	0.14
(1,153)	1:15:A:ASP:H	1:17:A:THR:H	19	0.14
(1,142)	1:14:A:ALA:HA	1:15:A:ASP:H	3	0.14
(1,140)	1:13:A:TYR:HB3	1:15:A:ASP:H	19	0.14
(1,128)	1:11:A:GLY:H	1:12:A:CYS:H	8	0.14
(1,127)	1:11:A:GLY:HA2	1:12:A:CYS:H	6	0.14
(1,112)	1:9:A:PRO:HG3	1:10:A:ASP:H	3	0.14
(1,112)	1:9:A:PRO:HG3	1:10:A:ASP:H	11	0.14
(1,102)	1:8:A:MET:HB3	1:12:A:CYS:H	20	0.14
(1,89)	1:8:A:MET:H	1:8:A:MET:HG2	4	0.14
(1,87)	1:7:A:ARG:HG3	1:10:A:ASP:H	14	0.14
(1,87)	1:7:A:ARG:HG3	1:10:A:ASP:H	17	0.14
(1,85)	1:7:A:ARG:HD3	1:8:A:MET:H	2	0.14
(1,85)	1:7:A:ARG:HD3	1:8:A:MET:H	4	0.14
(1,82)	1:7:A:ARG:HB2	1:8:A:MET:H	10	0.14
(1,67)	1:6:A:ILE:H	1:10:A:ASP:H	18	0.14
(1,65)	1:6:A:ILE:HA	1:7:A:ARG:H	4	0.14
(1,65)	1:6:A:ILE:HA	1:7:A:ARG:H	14	0.14
(1,58)	1:6:A:ILE:H	1:6:A:ILE:HG21	11	0.14
(1,58)	1:6:A:ILE:H	1:6:A:ILE:HG22	11	0.14
(1,58)	1:6:A:ILE:H	1:6:A:ILE:HG23	11	0.14
(1,49)	1:5:A:GLY:HA3	1:6:A:ILE:HB	4	0.14
(1,49)	1:5:A:GLY:HA3	1:6:A:ILE:HB	20	0.14
(1,39)	1:4:A:ASP:H	1:4:A:ASP:HB3	5	0.14
(3,16)	1:42:A:GLY:O	1:46:A:LEU:H	2	0.13
(3,16)	1:42:A:GLY:O	1:46:A:LEU:H	3	0.13
(3,16)	1:42:A:GLY:O	1:46:A:LEU:H	9	0.13
(3,16)	1:42:A:GLY:O	1:46:A:LEU:H	10	0.13
(3,13)	1:92:A:PHE:O	1:64:A:TRP:H	1	0.13
(3,13)	1:92:A:PHE:O	1:64:A:TRP:H	2	0.13
(3,13)	1:92:A:PHE:O	1:64:A:TRP:H	4	0.13
(3,13)	1:92:A:PHE:O	1:64:A:TRP:H	6	0.13
(3,13)	1:92:A:PHE:O	1:64:A:TRP:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,13)	1:92:A:PHE:O	1:64:A:TRP:H	8	0.13
(3,13)	1:92:A:PHE:O	1:64:A:TRP:H	16	0.13
(3,13)	1:92:A:PHE:O	1:64:A:TRP:H	19	0.13
(2,25)	1:77:A:TRP:O	1:81:A:LYS:N	2	0.13
(2,24)	1:45:A:MET:O	1:49:A:VAL:N	5	0.13
(2,24)	1:45:A:MET:O	1:49:A:VAL:N	6	0.13
(2,24)	1:45:A:MET:O	1:49:A:VAL:N	7	0.13
(2,24)	1:45:A:MET:O	1:49:A:VAL:N	18	0.13
(2,21)	1:39:A:VAL:O	1:43:A:GLY:N	7	0.13
(2,21)	1:39:A:VAL:O	1:43:A:GLY:N	9	0.13
(2,21)	1:39:A:VAL:O	1:43:A:GLY:N	10	0.13
(1,1408)	1:92:A:PHE:HB3	1:93:A:THR:H	5	0.13
(1,1408)	1:92:A:PHE:HB3	1:93:A:THR:H	16	0.13
(1,1408)	1:92:A:PHE:HB3	1:93:A:THR:H	20	0.13
(1,1397)	1:91:A:GLN:HB2	1:92:A:PHE:HA	11	0.13
(1,1382)	1:91:A:GLN:HG2	1:91:A:GLN:HE21	2	0.13
(1,1382)	1:91:A:GLN:HG2	1:91:A:GLN:HE21	7	0.13
(1,1382)	1:91:A:GLN:HG2	1:91:A:GLN:HE21	8	0.13
(1,1382)	1:91:A:GLN:HG2	1:91:A:GLN:HE21	14	0.13
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD11	11	0.13
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD12	11	0.13
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD13	11	0.13
(1,1329)	1:87:A:ASP:HB3	1:88:A:ALA:H	1	0.13
(1,1329)	1:87:A:ASP:HB3	1:88:A:ALA:H	3	0.13
(1,1329)	1:87:A:ASP:HB3	1:88:A:ALA:H	5	0.13
(1,1329)	1:87:A:ASP:HB3	1:88:A:ALA:H	12	0.13
(1,1329)	1:87:A:ASP:HB3	1:88:A:ALA:H	13	0.13
(1,1313)	1:85:A:GLN:HB3	1:87:A:ASP:H	11	0.13
(1,1294)	1:85:A:GLN:H	1:85:A:GLN:HG3	9	0.13
(1,1294)	1:85:A:GLN:H	1:85:A:GLN:HG3	17	0.13
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG21	12	0.13
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG22	12	0.13
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG23	12	0.13
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG21	2	0.13
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG22	2	0.13
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG23	2	0.13
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG21	17	0.13
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG22	17	0.13
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG23	17	0.13
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG21	18	0.13
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG22	18	0.13
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG23	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG21	2	0.13
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG22	2	0.13
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG23	2	0.13
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG21	18	0.13
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG22	18	0.13
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG23	18	0.13
(1,1246)	1:81:A:LYS:HE3	1:82:A:TYR:H	17	0.13
(1,1246)	1:81:A:LYS:HE3	1:82:A:TYR:H	19	0.13
(1,1225)	1:81:A:LYS:HA	1:81:A:LYS:HG2	1	0.13
(1,1225)	1:81:A:LYS:HA	1:81:A:LYS:HG2	6	0.13
(1,1225)	1:81:A:LYS:HA	1:81:A:LYS:HG2	7	0.13
(1,1225)	1:81:A:LYS:HA	1:81:A:LYS:HG2	10	0.13
(1,1225)	1:81:A:LYS:HA	1:81:A:LYS:HG2	14	0.13
(1,1225)	1:81:A:LYS:HA	1:81:A:LYS:HG2	17	0.13
(1,1216)	1:80:A:ASP:H	1:81:A:LYS:HD2	3	0.13
(1,1215)	1:80:A:ASP:HB2	1:81:A:LYS:H	7	0.13
(1,1215)	1:80:A:ASP:HB2	1:81:A:LYS:H	9	0.13
(1,1215)	1:80:A:ASP:HB2	1:81:A:LYS:H	10	0.13
(1,1215)	1:80:A:ASP:HB2	1:81:A:LYS:H	18	0.13
(1,1202)	1:79:A:LEU:HA	1:82:A:TYR:H	18	0.13
(1,1197)	1:79:A:LEU:HB3	1:80:A:ASP:H	2	0.13
(1,1197)	1:79:A:LEU:HB3	1:80:A:ASP:H	9	0.13
(1,1196)	1:79:A:LEU:HD21	1:80:A:ASP:H	4	0.13
(1,1196)	1:79:A:LEU:HD22	1:80:A:ASP:H	4	0.13
(1,1196)	1:79:A:LEU:HD23	1:80:A:ASP:H	4	0.13
(1,1196)	1:79:A:LEU:HD21	1:80:A:ASP:H	15	0.13
(1,1196)	1:79:A:LEU:HD22	1:80:A:ASP:H	15	0.13
(1,1196)	1:79:A:LEU:HD23	1:80:A:ASP:H	15	0.13
(1,1193)	1:79:A:LEU:HA	1:80:A:ASP:H	1	0.13
(1,1193)	1:79:A:LEU:HA	1:80:A:ASP:H	2	0.13
(1,1193)	1:79:A:LEU:HA	1:80:A:ASP:H	3	0.13
(1,1193)	1:79:A:LEU:HA	1:80:A:ASP:H	4	0.13
(1,1193)	1:79:A:LEU:HA	1:80:A:ASP:H	5	0.13
(1,1193)	1:79:A:LEU:HA	1:80:A:ASP:H	10	0.13
(1,1193)	1:79:A:LEU:HA	1:80:A:ASP:H	11	0.13
(1,1193)	1:79:A:LEU:HA	1:80:A:ASP:H	12	0.13
(1,1193)	1:79:A:LEU:HA	1:80:A:ASP:H	16	0.13
(1,1193)	1:79:A:LEU:HA	1:80:A:ASP:H	18	0.13
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD11	18	0.13
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD12	18	0.13
(1,1188)	1:79:A:LEU:H	1:79:A:LEU:HD13	18	0.13
(1,1177)	1:78:A:THR:H	1:81:A:LYS:H	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1176)	1:78:A:THR:H	1:81:A:LYS:HA	7	0.13
(1,1176)	1:78:A:THR:H	1:81:A:LYS:HA	10	0.13
(1,1176)	1:78:A:THR:H	1:81:A:LYS:HA	17	0.13
(1,1169)	1:78:A:THR:HB	1:79:A:LEU:H	8	0.13
(1,1169)	1:78:A:THR:HB	1:79:A:LEU:H	18	0.13
(1,1164)	1:78:A:THR:HG21	1:78:A:THR:H	2	0.13
(1,1164)	1:78:A:THR:HG22	1:78:A:THR:H	2	0.13
(1,1164)	1:78:A:THR:HG23	1:78:A:THR:H	2	0.13
(1,1161)	1:77:A:TRP:H	1:81:A:LYS:HD3	1	0.13
(1,1161)	1:77:A:TRP:H	1:81:A:LYS:HD3	9	0.13
(1,1161)	1:77:A:TRP:H	1:81:A:LYS:HD3	10	0.13
(1,1157)	1:77:A:TRP:H	1:77:A:TRP:HB3	20	0.13
(1,1153)	1:76:A:HIS:HB3	1:77:A:TRP:H	8	0.13
(1,1148)	1:75:A:THR:HG21	1:77:A:TRP:H	3	0.13
(1,1148)	1:75:A:THR:HG22	1:77:A:TRP:H	3	0.13
(1,1148)	1:75:A:THR:HG23	1:77:A:TRP:H	3	0.13
(1,1148)	1:75:A:THR:HG21	1:77:A:TRP:H	4	0.13
(1,1148)	1:75:A:THR:HG22	1:77:A:TRP:H	4	0.13
(1,1148)	1:75:A:THR:HG23	1:77:A:TRP:H	4	0.13
(1,1148)	1:75:A:THR:HG21	1:77:A:TRP:H	16	0.13
(1,1148)	1:75:A:THR:HG22	1:77:A:TRP:H	16	0.13
(1,1148)	1:75:A:THR:HG23	1:77:A:TRP:H	16	0.13
(1,1148)	1:75:A:THR:HG21	1:77:A:TRP:H	19	0.13
(1,1148)	1:75:A:THR:HG22	1:77:A:TRP:H	19	0.13
(1,1148)	1:75:A:THR:HG23	1:77:A:TRP:H	19	0.13
(1,1138)	1:74:A:LYS:HD3	1:77:A:TRP:H	17	0.13
(1,1134)	1:74:A:LYS:HG2	1:75:A:THR:H	4	0.13
(1,1134)	1:74:A:LYS:HG2	1:75:A:THR:H	8	0.13
(1,1129)	1:74:A:LYS:HE2	1:74:A:LYS:HB3	15	0.13
(1,1128)	1:74:A:LYS:HE3	1:74:A:LYS:HB3	11	0.13
(1,1121)	1:74:A:LYS:H	1:74:A:LYS:HG3	11	0.13
(1,1113)	1:74:A:LYS:HA	1:74:A:LYS:HE3	7	0.13
(1,1112)	1:74:A:LYS:HA	1:74:A:LYS:HE2	5	0.13
(1,1112)	1:74:A:LYS:HA	1:74:A:LYS:HE2	16	0.13
(1,1112)	1:74:A:LYS:HA	1:74:A:LYS:HE2	17	0.13
(1,1105)	1:73:A:LEU:H	1:73:A:LEU:HB3	20	0.13
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD11	18	0.13
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD12	18	0.13
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD13	18	0.13
(1,1081)	1:71:A:TRP:HB2	1:72:A:LEU:H	7	0.13
(1,1080)	1:71:A:TRP:HB3	1:72:A:LEU:H	7	0.13
(1,1076)	1:71:A:TRP:H	1:71:A:TRP:HB3	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1076)	1:71:A:TRP:H	1:71:A:TRP:HB3	14	0.13
(1,1075)	1:71:A:TRP:H	1:71:A:TRP:HB2	7	0.13
(1,1074)	1:70:A:THR:HG21	1:72:A:LEU:H	20	0.13
(1,1074)	1:70:A:THR:HG22	1:72:A:LEU:H	20	0.13
(1,1074)	1:70:A:THR:HG23	1:72:A:LEU:H	20	0.13
(1,1066)	1:70:A:THR:HB	1:70:A:THR:H	2	0.13
(1,1064)	1:69:A:ARG:HB2	1:70:A:THR:H	5	0.13
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD21	12	0.13
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD22	12	0.13
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD23	12	0.13
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD21	13	0.13
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD22	13	0.13
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD23	13	0.13
(1,1053)	1:67:A:LYS:H	1:88:A:ALA:HA	15	0.13
(1,1038)	1:67:A:LYS:H	1:67:A:LYS:HG3	5	0.13
(1,1038)	1:67:A:LYS:H	1:67:A:LYS:HG3	6	0.13
(1,1038)	1:67:A:LYS:H	1:67:A:LYS:HG3	11	0.13
(1,1038)	1:67:A:LYS:H	1:67:A:LYS:HG3	14	0.13
(1,1036)	1:67:A:LYS:HE3	1:67:A:LYS:H	15	0.13
(1,1018)	1:65:A:TRP:HB2	1:91:A:GLN:HG3	10	0.13
(1,1016)	1:65:A:TRP:HB2	1:90:A:LEU:HD21	16	0.13
(1,1016)	1:65:A:TRP:HB2	1:90:A:LEU:HD22	16	0.13
(1,1016)	1:65:A:TRP:HB2	1:90:A:LEU:HD23	16	0.13
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD21	1	0.13
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD22	1	0.13
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD23	1	0.13
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG21	18	0.13
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG22	18	0.13
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG23	18	0.13
(1,1003)	1:65:A:TRP:H	1:70:A:THR:H	15	0.13
(1,999)	1:65:A:TRP:HA	1:67:A:LYS:H	18	0.13
(1,997)	1:65:A:TRP:HB3	1:66:A:GLU:H	15	0.13
(1,997)	1:65:A:TRP:HB3	1:66:A:GLU:H	16	0.13
(1,994)	1:65:A:TRP:H	1:65:A:TRP:HB2	20	0.13
(1,988)	1:64:A:TRP:H	1:92:A:PHE:HB3	2	0.13
(1,988)	1:64:A:TRP:H	1:92:A:PHE:HB3	13	0.13
(1,985)	1:64:A:TRP:H	1:90:A:LEU:HA	11	0.13
(1,972)	1:63:A:LEU:HD11	1:91:A:GLN:H	3	0.13
(1,972)	1:63:A:LEU:HD12	1:91:A:GLN:H	3	0.13
(1,972)	1:63:A:LEU:HD13	1:91:A:GLN:H	3	0.13
(1,972)	1:63:A:LEU:HD11	1:91:A:GLN:H	5	0.13
(1,972)	1:63:A:LEU:HD12	1:91:A:GLN:H	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,972)	1:63:A:LEU:HD13	1:91:A:GLN:H	5	0.13
(1,972)	1:63:A:LEU:HD11	1:91:A:GLN:H	10	0.13
(1,972)	1:63:A:LEU:HD12	1:91:A:GLN:H	10	0.13
(1,972)	1:63:A:LEU:HD13	1:91:A:GLN:H	10	0.13
(1,968)	1:63:A:LEU:HG	1:90:A:LEU:HA	11	0.13
(1,968)	1:63:A:LEU:HG	1:90:A:LEU:HA	18	0.13
(1,968)	1:63:A:LEU:HG	1:90:A:LEU:HA	20	0.13
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD11	20	0.13
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD12	20	0.13
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD13	20	0.13
(1,961)	1:63:A:LEU:H	1:70:A:THR:HG21	19	0.13
(1,961)	1:63:A:LEU:H	1:70:A:THR:HG22	19	0.13
(1,961)	1:63:A:LEU:H	1:70:A:THR:HG23	19	0.13
(1,959)	1:63:A:LEU:H	1:64:A:TRP:H	10	0.13
(1,959)	1:63:A:LEU:H	1:64:A:TRP:H	12	0.13
(1,950)	1:63:A:LEU:H	1:63:A:LEU:HG	15	0.13
(1,946)	1:62:A:ALA:H	1:94:A:PRO:HA	7	0.13
(1,945)	1:62:A:ALA:HB1	1:93:A:THR:HA	2	0.13
(1,945)	1:62:A:ALA:HB2	1:93:A:THR:HA	2	0.13
(1,945)	1:62:A:ALA:HB3	1:93:A:THR:HA	2	0.13
(1,945)	1:62:A:ALA:HB1	1:93:A:THR:HA	13	0.13
(1,945)	1:62:A:ALA:HB2	1:93:A:THR:HA	13	0.13
(1,945)	1:62:A:ALA:HB3	1:93:A:THR:HA	13	0.13
(1,942)	1:62:A:ALA:HB1	1:92:A:PHE:HA	1	0.13
(1,942)	1:62:A:ALA:HB2	1:92:A:PHE:HA	1	0.13
(1,942)	1:62:A:ALA:HB3	1:92:A:PHE:HA	1	0.13
(1,941)	1:62:A:ALA:H	1:92:A:PHE:HA	12	0.13
(1,940)	1:62:A:ALA:HB1	1:92:A:PHE:H	19	0.13
(1,940)	1:62:A:ALA:HB2	1:92:A:PHE:H	19	0.13
(1,940)	1:62:A:ALA:HB3	1:92:A:PHE:H	19	0.13
(1,930)	1:61:A:HIS:HB2	1:63:A:LEU:H	18	0.13
(1,924)	1:61:A:HIS:H	1:61:A:HIS:HB2	9	0.13
(1,923)	1:61:A:HIS:H	1:61:A:HIS:HB3	19	0.13
(1,920)	1:60:A:ASP:H	1:60:A:ASP:HB3	10	0.13
(1,904)	1:58:A:TRP:H	1:58:A:TRP:HB3	6	0.13
(1,904)	1:58:A:TRP:H	1:58:A:TRP:HB3	18	0.13
(1,893)	1:56:A:LYS:HB3	1:57:A:ASP:H	2	0.13
(1,889)	1:56:A:LYS:HA	1:57:A:ASP:HB3	9	0.13
(1,889)	1:56:A:LYS:HA	1:57:A:ASP:HB3	19	0.13
(1,869)	1:52:A:LEU:H	1:52:A:LEU:HD21	6	0.13
(1,869)	1:52:A:LEU:H	1:52:A:LEU:HD22	6	0.13
(1,869)	1:52:A:LEU:H	1:52:A:LEU:HD23	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:51:A:LYS:H	1:51:A:LYS:HD3	1	0.13
(1,858)	1:51:A:LYS:H	1:51:A:LYS:HD3	11	0.13
(1,858)	1:51:A:LYS:H	1:51:A:LYS:HD3	15	0.13
(1,856)	1:51:A:LYS:HE3	1:51:A:LYS:H	14	0.13
(1,852)	1:51:A:LYS:HA	1:51:A:LYS:HD3	5	0.13
(1,852)	1:51:A:LYS:HA	1:51:A:LYS:HD3	11	0.13
(1,838)	1:49:A:VAL:HG21	1:58:A:TRP:H	4	0.13
(1,838)	1:49:A:VAL:HG22	1:58:A:TRP:H	4	0.13
(1,838)	1:49:A:VAL:HG23	1:58:A:TRP:H	4	0.13
(1,838)	1:49:A:VAL:HG21	1:58:A:TRP:H	18	0.13
(1,838)	1:49:A:VAL:HG22	1:58:A:TRP:H	18	0.13
(1,838)	1:49:A:VAL:HG23	1:58:A:TRP:H	18	0.13
(1,821)	1:48:A:LEU:HD21	1:63:A:LEU:H	20	0.13
(1,821)	1:48:A:LEU:HD22	1:63:A:LEU:H	20	0.13
(1,821)	1:48:A:LEU:HD23	1:63:A:LEU:H	20	0.13
(1,813)	1:48:A:LEU:H	1:51:A:LYS:H	3	0.13
(1,813)	1:48:A:LEU:H	1:51:A:LYS:H	5	0.13
(1,812)	1:48:A:LEU:HA	1:51:A:LYS:HB3	4	0.13
(1,812)	1:48:A:LEU:HA	1:51:A:LYS:HB3	5	0.13
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG21	19	0.13
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG22	19	0.13
(1,800)	1:48:A:LEU:HA	1:49:A:VAL:HG23	19	0.13
(1,794)	1:48:A:LEU:H	1:48:A:LEU:HD11	18	0.13
(1,794)	1:48:A:LEU:H	1:48:A:LEU:HD12	18	0.13
(1,794)	1:48:A:LEU:H	1:48:A:LEU:HD13	18	0.13
(1,695)	1:43:A:GLY:HA2	1:46:A:LEU:H	16	0.13
(1,694)	1:43:A:GLY:H	1:45:A:MET:H	14	0.13
(1,692)	1:43:A:GLY:H	1:44:A:VAL:HB	15	0.13
(1,688)	1:42:A:GLY:H	1:75:A:THR:HG21	20	0.13
(1,688)	1:42:A:GLY:H	1:75:A:THR:HG22	20	0.13
(1,688)	1:42:A:GLY:H	1:75:A:THR:HG23	20	0.13
(1,684)	1:42:A:GLY:HA3	1:75:A:THR:HB	2	0.13
(1,684)	1:42:A:GLY:HA3	1:75:A:THR:HB	15	0.13
(1,683)	1:42:A:GLY:H	1:74:A:LYS:HE3	2	0.13
(1,683)	1:42:A:GLY:H	1:74:A:LYS:HE3	5	0.13
(1,683)	1:42:A:GLY:H	1:74:A:LYS:HE3	8	0.13
(1,676)	1:41:A:ILE:HG13	1:78:A:THR:H	3	0.13
(1,671)	1:41:A:ILE:HD11	1:75:A:THR:HA	7	0.13
(1,671)	1:41:A:ILE:HD12	1:75:A:THR:HA	7	0.13
(1,671)	1:41:A:ILE:HD13	1:75:A:THR:HA	7	0.13
(1,671)	1:41:A:ILE:HD11	1:75:A:THR:HA	11	0.13
(1,671)	1:41:A:ILE:HD12	1:75:A:THR:HA	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,671)	1:41:A:ILE:HD13	1:75:A:THR:HA	11	0.13
(1,663)	1:41:A:ILE:HG21	1:72:A:LEU:HG	13	0.13
(1,663)	1:41:A:ILE:HG22	1:72:A:LEU:HG	13	0.13
(1,663)	1:41:A:ILE:HG23	1:72:A:LEU:HG	13	0.13
(1,641)	1:41:A:ILE:H	1:41:A:ILE:HD11	17	0.13
(1,641)	1:41:A:ILE:H	1:41:A:ILE:HD12	17	0.13
(1,641)	1:41:A:ILE:H	1:41:A:ILE:HD13	17	0.13
(1,640)	1:41:A:ILE:H	1:41:A:ILE:HG12	9	0.13
(1,640)	1:41:A:ILE:H	1:41:A:ILE:HG12	15	0.13
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG11	7	0.13
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG12	7	0.13
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG13	7	0.13
(1,617)	1:40:A:HIS:HB3	1:41:A:ILE:H	6	0.13
(1,611)	1:39:A:VAL:HG11	1:78:A:THR:H	16	0.13
(1,611)	1:39:A:VAL:HG12	1:78:A:THR:H	16	0.13
(1,611)	1:39:A:VAL:HG13	1:78:A:THR:H	16	0.13
(1,610)	1:39:A:VAL:HG21	1:80:A:ASP:H	4	0.13
(1,610)	1:39:A:VAL:HG22	1:80:A:ASP:H	4	0.13
(1,610)	1:39:A:VAL:HG23	1:80:A:ASP:H	4	0.13
(1,610)	1:39:A:VAL:HG21	1:80:A:ASP:H	7	0.13
(1,610)	1:39:A:VAL:HG22	1:80:A:ASP:H	7	0.13
(1,610)	1:39:A:VAL:HG23	1:80:A:ASP:H	7	0.13
(1,610)	1:39:A:VAL:HG21	1:80:A:ASP:H	14	0.13
(1,610)	1:39:A:VAL:HG22	1:80:A:ASP:H	14	0.13
(1,610)	1:39:A:VAL:HG23	1:80:A:ASP:H	14	0.13
(1,610)	1:39:A:VAL:HG21	1:80:A:ASP:H	17	0.13
(1,610)	1:39:A:VAL:HG22	1:80:A:ASP:H	17	0.13
(1,610)	1:39:A:VAL:HG23	1:80:A:ASP:H	17	0.13
(1,607)	1:39:A:VAL:H	1:79:A:LEU:H	11	0.13
(1,607)	1:39:A:VAL:H	1:79:A:LEU:H	16	0.13
(1,602)	1:39:A:VAL:HG21	1:43:A:GLY:H	8	0.13
(1,602)	1:39:A:VAL:HG22	1:43:A:GLY:H	8	0.13
(1,602)	1:39:A:VAL:HG23	1:43:A:GLY:H	8	0.13
(1,602)	1:39:A:VAL:HG21	1:43:A:GLY:H	10	0.13
(1,602)	1:39:A:VAL:HG22	1:43:A:GLY:H	10	0.13
(1,602)	1:39:A:VAL:HG23	1:43:A:GLY:H	10	0.13
(1,602)	1:39:A:VAL:HG21	1:43:A:GLY:H	18	0.13
(1,602)	1:39:A:VAL:HG22	1:43:A:GLY:H	18	0.13
(1,602)	1:39:A:VAL:HG23	1:43:A:GLY:H	18	0.13
(1,599)	1:39:A:VAL:H	1:40:A:HIS:H	15	0.13
(1,588)	1:38:A:GLU:HA	1:80:A:ASP:H	18	0.13
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG21	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG22	6	0.13
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG23	6	0.13
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG21	10	0.13
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG22	10	0.13
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG23	10	0.13
(1,580)	1:38:A:GLU:HB3	1:39:A:VAL:H	19	0.13
(1,561)	1:37:A:GLY:H	1:38:A:GLU:HG3	5	0.13
(1,561)	1:37:A:GLY:H	1:38:A:GLU:HG3	15	0.13
(1,561)	1:37:A:GLY:H	1:38:A:GLU:HG3	20	0.13
(1,554)	1:36:A:THR:H	1:38:A:GLU:HB3	1	0.13
(1,554)	1:36:A:THR:H	1:38:A:GLU:HB3	18	0.13
(1,527)	1:34:A:ARG:H	1:51:A:LYS:HD3	1	0.13
(1,527)	1:34:A:ARG:H	1:51:A:LYS:HD3	2	0.13
(1,527)	1:34:A:ARG:H	1:51:A:LYS:HD3	9	0.13
(1,527)	1:34:A:ARG:H	1:51:A:LYS:HD3	12	0.13
(1,527)	1:34:A:ARG:H	1:51:A:LYS:HD3	13	0.13
(1,527)	1:34:A:ARG:H	1:51:A:LYS:HD3	20	0.13
(1,514)	1:33:A:LEU:HD21	1:50:A:GLU:H	12	0.13
(1,514)	1:33:A:LEU:HD22	1:50:A:GLU:H	12	0.13
(1,514)	1:33:A:LEU:HD23	1:50:A:GLU:H	12	0.13
(1,499)	1:33:A:LEU:HD21	1:34:A:ARG:H	2	0.13
(1,499)	1:33:A:LEU:HD22	1:34:A:ARG:H	2	0.13
(1,499)	1:33:A:LEU:HD23	1:34:A:ARG:H	2	0.13
(1,499)	1:33:A:LEU:HD21	1:34:A:ARG:H	20	0.13
(1,499)	1:33:A:LEU:HD22	1:34:A:ARG:H	20	0.13
(1,499)	1:33:A:LEU:HD23	1:34:A:ARG:H	20	0.13
(1,497)	1:33:A:LEU:HB3	1:34:A:ARG:H	13	0.13
(1,483)	1:32:A:THR:H	1:34:A:ARG:H	20	0.13
(1,473)	1:32:A:THR:HB	1:32:A:THR:H	10	0.13
(1,473)	1:32:A:THR:HB	1:32:A:THR:H	11	0.13
(1,473)	1:32:A:THR:HB	1:32:A:THR:H	13	0.13
(1,473)	1:32:A:THR:HB	1:32:A:THR:H	14	0.13
(1,473)	1:32:A:THR:HB	1:32:A:THR:H	15	0.13
(1,473)	1:32:A:THR:HB	1:32:A:THR:H	17	0.13
(1,473)	1:32:A:THR:HB	1:32:A:THR:H	19	0.13
(1,473)	1:32:A:THR:HB	1:32:A:THR:H	20	0.13
(1,438)	1:29:A:ARG:HD3	1:29:A:ARG:HA	8	0.13
(1,431)	1:27:A:VAL:H	1:93:A:THR:HB	14	0.13
(1,426)	1:27:A:VAL:H	1:28:A:ASN:HB2	3	0.13
(1,426)	1:27:A:VAL:H	1:28:A:ASN:HB2	13	0.13
(1,414)	1:25:A:THR:H	1:93:A:THR:HG21	5	0.13
(1,414)	1:25:A:THR:H	1:93:A:THR:HG22	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,414)	1:25:A:THR:H	1:93:A:THR:HG23	5	0.13
(1,414)	1:25:A:THR:H	1:93:A:THR:HG21	9	0.13
(1,414)	1:25:A:THR:H	1:93:A:THR:HG22	9	0.13
(1,414)	1:25:A:THR:H	1:93:A:THR:HG23	9	0.13
(1,414)	1:25:A:THR:H	1:93:A:THR:HG21	13	0.13
(1,414)	1:25:A:THR:H	1:93:A:THR:HG22	13	0.13
(1,414)	1:25:A:THR:H	1:93:A:THR:HG23	13	0.13
(1,392)	1:24:A:VAL:HB	1:92:A:PHE:H	9	0.13
(1,392)	1:24:A:VAL:HB	1:92:A:PHE:H	16	0.13
(1,390)	1:24:A:VAL:HG21	1:91:A:GLN:H	10	0.13
(1,390)	1:24:A:VAL:HG22	1:91:A:GLN:H	10	0.13
(1,390)	1:24:A:VAL:HG23	1:91:A:GLN:H	10	0.13
(1,383)	1:24:A:VAL:HA	1:31:A:VAL:H	7	0.13
(1,383)	1:24:A:VAL:HA	1:31:A:VAL:H	13	0.13
(1,377)	1:24:A:VAL:HA	1:30:A:ASP:HA	1	0.13
(1,377)	1:24:A:VAL:HA	1:30:A:ASP:HA	13	0.13
(1,371)	1:24:A:VAL:HG11	1:29:A:ARG:H	7	0.13
(1,371)	1:24:A:VAL:HG12	1:29:A:ARG:H	7	0.13
(1,371)	1:24:A:VAL:HG13	1:29:A:ARG:H	7	0.13
(1,370)	1:24:A:VAL:H	1:29:A:ARG:H	13	0.13
(1,369)	1:24:A:VAL:H	1:29:A:ARG:HG3	8	0.13
(1,350)	1:23:A:HIS:HB2	1:91:A:GLN:HG3	15	0.13
(1,339)	1:23:A:HIS:H	1:90:A:LEU:H	6	0.13
(1,339)	1:23:A:HIS:H	1:90:A:LEU:H	17	0.13
(1,339)	1:23:A:HIS:H	1:90:A:LEU:H	20	0.13
(1,312)	1:22:A:VAL:HG21	1:90:A:LEU:H	5	0.13
(1,312)	1:22:A:VAL:HG22	1:90:A:LEU:H	5	0.13
(1,312)	1:22:A:VAL:HG23	1:90:A:LEU:H	5	0.13
(1,312)	1:22:A:VAL:HG21	1:90:A:LEU:H	8	0.13
(1,312)	1:22:A:VAL:HG22	1:90:A:LEU:H	8	0.13
(1,312)	1:22:A:VAL:HG23	1:90:A:LEU:H	8	0.13
(1,312)	1:22:A:VAL:HG21	1:90:A:LEU:H	10	0.13
(1,312)	1:22:A:VAL:HG22	1:90:A:LEU:H	10	0.13
(1,312)	1:22:A:VAL:HG23	1:90:A:LEU:H	10	0.13
(1,312)	1:22:A:VAL:HG21	1:90:A:LEU:H	13	0.13
(1,312)	1:22:A:VAL:HG22	1:90:A:LEU:H	13	0.13
(1,312)	1:22:A:VAL:HG23	1:90:A:LEU:H	13	0.13
(1,312)	1:22:A:VAL:HG21	1:90:A:LEU:H	18	0.13
(1,312)	1:22:A:VAL:HG22	1:90:A:LEU:H	18	0.13
(1,312)	1:22:A:VAL:HG23	1:90:A:LEU:H	18	0.13
(1,299)	1:22:A:VAL:H	1:32:A:THR:HB	2	0.13
(1,299)	1:22:A:VAL:H	1:32:A:THR:HB	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:22:A:VAL:H	1:32:A:THR:HB	7	0.13
(1,299)	1:22:A:VAL:H	1:32:A:THR:HB	10	0.13
(1,299)	1:22:A:VAL:H	1:32:A:THR:HB	12	0.13
(1,299)	1:22:A:VAL:H	1:32:A:THR:HB	16	0.13
(1,280)	1:21:A:SER:HB3	1:90:A:LEU:H	2	0.13
(1,280)	1:21:A:SER:HB3	1:90:A:LEU:H	15	0.13
(1,259)	1:20:A:LEU:HD21	1:88:A:ALA:H	4	0.13
(1,259)	1:20:A:LEU:HD22	1:88:A:ALA:H	4	0.13
(1,259)	1:20:A:LEU:HD23	1:88:A:ALA:H	4	0.13
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB1	1	0.13
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB2	1	0.13
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB3	1	0.13
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB1	1	0.13
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB2	1	0.13
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB3	1	0.13
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB1	1	0.13
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB2	1	0.13
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB3	1	0.13
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB1	10	0.13
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB2	10	0.13
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB3	10	0.13
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB1	10	0.13
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB2	10	0.13
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB3	10	0.13
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB1	10	0.13
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB2	10	0.13
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB3	10	0.13
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB1	14	0.13
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB2	14	0.13
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB3	14	0.13
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB1	14	0.13
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB2	14	0.13
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB3	14	0.13
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB1	14	0.13
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB2	14	0.13
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB3	14	0.13
(1,251)	1:20:A:LEU:HG	1:35:A:VAL:H	7	0.13
(1,251)	1:20:A:LEU:HG	1:35:A:VAL:H	9	0.13
(1,251)	1:20:A:LEU:HG	1:35:A:VAL:H	11	0.13
(1,250)	1:20:A:LEU:H	1:35:A:VAL:H	14	0.13
(1,249)	1:20:A:LEU:HB2	1:34:A:ARG:H	15	0.13
(1,242)	1:20:A:LEU:HB3	1:33:A:LEU:H	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:20:A:LEU:HB3	1:33:A:LEU:H	13	0.13
(1,236)	1:20:A:LEU:HD21	1:21:A:SER:H	19	0.13
(1,236)	1:20:A:LEU:HD22	1:21:A:SER:H	19	0.13
(1,236)	1:20:A:LEU:HD23	1:21:A:SER:H	19	0.13
(1,212)	1:19:A:GLU:HB2	1:33:A:LEU:H	5	0.13
(1,212)	1:19:A:GLU:HB2	1:33:A:LEU:H	17	0.13
(1,208)	1:19:A:GLU:HG2	1:32:A:THR:HB	13	0.13
(1,204)	1:19:A:GLU:HG2	1:20:A:LEU:H	15	0.13
(1,204)	1:19:A:GLU:HG2	1:20:A:LEU:H	20	0.13
(1,176)	1:18:A:TRP:H	1:36:A:THR:H	16	0.13
(1,176)	1:18:A:TRP:H	1:36:A:THR:H	17	0.13
(1,148)	1:15:A:ASP:HA	1:16:A:GLY:H	6	0.13
(1,147)	1:15:A:ASP:H	1:15:A:ASP:HB2	3	0.13
(1,147)	1:15:A:ASP:H	1:15:A:ASP:HB2	16	0.13
(1,127)	1:11:A:GLY:HA2	1:12:A:CYS:H	9	0.13
(1,115)	1:9:A:PRO:HA	1:13:A:TYR:H	4	0.13
(1,102)	1:8:A:MET:HB3	1:12:A:CYS:H	1	0.13
(1,102)	1:8:A:MET:HB3	1:12:A:CYS:H	19	0.13
(1,100)	1:8:A:MET:H	1:12:A:CYS:HA	9	0.13
(1,95)	1:8:A:MET:HA	1:10:A:ASP:H	17	0.13
(1,94)	1:8:A:MET:H	1:10:A:ASP:HA	6	0.13
(1,90)	1:8:A:MET:H	1:8:A:MET:HG3	20	0.13
(1,89)	1:8:A:MET:H	1:8:A:MET:HG2	17	0.13
(1,87)	1:7:A:ARG:HG3	1:10:A:ASP:H	5	0.13
(1,86)	1:7:A:ARG:HA	1:10:A:ASP:H	6	0.13
(1,85)	1:7:A:ARG:HD3	1:8:A:MET:H	7	0.13
(1,62)	1:6:A:ILE:HG21	1:7:A:ARG:H	6	0.13
(1,62)	1:6:A:ILE:HG22	1:7:A:ARG:H	6	0.13
(1,62)	1:6:A:ILE:HG23	1:7:A:ARG:H	6	0.13
(1,62)	1:6:A:ILE:HG21	1:7:A:ARG:H	17	0.13
(1,62)	1:6:A:ILE:HG22	1:7:A:ARG:H	17	0.13
(1,62)	1:6:A:ILE:HG23	1:7:A:ARG:H	17	0.13
(1,43)	1:4:A:ASP:HB3	1:5:A:GLY:H	8	0.13
(1,42)	1:4:A:ASP:H	1:5:A:GLY:HA3	13	0.13
(1,40)	1:4:A:ASP:HA	1:5:A:GLY:H	19	0.13
(1,39)	1:4:A:ASP:H	1:4:A:ASP:HB3	11	0.13
(1,36)	1:3:A:LEU:HB3	1:4:A:ASP:H	12	0.13
(1,34)	1:3:A:LEU:HD21	1:4:A:ASP:H	20	0.13
(1,34)	1:3:A:LEU:HD22	1:4:A:ASP:H	20	0.13
(1,34)	1:3:A:LEU:HD23	1:4:A:ASP:H	20	0.13
(1,28)	1:3:A:LEU:H	1:3:A:LEU:HB2	14	0.13
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD11	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD12	11	0.13
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD13	11	0.13
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD11	13	0.13
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD12	13	0.13
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD13	13	0.13
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD11	16	0.13
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD12	16	0.13
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD13	16	0.13
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD11	17	0.13
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD12	17	0.13
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD13	17	0.13
(1,20)	1:2:A:ALA:HB1	1:4:A:ASP:H	6	0.13
(1,20)	1:2:A:ALA:HB2	1:4:A:ASP:H	6	0.13
(1,20)	1:2:A:ALA:HB3	1:4:A:ASP:H	6	0.13
(1,20)	1:2:A:ALA:HB1	1:4:A:ASP:H	7	0.13
(1,20)	1:2:A:ALA:HB2	1:4:A:ASP:H	7	0.13
(1,20)	1:2:A:ALA:HB3	1:4:A:ASP:H	7	0.13
(1,16)	1:2:A:ALA:H	1:3:A:LEU:HB3	2	0.13
(1,1)	1:1:A:MET:HA	1:1:A:MET:HG3	14	0.13
(1,1)	1:1:A:MET:HA	1:1:A:MET:HG3	19	0.13
(3,16)	1:42:A:GLY:O	1:46:A:LEU:H	5	0.12
(3,16)	1:42:A:GLY:O	1:46:A:LEU:H	11	0.12
(3,16)	1:42:A:GLY:O	1:46:A:LEU:H	14	0.12
(3,16)	1:42:A:GLY:O	1:46:A:LEU:H	16	0.12
(3,14)	1:91:A:GLN:O	1:23:A:HIS:H	6	0.12
(2,25)	1:77:A:TRP:O	1:81:A:LYS:N	11	0.12
(2,24)	1:45:A:MET:O	1:49:A:VAL:N	3	0.12
(2,24)	1:45:A:MET:O	1:49:A:VAL:N	8	0.12
(2,21)	1:39:A:VAL:O	1:43:A:GLY:N	17	0.12
(2,14)	1:64:A:TRP:O	1:92:A:PHE:N	6	0.12
(2,3)	1:20:A:LEU:O	1:33:A:LEU:N	5	0.12
(1,1397)	1:91:A:GLN:HB2	1:92:A:PHE:HA	5	0.12
(1,1388)	1:91:A:GLN:HE21	1:91:A:GLN:HB2	15	0.12
(1,1382)	1:91:A:GLN:HG2	1:91:A:GLN:HE21	18	0.12
(1,1381)	1:91:A:GLN:H	1:91:A:GLN:HG2	9	0.12
(1,1381)	1:91:A:GLN:H	1:91:A:GLN:HG2	14	0.12
(1,1355)	1:90:A:LEU:H	1:90:A:LEU:HD21	20	0.12
(1,1355)	1:90:A:LEU:H	1:90:A:LEU:HD22	20	0.12
(1,1355)	1:90:A:LEU:H	1:90:A:LEU:HD23	20	0.12
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD11	6	0.12
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD12	6	0.12
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD13	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD11	9	0.12
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD12	9	0.12
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD13	9	0.12
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD11	15	0.12
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD12	15	0.12
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD13	15	0.12
(1,1330)	1:87:A:ASP:H	1:88:A:ALA:HA	8	0.12
(1,1329)	1:87:A:ASP:HB3	1:88:A:ALA:H	4	0.12
(1,1329)	1:87:A:ASP:HB3	1:88:A:ALA:H	7	0.12
(1,1329)	1:87:A:ASP:HB3	1:88:A:ALA:H	20	0.12
(1,1326)	1:87:A:ASP:HB2	1:88:A:ALA:H	19	0.12
(1,1313)	1:85:A:GLN:HB3	1:87:A:ASP:H	2	0.12
(1,1313)	1:85:A:GLN:HB3	1:87:A:ASP:H	6	0.12
(1,1294)	1:85:A:GLN:H	1:85:A:GLN:HG3	6	0.12
(1,1294)	1:85:A:GLN:H	1:85:A:GLN:HG3	8	0.12
(1,1294)	1:85:A:GLN:H	1:85:A:GLN:HG3	11	0.12
(1,1294)	1:85:A:GLN:H	1:85:A:GLN:HG3	12	0.12
(1,1294)	1:85:A:GLN:H	1:85:A:GLN:HG3	14	0.12
(1,1294)	1:85:A:GLN:H	1:85:A:GLN:HG3	19	0.12
(1,1289)	1:84:A:ILE:HA	1:88:A:ALA:HB1	6	0.12
(1,1289)	1:84:A:ILE:HA	1:88:A:ALA:HB2	6	0.12
(1,1289)	1:84:A:ILE:HA	1:88:A:ALA:HB3	6	0.12
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG21	6	0.12
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG22	6	0.12
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG23	6	0.12
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG21	11	0.12
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG22	11	0.12
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG23	11	0.12
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG21	10	0.12
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG22	10	0.12
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG23	10	0.12
(1,1255)	1:82:A:TYR:HB3	1:83:A:GLY:H	16	0.12
(1,1246)	1:81:A:LYS:HE3	1:82:A:TYR:H	3	0.12
(1,1225)	1:81:A:LYS:HA	1:81:A:LYS:HG2	2	0.12
(1,1225)	1:81:A:LYS:HA	1:81:A:LYS:HG2	4	0.12
(1,1225)	1:81:A:LYS:HA	1:81:A:LYS:HG2	5	0.12
(1,1225)	1:81:A:LYS:HA	1:81:A:LYS:HG2	8	0.12
(1,1225)	1:81:A:LYS:HA	1:81:A:LYS:HG2	9	0.12
(1,1225)	1:81:A:LYS:HA	1:81:A:LYS:HG2	11	0.12
(1,1225)	1:81:A:LYS:HA	1:81:A:LYS:HG2	12	0.12
(1,1225)	1:81:A:LYS:HA	1:81:A:LYS:HG2	16	0.12
(1,1225)	1:81:A:LYS:HA	1:81:A:LYS:HG2	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1221)	1:80:A:ASP:HB3	1:83:A:GLY:H	19	0.12
(1,1218)	1:80:A:ASP:HB2	1:82:A:TYR:H	8	0.12
(1,1218)	1:80:A:ASP:HB2	1:82:A:TYR:H	13	0.12
(1,1218)	1:80:A:ASP:HB2	1:82:A:TYR:H	19	0.12
(1,1215)	1:80:A:ASP:HB2	1:81:A:LYS:H	8	0.12
(1,1211)	1:80:A:ASP:H	1:80:A:ASP:HB2	13	0.12
(1,1197)	1:79:A:LEU:HB3	1:80:A:ASP:H	10	0.12
(1,1196)	1:79:A:LEU:HD21	1:80:A:ASP:H	5	0.12
(1,1196)	1:79:A:LEU:HD22	1:80:A:ASP:H	5	0.12
(1,1196)	1:79:A:LEU:HD23	1:80:A:ASP:H	5	0.12
(1,1196)	1:79:A:LEU:HD21	1:80:A:ASP:H	9	0.12
(1,1196)	1:79:A:LEU:HD22	1:80:A:ASP:H	9	0.12
(1,1196)	1:79:A:LEU:HD23	1:80:A:ASP:H	9	0.12
(1,1196)	1:79:A:LEU:HD21	1:80:A:ASP:H	18	0.12
(1,1196)	1:79:A:LEU:HD22	1:80:A:ASP:H	18	0.12
(1,1196)	1:79:A:LEU:HD23	1:80:A:ASP:H	18	0.12
(1,1193)	1:79:A:LEU:HA	1:80:A:ASP:H	20	0.12
(1,1180)	1:78:A:THR:H	1:81:A:LYS:HB3	18	0.12
(1,1176)	1:78:A:THR:H	1:81:A:LYS:HA	1	0.12
(1,1176)	1:78:A:THR:H	1:81:A:LYS:HA	9	0.12
(1,1176)	1:78:A:THR:H	1:81:A:LYS:HA	14	0.12
(1,1171)	1:78:A:THR:HB	1:80:A:ASP:H	3	0.12
(1,1171)	1:78:A:THR:HB	1:80:A:ASP:H	4	0.12
(1,1164)	1:78:A:THR:HG21	1:78:A:THR:H	11	0.12
(1,1164)	1:78:A:THR:HG22	1:78:A:THR:H	11	0.12
(1,1164)	1:78:A:THR:HG23	1:78:A:THR:H	11	0.12
(1,1162)	1:77:A:TRP:H	1:81:A:LYS:HE3	13	0.12
(1,1161)	1:77:A:TRP:H	1:81:A:LYS:HD3	7	0.12
(1,1161)	1:77:A:TRP:H	1:81:A:LYS:HD3	14	0.12
(1,1161)	1:77:A:TRP:H	1:81:A:LYS:HD3	17	0.12
(1,1160)	1:77:A:TRP:HB2	1:78:A:THR:H	18	0.12
(1,1158)	1:77:A:TRP:H	1:78:A:THR:H	13	0.12
(1,1157)	1:77:A:TRP:H	1:77:A:TRP:HB3	18	0.12
(1,1157)	1:77:A:TRP:H	1:77:A:TRP:HB3	19	0.12
(1,1153)	1:76:A:HIS:HB3	1:77:A:TRP:H	15	0.12
(1,1148)	1:75:A:THR:HG21	1:77:A:TRP:H	5	0.12
(1,1148)	1:75:A:THR:HG22	1:77:A:TRP:H	5	0.12
(1,1148)	1:75:A:THR:HG23	1:77:A:TRP:H	5	0.12
(1,1144)	1:75:A:THR:H	1:75:A:THR:HG21	20	0.12
(1,1144)	1:75:A:THR:H	1:75:A:THR:HG22	20	0.12
(1,1144)	1:75:A:THR:H	1:75:A:THR:HG23	20	0.12
(1,1140)	1:74:A:LYS:HA	1:77:A:TRP:H	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1140)	1:74:A:LYS:HA	1:77:A:TRP:H	8	0.12
(1,1132)	1:74:A:LYS:HG3	1:75:A:THR:H	7	0.12
(1,1129)	1:74:A:LYS:HE2	1:74:A:LYS:HB3	9	0.12
(1,1129)	1:74:A:LYS:HE2	1:74:A:LYS:HB3	17	0.12
(1,1129)	1:74:A:LYS:HE2	1:74:A:LYS:HB3	18	0.12
(1,1121)	1:74:A:LYS:H	1:74:A:LYS:HG3	2	0.12
(1,1121)	1:74:A:LYS:H	1:74:A:LYS:HG3	5	0.12
(1,1121)	1:74:A:LYS:H	1:74:A:LYS:HG3	10	0.12
(1,1121)	1:74:A:LYS:H	1:74:A:LYS:HG3	18	0.12
(1,1121)	1:74:A:LYS:H	1:74:A:LYS:HG3	19	0.12
(1,1120)	1:74:A:LYS:H	1:74:A:LYS:HG2	13	0.12
(1,1105)	1:73:A:LEU:H	1:73:A:LEU:HB3	18	0.12
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD11	20	0.12
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD12	20	0.12
(1,1103)	1:73:A:LEU:H	1:73:A:LEU:HD13	20	0.12
(1,1081)	1:71:A:TRP:HB2	1:72:A:LEU:H	2	0.12
(1,1078)	1:71:A:TRP:H	1:72:A:LEU:HD11	13	0.12
(1,1078)	1:71:A:TRP:H	1:72:A:LEU:HD12	13	0.12
(1,1078)	1:71:A:TRP:H	1:72:A:LEU:HD13	13	0.12
(1,1078)	1:71:A:TRP:H	1:72:A:LEU:HD11	20	0.12
(1,1078)	1:71:A:TRP:H	1:72:A:LEU:HD12	20	0.12
(1,1078)	1:71:A:TRP:H	1:72:A:LEU:HD13	20	0.12
(1,1076)	1:71:A:TRP:H	1:71:A:TRP:HB3	13	0.12
(1,1076)	1:71:A:TRP:H	1:71:A:TRP:HB3	16	0.12
(1,1076)	1:71:A:TRP:H	1:71:A:TRP:HB3	19	0.12
(1,1066)	1:70:A:THR:HB	1:70:A:THR:H	14	0.12
(1,1063)	1:69:A:ARG:H	1:70:A:THR:H	14	0.12
(1,1063)	1:69:A:ARG:H	1:70:A:THR:H	19	0.12
(1,1061)	1:69:A:ARG:HD3	1:70:A:THR:HB	10	0.12
(1,1061)	1:69:A:ARG:HD3	1:70:A:THR:HB	20	0.12
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD21	1	0.12
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD22	1	0.12
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD23	1	0.12
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD21	3	0.12
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD22	3	0.12
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD23	3	0.12
(1,1053)	1:67:A:LYS:H	1:88:A:ALA:HA	19	0.12
(1,1052)	1:67:A:LYS:H	1:72:A:LEU:HD11	13	0.12
(1,1052)	1:67:A:LYS:H	1:72:A:LEU:HD12	13	0.12
(1,1052)	1:67:A:LYS:H	1:72:A:LEU:HD13	13	0.12
(1,1051)	1:67:A:LYS:HG2	1:69:A:ARG:H	7	0.12
(1,1051)	1:67:A:LYS:HG2	1:69:A:ARG:H	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1051)	1:67:A:LYS:HG2	1:69:A:ARG:H	9	0.12
(1,1051)	1:67:A:LYS:HG2	1:69:A:ARG:H	10	0.12
(1,1051)	1:67:A:LYS:HG2	1:69:A:ARG:H	13	0.12
(1,1049)	1:67:A:LYS:HB3	1:69:A:ARG:HA	3	0.12
(1,1038)	1:67:A:LYS:H	1:67:A:LYS:HG3	12	0.12
(1,1038)	1:67:A:LYS:H	1:67:A:LYS:HG3	16	0.12
(1,1038)	1:67:A:LYS:H	1:67:A:LYS:HG3	19	0.12
(1,1036)	1:67:A:LYS:HE3	1:67:A:LYS:H	6	0.12
(1,1036)	1:67:A:LYS:HE3	1:67:A:LYS:H	19	0.12
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD21	2	0.12
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD22	2	0.12
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD23	2	0.12
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD21	15	0.12
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD22	15	0.12
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD23	15	0.12
(1,1010)	1:65:A:TRP:H	1:72:A:LEU:H	1	0.12
(1,1003)	1:65:A:TRP:H	1:70:A:THR:H	8	0.12
(1,992)	1:64:A:TRP:H	1:93:A:THR:HG1	15	0.12
(1,988)	1:64:A:TRP:H	1:92:A:PHE:HB3	1	0.12
(1,988)	1:64:A:TRP:H	1:92:A:PHE:HB3	9	0.12
(1,988)	1:64:A:TRP:H	1:92:A:PHE:HB3	11	0.12
(1,988)	1:64:A:TRP:H	1:92:A:PHE:HB3	19	0.12
(1,985)	1:64:A:TRP:H	1:90:A:LEU:HA	7	0.12
(1,985)	1:64:A:TRP:H	1:90:A:LEU:HA	10	0.12
(1,985)	1:64:A:TRP:H	1:90:A:LEU:HA	13	0.12
(1,985)	1:64:A:TRP:H	1:90:A:LEU:HA	14	0.12
(1,983)	1:64:A:TRP:HB2	1:65:A:TRP:H	13	0.12
(1,976)	1:63:A:LEU:HG	1:93:A:THR:H	13	0.12
(1,968)	1:63:A:LEU:HG	1:90:A:LEU:HA	4	0.12
(1,968)	1:63:A:LEU:HG	1:90:A:LEU:HA	7	0.12
(1,968)	1:63:A:LEU:HG	1:90:A:LEU:HA	12	0.12
(1,962)	1:63:A:LEU:HD21	1:72:A:LEU:H	3	0.12
(1,962)	1:63:A:LEU:HD22	1:72:A:LEU:H	3	0.12
(1,962)	1:63:A:LEU:HD23	1:72:A:LEU:H	3	0.12
(1,960)	1:67:A:LYS:HG2	1:69:A:ARG:H	7	0.12
(1,960)	1:67:A:LYS:HG2	1:69:A:ARG:H	8	0.12
(1,960)	1:67:A:LYS:HG2	1:69:A:ARG:H	9	0.12
(1,960)	1:67:A:LYS:HG2	1:69:A:ARG:H	10	0.12
(1,960)	1:67:A:LYS:HG2	1:69:A:ARG:H	13	0.12
(1,959)	1:63:A:LEU:H	1:64:A:TRP:H	5	0.12
(1,946)	1:62:A:ALA:H	1:94:A:PRO:HA	3	0.12
(1,945)	1:62:A:ALA:HB1	1:93:A:THR:HA	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,945)	1:62:A:ALA:HB2	1:93:A:THR:HA	18	0.12
(1,945)	1:62:A:ALA:HB3	1:93:A:THR:HA	18	0.12
(1,942)	1:62:A:ALA:HB1	1:92:A:PHE:HA	15	0.12
(1,942)	1:62:A:ALA:HB2	1:92:A:PHE:HA	15	0.12
(1,942)	1:62:A:ALA:HB3	1:92:A:PHE:HA	15	0.12
(1,924)	1:61:A:HIS:H	1:61:A:HIS:HB2	14	0.12
(1,923)	1:61:A:HIS:H	1:61:A:HIS:HB3	1	0.12
(1,923)	1:61:A:HIS:H	1:61:A:HIS:HB3	15	0.12
(1,904)	1:58:A:TRP:H	1:58:A:TRP:HB3	3	0.12
(1,904)	1:58:A:TRP:H	1:58:A:TRP:HB3	13	0.12
(1,899)	1:57:A:ASP:HB2	1:58:A:TRP:H	14	0.12
(1,890)	1:56:A:LYS:HA	1:57:A:ASP:HB2	4	0.12
(1,890)	1:56:A:LYS:HA	1:57:A:ASP:HB2	15	0.12
(1,884)	1:56:A:LYS:HE3	1:56:A:LYS:HB3	9	0.12
(1,884)	1:56:A:LYS:HE3	1:56:A:LYS:HB3	13	0.12
(1,884)	1:56:A:LYS:HE3	1:56:A:LYS:HB3	18	0.12
(1,884)	1:56:A:LYS:HE3	1:56:A:LYS:HB3	20	0.12
(1,878)	1:56:A:LYS:H	1:56:A:LYS:HD3	8	0.12
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD11	18	0.12
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD12	18	0.12
(1,868)	1:52:A:LEU:H	1:52:A:LEU:HD13	18	0.12
(1,858)	1:51:A:LYS:H	1:51:A:LYS:HD3	4	0.12
(1,858)	1:51:A:LYS:H	1:51:A:LYS:HD3	6	0.12
(1,852)	1:51:A:LYS:HA	1:51:A:LYS:HD3	2	0.12
(1,852)	1:51:A:LYS:HA	1:51:A:LYS:HD3	3	0.12
(1,852)	1:51:A:LYS:HA	1:51:A:LYS:HD3	4	0.12
(1,852)	1:51:A:LYS:HA	1:51:A:LYS:HD3	6	0.12
(1,852)	1:51:A:LYS:HA	1:51:A:LYS:HD3	7	0.12
(1,852)	1:51:A:LYS:HA	1:51:A:LYS:HD3	8	0.12
(1,852)	1:51:A:LYS:HA	1:51:A:LYS:HD3	13	0.12
(1,852)	1:51:A:LYS:HA	1:51:A:LYS:HD3	16	0.12
(1,852)	1:51:A:LYS:HA	1:51:A:LYS:HD3	17	0.12
(1,852)	1:51:A:LYS:HA	1:51:A:LYS:HD3	19	0.12
(1,841)	1:50:A:GLU:HA	1:50:A:GLU:HG3	1	0.12
(1,841)	1:50:A:GLU:HA	1:50:A:GLU:HG3	7	0.12
(1,841)	1:50:A:GLU:HA	1:50:A:GLU:HG3	8	0.12
(1,841)	1:50:A:GLU:HA	1:50:A:GLU:HG3	10	0.12
(1,841)	1:50:A:GLU:HA	1:50:A:GLU:HG3	20	0.12
(1,838)	1:49:A:VAL:HG21	1:58:A:TRP:H	3	0.12
(1,838)	1:49:A:VAL:HG22	1:58:A:TRP:H	3	0.12
(1,838)	1:49:A:VAL:HG23	1:58:A:TRP:H	3	0.12
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD21	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD22	1	0.12
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD23	1	0.12
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD21	1	0.12
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD22	1	0.12
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD23	1	0.12
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD21	1	0.12
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD22	1	0.12
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD23	1	0.12
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD21	7	0.12
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD22	7	0.12
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD23	7	0.12
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD21	7	0.12
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD22	7	0.12
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD23	7	0.12
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD21	7	0.12
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD22	7	0.12
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD23	7	0.12
(1,821)	1:48:A:LEU:HD21	1:63:A:LEU:H	17	0.12
(1,821)	1:48:A:LEU:HD22	1:63:A:LEU:H	17	0.12
(1,821)	1:48:A:LEU:HD23	1:63:A:LEU:H	17	0.12
(1,813)	1:48:A:LEU:H	1:51:A:LYS:H	4	0.12
(1,812)	1:48:A:LEU:HA	1:51:A:LYS:HB3	10	0.12
(1,805)	1:48:A:LEU:HG	1:49:A:VAL:H	2	0.12
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD21	11	0.12
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD22	11	0.12
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD23	11	0.12
(1,766)	1:46:A:LEU:HA	1:50:A:GLU:H	10	0.12
(1,746)	1:45:A:MET:HG3	1:63:A:LEU:HD21	7	0.12
(1,746)	1:45:A:MET:HG3	1:63:A:LEU:HD22	7	0.12
(1,746)	1:45:A:MET:HG3	1:63:A:LEU:HD23	7	0.12
(1,741)	1:45:A:MET:H	1:48:A:LEU:HD11	7	0.12
(1,741)	1:45:A:MET:H	1:48:A:LEU:HD12	7	0.12
(1,741)	1:45:A:MET:H	1:48:A:LEU:HD13	7	0.12
(1,738)	1:45:A:MET:HA	1:48:A:LEU:H	14	0.12
(1,723)	1:45:A:MET:H	1:45:A:MET:HB3	3	0.12
(1,723)	1:45:A:MET:H	1:45:A:MET:HB3	10	0.12
(1,723)	1:45:A:MET:H	1:45:A:MET:HB3	20	0.12
(1,719)	1:44:A:VAL:HG11	1:90:A:LEU:H	13	0.12
(1,719)	1:44:A:VAL:HG12	1:90:A:LEU:H	13	0.12
(1,719)	1:44:A:VAL:HG13	1:90:A:LEU:H	13	0.12
(1,712)	1:44:A:VAL:H	1:46:A:LEU:HG	9	0.12
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG11	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG12	3	0.12
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG13	3	0.12
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG11	20	0.12
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG12	20	0.12
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG13	20	0.12
(1,688)	1:42:A:GLY:H	1:75:A:THR:HG21	16	0.12
(1,688)	1:42:A:GLY:H	1:75:A:THR:HG22	16	0.12
(1,688)	1:42:A:GLY:H	1:75:A:THR:HG23	16	0.12
(1,684)	1:42:A:GLY:HA3	1:75:A:THR:HB	19	0.12
(1,683)	1:42:A:GLY:H	1:74:A:LYS:HE3	11	0.12
(1,683)	1:42:A:GLY:H	1:74:A:LYS:HE3	19	0.12
(1,676)	1:41:A:ILE:HG13	1:78:A:THR:H	6	0.12
(1,676)	1:41:A:ILE:HG13	1:78:A:THR:H	7	0.12
(1,676)	1:41:A:ILE:HG13	1:78:A:THR:H	19	0.12
(1,671)	1:41:A:ILE:HD11	1:75:A:THR:HA	3	0.12
(1,671)	1:41:A:ILE:HD12	1:75:A:THR:HA	3	0.12
(1,671)	1:41:A:ILE:HD13	1:75:A:THR:HA	3	0.12
(1,641)	1:41:A:ILE:H	1:41:A:ILE:HD11	6	0.12
(1,641)	1:41:A:ILE:H	1:41:A:ILE:HD12	6	0.12
(1,641)	1:41:A:ILE:H	1:41:A:ILE:HD13	6	0.12
(1,640)	1:41:A:ILE:H	1:41:A:ILE:HG12	1	0.12
(1,640)	1:41:A:ILE:H	1:41:A:ILE:HG12	19	0.12
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG11	1	0.12
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG12	1	0.12
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG13	1	0.12
(1,628)	1:40:A:HIS:H	1:44:A:VAL:HB	2	0.12
(1,628)	1:40:A:HIS:H	1:44:A:VAL:HB	12	0.12
(1,617)	1:40:A:HIS:HB3	1:41:A:ILE:H	1	0.12
(1,611)	1:39:A:VAL:HG11	1:78:A:THR:H	3	0.12
(1,611)	1:39:A:VAL:HG12	1:78:A:THR:H	3	0.12
(1,611)	1:39:A:VAL:HG13	1:78:A:THR:H	3	0.12
(1,611)	1:39:A:VAL:HG11	1:78:A:THR:H	4	0.12
(1,611)	1:39:A:VAL:HG12	1:78:A:THR:H	4	0.12
(1,611)	1:39:A:VAL:HG13	1:78:A:THR:H	4	0.12
(1,611)	1:39:A:VAL:HG11	1:78:A:THR:H	20	0.12
(1,611)	1:39:A:VAL:HG12	1:78:A:THR:H	20	0.12
(1,611)	1:39:A:VAL:HG13	1:78:A:THR:H	20	0.12
(1,610)	1:39:A:VAL:HG21	1:80:A:ASP:H	5	0.12
(1,610)	1:39:A:VAL:HG22	1:80:A:ASP:H	5	0.12
(1,610)	1:39:A:VAL:HG23	1:80:A:ASP:H	5	0.12
(1,602)	1:39:A:VAL:HG21	1:43:A:GLY:H	1	0.12
(1,602)	1:39:A:VAL:HG22	1:43:A:GLY:H	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,602)	1:39:A:VAL:HG23	1:43:A:GLY:H	1	0.12
(1,602)	1:39:A:VAL:HG21	1:43:A:GLY:H	14	0.12
(1,602)	1:39:A:VAL:HG22	1:43:A:GLY:H	14	0.12
(1,602)	1:39:A:VAL:HG23	1:43:A:GLY:H	14	0.12
(1,602)	1:39:A:VAL:HG21	1:43:A:GLY:H	19	0.12
(1,602)	1:39:A:VAL:HG22	1:43:A:GLY:H	19	0.12
(1,602)	1:39:A:VAL:HG23	1:43:A:GLY:H	19	0.12
(1,602)	1:39:A:VAL:HG21	1:43:A:GLY:H	20	0.12
(1,602)	1:39:A:VAL:HG22	1:43:A:GLY:H	20	0.12
(1,602)	1:39:A:VAL:HG23	1:43:A:GLY:H	20	0.12
(1,599)	1:39:A:VAL:H	1:40:A:HIS:H	18	0.12
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG21	1	0.12
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG22	1	0.12
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG23	1	0.12
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG21	17	0.12
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG22	17	0.12
(1,586)	1:38:A:GLU:HG3	1:78:A:THR:HG23	17	0.12
(1,580)	1:38:A:GLU:HB3	1:39:A:VAL:H	13	0.12
(1,563)	1:37:A:GLY:HA3	1:38:A:GLU:H	6	0.12
(1,561)	1:37:A:GLY:H	1:38:A:GLU:HG3	3	0.12
(1,561)	1:37:A:GLY:H	1:38:A:GLU:HG3	8	0.12
(1,561)	1:37:A:GLY:H	1:38:A:GLU:HG3	17	0.12
(1,561)	1:37:A:GLY:H	1:38:A:GLU:HG3	18	0.12
(1,554)	1:36:A:THR:H	1:38:A:GLU:HB3	2	0.12
(1,554)	1:36:A:THR:H	1:38:A:GLU:HB3	13	0.12
(1,554)	1:36:A:THR:H	1:38:A:GLU:HB3	19	0.12
(1,552)	1:36:A:THR:HB	1:38:A:GLU:H	19	0.12
(1,548)	1:36:A:THR:HG21	1:37:A:GLY:H	16	0.12
(1,548)	1:36:A:THR:HG22	1:37:A:GLY:H	16	0.12
(1,548)	1:36:A:THR:HG23	1:37:A:GLY:H	16	0.12
(1,527)	1:34:A:ARG:H	1:51:A:LYS:HD3	3	0.12
(1,527)	1:34:A:ARG:H	1:51:A:LYS:HD3	18	0.12
(1,516)	1:34:A:ARG:H	1:34:A:ARG:HG3	17	0.12
(1,511)	1:33:A:LEU:HD21	1:48:A:LEU:HB3	19	0.12
(1,511)	1:33:A:LEU:HD22	1:48:A:LEU:HB3	19	0.12
(1,511)	1:33:A:LEU:HD23	1:48:A:LEU:HB3	19	0.12
(1,505)	1:33:A:LEU:HD21	1:47:A:LYS:H	13	0.12
(1,505)	1:33:A:LEU:HD22	1:47:A:LYS:H	13	0.12
(1,505)	1:33:A:LEU:HD23	1:47:A:LYS:H	13	0.12
(1,503)	1:33:A:LEU:HB2	1:35:A:VAL:HG11	8	0.12
(1,503)	1:33:A:LEU:HB2	1:35:A:VAL:HG12	8	0.12
(1,503)	1:33:A:LEU:HB2	1:35:A:VAL:HG13	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,503)	1:33:A:LEU:HB2	1:35:A:VAL:HG11	10	0.12
(1,503)	1:33:A:LEU:HB2	1:35:A:VAL:HG12	10	0.12
(1,503)	1:33:A:LEU:HB2	1:35:A:VAL:HG13	10	0.12
(1,499)	1:33:A:LEU:HD21	1:34:A:ARG:H	9	0.12
(1,499)	1:33:A:LEU:HD22	1:34:A:ARG:H	9	0.12
(1,499)	1:33:A:LEU:HD23	1:34:A:ARG:H	9	0.12
(1,499)	1:33:A:LEU:HD21	1:34:A:ARG:H	18	0.12
(1,499)	1:33:A:LEU:HD22	1:34:A:ARG:H	18	0.12
(1,499)	1:33:A:LEU:HD23	1:34:A:ARG:H	18	0.12
(1,497)	1:33:A:LEU:HB3	1:34:A:ARG:H	9	0.12
(1,497)	1:33:A:LEU:HB3	1:34:A:ARG:H	16	0.12
(1,487)	1:33:A:LEU:H	1:33:A:LEU:HD11	5	0.12
(1,487)	1:33:A:LEU:H	1:33:A:LEU:HD12	5	0.12
(1,487)	1:33:A:LEU:H	1:33:A:LEU:HD13	5	0.12
(1,487)	1:33:A:LEU:H	1:33:A:LEU:HD11	14	0.12
(1,487)	1:33:A:LEU:H	1:33:A:LEU:HD12	14	0.12
(1,487)	1:33:A:LEU:H	1:33:A:LEU:HD13	14	0.12
(1,487)	1:33:A:LEU:H	1:33:A:LEU:HD11	16	0.12
(1,487)	1:33:A:LEU:H	1:33:A:LEU:HD12	16	0.12
(1,487)	1:33:A:LEU:H	1:33:A:LEU:HD13	16	0.12
(1,482)	1:32:A:THR:HA	1:34:A:ARG:H	20	0.12
(1,480)	1:32:A:THR:HG21	1:33:A:LEU:H	16	0.12
(1,480)	1:32:A:THR:HG22	1:33:A:LEU:H	16	0.12
(1,480)	1:32:A:THR:HG23	1:33:A:LEU:H	16	0.12
(1,473)	1:32:A:THR:HB	1:32:A:THR:H	3	0.12
(1,473)	1:32:A:THR:HB	1:32:A:THR:H	8	0.12
(1,473)	1:32:A:THR:HB	1:32:A:THR:H	16	0.12
(1,473)	1:32:A:THR:HB	1:32:A:THR:H	18	0.12
(1,443)	1:29:A:ARG:HB2	1:29:A:ARG:H	5	0.12
(1,443)	1:29:A:ARG:HB2	1:29:A:ARG:H	12	0.12
(1,443)	1:29:A:ARG:HB2	1:29:A:ARG:H	14	0.12
(1,431)	1:27:A:VAL:H	1:93:A:THR:HB	9	0.12
(1,427)	1:27:A:VAL:H	1:29:A:ARG:H	12	0.12
(1,426)	1:27:A:VAL:H	1:28:A:ASN:HB2	10	0.12
(1,422)	1:27:A:VAL:H	1:28:A:ASN:H	11	0.12
(1,414)	1:25:A:THR:H	1:93:A:THR:HG21	3	0.12
(1,414)	1:25:A:THR:H	1:93:A:THR:HG22	3	0.12
(1,414)	1:25:A:THR:H	1:93:A:THR:HG23	3	0.12
(1,414)	1:25:A:THR:H	1:93:A:THR:HG21	17	0.12
(1,414)	1:25:A:THR:H	1:93:A:THR:HG22	17	0.12
(1,414)	1:25:A:THR:H	1:93:A:THR:HG23	17	0.12
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG21	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG22	5	0.12
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG23	5	0.12
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG21	9	0.12
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG22	9	0.12
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG23	9	0.12
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG21	13	0.12
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG22	13	0.12
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG23	13	0.12
(1,392)	1:24:A:VAL:HB	1:92:A:PHE:H	3	0.12
(1,392)	1:24:A:VAL:HB	1:92:A:PHE:H	7	0.12
(1,392)	1:24:A:VAL:HB	1:92:A:PHE:H	12	0.12
(1,392)	1:24:A:VAL:HB	1:92:A:PHE:H	17	0.12
(1,383)	1:24:A:VAL:HA	1:31:A:VAL:H	8	0.12
(1,383)	1:24:A:VAL:HA	1:31:A:VAL:H	16	0.12
(1,372)	1:24:A:VAL:HG21	1:29:A:ARG:H	12	0.12
(1,372)	1:24:A:VAL:HG22	1:29:A:ARG:H	12	0.12
(1,372)	1:24:A:VAL:HG23	1:29:A:ARG:H	12	0.12
(1,312)	1:22:A:VAL:HG21	1:90:A:LEU:H	17	0.12
(1,312)	1:22:A:VAL:HG22	1:90:A:LEU:H	17	0.12
(1,312)	1:22:A:VAL:HG23	1:90:A:LEU:H	17	0.12
(1,306)	1:22:A:VAL:HB	1:48:A:LEU:HD21	14	0.12
(1,306)	1:22:A:VAL:HB	1:48:A:LEU:HD22	14	0.12
(1,306)	1:22:A:VAL:HB	1:48:A:LEU:HD23	14	0.12
(1,299)	1:22:A:VAL:H	1:32:A:THR:HB	1	0.12
(1,299)	1:22:A:VAL:H	1:32:A:THR:HB	17	0.12
(1,293)	1:22:A:VAL:HG21	1:24:A:VAL:H	6	0.12
(1,293)	1:22:A:VAL:HG22	1:24:A:VAL:H	6	0.12
(1,293)	1:22:A:VAL:HG23	1:24:A:VAL:H	6	0.12
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG21	5	0.12
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG22	5	0.12
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG23	5	0.12
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG21	8	0.12
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG22	8	0.12
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG23	8	0.12
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB1	12	0.12
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB2	12	0.12
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB3	12	0.12
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB1	12	0.12
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB2	12	0.12
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB3	12	0.12
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB1	12	0.12
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB2	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB3	12	0.12
(1,251)	1:20:A:LEU:HG	1:35:A:VAL:H	3	0.12
(1,251)	1:20:A:LEU:HG	1:35:A:VAL:H	6	0.12
(1,251)	1:20:A:LEU:HG	1:35:A:VAL:H	10	0.12
(1,251)	1:20:A:LEU:HG	1:35:A:VAL:H	19	0.12
(1,250)	1:20:A:LEU:H	1:35:A:VAL:H	11	0.12
(1,244)	1:20:A:LEU:HD21	1:33:A:LEU:HA	4	0.12
(1,244)	1:20:A:LEU:HD22	1:33:A:LEU:HA	4	0.12
(1,244)	1:20:A:LEU:HD23	1:33:A:LEU:HA	4	0.12
(1,244)	1:20:A:LEU:HD21	1:33:A:LEU:HA	5	0.12
(1,244)	1:20:A:LEU:HD22	1:33:A:LEU:HA	5	0.12
(1,244)	1:20:A:LEU:HD23	1:33:A:LEU:HA	5	0.12
(1,242)	1:20:A:LEU:HB3	1:33:A:LEU:H	7	0.12
(1,242)	1:20:A:LEU:HB3	1:33:A:LEU:H	8	0.12
(1,242)	1:20:A:LEU:HB3	1:33:A:LEU:H	11	0.12
(1,242)	1:20:A:LEU:HB3	1:33:A:LEU:H	17	0.12
(1,236)	1:20:A:LEU:HD21	1:21:A:SER:H	6	0.12
(1,236)	1:20:A:LEU:HD22	1:21:A:SER:H	6	0.12
(1,236)	1:20:A:LEU:HD23	1:21:A:SER:H	6	0.12
(1,232)	1:20:A:LEU:HG	1:21:A:SER:H	5	0.12
(1,212)	1:19:A:GLU:HB2	1:33:A:LEU:H	19	0.12
(1,204)	1:19:A:GLU:HG2	1:20:A:LEU:H	1	0.12
(1,189)	1:18:A:TRP:HD1	1:85:A:GLN:HB3	8	0.12
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG21	9	0.12
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG22	9	0.12
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG23	9	0.12
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG21	14	0.12
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG22	14	0.12
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG23	14	0.12
(1,176)	1:18:A:TRP:H	1:36:A:THR:H	13	0.12
(1,169)	1:18:A:TRP:H	1:18:A:TRP:HD1	13	0.12
(1,166)	1:17:A:THR:HG21	1:18:A:TRP:H	1	0.12
(1,166)	1:17:A:THR:HG22	1:18:A:TRP:H	1	0.12
(1,166)	1:17:A:THR:HG23	1:18:A:TRP:H	1	0.12
(1,166)	1:17:A:THR:HG21	1:18:A:TRP:H	17	0.12
(1,166)	1:17:A:THR:HG22	1:18:A:TRP:H	17	0.12
(1,166)	1:17:A:THR:HG23	1:18:A:TRP:H	17	0.12
(1,148)	1:15:A:ASP:HA	1:16:A:GLY:H	13	0.12
(1,147)	1:15:A:ASP:H	1:15:A:ASP:HB2	7	0.12
(1,135)	1:13:A:TYR:H	1:13:A:TYR:HB3	6	0.12
(1,127)	1:11:A:GLY:HA2	1:12:A:CYS:H	17	0.12
(1,127)	1:11:A:GLY:HA2	1:12:A:CYS:H	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,112)	1:9:A:PRO:HG3	1:10:A:ASP:H	7	0.12
(1,111)	1:9:A:PRO:HB3	1:10:A:ASP:H	12	0.12
(1,103)	1:8:A:MET:HG3	1:12:A:CYS:HB3	7	0.12
(1,102)	1:8:A:MET:HB3	1:12:A:CYS:H	16	0.12
(1,100)	1:8:A:MET:H	1:12:A:CYS:HA	5	0.12
(1,96)	1:8:A:MET:HG3	1:10:A:ASP:H	7	0.12
(1,79)	1:7:A:ARG:HD3	1:7:A:ARG:HB2	17	0.12
(1,78)	1:7:A:ARG:HD3	1:7:A:ARG:HB3	2	0.12
(1,78)	1:7:A:ARG:HD3	1:7:A:ARG:HB3	8	0.12
(1,66)	1:6:A:ILE:HB	1:8:A:MET:H	18	0.12
(1,61)	1:6:A:ILE:H	1:7:A:ARG:H	9	0.12
(1,56)	1:6:A:ILE:H	1:6:A:ILE:HG12	19	0.12
(1,45)	1:4:A:ASP:HB3	1:6:A:ILE:H	13	0.12
(1,42)	1:4:A:ASP:H	1:5:A:GLY:HA3	18	0.12
(1,40)	1:4:A:ASP:HA	1:5:A:GLY:H	1	0.12
(1,40)	1:4:A:ASP:HA	1:5:A:GLY:H	16	0.12
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD11	7	0.12
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD12	7	0.12
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD13	7	0.12
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD11	8	0.12
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD12	8	0.12
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD13	8	0.12
(1,24)	1:3:A:LEU:H	1:3:A:LEU:HD21	1	0.12
(1,24)	1:3:A:LEU:H	1:3:A:LEU:HD22	1	0.12
(1,24)	1:3:A:LEU:H	1:3:A:LEU:HD23	1	0.12
(1,20)	1:2:A:ALA:HB1	1:4:A:ASP:H	11	0.12
(1,20)	1:2:A:ALA:HB2	1:4:A:ASP:H	11	0.12
(1,20)	1:2:A:ALA:HB3	1:4:A:ASP:H	11	0.12
(1,20)	1:2:A:ALA:HB1	1:4:A:ASP:H	12	0.12
(1,20)	1:2:A:ALA:HB2	1:4:A:ASP:H	12	0.12
(1,20)	1:2:A:ALA:HB3	1:4:A:ASP:H	12	0.12
(1,19)	1:2:A:ALA:HB1	1:3:A:LEU:H	17	0.12
(1,19)	1:2:A:ALA:HB2	1:3:A:LEU:H	17	0.12
(1,19)	1:2:A:ALA:HB3	1:3:A:LEU:H	17	0.12
(3,16)	1:42:A:GLY:O	1:46:A:LEU:H	4	0.11
(3,16)	1:42:A:GLY:O	1:46:A:LEU:H	8	0.11
(3,14)	1:91:A:GLN:O	1:23:A:HIS:H	19	0.11
(3,13)	1:92:A:PHE:O	1:64:A:TRP:H	9	0.11
(3,13)	1:92:A:PHE:O	1:64:A:TRP:H	10	0.11
(3,12)	1:72:A:LEU:O	1:63:A:LEU:H	13	0.11
(2,25)	1:77:A:TRP:O	1:81:A:LYS:N	5	0.11
(2,25)	1:77:A:TRP:O	1:81:A:LYS:N	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,25)	1:77:A:TRP:O	1:81:A:LYS:N	20	0.11
(2,24)	1:45:A:MET:O	1:49:A:VAL:N	1	0.11
(2,24)	1:45:A:MET:O	1:49:A:VAL:N	2	0.11
(2,24)	1:45:A:MET:O	1:49:A:VAL:N	4	0.11
(2,24)	1:45:A:MET:O	1:49:A:VAL:N	12	0.11
(2,24)	1:45:A:MET:O	1:49:A:VAL:N	13	0.11
(2,24)	1:45:A:MET:O	1:49:A:VAL:N	15	0.11
(2,24)	1:45:A:MET:O	1:49:A:VAL:N	16	0.11
(2,24)	1:45:A:MET:O	1:49:A:VAL:N	17	0.11
(2,24)	1:45:A:MET:O	1:49:A:VAL:N	20	0.11
(2,21)	1:39:A:VAL:O	1:43:A:GLY:N	1	0.11
(2,19)	1:23:A:HIS:O	1:93:A:THR:H	14	0.11
(2,14)	1:64:A:TRP:O	1:92:A:PHE:N	10	0.11
(2,14)	1:64:A:TRP:O	1:92:A:PHE:N	13	0.11
(2,13)	1:92:A:PHE:O	1:64:A:TRP:N	12	0.11
(2,3)	1:20:A:LEU:O	1:33:A:LEU:N	12	0.11
(2,3)	1:20:A:LEU:O	1:33:A:LEU:N	20	0.11
(1,1407)	1:92:A:PHE:HB2	1:93:A:THR:H	6	0.11
(1,1397)	1:91:A:GLN:HB2	1:92:A:PHE:HA	2	0.11
(1,1397)	1:91:A:GLN:HB2	1:92:A:PHE:HA	8	0.11
(1,1397)	1:91:A:GLN:HB2	1:92:A:PHE:HA	10	0.11
(1,1397)	1:91:A:GLN:HB2	1:92:A:PHE:HA	14	0.11
(1,1381)	1:91:A:GLN:H	1:91:A:GLN:HG2	2	0.11
(1,1381)	1:91:A:GLN:H	1:91:A:GLN:HG2	5	0.11
(1,1381)	1:91:A:GLN:H	1:91:A:GLN:HG2	11	0.11
(1,1380)	1:91:A:GLN:H	1:91:A:GLN:HE22	9	0.11
(1,1376)	1:91:A:GLN:HA	1:91:A:GLN:HE22	7	0.11
(1,1376)	1:91:A:GLN:HA	1:91:A:GLN:HE22	8	0.11
(1,1376)	1:91:A:GLN:HA	1:91:A:GLN:HE22	14	0.11
(1,1376)	1:91:A:GLN:HA	1:91:A:GLN:HE22	18	0.11
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD11	18	0.11
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD12	18	0.11
(1,1354)	1:89:A:LYS:H	1:90:A:LEU:HD13	18	0.11
(1,1330)	1:87:A:ASP:H	1:88:A:ALA:HA	11	0.11
(1,1329)	1:87:A:ASP:HB3	1:88:A:ALA:H	2	0.11
(1,1329)	1:87:A:ASP:HB3	1:88:A:ALA:H	9	0.11
(1,1329)	1:87:A:ASP:HB3	1:88:A:ALA:H	10	0.11
(1,1329)	1:87:A:ASP:HB3	1:88:A:ALA:H	17	0.11
(1,1323)	1:86:A:ALA:HB1	1:88:A:ALA:H	4	0.11
(1,1323)	1:86:A:ALA:HB2	1:88:A:ALA:H	4	0.11
(1,1323)	1:86:A:ALA:HB3	1:88:A:ALA:H	4	0.11
(1,1313)	1:85:A:GLN:HB3	1:87:A:ASP:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1313)	1:85:A:GLN:HB3	1:87:A:ASP:H	7	0.11
(1,1313)	1:85:A:GLN:HB3	1:87:A:ASP:H	13	0.11
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB1	2	0.11
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB2	2	0.11
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB3	2	0.11
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB1	4	0.11
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB2	4	0.11
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB3	4	0.11
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB1	5	0.11
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB2	5	0.11
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB3	5	0.11
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB1	12	0.11
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB2	12	0.11
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB3	12	0.11
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB1	15	0.11
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB2	15	0.11
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB3	15	0.11
(1,1294)	1:85:A:GLN:H	1:85:A:GLN:HG3	2	0.11
(1,1294)	1:85:A:GLN:H	1:85:A:GLN:HG3	3	0.11
(1,1294)	1:85:A:GLN:H	1:85:A:GLN:HG3	4	0.11
(1,1294)	1:85:A:GLN:H	1:85:A:GLN:HG3	5	0.11
(1,1294)	1:85:A:GLN:H	1:85:A:GLN:HG3	16	0.11
(1,1293)	1:85:A:GLN:H	1:85:A:GLN:HE22	13	0.11
(1,1289)	1:84:A:ILE:HA	1:88:A:ALA:HB1	16	0.11
(1,1289)	1:84:A:ILE:HA	1:88:A:ALA:HB2	16	0.11
(1,1289)	1:84:A:ILE:HA	1:88:A:ALA:HB3	16	0.11
(1,1289)	1:84:A:ILE:HA	1:88:A:ALA:HB1	19	0.11
(1,1289)	1:84:A:ILE:HA	1:88:A:ALA:HB2	19	0.11
(1,1289)	1:84:A:ILE:HA	1:88:A:ALA:HB3	19	0.11
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG21	9	0.11
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG22	9	0.11
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG23	9	0.11
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG21	11	0.11
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG22	11	0.11
(1,1278)	1:84:A:ILE:H	1:84:A:ILE:HG23	11	0.11
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG21	6	0.11
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG22	6	0.11
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG23	6	0.11
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG21	6	0.11
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG22	6	0.11
(1,1259)	1:82:A:TYR:H	1:84:A:ILE:HG23	6	0.11
(1,1245)	1:81:A:LYS:HB2	1:82:A:TYR:H	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1244)	1:81:A:LYS:HB3	1:82:A:TYR:H	9	0.11
(1,1235)	1:81:A:LYS:HE3	1:81:A:LYS:HG3	13	0.11
(1,1225)	1:81:A:LYS:HA	1:81:A:LYS:HG2	3	0.11
(1,1225)	1:81:A:LYS:HA	1:81:A:LYS:HG2	13	0.11
(1,1225)	1:81:A:LYS:HA	1:81:A:LYS:HG2	15	0.11
(1,1215)	1:80:A:ASP:HB2	1:81:A:LYS:H	17	0.11
(1,1211)	1:80:A:ASP:H	1:80:A:ASP:HB2	19	0.11
(1,1208)	1:79:A:LEU:HA	1:84:A:ILE:H	19	0.11
(1,1196)	1:79:A:LEU:HD21	1:80:A:ASP:H	3	0.11
(1,1196)	1:79:A:LEU:HD22	1:80:A:ASP:H	3	0.11
(1,1196)	1:79:A:LEU:HD23	1:80:A:ASP:H	3	0.11
(1,1196)	1:79:A:LEU:HD21	1:80:A:ASP:H	6	0.11
(1,1196)	1:79:A:LEU:HD22	1:80:A:ASP:H	6	0.11
(1,1196)	1:79:A:LEU:HD23	1:80:A:ASP:H	6	0.11
(1,1193)	1:79:A:LEU:HA	1:80:A:ASP:H	13	0.11
(1,1171)	1:78:A:THR:HB	1:80:A:ASP:H	5	0.11
(1,1171)	1:78:A:THR:HB	1:80:A:ASP:H	12	0.11
(1,1157)	1:77:A:TRP:H	1:77:A:TRP:HB3	1	0.11
(1,1157)	1:77:A:TRP:H	1:77:A:TRP:HB3	8	0.11
(1,1153)	1:76:A:HIS:HB3	1:77:A:TRP:H	18	0.11
(1,1132)	1:74:A:LYS:HG3	1:75:A:THR:H	18	0.11
(1,1129)	1:74:A:LYS:HE2	1:74:A:LYS:HB3	3	0.11
(1,1129)	1:74:A:LYS:HE2	1:74:A:LYS:HB3	4	0.11
(1,1129)	1:74:A:LYS:HE2	1:74:A:LYS:HB3	12	0.11
(1,1129)	1:74:A:LYS:HE2	1:74:A:LYS:HB3	13	0.11
(1,1129)	1:74:A:LYS:HE2	1:74:A:LYS:HB3	14	0.11
(1,1121)	1:74:A:LYS:H	1:74:A:LYS:HG3	6	0.11
(1,1121)	1:74:A:LYS:H	1:74:A:LYS:HG3	15	0.11
(1,1121)	1:74:A:LYS:H	1:74:A:LYS:HG3	16	0.11
(1,1119)	1:74:A:LYS:H	1:74:A:LYS:HE2	10	0.11
(1,1112)	1:74:A:LYS:HA	1:74:A:LYS:HE2	14	0.11
(1,1097)	1:72:A:LEU:HD21	1:73:A:LEU:H	2	0.11
(1,1097)	1:72:A:LEU:HD22	1:73:A:LEU:H	2	0.11
(1,1097)	1:72:A:LEU:HD23	1:73:A:LEU:H	2	0.11
(1,1097)	1:72:A:LEU:HD21	1:73:A:LEU:H	4	0.11
(1,1097)	1:72:A:LEU:HD22	1:73:A:LEU:H	4	0.11
(1,1097)	1:72:A:LEU:HD23	1:73:A:LEU:H	4	0.11
(1,1097)	1:72:A:LEU:HD21	1:73:A:LEU:H	5	0.11
(1,1097)	1:72:A:LEU:HD22	1:73:A:LEU:H	5	0.11
(1,1097)	1:72:A:LEU:HD23	1:73:A:LEU:H	5	0.11
(1,1097)	1:72:A:LEU:HD21	1:73:A:LEU:H	12	0.11
(1,1097)	1:72:A:LEU:HD22	1:73:A:LEU:H	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1097)	1:72:A:LEU:HD23	1:73:A:LEU:H	12	0.11
(1,1081)	1:71:A:TRP:HB2	1:72:A:LEU:H	20	0.11
(1,1076)	1:71:A:TRP:H	1:71:A:TRP:HB3	10	0.11
(1,1074)	1:70:A:THR:HG21	1:72:A:LEU:H	10	0.11
(1,1074)	1:70:A:THR:HG22	1:72:A:LEU:H	10	0.11
(1,1074)	1:70:A:THR:HG23	1:72:A:LEU:H	10	0.11
(1,1074)	1:70:A:THR:HG21	1:72:A:LEU:H	11	0.11
(1,1074)	1:70:A:THR:HG22	1:72:A:LEU:H	11	0.11
(1,1074)	1:70:A:THR:HG23	1:72:A:LEU:H	11	0.11
(1,1066)	1:70:A:THR:HB	1:70:A:THR:H	20	0.11
(1,1064)	1:69:A:ARG:HB2	1:70:A:THR:H	18	0.11
(1,1063)	1:69:A:ARG:H	1:70:A:THR:H	8	0.11
(1,1053)	1:67:A:LYS:H	1:88:A:ALA:HA	5	0.11
(1,1053)	1:67:A:LYS:H	1:88:A:ALA:HA	11	0.11
(1,1053)	1:67:A:LYS:H	1:88:A:ALA:HA	14	0.11
(1,1049)	1:67:A:LYS:HB3	1:69:A:ARG:HA	7	0.11
(1,1049)	1:67:A:LYS:HB3	1:69:A:ARG:HA	10	0.11
(1,1038)	1:67:A:LYS:H	1:67:A:LYS:HG3	9	0.11
(1,1035)	1:67:A:LYS:HE3	1:67:A:LYS:HG3	10	0.11
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG21	10	0.11
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG22	10	0.11
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG23	10	0.11
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG21	11	0.11
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG22	11	0.11
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG23	11	0.11
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG21	14	0.11
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG22	14	0.11
(1,1006)	1:65:A:TRP:H	1:70:A:THR:HG23	14	0.11
(1,999)	1:65:A:TRP:HA	1:67:A:LYS:H	13	0.11
(1,997)	1:65:A:TRP:HB3	1:66:A:GLU:H	10	0.11
(1,997)	1:65:A:TRP:HB3	1:66:A:GLU:H	18	0.11
(1,988)	1:64:A:TRP:H	1:92:A:PHE:HB3	7	0.11
(1,988)	1:64:A:TRP:H	1:92:A:PHE:HB3	12	0.11
(1,981)	1:64:A:TRP:H	1:64:A:TRP:HB3	2	0.11
(1,981)	1:64:A:TRP:H	1:64:A:TRP:HB3	13	0.11
(1,981)	1:64:A:TRP:H	1:64:A:TRP:HB3	16	0.11
(1,981)	1:64:A:TRP:H	1:64:A:TRP:HB3	17	0.11
(1,978)	1:63:A:LEU:HA	1:93:A:THR:H	3	0.11
(1,976)	1:63:A:LEU:HG	1:93:A:THR:H	8	0.11
(1,976)	1:63:A:LEU:HG	1:93:A:THR:H	10	0.11
(1,968)	1:63:A:LEU:HG	1:90:A:LEU:HA	3	0.11
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD11	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD12	18	0.11
(1,965)	1:63:A:LEU:H	1:72:A:LEU:HD13	18	0.11
(1,962)	1:63:A:LEU:HD21	1:72:A:LEU:H	12	0.11
(1,962)	1:63:A:LEU:HD22	1:72:A:LEU:H	12	0.11
(1,962)	1:63:A:LEU:HD23	1:72:A:LEU:H	12	0.11
(1,959)	1:63:A:LEU:H	1:64:A:TRP:H	3	0.11
(1,959)	1:63:A:LEU:H	1:64:A:TRP:H	6	0.11
(1,959)	1:63:A:LEU:H	1:64:A:TRP:H	13	0.11
(1,959)	1:63:A:LEU:H	1:64:A:TRP:H	18	0.11
(1,945)	1:62:A:ALA:HB1	1:93:A:THR:HA	6	0.11
(1,945)	1:62:A:ALA:HB2	1:93:A:THR:HA	6	0.11
(1,945)	1:62:A:ALA:HB3	1:93:A:THR:HA	6	0.11
(1,942)	1:62:A:ALA:HB1	1:92:A:PHE:HA	4	0.11
(1,942)	1:62:A:ALA:HB2	1:92:A:PHE:HA	4	0.11
(1,942)	1:62:A:ALA:HB3	1:92:A:PHE:HA	4	0.11
(1,942)	1:62:A:ALA:HB1	1:92:A:PHE:HA	5	0.11
(1,942)	1:62:A:ALA:HB2	1:92:A:PHE:HA	5	0.11
(1,942)	1:62:A:ALA:HB3	1:92:A:PHE:HA	5	0.11
(1,940)	1:62:A:ALA:HB1	1:92:A:PHE:H	12	0.11
(1,940)	1:62:A:ALA:HB2	1:92:A:PHE:H	12	0.11
(1,940)	1:62:A:ALA:HB3	1:92:A:PHE:H	12	0.11
(1,940)	1:62:A:ALA:HB1	1:92:A:PHE:H	15	0.11
(1,940)	1:62:A:ALA:HB2	1:92:A:PHE:H	15	0.11
(1,940)	1:62:A:ALA:HB3	1:92:A:PHE:H	15	0.11
(1,930)	1:61:A:HIS:HB2	1:63:A:LEU:H	4	0.11
(1,924)	1:61:A:HIS:H	1:61:A:HIS:HB2	2	0.11
(1,924)	1:61:A:HIS:H	1:61:A:HIS:HB2	12	0.11
(1,908)	1:58:A:TRP:HB2	1:59:A:SER:H	19	0.11
(1,906)	1:58:A:TRP:H	1:59:A:SER:H	11	0.11
(1,906)	1:58:A:TRP:H	1:59:A:SER:H	20	0.11
(1,899)	1:57:A:ASP:HB2	1:58:A:TRP:H	9	0.11
(1,899)	1:57:A:ASP:HB2	1:58:A:TRP:H	15	0.11
(1,890)	1:56:A:LYS:HA	1:57:A:ASP:HB2	17	0.11
(1,889)	1:56:A:LYS:HA	1:57:A:ASP:HB3	6	0.11
(1,889)	1:56:A:LYS:HA	1:57:A:ASP:HB3	12	0.11
(1,889)	1:56:A:LYS:HA	1:57:A:ASP:HB3	15	0.11
(1,889)	1:56:A:LYS:HA	1:57:A:ASP:HB3	17	0.11
(1,852)	1:51:A:LYS:HA	1:51:A:LYS:HD3	1	0.11
(1,852)	1:51:A:LYS:HA	1:51:A:LYS:HD3	9	0.11
(1,852)	1:51:A:LYS:HA	1:51:A:LYS:HD3	10	0.11
(1,852)	1:51:A:LYS:HA	1:51:A:LYS:HD3	12	0.11
(1,852)	1:51:A:LYS:HA	1:51:A:LYS:HD3	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:50:A:GLU:HB3	1:51:A:LYS:H	6	0.11
(1,841)	1:50:A:GLU:HA	1:50:A:GLU:HG3	3	0.11
(1,841)	1:50:A:GLU:HA	1:50:A:GLU:HG3	9	0.11
(1,841)	1:50:A:GLU:HA	1:50:A:GLU:HG3	14	0.11
(1,841)	1:50:A:GLU:HA	1:50:A:GLU:HG3	16	0.11
(1,837)	1:49:A:VAL:HA	1:52:A:LEU:H	6	0.11
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD21	12	0.11
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD22	12	0.11
(1,822)	1:48:A:LEU:HD21	1:90:A:LEU:HD23	12	0.11
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD21	12	0.11
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD22	12	0.11
(1,822)	1:48:A:LEU:HD22	1:90:A:LEU:HD23	12	0.11
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD21	12	0.11
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD22	12	0.11
(1,822)	1:48:A:LEU:HD23	1:90:A:LEU:HD23	12	0.11
(1,821)	1:48:A:LEU:HD21	1:63:A:LEU:H	1	0.11
(1,821)	1:48:A:LEU:HD22	1:63:A:LEU:H	1	0.11
(1,821)	1:48:A:LEU:HD23	1:63:A:LEU:H	1	0.11
(1,821)	1:48:A:LEU:HD21	1:63:A:LEU:H	6	0.11
(1,821)	1:48:A:LEU:HD22	1:63:A:LEU:H	6	0.11
(1,821)	1:48:A:LEU:HD23	1:63:A:LEU:H	6	0.11
(1,813)	1:48:A:LEU:H	1:51:A:LYS:H	16	0.11
(1,812)	1:48:A:LEU:HA	1:51:A:LYS:HB3	3	0.11
(1,805)	1:48:A:LEU:HG	1:49:A:VAL:H	10	0.11
(1,799)	1:48:A:LEU:HA	1:49:A:VAL:H	7	0.11
(1,799)	1:48:A:LEU:HA	1:49:A:VAL:H	14	0.11
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD21	1	0.11
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD22	1	0.11
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD23	1	0.11
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD21	2	0.11
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD22	2	0.11
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD23	2	0.11
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD21	3	0.11
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD22	3	0.11
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD23	3	0.11
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD21	7	0.11
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD22	7	0.11
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD23	7	0.11
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD21	10	0.11
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD22	10	0.11
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD23	10	0.11
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD21	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD22	12	0.11
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD23	12	0.11
(1,756)	1:46:A:LEU:HD11	1:47:A:LYS:H	9	0.11
(1,756)	1:46:A:LEU:HD12	1:47:A:LYS:H	9	0.11
(1,756)	1:46:A:LEU:HD13	1:47:A:LYS:H	9	0.11
(1,746)	1:45:A:MET:HG3	1:63:A:LEU:HD21	2	0.11
(1,746)	1:45:A:MET:HG3	1:63:A:LEU:HD22	2	0.11
(1,746)	1:45:A:MET:HG3	1:63:A:LEU:HD23	2	0.11
(1,744)	1:45:A:MET:HE1	1:63:A:LEU:H	9	0.11
(1,744)	1:45:A:MET:HE2	1:63:A:LEU:H	9	0.11
(1,744)	1:45:A:MET:HE3	1:63:A:LEU:H	9	0.11
(1,741)	1:45:A:MET:H	1:48:A:LEU:HD11	14	0.11
(1,741)	1:45:A:MET:H	1:48:A:LEU:HD12	14	0.11
(1,741)	1:45:A:MET:H	1:48:A:LEU:HD13	14	0.11
(1,738)	1:45:A:MET:HA	1:48:A:LEU:H	12	0.11
(1,738)	1:45:A:MET:HA	1:48:A:LEU:H	16	0.11
(1,731)	1:45:A:MET:H	1:46:A:LEU:HG	2	0.11
(1,731)	1:45:A:MET:H	1:46:A:LEU:HG	7	0.11
(1,731)	1:45:A:MET:H	1:46:A:LEU:HG	11	0.11
(1,731)	1:45:A:MET:H	1:46:A:LEU:HG	12	0.11
(1,723)	1:45:A:MET:H	1:45:A:MET:HB3	5	0.11
(1,723)	1:45:A:MET:H	1:45:A:MET:HB3	11	0.11
(1,718)	1:44:A:VAL:HG11	1:48:A:LEU:HD21	19	0.11
(1,718)	1:44:A:VAL:HG11	1:48:A:LEU:HD22	19	0.11
(1,718)	1:44:A:VAL:HG11	1:48:A:LEU:HD23	19	0.11
(1,718)	1:44:A:VAL:HG12	1:48:A:LEU:HD21	19	0.11
(1,718)	1:44:A:VAL:HG12	1:48:A:LEU:HD22	19	0.11
(1,718)	1:44:A:VAL:HG12	1:48:A:LEU:HD23	19	0.11
(1,718)	1:44:A:VAL:HG13	1:48:A:LEU:HD21	19	0.11
(1,718)	1:44:A:VAL:HG13	1:48:A:LEU:HD22	19	0.11
(1,718)	1:44:A:VAL:HG13	1:48:A:LEU:HD23	19	0.11
(1,717)	1:44:A:VAL:HB	1:47:A:LYS:H	6	0.11
(1,717)	1:44:A:VAL:HB	1:47:A:LYS:H	18	0.11
(1,717)	1:44:A:VAL:HB	1:47:A:LYS:H	20	0.11
(1,712)	1:44:A:VAL:H	1:46:A:LEU:HG	4	0.11
(1,712)	1:44:A:VAL:H	1:46:A:LEU:HG	14	0.11
(1,712)	1:44:A:VAL:H	1:46:A:LEU:HG	15	0.11
(1,712)	1:44:A:VAL:H	1:46:A:LEU:HG	16	0.11
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG11	4	0.11
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG12	4	0.11
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG13	4	0.11
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG11	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG12	5	0.11
(1,706)	1:44:A:VAL:H	1:44:A:VAL:HG13	5	0.11
(1,695)	1:43:A:GLY:HA2	1:46:A:LEU:H	2	0.11
(1,688)	1:42:A:GLY:H	1:75:A:THR:HG21	11	0.11
(1,688)	1:42:A:GLY:H	1:75:A:THR:HG22	11	0.11
(1,688)	1:42:A:GLY:H	1:75:A:THR:HG23	11	0.11
(1,684)	1:42:A:GLY:HA3	1:75:A:THR:HB	8	0.11
(1,641)	1:41:A:ILE:H	1:41:A:ILE:HD11	7	0.11
(1,641)	1:41:A:ILE:H	1:41:A:ILE:HD12	7	0.11
(1,641)	1:41:A:ILE:H	1:41:A:ILE:HD13	7	0.11
(1,640)	1:41:A:ILE:H	1:41:A:ILE:HG12	6	0.11
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG11	9	0.11
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG12	9	0.11
(1,629)	1:40:A:HIS:H	1:44:A:VAL:HG13	9	0.11
(1,628)	1:40:A:HIS:H	1:44:A:VAL:HB	10	0.11
(1,617)	1:40:A:HIS:HB3	1:41:A:ILE:H	10	0.11
(1,617)	1:40:A:HIS:HB3	1:41:A:ILE:H	17	0.11
(1,611)	1:39:A:VAL:HG11	1:78:A:THR:H	5	0.11
(1,611)	1:39:A:VAL:HG12	1:78:A:THR:H	5	0.11
(1,611)	1:39:A:VAL:HG13	1:78:A:THR:H	5	0.11
(1,611)	1:39:A:VAL:HG11	1:78:A:THR:H	14	0.11
(1,611)	1:39:A:VAL:HG12	1:78:A:THR:H	14	0.11
(1,611)	1:39:A:VAL:HG13	1:78:A:THR:H	14	0.11
(1,602)	1:39:A:VAL:HG21	1:43:A:GLY:H	4	0.11
(1,602)	1:39:A:VAL:HG22	1:43:A:GLY:H	4	0.11
(1,602)	1:39:A:VAL:HG23	1:43:A:GLY:H	4	0.11
(1,602)	1:39:A:VAL:HG21	1:43:A:GLY:H	9	0.11
(1,602)	1:39:A:VAL:HG22	1:43:A:GLY:H	9	0.11
(1,602)	1:39:A:VAL:HG23	1:43:A:GLY:H	9	0.11
(1,602)	1:39:A:VAL:HG21	1:43:A:GLY:H	15	0.11
(1,602)	1:39:A:VAL:HG22	1:43:A:GLY:H	15	0.11
(1,602)	1:39:A:VAL:HG23	1:43:A:GLY:H	15	0.11
(1,599)	1:39:A:VAL:H	1:40:A:HIS:H	20	0.11
(1,588)	1:38:A:GLU:HA	1:80:A:ASP:H	3	0.11
(1,580)	1:38:A:GLU:HB3	1:39:A:VAL:H	11	0.11
(1,561)	1:37:A:GLY:H	1:38:A:GLU:HG3	1	0.11
(1,561)	1:37:A:GLY:H	1:38:A:GLU:HG3	2	0.11
(1,561)	1:37:A:GLY:H	1:38:A:GLU:HG3	19	0.11
(1,554)	1:36:A:THR:H	1:38:A:GLU:HB3	6	0.11
(1,552)	1:36:A:THR:HB	1:38:A:GLU:H	6	0.11
(1,548)	1:36:A:THR:HG21	1:37:A:GLY:H	13	0.11
(1,548)	1:36:A:THR:HG22	1:37:A:GLY:H	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,548)	1:36:A:THR:HG23	1:37:A:GLY:H	13	0.11
(1,526)	1:34:A:ARG:H	1:44:A:VAL:HG11	20	0.11
(1,526)	1:34:A:ARG:H	1:44:A:VAL:HG12	20	0.11
(1,526)	1:34:A:ARG:H	1:44:A:VAL:HG13	20	0.11
(1,514)	1:33:A:LEU:HD21	1:50:A:GLU:H	3	0.11
(1,514)	1:33:A:LEU:HD22	1:50:A:GLU:H	3	0.11
(1,514)	1:33:A:LEU:HD23	1:50:A:GLU:H	3	0.11
(1,506)	1:33:A:LEU:HD21	1:48:A:LEU:HA	19	0.11
(1,506)	1:33:A:LEU:HD22	1:48:A:LEU:HA	19	0.11
(1,506)	1:33:A:LEU:HD23	1:48:A:LEU:HA	19	0.11
(1,505)	1:33:A:LEU:HD21	1:47:A:LYS:H	7	0.11
(1,505)	1:33:A:LEU:HD22	1:47:A:LYS:H	7	0.11
(1,505)	1:33:A:LEU:HD23	1:47:A:LYS:H	7	0.11
(1,505)	1:33:A:LEU:HD21	1:47:A:LYS:H	10	0.11
(1,505)	1:33:A:LEU:HD22	1:47:A:LYS:H	10	0.11
(1,505)	1:33:A:LEU:HD23	1:47:A:LYS:H	10	0.11
(1,505)	1:33:A:LEU:HD21	1:47:A:LYS:H	17	0.11
(1,505)	1:33:A:LEU:HD22	1:47:A:LYS:H	17	0.11
(1,505)	1:33:A:LEU:HD23	1:47:A:LYS:H	17	0.11
(1,503)	1:33:A:LEU:HB2	1:35:A:VAL:HG11	9	0.11
(1,503)	1:33:A:LEU:HB2	1:35:A:VAL:HG12	9	0.11
(1,503)	1:33:A:LEU:HB2	1:35:A:VAL:HG13	9	0.11
(1,503)	1:33:A:LEU:HB2	1:35:A:VAL:HG11	19	0.11
(1,503)	1:33:A:LEU:HB2	1:35:A:VAL:HG12	19	0.11
(1,503)	1:33:A:LEU:HB2	1:35:A:VAL:HG13	19	0.11
(1,499)	1:33:A:LEU:HD21	1:34:A:ARG:H	4	0.11
(1,499)	1:33:A:LEU:HD22	1:34:A:ARG:H	4	0.11
(1,499)	1:33:A:LEU:HD23	1:34:A:ARG:H	4	0.11
(1,499)	1:33:A:LEU:HD21	1:34:A:ARG:H	11	0.11
(1,499)	1:33:A:LEU:HD22	1:34:A:ARG:H	11	0.11
(1,499)	1:33:A:LEU:HD23	1:34:A:ARG:H	11	0.11
(1,499)	1:33:A:LEU:HD21	1:34:A:ARG:H	13	0.11
(1,499)	1:33:A:LEU:HD22	1:34:A:ARG:H	13	0.11
(1,499)	1:33:A:LEU:HD23	1:34:A:ARG:H	13	0.11
(1,497)	1:33:A:LEU:HB3	1:34:A:ARG:H	7	0.11
(1,480)	1:32:A:THR:HG21	1:33:A:LEU:H	1	0.11
(1,480)	1:32:A:THR:HG22	1:33:A:LEU:H	1	0.11
(1,480)	1:32:A:THR:HG23	1:33:A:LEU:H	1	0.11
(1,480)	1:32:A:THR:HG21	1:33:A:LEU:H	2	0.11
(1,480)	1:32:A:THR:HG22	1:33:A:LEU:H	2	0.11
(1,480)	1:32:A:THR:HG23	1:33:A:LEU:H	2	0.11
(1,480)	1:32:A:THR:HG21	1:33:A:LEU:H	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,480)	1:32:A:THR:HG22	1:33:A:LEU:H	4	0.11
(1,480)	1:32:A:THR:HG23	1:33:A:LEU:H	4	0.11
(1,480)	1:32:A:THR:HG21	1:33:A:LEU:H	6	0.11
(1,480)	1:32:A:THR:HG22	1:33:A:LEU:H	6	0.11
(1,480)	1:32:A:THR:HG23	1:33:A:LEU:H	6	0.11
(1,480)	1:32:A:THR:HG21	1:33:A:LEU:H	9	0.11
(1,480)	1:32:A:THR:HG22	1:33:A:LEU:H	9	0.11
(1,480)	1:32:A:THR:HG23	1:33:A:LEU:H	9	0.11
(1,480)	1:32:A:THR:HG21	1:33:A:LEU:H	10	0.11
(1,480)	1:32:A:THR:HG22	1:33:A:LEU:H	10	0.11
(1,480)	1:32:A:THR:HG23	1:33:A:LEU:H	10	0.11
(1,480)	1:32:A:THR:HG21	1:33:A:LEU:H	12	0.11
(1,480)	1:32:A:THR:HG22	1:33:A:LEU:H	12	0.11
(1,480)	1:32:A:THR:HG23	1:33:A:LEU:H	12	0.11
(1,480)	1:32:A:THR:HG21	1:33:A:LEU:H	17	0.11
(1,480)	1:32:A:THR:HG22	1:33:A:LEU:H	17	0.11
(1,480)	1:32:A:THR:HG23	1:33:A:LEU:H	17	0.11
(1,480)	1:32:A:THR:HG21	1:33:A:LEU:H	20	0.11
(1,480)	1:32:A:THR:HG22	1:33:A:LEU:H	20	0.11
(1,480)	1:32:A:THR:HG23	1:33:A:LEU:H	20	0.11
(1,473)	1:32:A:THR:HB	1:32:A:THR:H	6	0.11
(1,454)	1:30:A:ASP:H	1:30:A:ASP:HB3	20	0.11
(1,443)	1:29:A:ARG:HB2	1:29:A:ARG:H	3	0.11
(1,443)	1:29:A:ARG:HB2	1:29:A:ARG:H	15	0.11
(1,431)	1:27:A:VAL:H	1:93:A:THR:HB	8	0.11
(1,427)	1:27:A:VAL:H	1:29:A:ARG:H	6	0.11
(1,427)	1:27:A:VAL:H	1:29:A:ARG:H	7	0.11
(1,426)	1:27:A:VAL:H	1:28:A:ASN:HB2	5	0.11
(1,414)	1:25:A:THR:H	1:93:A:THR:HG21	12	0.11
(1,414)	1:25:A:THR:H	1:93:A:THR:HG22	12	0.11
(1,414)	1:25:A:THR:H	1:93:A:THR:HG23	12	0.11
(1,414)	1:25:A:THR:H	1:93:A:THR:HG21	20	0.11
(1,414)	1:25:A:THR:H	1:93:A:THR:HG22	20	0.11
(1,414)	1:25:A:THR:H	1:93:A:THR:HG23	20	0.11
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG21	14	0.11
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG22	14	0.11
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG23	14	0.11
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG21	15	0.11
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG22	15	0.11
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG23	15	0.11
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG21	18	0.11
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG22	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,413)	1:25:A:THR:HA	1:93:A:THR:HG23	18	0.11
(1,405)	1:25:A:THR:H	1:64:A:TRP:HB2	14	0.11
(1,402)	1:25:A:THR:HA	1:29:A:ARG:H	14	0.11
(1,395)	1:25:A:THR:HB	1:25:A:THR:H	9	0.11
(1,395)	1:25:A:THR:HB	1:25:A:THR:H	11	0.11
(1,392)	1:24:A:VAL:HB	1:92:A:PHE:H	5	0.11
(1,392)	1:24:A:VAL:HB	1:92:A:PHE:H	6	0.11
(1,392)	1:24:A:VAL:HB	1:92:A:PHE:H	18	0.11
(1,392)	1:24:A:VAL:HB	1:92:A:PHE:H	19	0.11
(1,390)	1:24:A:VAL:HG21	1:91:A:GLN:H	19	0.11
(1,390)	1:24:A:VAL:HG22	1:91:A:GLN:H	19	0.11
(1,390)	1:24:A:VAL:HG23	1:91:A:GLN:H	19	0.11
(1,386)	1:24:A:VAL:HG21	1:31:A:VAL:HB	15	0.11
(1,386)	1:24:A:VAL:HG22	1:31:A:VAL:HB	15	0.11
(1,386)	1:24:A:VAL:HG23	1:31:A:VAL:HB	15	0.11
(1,386)	1:24:A:VAL:HG21	1:31:A:VAL:HB	20	0.11
(1,386)	1:24:A:VAL:HG22	1:31:A:VAL:HB	20	0.11
(1,386)	1:24:A:VAL:HG23	1:31:A:VAL:HB	20	0.11
(1,383)	1:24:A:VAL:HA	1:31:A:VAL:H	1	0.11
(1,383)	1:24:A:VAL:HA	1:31:A:VAL:H	3	0.11
(1,383)	1:24:A:VAL:HA	1:31:A:VAL:H	6	0.11
(1,383)	1:24:A:VAL:HA	1:31:A:VAL:H	9	0.11
(1,383)	1:24:A:VAL:HA	1:31:A:VAL:H	12	0.11
(1,383)	1:24:A:VAL:HA	1:31:A:VAL:H	20	0.11
(1,377)	1:24:A:VAL:HA	1:30:A:ASP:HA	19	0.11
(1,372)	1:24:A:VAL:HG21	1:29:A:ARG:H	15	0.11
(1,372)	1:24:A:VAL:HG22	1:29:A:ARG:H	15	0.11
(1,372)	1:24:A:VAL:HG23	1:29:A:ARG:H	15	0.11
(1,371)	1:24:A:VAL:HG11	1:29:A:ARG:H	6	0.11
(1,371)	1:24:A:VAL:HG12	1:29:A:ARG:H	6	0.11
(1,371)	1:24:A:VAL:HG13	1:29:A:ARG:H	6	0.11
(1,371)	1:24:A:VAL:HG11	1:29:A:ARG:H	9	0.11
(1,371)	1:24:A:VAL:HG12	1:29:A:ARG:H	9	0.11
(1,371)	1:24:A:VAL:HG13	1:29:A:ARG:H	9	0.11
(1,339)	1:23:A:HIS:H	1:90:A:LEU:H	10	0.11
(1,339)	1:23:A:HIS:H	1:90:A:LEU:H	15	0.11
(1,323)	1:23:A:HIS:HB2	1:24:A:VAL:H	6	0.11
(1,323)	1:23:A:HIS:HB2	1:24:A:VAL:H	11	0.11
(1,316)	1:22:A:VAL:HG21	1:91:A:GLN:H	5	0.11
(1,316)	1:22:A:VAL:HG22	1:91:A:GLN:H	5	0.11
(1,316)	1:22:A:VAL:HG23	1:91:A:GLN:H	5	0.11
(1,306)	1:22:A:VAL:HB	1:48:A:LEU:HD21	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:22:A:VAL:HB	1:48:A:LEU:HD22	10	0.11
(1,306)	1:22:A:VAL:HB	1:48:A:LEU:HD23	10	0.11
(1,299)	1:22:A:VAL:H	1:32:A:THR:HB	4	0.11
(1,293)	1:22:A:VAL:HG21	1:24:A:VAL:H	7	0.11
(1,293)	1:22:A:VAL:HG22	1:24:A:VAL:H	7	0.11
(1,293)	1:22:A:VAL:HG23	1:24:A:VAL:H	7	0.11
(1,293)	1:22:A:VAL:HG21	1:24:A:VAL:H	17	0.11
(1,293)	1:22:A:VAL:HG22	1:24:A:VAL:H	17	0.11
(1,293)	1:22:A:VAL:HG23	1:24:A:VAL:H	17	0.11
(1,293)	1:22:A:VAL:HG21	1:24:A:VAL:H	20	0.11
(1,293)	1:22:A:VAL:HG22	1:24:A:VAL:H	20	0.11
(1,293)	1:22:A:VAL:HG23	1:24:A:VAL:H	20	0.11
(1,280)	1:21:A:SER:HB3	1:90:A:LEU:H	7	0.11
(1,280)	1:21:A:SER:HB3	1:90:A:LEU:H	11	0.11
(1,280)	1:21:A:SER:HB3	1:90:A:LEU:H	17	0.11
(1,270)	1:21:A:SER:HB3	1:32:A:THR:HA	11	0.11
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG21	3	0.11
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG22	3	0.11
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG23	3	0.11
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG21	6	0.11
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG22	6	0.11
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG23	6	0.11
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG21	10	0.11
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG22	10	0.11
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG23	10	0.11
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB1	4	0.11
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB2	4	0.11
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB3	4	0.11
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB1	4	0.11
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB2	4	0.11
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB3	4	0.11
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB1	4	0.11
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB2	4	0.11
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB3	4	0.11
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB1	8	0.11
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB2	8	0.11
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB3	8	0.11
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB1	8	0.11
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB2	8	0.11
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB3	8	0.11
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB1	8	0.11
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB2	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB3	8	0.11
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB1	18	0.11
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB2	18	0.11
(1,257)	1:20:A:LEU:HD11	1:86:A:ALA:HB3	18	0.11
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB1	18	0.11
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB2	18	0.11
(1,257)	1:20:A:LEU:HD12	1:86:A:ALA:HB3	18	0.11
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB1	18	0.11
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB2	18	0.11
(1,257)	1:20:A:LEU:HD13	1:86:A:ALA:HB3	18	0.11
(1,250)	1:20:A:LEU:H	1:35:A:VAL:H	1	0.11
(1,250)	1:20:A:LEU:H	1:35:A:VAL:H	6	0.11
(1,250)	1:20:A:LEU:H	1:35:A:VAL:H	12	0.11
(1,250)	1:20:A:LEU:H	1:35:A:VAL:H	19	0.11
(1,250)	1:20:A:LEU:H	1:35:A:VAL:H	20	0.11
(1,242)	1:20:A:LEU:HB3	1:33:A:LEU:H	9	0.11
(1,242)	1:20:A:LEU:HB3	1:33:A:LEU:H	10	0.11
(1,242)	1:20:A:LEU:HB3	1:33:A:LEU:H	18	0.11
(1,232)	1:20:A:LEU:HG	1:21:A:SER:H	3	0.11
(1,232)	1:20:A:LEU:HG	1:21:A:SER:H	4	0.11
(1,232)	1:20:A:LEU:HG	1:21:A:SER:H	12	0.11
(1,212)	1:19:A:GLU:HB2	1:33:A:LEU:H	11	0.11
(1,212)	1:19:A:GLU:HB2	1:33:A:LEU:H	13	0.11
(1,208)	1:19:A:GLU:HG2	1:32:A:THR:HB	14	0.11
(1,204)	1:19:A:GLU:HG2	1:20:A:LEU:H	8	0.11
(1,204)	1:19:A:GLU:HG2	1:20:A:LEU:H	9	0.11
(1,204)	1:19:A:GLU:HG2	1:20:A:LEU:H	18	0.11
(1,189)	1:18:A:TRP:HD1	1:85:A:GLN:HB3	13	0.11
(1,189)	1:18:A:TRP:HD1	1:85:A:GLN:HB3	19	0.11
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG21	12	0.11
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG22	12	0.11
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG23	12	0.11
(1,176)	1:18:A:TRP:H	1:36:A:THR:H	3	0.11
(1,169)	1:18:A:TRP:H	1:18:A:TRP:HD1	6	0.11
(1,156)	1:16:A:GLY:HA2	1:17:A:THR:H	16	0.11
(1,153)	1:15:A:ASP:H	1:17:A:THR:H	2	0.11
(1,152)	1:15:A:ASP:HB3	1:16:A:GLY:H	16	0.11
(1,142)	1:14:A:ALA:HA	1:15:A:ASP:H	2	0.11
(1,140)	1:13:A:TYR:HB3	1:15:A:ASP:H	10	0.11
(1,135)	1:13:A:TYR:H	1:13:A:TYR:HB3	19	0.11
(1,127)	1:11:A:GLY:HA2	1:12:A:CYS:H	2	0.11
(1,127)	1:11:A:GLY:HA2	1:12:A:CYS:H	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,110)	1:9:A:PRO:HB2	1:10:A:ASP:H	5	0.11
(1,103)	1:8:A:MET:HG3	1:12:A:CYS:HB3	11	0.11
(1,102)	1:8:A:MET:HB3	1:12:A:CYS:H	12	0.11
(1,100)	1:8:A:MET:H	1:12:A:CYS:HA	3	0.11
(1,100)	1:8:A:MET:H	1:12:A:CYS:HA	20	0.11
(1,96)	1:8:A:MET:HG3	1:10:A:ASP:H	14	0.11
(1,87)	1:7:A:ARG:HG3	1:10:A:ASP:H	16	0.11
(1,85)	1:7:A:ARG:HD3	1:8:A:MET:H	20	0.11
(1,79)	1:7:A:ARG:HD3	1:7:A:ARG:HB2	20	0.11
(1,78)	1:7:A:ARG:HD3	1:7:A:ARG:HB3	6	0.11
(1,78)	1:7:A:ARG:HD3	1:7:A:ARG:HB3	18	0.11
(1,76)	1:7:A:ARG:HA	1:7:A:ARG:HG3	20	0.11
(1,67)	1:6:A:ILE:H	1:10:A:ASP:H	5	0.11
(1,67)	1:6:A:ILE:H	1:10:A:ASP:H	8	0.11
(1,66)	1:6:A:ILE:HB	1:8:A:MET:H	2	0.11
(1,66)	1:6:A:ILE:HB	1:8:A:MET:H	10	0.11
(1,66)	1:6:A:ILE:HB	1:8:A:MET:H	20	0.11
(1,49)	1:5:A:GLY:HA3	1:6:A:ILE:HB	8	0.11
(1,43)	1:4:A:ASP:HB3	1:5:A:GLY:H	3	0.11
(1,43)	1:4:A:ASP:HB3	1:5:A:GLY:H	18	0.11
(1,42)	1:4:A:ASP:H	1:5:A:GLY:HA3	4	0.11
(1,40)	1:4:A:ASP:HA	1:5:A:GLY:H	6	0.11
(1,40)	1:4:A:ASP:HA	1:5:A:GLY:H	14	0.11
(1,39)	1:4:A:ASP:H	1:4:A:ASP:HB3	6	0.11
(1,34)	1:3:A:LEU:HD21	1:4:A:ASP:H	16	0.11
(1,34)	1:3:A:LEU:HD22	1:4:A:ASP:H	16	0.11
(1,34)	1:3:A:LEU:HD23	1:4:A:ASP:H	16	0.11
(1,34)	1:3:A:LEU:HD21	1:4:A:ASP:H	18	0.11
(1,34)	1:3:A:LEU:HD22	1:4:A:ASP:H	18	0.11
(1,34)	1:3:A:LEU:HD23	1:4:A:ASP:H	18	0.11
(1,33)	1:3:A:LEU:H	1:4:A:ASP:HB3	6	0.11
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD11	4	0.11
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD12	4	0.11
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD13	4	0.11
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD11	5	0.11
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD12	5	0.11
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD13	5	0.11
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD11	12	0.11
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD12	12	0.11
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD13	12	0.11
(1,16)	1:2:A:ALA:H	1:3:A:LEU:HB3	18	0.11
(1,16)	1:2:A:ALA:H	1:3:A:LEU:HB3	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:1:A:MET:HA	1:1:A:MET:HG3	2	0.11
(1,1)	1:1:A:MET:HA	1:1:A:MET:HG3	3	0.11
(1,1)	1:1:A:MET:HA	1:1:A:MET:HG3	8	0.11
(1,1)	1:1:A:MET:HA	1:1:A:MET:HG3	13	0.11
(1,1)	1:1:A:MET:HA	1:1:A:MET:HG3	16	0.11
(1,1)	1:1:A:MET:HA	1:1:A:MET:HG3	17	0.11
(3,16)	1:42:A:GLY:O	1:46:A:LEU:H	13	0.1
(3,16)	1:42:A:GLY:O	1:46:A:LEU:H	15	0.1
(3,14)	1:91:A:GLN:O	1:23:A:HIS:H	12	0.1
(3,7)	1:29:A:ARG:O	1:24:A:VAL:H	11	0.1
(3,4)	1:33:A:LEU:O	1:20:A:LEU:H	15	0.1
(2,16)	1:21:A:SER:O	1:91:A:GLN:N	6	0.1
(2,14)	1:64:A:TRP:O	1:92:A:PHE:N	19	0.1
(2,3)	1:20:A:LEU:O	1:33:A:LEU:N	3	0.1
(2,3)	1:20:A:LEU:O	1:33:A:LEU:N	4	0.1
(2,3)	1:20:A:LEU:O	1:33:A:LEU:N	8	0.1
(2,3)	1:20:A:LEU:O	1:33:A:LEU:N	14	0.1
(2,3)	1:20:A:LEU:O	1:33:A:LEU:N	15	0.1
(2,3)	1:20:A:LEU:O	1:33:A:LEU:N	17	0.1
(1,1407)	1:92:A:PHE:HB2	1:93:A:THR:H	16	0.1
(1,1397)	1:91:A:GLN:HB2	1:92:A:PHE:HA	12	0.1
(1,1397)	1:91:A:GLN:HB2	1:92:A:PHE:HA	16	0.1
(1,1381)	1:91:A:GLN:H	1:91:A:GLN:HG2	7	0.1
(1,1355)	1:90:A:LEU:H	1:90:A:LEU:HD21	8	0.1
(1,1355)	1:90:A:LEU:H	1:90:A:LEU:HD22	8	0.1
(1,1355)	1:90:A:LEU:H	1:90:A:LEU:HD23	8	0.1
(1,1355)	1:90:A:LEU:H	1:90:A:LEU:HD21	18	0.1
(1,1355)	1:90:A:LEU:H	1:90:A:LEU:HD22	18	0.1
(1,1355)	1:90:A:LEU:H	1:90:A:LEU:HD23	18	0.1
(1,1330)	1:87:A:ASP:H	1:88:A:ALA:HA	9	0.1
(1,1330)	1:87:A:ASP:H	1:88:A:ALA:HA	12	0.1
(1,1330)	1:87:A:ASP:H	1:88:A:ALA:HA	14	0.1
(1,1329)	1:87:A:ASP:HB3	1:88:A:ALA:H	8	0.1
(1,1329)	1:87:A:ASP:HB3	1:88:A:ALA:H	11	0.1
(1,1329)	1:87:A:ASP:HB3	1:88:A:ALA:H	18	0.1
(1,1323)	1:86:A:ALA:HB1	1:88:A:ALA:H	3	0.1
(1,1323)	1:86:A:ALA:HB2	1:88:A:ALA:H	3	0.1
(1,1323)	1:86:A:ALA:HB3	1:88:A:ALA:H	3	0.1
(1,1313)	1:85:A:GLN:HB3	1:87:A:ASP:H	8	0.1
(1,1313)	1:85:A:GLN:HB3	1:87:A:ASP:H	15	0.1
(1,1313)	1:85:A:GLN:HB3	1:87:A:ASP:H	19	0.1
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB1	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB2	3	0.1
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB3	3	0.1
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB1	7	0.1
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB2	7	0.1
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB3	7	0.1
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB1	8	0.1
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB2	8	0.1
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB3	8	0.1
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB1	11	0.1
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB2	11	0.1
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB3	11	0.1
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB1	16	0.1
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB2	16	0.1
(1,1310)	1:85:A:GLN:HG3	1:86:A:ALA:HB3	16	0.1
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG21	1	0.1
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG22	1	0.1
(1,1267)	1:83:A:GLY:H	1:84:A:ILE:HG23	1	0.1
(1,1230)	1:81:A:LYS:H	1:81:A:LYS:HG3	20	0.1
(1,1225)	1:81:A:LYS:HA	1:81:A:LYS:HG2	18	0.1
(1,1220)	1:80:A:ASP:H	1:83:A:GLY:H	18	0.1
(1,1215)	1:80:A:ASP:HB2	1:81:A:LYS:H	15	0.1
(1,1202)	1:79:A:LEU:HA	1:82:A:TYR:H	4	0.1
(1,1177)	1:78:A:THR:H	1:81:A:LYS:H	15	0.1
(1,1144)	1:75:A:THR:H	1:75:A:THR:HG21	18	0.1
(1,1144)	1:75:A:THR:H	1:75:A:THR:HG22	18	0.1
(1,1144)	1:75:A:THR:H	1:75:A:THR:HG23	18	0.1
(1,1134)	1:74:A:LYS:HG2	1:75:A:THR:H	20	0.1
(1,1132)	1:74:A:LYS:HG3	1:75:A:THR:H	1	0.1
(1,1129)	1:74:A:LYS:HE2	1:74:A:LYS:HB3	1	0.1
(1,1129)	1:74:A:LYS:HE2	1:74:A:LYS:HB3	8	0.1
(1,1121)	1:74:A:LYS:H	1:74:A:LYS:HG3	3	0.1
(1,1121)	1:74:A:LYS:H	1:74:A:LYS:HG3	8	0.1
(1,1120)	1:74:A:LYS:H	1:74:A:LYS:HG2	19	0.1
(1,1119)	1:74:A:LYS:H	1:74:A:LYS:HE2	11	0.1
(1,1112)	1:74:A:LYS:HA	1:74:A:LYS:HE2	3	0.1
(1,1112)	1:74:A:LYS:HA	1:74:A:LYS:HE2	4	0.1
(1,1097)	1:72:A:LEU:HD21	1:73:A:LEU:H	1	0.1
(1,1097)	1:72:A:LEU:HD22	1:73:A:LEU:H	1	0.1
(1,1097)	1:72:A:LEU:HD23	1:73:A:LEU:H	1	0.1
(1,1097)	1:72:A:LEU:HD21	1:73:A:LEU:H	9	0.1
(1,1097)	1:72:A:LEU:HD22	1:73:A:LEU:H	9	0.1
(1,1097)	1:72:A:LEU:HD23	1:73:A:LEU:H	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1097)	1:72:A:LEU:HD21	1:73:A:LEU:H	17	0.1
(1,1097)	1:72:A:LEU:HD22	1:73:A:LEU:H	17	0.1
(1,1097)	1:72:A:LEU:HD23	1:73:A:LEU:H	17	0.1
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD21	7	0.1
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD22	7	0.1
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD23	7	0.1
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD21	16	0.1
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD22	16	0.1
(1,1054)	1:67:A:LYS:H	1:90:A:LEU:HD23	16	0.1
(1,1052)	1:67:A:LYS:H	1:72:A:LEU:HD11	9	0.1
(1,1052)	1:67:A:LYS:H	1:72:A:LEU:HD12	9	0.1
(1,1052)	1:67:A:LYS:H	1:72:A:LEU:HD13	9	0.1
(1,1036)	1:67:A:LYS:HE3	1:67:A:LYS:H	16	0.1
(1,1029)	1:66:A:GLU:HB3	1:69:A:ARG:HA	18	0.1
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD21	7	0.1
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD22	7	0.1
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD23	7	0.1
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD21	12	0.1
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD22	12	0.1
(1,1014)	1:65:A:TRP:H	1:73:A:LEU:HD23	12	0.1
(1,981)	1:64:A:TRP:H	1:64:A:TRP:HB3	9	0.1
(1,976)	1:63:A:LEU:HG	1:93:A:THR:H	11	0.1
(1,968)	1:63:A:LEU:HG	1:90:A:LEU:HA	15	0.1
(1,959)	1:63:A:LEU:H	1:64:A:TRP:H	4	0.1
(1,959)	1:63:A:LEU:H	1:64:A:TRP:H	7	0.1
(1,959)	1:63:A:LEU:H	1:64:A:TRP:H	11	0.1
(1,950)	1:63:A:LEU:H	1:63:A:LEU:HG	19	0.1
(1,942)	1:62:A:ALA:HB1	1:92:A:PHE:HA	12	0.1
(1,942)	1:62:A:ALA:HB2	1:92:A:PHE:HA	12	0.1
(1,942)	1:62:A:ALA:HB3	1:92:A:PHE:HA	12	0.1
(1,932)	1:62:A:ALA:H	1:63:A:LEU:HD11	8	0.1
(1,932)	1:62:A:ALA:H	1:63:A:LEU:HD12	8	0.1
(1,932)	1:62:A:ALA:H	1:63:A:LEU:HD13	8	0.1
(1,924)	1:61:A:HIS:H	1:61:A:HIS:HB2	5	0.1
(1,924)	1:61:A:HIS:H	1:61:A:HIS:HB2	7	0.1
(1,924)	1:61:A:HIS:H	1:61:A:HIS:HB2	16	0.1
(1,923)	1:61:A:HIS:H	1:61:A:HIS:HB3	10	0.1
(1,923)	1:61:A:HIS:H	1:61:A:HIS:HB3	13	0.1
(1,923)	1:61:A:HIS:H	1:61:A:HIS:HB3	20	0.1
(1,906)	1:58:A:TRP:H	1:59:A:SER:H	16	0.1
(1,903)	1:57:A:ASP:HB2	1:61:A:HIS:H	4	0.1
(1,903)	1:57:A:ASP:HB2	1:61:A:HIS:H	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,889)	1:56:A:LYS:HA	1:57:A:ASP:HB3	1	0.1
(1,884)	1:56:A:LYS:HE3	1:56:A:LYS:HB3	3	0.1
(1,878)	1:56:A:LYS:H	1:56:A:LYS:HD3	5	0.1
(1,859)	1:51:A:LYS:H	1:51:A:LYS:HB3	4	0.1
(1,852)	1:51:A:LYS:HA	1:51:A:LYS:HD3	14	0.1
(1,852)	1:51:A:LYS:HA	1:51:A:LYS:HD3	18	0.1
(1,852)	1:51:A:LYS:HA	1:51:A:LYS:HD3	20	0.1
(1,838)	1:49:A:VAL:HG21	1:58:A:TRP:H	8	0.1
(1,838)	1:49:A:VAL:HG22	1:58:A:TRP:H	8	0.1
(1,838)	1:49:A:VAL:HG23	1:58:A:TRP:H	8	0.1
(1,837)	1:49:A:VAL:HA	1:52:A:LEU:H	14	0.1
(1,812)	1:48:A:LEU:HA	1:51:A:LYS:HB3	20	0.1
(1,805)	1:48:A:LEU:HG	1:49:A:VAL:H	3	0.1
(1,805)	1:48:A:LEU:HG	1:49:A:VAL:H	7	0.1
(1,799)	1:48:A:LEU:HA	1:49:A:VAL:H	1	0.1
(1,799)	1:48:A:LEU:HA	1:49:A:VAL:H	2	0.1
(1,799)	1:48:A:LEU:HA	1:49:A:VAL:H	6	0.1
(1,799)	1:48:A:LEU:HA	1:49:A:VAL:H	8	0.1
(1,799)	1:48:A:LEU:HA	1:49:A:VAL:H	11	0.1
(1,799)	1:48:A:LEU:HA	1:49:A:VAL:H	16	0.1
(1,794)	1:48:A:LEU:H	1:48:A:LEU:HD11	17	0.1
(1,794)	1:48:A:LEU:H	1:48:A:LEU:HD12	17	0.1
(1,794)	1:48:A:LEU:H	1:48:A:LEU:HD13	17	0.1
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD21	15	0.1
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD22	15	0.1
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD23	15	0.1
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD21	19	0.1
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD22	19	0.1
(1,792)	1:48:A:LEU:H	1:48:A:LEU:HD23	19	0.1
(1,738)	1:45:A:MET:HA	1:48:A:LEU:H	5	0.1
(1,738)	1:45:A:MET:HA	1:48:A:LEU:H	11	0.1
(1,736)	1:45:A:MET:H	1:48:A:LEU:H	20	0.1
(1,723)	1:45:A:MET:H	1:45:A:MET:HB3	14	0.1
(1,717)	1:44:A:VAL:HB	1:47:A:LYS:H	3	0.1
(1,714)	1:44:A:VAL:HA	1:47:A:LYS:HB2	19	0.1
(1,695)	1:43:A:GLY:HA2	1:46:A:LEU:H	5	0.1
(1,695)	1:43:A:GLY:HA2	1:46:A:LEU:H	11	0.1
(1,695)	1:43:A:GLY:HA2	1:46:A:LEU:H	19	0.1
(1,695)	1:43:A:GLY:HA2	1:46:A:LEU:H	20	0.1
(1,688)	1:42:A:GLY:H	1:75:A:THR:HG21	2	0.1
(1,688)	1:42:A:GLY:H	1:75:A:THR:HG22	2	0.1
(1,688)	1:42:A:GLY:H	1:75:A:THR:HG23	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,681)	1:42:A:GLY:HA3	1:45:A:MET:H	19	0.1
(1,676)	1:41:A:ILE:HG13	1:78:A:THR:H	12	0.1
(1,663)	1:41:A:ILE:HG21	1:72:A:LEU:HG	20	0.1
(1,663)	1:41:A:ILE:HG22	1:72:A:LEU:HG	20	0.1
(1,663)	1:41:A:ILE:HG23	1:72:A:LEU:HG	20	0.1
(1,641)	1:41:A:ILE:H	1:41:A:ILE:HD11	1	0.1
(1,641)	1:41:A:ILE:H	1:41:A:ILE:HD12	1	0.1
(1,641)	1:41:A:ILE:H	1:41:A:ILE:HD13	1	0.1
(1,641)	1:41:A:ILE:H	1:41:A:ILE:HD11	14	0.1
(1,641)	1:41:A:ILE:H	1:41:A:ILE:HD12	14	0.1
(1,641)	1:41:A:ILE:H	1:41:A:ILE:HD13	14	0.1
(1,640)	1:41:A:ILE:H	1:41:A:ILE:HG12	8	0.1
(1,640)	1:41:A:ILE:H	1:41:A:ILE:HG12	14	0.1
(1,627)	1:40:A:HIS:HB3	1:43:A:GLY:H	16	0.1
(1,617)	1:40:A:HIS:HB3	1:41:A:ILE:H	7	0.1
(1,617)	1:40:A:HIS:HB3	1:41:A:ILE:H	15	0.1
(1,617)	1:40:A:HIS:HB3	1:41:A:ILE:H	18	0.1
(1,599)	1:39:A:VAL:H	1:40:A:HIS:H	7	0.1
(1,588)	1:38:A:GLU:HA	1:80:A:ASP:H	19	0.1
(1,584)	1:38:A:GLU:H	1:39:A:VAL:HG11	4	0.1
(1,584)	1:38:A:GLU:H	1:39:A:VAL:HG12	4	0.1
(1,584)	1:38:A:GLU:H	1:39:A:VAL:HG13	4	0.1
(1,584)	1:38:A:GLU:H	1:39:A:VAL:HG11	13	0.1
(1,584)	1:38:A:GLU:H	1:39:A:VAL:HG12	13	0.1
(1,584)	1:38:A:GLU:H	1:39:A:VAL:HG13	13	0.1
(1,563)	1:37:A:GLY:HA3	1:38:A:GLU:H	19	0.1
(1,561)	1:37:A:GLY:H	1:38:A:GLU:HG3	9	0.1
(1,561)	1:37:A:GLY:H	1:38:A:GLU:HG3	13	0.1
(1,515)	1:34:A:ARG:H	1:34:A:ARG:HB3	9	0.1
(1,514)	1:33:A:LEU:HD21	1:50:A:GLU:H	2	0.1
(1,514)	1:33:A:LEU:HD22	1:50:A:GLU:H	2	0.1
(1,514)	1:33:A:LEU:HD23	1:50:A:GLU:H	2	0.1
(1,514)	1:33:A:LEU:HD21	1:50:A:GLU:H	8	0.1
(1,514)	1:33:A:LEU:HD22	1:50:A:GLU:H	8	0.1
(1,514)	1:33:A:LEU:HD23	1:50:A:GLU:H	8	0.1
(1,514)	1:33:A:LEU:HD21	1:50:A:GLU:H	9	0.1
(1,514)	1:33:A:LEU:HD22	1:50:A:GLU:H	9	0.1
(1,514)	1:33:A:LEU:HD23	1:50:A:GLU:H	9	0.1
(1,514)	1:33:A:LEU:HD21	1:50:A:GLU:H	11	0.1
(1,514)	1:33:A:LEU:HD22	1:50:A:GLU:H	11	0.1
(1,514)	1:33:A:LEU:HD23	1:50:A:GLU:H	11	0.1
(1,514)	1:33:A:LEU:HD21	1:50:A:GLU:H	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,514)	1:33:A:LEU:HD22	1:50:A:GLU:H	17	0.1
(1,514)	1:33:A:LEU:HD23	1:50:A:GLU:H	17	0.1
(1,505)	1:33:A:LEU:HD21	1:47:A:LYS:H	6	0.1
(1,505)	1:33:A:LEU:HD22	1:47:A:LYS:H	6	0.1
(1,505)	1:33:A:LEU:HD23	1:47:A:LYS:H	6	0.1
(1,499)	1:33:A:LEU:HD21	1:34:A:ARG:H	19	0.1
(1,499)	1:33:A:LEU:HD22	1:34:A:ARG:H	19	0.1
(1,499)	1:33:A:LEU:HD23	1:34:A:ARG:H	19	0.1
(1,487)	1:33:A:LEU:H	1:33:A:LEU:HD11	11	0.1
(1,487)	1:33:A:LEU:H	1:33:A:LEU:HD12	11	0.1
(1,487)	1:33:A:LEU:H	1:33:A:LEU:HD13	11	0.1
(1,480)	1:32:A:THR:HG21	1:33:A:LEU:H	3	0.1
(1,480)	1:32:A:THR:HG22	1:33:A:LEU:H	3	0.1
(1,480)	1:32:A:THR:HG23	1:33:A:LEU:H	3	0.1
(1,480)	1:32:A:THR:HG21	1:33:A:LEU:H	7	0.1
(1,480)	1:32:A:THR:HG22	1:33:A:LEU:H	7	0.1
(1,480)	1:32:A:THR:HG23	1:33:A:LEU:H	7	0.1
(1,480)	1:32:A:THR:HG21	1:33:A:LEU:H	19	0.1
(1,480)	1:32:A:THR:HG22	1:33:A:LEU:H	19	0.1
(1,480)	1:32:A:THR:HG23	1:33:A:LEU:H	19	0.1
(1,473)	1:32:A:THR:HB	1:32:A:THR:H	5	0.1
(1,464)	1:31:A:VAL:HA	1:32:A:THR:HB	17	0.1
(1,464)	1:31:A:VAL:HA	1:32:A:THR:HB	20	0.1
(1,454)	1:30:A:ASP:H	1:30:A:ASP:HB3	2	0.1
(1,454)	1:30:A:ASP:H	1:30:A:ASP:HB3	17	0.1
(1,430)	1:27:A:VAL:HG21	1:92:A:PHE:H	9	0.1
(1,430)	1:27:A:VAL:HG22	1:92:A:PHE:H	9	0.1
(1,430)	1:27:A:VAL:HG23	1:92:A:PHE:H	9	0.1
(1,422)	1:27:A:VAL:H	1:28:A:ASN:H	5	0.1
(1,422)	1:27:A:VAL:H	1:28:A:ASN:H	8	0.1
(1,422)	1:27:A:VAL:H	1:28:A:ASN:H	9	0.1
(1,422)	1:27:A:VAL:H	1:28:A:ASN:H	10	0.1
(1,422)	1:27:A:VAL:H	1:28:A:ASN:H	16	0.1
(1,395)	1:25:A:THR:HB	1:25:A:THR:H	4	0.1
(1,395)	1:25:A:THR:HB	1:25:A:THR:H	19	0.1
(1,392)	1:24:A:VAL:HB	1:92:A:PHE:H	2	0.1
(1,392)	1:24:A:VAL:HB	1:92:A:PHE:H	13	0.1
(1,392)	1:24:A:VAL:HB	1:92:A:PHE:H	14	0.1
(1,392)	1:24:A:VAL:HB	1:92:A:PHE:H	20	0.1
(1,339)	1:23:A:HIS:H	1:90:A:LEU:H	16	0.1
(1,339)	1:23:A:HIS:H	1:90:A:LEU:H	18	0.1
(1,329)	1:23:A:HIS:HB2	1:24:A:VAL:HA	14	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,312)	1:22:A:VAL:HG21	1:90:A:LEU:H	16	0.1
(1,312)	1:22:A:VAL:HG22	1:90:A:LEU:H	16	0.1
(1,312)	1:22:A:VAL:HG23	1:90:A:LEU:H	16	0.1
(1,312)	1:22:A:VAL:HG21	1:90:A:LEU:H	20	0.1
(1,312)	1:22:A:VAL:HG22	1:90:A:LEU:H	20	0.1
(1,312)	1:22:A:VAL:HG23	1:90:A:LEU:H	20	0.1
(1,299)	1:22:A:VAL:H	1:32:A:THR:HB	9	0.1
(1,299)	1:22:A:VAL:H	1:32:A:THR:HB	13	0.1
(1,293)	1:22:A:VAL:HG21	1:24:A:VAL:H	13	0.1
(1,293)	1:22:A:VAL:HG22	1:24:A:VAL:H	13	0.1
(1,293)	1:22:A:VAL:HG23	1:24:A:VAL:H	13	0.1
(1,280)	1:21:A:SER:HB3	1:90:A:LEU:H	13	0.1
(1,280)	1:21:A:SER:HB3	1:90:A:LEU:H	20	0.1
(1,270)	1:21:A:SER:HB3	1:32:A:THR:HA	2	0.1
(1,270)	1:21:A:SER:HB3	1:32:A:THR:HA	7	0.1
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG21	1	0.1
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG22	1	0.1
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG23	1	0.1
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG21	12	0.1
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG22	12	0.1
(1,263)	1:21:A:SER:HB3	1:22:A:VAL:HG23	12	0.1
(1,259)	1:20:A:LEU:HD21	1:88:A:ALA:H	11	0.1
(1,259)	1:20:A:LEU:HD22	1:88:A:ALA:H	11	0.1
(1,259)	1:20:A:LEU:HD23	1:88:A:ALA:H	11	0.1
(1,250)	1:20:A:LEU:H	1:35:A:VAL:H	4	0.1
(1,250)	1:20:A:LEU:H	1:35:A:VAL:H	15	0.1
(1,232)	1:20:A:LEU:HG	1:21:A:SER:H	1	0.1
(1,232)	1:20:A:LEU:HG	1:21:A:SER:H	17	0.1
(1,208)	1:19:A:GLU:HG2	1:32:A:THR:HB	6	0.1
(1,208)	1:19:A:GLU:HG2	1:32:A:THR:HB	17	0.1
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG21	7	0.1
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG22	7	0.1
(1,186)	1:18:A:TRP:HZ2	1:84:A:ILE:HG23	7	0.1
(1,177)	1:18:A:TRP:HE1	1:36:A:THR:HB	12	0.1
(1,176)	1:18:A:TRP:H	1:36:A:THR:H	7	0.1
(1,176)	1:18:A:TRP:H	1:36:A:THR:H	11	0.1
(1,176)	1:18:A:TRP:H	1:36:A:THR:H	12	0.1
(1,176)	1:18:A:TRP:H	1:36:A:THR:H	14	0.1
(1,166)	1:17:A:THR:HG21	1:18:A:TRP:H	3	0.1
(1,166)	1:17:A:THR:HG22	1:18:A:TRP:H	3	0.1
(1,166)	1:17:A:THR:HG23	1:18:A:TRP:H	3	0.1
(1,153)	1:15:A:ASP:H	1:17:A:THR:H	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,147)	1:15:A:ASP:H	1:15:A:ASP:HB2	8	0.1
(1,142)	1:14:A:ALA:HA	1:15:A:ASP:H	18	0.1
(1,135)	1:13:A:TYR:H	1:13:A:TYR:HB3	4	0.1
(1,103)	1:8:A:MET:HG3	1:12:A:CYS:HB3	14	0.1
(1,102)	1:8:A:MET:HB3	1:12:A:CYS:H	8	0.1
(1,100)	1:8:A:MET:H	1:12:A:CYS:HA	6	0.1
(1,95)	1:8:A:MET:HA	1:10:A:ASP:H	4	0.1
(1,94)	1:8:A:MET:H	1:10:A:ASP:HA	11	0.1
(1,85)	1:7:A:ARG:HD3	1:8:A:MET:H	10	0.1
(1,75)	1:7:A:ARG:H	1:7:A:ARG:HB2	4	0.1
(1,67)	1:6:A:ILE:H	1:10:A:ASP:H	9	0.1
(1,66)	1:6:A:ILE:HB	1:8:A:MET:H	8	0.1
(1,62)	1:6:A:ILE:HG21	1:7:A:ARG:H	11	0.1
(1,62)	1:6:A:ILE:HG22	1:7:A:ARG:H	11	0.1
(1,62)	1:6:A:ILE:HG23	1:7:A:ARG:H	11	0.1
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD11	14	0.1
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD12	14	0.1
(1,25)	1:3:A:LEU:H	1:3:A:LEU:HD13	14	0.1
(1,16)	1:2:A:ALA:H	1:3:A:LEU:HB3	16	0.1
(1,1)	1:1:A:MET:HA	1:1:A:MET:HG3	4	0.1
(1,1)	1:1:A:MET:HA	1:1:A:MET:HG3	5	0.1
(1,1)	1:1:A:MET:HA	1:1:A:MET:HG3	10	0.1
(1,1)	1:1:A:MET:HA	1:1:A:MET:HG3	15	0.1

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

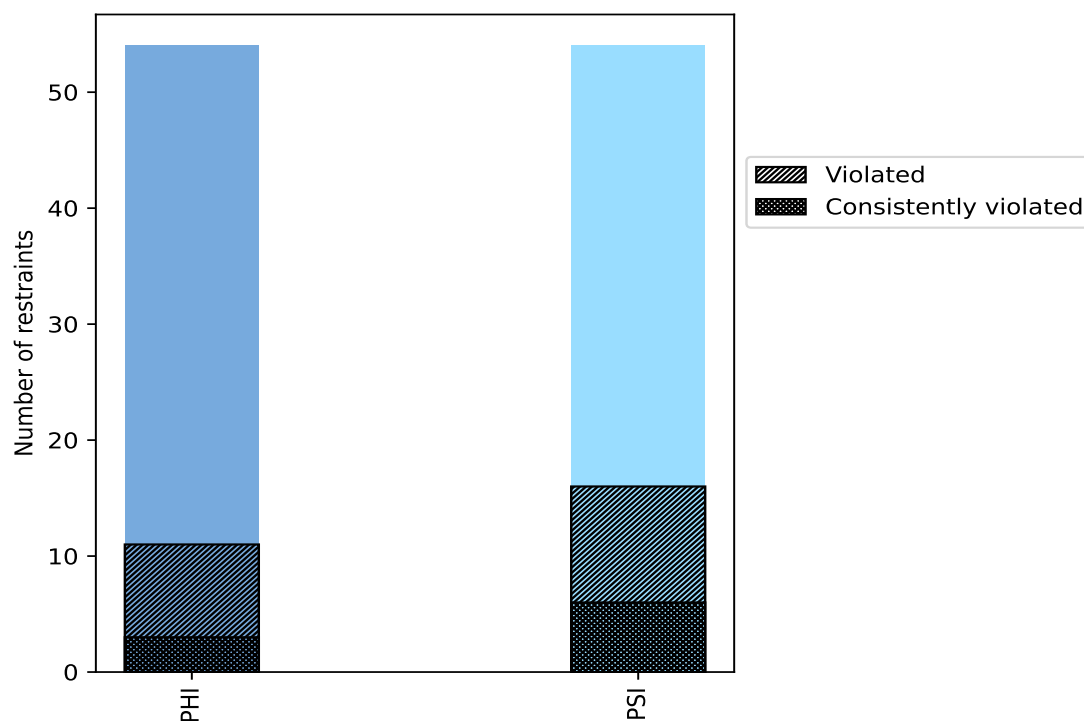
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	54	50.0	11	20.4	10.2	3	5.6	2.8
PSI	54	50.0	16	29.6	14.8	6	11.1	5.6
Total	108	100.0	27	25.0	25.0	9	8.3	8.3

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

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



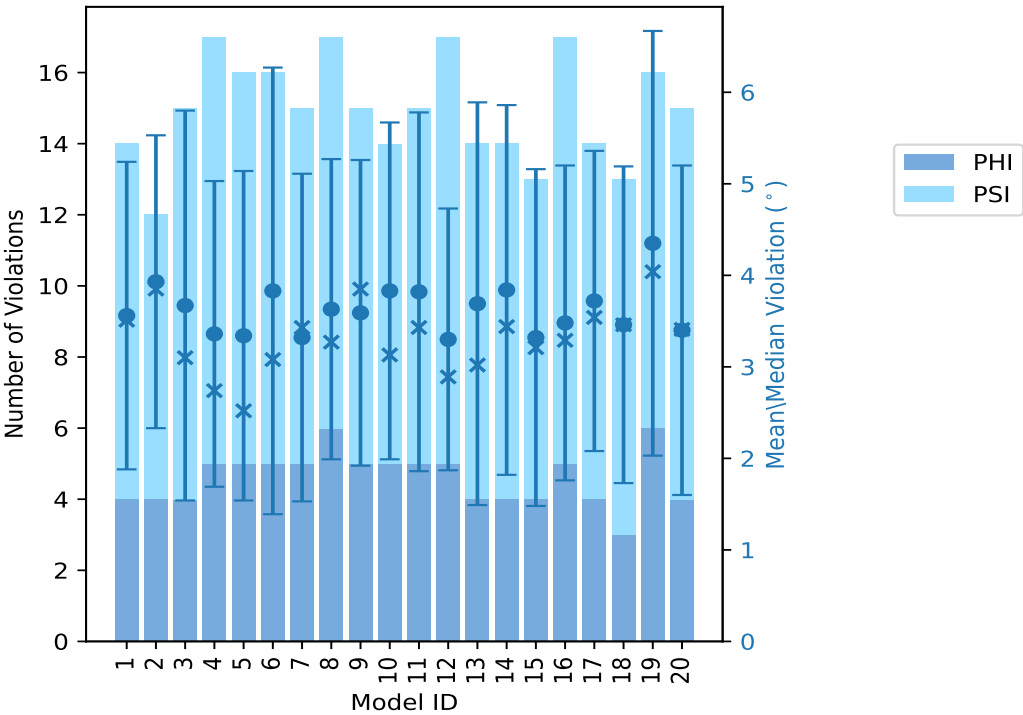
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	4	10	14	3.56	6.41	1.68	3.51
2	4	8	12	3.93	6.8	1.6	3.85
3	4	11	15	3.67	9.19	2.13	3.1
4	5	12	17	3.36	6.97	1.67	2.74
5	5	11	16	3.34	7.35	1.8	2.52
6	5	11	16	3.83	10.58	2.44	3.08
7	5	10	15	3.32	6.89	1.79	3.43
8	6	11	17	3.63	7.15	1.64	3.27
9	5	10	15	3.59	7.13	1.67	3.85
10	5	9	14	3.83	7.59	1.84	3.13
11	5	10	15	3.82	8.28	1.96	3.43
12	5	12	17	3.3	6.36	1.43	2.89
13	4	10	14	3.69	8.35	2.2	3.02
14	4	10	14	3.84	7.26	2.02	3.44
15	4	9	13	3.32	7.63	1.84	3.21
16	5	12	17	3.48	7.02	1.72	3.29
17	4	10	14	3.72	6.62	1.64	3.54
18	3	10	13	3.46	7.41	1.73	3.46
19	6	10	16	4.35	11.3	2.32	4.04
20	4	11	15	3.4	7.39	1.8	3.41

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

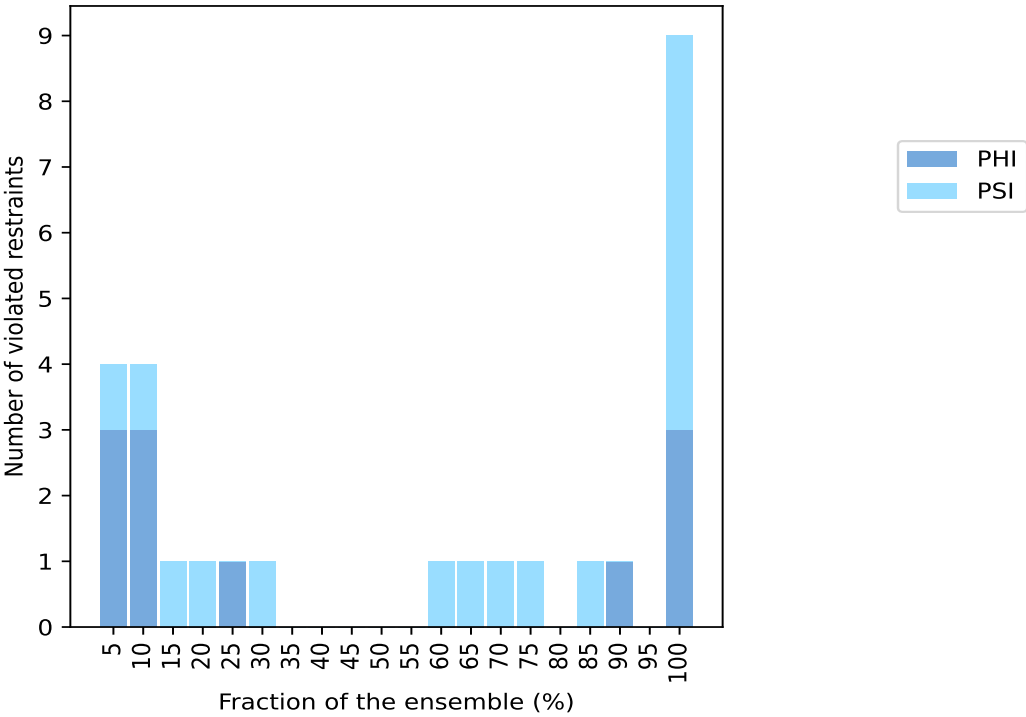
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	1	1	12	60.0
0	1	1	13	65.0
0	1	1	14	70.0
0	1	1	15	75.0
0	0	0	16	80.0
0	1	1	17	85.0
1	0	1	18	90.0
0	0	0	19	95.0
3	6	9	20	100.0

¹ Number of models with violations

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

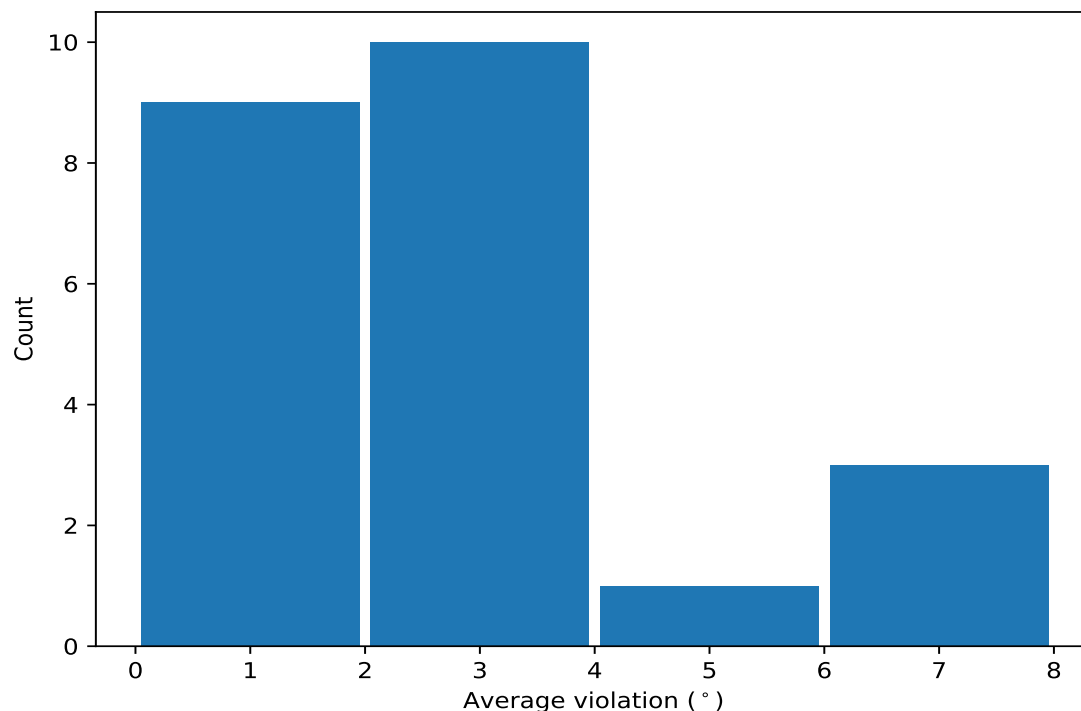


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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
(1,6)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:SER:N	20	7.17	1.32	6.79
(1,81)	1:74:A:LYS:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	20	6.22	1.01	6.47
(1,107)	1:92:A:PHE:C	1:93:A:THR:N	1:93:A:THR:CA	1:93:A:THR:C	20	6.15	1.4	5.84
(1,26)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:VAL:N	20	4.52	0.62	4.36
(1,104)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:PHE:N	20	3.91	0.99	3.83
(1,20)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:THR:N	20	3.75	0.55	3.74
(1,67)	1:63:A:LEU:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	20	3.68	0.71	3.69
(1,16)	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1:30:A:ASP:N	20	3.37	0.92	3.67
(1,10)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:HIS:N	20	2.43	0.31	2.45
(1,83)	1:77:A:TRP:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	18	3.0	0.45	3.09
(1,102)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:GLN:N	17	1.88	0.54	1.81
(1,58)	1:57:A:ASP:N	1:57:A:ASP:CA	1:57:A:ASP:C	1:58:A:TRP:N	15	1.59	0.63	1.28
(1,74)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:LYS:N	14	3.14	0.74	3.1
(1,30)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	13	2.13	0.62	2.07
(1,62)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:ALA:N	12	2.19	0.87	2.06
(1,54)	1:51:A:LYS:N	1:51:A:LYS:CA	1:51:A:LYS:C	1:52:A:LEU:N	6	1.98	0.77	1.98
(1,61)	1:60:A:ASP:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	5	1.91	0.75	1.69
(1,60)	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	1:60:A:ASP:N	4	1.27	0.19	1.27
(1,4)	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1:18:A:TRP:N	3	1.61	0.36	1.63
(1,5)	1:19:A:GLU:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	2	2.38	0.19	2.38

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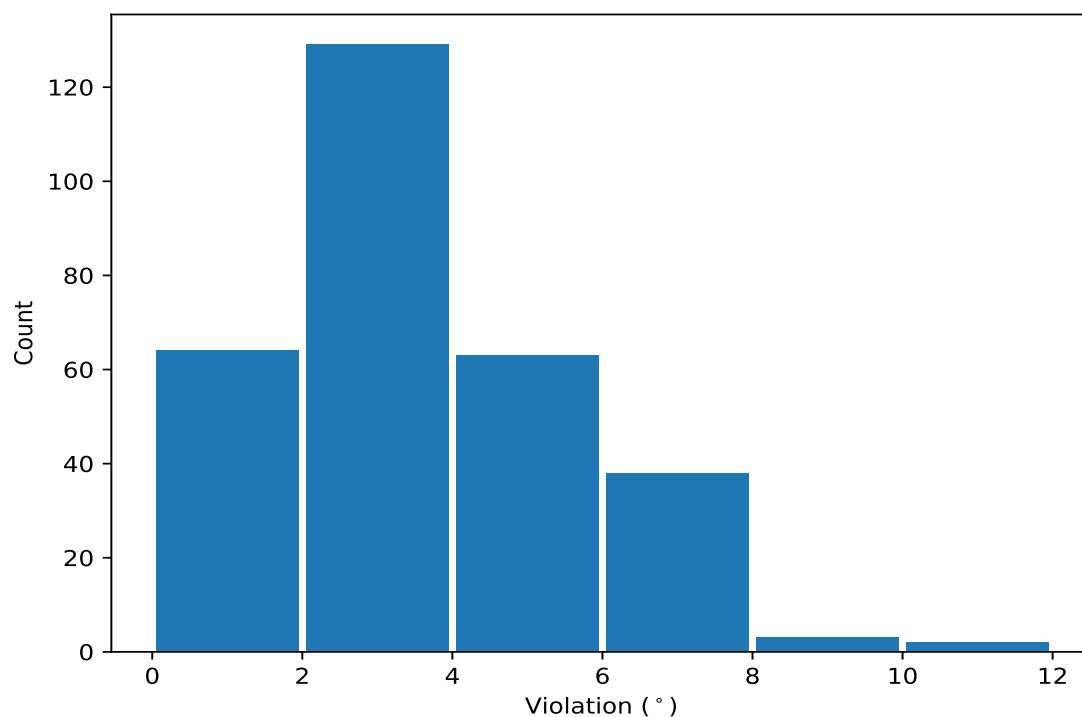
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,59)	1:58:A:TRP:C	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	2	1.48	0.36	1.48
(1,11)	1:22:A:VAL:C	1:23:A:HIS:N	1:23:A:HIS:CA	1:23:A:HIS:C	2	1.36	0.3	1.36
(1,98)	1:88:A:ALA:N	1:88:A:ALA:CA	1:88:A:ALA:C	1:89:A:LYS:N	2	1.33	0.2	1.33

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,6)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:SER:N	19	11.3
(1,6)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:SER:N	6	10.58
(1,107)	1:92:A:PHE:C	1:93:A:THR:N	1:93:A:THR:CA	1:93:A:THR:C	3	9.19
(1,81)	1:74:A:LYS:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	13	8.35

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,107)	1:92:A:PHE:C	1:93:A:THR:N	1:93:A:THR:CA	1:93:A:THR:C	11	8.28
(1,107)	1:92:A:PHE:C	1:93:A:THR:N	1:93:A:THR:CA	1:93:A:THR:C	13	7.7
(1,6)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:SER:N	15	7.63
(1,107)	1:92:A:PHE:C	1:93:A:THR:N	1:93:A:THR:CA	1:93:A:THR:C	10	7.59
(1,81)	1:74:A:LYS:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	19	7.43
(1,6)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:SER:N	18	7.41
(1,107)	1:92:A:PHE:C	1:93:A:THR:N	1:93:A:THR:CA	1:93:A:THR:C	20	7.39
(1,107)	1:92:A:PHE:C	1:93:A:THR:N	1:93:A:THR:CA	1:93:A:THR:C	5	7.35
(1,107)	1:92:A:PHE:C	1:93:A:THR:N	1:93:A:THR:CA	1:93:A:THR:C	14	7.26
(1,6)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:SER:N	8	7.15
(1,6)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:SER:N	9	7.13
(1,6)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:SER:N	16	7.02
(1,6)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:SER:N	4	6.97
(1,81)	1:74:A:LYS:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	6	6.89
(1,81)	1:74:A:LYS:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	7	6.89
(1,6)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:SER:N	11	6.85
(1,81)	1:74:A:LYS:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	8	6.83
(1,6)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:SER:N	2	6.8
(1,6)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:SER:N	20	6.78
(1,81)	1:74:A:LYS:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	3	6.75
(1,6)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:SER:N	14	6.73
(1,6)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:SER:N	13	6.65
(1,6)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:SER:N	17	6.62
(1,81)	1:74:A:LYS:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	10	6.54
(1,81)	1:74:A:LYS:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	9	6.51
(1,81)	1:74:A:LYS:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	17	6.49
(1,81)	1:74:A:LYS:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	14	6.48
(1,81)	1:74:A:LYS:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	11	6.46
(1,104)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:PHE:N	14	6.41
(1,81)	1:74:A:LYS:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	1	6.41
(1,6)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:SER:N	10	6.41
(1,6)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:SER:N	1	6.37
(1,6)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:SER:N	12	6.36
(1,81)	1:74:A:LYS:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	2	6.34
(1,6)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:SER:N	5	6.33
(1,6)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:SER:N	7	6.29
(1,81)	1:74:A:LYS:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	16	6.23
(1,6)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:SER:N	3	6.11
(1,107)	1:92:A:PHE:C	1:93:A:THR:N	1:93:A:THR:CA	1:93:A:THR:C	17	6.07
(1,81)	1:74:A:LYS:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	12	5.92
(1,107)	1:92:A:PHE:C	1:93:A:THR:N	1:93:A:THR:CA	1:93:A:THR:C	2	5.9
(1,107)	1:92:A:PHE:C	1:93:A:THR:N	1:93:A:THR:CA	1:93:A:THR:C	8	5.84
(1,107)	1:92:A:PHE:C	1:93:A:THR:N	1:93:A:THR:CA	1:93:A:THR:C	16	5.84
(1,107)	1:92:A:PHE:C	1:93:A:THR:N	1:93:A:THR:CA	1:93:A:THR:C	7	5.79
(1,104)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:PHE:N	6	5.52
(1,81)	1:74:A:LYS:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	5	5.49
(1,107)	1:92:A:PHE:C	1:93:A:THR:N	1:93:A:THR:CA	1:93:A:THR:C	4	5.48
(1,26)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:VAL:N	6	5.47
(1,81)	1:74:A:LYS:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	4	5.46
(1,26)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:VAL:N	19	5.44
(1,107)	1:92:A:PHE:C	1:93:A:THR:N	1:93:A:THR:CA	1:93:A:THR:C	18	5.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,26)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:VAL:N	5	5.4
(1,107)	1:92:A:PHE:C	1:93:A:THR:N	1:93:A:THR:CA	1:93:A:THR:C	6	5.18
(1,26)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:VAL:N	1	5.15
(1,26)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:VAL:N	15	5.15
(1,104)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:PHE:N	12	5.06
(1,26)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:VAL:N	4	5.06
(1,107)	1:92:A:PHE:C	1:93:A:THR:N	1:93:A:THR:CA	1:93:A:THR:C	1	5.04
(1,26)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:VAL:N	20	5.03
(1,107)	1:92:A:PHE:C	1:93:A:THR:N	1:93:A:THR:CA	1:93:A:THR:C	15	5.02
(1,20)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:THR:N	19	5.02
(1,107)	1:92:A:PHE:C	1:93:A:THR:N	1:93:A:THR:CA	1:93:A:THR:C	19	4.94
(1,26)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:VAL:N	18	4.89
(1,67)	1:63:A:LEU:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	10	4.87
(1,74)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:LYS:N	19	4.65
(1,26)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:VAL:N	14	4.61
(1,104)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:PHE:N	19	4.54
(1,81)	1:74:A:LYS:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	18	4.54
(1,67)	1:63:A:LEU:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	3	4.54
(1,16)	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1:30:A:ASP:N	15	4.53
(1,67)	1:63:A:LEU:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	8	4.49
(1,67)	1:63:A:LEU:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	16	4.49
(1,16)	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1:30:A:ASP:N	10	4.47
(1,16)	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1:30:A:ASP:N	19	4.46
(1,26)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:VAL:N	17	4.41
(1,20)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:THR:N	6	4.41
(1,16)	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1:30:A:ASP:N	16	4.37
(1,62)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:ALA:N	12	4.36
(1,20)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:THR:N	9	4.36
(1,67)	1:63:A:LEU:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	6	4.35
(1,26)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:VAL:N	11	4.32
(1,16)	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1:30:A:ASP:N	4	4.32
(1,81)	1:74:A:LYS:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	20	4.31
(1,26)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:VAL:N	8	4.27
(1,26)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:VAL:N	3	4.25
(1,26)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:VAL:N	16	4.25
(1,104)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:PHE:N	4	4.23
(1,104)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:PHE:N	11	4.23
(1,67)	1:63:A:LEU:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	9	4.18
(1,26)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:VAL:N	2	4.18
(1,20)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:THR:N	2	4.16
(1,20)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:THR:N	4	4.14
(1,74)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:LYS:N	9	4.11
(1,67)	1:63:A:LEU:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	11	4.08
(1,20)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:THR:N	1	4.05
(1,16)	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1:30:A:ASP:N	2	4.05
(1,16)	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1:30:A:ASP:N	17	4.05
(1,20)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:THR:N	11	4.04
(1,20)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:THR:N	12	4.01
(1,107)	1:92:A:PHE:C	1:93:A:THR:N	1:93:A:THR:CA	1:93:A:THR:C	9	4.0
(1,81)	1:74:A:LYS:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	15	4.0
(1,67)	1:63:A:LEU:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	5	4.0

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,104)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:PHE:N	18	3.99
(1,104)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:PHE:N	13	3.98
(1,67)	1:63:A:LEU:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	17	3.97
(1,16)	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1:30:A:ASP:N	8	3.95
(1,104)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:PHE:N	16	3.92
(1,104)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:PHE:N	9	3.86
(1,16)	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1:30:A:ASP:N	9	3.85
(1,26)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:VAL:N	9	3.83
(1,26)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:VAL:N	10	3.83
(1,104)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:PHE:N	1	3.8
(1,83)	1:77:A:TRP:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	8	3.8
(1,20)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:THR:N	7	3.79
(1,104)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:PHE:N	7	3.78
(1,104)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:PHE:N	8	3.76
(1,20)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:THR:N	14	3.76
(1,67)	1:63:A:LEU:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	20	3.73
(1,20)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:THR:N	13	3.72
(1,16)	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1:30:A:ASP:N	20	3.72
(1,107)	1:92:A:PHE:C	1:93:A:THR:N	1:93:A:THR:CA	1:93:A:THR:C	12	3.71
(1,26)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:VAL:N	12	3.68
(1,104)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:PHE:N	2	3.65
(1,67)	1:63:A:LEU:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	1	3.65
(1,20)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:THR:N	17	3.64
(1,20)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:THR:N	16	3.63
(1,20)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:THR:N	20	3.63
(1,20)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:THR:N	15	3.62
(1,16)	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1:30:A:ASP:N	3	3.62
(1,83)	1:77:A:TRP:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	19	3.61
(1,26)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:VAL:N	13	3.61
(1,26)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:VAL:N	7	3.6
(1,74)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:LYS:N	7	3.58
(1,58)	1:57:A:ASP:N	1:57:A:ASP:CA	1:57:A:ASP:C	1:58:A:TRP:N	19	3.57
(1,16)	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1:30:A:ASP:N	18	3.57
(1,74)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:LYS:N	14	3.47
(1,83)	1:77:A:TRP:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	13	3.46
(1,67)	1:63:A:LEU:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	18	3.46
(1,104)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:PHE:N	17	3.45
(1,67)	1:63:A:LEU:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	4	3.44
(1,74)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:LYS:N	11	3.43
(1,67)	1:63:A:LEU:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	7	3.43
(1,104)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:PHE:N	20	3.41
(1,83)	1:77:A:TRP:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	14	3.4
(1,104)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:PHE:N	5	3.38
(1,74)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:LYS:N	1	3.38
(1,20)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:THR:N	5	3.34
(1,102)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:GLN:N	16	3.29
(1,67)	1:63:A:LEU:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	12	3.29
(1,67)	1:63:A:LEU:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	19	3.27
(1,20)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:THR:N	8	3.27
(1,83)	1:77:A:TRP:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	7	3.26
(1,104)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:PHE:N	15	3.21

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,83)	1:77:A:TRP:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	6	3.19
(1,61)	1:60:A:ASP:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	10	3.19
(1,83)	1:77:A:TRP:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	1	3.18
(1,30)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	11	3.18
(1,74)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:LYS:N	3	3.16
(1,83)	1:77:A:TRP:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	9	3.13
(1,83)	1:77:A:TRP:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	3	3.1
(1,83)	1:77:A:TRP:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	16	3.08
(1,20)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:THR:N	10	3.07
(1,74)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:LYS:N	16	3.04
(1,54)	1:51:A:LYS:N	1:51:A:LYS:CA	1:51:A:LYS:C	1:52:A:LEU:N	6	2.96
(1,67)	1:63:A:LEU:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	2	2.95
(1,83)	1:77:A:TRP:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	11	2.94
(1,74)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:LYS:N	10	2.93
(1,10)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:HIS:N	6	2.93
(1,30)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	8	2.92
(1,102)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:GLN:N	10	2.91
(1,62)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:ALA:N	9	2.91
(1,62)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:ALA:N	8	2.9
(1,10)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:HIS:N	19	2.9
(1,54)	1:51:A:LYS:N	1:51:A:LYS:CA	1:51:A:LYS:C	1:52:A:LEU:N	12	2.89
(1,83)	1:77:A:TRP:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	17	2.88
(1,83)	1:77:A:TRP:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	2	2.86
(1,30)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	19	2.86
(1,10)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:HIS:N	18	2.86
(1,20)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:THR:N	3	2.83
(1,74)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:LYS:N	8	2.82
(1,74)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:LYS:N	12	2.76
(1,10)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:HIS:N	4	2.74
(1,83)	1:77:A:TRP:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	4	2.7
(1,74)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:LYS:N	4	2.69
(1,83)	1:77:A:TRP:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	5	2.64
(1,30)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	4	2.62
(1,10)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:HIS:N	1	2.61
(1,83)	1:77:A:TRP:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	10	2.6
(1,62)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:ALA:N	17	2.59
(1,16)	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1:30:A:ASP:N	11	2.59
(1,10)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:HIS:N	13	2.59
(1,20)	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1:32:A:THR:N	18	2.58
(1,5)	1:19:A:GLU:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	19	2.57
(1,10)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:HIS:N	16	2.54
(1,10)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:HIS:N	12	2.51
(1,74)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:LYS:N	17	2.49
(1,67)	1:63:A:LEU:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	13	2.49
(1,10)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:HIS:N	17	2.49
(1,67)	1:63:A:LEU:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	14	2.48
(1,10)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:HIS:N	3	2.45
(1,104)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:PHE:N	3	2.44
(1,10)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:HIS:N	2	2.44
(1,16)	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1:30:A:ASP:N	12	2.43
(1,16)	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1:30:A:ASP:N	5	2.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,10)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:HIS:N	8	2.38
(1,16)	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1:30:A:ASP:N	13	2.37
(1,10)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:HIS:N	9	2.37
(1,10)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:HIS:N	10	2.36
(1,102)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:GLN:N	8	2.35
(1,16)	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1:30:A:ASP:N	1	2.35
(1,10)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:HIS:N	20	2.35
(1,67)	1:63:A:LEU:C	1:64:A:TRP:N	1:64:A:TRP:CA	1:64:A:TRP:C	15	2.34
(1,83)	1:77:A:TRP:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	12	2.29
(1,30)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	12	2.28
(1,61)	1:60:A:ASP:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	5	2.26
(1,102)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:GLN:N	2	2.21
(1,62)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:ALA:N	13	2.21
(1,30)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	16	2.21
(1,10)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:HIS:N	7	2.21
(1,10)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:HIS:N	5	2.2
(1,58)	1:57:A:ASP:N	1:57:A:ASP:CA	1:57:A:ASP:C	1:58:A:TRP:N	8	2.19
(1,10)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:HIS:N	14	2.19
(1,54)	1:51:A:LYS:N	1:51:A:LYS:CA	1:51:A:LYS:C	1:52:A:LEU:N	14	2.18
(1,5)	1:19:A:GLU:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	6	2.18
(1,62)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:ALA:N	18	2.16
(1,16)	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1:30:A:ASP:N	6	2.11
(1,30)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	20	2.07
(1,16)	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1:30:A:ASP:N	7	2.07
(1,30)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	5	2.06
(1,16)	1:29:A:ARG:N	1:29:A:ARG:CA	1:29:A:ARG:C	1:30:A:ASP:N	14	2.04
(1,4)	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1:18:A:TRP:N	3	2.04
(1,102)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:GLN:N	20	1.98
(1,102)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:GLN:N	11	1.95
(1,62)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:ALA:N	20	1.95
(1,102)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:GLN:N	7	1.93
(1,83)	1:77:A:TRP:C	1:78:A:THR:N	1:78:A:THR:CA	1:78:A:THR:C	20	1.92
(1,58)	1:57:A:ASP:N	1:57:A:ASP:CA	1:57:A:ASP:C	1:58:A:TRP:N	11	1.92
(1,58)	1:57:A:ASP:N	1:57:A:ASP:CA	1:57:A:ASP:C	1:58:A:TRP:N	12	1.92
(1,30)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	3	1.9
(1,77)	1:70:A:THR:C	1:71:A:TRP:N	1:71:A:TRP:CA	1:71:A:TRP:C	4	1.84
(1,59)	1:58:A:TRP:C	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	19	1.84
(1,62)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:ALA:N	4	1.82
(1,102)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:GLN:N	5	1.81
(1,102)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:GLN:N	13	1.81
(1,10)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:HIS:N	15	1.79
(1,54)	1:51:A:LYS:N	1:51:A:LYS:CA	1:51:A:LYS:C	1:52:A:LEU:N	16	1.77
(1,102)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:GLN:N	17	1.76
(1,10)	1:22:A:VAL:N	1:22:A:VAL:CA	1:22:A:VAL:C	1:23:A:HIS:N	11	1.71
(1,61)	1:60:A:ASP:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	8	1.69
(1,11)	1:22:A:VAL:C	1:23:A:HIS:N	1:23:A:HIS:CA	1:23:A:HIS:C	15	1.66
(1,58)	1:57:A:ASP:N	1:57:A:ASP:CA	1:57:A:ASP:C	1:58:A:TRP:N	15	1.64
(1,4)	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1:18:A:TRP:N	5	1.63
(1,104)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:PHE:N	10	1.62
(1,58)	1:57:A:ASP:N	1:57:A:ASP:CA	1:57:A:ASP:C	1:58:A:TRP:N	20	1.62
(1,58)	1:57:A:ASP:N	1:57:A:ASP:CA	1:57:A:ASP:C	1:58:A:TRP:N	5	1.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,30)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	2	1.59
(1,30)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	13	1.59
(1,102)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:GLN:N	9	1.56
(1,62)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:ALA:N	1	1.56
(1,98)	1:88:A:ALA:N	1:88:A:ALA:CA	1:88:A:ALA:C	1:89:A:LYS:N	6	1.53
(1,102)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:GLN:N	3	1.5
(1,102)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:GLN:N	18	1.5
(1,60)	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	1:60:A:ASP:N	5	1.48
(1,62)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:ALA:N	6	1.45
(1,102)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:GLN:N	12	1.44
(1,60)	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	1:60:A:ASP:N	14	1.42
(1,74)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:LYS:N	6	1.41
(1,30)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	18	1.35
(1,102)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:GLN:N	15	1.34
(1,102)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:GLN:N	14	1.33
(1,61)	1:60:A:ASP:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	16	1.31
(1,62)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:ALA:N	15	1.28
(1,58)	1:57:A:ASP:N	1:57:A:ASP:CA	1:57:A:ASP:C	1:58:A:TRP:N	4	1.28
(1,58)	1:57:A:ASP:N	1:57:A:ASP:CA	1:57:A:ASP:C	1:58:A:TRP:N	10	1.28
(1,102)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:GLN:N	4	1.27
(1,1)	1:15:A:ASP:C	1:16:A:GLY:N	1:16:A:GLY:CA	1:16:A:GLY:C	11	1.26
(1,58)	1:57:A:ASP:N	1:57:A:ASP:CA	1:57:A:ASP:C	1:58:A:TRP:N	18	1.23
(1,28)	1:35:A:VAL:N	1:35:A:VAL:CA	1:35:A:VAL:C	1:36:A:THR:N	19	1.2
(1,58)	1:57:A:ASP:N	1:57:A:ASP:CA	1:57:A:ASP:C	1:58:A:TRP:N	3	1.19
(1,7)	1:20:A:LEU:C	1:21:A:SER:N	1:21:A:SER:CA	1:21:A:SER:C	12	1.19
(1,58)	1:57:A:ASP:N	1:57:A:ASP:CA	1:57:A:ASP:C	1:58:A:TRP:N	17	1.16
(1,4)	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1:18:A:TRP:N	1	1.16
(1,98)	1:88:A:ALA:N	1:88:A:ALA:CA	1:88:A:ALA:C	1:89:A:LYS:N	4	1.13
(1,60)	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	1:60:A:ASP:N	16	1.13
(1,59)	1:58:A:TRP:C	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	8	1.12
(1,62)	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	1:62:A:ALA:N	7	1.11
(1,58)	1:57:A:ASP:N	1:57:A:ASP:CA	1:57:A:ASP:C	1:58:A:TRP:N	1	1.11
(1,58)	1:57:A:ASP:N	1:57:A:ASP:CA	1:57:A:ASP:C	1:58:A:TRP:N	13	1.11
(1,61)	1:60:A:ASP:C	1:61:A:HIS:N	1:61:A:HIS:CA	1:61:A:HIS:C	7	1.1
(1,58)	1:57:A:ASP:N	1:57:A:ASP:CA	1:57:A:ASP:C	1:58:A:TRP:N	16	1.08
(1,54)	1:51:A:LYS:N	1:51:A:LYS:CA	1:51:A:LYS:C	1:52:A:LEU:N	20	1.08
(1,30)	1:36:A:THR:N	1:36:A:THR:CA	1:36:A:THR:C	1:37:A:GLY:N	6	1.06
(1,11)	1:22:A:VAL:C	1:23:A:HIS:N	1:23:A:HIS:CA	1:23:A:HIS:C	9	1.05
(1,60)	1:59:A:SER:N	1:59:A:SER:CA	1:59:A:SER:C	1:60:A:ASP:N	7	1.04
(1,54)	1:51:A:LYS:N	1:51:A:LYS:CA	1:51:A:LYS:C	1:52:A:LEU:N	9	1.03