



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 03:54 PM UTC

PDB ID : 2MH3 / pdb_00002mh3
BMRB ID : 19614
Title : NMR structure of the basic helix-loop-helix region of the transcriptional repressor HES-1
Authors : Wienk, H.; Popovic, M.; Cogliervina, M.; Boelens, R.; Pongor, S.; Pintar, A.
Deposited on : 2013-11-15

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

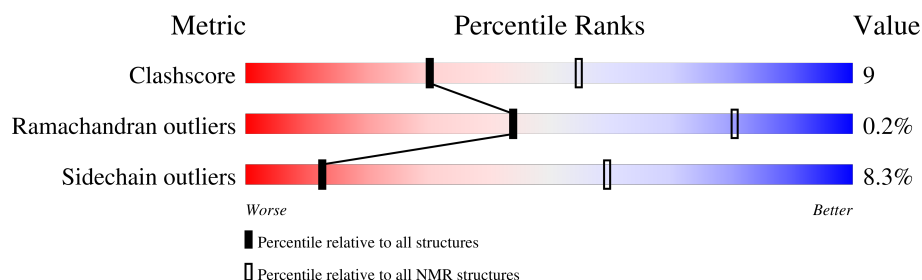
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 41%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	70	51% 24% 24%
1	B	70	54% 21% 24%

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 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:42-A:94, B:43-B:95 (106)	0.66	11

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 9 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2398 atoms, of which 1254 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcription factor HES-1.

Mol	Chain	Residues	Atoms						Trace
1	A	70	Total	C	H	N	O	S	0
			1199	351	627	116	102	3	
1	B	70	Total	C	H	N	O	S	0
			1199	351	627	116	102	3	

There are 2 discrepancies between the modelled and reference sequences:

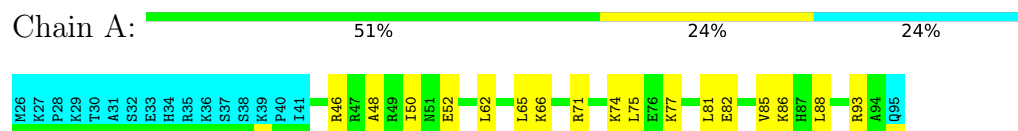
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	initiating methionine	UNP Q14469
B	26	MET	-	initiating methionine	UNP Q14469

4 Residue-property plots

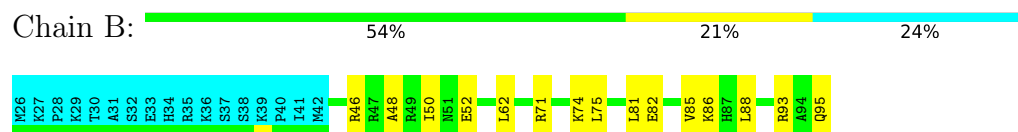
4.1 Average score per residue in the NMR ensemble

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: Transcription factor HES-1



- Molecule 1: Transcription factor HES-1

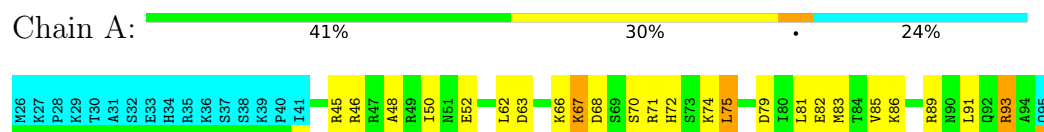


4.2 Scores per residue for each member of the ensemble

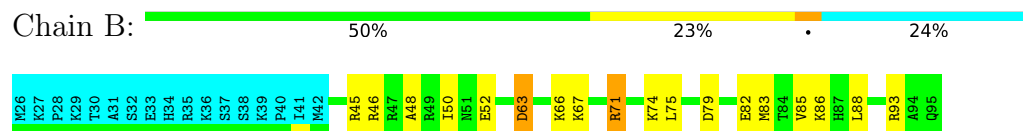
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Transcription factor HES-1

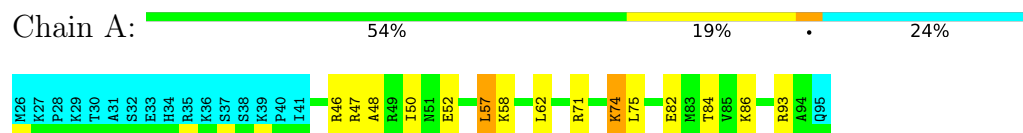


- Molecule 1: Transcription factor HES-1

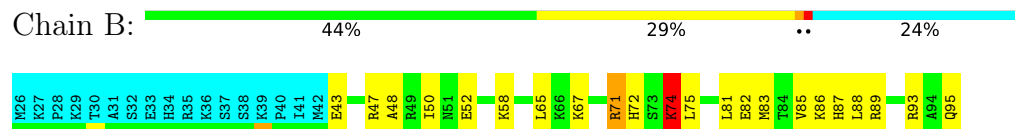


4.2.2 Score per residue for model 2

- Molecule 1: Transcription factor HES-1

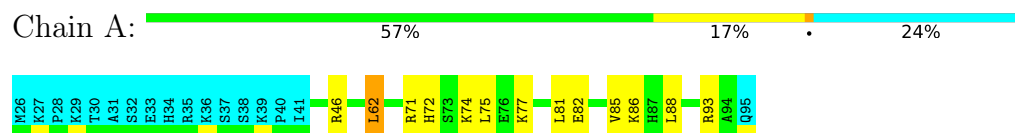


- Molecule 1: Transcription factor HES-1

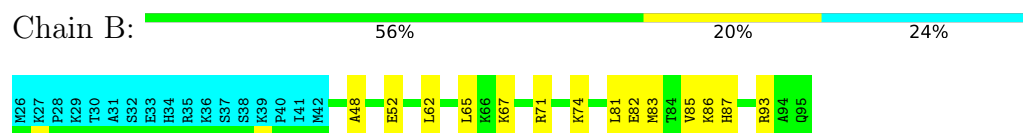


4.2.3 Score per residue for model 3

- Molecule 1: Transcription factor HES-1

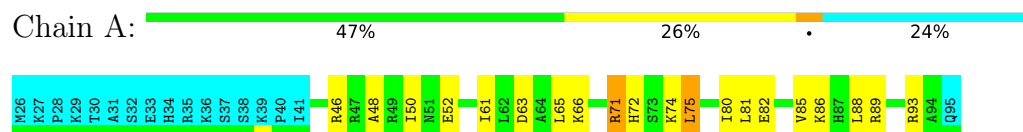


- Molecule 1: Transcription factor HES-1

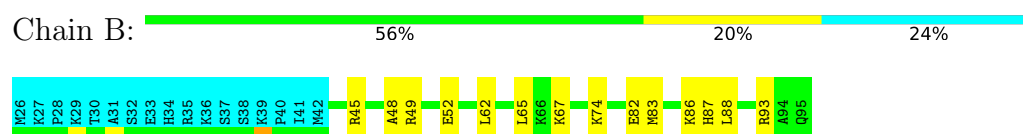


4.2.4 Score per residue for model 4

- Molecule 1: Transcription factor HES-1

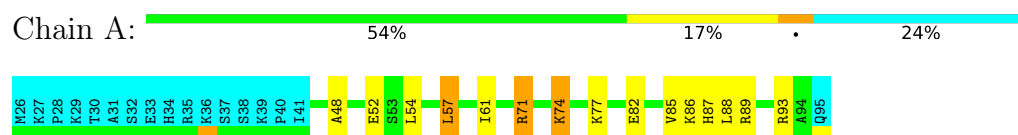


- Molecule 1: Transcription factor HES-1

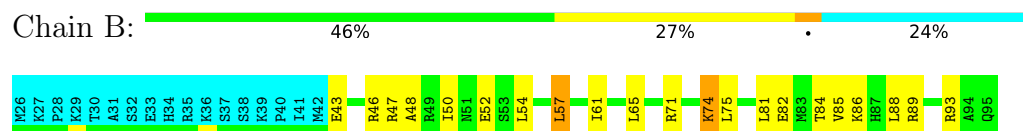


4.2.5 Score per residue for model 5

- Molecule 1: Transcription factor HES-1

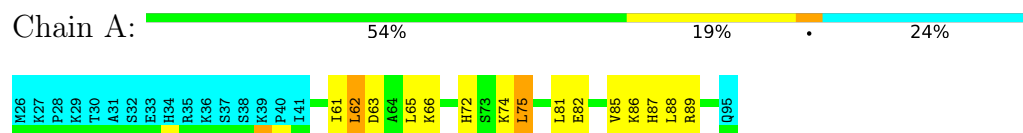


- Molecule 1: Transcription factor HES-1

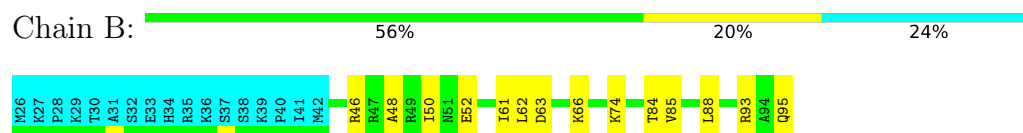


4.2.6 Score per residue for model 6

- Molecule 1: Transcription factor HES-1

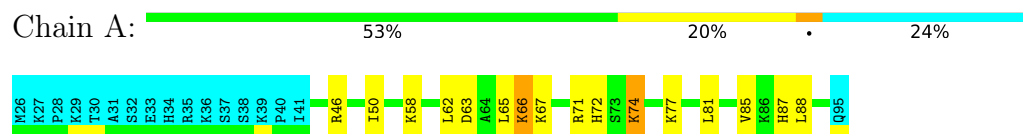


- Molecule 1: Transcription factor HES-1

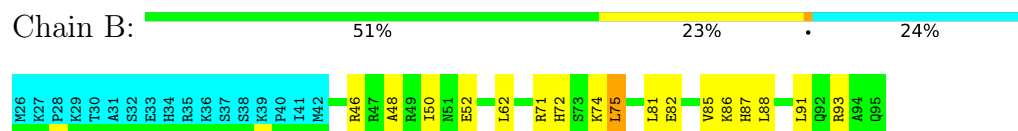


4.2.7 Score per residue for model 7

- Molecule 1: Transcription factor HES-1

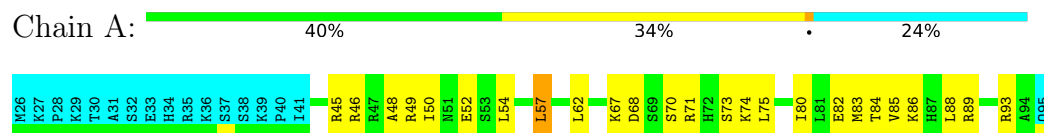


- Molecule 1: Transcription factor HES-1

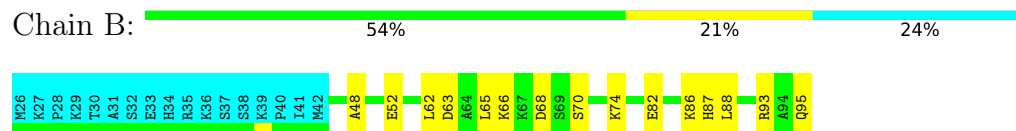


4.2.8 Score per residue for model 8

- Molecule 1: Transcription factor HES-1

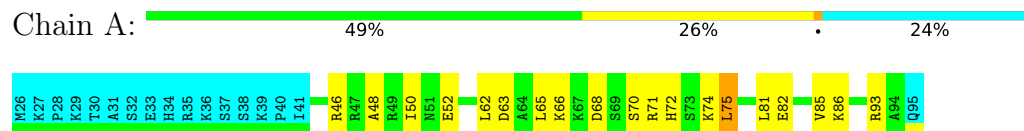


- Molecule 1: Transcription factor HES-1

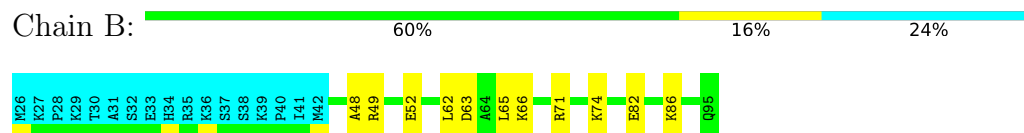


4.2.9 Score per residue for model 9

- Molecule 1: Transcription factor HES-1

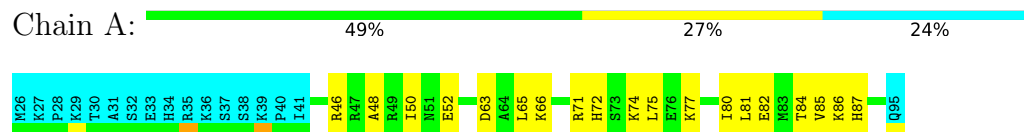


- Molecule 1: Transcription factor HES-1

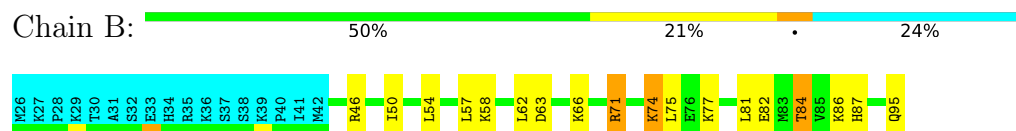


4.2.10 Score per residue for model 10

- Molecule 1: Transcription factor HES-1

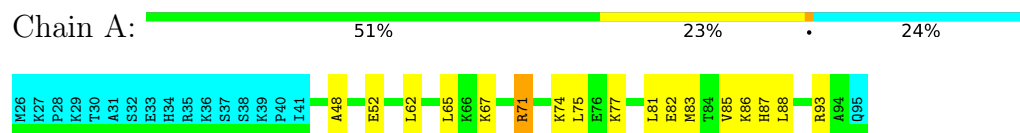


- Molecule 1: Transcription factor HES-1

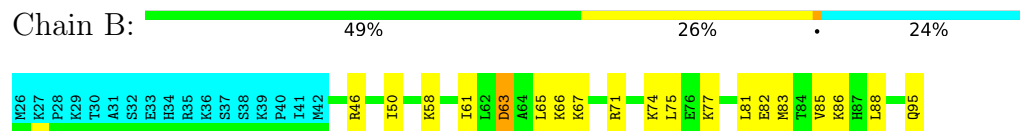


4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Transcription factor HES-1

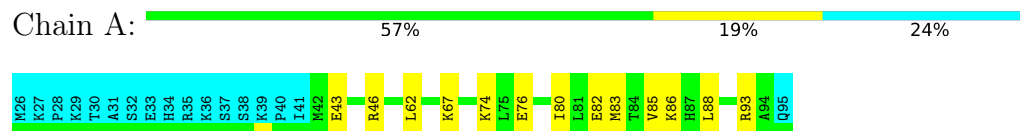


- Molecule 1: Transcription factor HES-1

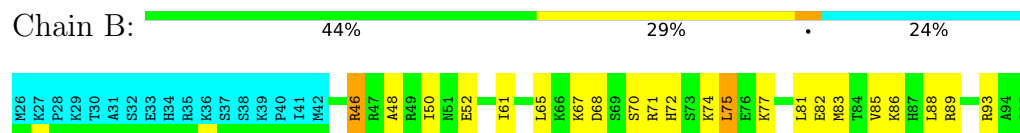


4.2.12 Score per residue for model 12

- Molecule 1: Transcription factor HES-1

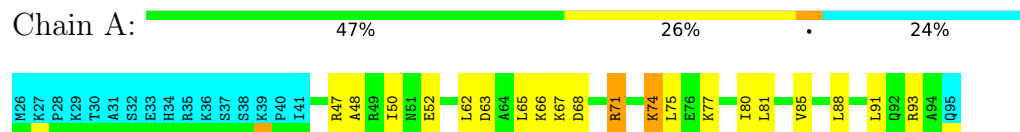


- Molecule 1: Transcription factor HES-1

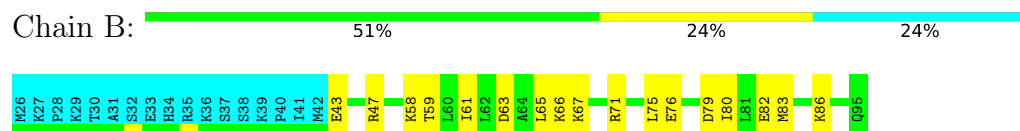


4.2.13 Score per residue for model 13

- Molecule 1: Transcription factor HES-1

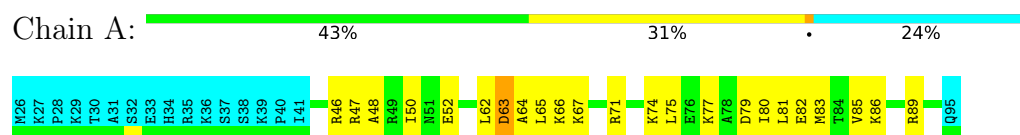


- Molecule 1: Transcription factor HES-1

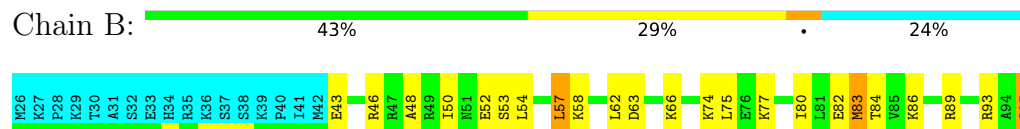


4.2.14 Score per residue for model 14

- Molecule 1: Transcription factor HES-1

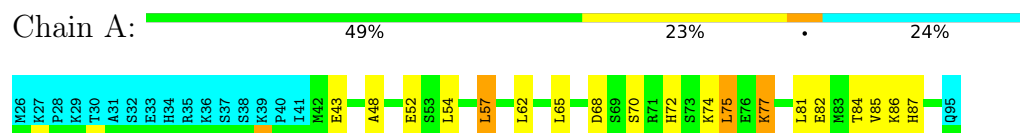


- Molecule 1: Transcription factor HES-1

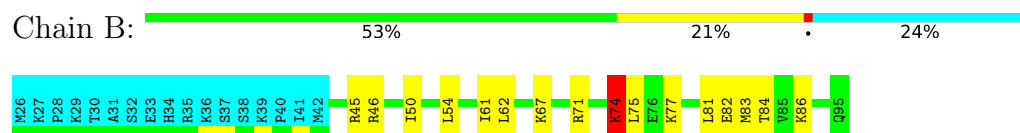


4.2.15 Score per residue for model 15

- Molecule 1: Transcription factor HES-1

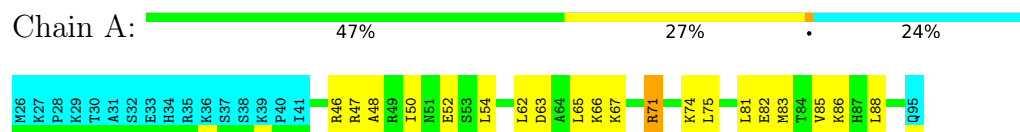


- Molecule 1: Transcription factor HES-1

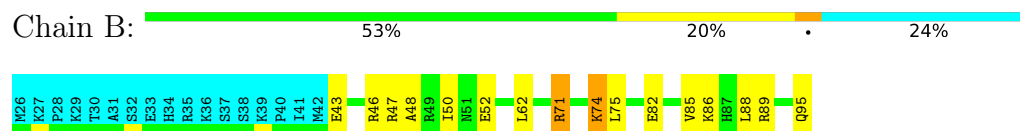


4.2.16 Score per residue for model 16

- Molecule 1: Transcription factor HES-1

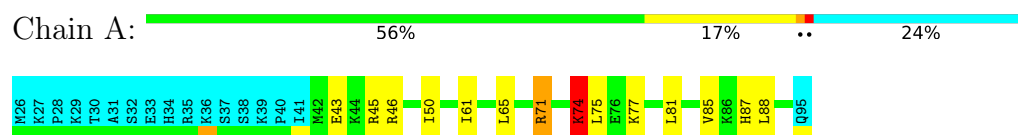


- Molecule 1: Transcription factor HES-1

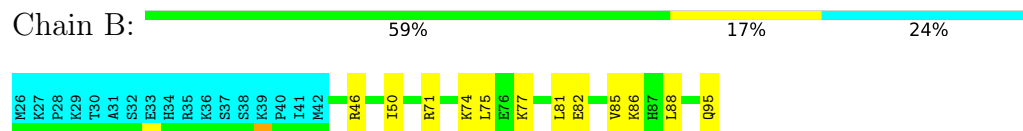


4.2.17 Score per residue for model 17

- Molecule 1: Transcription factor HES-1

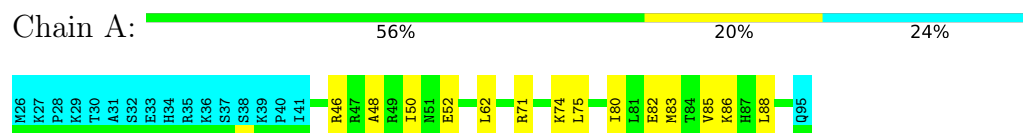


- Molecule 1: Transcription factor HES-1

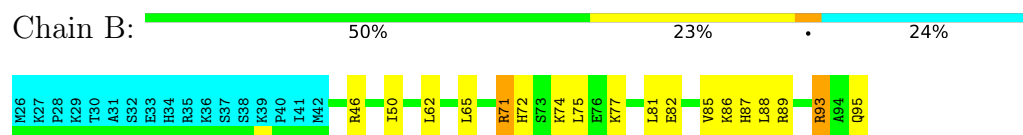


4.2.18 Score per residue for model 18

- Molecule 1: Transcription factor HES-1

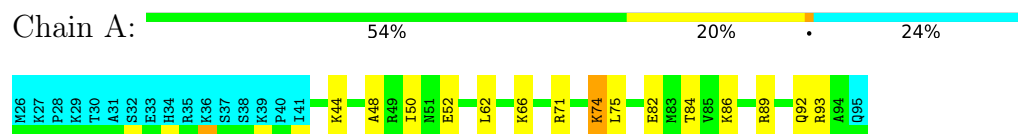


- Molecule 1: Transcription factor HES-1

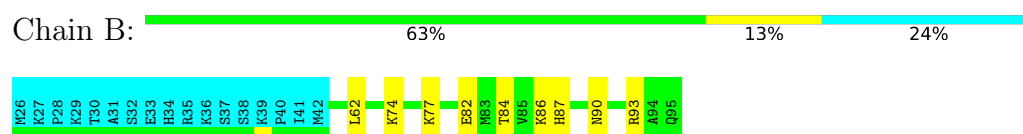


4.2.19 Score per residue for model 19

- Molecule 1: Transcription factor HES-1

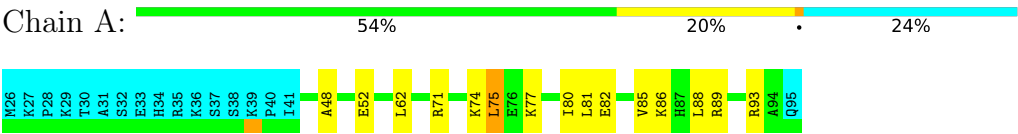


- Molecule 1: Transcription factor HES-1

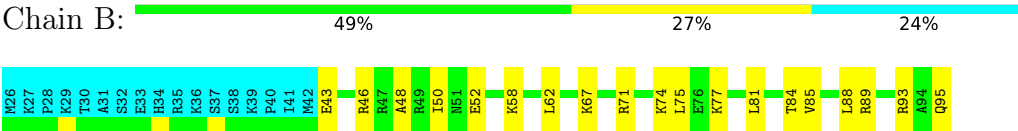


4.2.20 Score per residue for model 20

● Molecule 1: Transcription factor HES-1



● Molecule 1: Transcription factor HES-1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *restrained molecular dynamics*.

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
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	861
Number of shifts mapped to atoms	861
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	41%

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.05±0.04	0±0/439 (0.0± 0.1%)	1.08±0.04	0±0/582 (0.0± 0.1%)
1	B	1.07±0.05	0±0/439 (0.0± 0.1%)	1.07±0.04	0±0/581 (0.0± 0.0%)
All	All	1.06	6/17560 (0.0%)	1.08	3/23260 (0.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.3±0.5
1	B	0.0±0.0	0.1±0.3
All	All	0	8

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	75	LEU	N-CA	-5.93	1.39	1.46	20	1
1	A	63	ASP	C-O	-5.65	1.17	1.24	14	1
1	A	73	SER	C-N	-5.58	1.27	1.33	8	1
1	B	75	LEU	N-CA	-5.44	1.39	1.46	2	2
1	B	74	LYS	C-N	-5.25	1.26	1.33	15	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	74	LYS	N-CA-C	-5.33	105.06	112.30	17	1
1	A	88	LEU	N-CA-C	-5.32	105.56	111.36	4	1
1	B	74	LYS	N-CA-C	-5.25	106.88	113.28	2	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	71	ARG	Sidechain	3
1	A	46	ARG	Sidechain	2
1	B	71	ARG	Sidechain	1
1	B	46	ARG	Sidechain	1
1	A	47	ARG	Sidechain	1

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	437	478	478	9±3
1	B	438	477	477	8±3
All	All	17500	19100	19100	329

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:LYS:HE2	1:A:83:MET:SD	0.71	2.24	1	2
1:A:63:ASP:O	1:A:66:LYS:HE3	0.67	1.89	9	4
1:B:63:ASP:O	1:B:66:LYS:HE2	0.66	1.91	9	3
1:A:75:LEU:HG	1:A:80:ILE:CG1	0.64	2.22	20	4
1:A:72:HIS:HA	1:A:75:LEU:HD23	0.64	1.69	9	1
1:A:85:VAL:O	1:A:88:LEU:HG	0.63	1.94	16	5
1:B:67:LYS:HE3	1:B:83:MET:SD	0.63	2.33	11	7
1:A:72:HIS:HA	1:A:75:LEU:HD12	0.63	1.71	15	2
1:A:63:ASP:O	1:A:66:LYS:HE2	0.61	1.96	14	5
1:A:82:GLU:O	1:A:86:LYS:HG2	0.60	1.95	10	1
1:B:82:GLU:O	1:B:86:LYS:HG3	0.59	1.97	2	18
1:B:85:VAL:O	1:B:88:LEU:HG	0.59	1.97	17	3
1:A:67:LYS:HE3	1:A:83:MET:SD	0.58	2.38	12	3
1:A:61:ILE:O	1:A:65:LEU:HG	0.58	1.99	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:VAL:HG22	1:B:57:LEU:HD23	0.57	1.77	10	1
1:A:82:GLU:O	1:A:86:LYS:HG3	0.57	2.00	11	16
1:B:89:ARG:O	1:B:93:ARG:HG3	0.56	2.00	18	5
1:A:71:ARG:O	1:A:75:LEU:HG	0.56	2.00	11	5
1:B:61:ILE:O	1:B:65:LEU:HG	0.56	2.01	13	3
1:A:63:ASP:HA	1:A:66:LYS:HE3	0.55	1.78	16	2
1:A:77:LYS:O	1:A:81:LEU:HG	0.55	2.02	10	8
1:A:47:ARG:HA	1:A:50:ILE:HD12	0.55	1.78	16	3
1:A:65:LEU:HD21	1:A:87:HIS:CD2	0.54	2.37	15	2
1:B:85:VAL:O	1:B:88:LEU:HB3	0.54	2.03	1	8
1:B:63:ASP:O	1:B:66:LYS:HE3	0.54	2.03	10	5
1:B:63:ASP:HA	1:B:66:LYS:HE3	0.53	1.79	1	4
1:B:72:HIS:HA	1:B:75:LEU:HD23	0.53	1.79	7	2
1:A:89:ARG:O	1:A:93:ARG:HG3	0.53	2.02	1	6
1:B:71:ARG:O	1:B:75:LEU:HG	0.53	2.03	18	6
1:B:67:LYS:HE2	1:B:83:MET:SD	0.53	2.44	4	1
1:B:63:ASP:HA	1:B:66:LYS:CE	0.52	2.34	6	4
1:B:46:ARG:O	1:B:50:ILE:HG13	0.52	2.04	7	13
1:A:48:ALA:O	1:A:52:GLU:HG2	0.51	2.06	14	9
1:B:48:ALA:O	1:B:52:GLU:HG2	0.50	2.07	14	9
1:A:85:VAL:O	1:A:88:LEU:HB3	0.50	2.06	5	7
1:A:71:ARG:NH1	1:A:75:LEU:HD13	0.50	2.22	14	1
1:A:83:MET:HE3	1:A:83:MET:HA	0.50	1.83	16	1
1:B:48:ALA:O	1:B:52:GLU:HG3	0.50	2.07	16	4
1:B:61:ILE:O	1:B:65:LEU:HD12	0.50	2.06	11	1
1:A:62:LEU:HD21	1:A:72:HIS:CG	0.50	2.41	6	1
1:B:74:LYS:HE2	1:B:74:LYS:O	0.50	2.06	15	1
1:A:48:ALA:O	1:A:52:GLU:HG3	0.50	2.06	19	6
1:A:75:LEU:HG	1:A:80:ILE:HG12	0.49	1.84	14	2
1:B:57:LEU:HD21	1:B:84:THR:CG2	0.49	2.36	10	1
1:B:77:LYS:O	1:B:81:LEU:HG	0.49	2.08	20	6
1:B:43:GLU:O	1:B:47:ARG:HG3	0.48	2.07	13	2
1:B:75:LEU:HG	1:B:80:ILE:CG1	0.48	2.39	14	1
1:A:54:LEU:O	1:A:57:LEU:HB3	0.48	2.09	8	3
1:B:47:ARG:HA	1:B:50:ILE:HD12	0.47	1.86	2	1
1:A:68:ASP:OD2	1:A:70:SER:HB2	0.47	2.09	8	3
1:B:65:LEU:HD12	1:B:65:LEU:N	0.47	2.24	9	1
1:B:65:LEU:HD11	1:B:87:HIS:CD2	0.47	2.45	4	2
1:B:68:ASP:OD2	1:B:70:SER:HB3	0.47	2.10	12	1
1:A:63:ASP:O	1:A:66:LYS:HG2	0.47	2.09	14	1
1:B:61:ILE:HG21	1:B:83:MET:HB3	0.47	1.87	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:58:LYS:HB3	1:B:80:ILE:HG23	0.47	1.86	13	1
1:B:58:LYS:HD2	1:B:59:THR:N	0.47	2.24	13	1
1:A:65:LEU:HD21	1:A:87:HIS:ND1	0.47	2.24	17	1
1:A:81:LEU:O	1:A:85:VAL:HG23	0.46	2.11	14	10
1:B:74:LYS:HE3	1:B:74:LYS:HA	0.46	1.87	10	1
1:B:76:GLU:HB2	1:B:79:ASP:OD1	0.46	2.10	13	1
1:A:68:ASP:OD2	1:A:70:SER:HB3	0.46	2.10	1	1
1:B:74:LYS:HE2	1:B:74:LYS:HA	0.46	1.86	16	2
1:A:65:LEU:HD12	1:A:65:LEU:N	0.46	2.26	9	1
1:A:65:LEU:HD11	1:A:87:HIS:CG	0.46	2.45	11	1
1:A:46:ARG:O	1:A:50:ILE:HG13	0.46	2.11	17	11
1:A:50:ILE:HD13	1:B:77:LYS:HE3	0.46	1.88	19	2
1:B:65:LEU:HD11	1:B:87:HIS:CG	0.46	2.46	2	3
1:B:72:HIS:HA	1:B:75:LEU:CD2	0.46	2.41	7	1
1:A:57:LEU:CD2	1:A:84:THR:HG21	0.46	2.41	8	3
1:A:74:LYS:HA	1:A:74:LYS:HE3	0.46	1.86	17	2
1:A:75:LEU:HB3	1:A:80:ILE:CG1	0.46	2.41	4	3
1:A:68:ASP:HB2	1:A:71:ARG:CG	0.46	2.41	13	1
1:B:74:LYS:HA	1:B:74:LYS:HE3	0.45	1.87	5	1
1:A:74:LYS:O	1:A:74:LYS:HE2	0.45	2.11	19	1
1:B:85:VAL:O	1:B:89:ARG:HG2	0.45	2.11	2	1
1:A:75:LEU:HG	1:A:80:ILE:HG13	0.45	1.88	8	2
1:A:63:ASP:HA	1:A:66:LYS:CE	0.45	2.41	16	3
1:A:86:LYS:HA	1:A:89:ARG:HG2	0.44	1.88	14	1
1:A:79:ASP:O	1:A:83:MET:HB2	0.44	2.12	14	2
1:B:81:LEU:O	1:B:85:VAL:HG23	0.44	2.12	2	6
1:A:71:ARG:NH1	1:A:75:LEU:HG	0.44	2.27	4	1
1:B:45:ARG:O	1:B:49:ARG:HD3	0.44	2.13	4	1
1:A:64:ALA:C	1:A:65:LEU:HD12	0.44	2.38	14	1
1:B:95:GLN:NE2	1:B:95:GLN:H	0.44	2.11	14	1
1:A:62:LEU:HG	1:A:72:HIS:CD2	0.44	2.48	3	1
1:B:54:LEU:O	1:B:57:LEU:HB3	0.44	2.13	14	2
1:A:61:ILE:HG23	1:A:87:HIS:ND1	0.43	2.28	5	1
1:A:74:LYS:HA	1:A:74:LYS:HE2	0.43	1.89	13	1
1:B:43:GLU:O	1:B:47:ARG:HG2	0.43	2.13	5	1
1:B:68:ASP:OD2	1:B:70:SER:HB2	0.42	2.13	8	1
1:A:71:ARG:HG3	1:A:72:HIS:N	0.42	2.28	10	2
1:A:72:HIS:HA	1:A:75:LEU:HD13	0.42	1.91	1	1
1:A:68:ASP:HB2	1:A:71:ARG:HG2	0.42	1.89	13	1
1:A:72:HIS:HA	1:A:75:LEU:CD1	0.42	2.45	1	2
1:B:57:LEU:CD2	1:B:84:THR:HG21	0.42	2.45	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:ASP:CA	1:A:66:LYS:HE3	0.42	2.43	16	1
1:A:74:LYS:HE2	1:A:74:LYS:HA	0.42	1.91	7	2
1:A:65:LEU:HB2	1:A:67:LYS:HD2	0.41	1.92	13	1
1:A:65:LEU:HD11	1:A:87:HIS:CD2	0.41	2.50	7	1
1:B:53:SER:O	1:B:57:LEU:HB2	0.41	2.15	14	1
1:A:68:ASP:HB3	1:A:71:ARG:CG	0.41	2.45	8	1
1:B:83:MET:HE3	1:B:83:MET:HA	0.41	1.91	14	1
1:B:71:ARG:HG3	1:B:72:HIS:N	0.41	2.31	2	1
1:B:63:ASP:CA	1:B:66:LYS:HE3	0.41	2.45	1	1
1:A:45:ARG:O	1:A:49:ARG:HG3	0.41	2.16	8	1
1:A:85:VAL:O	1:A:89:ARG:HG2	0.41	2.15	4	1
1:B:58:LYS:HE3	1:B:72:HIS:NE2	0.41	2.30	2	1
1:A:72:HIS:HD1	1:A:75:LEU:HD22	0.41	1.75	6	1
1:A:65:LEU:HD11	1:A:87:HIS:ND1	0.41	2.31	10	1
1:B:90:ASN:O	1:B:93:ARG:HG3	0.40	2.16	19	1
1:B:79:ASP:O	1:B:83:MET:HB2	0.40	2.17	1	1
1:B:61:ILE:CD1	1:B:84:THR:HA	0.40	2.47	6	1
1:B:87:HIS:CE1	1:B:91:LEU:HD11	0.40	2.52	7	1
1:A:57:LEU:HD22	1:A:84:THR:HG21	0.40	1.92	8	1
1:A:92:GLN:OE1	1:A:92:GLN:HA	0.40	2.16	19	1
1:B:66:LYS:HA	1:B:66:LYS:HE2	0.40	1.94	13	1
1:B:58:LYS:C	1:B:58:LYS:HD2	0.40	2.42	14	1
1:A:62:LEU:O	1:A:66:LYS:HA	0.40	2.16	19	1
1:B:62:LEU:HG	1:B:72:HIS:CG	0.40	2.51	18	1
1:A:76:GLU:O	1:A:80:ILE:HD12	0.40	2.16	12	1
1:A:65:LEU:N	1:A:65:LEU:HD12	0.40	2.32	16	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	53/70 (76%)	50±1 (95±2%)	2±1 (4±2%)	0±0 (0±1%)	31	76
1	B	52/70 (74%)	49±1 (94±1%)	3±1 (6±1%)	0±0 (0±0%)	49	83
All	All	2100/2800 (75%)	1990 (95%)	105 (5%)	5 (0%)	44	80

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

Mol	Chain	Res	Type	Models (Total)
1	A	67	LYS	3
1	A	75	LEU	1
1	B	67	LYS	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	49/65 (75%)	45±1 (92±3%)	4±1 (8±3%)	14	61
1	B	49/65 (75%)	45±2 (91±3%)	4±2 (9±3%)	11	57
All	All	1960/2600 (75%)	1798 (92%)	162 (8%)	12	59

All 30 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	74	LYS	20
1	B	74	LYS	19
1	A	62	LEU	15
1	B	71	ARG	12
1	B	62	LEU	12
1	A	71	ARG	11
1	B	95	GLN	10
1	B	93	ARG	8
1	A	75	LEU	7
1	A	93	ARG	7
1	B	75	LEU	5
1	A	57	LEU	4
1	B	84	THR	4
1	A	77	LYS	3
1	B	58	LYS	3
1	B	63	ASP	2
1	A	58	LYS	2
1	B	88	LEU	2
1	B	57	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	84	THR	2
1	B	54	LEU	2
1	B	87	HIS	2
1	A	89	ARG	1
1	A	66	LYS	1
1	B	49	ARG	1
1	B	83	MET	1
1	A	54	LEU	1
1	B	89	ARG	1
1	A	83	MET	1
1	B	77	LYS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 41% for the well-defined parts and 41% 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	861
Number of shifts mapped to atoms	861
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	70	-0.35 ± 0.19	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	69	0.26 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	68	-0.38 ± 0.12	None needed (< 0.5 ppm)
^{15}N	66	-0.48 ± 0.27	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 41%, i.e. 655 atoms were assigned a chemical shift out of a possible 1610. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	261/530 (49%)	102/212 (48%)	106/212 (50%)	53/106 (50%)
Sidechain	394/1052 (37%)	268/675 (40%)	122/312 (39%)	4/65 (6%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/28 (0%)	0/16 (0%)	0/8 (0%)	0/4 (0%)
Overall	655/1610 (41%)	370/903 (41%)	228/532 (43%)	57/175 (33%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 41%, i.e. 861 atoms were assigned a chemical shift out of a possible 2086. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	336/692 (49%)	132/276 (48%)	138/280 (49%)	66/136 (49%)
Sidechain	525/1352 (39%)	356/868 (41%)	164/404 (41%)	5/80 (6%)
Aromatic	0/42 (0%)	0/24 (0%)	0/12 (0%)	0/6 (0%)
Overall	861/2086 (41%)	488/1168 (42%)	302/696 (43%)	71/222 (32%)

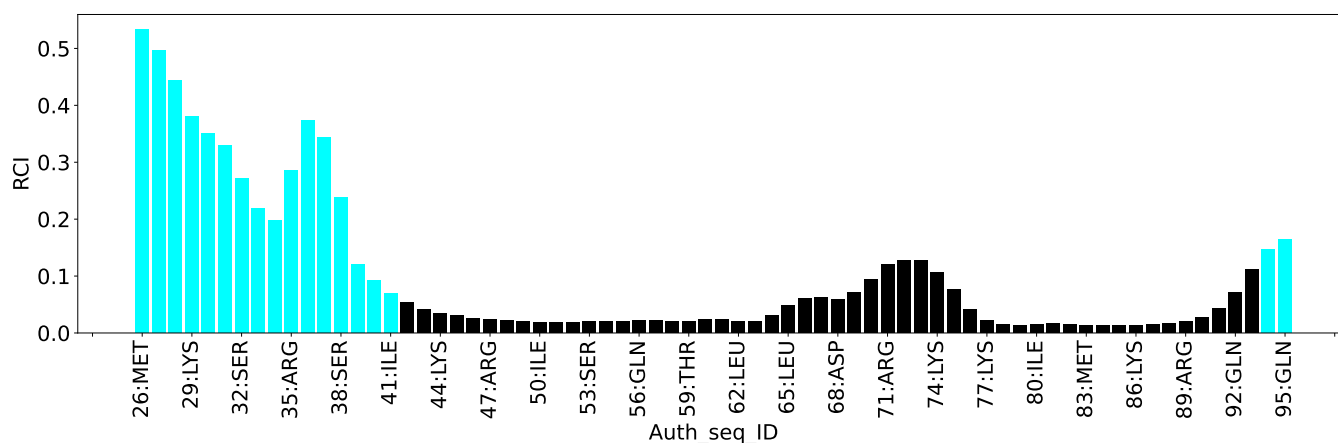
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



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	991
Intra-residue ($ i-j =0$)	210
Sequential ($ i-j =1$)	251
Medium range ($ i-j >1$ and $ i-j <5$)	257
Long range ($ i-j \geq 5$)	204
Inter-chain	2
Hydrogen bond restraints	67
Disulfide bond restraints	0
Total dihedral-angle restraints	122
Number of unmapped restraints	0
Number of restraints per residue	8.0
Number of long range restraints per residue ¹	1.5

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	18.4	0.2
0.2-0.5 (Medium)	43.0	0.5
>0.5 (Large)	318.9	33.68

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)	6.4	9.82
10.0-20.0 (Medium)	3.7	19.88
>20.0 (Large)	18.3	155.78

9 Distance violation analysis ⓘ

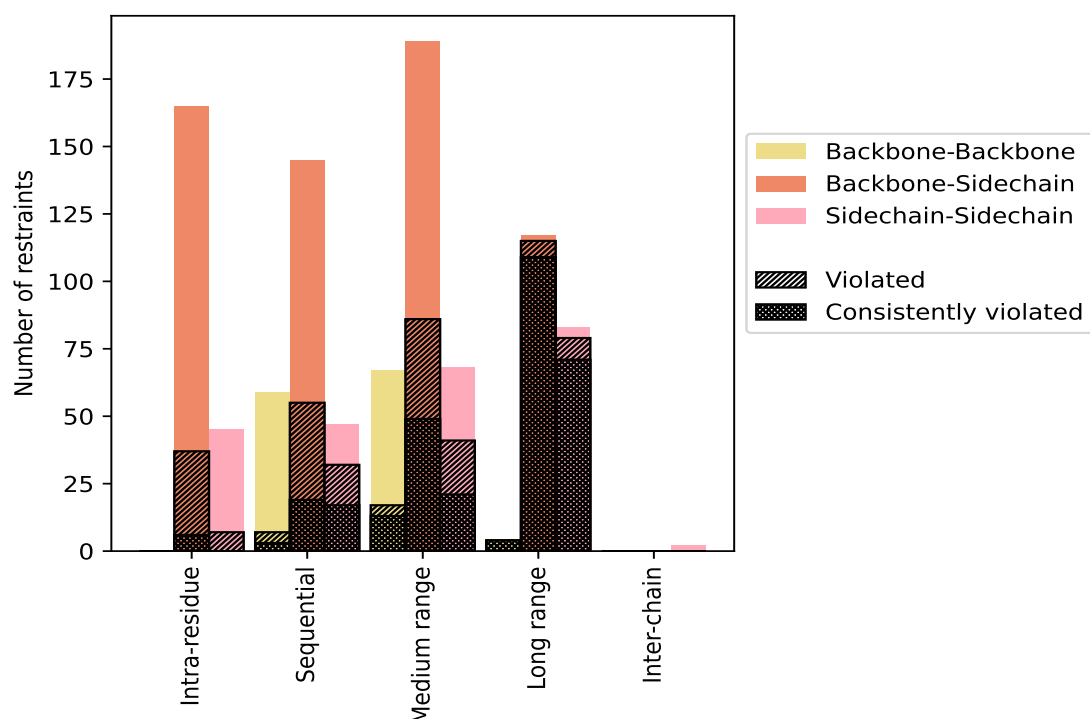
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	210	21.2	44	21.0	4.4	6	2.9	0.6
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	165	16.6	37	22.4	3.7	6	3.6	0.6
Sidechain-Sidechain	45	4.5	7	15.6	0.7	0	0.0	0.0
Sequential ($i-j =1$)	251	25.3	94	37.5	9.5	39	15.5	3.9
Backbone-Backbone	59	6.0	7	11.9	0.7	3	5.1	0.3
Backbone-Sidechain	145	14.6	55	37.9	5.5	19	13.1	1.9
Sidechain-Sidechain	47	4.7	32	68.1	3.2	17	36.2	1.7
Medium range ($i-j >1$ & $i-j <5$)	257	25.9	125	48.6	12.6	72	28.0	7.3
Backbone-Backbone	67	6.8	17	25.4	1.7	13	19.4	1.3
Backbone-Sidechain	122	12.3	67	54.9	6.8	38	31.1	3.8
Sidechain-Sidechain	68	6.9	41	60.3	4.1	21	30.9	2.1
Long range ($i-j \geq 5$)	204	20.6	198	97.1	20.0	184	90.2	18.6
Backbone-Backbone	4	0.4	4	100.0	0.4	4	100.0	0.4
Backbone-Sidechain	117	11.8	115	98.3	11.6	109	93.2	11.0
Sidechain-Sidechain	83	8.4	79	95.2	8.0	71	85.5	7.2
Inter-chain	2	0.2	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	2	0.2	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	67	6.8	19	28.4	1.9	11	16.4	1.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	991	100.0	480	48.4	48.4	312	31.5	31.5
Backbone-Backbone	130	13.1	28	21.5	2.8	20	15.4	2.0
Backbone-Sidechain	616	62.2	293	47.6	29.6	183	29.7	18.5
Sidechain-Sidechain	245	24.7	159	64.9	16.0	109	44.5	11.0

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	27	69	109	64	127	396	7.69	31.5	8.85	3.3
2	20	64	101	63	126	374	8.16	31.8	9.17	3.75
3	21	59	109	62	127	378	8.09	32.66	9.25	3.56
4	24	64	108	66	123	385	8.04	32.88	9.27	3.61
5	21	60	104	66	126	377	8.1	32.16	9.23	3.8
6	22	60	109	66	126	383	7.97	32.6	8.98	3.72
7	24	64	104	62	128	382	7.86	32.19	8.85	3.61
8	19	61	101	66	125	372	8.48	33.68	9.64	3.64
9	22	61	103	66	124	376	8.37	32.85	9.57	3.44
10	19	61	99	62	129	370	8.15	32.08	9.06	3.7

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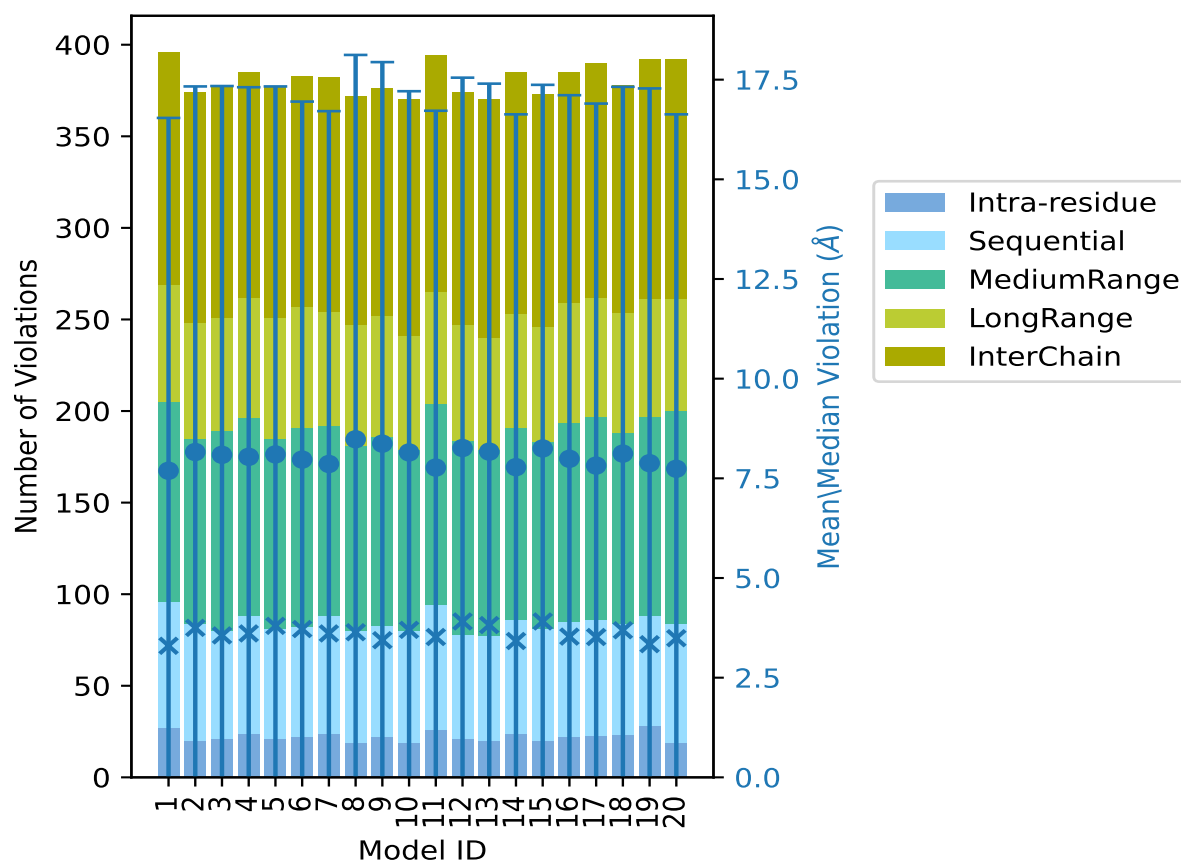
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	26	68	110	61	129	394	7.77	32.35	8.95	3.52
12	21	57	106	63	127	374	8.26	32.23	9.29	3.91
13	20	57	102	61	130	370	8.17	31.84	9.23	3.82
14	24	62	105	62	132	385	7.78	32.25	8.85	3.42
15	20	61	102	63	127	373	8.25	32.47	9.12	3.91
16	22	63	109	65	126	385	7.99	31.96	9.12	3.53
17	23	63	111	65	128	390	7.82	32.99	9.08	3.52
18	23	61	104	66	124	378	8.12	33.34	9.2	3.69
19	28	60	109	64	131	392	7.88	33.52	9.4	3.34
20	19	65	116	61	131	392	7.74	32.24	8.89	3.49

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

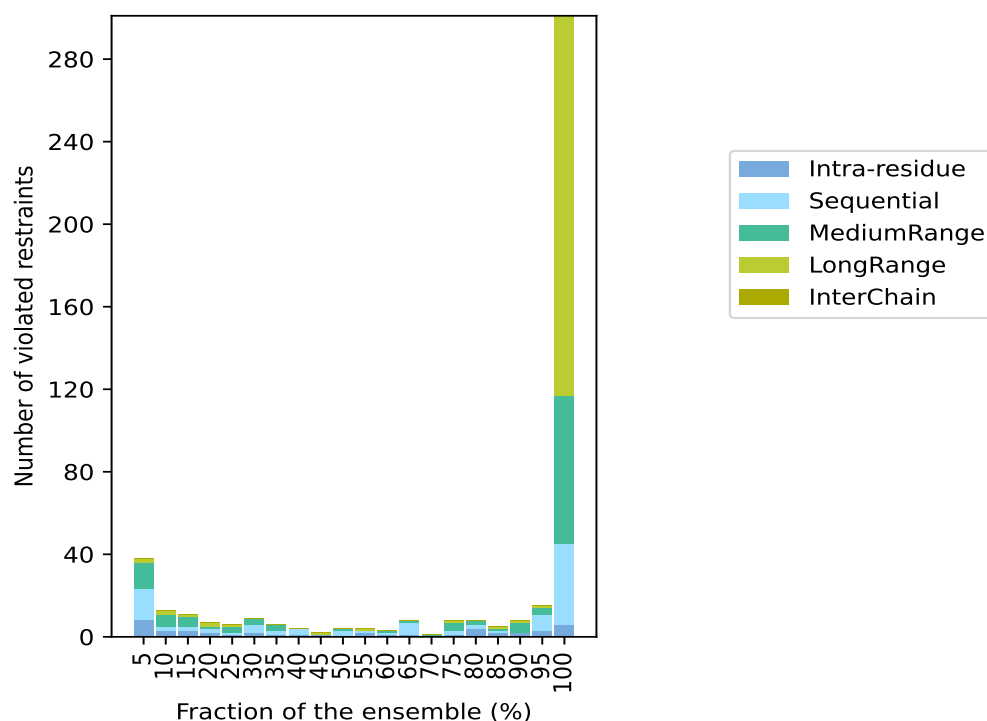
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 463(IR:166, SQ:157, MR:132, LR:6, IC:2) restraints are not 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	%
8	15	13	2	0	38	1	5.0
3	2	6	2	0	13	2	10.0
3	2	5	1	0	11	3	15.0
2	2	1	2	0	7	4	20.0
1	1	3	1	0	6	5	25.0
2	4	3	0	0	9	6	30.0
1	2	3	0	0	6	7	35.0
1	3	0	0	0	4	8	40.0
1	0	0	1	0	2	9	45.0
0	3	1	0	0	4	10	50.0
2	1	0	1	0	4	11	55.0
1	1	1	0	0	3	12	60.0
1	6	1	0	0	8	13	65.0
0	0	1	0	0	1	14	70.0
1	2	4	1	0	8	15	75.0
4	2	2	0	0	8	16	80.0
2	1	1	1	0	5	17	85.0
2	0	5	1	0	8	18	90.0
3	8	3	1	0	15	19	95.0
6	39	72	184	0	301	20	100.0

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

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

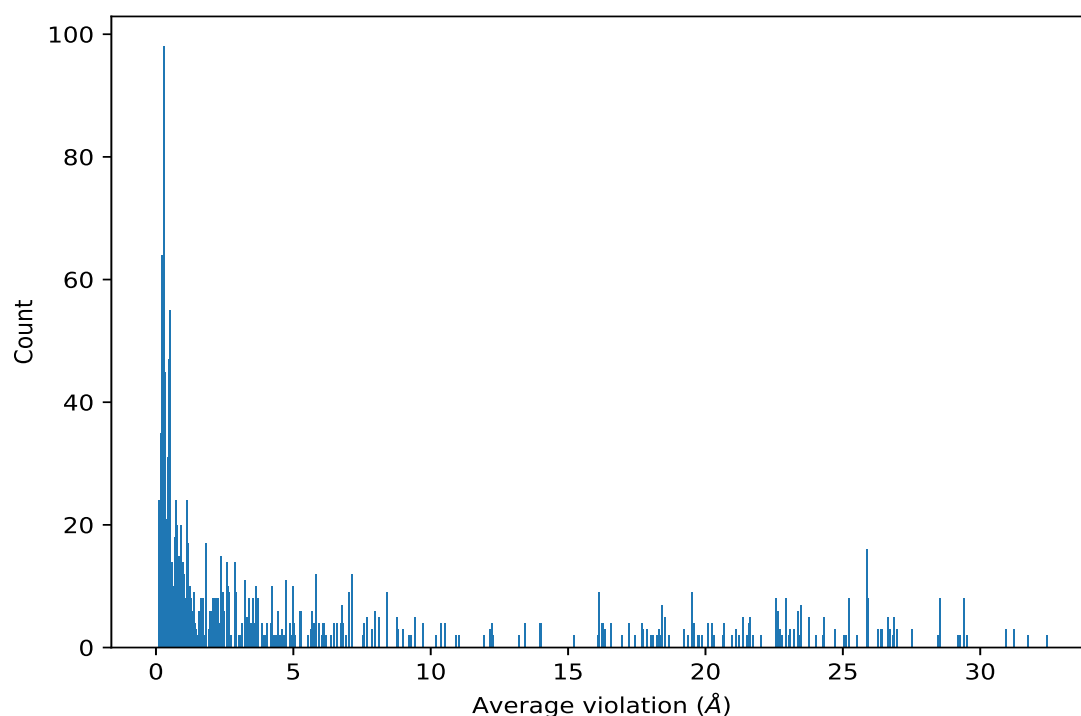
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,410)	1:64:B:ALA:HA	1:40:A:PRO:HG3	20	32.44	0.6	32.3
(1,410)	1:64:A:ALA:HA	1:40:B:PRO:HG3	20	32.44	0.6	32.3
(1,411)	1:64:B:ALA:HA	1:40:A:PRO:HG2	20	31.72	0.51	31.69
(1,411)	1:64:A:ALA:HA	1:40:B:PRO:HG2	20	31.72	0.51	31.69
(1,544)	1:64:B:ALA:HA	1:39:A:LYS:HE2	20	31.22	1.35	31.27
(1,544)	1:64:A:ALA:HA	1:39:B:LYS:HE3	20	31.22	1.35	31.27
(1,544)	1:64:A:ALA:HA	1:39:B:LYS:HE2	20	31.22	1.35	31.27
(1,733)	1:64:B:ALA:HA	1:39:A:LYS:HD2	20	30.92	1.1	31.03
(1,733)	1:64:A:ALA:HA	1:39:B:LYS:HD2	20	30.92	1.1	31.03
(1,733)	1:64:A:ALA:HA	1:39:B:LYS:HD3	20	30.92	1.1	31.03
(1,632)	1:66:B:LYS:HG2	1:41:A:ILE:HG13	20	29.51	0.74	29.62
(1,632)	1:66:A:LYS:HG2	1:41:B:ILE:HG13	20	29.51	0.74	29.62
(1,780)	1:64:B:ALA:HB3	1:39:A:LYS:HE2	20	29.43	1.32	29.62
(1,780)	1:64:A:ALA:HB3	1:39:B:LYS:HE3	20	29.43	1.32	29.62
(1,780)	1:64:A:ALA:HB3	1:39:B:LYS:HE2	20	29.43	1.32	29.62
(1,780)	1:64:A:ALA:HB1	1:39:B:LYS:HE2	20	29.43	1.32	29.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,780)	1:64:B:ALA:HB2	1:39:A:LYS:HE2	20	29.43	1.32	29.62
(1,780)	1:64:A:ALA:HB2	1:39:B:LYS:HE3	20	29.43	1.32	29.62
(1,780)	1:64:B:ALA:HB1	1:39:A:LYS:HE2	20	29.43	1.32	29.62
(1,780)	1:64:A:ALA:HB1	1:39:B:LYS:HE3	20	29.43	1.32	29.62
(1,526)	1:40:A:PRO:HG3	1:66:B:LYS:H	20	29.26	0.68	29.18
(1,526)	1:40:B:PRO:HG3	1:66:A:LYS:H	20	29.26	0.68	29.18
(1,732)	1:64:B:ALA:HA	1:39:A:LYS:HG2	20	29.19	0.87	29.06
(1,732)	1:64:A:ALA:HA	1:39:B:LYS:HG2	20	29.19	0.87	29.06
(1,288)	1:40:A:PRO:HG2	1:66:B:LYS:H	20	28.5	0.64	28.36
(1,288)	1:40:B:PRO:HG2	1:66:A:LYS:H	20	28.5	0.64	28.36
(1,779)	1:64:B:ALA:HB3	1:39:A:LYS:HG2	20	28.5	0.85	28.42
(1,779)	1:64:B:ALA:HB1	1:39:A:LYS:HG2	20	28.5	0.85	28.42
(1,779)	1:64:A:ALA:HB3	1:39:B:LYS:HG2	20	28.5	0.85	28.42
(1,779)	1:64:A:ALA:HB1	1:39:B:LYS:HG2	20	28.5	0.85	28.42
(1,779)	1:64:B:ALA:HB2	1:39:A:LYS:HG2	20	28.5	0.85	28.42
(1,779)	1:64:A:ALA:HB2	1:39:B:LYS:HG2	20	28.5	0.85	28.42
(1,734)	1:64:B:ALA:HA	1:39:A:LYS:HG3	20	28.48	0.71	28.33
(1,734)	1:64:A:ALA:HA	1:39:B:LYS:HG3	20	28.48	0.71	28.33
(1,21)	1:64:B:ALA:H	1:39:A:LYS:HE2	20	27.51	1.36	27.6
(1,21)	1:64:A:ALA:H	1:39:B:LYS:HE3	20	27.51	1.36	27.6
(1,21)	1:64:A:ALA:H	1:39:B:LYS:HE2	20	27.51	1.36	27.6
(1,786)	1:39:A:LYS:HE2	1:65:B:LEU:HG	20	26.99	1.35	27.04
(1,786)	1:39:B:LYS:HE3	1:65:A:LEU:HG	20	26.99	1.35	27.04
(1,786)	1:39:B:LYS:HE2	1:65:A:LEU:HG	20	26.99	1.35	27.04
(1,703)	1:66:A:LYS:HA	1:41:B:ILE:HG13	20	26.89	0.82	27.02
(1,703)	1:66:B:LYS:HA	1:41:A:ILE:HG13	20	26.89	0.82	27.02
(1,527)	1:39:A:LYS:HE2	1:66:B:LYS:H	20	26.85	1.25	26.98
(1,527)	1:39:B:LYS:HE3	1:66:A:LYS:H	20	26.85	1.25	26.98
(1,527)	1:39:B:LYS:HE2	1:66:A:LYS:H	20	26.85	1.25	26.98
(1,317)	1:64:B:ALA:H	1:39:A:LYS:HG2	20	26.81	0.86	26.76
(1,317)	1:64:A:ALA:H	1:39:B:LYS:HG2	20	26.81	0.86	26.76
(1,565)	1:66:A:LYS:HA	1:44:B:LYS:HE2	20	26.72	0.86	26.88
(1,565)	1:66:B:LYS:HA	1:44:A:LYS:HE2	20	26.72	0.86	26.88
(1,565)	1:66:A:LYS:HA	1:44:B:LYS:HE3	20	26.72	0.86	26.88
(1,792)	1:69:A:SER:HG	1:44:B:LYS:HE2	20	26.61	0.91	26.84
(1,792)	1:69:A:SER:HG	1:44:A:LYS:HE2	20	26.61	0.91	26.84
(1,792)	1:69:A:SER:HG	1:44:B:LYS:HE3	20	26.61	0.91	26.84
(1,792)	1:69:B:SER:HG	1:44:A:LYS:HE2	20	26.61	0.91	26.84
(1,792)	1:69:B:SER:HG	1:44:B:LYS:HE3	20	26.61	0.91	26.84
(1,301)	1:64:B:ALA:H	1:39:A:LYS:HD2	20	26.45	1.12	26.56
(1,301)	1:64:A:ALA:H	1:39:B:LYS:HD2	20	26.45	1.12	26.56
(1,301)	1:64:A:ALA:H	1:39:B:LYS:HD3	20	26.45	1.12	26.56

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,305)	1:39:A:LYS:HD2	1:66:B:LYS:H	20	26.4	1.04	26.36
(1,305)	1:39:B:LYS:HD3	1:66:A:LYS:H	20	26.4	1.04	26.36
(1,305)	1:39:B:LYS:HD2	1:66:A:LYS:H	20	26.4	1.04	26.36
(1,547)	1:65:B:LEU:HA	1:43:A:GLU:HG2	20	26.25	0.69	26.34
(1,547)	1:65:A:LEU:HA	1:43:B:GLU:HG3	20	26.25	0.69	26.34
(1,547)	1:65:A:LEU:HA	1:43:B:GLU:HG2	20	26.25	0.69	26.34
(1,571)	1:39:A:LYS:HE2	1:65:B:LEU:HD12	20	25.93	1.35	25.88
(1,571)	1:39:B:LYS:HE3	1:65:A:LEU:HD13	20	25.93	1.35	25.88
(1,571)	1:39:B:LYS:HE2	1:65:A:LEU:HD12	20	25.93	1.35	25.88
(1,571)	1:39:B:LYS:HE3	1:65:A:LEU:HD12	20	25.93	1.35	25.88
(1,571)	1:39:A:LYS:HE2	1:65:B:LEU:HD11	20	25.93	1.35	25.88
(1,571)	1:39:A:LYS:HE2	1:65:B:LEU:HD13	20	25.93	1.35	25.88
(1,571)	1:39:B:LYS:HE3	1:65:A:LEU:HD11	20	25.93	1.35	25.88
(1,571)	1:39:B:LYS:HE2	1:65:A:LEU:HD13	20	25.93	1.35	25.88
(1,572)	1:39:A:LYS:HE2	1:65:B:LEU:HD22	20	25.88	1.73	25.64
(1,572)	1:39:B:LYS:HE3	1:65:A:LEU:HD23	20	25.88	1.73	25.64
(1,572)	1:39:A:LYS:HE2	1:65:B:LEU:HD21	20	25.88	1.73	25.64
(1,572)	1:39:B:LYS:HE3	1:65:A:LEU:HD22	20	25.88	1.73	25.64
(1,572)	1:39:B:LYS:HE2	1:65:A:LEU:HD22	20	25.88	1.73	25.64
(1,572)	1:39:A:LYS:HE2	1:65:B:LEU:HD23	20	25.88	1.73	25.64
(1,572)	1:39:B:LYS:HE3	1:65:A:LEU:HD21	20	25.88	1.73	25.64
(1,599)	1:69:A:SER:HB3	1:44:B:LYS:HE2	20	25.88	0.76	25.94
(1,599)	1:69:B:SER:HB2	1:44:B:LYS:HE3	20	25.88	0.76	25.94
(1,599)	1:69:B:SER:HB3	1:44:A:LYS:HE2	20	25.88	0.76	25.94
(1,599)	1:69:A:SER:HB3	1:44:B:LYS:HE3	20	25.88	0.76	25.94
(1,599)	1:69:A:SER:HB2	1:44:B:LYS:HE2	20	25.88	0.76	25.94
(1,599)	1:69:B:SER:HB2	1:44:A:LYS:HE2	20	25.88	0.76	25.94
(1,599)	1:69:A:SER:HB2	1:44:B:LYS:HE3	20	25.88	0.76	25.94
(1,24)	1:64:B:ALA:H	1:39:A:LYS:HG3	20	25.86	0.69	25.74
(1,24)	1:64:A:ALA:H	1:39:B:LYS:HG3	20	25.86	0.69	25.74
(1,434)	1:63:B:ASP:HB2	1:39:A:LYS:HG2	20	25.54	0.78	25.6
(1,434)	1:63:A:ASP:HB2	1:39:B:LYS:HG2	20	25.54	0.78	25.6
(1,724)	1:39:A:LYS:HD2	1:65:B:LEU:HD22	20	25.21	1.51	25.32
(1,724)	1:39:A:LYS:HD2	1:65:B:LEU:HD23	20	25.21	1.51	25.32
(1,724)	1:39:A:LYS:HD2	1:65:B:LEU:HD21	20	25.21	1.51	25.32
(1,724)	1:39:B:LYS:HD3	1:65:A:LEU:HD22	20	25.21	1.51	25.32
(1,724)	1:39:B:LYS:HD3	1:65:A:LEU:HD23	20	25.21	1.51	25.32
(1,724)	1:39:B:LYS:HD2	1:65:A:LEU:HD23	20	25.21	1.51	25.32
(1,724)	1:39:B:LYS:HD2	1:65:A:LEU:HD21	20	25.21	1.51	25.32
(1,724)	1:39:B:LYS:HD3	1:65:A:LEU:HD21	20	25.21	1.51	25.32
(1,702)	1:66:A:LYS:HA	1:41:B:ILE:HG12	20	25.12	0.83	25.22
(1,702)	1:66:B:LYS:HA	1:41:A:ILE:HG12	20	25.12	0.83	25.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,686)	1:66:A:LYS:HG2	1:45:B:ARG:HD3	20	25.04	0.77	24.96
(1,686)	1:66:B:LYS:HG2	1:45:A:ARG:HD2	20	25.04	0.77	24.96
(1,328)	1:69:A:SER:H	1:44:B:LYS:HE2	20	24.74	0.87	24.87
(1,328)	1:69:B:SER:H	1:44:A:LYS:HE2	20	24.74	0.87	24.87
(1,328)	1:69:A:SER:H	1:44:B:LYS:HE3	20	24.74	0.87	24.87
(1,32)	1:66:B:LYS:H	1:41:A:ILE:HG12	20	24.32	0.76	24.36
(1,32)	1:66:A:LYS:H	1:41:B:ILE:HG12	20	24.32	0.76	24.36
(1,302)	1:39:A:LYS:HD2	1:67:B:LYS:H	20	24.31	0.99	24.3
(1,302)	1:39:B:LYS:HD3	1:67:A:LYS:H	20	24.31	0.99	24.3
(1,302)	1:39:B:LYS:HD2	1:67:A:LYS:H	20	24.31	0.99	24.3
(1,45)	1:69:B:SER:H	1:44:A:LYS:HG3	20	24.25	0.7	24.24
(1,45)	1:69:A:SER:H	1:44:B:LYS:HG3	20	24.25	0.7	24.24
(1,750)	1:69:B:SER:H	1:44:A:LYS:HG2	20	24.02	0.6	24.04
(1,750)	1:69:A:SER:H	1:44:B:LYS:HG2	20	24.02	0.6	24.04
(1,429)	1:69:A:SER:HA	1:44:B:LYS:HD2	20	23.78	1.17	23.6
(1,429)	1:69:B:SER:HA	1:44:A:LYS:HD2	20	23.78	1.17	23.6
(1,429)	1:69:A:SER:HA	1:44:A:LYS:HD2	20	23.78	1.17	23.6
(1,429)	1:69:B:SER:HA	1:44:B:LYS:HD2	20	23.78	1.17	23.6
(1,429)	1:69:A:SER:HA	1:44:B:LYS:HD3	20	23.78	1.17	23.6
(1,722)	1:39:A:LYS:HG2	1:65:B:LEU:HD22	20	23.48	1.31	23.43
(1,722)	1:39:A:LYS:HG2	1:65:B:LEU:HD23	20	23.48	1.31	23.43
(1,722)	1:39:A:LYS:HG2	1:65:B:LEU:HD21	20	23.48	1.31	23.43
(1,722)	1:39:B:LYS:HG2	1:65:A:LEU:HD22	20	23.48	1.31	23.43
(1,722)	1:39:B:LYS:HG2	1:65:A:LEU:HD23	20	23.48	1.31	23.43
(1,323)	1:41:B:ILE:HG13	1:67:A:LYS:H	20	23.47	0.79	23.55
(1,323)	1:41:A:ILE:HG13	1:67:B:LYS:H	20	23.47	0.79	23.55
(1,773)	1:63:A:ASP:H	1:39:B:LYS:HG2	20	23.42	0.82	23.42
(1,773)	1:63:B:ASP:H	1:39:A:LYS:HG2	20	23.42	0.82	23.42
(1,605)	1:39:B:LYS:HD2	1:67:A:LYS:HG2	20	23.4	1.06	23.38
(1,605)	1:39:A:LYS:HD2	1:67:B:LYS:HG2	20	23.4	1.06	23.38
(1,605)	1:39:B:LYS:HD3	1:67:A:LYS:HG2	20	23.4	1.06	23.38
(1,336)	1:66:B:LYS:H	1:43:A:GLU:HG2	20	23.36	0.62	23.36
(1,336)	1:66:A:LYS:H	1:43:B:GLU:HG3	20	23.36	0.62	23.36
(1,336)	1:66:A:LYS:H	1:43:B:GLU:HG2	20	23.36	0.62	23.36
(1,441)	1:68:B:ASP:HA	1:43:A:GLU:HG2	20	23.21	0.78	23.36
(1,441)	1:68:A:ASP:HA	1:43:B:GLU:HG2	20	23.21	0.78	23.36
(1,441)	1:68:A:ASP:HA	1:43:B:GLU:HG3	20	23.21	0.78	23.36
(1,22)	1:64:B:ALA:H	1:43:A:GLU:HG2	20	23.05	0.56	23.04
(1,22)	1:64:A:ALA:H	1:43:B:GLU:HG3	20	23.05	0.56	23.04
(1,22)	1:64:A:ALA:H	1:43:B:GLU:HG2	20	23.05	0.56	23.04
(1,693)	1:41:B:ILE:HG12	1:67:A:LYS:HA	20	23.01	0.81	22.88
(1,693)	1:41:A:ILE:HG12	1:67:B:LYS:HA	20	23.01	0.81	22.88

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,310)	1:41:B:ILE:HG12	1:67:A:LYS:H	20	22.95	0.78	23.0
(1,310)	1:41:A:ILE:HG12	1:67:B:LYS:H	20	22.95	0.78	23.0
(1,457)	1:69:A:SER:HA	1:44:B:LYS:HE2	20	22.94	0.81	23.02
(1,457)	1:69:B:SER:HA	1:44:A:LYS:HE2	20	22.94	0.81	23.02
(1,457)	1:69:A:SER:HA	1:44:B:LYS:HE3	20	22.94	0.81	23.02
(1,606)	1:39:A:LYS:HD2	1:67:B:LYS:HG3	20	22.92	1.03	22.91
(1,606)	1:39:B:LYS:HD2	1:67:A:LYS:HG3	20	22.92	1.03	22.91
(1,606)	1:39:B:LYS:HD3	1:67:A:LYS:HG3	20	22.92	1.03	22.91
(1,694)	1:41:B:ILE:HG13	1:67:A:LYS:HA	20	22.76	0.82	22.68
(1,694)	1:41:A:ILE:HG13	1:67:B:LYS:HA	20	22.76	0.82	22.68
(1,525)	1:44:B:LYS:HE2	1:70:A:SER:H	20	22.72	0.92	22.89
(1,525)	1:44:A:LYS:HE2	1:70:B:SER:H	20	22.72	0.92	22.89
(1,525)	1:44:B:LYS:HE3	1:70:A:SER:H	20	22.72	0.92	22.89
(1,723)	1:39:A:LYS:HG3	1:65:B:LEU:HD22	20	22.6	1.27	22.54
(1,723)	1:39:A:LYS:HG3	1:65:B:LEU:HD23	20	22.6	1.27	22.54
(1,723)	1:39:A:LYS:HG3	1:65:B:LEU:HD21	20	22.6	1.27	22.54
(1,723)	1:39:B:LYS:HG3	1:65:A:LEU:HD22	20	22.6	1.27	22.54
(1,723)	1:39:B:LYS:HG3	1:65:A:LEU:HD23	20	22.6	1.27	22.54
(1,723)	1:39:B:LYS:HG3	1:65:A:LEU:HD21	20	22.6	1.27	22.54
(1,604)	1:61:B:ILE:HD13	1:36:A:LYS:HE2	20	22.56	3.33	22.06
(1,604)	1:61:A:ILE:HD12	1:36:B:LYS:HE3	20	22.56	3.33	22.06
(1,604)	1:61:B:ILE:HD12	1:36:A:LYS:HE2	20	22.56	3.33	22.06
(1,604)	1:61:A:ILE:HD13	1:36:B:LYS:HE2	20	22.56	3.33	22.06
(1,604)	1:61:A:ILE:HD12	1:36:B:LYS:HE2	20	22.56	3.33	22.06
(1,604)	1:61:A:ILE:HD11	1:36:B:LYS:HE3	20	22.56	3.33	22.06
(1,604)	1:61:B:ILE:HD11	1:36:A:LYS:HE2	20	22.56	3.33	22.06
(1,604)	1:61:A:ILE:HD11	1:36:B:LYS:HE2	20	22.56	3.33	22.06
(1,42)	1:43:A:GLU:HG2	1:69:B:SER:H	20	22.02	0.77	22.17
(1,42)	1:43:B:GLU:HG2	1:69:A:SER:H	20	22.02	0.77	22.17
(1,477)	1:66:A:LYS:HA	1:45:B:ARG:HD3	20	21.71	0.87	21.67
(1,477)	1:66:B:LYS:HA	1:45:A:ARG:HD2	20	21.71	0.87	21.67
(1,518)	1:68:B:ASP:H	1:43:A:GLU:HG2	20	21.62	0.72	21.78
(1,518)	1:68:A:ASP:H	1:43:B:GLU:HG2	20	21.62	0.72	21.78
(1,518)	1:68:A:ASP:H	1:43:B:GLU:HG3	20	21.62	0.72	21.78
(1,672)	1:39:B:LYS:HG2	1:67:A:LYS:HG2	20	21.62	0.96	21.47
(1,672)	1:39:A:LYS:HG2	1:67:B:LYS:HG2	20	21.62	0.96	21.47
(1,17)	1:95:A:GLN:H	1:71:A:ARG:H	20	21.55	0.79	21.72
(1,17)	1:95:B:GLN:H	1:71:B:ARG:H	20	21.55	0.79	21.72
(1,17)	1:95:B:GLN:H	1:71:A:ARG:H	20	21.55	0.79	21.72
(1,17)	1:95:A:GLN:H	1:71:B:ARG:H	20	21.55	0.79	21.72
(1,617)	1:39:A:LYS:HG2	1:67:B:LYS:HG3	20	21.53	1.02	21.52
(1,617)	1:39:B:LYS:HG2	1:67:A:LYS:HG3	20	21.53	1.02	21.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,589)	1:68:B:ASP:HB3	1:43:A:GLU:HG2	20	21.38	0.84	21.55
(1,589)	1:68:B:ASP:HB2	1:43:A:GLU:HG2	20	21.38	0.84	21.55
(1,589)	1:68:A:ASP:HB3	1:43:B:GLU:HG2	20	21.38	0.84	21.55
(1,589)	1:68:A:ASP:HB2	1:43:B:GLU:HG2	20	21.38	0.84	21.55
(1,589)	1:68:A:ASP:HB3	1:43:B:GLU:HG3	20	21.38	0.84	21.55
(1,611)	1:39:B:LYS:HG3	1:67:A:LYS:HG2	20	21.22	0.88	21.21
(1,611)	1:39:A:LYS:HG3	1:67:B:LYS:HG2	20	21.22	0.88	21.21
(1,465)	1:61:B:ILE:HA	1:36:A:LYS:HE2	20	21.15	3.27	20.87
(1,465)	1:61:A:ILE:HA	1:36:B:LYS:HE3	20	21.15	3.27	20.87
(1,465)	1:61:A:ILE:HA	1:36:B:LYS:HE2	20	21.15	3.27	20.87
(1,677)	1:39:A:LYS:HG3	1:67:B:LYS:HG3	20	20.98	0.93	21.06
(1,677)	1:39:B:LYS:HG3	1:67:A:LYS:HG3	20	20.98	0.93	21.06
(1,863)	1:95:B:GLN:HB3	1:71:A:ARG:H	20	20.69	1.33	20.85
(1,863)	1:95:A:GLN:HB2	1:71:B:ARG:H	20	20.69	1.33	20.85
(1,863)	1:95:B:GLN:HB2	1:71:A:ARG:H	20	20.69	1.33	20.85
(1,863)	1:95:A:GLN:HB3	1:71:A:ARG:H	20	20.69	1.33	20.85
(1,297)	1:70:B:SER:H	1:45:A:ARG:HG3	20	20.63	0.9	20.56
(1,297)	1:70:A:SER:H	1:45:B:ARG:HG3	20	20.63	0.9	20.56
(1,612)	1:41:B:ILE:HG12	1:67:A:LYS:HG2	20	20.3	0.84	20.32
(1,612)	1:41:A:ILE:HG12	1:67:B:LYS:HG2	20	20.3	0.84	20.32
(1,330)	1:93:B:ARG:HB3	1:71:B:ARG:H	20	20.21	0.53	20.1
(1,330)	1:93:B:ARG:HB3	1:71:A:ARG:H	20	20.21	0.53	20.1
(1,330)	1:93:A:ARG:HB3	1:71:A:ARG:H	20	20.21	0.53	20.1
(1,330)	1:93:A:ARG:HB3	1:71:B:ARG:H	20	20.21	0.53	20.1
(1,474)	1:67:A:LYS:HA	1:45:B:ARG:HD3	20	20.07	0.89	19.86
(1,474)	1:67:B:LYS:HA	1:45:A:ARG:HD2	20	20.07	0.89	19.86
(1,303)	1:70:B:SER:H	1:45:A:ARG:HG2	20	20.05	0.97	20.18
(1,303)	1:70:A:SER:H	1:45:B:ARG:HG2	20	20.05	0.97	20.18
(1,697)	1:70:B:SER:HA	1:45:A:ARG:HG2	20	19.86	1.03	19.94
(1,697)	1:70:A:SER:HA	1:45:B:ARG:HG2	20	19.86	1.03	19.94
(1,595)	1:39:A:LYS:HG3	1:67:B:LYS:HB2	20	19.79	0.79	19.7
(1,595)	1:39:B:LYS:HG3	1:67:A:LYS:HB2	20	19.79	0.79	19.7
(1,426)	1:70:B:SER:HA	1:45:A:ARG:HG3	20	19.74	0.95	19.56
(1,426)	1:70:A:SER:HA	1:45:B:ARG:HG3	20	19.74	0.95	19.56
(1,47)	1:43:A:GLU:HG2	1:70:B:SER:H	20	19.59	0.82	19.6
(1,47)	1:43:B:GLU:HG2	1:70:A:SER:H	20	19.59	0.82	19.6
(1,347)	1:67:A:LYS:H	1:45:B:ARG:HD3	20	19.58	0.85	19.58
(1,347)	1:67:B:LYS:H	1:45:A:ARG:HD2	20	19.58	0.85	19.58
(1,613)	1:61:B:ILE:HG21	1:36:A:LYS:HE2	20	19.52	3.41	19.06
(1,613)	1:61:A:ILE:HG21	1:36:B:LYS:HE3	20	19.52	3.41	19.06
(1,613)	1:61:B:ILE:HG22	1:36:A:LYS:HE2	20	19.52	3.41	19.06
(1,613)	1:61:A:ILE:HG21	1:36:B:LYS:HE2	20	19.52	3.41	19.06

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,613)	1:61:A:ILE:HG22	1:36:B:LYS:HE2	20	19.52	3.41	19.06
(1,613)	1:61:A:ILE:HG13	1:36:B:LYS:HE3	20	19.52	3.41	19.06
(1,613)	1:61:A:ILE:HG22	1:36:B:LYS:HE3	20	19.52	3.41	19.06
(1,613)	1:61:B:ILE:HG13	1:36:A:LYS:HE2	20	19.52	3.41	19.06
(1,613)	1:61:A:ILE:HG23	1:36:B:LYS:HE3	20	19.52	3.41	19.06
(1,40)	1:69:A:SER:H	1:45:B:ARG:HD3	20	19.35	0.98	19.24
(1,40)	1:69:B:SER:H	1:45:A:ARG:HD2	20	19.35	0.98	19.24
(1,579)	1:61:B:ILE:HB	1:36:A:LYS:HE2	20	19.21	3.22	19.03
(1,579)	1:61:A:ILE:HB	1:36:B:LYS:HE3	20	19.21	3.22	19.03
(1,579)	1:61:A:ILE:HB	1:36:B:LYS:HE2	20	19.21	3.22	19.03
(1,500)	1:70:A:SER:H	1:45:B:ARG:HD3	20	18.69	1.06	18.4
(1,500)	1:70:B:SER:H	1:45:A:ARG:HD2	20	18.69	1.06	18.4
(1,109)	1:95:A:GLN:H	1:71:A:ARG:HG2	20	18.52	0.79	18.68
(1,109)	1:95:B:GLN:H	1:71:B:ARG:HG3	20	18.52	0.79	18.68
(1,109)	1:95:B:GLN:H	1:71:A:ARG:HG3	20	18.52	0.79	18.68
(1,109)	1:95:B:GLN:H	1:71:B:ARG:HG2	20	18.52	0.79	18.68
(1,109)	1:95:A:GLN:H	1:71:B:ARG:HG3	20	18.52	0.79	18.68
(1,860)	1:94:A:ALA:HA	1:72:A:HIS:HB2	20	18.42	0.59	18.45
(1,860)	1:94:B:ALA:HA	1:72:B:HIS:HB2	20	18.42	0.59	18.45
(1,727)	1:93:B:ARG:HA	1:71:B:ARG:HG2	20	18.42	0.59	18.4
(1,727)	1:93:A:ARG:HA	1:71:B:ARG:HG3	20	18.42	0.59	18.4
(1,727)	1:93:A:ARG:HA	1:71:A:ARG:HG2	20	18.42	0.59	18.4
(1,727)	1:93:B:ARG:HA	1:71:B:ARG:HG3	20	18.42	0.59	18.4
(1,727)	1:93:B:ARG:HA	1:71:A:ARG:HG3	20	18.42	0.59	18.4
(1,352)	1:93:A:ARG:HA	1:72:B:HIS:H	20	18.37	0.48	18.44
(1,352)	1:93:B:ARG:HA	1:72:A:HIS:H	20	18.37	0.48	18.44
(1,515)	1:36:A:LYS:HE2	1:62:B:LEU:H	20	18.3	3.13	18.04
(1,515)	1:36:B:LYS:HE3	1:62:A:LEU:H	20	18.3	3.13	18.04
(1,515)	1:36:B:LYS:HE2	1:62:A:LEU:H	20	18.3	3.13	18.04
(1,393)	1:93:B:ARG:H	1:71:B:ARG:H	20	18.22	0.42	18.2
(1,393)	1:93:A:ARG:H	1:71:A:ARG:H	20	18.22	0.42	18.2
(1,453)	1:67:A:LYS:HG2	1:45:B:ARG:HD3	20	18.09	0.96	18.16
(1,453)	1:67:B:LYS:HG2	1:45:A:ARG:HD2	20	18.09	0.96	18.16
(1,670)	1:93:B:ARG:HB3	1:71:B:ARG:HB2	20	18.02	0.9	17.96
(1,670)	1:93:A:ARG:HB3	1:71:A:ARG:HB2	20	18.02	0.9	17.96
(1,422)	1:70:A:SER:HB3	1:45:B:ARG:HD3	20	17.85	1.2	17.47
(1,422)	1:70:B:SER:HB3	1:45:A:ARG:HD2	20	17.85	1.2	17.47
(1,422)	1:70:A:SER:HB2	1:45:B:ARG:HD3	20	17.85	1.2	17.47
(1,614)	1:93:B:ARG:HB2	1:71:B:ARG:HG2	20	17.71	0.66	17.8
(1,614)	1:93:A:ARG:HB2	1:71:A:ARG:HG2	20	17.71	0.66	17.8
(1,614)	1:93:B:ARG:HB2	1:71:B:ARG:HG3	20	17.71	0.66	17.8
(1,103)	1:93:B:ARG:H	1:72:B:HIS:H	20	17.67	0.43	17.64

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,103)	1:93:A:ARG:H	1:72:B:HIS:H	20	17.67	0.43	17.64
(1,103)	1:93:A:ARG:H	1:72:A:HIS:H	20	17.67	0.43	17.64
(1,103)	1:93:B:ARG:H	1:72:A:HIS:H	20	17.67	0.43	17.64
(1,468)	1:70:B:SER:HA	1:45:A:ARG:HD2	20	17.41	1.16	17.14
(1,468)	1:70:A:SER:HA	1:45:B:ARG:HD3	20	17.41	1.16	17.14
(1,668)	1:93:B:ARG:HB3	1:71:B:ARG:HG2	20	17.22	0.74	17.16
(1,668)	1:93:A:ARG:HB3	1:71:A:ARG:HG2	20	17.22	0.74	17.16
(1,668)	1:93:B:ARG:HB3	1:71:B:ARG:HG3	20	17.22	0.74	17.16
(1,668)	1:93:A:ARG:HB3	1:71:A:ARG:HG3	20	17.22	0.74	17.16
(1,775)	1:67:A:LYS:HG3	1:45:B:ARG:HD3	20	16.98	0.94	17.01
(1,775)	1:67:B:LYS:HG3	1:45:A:ARG:HD2	20	16.98	0.94	17.01
(1,772)	1:94:B:ALA:H	1:71:B:ARG:HG2	20	16.56	0.55	16.6
(1,772)	1:94:B:ALA:H	1:71:B:ARG:HG3	20	16.56	0.55	16.6
(1,772)	1:94:A:ALA:H	1:71:A:ARG:HG2	20	16.56	0.55	16.6
(1,772)	1:94:A:ALA:H	1:71:A:ARG:HG3	20	16.56	0.55	16.6
(1,856)	1:93:A:ARG:HA	1:72:B:HIS:HB2	20	16.33	0.5	16.34
(1,856)	1:93:B:ARG:HA	1:72:A:HIS:HB2	20	16.33	0.5	16.34
(1,856)	1:93:B:ARG:HA	1:72:A:HIS:HB3	20	16.33	0.5	16.34
(1,578)	1:43:A:GLU:HG2	1:72:B:HIS:HD2	20	16.26	0.84	16.34
(1,578)	1:43:B:GLU:HG3	1:72:A:HIS:HD2	20	16.26	0.84	16.34
(1,578)	1:43:A:GLU:HG2	1:72:B:HIS:HD1	20	16.26	0.84	16.34
(1,578)	1:43:B:GLU:HG2	1:72:A:HIS:HD2	20	16.26	0.84	16.34
(1,313)	1:93:B:ARG:H	1:71:B:ARG:HG2	20	16.23	0.59	16.16
(1,313)	1:93:A:ARG:H	1:71:A:ARG:HG2	20	16.23	0.59	16.16
(1,313)	1:93:B:ARG:H	1:71:B:ARG:HG3	20	16.23	0.59	16.16
(1,313)	1:93:A:ARG:H	1:71:A:ARG:HG3	20	16.23	0.59	16.16
(1,861)	1:94:A:ALA:HB3	1:72:A:HIS:HB2	20	16.13	0.64	16.16
(1,861)	1:94:B:ALA:HB2	1:72:B:HIS:HB2	20	16.13	0.64	16.16
(1,861)	1:94:A:ALA:HB2	1:72:A:HIS:HB2	20	16.13	0.64	16.16
(1,861)	1:94:A:ALA:HB3	1:72:A:HIS:HB3	20	16.13	0.64	16.16
(1,861)	1:94:A:ALA:HB1	1:72:A:HIS:HB2	20	16.13	0.64	16.16
(1,861)	1:94:B:ALA:HB1	1:72:B:HIS:HB2	20	16.13	0.64	16.16
(1,861)	1:94:B:ALA:HB3	1:72:B:HIS:HB2	20	16.13	0.64	16.16
(1,454)	1:93:B:ARG:HB2	1:71:B:ARG:HD2	20	16.11	0.56	16.12
(1,454)	1:93:A:ARG:HB2	1:71:A:ARG:HD2	20	16.11	0.56	16.12
(1,51)	1:43:A:GLU:HG2	1:72:B:HIS:H	20	16.09	0.72	16.22
(1,51)	1:43:B:GLU:HG2	1:72:A:HIS:H	20	16.09	0.72	16.22
(1,452)	1:93:B:ARG:HB3	1:71:B:ARG:HD2	20	15.24	0.63	15.18
(1,452)	1:93:A:ARG:HB3	1:71:A:ARG:HD2	20	15.24	0.63	15.18
(1,219)	1:72:A:HIS:HB3	1:51:A:ASN:HD21	20	14.02	0.47	14.12
(1,219)	1:72:B:HIS:HB3	1:51:B:ASN:HD21	20	14.02	0.47	14.12
(1,219)	1:72:A:HIS:HB2	1:51:A:ASN:HD21	20	14.02	0.47	14.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,219)	1:72:B:HIS:HB2	1:51:B:ASN:HD21	20	14.02	0.47	14.12
(1,542)	1:72:A:HIS:HB3	1:51:A:ASN:HD22	20	13.99	0.46	14.06
(1,542)	1:72:B:HIS:HB3	1:51:B:ASN:HD22	20	13.99	0.46	14.06
(1,542)	1:72:A:HIS:HB2	1:51:A:ASN:HD22	20	13.99	0.46	14.06
(1,542)	1:72:B:HIS:HB2	1:51:B:ASN:HD22	20	13.99	0.46	14.06
(1,220)	1:73:A:SER:HB2	1:51:A:ASN:HD21	20	13.43	1.34	13.86
(1,220)	1:73:B:SER:HB3	1:51:B:ASN:HD21	20	13.43	1.34	13.86
(1,220)	1:73:A:SER:HB3	1:51:A:ASN:HD21	20	13.43	1.34	13.86
(1,220)	1:73:B:SER:HB2	1:51:B:ASN:HD21	20	13.43	1.34	13.86
(1,56)	1:73:A:SER:H	1:51:A:ASN:HD22	20	13.24	1.15	13.64
(1,56)	1:73:B:SER:H	1:51:B:ASN:HD22	20	13.24	1.15	13.64
(1,217)	1:73:A:SER:HA	1:51:A:ASN:HD21	20	12.28	0.97	12.53
(1,217)	1:73:B:SER:HA	1:51:B:ASN:HD21	20	12.28	0.97	12.53
(1,229)	1:73:A:SER:HB2	1:51:A:ASN:HD22	20	12.24	1.24	12.65
(1,229)	1:73:B:SER:HB3	1:51:B:ASN:HD22	20	12.24	1.24	12.65
(1,229)	1:73:A:SER:HB3	1:51:A:ASN:HD22	20	12.24	1.24	12.65
(1,229)	1:73:B:SER:HB2	1:51:B:ASN:HD22	20	12.24	1.24	12.65
(1,494)	1:72:B:HIS:HD2	1:51:B:ASN:HD22	20	12.19	0.59	12.24
(1,494)	1:72:A:HIS:HD2	1:51:A:ASN:HD22	20	12.19	0.59	12.24
(1,494)	1:72:B:HIS:HD1	1:51:B:ASN:HD22	20	12.19	0.59	12.24
(1,227)	1:73:A:SER:HA	1:51:A:ASN:HD22	20	11.94	0.93	12.18
(1,227)	1:73:B:SER:HA	1:51:B:ASN:HD22	20	11.94	0.93	12.18
(1,218)	1:72:B:HIS:HD2	1:51:B:ASN:HD21	20	11.03	0.58	11.06
(1,218)	1:72:A:HIS:HD2	1:51:A:ASN:HD21	20	11.03	0.58	11.06
(1,438)	1:92:A:GLN:HG3	1:71:B:ARG:HD2	20	10.94	0.62	10.8
(1,438)	1:92:B:GLN:HG3	1:71:A:ARG:HD2	20	10.94	0.62	10.8
(1,594)	1:73:A:SER:HB2	1:77:A:LYS:HG3	20	10.51	0.89	10.72
(1,594)	1:73:B:SER:HB3	1:77:B:LYS:HG3	20	10.51	0.89	10.72
(1,594)	1:73:A:SER:HB3	1:77:A:LYS:HG3	20	10.51	0.89	10.72
(1,594)	1:73:B:SER:HB2	1:77:B:LYS:HG3	20	10.51	0.89	10.72
(1,309)	1:92:A:GLN:H	1:67:A:LYS:HD2	20	10.39	0.76	10.51
(1,309)	1:92:B:GLN:H	1:67:B:LYS:HD2	20	10.39	0.76	10.51
(1,309)	1:92:B:GLN:H	1:67:B:LYS:HD3	20	10.39	0.76	10.51
(1,309)	1:92:A:GLN:H	1:67:B:LYS:HD2	20	10.39	0.76	10.51
(1,401)	1:75:B:LEU:HB3	1:51:B:ASN:HD22	20	10.16	0.51	10.1
(1,401)	1:75:A:LEU:HB3	1:51:A:ASN:HD22	20	10.16	0.51	10.1
(1,839)	1:87:B:HIS:HD1	1:72:B:HIS:H	20	9.71	1.2	10.23
(1,839)	1:87:A:HIS:HD2	1:72:A:HIS:H	20	9.71	1.2	10.23
(1,839)	1:87:A:HIS:HD1	1:72:A:HIS:H	20	9.71	1.2	10.23
(1,839)	1:87:B:HIS:HD2	1:72:B:HIS:H	20	9.71	1.2	10.23
(1,327)	1:90:B:ASN:H	1:66:B:LYS:HE3	20	9.45	0.51	9.34
(1,327)	1:90:B:ASN:H	1:66:B:LYS:HE2	20	9.45	0.51	9.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,327)	1:90:A:ASN:H	1:66:A:LYS:HE2	20	9.45	0.51	9.34
(1,327)	1:90:A:ASN:H	1:66:B:LYS:HE2	20	9.45	0.51	9.34
(1,327)	1:90:B:ASN:H	1:66:A:LYS:HE2	20	9.45	0.51	9.34
(1,755)	1:87:B:HIS:HD1	1:72:B:HIS:H	20	9.25	0.86	9.52
(1,755)	1:87:A:HIS:HD1	1:72:A:HIS:H	20	9.25	0.86	9.52
(1,283)	1:87:B:HIS:HD2	1:72:B:HIS:H	20	9.22	1.34	9.75
(1,283)	1:87:A:HIS:HD2	1:72:A:HIS:H	20	9.22	1.34	9.75
(1,536)	1:89:A:ARG:H	1:66:B:LYS:HE3	20	8.99	0.47	8.98
(1,536)	1:89:B:ARG:H	1:66:A:LYS:HE2	20	8.99	0.47	8.98
(1,536)	1:89:A:ARG:H	1:66:B:LYS:HE2	20	8.99	0.47	8.98
(1,664)	1:86:B:LYS:HG2	1:92:B:GLN:HE21	20	8.8	0.4	8.95
(1,664)	1:86:A:LYS:HG2	1:92:B:GLN:HE21	20	8.8	0.4	8.95
(1,664)	1:86:A:LYS:HG2	1:92:A:GLN:HE21	20	8.8	0.4	8.95
(1,841)	1:87:A:HIS:HD2	1:72:A:HIS:HB2	20	8.78	1.05	9.07
(1,841)	1:87:B:HIS:HD2	1:72:B:HIS:HB2	20	8.78	1.05	9.07
(1,841)	1:87:B:HIS:HD1	1:72:B:HIS:HB2	20	8.78	1.05	9.07
(1,841)	1:87:A:HIS:HD1	1:72:A:HIS:HB2	20	8.78	1.05	9.07
(1,841)	1:87:A:HIS:HD1	1:72:A:HIS:HB3	20	8.78	1.05	9.07
(1,560)	1:91:B:LEU:HA	1:66:B:LYS:HE3	20	8.45	0.66	8.39
(1,560)	1:91:B:LEU:HA	1:66:B:LYS:HE2	20	8.45	0.66	8.39
(1,560)	1:91:A:LEU:HA	1:66:A:LYS:HE2	20	8.45	0.66	8.39
(1,537)	1:91:B:LEU:H	1:66:B:LYS:HE3	20	8.43	0.54	8.36
(1,537)	1:91:B:LEU:H	1:66:B:LYS:HE2	20	8.43	0.54	8.36
(1,537)	1:91:A:LEU:H	1:66:A:LYS:HE2	20	8.43	0.54	8.36
(1,546)	1:88:A:LEU:HA	1:66:B:LYS:HE3	20	8.43	0.61	8.42
(1,546)	1:88:A:LEU:HA	1:66:B:LYS:HE2	20	8.43	0.61	8.42
(1,546)	1:88:B:LEU:HA	1:66:A:LYS:HE2	20	8.43	0.61	8.42
(1,228)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	20	8.11	0.22	8.13
(1,228)	1:76:B:GLU:HB3	1:51:A:ASN:HD22	20	8.11	0.22	8.13
(1,354)	1:76:A:GLU:HA	1:51:B:ASN:HD21	20	8.11	0.31	8.09
(1,354)	1:76:B:GLU:HA	1:51:A:ASN:HD21	20	8.11	0.31	8.09
(1,354)	1:76:A:GLU:HA	1:51:A:ASN:HD21	20	8.11	0.31	8.09
(1,725)	1:75:A:LEU:HA	1:50:B:ILE:HG23	20	7.98	0.19	8.0
(1,725)	1:75:A:LEU:HA	1:50:B:ILE:HG21	20	7.98	0.19	8.0
(1,725)	1:75:A:LEU:HA	1:50:B:ILE:HG22	20	7.98	0.19	8.0
(1,725)	1:75:B:LEU:HA	1:50:A:ILE:HG21	20	7.98	0.19	8.0
(1,57)	1:73:B:SER:H	1:77:B:LYS:HG3	20	7.96	1.1	8.33
(1,57)	1:73:A:SER:H	1:77:A:LYS:HG3	20	7.96	1.1	8.33
(1,557)	1:89:A:ARG:HA	1:66:B:LYS:HE3	20	7.86	0.54	7.73
(1,557)	1:89:B:ARG:HA	1:66:A:LYS:HE2	20	7.86	0.54	7.73
(1,557)	1:89:A:ARG:HA	1:66:B:LYS:HE2	20	7.86	0.54	7.73
(1,216)	1:76:A:GLU:HB3	1:51:B:ASN:HD21	20	7.68	0.33	7.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,216)	1:76:B:GLU:HB3	1:51:A:ASN:HD21	20	7.68	0.33	7.6
(1,615)	1:91:B:LEU:HG	1:66:B:LYS:HE3	20	7.65	0.58	7.6
(1,615)	1:91:B:LEU:HG	1:66:B:LYS:HE2	20	7.65	0.58	7.6
(1,615)	1:91:A:LEU:HG	1:66:A:LYS:HE2	20	7.65	0.58	7.6
(1,840)	1:87:B:HIS:HD2	1:72:B:HIS:HA	20	7.59	1.23	8.16
(1,840)	1:87:A:HIS:HD2	1:72:A:HIS:HA	20	7.59	1.23	8.16
(1,840)	1:87:A:HIS:HD1	1:72:A:HIS:HA	20	7.59	1.23	8.16
(1,840)	1:87:B:HIS:HD1	1:72:B:HIS:HA	20	7.59	1.23	8.16
(1,399)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	20	7.54	0.22	7.56
(1,399)	1:76:B:GLU:HB3	1:51:A:ASN:HD22	20	7.54	0.22	7.56
(1,842)	1:87:A:HIS:HD2	1:75:A:LEU:HD23	20	7.11	1.5	7.91
(1,842)	1:87:B:HIS:HD2	1:75:B:LEU:HD23	20	7.11	1.5	7.91
(1,842)	1:87:A:HIS:HD2	1:75:A:LEU:HD12	20	7.11	1.5	7.91
(1,842)	1:87:A:HIS:HD1	1:75:A:LEU:HD11	20	7.11	1.5	7.91
(1,842)	1:87:A:HIS:HD1	1:75:A:LEU:HD22	20	7.11	1.5	7.91
(1,842)	1:87:B:HIS:HD1	1:75:B:LEU:HD13	20	7.11	1.5	7.91
(1,842)	1:87:B:HIS:HD2	1:75:B:LEU:HD12	20	7.11	1.5	7.91
(1,842)	1:87:A:HIS:HD2	1:75:A:LEU:HD13	20	7.11	1.5	7.91
(1,842)	1:87:A:HIS:HD2	1:75:A:LEU:HD21	20	7.11	1.5	7.91
(1,842)	1:87:A:HIS:HD1	1:75:A:LEU:HD23	20	7.11	1.5	7.91
(1,842)	1:87:B:HIS:HD1	1:75:B:LEU:HD11	20	7.11	1.5	7.91
(1,842)	1:87:A:HIS:HD1	1:75:A:LEU:HD21	20	7.11	1.5	7.91
(1,640)	1:86:B:LYS:HD3	1:84:B:THR:HG21	20	7.05	0.3	7.09
(1,640)	1:86:B:LYS:HD3	1:84:B:THR:HG22	20	7.05	0.3	7.09
(1,640)	1:86:A:LYS:HD3	1:84:A:THR:HG23	20	7.05	0.3	7.09
(1,640)	1:86:B:LYS:HD3	1:84:B:THR:HG23	20	7.05	0.3	7.09
(1,640)	1:86:A:LYS:HD3	1:84:A:THR:HG21	20	7.05	0.3	7.09
(1,640)	1:86:A:LYS:HD3	1:84:B:THR:HG22	20	7.05	0.3	7.09
(1,640)	1:86:A:LYS:HD3	1:84:A:THR:HG22	20	7.05	0.3	7.09
(1,925)	1:69:A:SER:H	1:65:A:LEU:O	20	7.02	0.27	7.02
(1,925)	1:69:B:SER:H	1:65:B:LEU:O	20	7.02	0.27	7.02
(1,503)	1:65:A:LEU:HA	1:69:A:SER:H	20	6.92	0.25	6.91
(1,503)	1:65:B:LEU:HA	1:69:B:SER:H	20	6.92	0.25	6.91
(1,23)	1:64:A:ALA:H	1:68:A:ASP:HB3	20	6.81	0.2	6.8
(1,23)	1:64:B:ALA:H	1:68:B:ASP:HB2	20	6.81	0.2	6.8
(1,23)	1:64:B:ALA:H	1:68:B:ASP:HB3	20	6.81	0.2	6.8
(1,23)	1:64:A:ALA:H	1:68:A:ASP:HB2	20	6.81	0.2	6.8
(1,650)	1:79:A:ASP:HB2	1:54:A:LEU:HD11	20	6.76	0.61	6.74
(1,650)	1:79:B:ASP:HB2	1:54:B:LEU:HD11	20	6.76	0.61	6.74
(1,650)	1:79:B:ASP:HB2	1:54:B:LEU:HD13	20	6.76	0.61	6.74
(1,650)	1:79:B:ASP:HB2	1:54:B:LEU:HD12	20	6.76	0.61	6.74
(1,99)	1:66:B:LYS:HE3	1:92:A:GLN:H	20	6.75	0.57	6.78

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,99)	1:66:A:LYS:HE2	1:92:B:GLN:H	20	6.75	0.57	6.78
(1,99)	1:66:B:LYS:HE2	1:92:A:GLN:H	20	6.75	0.57	6.78
(1,446)	1:77:A:LYS:HA	1:56:B:GLN:HG2	20	6.72	0.24	6.68
(1,446)	1:77:B:LYS:HA	1:56:B:GLN:HG2	20	6.72	0.24	6.68
(1,446)	1:77:B:LYS:HA	1:56:A:GLN:HG2	20	6.72	0.24	6.68
(1,446)	1:77:A:LYS:HA	1:56:A:GLN:HG2	20	6.72	0.24	6.68
(1,642)	1:79:A:ASP:HB3	1:54:A:LEU:HD11	20	6.58	0.56	6.62
(1,642)	1:79:B:ASP:HB3	1:54:B:LEU:HD11	20	6.58	0.56	6.62
(1,642)	1:79:B:ASP:HB3	1:54:B:LEU:HD12	20	6.58	0.56	6.62
(1,642)	1:79:B:ASP:HB3	1:54:B:LEU:HD13	20	6.58	0.56	6.62
(1,838)	1:87:B:HIS:HD1	1:71:B:ARG:HD2	20	6.46	1.35	7.16
(1,838)	1:87:A:HIS:HD2	1:71:A:ARG:HD2	20	6.46	1.35	7.16
(1,838)	1:87:B:HIS:HD2	1:71:B:ARG:HD2	20	6.46	1.35	7.16
(1,838)	1:87:A:HIS:HD1	1:71:A:ARG:HD2	20	6.46	1.35	7.16
(1,524)	1:78:A:ALA:H	1:56:B:GLN:HG2	20	6.39	0.18	6.42
(1,524)	1:78:B:ALA:H	1:56:A:GLN:HG2	20	6.39	0.18	6.42
(1,1)	1:80:A:ILE:H	1:56:B:GLN:HG2	20	6.19	0.2	6.16
(1,1)	1:80:B:ILE:H	1:56:A:GLN:HG2	20	6.19	0.2	6.16
(1,687)	1:87:B:HIS:HD1	1:71:B:ARG:HD2	20	6.11	1.05	6.54
(1,687)	1:87:A:HIS:HD1	1:71:A:ARG:HD2	20	6.11	1.05	6.54
(1,691)	1:87:B:HIS:HD2	1:71:B:ARG:HD2	20	6.11	1.55	6.75
(1,691)	1:87:A:HIS:HD2	1:71:A:ARG:HD2	20	6.11	1.55	6.75
(1,679)	1:92:A:GLN:HG3	1:83:B:MET:HG2	20	6.09	0.66	5.96
(1,679)	1:92:B:GLN:HG3	1:83:A:MET:HG2	20	6.09	0.66	5.96
(1,679)	1:92:A:GLN:HG2	1:83:B:MET:HG2	20	6.09	0.66	5.96
(1,679)	1:92:B:GLN:HG2	1:83:A:MET:HG2	20	6.09	0.66	5.96
(1,927)	1:70:A:SER:H	1:66:A:LYS:O	20	6.05	0.34	6.1
(1,927)	1:70:B:SER:H	1:66:B:LYS:O	20	6.05	0.34	6.1
(1,926)	1:69:A:SER:N	1:65:A:LEU:O	20	5.94	0.26	5.94
(1,926)	1:69:B:SER:N	1:65:B:LEU:O	20	5.94	0.26	5.94
(1,561)	1:92:A:GLN:HE21	1:83:B:MET:HA	20	5.94	0.27	5.85
(1,561)	1:92:B:GLN:HE21	1:83:A:MET:HA	20	5.94	0.27	5.85
(1,671)	1:92:A:GLN:HG2	1:83:B:MET:HG3	20	5.85	0.47	5.69
(1,671)	1:92:B:GLN:HG3	1:83:A:MET:HG3	20	5.85	0.47	5.69
(1,671)	1:92:A:GLN:HG3	1:83:B:MET:HG3	20	5.85	0.47	5.69
(1,671)	1:92:B:GLN:HG2	1:83:A:MET:HG3	20	5.85	0.47	5.69
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD23	20	5.82	0.63	6.02
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD13	20	5.82	0.63	6.02
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD21	20	5.82	0.63	6.02
(1,811)	1:84:B:THR:HB	1:60:A:LEU:HD11	20	5.82	0.63	6.02
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD22	20	5.82	0.63	6.02
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD11	20	5.82	0.63	6.02

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,635)	1:89:B:ARG:HB2	1:65:B:LEU:HG	20	5.81	0.61	5.72
(1,635)	1:89:A:ARG:HB2	1:65:A:LEU:HG	20	5.81	0.61	5.72
(1,939)	1:77:A:LYS:N	1:73:A:SER:O	20	5.77	0.67	5.95
(1,939)	1:77:B:LYS:N	1:73:B:SER:O	20	5.77	0.67	5.95
(1,940)	1:78:B:ALA:H	1:74:B:LYS:O	20	5.75	0.34	5.7
(1,940)	1:78:A:ALA:H	1:74:A:LYS:O	20	5.75	0.34	5.7
(1,445)	1:65:B:LEU:HA	1:68:B:ASP:HB2	20	5.72	0.23	5.72
(1,445)	1:65:A:LEU:HA	1:68:A:ASP:HB2	20	5.72	0.23	5.72
(1,928)	1:70:A:SER:N	1:66:A:LYS:O	20	5.71	0.33	5.75
(1,928)	1:70:B:SER:N	1:66:B:LYS:O	20	5.71	0.33	5.75
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD23	20	5.65	0.73	6.04
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD13	20	5.65	0.73	6.04
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD21	20	5.65	0.73	6.04
(1,809)	1:84:B:THR:H	1:60:A:LEU:HD11	20	5.65	0.73	6.04
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD22	20	5.65	0.73	6.04
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD11	20	5.65	0.73	6.04
(1,848)	1:90:B:ASN:HD21	1:66:B:LYS:HE2	20	5.61	0.61	5.4
(1,848)	1:90:B:ASN:HD21	1:66:B:LYS:HE3	20	5.61	0.61	5.4
(1,848)	1:90:A:ASN:HD21	1:66:A:LYS:HE2	20	5.61	0.61	5.4
(1,460)	1:73:B:SER:HA	1:76:B:GLU:HB2	20	5.51	0.4	5.56
(1,460)	1:73:A:SER:HA	1:76:A:GLU:HB2	20	5.51	0.4	5.56
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD23	20	5.3	0.31	5.36
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD13	20	5.3	0.31	5.36
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD21	20	5.3	0.31	5.36
(1,802)	1:81:B:LEU:HB3	1:60:A:LEU:HD11	20	5.3	0.31	5.36
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD22	20	5.3	0.31	5.36
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD11	20	5.3	0.31	5.36
(1,784)	1:64:A:ALA:HB1	1:67:A:LYS:HB2	20	5.21	0.3	5.26
(1,784)	1:64:B:ALA:HB1	1:67:B:LYS:HB2	20	5.21	0.3	5.26
(1,784)	1:64:A:ALA:HB3	1:67:A:LYS:HB2	20	5.21	0.3	5.26
(1,784)	1:64:B:ALA:HB2	1:67:B:LYS:HB2	20	5.21	0.3	5.26
(1,784)	1:64:A:ALA:HB2	1:67:A:LYS:HB2	20	5.21	0.3	5.26
(1,784)	1:64:B:ALA:HB3	1:67:B:LYS:HB2	20	5.21	0.3	5.26
(1,941)	1:78:B:ALA:N	1:74:B:LYS:O	20	5.07	0.31	5.03
(1,941)	1:78:A:ALA:N	1:74:A:LYS:O	20	5.07	0.31	5.03
(1,333)	1:81:A:LEU:H	1:56:B:GLN:HG3	20	5.05	0.17	4.99
(1,333)	1:81:B:LEU:H	1:56:A:GLN:HG3	20	5.05	0.17	4.99
(1,62)	1:81:A:LEU:H	1:56:B:GLN:HG2	20	5.0	0.19	4.96
(1,62)	1:81:B:LEU:H	1:56:A:GLN:HG2	20	5.0	0.19	4.96
(1,714)	1:86:A:LYS:HD3	1:84:A:THR:HA	20	4.98	0.25	5.02
(1,714)	1:86:B:LYS:HD3	1:84:B:THR:HA	20	4.98	0.25	5.02
(1,823)	1:86:B:LYS:HG3	1:84:B:THR:HG21	20	4.97	0.13	4.96

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,823)	1:86:B:LYS:HG3	1:84:B:THR:HG22	20	4.97	0.13	4.96
(1,823)	1:86:B:LYS:HG3	1:84:B:THR:HG23	20	4.97	0.13	4.96
(1,823)	1:86:A:LYS:HG3	1:84:A:THR:HG21	20	4.97	0.13	4.96
(1,823)	1:86:A:LYS:HG3	1:84:A:THR:HG23	20	4.97	0.13	4.96
(1,823)	1:86:A:LYS:HG3	1:84:A:THR:HG22	20	4.97	0.13	4.96
(1,226)	1:81:B:LEU:H	1:56:A:GLN:HE21	20	4.95	0.35	4.92
(1,226)	1:81:A:LEU:H	1:56:B:GLN:HE21	20	4.95	0.35	4.92
(1,432)	1:90:B:ASN:HA	1:65:B:LEU:HG	20	4.93	0.67	4.83
(1,432)	1:90:A:ASN:HA	1:65:A:LEU:HG	20	4.93	0.67	4.83
(1,739)	1:50:B:ILE:HG23	1:76:A:GLU:HA	20	4.89	0.14	4.89
(1,739)	1:50:A:ILE:HG21	1:76:B:GLU:HA	20	4.89	0.14	4.89
(1,739)	1:50:B:ILE:HG21	1:76:A:GLU:HA	20	4.89	0.14	4.89
(1,739)	1:50:B:ILE:HG22	1:76:A:GLU:HA	20	4.89	0.14	4.89
(1,812)	1:84:B:THR:HG23	1:60:B:LEU:HD23	20	4.7	0.51	4.81
(1,812)	1:84:B:THR:HG21	1:60:B:LEU:HD23	20	4.7	0.51	4.81
(1,812)	1:84:B:THR:HG23	1:60:B:LEU:HD13	20	4.7	0.51	4.81
(1,812)	1:84:B:THR:HG22	1:60:B:LEU:HD21	20	4.7	0.51	4.81
(1,812)	1:84:A:THR:HG21	1:60:A:LEU:HD11	20	4.7	0.51	4.81
(1,812)	1:84:B:THR:HG23	1:60:B:LEU:HD11	20	4.7	0.51	4.81
(1,812)	1:84:B:THR:HG21	1:60:B:LEU:HD21	20	4.7	0.51	4.81
(1,812)	1:84:B:THR:HG21	1:60:B:LEU:HD11	20	4.7	0.51	4.81
(1,812)	1:84:B:THR:HG23	1:60:B:LEU:HD21	20	4.7	0.51	4.81
(1,812)	1:84:B:THR:HG22	1:60:B:LEU:HD22	20	4.7	0.51	4.81
(1,812)	1:84:B:THR:HG23	1:60:B:LEU:HD22	20	4.7	0.51	4.81
(1,510)	1:79:A:ASP:H	1:54:A:LEU:HG	20	4.65	0.22	4.64
(1,510)	1:79:B:ASP:H	1:54:B:LEU:HG	20	4.65	0.22	4.64
(1,849)	1:90:A:ASN:HD21	1:92:B:GLN:HG2	20	4.59	0.21	4.61
(1,849)	1:90:B:ASN:HD21	1:92:A:GLN:HG2	20	4.59	0.21	4.61
(1,849)	1:90:B:ASN:HD21	1:92:B:GLN:HG2	20	4.59	0.21	4.61
(1,409)	1:64:A:ALA:HA	1:67:A:LYS:HB2	20	4.5	0.3	4.46
(1,409)	1:64:B:ALA:HA	1:67:B:LYS:HB2	20	4.5	0.3	4.46
(1,603)	1:64:B:ALA:HB2	1:67:B:LYS:HG2	20	4.44	0.8	4.36
(1,603)	1:64:A:ALA:HB2	1:67:A:LYS:HG2	20	4.44	0.8	4.36
(1,820)	1:86:A:LYS:HG2	1:87:A:HIS:HD1	20	4.44	1.46	5.48
(1,820)	1:86:A:LYS:HG2	1:87:A:HIS:HD2	20	4.44	1.46	5.48
(1,820)	1:86:B:LYS:HG2	1:87:B:HIS:HD2	20	4.44	1.46	5.48
(1,820)	1:86:B:LYS:HG2	1:87:B:HIS:HD1	20	4.44	1.46	5.48
(1,246)	1:81:B:LEU:H	1:56:A:GLN:HE22	20	4.37	0.31	4.38
(1,246)	1:81:A:LEU:H	1:56:B:GLN:HE22	20	4.37	0.31	4.38
(1,357)	1:67:B:LYS:HA	1:70:B:SER:H	20	4.32	0.09	4.34
(1,357)	1:67:A:LYS:HA	1:70:A:SER:H	20	4.32	0.09	4.34
(1,415)	1:86:B:LYS:HD3	1:84:B:THR:HB	20	4.29	0.42	4.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,415)	1:86:A:LYS:HD3	1:84:A:THR:HB	20	4.29	0.42	4.18
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD23	20	4.24	0.72	4.56
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD13	20	4.24	0.72	4.56
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD21	20	4.24	0.72	4.56
(1,813)	1:85:B:VAL:H	1:60:A:LEU:HD11	20	4.24	0.72	4.56
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD22	20	4.24	0.72	4.56
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD11	20	4.24	0.72	4.56
(1,601)	1:64:A:ALA:HB1	1:67:A:LYS:HG2	20	4.23	0.81	4.2
(1,601)	1:64:B:ALA:HB1	1:67:B:LYS:HG2	20	4.23	0.81	4.2
(1,684)	1:86:A:LYS:HD3	1:87:A:HIS:HB3	20	4.23	0.29	4.21
(1,684)	1:86:B:LYS:HD3	1:87:B:HIS:HB3	20	4.23	0.29	4.21
(1,76)	1:86:A:LYS:H	1:61:A:ILE:HG12	20	4.16	0.11	4.18
(1,76)	1:86:A:LYS:H	1:61:B:ILE:HG12	20	4.16	0.11	4.18
(1,76)	1:86:B:LYS:H	1:61:B:ILE:HG12	20	4.16	0.11	4.18
(1,76)	1:86:B:LYS:H	1:61:A:ILE:HG12	20	4.16	0.11	4.18
(1,633)	1:90:A:ASN:HB2	1:92:A:GLN:HG2	20	4.0	0.12	4.01
(1,633)	1:90:B:ASN:HB2	1:92:B:GLN:HG2	20	4.0	0.12	4.01
(1,633)	1:90:B:ASN:HB2	1:92:B:GLN:HG3	20	4.0	0.12	4.01
(1,633)	1:90:A:ASN:HB2	1:92:A:GLN:HG3	20	4.0	0.12	4.01
(1,308)	1:90:B:ASN:H	1:65:B:LEU:HG	20	3.95	0.57	3.8
(1,308)	1:90:A:ASN:H	1:65:A:LEU:HG	20	3.95	0.57	3.8
(1,355)	1:65:B:LEU:HA	1:68:B:ASP:H	20	3.92	0.22	3.96
(1,355)	1:65:A:LEU:HA	1:68:A:ASP:H	20	3.92	0.22	3.96
(1,214)	1:81:B:LEU:HB2	1:56:A:GLN:HE22	20	3.86	0.28	3.88
(1,214)	1:81:A:LEU:HB3	1:56:B:GLN:HE22	20	3.86	0.28	3.88
(1,214)	1:81:B:LEU:HB3	1:56:A:GLN:HE22	20	3.86	0.28	3.88
(1,214)	1:81:A:LEU:HB2	1:56:B:GLN:HE22	20	3.86	0.28	3.88
(1,929)	1:71:B:ARG:N	1:67:B:LYS:O	20	3.74	0.22	3.72
(1,929)	1:71:A:ARG:N	1:67:A:LYS:O	20	3.74	0.22	3.72
(1,237)	1:79:A:ASP:H	1:54:A:LEU:HD11	20	3.71	0.31	3.76
(1,237)	1:79:B:ASP:H	1:54:B:LEU:HD11	20	3.71	0.31	3.76
(1,237)	1:79:B:ASP:H	1:54:B:LEU:HD13	20	3.71	0.31	3.76
(1,237)	1:79:B:ASP:H	1:54:B:LEU:HD12	20	3.71	0.31	3.76
(1,447)	1:81:A:LEU:HA	1:56:B:GLN:HG2	20	3.71	0.15	3.72
(1,447)	1:81:B:LEU:HA	1:56:A:GLN:HG2	20	3.71	0.15	3.72
(1,451)	1:81:A:LEU:HA	1:56:B:GLN:HG3	20	3.65	0.15	3.62
(1,451)	1:81:B:LEU:HA	1:56:A:GLN:HG3	20	3.65	0.15	3.62
(1,602)	1:64:B:ALA:HB2	1:67:B:LYS:HG3	20	3.65	0.76	4.07
(1,602)	1:64:A:ALA:HB2	1:67:A:LYS:HG3	20	3.65	0.76	4.07
(1,785)	1:64:A:ALA:HB1	1:67:A:LYS:HG3	20	3.61	0.31	3.71
(1,785)	1:64:B:ALA:HB1	1:67:B:LYS:HG3	20	3.61	0.31	3.71
(1,785)	1:64:B:ALA:HB3	1:67:B:LYS:HG3	20	3.61	0.31	3.71

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,785)	1:64:A:ALA:HB2	1:67:A:LYS:HG3	20	3.61	0.31	3.71
(1,785)	1:64:B:ALA:HB2	1:67:B:LYS:HG3	20	3.61	0.31	3.71
(1,785)	1:64:A:ALA:HB3	1:67:A:LYS:HG3	20	3.61	0.31	3.71
(1,834)	1:87:B:HIS:HD2	1:92:A:GLN:HB2	20	3.57	0.17	3.57
(1,834)	1:87:A:HIS:HD1	1:92:B:GLN:HB2	20	3.57	0.17	3.57
(1,834)	1:87:B:HIS:HD1	1:92:A:GLN:HB2	20	3.57	0.17	3.57
(1,834)	1:87:A:HIS:HD2	1:92:B:GLN:HB2	20	3.57	0.17	3.57
(1,835)	1:87:A:HIS:HD1	1:67:A:LYS:HD2	20	3.55	1.36	4.1
(1,835)	1:87:B:HIS:HD1	1:67:B:LYS:HD2	20	3.55	1.36	4.1
(1,835)	1:87:B:HIS:HD2	1:67:B:LYS:HD2	20	3.55	1.36	4.1
(1,835)	1:87:A:HIS:HD2	1:67:A:LYS:HD2	20	3.55	1.36	4.1
(1,688)	1:86:A:LYS:HD3	1:87:A:HIS:HB2	20	3.55	0.42	3.4
(1,688)	1:86:B:LYS:HD3	1:87:B:HIS:HB2	20	3.55	0.42	3.4
(1,408)	1:64:B:ALA:HA	1:67:B:LYS:HG2	20	3.5	0.65	3.78
(1,408)	1:64:A:ALA:HA	1:67:A:LYS:HG2	20	3.5	0.65	3.78
(1,224)	1:81:B:LEU:HB3	1:56:A:GLN:HE21	20	3.47	0.28	3.52
(1,224)	1:81:A:LEU:HB3	1:56:B:GLN:HE21	20	3.47	0.28	3.52
(1,224)	1:81:B:LEU:HB2	1:56:A:GLN:HE21	20	3.47	0.28	3.52
(1,224)	1:81:A:LEU:HB2	1:56:B:GLN:HE21	20	3.47	0.28	3.52
(1,564)	1:66:A:LYS:HA	1:69:A:SER:HB2	20	3.39	0.59	3.45
(1,564)	1:66:B:LYS:HA	1:69:B:SER:HB3	20	3.39	0.59	3.45
(1,564)	1:66:A:LYS:HA	1:69:A:SER:HB3	20	3.39	0.59	3.45
(1,564)	1:66:B:LYS:HA	1:69:B:SER:HB2	20	3.39	0.59	3.45
(1,837)	1:87:A:HIS:HD1	1:93:A:ARG:H	20	3.35	0.36	3.4
(1,837)	1:87:A:HIS:HD2	1:93:A:ARG:H	20	3.35	0.36	3.4
(1,837)	1:87:B:HIS:HD2	1:93:B:ARG:H	20	3.35	0.36	3.4
(1,837)	1:87:B:HIS:HD1	1:93:B:ARG:H	20	3.35	0.36	3.4
(1,585)	1:64:A:ALA:HB1	1:67:A:LYS:HG3	20	3.34	0.62	3.14
(1,585)	1:64:B:ALA:HB1	1:67:B:LYS:HG3	20	3.34	0.62	3.14
(1,821)	1:86:B:LYS:HG2	1:83:B:MET:HG3	20	3.33	0.37	3.42
(1,821)	1:86:A:LYS:HG2	1:83:A:MET:HG3	20	3.33	0.37	3.42
(1,821)	1:86:B:LYS:HG2	1:83:B:MET:HG2	20	3.33	0.37	3.42
(1,654)	1:86:A:LYS:HB2	1:84:A:THR:HG21	20	3.24	0.14	3.24
(1,654)	1:86:A:LYS:HB2	1:84:A:THR:HG23	20	3.24	0.14	3.24
(1,654)	1:86:B:LYS:HB2	1:84:B:THR:HG21	20	3.24	0.14	3.24
(1,654)	1:86:A:LYS:HB2	1:84:A:THR:HG22	20	3.24	0.14	3.24
(1,654)	1:86:B:LYS:HB2	1:84:B:THR:HG22	20	3.24	0.14	3.24
(1,439)	1:86:A:LYS:HA	1:84:A:THR:HG21	20	3.22	0.17	3.18
(1,439)	1:86:B:LYS:HA	1:84:B:THR:HG22	20	3.22	0.17	3.18
(1,439)	1:86:B:LYS:HA	1:84:B:THR:HG21	20	3.22	0.17	3.18
(1,439)	1:86:A:LYS:HA	1:84:A:THR:HG23	20	3.22	0.17	3.18
(1,439)	1:86:A:LYS:HA	1:84:A:THR:HG22	20	3.22	0.17	3.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,439)	1:86:B:LYS:HA	1:84:A:THR:HG21	20	3.22	0.17	3.18
(1,942)	1:79:A:ASP:H	1:75:A:LEU:O	20	3.13	0.12	3.13
(1,942)	1:79:B:ASP:H	1:75:B:LEU:O	20	3.13	0.12	3.13
(1,628)	1:66:A:LYS:HG2	1:67:A:LYS:HB2	20	3.1	0.23	3.1
(1,628)	1:66:B:LYS:HG2	1:67:B:LYS:HB2	20	3.1	0.23	3.1
(1,176)	1:75:B:LEU:HA	1:78:B:ALA:H	20	3.07	0.11	3.08
(1,176)	1:75:A:LEU:HA	1:78:A:ALA:H	20	3.07	0.11	3.08
(1,627)	1:66:B:LYS:HG2	1:67:B:LYS:HG2	20	3.05	0.61	3.16
(1,627)	1:66:A:LYS:HG2	1:67:A:LYS:HG2	20	3.05	0.61	3.16
(1,783)	1:64:A:ALA:HB1	1:67:A:LYS:H	20	2.94	0.23	3.01
(1,783)	1:64:A:ALA:HB3	1:67:A:LYS:H	20	2.94	0.23	3.01
(1,783)	1:64:B:ALA:HB1	1:67:B:LYS:H	20	2.94	0.23	3.01
(1,783)	1:64:B:ALA:HB2	1:67:B:LYS:H	20	2.94	0.23	3.01
(1,783)	1:64:A:ALA:HB2	1:67:A:LYS:H	20	2.94	0.23	3.01
(1,943)	1:79:A:ASP:N	1:75:A:LEU:O	20	2.93	0.12	2.92
(1,943)	1:79:B:ASP:N	1:75:B:LEU:O	20	2.93	0.12	2.92
(1,761)	1:86:B:LYS:HD3	1:84:B:THR:H	20	2.93	0.3	2.82
(1,761)	1:86:A:LYS:HD3	1:84:A:THR:H	20	2.93	0.3	2.82
(1,649)	1:71:A:ARG:HG2	1:75:A:LEU:HD13	20	2.9	0.45	2.7
(1,649)	1:71:B:ARG:HG2	1:75:B:LEU:HD11	20	2.9	0.45	2.7
(1,649)	1:71:B:ARG:HG2	1:75:B:LEU:HD13	20	2.9	0.45	2.7
(1,649)	1:71:A:ARG:HG2	1:75:A:LEU:HD11	20	2.9	0.45	2.7
(1,649)	1:71:B:ARG:HG2	1:75:B:LEU:HD12	20	2.9	0.45	2.7
(1,649)	1:71:A:ARG:HG2	1:75:A:LEU:HD12	20	2.9	0.45	2.7
(1,833)	1:87:B:HIS:HD2	1:92:A:GLN:H	20	2.88	0.5	3.0
(1,833)	1:87:A:HIS:HD2	1:92:A:GLN:H	20	2.88	0.5	3.0
(1,833)	1:87:B:HIS:HD2	1:92:B:GLN:H	20	2.88	0.5	3.0
(1,833)	1:87:A:HIS:HD1	1:92:A:GLN:H	20	2.88	0.5	3.0
(1,833)	1:87:B:HIS:HD1	1:92:B:GLN:H	20	2.88	0.5	3.0
(1,833)	1:87:B:HIS:HD1	1:92:A:GLN:H	20	2.88	0.5	3.0
(1,938)	1:76:B:GLU:N	1:72:B:HIS:O	20	2.87	0.39	2.78
(1,938)	1:76:A:GLU:N	1:72:A:HIS:O	20	2.87	0.39	2.78
(1,680)	1:66:B:LYS:HG2	1:67:B:LYS:HG3	20	2.73	0.44	2.94
(1,680)	1:66:A:LYS:HG2	1:67:A:LYS:HG3	20	2.73	0.44	2.94
(1,817)	1:60:B:LEU:HD23	1:88:A:LEU:HB2	20	2.68	0.61	2.76
(1,817)	1:60:B:LEU:HD13	1:88:A:LEU:HB2	20	2.68	0.61	2.76
(1,817)	1:60:A:LEU:HD11	1:88:B:LEU:HB2	20	2.68	0.61	2.76
(1,817)	1:60:B:LEU:HD11	1:88:A:LEU:HB2	20	2.68	0.61	2.76
(1,817)	1:60:B:LEU:HD21	1:88:A:LEU:HB2	20	2.68	0.61	2.76
(1,817)	1:60:B:LEU:HD12	1:88:A:LEU:HB2	20	2.68	0.61	2.76
(1,817)	1:60:B:LEU:HD22	1:88:A:LEU:HB2	20	2.68	0.61	2.76
(1,267)	1:86:A:LYS:H	1:61:A:ILE:HG13	20	2.67	0.16	2.66

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,267)	1:86:B:LYS:H	1:61:B:ILE:HG13	20	2.67	0.16	2.66
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD23	20	2.65	0.79	3.01
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD13	20	2.65	0.79	3.01
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD21	20	2.65	0.79	3.01
(1,815)	1:85:B:VAL:HA	1:60:A:LEU:HD11	20	2.65	0.79	3.01
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD22	20	2.65	0.79	3.01
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD11	20	2.65	0.79	3.01
(1,404)	1:64:A:ALA:HA	1:67:A:LYS:H	20	2.6	0.21	2.59
(1,404)	1:64:B:ALA:HA	1:67:B:LYS:H	20	2.6	0.21	2.59
(1,41)	1:67:A:LYS:HG3	1:69:A:SER:H	20	2.6	0.21	2.65
(1,41)	1:67:B:LYS:HG3	1:69:B:SER:H	20	2.6	0.21	2.65
(1,774)	1:86:A:LYS:HD3	1:88:A:LEU:H	20	2.56	0.38	2.51
(1,774)	1:86:B:LYS:HD3	1:88:B:LEU:H	20	2.56	0.38	2.51
(1,816)	1:60:B:LEU:HD23	1:86:A:LYS:H	20	2.45	0.84	2.88
(1,816)	1:60:B:LEU:HD13	1:86:A:LYS:H	20	2.45	0.84	2.88
(1,816)	1:60:B:LEU:HD21	1:86:A:LYS:H	20	2.45	0.84	2.88
(1,816)	1:60:A:LEU:HD11	1:86:B:LYS:H	20	2.45	0.84	2.88
(1,816)	1:60:B:LEU:HD22	1:86:A:LYS:H	20	2.45	0.84	2.88
(1,816)	1:60:B:LEU:HD11	1:86:A:LYS:H	20	2.45	0.84	2.88
(1,259)	1:56:B:GLN:HG3	1:82:A:GLU:H	20	2.44	0.2	2.38
(1,259)	1:56:A:GLN:HG3	1:82:B:GLU:H	20	2.44	0.2	2.38
(1,858)	1:93:B:ARG:HB3	1:95:B:GLN:HB2	20	2.42	0.45	2.48
(1,858)	1:93:A:ARG:HB3	1:95:A:GLN:HB2	20	2.42	0.45	2.48
(1,858)	1:93:B:ARG:HB3	1:95:B:GLN:HB3	20	2.42	0.45	2.48
(1,647)	1:90:B:ASN:HB2	1:65:B:LEU:HD11	20	2.41	0.43	2.46
(1,647)	1:90:B:ASN:HB2	1:65:B:LEU:HD13	20	2.41	0.43	2.46
(1,647)	1:90:A:ASN:HB2	1:65:A:LEU:HD11	20	2.41	0.43	2.46
(1,647)	1:90:B:ASN:HB2	1:65:B:LEU:HD12	20	2.41	0.43	2.46
(1,850)	1:90:B:ASN:HD21	1:83:B:MET:HG3	20	2.39	0.22	2.45
(1,850)	1:90:A:ASN:HD22	1:83:A:MET:HG3	20	2.39	0.22	2.45
(1,850)	1:90:B:ASN:HD22	1:83:B:MET:HG3	20	2.39	0.22	2.45
(1,850)	1:90:A:ASN:HD21	1:83:A:MET:HG3	20	2.39	0.22	2.45
(1,850)	1:90:A:ASN:HD21	1:83:A:MET:HG2	20	2.39	0.22	2.45
(1,769)	1:50:B:ILE:HG23	1:79:A:ASP:H	20	2.39	0.13	2.4
(1,769)	1:50:B:ILE:HG21	1:79:A:ASP:H	20	2.39	0.13	2.4
(1,769)	1:50:B:ILE:HG22	1:79:A:ASP:H	20	2.39	0.13	2.4
(1,769)	1:50:A:ILE:HG21	1:79:B:ASP:H	20	2.39	0.13	2.4
(1,394)	1:67:A:LYS:H	1:69:A:SER:H	20	2.38	0.18	2.42
(1,394)	1:67:B:LYS:H	1:69:B:SER:H	20	2.38	0.18	2.42
(1,583)	1:76:B:GLU:HB2	1:77:B:LYS:HG2	20	2.37	0.12	2.38
(1,583)	1:76:A:GLU:HB2	1:77:A:LYS:HG2	20	2.37	0.12	2.38
(1,358)	1:67:A:LYS:HA	1:69:A:SER:H	20	2.36	0.11	2.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,358)	1:67:B:LYS:HA	1:69:B:SER:H	20	2.36	0.11	2.36
(1,746)	1:87:B:HIS:HD1	1:92:B:GLN:H	20	2.34	0.58	2.48
(1,746)	1:87:A:HIS:HD1	1:92:B:GLN:H	20	2.34	0.58	2.48
(1,746)	1:87:B:HIS:HD1	1:92:A:GLN:H	20	2.34	0.58	2.48
(1,746)	1:87:A:HIS:HD1	1:92:A:GLN:H	20	2.34	0.58	2.48
(1,789)	1:66:A:LYS:HA	1:69:A:SER:HG	20	2.28	1.08	2.09
(1,789)	1:66:B:LYS:HA	1:69:B:SER:HG	20	2.28	1.08	2.09
(1,747)	1:87:B:HIS:HD2	1:92:A:GLN:H	20	2.27	0.37	2.26
(1,747)	1:87:A:HIS:HD2	1:92:A:GLN:H	20	2.27	0.37	2.26
(1,747)	1:87:B:HIS:HD2	1:92:B:GLN:H	20	2.27	0.37	2.26
(1,747)	1:87:A:HIS:HD2	1:92:B:GLN:H	20	2.27	0.37	2.26
(1,370)	1:66:A:LYS:HA	1:69:A:SER:H	20	2.26	0.25	2.32
(1,370)	1:66:B:LYS:HA	1:69:B:SER:H	20	2.26	0.25	2.32
(1,844)	1:89:B:ARG:HB2	1:90:B:ASN:HD22	20	2.2	0.15	2.2
(1,844)	1:89:A:ARG:HB2	1:90:A:ASN:HD22	20	2.2	0.15	2.2
(1,431)	1:71:B:ARG:HG2	1:75:B:LEU:HA	20	2.19	0.33	2.22
(1,431)	1:71:A:ARG:HG2	1:75:A:LEU:HA	20	2.19	0.33	2.22
(1,832)	1:87:A:HIS:HD1	1:91:A:LEU:HA	20	2.18	0.33	2.24
(1,832)	1:87:A:HIS:HD2	1:91:A:LEU:HA	20	2.18	0.33	2.24
(1,832)	1:87:B:HIS:HD2	1:91:B:LEU:HA	20	2.18	0.33	2.24
(1,832)	1:87:B:HIS:HD1	1:91:B:LEU:HA	20	2.18	0.33	2.24
(1,65)	1:56:B:GLN:HG2	1:82:A:GLU:H	20	2.16	0.21	2.15
(1,65)	1:56:A:GLN:HG2	1:82:B:GLU:H	20	2.16	0.21	2.15
(1,857)	1:93:B:ARG:HB2	1:95:B:GLN:HB2	20	2.11	0.58	2.11
(1,857)	1:93:A:ARG:HB2	1:95:A:GLN:HB2	20	2.11	0.58	2.11
(1,857)	1:93:B:ARG:HB2	1:95:B:GLN:HB3	20	2.11	0.58	2.11
(1,857)	1:93:A:ARG:HB2	1:95:A:GLN:HB3	20	2.11	0.58	2.11
(1,569)	1:87:B:HIS:HA	1:92:A:GLN:HE21	20	2.11	0.41	2.04
(1,569)	1:87:A:HIS:HA	1:92:B:GLN:HE21	20	2.11	0.41	2.04
(1,450)	1:56:B:GLN:HG3	1:84:A:THR:HB	20	2.1	0.12	2.15
(1,450)	1:56:A:GLN:HG3	1:84:B:THR:HB	20	2.1	0.12	2.15
(1,764)	1:86:A:LYS:HG2	1:90:A:ASN:H	20	2.07	0.13	2.07
(1,764)	1:86:B:LYS:HG2	1:90:B:ASN:H	20	2.07	0.13	2.07
(1,803)	1:57:B:LEU:HD22	1:83:B:MET:H	20	2.07	0.12	2.11
(1,803)	1:57:B:LEU:HD21	1:83:B:MET:H	20	2.07	0.12	2.11
(1,803)	1:57:B:LEU:HD13	1:83:B:MET:H	20	2.07	0.12	2.11
(1,803)	1:57:A:LEU:HD11	1:83:A:MET:H	20	2.07	0.12	2.11
(1,803)	1:57:B:LEU:HD23	1:83:B:MET:H	20	2.07	0.12	2.11
(1,803)	1:57:B:LEU:HD11	1:83:B:MET:H	20	2.07	0.12	2.11
(1,437)	1:90:A:ASN:HA	1:92:A:GLN:HG2	20	2.05	0.11	2.01
(1,437)	1:90:B:ASN:HA	1:92:B:GLN:HG2	20	2.05	0.11	2.01
(1,437)	1:90:B:ASN:HA	1:92:B:GLN:HG3	20	2.05	0.11	2.01

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,437)	1:90:A:ASN:HA	1:92:A:GLN:HG3	20	2.05	0.11	2.01
(1,843)	1:89:B:ARG:H	1:90:B:ASN:HD21	20	2.03	0.1	2.02
(1,843)	1:89:A:ARG:H	1:90:A:ASN:HD21	20	2.03	0.1	2.02
(1,669)	1:88:A:LEU:HB3	1:91:A:LEU:HG	20	1.95	0.4	2.06
(1,669)	1:88:B:LEU:HB3	1:91:B:LEU:HG	20	1.95	0.4	2.06
(1,669)	1:88:A:LEU:HB3	1:91:B:LEU:HG	20	1.95	0.4	2.06
(1,270)	1:79:A:ASP:H	1:54:A:LEU:HD21	20	1.83	0.25	1.83
(1,270)	1:79:B:ASP:H	1:54:B:LEU:HD22	20	1.83	0.25	1.83
(1,270)	1:79:B:ASP:H	1:54:B:LEU:HD21	20	1.83	0.25	1.83
(1,270)	1:79:B:ASP:H	1:54:B:LEU:HD23	20	1.83	0.25	1.83
(1,731)	1:86:A:LYS:HD3	1:87:A:HIS:HA	20	1.76	0.56	1.52
(1,731)	1:86:B:LYS:HD3	1:87:B:HIS:HA	20	1.76	0.56	1.52
(1,69)	1:83:B:MET:H	1:80:B:ILE:HG22	20	1.71	0.07	1.69
(1,69)	1:83:A:MET:H	1:80:A:ILE:HG21	20	1.71	0.07	1.69
(1,69)	1:83:A:MET:H	1:80:A:ILE:HG23	20	1.71	0.07	1.69
(1,69)	1:83:B:MET:H	1:80:B:ILE:HG21	20	1.71	0.07	1.69
(1,69)	1:83:B:MET:H	1:80:B:ILE:HG23	20	1.71	0.07	1.69
(1,69)	1:83:A:MET:H	1:80:A:ILE:HG22	20	1.71	0.07	1.69
(1,458)	1:76:B:GLU:HB3	1:80:B:ILE:HB	20	1.65	0.14	1.66
(1,458)	1:76:A:GLU:HB3	1:80:A:ILE:HB	20	1.65	0.14	1.66
(1,558)	1:81:A:LEU:HA	1:83:A:MET:HE3	20	1.56	0.79	1.86
(1,558)	1:81:B:LEU:HA	1:83:B:MET:HE2	20	1.56	0.79	1.86
(1,558)	1:81:B:LEU:HA	1:83:B:MET:HE3	20	1.56	0.79	1.86
(1,558)	1:81:A:LEU:HA	1:83:A:MET:HE2	20	1.56	0.79	1.86
(1,558)	1:81:A:LEU:HA	1:83:A:MET:HE1	20	1.56	0.79	1.86
(1,558)	1:81:B:LEU:HA	1:83:B:MET:HE1	20	1.56	0.79	1.86
(1,760)	1:86:B:LYS:HG2	1:87:B:HIS:H	20	1.53	0.19	1.58
(1,760)	1:86:A:LYS:HG2	1:87:A:HIS:H	20	1.53	0.19	1.58
(1,824)	1:86:B:LYS:HG3	1:87:B:HIS:HB2	20	1.48	0.18	1.48
(1,824)	1:86:A:LYS:HG3	1:87:A:HIS:HB2	20	1.48	0.18	1.48
(1,824)	1:86:B:LYS:HG3	1:87:B:HIS:HB3	20	1.48	0.18	1.48
(1,487)	1:88:A:LEU:HA	1:91:A:LEU:HA	20	1.42	0.21	1.48
(1,487)	1:88:B:LEU:HA	1:91:B:LEU:HA	20	1.42	0.21	1.48
(1,700)	1:87:A:HIS:HD1	1:91:A:LEU:HA	20	1.41	0.78	1.21
(1,700)	1:87:B:HIS:HD1	1:91:B:LEU:HA	20	1.41	0.78	1.21
(1,609)	1:92:A:GLN:HB3	1:93:A:ARG:HB2	20	1.38	0.2	1.45
(1,609)	1:92:B:GLN:HB3	1:93:B:ARG:HB2	20	1.38	0.2	1.45
(1,609)	1:92:A:GLN:HB2	1:93:A:ARG:HB2	20	1.38	0.2	1.45
(1,609)	1:92:B:GLN:HB2	1:93:B:ARG:HB2	20	1.38	0.2	1.45
(1,467)	1:68:B:ASP:HA	1:71:B:ARG:HD2	20	1.36	0.23	1.45
(1,467)	1:68:B:ASP:HA	1:71:B:ARG:HD3	20	1.36	0.23	1.45
(1,467)	1:68:A:ASP:HA	1:71:A:ARG:HD2	20	1.36	0.23	1.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,520)	1:68:B:ASP:H	1:69:B:SER:HB2	20	1.32	0.32	1.26
(1,520)	1:68:A:ASP:H	1:69:A:SER:HB2	20	1.32	0.32	1.26
(1,520)	1:68:B:ASP:H	1:69:B:SER:HB3	20	1.32	0.32	1.26
(1,520)	1:68:A:ASP:H	1:69:A:SER:HB3	20	1.32	0.32	1.26
(1,676)	1:88:A:LEU:HB2	1:89:A:ARG:HB2	20	1.32	0.19	1.34
(1,676)	1:88:B:LEU:HB2	1:89:B:ARG:HB2	20	1.32	0.19	1.34
(1,483)	1:76:B:GLU:HA	1:80:B:ILE:HB	20	1.28	0.15	1.32
(1,483)	1:76:A:GLU:HA	1:80:A:ILE:HB	20	1.28	0.15	1.32
(1,324)	1:83:B:MET:H	1:84:B:THR:HG23	20	1.26	0.18	1.34
(1,324)	1:83:A:MET:H	1:84:A:THR:HG22	20	1.26	0.18	1.34
(1,324)	1:83:A:MET:H	1:84:A:THR:HG23	20	1.26	0.18	1.34
(1,324)	1:83:B:MET:H	1:84:B:THR:HG22	20	1.26	0.18	1.34
(1,324)	1:83:B:MET:H	1:84:B:THR:HG21	20	1.26	0.18	1.34
(1,324)	1:83:A:MET:H	1:84:A:THR:HG21	20	1.26	0.18	1.34
(1,35)	1:66:B:LYS:HG2	1:67:B:LYS:H	20	1.24	0.21	1.27
(1,35)	1:66:A:LYS:HG2	1:67:A:LYS:H	20	1.24	0.21	1.27
(1,277)	1:54:A:LEU:HD21	1:80:A:ILE:H	20	1.23	0.25	1.22
(1,277)	1:54:B:LEU:HD22	1:80:B:ILE:H	20	1.23	0.25	1.22
(1,277)	1:54:B:LEU:HD21	1:80:B:ILE:H	20	1.23	0.25	1.22
(1,277)	1:54:B:LEU:HD23	1:80:B:ILE:H	20	1.23	0.25	1.22
(1,673)	1:56:B:GLN:HG2	1:82:A:GLU:HB2	20	1.19	0.27	1.14
(1,673)	1:56:A:GLN:HG2	1:82:B:GLU:HB2	20	1.19	0.27	1.14
(1,846)	1:90:A:ASN:HA	1:90:A:ASN:HD21	20	1.15	0.02	1.15
(1,846)	1:90:B:ASN:HA	1:90:B:ASN:HD21	20	1.15	0.02	1.15
(1,552)	1:93:A:ARG:HB3	1:94:A:ALA:HA	20	1.14	0.07	1.15
(1,552)	1:93:B:ARG:HB3	1:94:B:ALA:HA	20	1.14	0.07	1.15
(1,96)	1:90:B:ASN:HB2	1:92:B:GLN:H	20	1.12	0.08	1.14
(1,96)	1:90:A:ASN:HB2	1:92:A:GLN:H	20	1.12	0.08	1.14
(1,782)	1:64:A:ALA:HB1	1:66:A:LYS:H	20	1.1	0.06	1.1
(1,782)	1:64:A:ALA:HB3	1:66:A:LYS:H	20	1.1	0.06	1.1
(1,782)	1:64:B:ALA:HB1	1:66:B:LYS:H	20	1.1	0.06	1.1
(1,782)	1:64:B:ALA:HB2	1:66:B:LYS:H	20	1.1	0.06	1.1
(1,782)	1:64:A:ALA:HB2	1:66:A:LYS:H	20	1.1	0.06	1.1
(1,782)	1:64:B:ALA:HB3	1:66:B:LYS:H	20	1.1	0.06	1.1
(1,743)	1:61:A:ILE:HD11	1:62:A:LEU:H	20	1.1	0.04	1.1
(1,743)	1:61:B:ILE:HD12	1:62:B:LEU:H	20	1.1	0.04	1.1
(1,743)	1:61:A:ILE:HD13	1:62:A:LEU:H	20	1.1	0.04	1.1
(1,743)	1:61:B:ILE:HD13	1:62:B:LEU:H	20	1.1	0.04	1.1
(1,743)	1:61:A:ILE:HD12	1:62:A:LEU:H	20	1.1	0.04	1.1
(1,743)	1:61:B:ILE:HD11	1:62:B:LEU:H	20	1.1	0.04	1.1
(1,754)	1:86:A:LYS:HD3	1:87:A:HIS:H	20	1.09	0.29	1.0
(1,754)	1:86:B:LYS:HD3	1:87:B:HIS:H	20	1.09	0.29	1.0

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,268)	1:86:A:LYS:H	1:84:A:THR:HG21	20	1.05	0.17	1.01
(1,268)	1:86:A:LYS:H	1:84:A:THR:HG23	20	1.05	0.17	1.01
(1,268)	1:86:B:LYS:H	1:84:B:THR:HG21	20	1.05	0.17	1.01
(1,268)	1:86:B:LYS:H	1:84:B:THR:HG23	20	1.05	0.17	1.01
(1,268)	1:86:B:LYS:H	1:84:B:THR:HG22	20	1.05	0.17	1.01
(1,268)	1:86:A:LYS:H	1:84:A:THR:HG22	20	1.05	0.17	1.01
(1,181)	1:83:B:MET:H	1:84:B:THR:HG23	20	1.04	0.18	1.12
(1,181)	1:83:A:MET:H	1:84:A:THR:HG22	20	1.04	0.18	1.12
(1,181)	1:83:A:MET:H	1:84:A:THR:HG23	20	1.04	0.18	1.12
(1,181)	1:83:B:MET:H	1:84:B:THR:HG22	20	1.04	0.18	1.12
(1,181)	1:83:B:MET:H	1:84:B:THR:HG21	20	1.04	0.18	1.12
(1,181)	1:83:A:MET:H	1:84:A:THR:HG21	20	1.04	0.18	1.12
(1,322)	1:90:A:ASN:H	1:92:A:GLN:HG2	20	1.01	0.2	1.0
(1,322)	1:90:B:ASN:H	1:92:B:GLN:HG2	20	1.01	0.2	1.0
(1,322)	1:90:B:ASN:H	1:92:B:GLN:HG3	20	1.01	0.2	1.0
(1,322)	1:90:A:ASN:H	1:92:A:GLN:HG3	20	1.01	0.2	1.0
(1,598)	1:66:B:LYS:HB2	1:67:B:LYS:HG2	20	0.98	0.25	1.06
(1,598)	1:66:A:LYS:HB2	1:67:A:LYS:HG2	20	0.98	0.25	1.06
(1,886)	1:76:A:GLU:HG2	1:80:A:ILE:HD12	20	0.93	0.13	0.96
(1,886)	1:76:B:GLU:HG2	1:80:B:ILE:HD13	20	0.93	0.13	0.96
(1,886)	1:76:B:GLU:HG2	1:80:B:ILE:HD11	20	0.93	0.13	0.96
(1,886)	1:76:A:GLU:HG2	1:80:A:ILE:HD11	20	0.93	0.13	0.96
(1,886)	1:76:A:GLU:HG2	1:80:A:ILE:HD13	20	0.93	0.13	0.96
(1,886)	1:76:A:GLU:HG3	1:80:A:ILE:HD12	20	0.93	0.13	0.96
(1,886)	1:76:B:GLU:HG3	1:80:B:ILE:HD11	20	0.93	0.13	0.96
(1,886)	1:76:B:GLU:HG3	1:80:B:ILE:HD13	20	0.93	0.13	0.96
(1,886)	1:76:A:GLU:HG3	1:80:A:ILE:HD13	20	0.93	0.13	0.96
(1,274)	1:86:B:LYS:HG2	1:89:B:ARG:H	20	0.91	0.13	0.88
(1,274)	1:86:A:LYS:HG2	1:89:A:ARG:H	20	0.91	0.13	0.88
(1,788)	1:65:A:LEU:HG	1:66:A:LYS:H	20	0.91	0.48	1.15
(1,788)	1:65:B:LEU:HG	1:66:B:LYS:H	20	0.91	0.48	1.15
(1,275)	1:86:B:LYS:HG2	1:88:B:LEU:H	20	0.9	0.13	0.93
(1,275)	1:86:A:LYS:HG2	1:88:A:LEU:H	20	0.9	0.13	0.93
(1,52)	1:71:B:ARG:HB3	1:72:B:HIS:H	20	0.88	0.24	0.99
(1,52)	1:71:B:ARG:HB2	1:72:B:HIS:H	20	0.88	0.24	0.99
(1,52)	1:71:A:ARG:HB3	1:72:A:HIS:H	20	0.88	0.24	0.99
(1,52)	1:71:A:ARG:HB2	1:72:A:HIS:H	20	0.88	0.24	0.99
(1,50)	1:68:B:ASP:HA	1:71:B:ARG:H	20	0.86	0.14	0.86
(1,50)	1:68:A:ASP:HA	1:71:A:ARG:H	20	0.86	0.14	0.86
(1,484)	1:91:A:LEU:HA	1:93:A:ARG:HA	20	0.84	0.15	0.84
(1,484)	1:91:B:LEU:HA	1:93:B:ARG:HA	20	0.84	0.15	0.84
(1,652)	1:85:A:VAL:HG13	1:86:A:LYS:HB2	20	0.82	0.1	0.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,652)	1:85:B:VAL:HG11	1:86:B:LYS:HB2	20	0.82	0.1	0.82
(1,652)	1:85:B:VAL:HG13	1:86:B:LYS:HB2	20	0.82	0.1	0.82
(1,652)	1:85:A:VAL:HG11	1:86:A:LYS:HB2	20	0.82	0.1	0.82
(1,652)	1:85:A:VAL:HG12	1:86:A:LYS:HB2	20	0.82	0.1	0.82
(1,652)	1:85:A:VAL:HG11	1:86:A:LYS:HB3	20	0.82	0.1	0.82
(1,652)	1:85:B:VAL:HG12	1:86:B:LYS:HB2	20	0.82	0.1	0.82
(1,652)	1:85:A:VAL:HG13	1:86:A:LYS:HB3	20	0.82	0.1	0.82
(1,652)	1:85:A:VAL:HG12	1:86:A:LYS:HB3	20	0.82	0.1	0.82
(1,414)	1:88:A:LEU:HA	1:89:A:ARG:HB2	20	0.8	0.11	0.78
(1,414)	1:88:B:LEU:HA	1:89:B:ARG:HB2	20	0.8	0.11	0.78
(1,363)	1:68:A:ASP:HA	1:72:A:HIS:H	20	0.79	0.08	0.81
(1,363)	1:68:B:ASP:HA	1:72:B:HIS:H	20	0.79	0.08	0.81
(1,379)	1:65:B:LEU:HD22	1:66:B:LYS:H	20	0.77	0.45	1.0
(1,379)	1:65:A:LEU:HD23	1:66:A:LYS:H	20	0.77	0.45	1.0
(1,379)	1:65:B:LEU:HD23	1:66:B:LYS:H	20	0.77	0.45	1.0
(1,379)	1:65:B:LEU:HD21	1:66:B:LYS:H	20	0.77	0.45	1.0
(1,379)	1:65:A:LEU:HD22	1:66:A:LYS:H	20	0.77	0.45	1.0
(1,299)	1:82:B:GLU:HB3	1:84:B:THR:H	20	0.76	0.07	0.74
(1,299)	1:82:A:GLU:HB3	1:84:A:THR:H	20	0.76	0.07	0.74
(1,106)	1:92:A:GLN:HG2	1:93:A:ARG:H	20	0.76	0.06	0.76
(1,106)	1:92:B:GLN:HG2	1:93:B:ARG:H	20	0.76	0.06	0.76
(1,888)	1:77:A:LYS:HE2	1:81:A:LEU:HD23	20	0.72	0.15	0.74
(1,888)	1:77:A:LYS:HE2	1:81:A:LEU:HD12	20	0.72	0.15	0.74
(1,888)	1:77:A:LYS:HE2	1:81:A:LEU:HD22	20	0.72	0.15	0.74
(1,888)	1:77:A:LYS:HE2	1:81:A:LEU:HD11	20	0.72	0.15	0.74
(1,888)	1:77:A:LYS:HE3	1:81:A:LEU:HD13	20	0.72	0.15	0.74
(1,888)	1:77:B:LYS:HE2	1:81:B:LEU:HD11	20	0.72	0.15	0.74
(1,888)	1:77:A:LYS:HE3	1:81:A:LEU:HD23	20	0.72	0.15	0.74
(1,888)	1:77:B:LYS:HE2	1:81:B:LEU:HD21	20	0.72	0.15	0.74
(1,888)	1:77:A:LYS:HE3	1:81:A:LEU:HD11	20	0.72	0.15	0.74
(1,888)	1:77:B:LYS:HE2	1:81:B:LEU:HD12	20	0.72	0.15	0.74
(1,888)	1:77:B:LYS:HE2	1:81:B:LEU:HD22	20	0.72	0.15	0.74
(1,888)	1:77:A:LYS:HE2	1:81:A:LEU:HD21	20	0.72	0.15	0.74
(1,888)	1:77:B:LYS:HE3	1:81:B:LEU:HD11	20	0.72	0.15	0.74
(1,888)	1:77:B:LYS:HE3	1:81:B:LEU:HD12	20	0.72	0.15	0.74
(1,316)	1:90:A:ASN:H	1:91:A:LEU:HG	20	0.72	0.11	0.72
(1,316)	1:90:B:ASN:H	1:91:B:LEU:HG	20	0.72	0.11	0.72
(1,900)	1:81:B:LEU:HD23	1:83:B:MET:H	20	0.68	0.07	0.67
(1,900)	1:81:A:LEU:HD11	1:83:A:MET:H	20	0.68	0.07	0.67
(1,900)	1:81:B:LEU:HD13	1:83:B:MET:H	20	0.68	0.07	0.67
(1,900)	1:81:A:LEU:HD13	1:83:A:MET:H	20	0.68	0.07	0.67
(1,900)	1:81:A:LEU:HD12	1:83:A:MET:H	20	0.68	0.07	0.67

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,900)	1:81:B:LEU:HD22	1:83:B:MET:H	20	0.68	0.07	0.67
(1,900)	1:81:A:LEU:HD22	1:83:A:MET:H	20	0.68	0.07	0.67
(1,900)	1:81:A:LEU:HD23	1:83:A:MET:H	20	0.68	0.07	0.67
(1,900)	1:81:A:LEU:HD21	1:83:A:MET:H	20	0.68	0.07	0.67
(1,900)	1:81:B:LEU:HD12	1:83:B:MET:H	20	0.68	0.07	0.67
(1,900)	1:81:B:LEU:HD21	1:83:B:MET:H	20	0.68	0.07	0.67
(1,736)	1:84:B:THR:HB	1:85:B:VAL:HG13	20	0.66	0.13	0.7
(1,736)	1:84:A:THR:HB	1:85:A:VAL:HG11	20	0.66	0.13	0.7
(1,736)	1:84:B:THR:HB	1:85:B:VAL:HG11	20	0.66	0.13	0.7
(1,736)	1:84:A:THR:HB	1:85:A:VAL:HG13	20	0.66	0.13	0.7
(1,736)	1:84:B:THR:HB	1:85:B:VAL:HG12	20	0.66	0.13	0.7
(1,738)	1:76:B:GLU:HA	1:79:B:ASP:HB2	20	0.65	0.14	0.64
(1,738)	1:76:A:GLU:HA	1:79:A:ASP:HB2	20	0.65	0.14	0.64
(1,325)	1:85:B:VAL:H	1:85:B:VAL:HG13	20	0.63	0.03	0.64
(1,325)	1:85:A:VAL:H	1:85:A:VAL:HG13	20	0.63	0.03	0.64
(1,325)	1:85:B:VAL:H	1:85:B:VAL:HG11	20	0.63	0.03	0.64
(1,325)	1:85:A:VAL:H	1:85:A:VAL:HG12	20	0.63	0.03	0.64
(1,325)	1:85:A:VAL:H	1:85:A:VAL:HG11	20	0.63	0.03	0.64
(1,325)	1:85:B:VAL:H	1:85:B:VAL:HG12	20	0.63	0.03	0.64
(1,189)	1:75:B:LEU:HA	1:79:B:ASP:H	20	0.62	0.16	0.64
(1,189)	1:75:A:LEU:HA	1:79:A:ASP:H	20	0.62	0.16	0.64
(1,12)	1:61:A:ILE:HA	1:62:A:LEU:H	20	0.59	0.02	0.6
(1,12)	1:61:B:ILE:HA	1:62:B:LEU:H	20	0.59	0.02	0.6
(1,421)	1:79:B:ASP:HB3	1:80:B:ILE:HB	20	0.59	0.31	0.48
(1,421)	1:79:A:ASP:HB3	1:80:A:ILE:HB	20	0.59	0.31	0.48
(1,798)	1:77:B:LYS:HB3	1:81:B:LEU:H	20	0.58	0.09	0.58
(1,798)	1:77:A:LYS:HB3	1:81:A:LEU:H	20	0.58	0.09	0.58
(1,711)	1:71:B:ARG:HA	1:71:B:ARG:HG2	20	0.56	0.21	0.7
(1,711)	1:71:A:ARG:HA	1:71:A:ARG:HG2	20	0.56	0.21	0.7
(1,845)	1:90:B:ASN:H	1:90:B:ASN:HD21	20	0.54	0.07	0.55
(1,845)	1:90:A:ASN:H	1:90:A:ASN:HD21	20	0.54	0.07	0.55
(1,864)	1:71:A:ARG:HA	1:75:A:LEU:HD12	20	0.53	0.16	0.55
(1,864)	1:71:A:ARG:HA	1:75:A:LEU:HD11	20	0.53	0.16	0.55
(1,864)	1:71:B:ARG:HA	1:75:B:LEU:HD13	20	0.53	0.16	0.55
(1,864)	1:71:B:ARG:HA	1:75:B:LEU:HD21	20	0.53	0.16	0.55
(1,864)	1:71:B:ARG:HA	1:75:B:LEU:HD22	20	0.53	0.16	0.55
(1,864)	1:71:A:ARG:HA	1:75:A:LEU:HD13	20	0.53	0.16	0.55
(1,864)	1:71:A:ARG:HA	1:75:A:LEU:HD23	20	0.53	0.16	0.55
(1,864)	1:71:A:ARG:HA	1:75:A:LEU:HD21	20	0.53	0.16	0.55
(1,864)	1:71:B:ARG:HA	1:75:B:LEU:HD23	20	0.53	0.16	0.55
(1,667)	1:90:B:ASN:HB2	1:91:B:LEU:HD12	20	0.51	0.13	0.53
(1,667)	1:90:B:ASN:HB2	1:91:B:LEU:HD13	20	0.51	0.13	0.53

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,667)	1:90:A:ASN:HB2	1:91:A:LEU:HD13	20	0.51	0.13	0.53
(1,667)	1:90:A:ASN:HB2	1:91:A:LEU:HD12	20	0.51	0.13	0.53
(1,667)	1:90:B:ASN:HB2	1:91:B:LEU:HD11	20	0.51	0.13	0.53
(1,667)	1:90:A:ASN:HB2	1:91:A:LEU:HD11	20	0.51	0.13	0.53
(1,877)	1:75:A:LEU:HD21	1:79:A:ASP:HA	20	0.49	0.16	0.46
(1,877)	1:75:A:LEU:HD11	1:79:A:ASP:HA	20	0.49	0.16	0.46
(1,877)	1:75:B:LEU:HD11	1:79:B:ASP:HA	20	0.49	0.16	0.46
(1,877)	1:75:B:LEU:HD21	1:79:B:ASP:HA	20	0.49	0.16	0.46
(1,877)	1:75:A:LEU:HD23	1:79:A:ASP:HA	20	0.49	0.16	0.46
(1,877)	1:75:B:LEU:HD23	1:79:B:ASP:HA	20	0.49	0.16	0.46
(1,877)	1:75:B:LEU:HD22	1:79:B:ASP:HA	20	0.49	0.16	0.46
(1,877)	1:75:A:LEU:HD22	1:79:A:ASP:HA	20	0.49	0.16	0.46
(1,877)	1:75:A:LEU:HD13	1:79:A:ASP:HA	20	0.49	0.16	0.46
(1,242)	1:88:A:LEU:H	1:89:A:ARG:HB2	20	0.49	0.1	0.49
(1,242)	1:88:B:LEU:H	1:89:B:ARG:HB2	20	0.49	0.1	0.49
(1,756)	1:84:A:THR:HG21	1:85:A:VAL:H	20	0.46	0.15	0.44
(1,756)	1:84:B:THR:HG22	1:85:B:VAL:H	20	0.46	0.15	0.44
(1,756)	1:84:B:THR:HG21	1:85:B:VAL:H	20	0.46	0.15	0.44
(1,756)	1:84:A:THR:HG23	1:85:A:VAL:H	20	0.46	0.15	0.44
(1,756)	1:84:A:THR:HG22	1:85:A:VAL:H	20	0.46	0.15	0.44
(1,756)	1:84:B:THR:HG23	1:85:B:VAL:H	20	0.46	0.15	0.44
(1,756)	1:84:B:THR:HG22	1:85:A:VAL:H	20	0.46	0.15	0.44
(1,756)	1:84:A:THR:HG22	1:85:B:VAL:H	20	0.46	0.15	0.44
(1,566)	1:56:B:GLN:HG2	1:82:A:GLU:HA	20	0.43	0.2	0.45
(1,566)	1:56:A:GLN:HG2	1:82:B:GLU:HA	20	0.43	0.2	0.45
(1,770)	1:80:B:ILE:HG22	1:83:B:MET:H	20	0.43	0.07	0.42
(1,770)	1:80:A:ILE:HG21	1:83:A:MET:H	20	0.43	0.07	0.42
(1,770)	1:80:A:ILE:HG23	1:83:A:MET:H	20	0.43	0.07	0.42
(1,770)	1:80:B:ILE:HG21	1:83:B:MET:H	20	0.43	0.07	0.42
(1,770)	1:80:B:ILE:HG23	1:83:B:MET:H	20	0.43	0.07	0.42
(1,770)	1:80:A:ILE:HG22	1:83:A:MET:H	20	0.43	0.07	0.42
(1,39)	1:68:A:ASP:H	1:69:A:SER:H	20	0.42	0.07	0.43
(1,39)	1:68:B:ASP:H	1:69:B:SER:H	20	0.42	0.07	0.43
(1,482)	1:81:A:LEU:HA	1:84:A:THR:HB	20	0.4	0.3	0.32
(1,482)	1:81:B:LEU:HA	1:84:B:THR:HB	20	0.4	0.3	0.32
(1,796)	1:76:B:GLU:HB2	1:77:B:LYS:HB3	20	0.39	0.13	0.38
(1,796)	1:76:A:GLU:HB2	1:77:A:LYS:HB3	20	0.39	0.13	0.38
(1,461)	1:76:B:GLU:HB2	1:77:B:LYS:HA	20	0.39	0.07	0.41
(1,461)	1:76:A:GLU:HB2	1:77:A:LYS:HA	20	0.39	0.07	0.41
(1,155)	1:91:B:LEU:H	1:91:B:LEU:HD12	20	0.28	0.04	0.29
(1,155)	1:91:A:LEU:H	1:91:A:LEU:HD12	20	0.28	0.04	0.29
(1,155)	1:91:B:LEU:H	1:91:B:LEU:HD11	20	0.28	0.04	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,155)	1:91:A:LEU:H	1:91:A:LEU:HD11	20	0.28	0.04	0.29
(1,155)	1:91:A:LEU:H	1:91:A:LEU:HD13	20	0.28	0.04	0.29
(1,155)	1:91:B:LEU:H	1:91:B:LEU:HD13	20	0.28	0.04	0.29
(1,31)	1:66:B:LYS:H	1:66:B:LYS:HB2	20	0.26	0.06	0.26
(1,31)	1:66:A:LYS:H	1:66:A:LYS:HB2	20	0.26	0.06	0.26
(1,419)	1:75:B:LEU:HA	1:80:B:ILE:HD11	20	0.26	0.09	0.26
(1,419)	1:75:B:LEU:HA	1:80:B:ILE:HD13	20	0.26	0.09	0.26
(1,419)	1:75:A:LEU:HA	1:80:A:ILE:HD11	20	0.26	0.09	0.26
(1,419)	1:75:A:LEU:HA	1:80:A:ILE:HD12	20	0.26	0.09	0.26
(1,419)	1:75:A:LEU:HA	1:80:A:ILE:HD13	20	0.26	0.09	0.26
(1,419)	1:75:B:LEU:HA	1:80:B:ILE:HD12	20	0.26	0.09	0.26
(1,541)	1:77:B:LYS:HB3	1:79:B:ASP:H	20	0.23	0.07	0.26
(1,541)	1:77:A:LYS:HB3	1:79:A:ASP:H	20	0.23	0.07	0.26
(1,25)	1:63:A:ASP:HA	1:64:A:ALA:H	20	0.2	0.03	0.2
(1,25)	1:63:B:ASP:HA	1:64:B:ALA:H	20	0.2	0.03	0.2
(1,626)	1:83:A:MET:HE3	1:84:A:THR:HG23	19	2.56	1.46	2.88
(1,626)	1:83:A:MET:HE1	1:84:A:THR:HG22	19	2.56	1.46	2.88
(1,626)	1:83:A:MET:HE2	1:84:A:THR:HG23	19	2.56	1.46	2.88
(1,626)	1:83:A:MET:HE1	1:84:A:THR:HG21	19	2.56	1.46	2.88
(1,626)	1:83:A:MET:HE1	1:84:A:THR:HG23	19	2.56	1.46	2.88
(1,626)	1:83:B:MET:HE1	1:84:B:THR:HG22	19	2.56	1.46	2.88
(1,626)	1:83:B:MET:HE2	1:84:B:THR:HG21	19	2.56	1.46	2.88
(1,626)	1:83:B:MET:HE1	1:84:B:THR:HG23	19	2.56	1.46	2.88
(1,626)	1:83:B:MET:HE3	1:84:B:THR:HG21	19	2.56	1.46	2.88
(1,626)	1:83:B:MET:HE2	1:84:B:THR:HG23	19	2.56	1.46	2.88
(1,626)	1:83:A:MET:HE2	1:84:A:THR:HG22	19	2.56	1.46	2.88
(1,626)	1:83:B:MET:HE3	1:84:B:THR:HG23	19	2.56	1.46	2.88
(1,577)	1:68:A:ASP:HB3	1:72:A:HIS:HD2	19	1.99	0.22	2.02
(1,577)	1:68:B:ASP:HB2	1:72:B:HIS:HD1	19	1.99	0.22	2.02
(1,577)	1:68:B:ASP:HB3	1:72:B:HIS:HD1	19	1.99	0.22	2.02
(1,577)	1:68:B:ASP:HB3	1:72:B:HIS:HD2	19	1.99	0.22	2.02
(1,577)	1:68:A:ASP:HB2	1:72:A:HIS:HD1	19	1.99	0.22	2.02
(1,577)	1:68:A:ASP:HB3	1:72:A:HIS:HD1	19	1.99	0.22	2.02
(1,744)	1:66:B:LYS:HD3	1:67:B:LYS:H	19	1.72	0.73	2.23
(1,744)	1:66:A:LYS:HD3	1:67:A:LYS:H	19	1.72	0.73	2.23
(1,805)	1:57:B:LEU:HD13	1:86:A:LYS:H	19	1.2	0.14	1.17
(1,805)	1:57:B:LEU:HD11	1:86:A:LYS:H	19	1.2	0.14	1.17
(1,805)	1:57:B:LEU:HD12	1:86:A:LYS:H	19	1.2	0.14	1.17
(1,805)	1:57:A:LEU:HD11	1:86:B:LYS:H	19	1.2	0.14	1.17
(1,805)	1:57:B:LEU:HD21	1:86:A:LYS:H	19	1.2	0.14	1.17
(1,407)	1:93:B:ARG:HA	1:94:B:ALA:HB2	19	1.16	0.11	1.17
(1,407)	1:93:A:ARG:HA	1:94:A:ALA:HB3	19	1.16	0.11	1.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,407)	1:93:A:ARG:HA	1:94:A:ALA:HB2	19	1.16	0.11	1.17
(1,407)	1:93:A:ARG:HA	1:94:A:ALA:HB1	19	1.16	0.11	1.17
(1,407)	1:93:B:ARG:HA	1:94:B:ALA:HB1	19	1.16	0.11	1.17
(1,407)	1:93:B:ARG:HA	1:94:B:ALA:HB3	19	1.16	0.11	1.17
(1,745)	1:72:A:HIS:H	1:75:A:LEU:HD12	19	0.97	0.39	0.84
(1,745)	1:72:A:HIS:H	1:75:A:LEU:HD11	19	0.97	0.39	0.84
(1,745)	1:72:B:HIS:H	1:75:B:LEU:HD13	19	0.97	0.39	0.84
(1,745)	1:72:A:HIS:H	1:75:A:LEU:HD13	19	0.97	0.39	0.84
(1,745)	1:72:B:HIS:H	1:75:B:LEU:HD11	19	0.97	0.39	0.84
(1,745)	1:72:B:HIS:H	1:75:B:LEU:HD12	19	0.97	0.39	0.84
(1,488)	1:64:B:ALA:HA	1:65:B:LEU:HD13	19	0.97	0.86	0.69
(1,488)	1:64:B:ALA:HA	1:65:B:LEU:HD12	19	0.97	0.86	0.69
(1,488)	1:64:A:ALA:HA	1:65:A:LEU:HD13	19	0.97	0.86	0.69
(1,488)	1:64:A:ALA:HA	1:65:A:LEU:HD12	19	0.97	0.86	0.69
(1,488)	1:64:B:ALA:HA	1:65:B:LEU:HD11	19	0.97	0.86	0.69
(1,488)	1:64:A:ALA:HA	1:65:A:LEU:HD11	19	0.97	0.86	0.69
(1,709)	1:86:A:LYS:HA	1:86:A:LYS:HD3	19	0.86	0.28	0.7
(1,709)	1:86:B:LYS:HA	1:86:B:LYS:HD3	19	0.86	0.28	0.7
(1,934)	1:74:B:LYS:H	1:70:B:SER:O	19	0.81	0.4	0.79
(1,934)	1:74:A:LYS:H	1:70:A:SER:O	19	0.81	0.4	0.79
(1,894)	1:79:A:ASP:HB3	1:80:A:ILE:HD12	19	0.76	0.09	0.78
(1,894)	1:79:B:ASP:HB2	1:80:B:ILE:HD13	19	0.76	0.09	0.78
(1,894)	1:79:B:ASP:HB3	1:80:B:ILE:HD11	19	0.76	0.09	0.78
(1,894)	1:79:A:ASP:HB3	1:80:A:ILE:HD11	19	0.76	0.09	0.78
(1,894)	1:79:B:ASP:HB2	1:80:B:ILE:HD11	19	0.76	0.09	0.78
(1,894)	1:79:A:ASP:HB2	1:80:A:ILE:HD11	19	0.76	0.09	0.78
(1,894)	1:79:A:ASP:HB3	1:80:A:ILE:HD13	19	0.76	0.09	0.78
(1,894)	1:79:B:ASP:HB2	1:80:B:ILE:HD12	19	0.76	0.09	0.78
(1,894)	1:79:B:ASP:HB3	1:80:B:ILE:HD13	19	0.76	0.09	0.78
(1,768)	1:86:B:LYS:H	1:86:B:LYS:HD3	19	0.6	0.12	0.53
(1,768)	1:86:A:LYS:H	1:86:A:LYS:HD3	19	0.6	0.12	0.53
(1,740)	1:79:B:ASP:H	1:80:B:ILE:HD13	19	0.35	0.03	0.35
(1,740)	1:79:A:ASP:H	1:80:A:ILE:HD11	19	0.35	0.03	0.35
(1,740)	1:79:A:ASP:H	1:80:A:ILE:HD13	19	0.35	0.03	0.35
(1,740)	1:79:B:ASP:H	1:80:B:ILE:HD12	19	0.35	0.03	0.35
(1,740)	1:79:B:ASP:H	1:80:B:ILE:HD11	19	0.35	0.03	0.35
(1,740)	1:79:A:ASP:H	1:80:A:ILE:HD12	19	0.35	0.03	0.35
(1,930)	1:72:B:HIS:H	1:68:B:ASP:O	19	0.31	0.09	0.34
(1,930)	1:72:A:HIS:H	1:68:A:ASP:O	19	0.31	0.09	0.34
(1,540)	1:89:B:ARG:HB3	1:92:B:GLN:H	19	0.31	0.11	0.3
(1,540)	1:89:A:ARG:HB3	1:92:A:GLN:H	19	0.31	0.11	0.3
(1,540)	1:89:B:ARG:HB2	1:92:B:GLN:H	19	0.31	0.11	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,540)	1:89:A:ARG:HB2	1:92:A:GLN:H	19	0.31	0.11	0.3
(1,201)	1:85:B:VAL:HG21	1:86:B:LYS:H	19	0.3	0.04	0.31
(1,201)	1:85:A:VAL:HG22	1:86:A:LYS:H	19	0.3	0.04	0.31
(1,201)	1:85:B:VAL:HG23	1:86:B:LYS:H	19	0.3	0.04	0.31
(1,201)	1:85:B:VAL:HG22	1:86:B:LYS:H	19	0.3	0.04	0.31
(1,201)	1:85:A:VAL:HG23	1:86:A:LYS:H	19	0.3	0.04	0.31
(1,201)	1:85:A:VAL:HG21	1:86:A:LYS:H	19	0.3	0.04	0.31
(1,13)	1:88:B:LEU:H	1:89:B:ARG:HD2	19	0.29	0.09	0.3
(1,13)	1:88:A:LEU:H	1:89:A:ARG:HD2	19	0.29	0.09	0.3
(1,13)	1:88:A:LEU:H	1:89:A:ARG:HD3	19	0.29	0.09	0.3
(1,13)	1:88:B:LEU:H	1:89:B:ARG:HD3	19	0.29	0.09	0.3
(1,428)	1:86:A:LYS:HA	1:86:A:LYS:HD3	19	0.27	0.03	0.27
(1,428)	1:86:B:LYS:HA	1:86:B:LYS:HD2	19	0.27	0.03	0.27
(1,428)	1:86:A:LYS:HA	1:86:A:LYS:HD2	19	0.27	0.03	0.27
(1,428)	1:86:B:LYS:HA	1:86:B:LYS:HD3	19	0.27	0.03	0.27
(1,551)	1:67:A:LYS:HA	1:67:A:LYS:HE3	18	1.16	0.34	1.23
(1,551)	1:67:A:LYS:HA	1:67:A:LYS:HE2	18	1.16	0.34	1.23
(1,551)	1:67:B:LYS:HA	1:67:B:LYS:HE3	18	1.16	0.34	1.23
(1,551)	1:67:B:LYS:HA	1:67:B:LYS:HE2	18	1.16	0.34	1.23
(1,420)	1:87:B:HIS:HD2	1:91:B:LEU:HA	18	1.11	0.66	0.82
(1,420)	1:87:A:HIS:HD2	1:91:A:LEU:HA	18	1.11	0.66	0.82
(1,831)	1:87:A:HIS:HD1	1:91:A:LEU:H	18	0.58	0.28	0.57
(1,831)	1:87:A:HIS:HD2	1:91:A:LEU:H	18	0.58	0.28	0.57
(1,831)	1:87:B:HIS:HD2	1:91:B:LEU:H	18	0.58	0.28	0.57
(1,831)	1:87:B:HIS:HD1	1:91:B:LEU:H	18	0.58	0.28	0.57
(1,801)	1:54:B:LEU:HD23	1:81:B:LEU:HD23	18	0.51	0.18	0.55
(1,801)	1:54:B:LEU:HD21	1:81:B:LEU:HD11	18	0.51	0.18	0.55
(1,801)	1:54:A:LEU:HD21	1:81:A:LEU:HD13	18	0.51	0.18	0.55
(1,801)	1:54:B:LEU:HD22	1:81:B:LEU:HD12	18	0.51	0.18	0.55
(1,801)	1:54:B:LEU:HD23	1:81:B:LEU:HD13	18	0.51	0.18	0.55
(1,801)	1:54:B:LEU:HD22	1:81:B:LEU:HD13	18	0.51	0.18	0.55
(1,801)	1:54:B:LEU:HD21	1:81:B:LEU:HD22	18	0.51	0.18	0.55
(1,801)	1:54:A:LEU:HD21	1:81:A:LEU:HD21	18	0.51	0.18	0.55
(1,801)	1:54:B:LEU:HD22	1:81:B:LEU:HD22	18	0.51	0.18	0.55
(1,801)	1:54:B:LEU:HD23	1:81:B:LEU:HD11	18	0.51	0.18	0.55
(1,801)	1:54:B:LEU:HD22	1:81:B:LEU:HD23	18	0.51	0.18	0.55
(1,801)	1:54:A:LEU:HD21	1:81:A:LEU:HD22	18	0.51	0.18	0.55
(1,801)	1:54:A:LEU:HD21	1:81:A:LEU:HD23	18	0.51	0.18	0.55
(1,622)	1:82:A:GLU:HB2	1:85:A:VAL:HG11	18	0.46	0.12	0.48
(1,622)	1:82:A:GLU:HB2	1:85:A:VAL:HG13	18	0.46	0.12	0.48
(1,622)	1:82:B:GLU:HB2	1:85:B:VAL:HG13	18	0.46	0.12	0.48
(1,622)	1:82:B:GLU:HB2	1:85:B:VAL:HG12	18	0.46	0.12	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,622)	1:82:B:GLU:HB2	1:85:B:VAL:HG11	18	0.46	0.12	0.48
(1,622)	1:82:A:GLU:HB2	1:85:A:VAL:HG12	18	0.46	0.12	0.48
(1,416)	1:82:A:GLU:HA	1:85:A:VAL:HG11	18	0.31	0.09	0.31
(1,416)	1:82:A:GLU:HA	1:85:A:VAL:HG13	18	0.31	0.09	0.31
(1,416)	1:82:B:GLU:HA	1:85:B:VAL:HG13	18	0.31	0.09	0.31
(1,416)	1:82:B:GLU:HA	1:85:B:VAL:HG12	18	0.31	0.09	0.31
(1,416)	1:82:B:GLU:HA	1:85:B:VAL:HG11	18	0.31	0.09	0.31
(1,416)	1:82:A:GLU:HA	1:85:A:VAL:HG12	18	0.31	0.09	0.31
(1,763)	1:86:A:LYS:H	1:86:A:LYS:HD2	18	0.3	0.1	0.25
(1,763)	1:86:A:LYS:H	1:86:A:LYS:HD3	18	0.3	0.1	0.25
(1,763)	1:86:B:LYS:H	1:86:B:LYS:HD2	18	0.3	0.1	0.25
(1,903)	1:84:B:THR:H	1:87:B:HIS:HB3	18	0.3	0.12	0.34
(1,903)	1:84:A:THR:H	1:87:A:HIS:HB3	18	0.3	0.12	0.34
(1,903)	1:84:A:THR:H	1:87:A:HIS:HB2	18	0.3	0.12	0.34
(1,903)	1:84:B:THR:H	1:87:B:HIS:HB2	18	0.3	0.12	0.34
(1,936)	1:75:B:LEU:H	1:71:B:ARG:O	17	1.13	0.51	1.0
(1,936)	1:75:A:LEU:H	1:71:A:ARG:O	17	1.13	0.51	1.0
(1,276)	1:75:A:LEU:H	1:75:A:LEU:HD12	17	0.72	0.29	0.79
(1,276)	1:75:A:LEU:H	1:75:A:LEU:HD13	17	0.72	0.29	0.79
(1,276)	1:75:B:LEU:H	1:75:B:LEU:HD12	17	0.72	0.29	0.79
(1,276)	1:75:B:LEU:H	1:75:B:LEU:HD11	17	0.72	0.29	0.79
(1,276)	1:75:B:LEU:H	1:75:B:LEU:HD13	17	0.72	0.29	0.79
(1,881)	1:75:A:LEU:HD21	1:83:A:MET:H	17	0.51	0.15	0.51
(1,881)	1:75:A:LEU:HD11	1:83:A:MET:H	17	0.51	0.15	0.51
(1,881)	1:75:B:LEU:HD11	1:83:B:MET:H	17	0.51	0.15	0.51
(1,881)	1:75:A:LEU:HD22	1:83:A:MET:H	17	0.51	0.15	0.51
(1,881)	1:75:B:LEU:HD13	1:83:B:MET:H	17	0.51	0.15	0.51
(1,881)	1:75:A:LEU:HD12	1:83:A:MET:H	17	0.51	0.15	0.51
(1,881)	1:75:B:LEU:HD23	1:83:B:MET:H	17	0.51	0.15	0.51
(1,881)	1:75:B:LEU:HD21	1:83:B:MET:H	17	0.51	0.15	0.51
(1,881)	1:75:B:LEU:HD12	1:83:B:MET:H	17	0.51	0.15	0.51
(1,881)	1:75:A:LEU:HD23	1:83:A:MET:H	17	0.51	0.15	0.51
(1,881)	1:75:B:LEU:HD22	1:83:B:MET:H	17	0.51	0.15	0.51
(1,329)	1:92:A:GLN:H	1:92:A:GLN:HE21	17	0.38	0.2	0.31
(1,329)	1:92:B:GLN:H	1:92:B:GLN:HE21	17	0.38	0.2	0.31
(1,188)	1:76:B:GLU:HA	1:79:B:ASP:H	17	0.22	0.08	0.22
(1,188)	1:76:A:GLU:HA	1:79:A:ASP:H	17	0.22	0.08	0.22
(1,165)	1:93:B:ARG:HB2	1:94:B:ALA:H	17	0.2	0.05	0.21
(1,165)	1:93:B:ARG:HB3	1:94:B:ALA:H	17	0.2	0.05	0.21
(1,165)	1:93:A:ARG:HB2	1:94:A:ALA:H	17	0.2	0.05	0.21
(1,165)	1:93:A:ARG:HB3	1:94:A:ALA:H	17	0.2	0.05	0.21
(1,765)	1:84:B:THR:H	1:84:B:THR:HG23	16	0.45	0.07	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,765)	1:84:A:THR:H	1:84:A:THR:HG22	16	0.45	0.07	0.44
(1,765)	1:84:A:THR:H	1:84:A:THR:HG23	16	0.45	0.07	0.44
(1,765)	1:84:B:THR:H	1:84:B:THR:HG22	16	0.45	0.07	0.44
(1,765)	1:84:B:THR:H	1:84:B:THR:HG21	16	0.45	0.07	0.44
(1,765)	1:84:A:THR:H	1:84:A:THR:HG21	16	0.45	0.07	0.44
(1,867)	1:72:A:HIS:H	1:75:A:LEU:HD12	16	0.41	0.21	0.34
(1,867)	1:72:A:HIS:H	1:75:A:LEU:HD21	16	0.41	0.21	0.34
(1,867)	1:72:B:HIS:H	1:75:B:LEU:HD23	16	0.41	0.21	0.34
(1,867)	1:72:B:HIS:H	1:75:B:LEU:HD22	16	0.41	0.21	0.34
(1,867)	1:72:A:HIS:H	1:75:A:LEU:HD22	16	0.41	0.21	0.34
(1,867)	1:72:A:HIS:H	1:75:A:LEU:HD11	16	0.41	0.21	0.34
(1,867)	1:72:A:HIS:H	1:75:A:LEU:HD13	16	0.41	0.21	0.34
(1,867)	1:72:B:HIS:H	1:75:B:LEU:HD12	16	0.41	0.21	0.34
(1,867)	1:72:A:HIS:H	1:75:A:LEU:HD23	16	0.41	0.21	0.34
(1,867)	1:72:B:HIS:H	1:75:B:LEU:HD13	16	0.41	0.21	0.34
(1,759)	1:84:B:THR:H	1:84:B:THR:HG23	16	0.35	0.07	0.34
(1,759)	1:84:A:THR:H	1:84:A:THR:HG22	16	0.35	0.07	0.34
(1,759)	1:84:A:THR:H	1:84:A:THR:HG23	16	0.35	0.07	0.34
(1,759)	1:84:B:THR:H	1:84:B:THR:HG22	16	0.35	0.07	0.34
(1,759)	1:84:B:THR:H	1:84:B:THR:HG21	16	0.35	0.07	0.34
(1,759)	1:84:A:THR:H	1:84:A:THR:HG21	16	0.35	0.07	0.34
(1,87)	1:88:A:LEU:HB2	1:90:A:ASN:H	16	0.26	0.08	0.27
(1,87)	1:88:B:LEU:HB2	1:90:B:ASN:H	16	0.26	0.08	0.27
(1,637)	1:85:A:VAL:HG13	1:86:A:LYS:HG2	16	0.26	0.04	0.26
(1,637)	1:85:B:VAL:HG13	1:86:B:LYS:HG2	16	0.26	0.04	0.26
(1,637)	1:85:A:VAL:HG11	1:86:A:LYS:HG2	16	0.26	0.04	0.26
(1,637)	1:85:B:VAL:HG11	1:86:B:LYS:HG2	16	0.26	0.04	0.26
(1,637)	1:85:A:VAL:HG12	1:86:A:LYS:HG2	16	0.26	0.04	0.26
(1,637)	1:85:B:VAL:HG12	1:86:B:LYS:HG2	16	0.26	0.04	0.26
(1,486)	1:93:A:ARG:HA	1:94:A:ALA:HA	16	0.21	0.06	0.22
(1,486)	1:93:B:ARG:HA	1:94:B:ALA:HA	16	0.21	0.06	0.22
(1,901)	1:83:A:MET:H	1:83:A:MET:HG2	16	0.16	0.05	0.15
(1,901)	1:83:A:MET:H	1:83:A:MET:HG3	16	0.16	0.05	0.15
(1,901)	1:83:B:MET:H	1:83:B:MET:HG3	16	0.16	0.05	0.15
(1,757)	1:80:B:ILE:H	1:80:B:ILE:HD13	16	0.16	0.03	0.15
(1,757)	1:80:A:ILE:H	1:80:A:ILE:HD11	16	0.16	0.03	0.15
(1,757)	1:80:A:ILE:H	1:80:A:ILE:HD13	16	0.16	0.03	0.15
(1,757)	1:80:B:ILE:H	1:80:B:ILE:HD12	16	0.16	0.03	0.15
(1,757)	1:80:B:ILE:H	1:80:B:ILE:HD11	16	0.16	0.03	0.15
(1,757)	1:80:A:ILE:H	1:80:A:ILE:HD12	16	0.16	0.03	0.15
(1,498)	1:65:A:LEU:HD23	1:67:A:LYS:H	15	0.51	0.25	0.44
(1,498)	1:65:B:LEU:HD23	1:67:B:LYS:H	15	0.51	0.25	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,498)	1:65:B:LEU:HD21	1:67:B:LYS:H	15	0.51	0.25	0.44
(1,498)	1:65:A:LEU:HD22	1:67:A:LYS:H	15	0.51	0.25	0.44
(1,498)	1:65:B:LEU:HD22	1:67:B:LYS:H	15	0.51	0.25	0.44
(1,498)	1:65:A:LEU:HD21	1:67:A:LYS:H	15	0.51	0.25	0.44
(1,499)	1:65:A:LEU:HA	1:67:A:LYS:H	15	0.47	0.17	0.51
(1,499)	1:65:B:LEU:HA	1:67:B:LYS:H	15	0.47	0.17	0.51
(1,806)	1:57:B:LEU:HD22	1:84:B:THR:H	15	0.3	0.1	0.27
(1,806)	1:57:B:LEU:HD21	1:84:B:THR:H	15	0.3	0.1	0.27
(1,806)	1:57:B:LEU:HD13	1:84:B:THR:H	15	0.3	0.1	0.27
(1,806)	1:57:A:LEU:HD11	1:84:A:THR:H	15	0.3	0.1	0.27
(1,806)	1:57:B:LEU:HD23	1:84:B:THR:H	15	0.3	0.1	0.27
(1,206)	1:93:A:ARG:HG3	1:95:A:GLN:HE21	15	0.29	0.04	0.28
(1,206)	1:93:B:ARG:HG3	1:95:B:GLN:HE21	15	0.29	0.04	0.28
(1,206)	1:93:A:ARG:HG2	1:95:A:GLN:HE21	15	0.29	0.04	0.28
(1,206)	1:93:B:ARG:HG2	1:95:B:GLN:HE21	15	0.29	0.04	0.28
(1,516)	1:67:A:LYS:HG2	1:68:A:ASP:H	15	0.26	0.07	0.27
(1,516)	1:67:B:LYS:HG2	1:68:B:ASP:H	15	0.26	0.07	0.27
(1,271)	1:76:B:GLU:H	1:80:B:ILE:HD11	15	0.24	0.07	0.24
(1,271)	1:76:B:GLU:H	1:80:B:ILE:HD13	15	0.24	0.07	0.24
(1,271)	1:76:A:GLU:H	1:80:A:ILE:HD11	15	0.24	0.07	0.24
(1,271)	1:76:A:GLU:H	1:80:A:ILE:HD13	15	0.24	0.07	0.24
(1,271)	1:76:B:GLU:H	1:80:B:ILE:HD12	15	0.24	0.07	0.24
(1,101)	1:91:A:LEU:HA	1:92:A:GLN:H	15	0.13	0.02	0.13
(1,101)	1:91:B:LEU:HA	1:92:B:GLN:H	15	0.13	0.02	0.13
(1,215)	1:92:B:GLN:HB3	1:92:B:GLN:HE22	15	0.13	0.02	0.12
(1,215)	1:92:A:GLN:HB3	1:92:A:GLN:HE22	15	0.13	0.02	0.12
(1,674)	1:88:A:LEU:HB2	1:91:A:LEU:HG	14	0.95	0.36	0.96
(1,674)	1:88:B:LEU:HB2	1:91:B:LEU:HG	14	0.95	0.36	0.96
(1,674)	1:88:B:LEU:HB2	1:91:A:LEU:HG	14	0.95	0.36	0.96
(1,781)	1:64:A:ALA:HB1	1:65:A:LEU:HD21	13	1.83	0.41	1.88
(1,781)	1:64:A:ALA:HB3	1:65:A:LEU:HD21	13	1.83	0.41	1.88
(1,781)	1:64:A:ALA:HB3	1:65:A:LEU:HD22	13	1.83	0.41	1.88
(1,781)	1:64:A:ALA:HB2	1:65:A:LEU:HD23	13	1.83	0.41	1.88
(1,781)	1:64:A:ALA:HB1	1:65:A:LEU:HD23	13	1.83	0.41	1.88
(1,781)	1:64:B:ALA:HB2	1:65:B:LEU:HD22	13	1.83	0.41	1.88
(1,781)	1:64:A:ALA:HB3	1:65:A:LEU:HD23	13	1.83	0.41	1.88
(1,781)	1:64:B:ALA:HB1	1:65:B:LEU:HD23	13	1.83	0.41	1.88
(1,781)	1:64:B:ALA:HB2	1:65:B:LEU:HD23	13	1.83	0.41	1.88
(1,496)	1:64:B:ALA:H	1:65:B:LEU:HD22	13	1.68	0.28	1.71
(1,496)	1:64:A:ALA:H	1:65:A:LEU:HD23	13	1.68	0.28	1.71
(1,496)	1:64:B:ALA:H	1:65:B:LEU:HD23	13	1.68	0.28	1.71
(1,496)	1:64:B:ALA:H	1:65:B:LEU:HD21	13	1.68	0.28	1.71

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,496)	1:64:A:ALA:H	1:65:A:LEU:HD22	13	1.68	0.28	1.71
(1,496)	1:64:A:ALA:H	1:65:A:LEU:HD21	13	1.68	0.28	1.71
(1,573)	1:64:A:ALA:HB1	1:65:A:LEU:HD21	13	1.61	0.65	1.31
(1,573)	1:64:B:ALA:HB1	1:65:B:LEU:HD21	13	1.61	0.65	1.31
(1,573)	1:64:A:ALA:HB1	1:65:A:LEU:HD22	13	1.61	0.65	1.31
(1,573)	1:64:B:ALA:HB1	1:65:B:LEU:HD22	13	1.61	0.65	1.31
(1,573)	1:64:A:ALA:HB1	1:65:A:LEU:HD23	13	1.61	0.65	1.31
(1,573)	1:64:B:ALA:HB1	1:65:B:LEU:HD23	13	1.61	0.65	1.31
(1,741)	1:50:B:ILE:HG21	1:51:B:ASN:HD22	13	0.34	0.15	0.33
(1,741)	1:50:B:ILE:HG23	1:51:B:ASN:HD22	13	0.34	0.15	0.33
(1,741)	1:50:B:ILE:HG22	1:51:B:ASN:HD22	13	0.34	0.15	0.33
(1,741)	1:50:A:ILE:HG21	1:51:A:ASN:HD22	13	0.34	0.15	0.33
(1,321)	1:87:B:HIS:HB2	1:88:B:LEU:H	13	0.22	0.05	0.22
(1,321)	1:87:A:HIS:HB2	1:88:A:LEU:H	13	0.22	0.05	0.22
(1,425)	1:93:A:ARG:HA	1:93:A:ARG:HG3	13	0.15	0.03	0.15
(1,425)	1:93:B:ARG:HA	1:93:B:ARG:HG3	13	0.15	0.03	0.15
(1,19)	1:62:B:LEU:HA	1:63:B:ASP:H	13	0.15	0.03	0.14
(1,19)	1:62:A:LEU:HA	1:63:A:ASP:H	13	0.15	0.03	0.14
(1,656)	1:82:A:GLU:HB2	1:86:A:LYS:HG2	13	0.13	0.02	0.13
(1,656)	1:82:B:GLU:HB2	1:86:B:LYS:HG2	13	0.13	0.02	0.13
(1,574)	1:64:B:ALA:HB2	1:65:B:LEU:HD23	12	1.81	0.7	1.48
(1,574)	1:64:A:ALA:HB2	1:65:A:LEU:HD21	12	1.81	0.7	1.48
(1,574)	1:64:A:ALA:HB2	1:65:A:LEU:HD23	12	1.81	0.7	1.48
(1,574)	1:64:B:ALA:HB2	1:65:B:LEU:HD22	12	1.81	0.7	1.48
(1,826)	1:87:B:HIS:H	1:87:B:HIS:HD1	12	1.24	0.05	1.24
(1,826)	1:87:A:HIS:H	1:87:A:HIS:HD2	12	1.24	0.05	1.24
(1,826)	1:87:A:HIS:H	1:87:A:HIS:HD1	12	1.24	0.05	1.24
(1,826)	1:87:B:HIS:H	1:87:B:HIS:HD2	12	1.24	0.05	1.24
(1,876)	1:75:A:LEU:HD21	1:79:A:ASP:H	12	0.34	0.14	0.34
(1,876)	1:75:A:LEU:HD11	1:79:A:ASP:H	12	0.34	0.14	0.34
(1,876)	1:75:A:LEU:HD23	1:79:A:ASP:H	12	0.34	0.14	0.34
(1,876)	1:75:A:LEU:HD22	1:79:A:ASP:H	12	0.34	0.14	0.34
(1,876)	1:75:B:LEU:HD22	1:79:B:ASP:H	12	0.34	0.14	0.34
(1,876)	1:75:A:LEU:HD12	1:79:A:ASP:H	12	0.34	0.14	0.34
(1,876)	1:75:A:LEU:HD13	1:79:A:ASP:H	12	0.34	0.14	0.34
(1,935)	1:74:A:LYS:N	1:70:A:SER:O	11	0.48	0.38	0.38
(1,935)	1:74:B:LYS:N	1:70:B:SER:O	11	0.48	0.38	0.38
(1,563)	1:56:B:GLN:HG3	1:82:A:GLU:HA	11	0.32	0.15	0.3
(1,563)	1:56:A:GLN:HG3	1:82:B:GLU:HA	11	0.32	0.15	0.3
(1,225)	1:92:B:GLN:HB3	1:92:B:GLN:HE21	11	0.27	0.14	0.37
(1,225)	1:92:A:GLN:HB3	1:92:A:GLN:HE21	11	0.27	0.14	0.37
(1,348)	1:71:A:ARG:H	1:71:A:ARG:HD3	11	0.26	0.12	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,348)	1:71:B:ARG:H	1:71:B:ARG:HD3	11	0.26	0.12	0.25
(1,348)	1:71:A:ARG:H	1:71:A:ARG:HD2	11	0.26	0.12	0.25
(1,112)	1:71:A:ARG:HD3	1:72:A:HIS:H	11	0.24	0.1	0.19
(1,112)	1:71:B:ARG:HD3	1:72:B:HIS:H	11	0.24	0.1	0.19
(1,284)	1:87:A:HIS:HD2	1:88:A:LEU:H	10	0.46	0.21	0.5
(1,284)	1:87:B:HIS:HD2	1:88:B:LEU:H	10	0.46	0.21	0.5
(1,895)	1:80:A:ILE:HA	1:81:A:LEU:HD21	10	0.29	0.11	0.3
(1,895)	1:80:A:ILE:HA	1:81:A:LEU:HD11	10	0.29	0.11	0.3
(1,895)	1:80:A:ILE:HA	1:81:A:LEU:HD12	10	0.29	0.11	0.3
(1,895)	1:80:A:ILE:HA	1:81:A:LEU:HD22	10	0.29	0.11	0.3
(1,895)	1:80:A:ILE:HA	1:81:A:LEU:HD23	10	0.29	0.11	0.3
(1,895)	1:80:B:ILE:HA	1:81:B:LEU:HD13	10	0.29	0.11	0.3
(1,895)	1:80:B:ILE:HA	1:81:B:LEU:HD23	10	0.29	0.11	0.3
(1,895)	1:80:B:ILE:HA	1:81:B:LEU:HD21	10	0.29	0.11	0.3
(1,914)	1:88:A:LEU:HD23	1:92:A:GLN:HB2	10	0.27	0.09	0.29
(1,914)	1:88:B:LEU:HD12	1:92:B:GLN:HB2	10	0.27	0.09	0.29
(1,914)	1:88:B:LEU:HD13	1:92:B:GLN:HB2	10	0.27	0.09	0.29
(1,914)	1:88:B:LEU:HD11	1:92:B:GLN:HB2	10	0.27	0.09	0.29
(1,914)	1:88:A:LEU:HD11	1:92:A:GLN:HB2	10	0.27	0.09	0.29
(1,914)	1:88:A:LEU:HD13	1:92:A:GLN:HB2	10	0.27	0.09	0.29
(1,70)	1:83:A:MET:HE3	1:84:A:THR:H	10	0.23	0.1	0.2
(1,70)	1:83:B:MET:HE2	1:84:B:THR:H	10	0.23	0.1	0.2
(1,70)	1:83:B:MET:HE3	1:84:B:THR:H	10	0.23	0.1	0.2
(1,70)	1:83:A:MET:HE1	1:84:A:THR:H	10	0.23	0.1	0.2
(1,70)	1:83:B:MET:HE1	1:84:B:THR:H	10	0.23	0.1	0.2
(1,871)	1:75:A:LEU:H	1:75:A:LEU:HD13	9	0.48	0.2	0.45
(1,871)	1:75:B:LEU:H	1:75:B:LEU:HD22	9	0.48	0.2	0.45
(1,871)	1:75:A:LEU:H	1:75:A:LEU:HD23	9	0.48	0.2	0.45
(1,871)	1:75:B:LEU:H	1:75:B:LEU:HD13	9	0.48	0.2	0.45
(1,871)	1:75:B:LEU:H	1:75:B:LEU:HD23	9	0.48	0.2	0.45
(1,871)	1:75:B:LEU:H	1:75:B:LEU:HD21	9	0.48	0.2	0.45
(1,871)	1:75:A:LEU:H	1:75:A:LEU:HD12	9	0.48	0.2	0.45
(1,879)	1:75:A:LEU:HD21	1:80:A:ILE:H	9	0.23	0.12	0.19
(1,879)	1:75:A:LEU:HD23	1:80:A:ILE:H	9	0.23	0.12	0.19
(1,879)	1:75:B:LEU:HD23	1:80:B:ILE:H	9	0.23	0.12	0.19
(1,879)	1:75:B:LEU:HD21	1:80:B:ILE:H	9	0.23	0.12	0.19
(1,879)	1:75:A:LEU:HD11	1:80:A:ILE:H	9	0.23	0.12	0.19
(1,879)	1:75:B:LEU:HD22	1:80:B:ILE:H	9	0.23	0.12	0.19
(1,879)	1:75:A:LEU:HD13	1:80:A:ILE:H	9	0.23	0.12	0.19
(1,879)	1:75:B:LEU:HD11	1:80:B:ILE:H	9	0.23	0.12	0.19
(1,910)	1:88:A:LEU:HD21	1:89:A:ARG:H	8	0.5	0.19	0.58
(1,910)	1:88:B:LEU:HD12	1:89:B:ARG:H	8	0.5	0.19	0.58

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,910)	1:88:A:LEU:HD12	1:89:A:ARG:H	8	0.5	0.19	0.58
(1,910)	1:88:B:LEU:HD13	1:89:B:ARG:H	8	0.5	0.19	0.58
(1,910)	1:88:B:LEU:HD23	1:89:B:ARG:H	8	0.5	0.19	0.58
(1,910)	1:88:B:LEU:HD21	1:89:B:ARG:H	8	0.5	0.19	0.58
(1,909)	1:88:A:LEU:H	1:88:A:LEU:HD12	8	0.38	0.05	0.4
(1,909)	1:88:B:LEU:H	1:88:B:LEU:HD23	8	0.38	0.05	0.4
(1,909)	1:88:B:LEU:H	1:88:B:LEU:HD22	8	0.38	0.05	0.4
(1,909)	1:88:A:LEU:H	1:88:A:LEU:HD23	8	0.38	0.05	0.4
(1,909)	1:88:A:LEU:H	1:88:A:LEU:HD22	8	0.38	0.05	0.4
(1,762)	1:87:B:HIS:HD1	1:88:B:LEU:H	8	0.38	0.27	0.27
(1,762)	1:87:A:HIS:HD1	1:88:A:LEU:H	8	0.38	0.27	0.27
(1,534)	1:74:A:LYS:HE3	1:75:A:LEU:H	8	0.17	0.05	0.17
(1,534)	1:74:B:LYS:HE2	1:75:B:LEU:H	8	0.17	0.05	0.17
(1,534)	1:74:B:LYS:HE3	1:75:B:LEU:H	8	0.17	0.05	0.17
(1,534)	1:74:A:LYS:HE2	1:75:A:LEU:H	8	0.17	0.05	0.17
(1,891)	1:79:A:ASP:H	1:81:A:LEU:HD13	7	0.4	0.18	0.45
(1,891)	1:79:A:ASP:H	1:81:A:LEU:HD11	7	0.4	0.18	0.45
(1,891)	1:79:B:ASP:H	1:81:B:LEU:HD13	7	0.4	0.18	0.45
(1,891)	1:79:B:ASP:H	1:81:B:LEU:HD11	7	0.4	0.18	0.45
(1,932)	1:73:A:SER:H	1:69:A:SER:O	7	0.39	0.25	0.23
(1,932)	1:73:B:SER:H	1:69:B:SER:O	7	0.39	0.25	0.23
(1,621)	1:82:B:GLU:HG3	1:85:B:VAL:HG12	7	0.38	0.15	0.32
(1,621)	1:82:A:GLU:HG3	1:85:A:VAL:HG12	7	0.38	0.15	0.32
(1,621)	1:82:B:GLU:HG3	1:85:B:VAL:HG11	7	0.38	0.15	0.32
(1,621)	1:82:A:GLU:HG3	1:85:A:VAL:HG11	7	0.38	0.15	0.32
(1,771)	1:83:B:MET:H	1:86:B:LYS:HD3	7	0.27	0.1	0.32
(1,771)	1:83:A:MET:H	1:86:A:LYS:HD3	7	0.27	0.1	0.32
(1,771)	1:83:A:MET:H	1:86:A:LYS:HD2	7	0.27	0.1	0.32
(1,865)	1:71:B:ARG:HD2	1:72:B:HIS:HB2	7	0.26	0.1	0.26
(1,865)	1:71:B:ARG:HD3	1:72:B:HIS:HB2	7	0.26	0.1	0.26
(1,865)	1:71:A:ARG:HD3	1:72:A:HIS:HB2	7	0.26	0.1	0.26
(1,865)	1:71:A:ARG:HD2	1:72:A:HIS:HB2	7	0.26	0.1	0.26
(1,162)	1:93:B:ARG:H	1:94:B:ALA:HB3	7	0.2	0.07	0.19
(1,162)	1:93:A:ARG:H	1:94:A:ALA:HB3	7	0.2	0.07	0.19
(1,162)	1:93:B:ARG:H	1:94:B:ALA:HB2	7	0.2	0.07	0.19
(1,162)	1:93:B:ARG:H	1:94:B:ALA:HB1	7	0.2	0.07	0.19
(1,162)	1:93:A:ARG:H	1:94:A:ALA:HB2	7	0.2	0.07	0.19
(1,466)	1:93:A:ARG:HA	1:93:A:ARG:HD3	7	0.13	0.04	0.12
(1,466)	1:93:A:ARG:HA	1:93:A:ARG:HD2	7	0.13	0.04	0.12
(1,466)	1:93:B:ARG:HA	1:93:B:ARG:HD3	7	0.13	0.04	0.12
(1,531)	1:87:B:HIS:H	1:88:B:LEU:HB2	6	0.51	0.47	0.3
(1,531)	1:87:A:HIS:H	1:88:A:LEU:HB2	6	0.51	0.47	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,580)	1:75:A:LEU:HB3	1:76:A:GLU:HB2	6	0.31	0.24	0.18
(1,580)	1:75:B:LEU:HB3	1:76:B:GLU:HB2	6	0.31	0.24	0.18
(1,896)	1:80:A:ILE:HB	1:81:A:LEU:HD21	6	0.26	0.06	0.28
(1,896)	1:80:B:ILE:HB	1:81:B:LEU:HD23	6	0.26	0.06	0.28
(1,896)	1:80:A:ILE:HB	1:81:A:LEU:HD23	6	0.26	0.06	0.28
(1,108)	1:93:A:ARG:HB2	1:95:A:GLN:H	6	0.24	0.16	0.15
(1,108)	1:93:B:ARG:HB2	1:95:B:GLN:H	6	0.24	0.16	0.15
(1,660)	1:74:B:LYS:HG3	1:76:B:GLU:HG3	6	0.2	0.02	0.21
(1,660)	1:74:A:LYS:HG3	1:76:A:GLU:HG3	6	0.2	0.02	0.21
(1,644)	1:86:B:LYS:HB3	1:86:B:LYS:HD3	6	0.2	0.04	0.21
(1,644)	1:86:A:LYS:HB3	1:86:A:LYS:HD3	6	0.2	0.04	0.21
(1,624)	1:84:B:THR:HG21	1:88:B:LEU:HB3	6	0.18	0.08	0.16
(1,624)	1:84:B:THR:HG23	1:88:B:LEU:HB3	6	0.18	0.08	0.16
(1,624)	1:84:B:THR:HG21	1:88:A:LEU:HB3	6	0.18	0.08	0.16
(1,624)	1:84:B:THR:HG22	1:88:B:LEU:HB3	6	0.18	0.08	0.16
(1,624)	1:84:A:THR:HG21	1:88:B:LEU:HB3	6	0.18	0.08	0.16
(1,624)	1:84:B:THR:HG23	1:88:A:LEU:HB3	6	0.18	0.08	0.16
(1,751)	1:73:B:SER:HB2	1:74:B:LYS:H	6	0.16	0.05	0.16
(1,751)	1:73:A:SER:HB2	1:74:A:LYS:H	6	0.16	0.05	0.16
(1,751)	1:73:A:SER:HB3	1:74:A:LYS:H	6	0.16	0.05	0.16
(1,751)	1:73:B:SER:HB3	1:74:B:LYS:H	6	0.16	0.05	0.16
(1,828)	1:87:A:HIS:HB3	1:87:A:HIS:HD2	6	0.15	0.02	0.16
(1,828)	1:87:B:HIS:HB3	1:87:B:HIS:HD1	6	0.15	0.02	0.16
(1,828)	1:87:B:HIS:HB3	1:87:B:HIS:HD2	6	0.15	0.02	0.16
(1,828)	1:87:A:HIS:HB2	1:87:A:HIS:HD1	6	0.15	0.02	0.16
(1,836)	1:87:B:HIS:HD1	1:92:A:GLN:HE21	5	0.72	0.55	0.64
(1,836)	1:87:B:HIS:HD2	1:92:A:GLN:HE21	5	0.72	0.55	0.64
(1,836)	1:87:A:HIS:HD1	1:92:B:GLN:HE21	5	0.72	0.55	0.64
(1,937)	1:75:B:LEU:N	1:71:B:ARG:O	5	0.49	0.24	0.46
(1,937)	1:75:A:LEU:N	1:71:A:ARG:O	5	0.49	0.24	0.46
(1,616)	1:86:A:LYS:HG2	1:86:A:LYS:HE2	5	0.3	0.02	0.3
(1,616)	1:86:B:LYS:HG2	1:86:B:LYS:HE2	5	0.3	0.02	0.3
(1,889)	1:78:A:ALA:H	1:81:A:LEU:HD13	5	0.3	0.14	0.3
(1,889)	1:78:B:ALA:H	1:81:B:LEU:HD13	5	0.3	0.14	0.3
(1,889)	1:78:B:ALA:H	1:81:B:LEU:HD11	5	0.3	0.14	0.3
(1,46)	1:73:B:SER:HB2	1:75:B:LEU:H	5	0.26	0.2	0.15
(1,46)	1:73:A:SER:HB3	1:75:A:LEU:H	5	0.26	0.2	0.15
(1,46)	1:73:A:SER:HB2	1:75:A:LEU:H	5	0.26	0.2	0.15
(1,81)	1:88:A:LEU:HB2	1:89:A:ARG:H	5	0.21	0.08	0.17
(1,81)	1:88:B:LEU:HB2	1:89:B:ARG:H	5	0.21	0.08	0.17
(1,588)	1:82:A:GLU:HB2	1:86:A:LYS:HE2	5	0.15	0.02	0.16
(1,588)	1:82:B:GLU:HB2	1:86:B:LYS:HE2	5	0.15	0.02	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,713)	1:87:B:HIS:HA	1:87:B:HIS:HD2	4	1.36	0.08	1.36
(1,713)	1:87:A:HIS:HA	1:87:A:HIS:HD2	4	1.36	0.08	1.36
(1,710)	1:87:A:HIS:HA	1:87:A:HIS:HD1	4	1.1	0.41	1.3
(1,710)	1:87:B:HIS:HA	1:87:B:HIS:HD1	4	1.1	0.41	1.3
(1,793)	1:69:A:SER:HG	1:70:A:SER:H	4	0.31	0.1	0.33
(1,793)	1:69:B:SER:HG	1:70:B:SER:H	4	0.31	0.1	0.33
(1,630)	1:75:B:LEU:HB2	1:80:B:ILE:HG13	4	0.26	0.16	0.2
(1,630)	1:75:A:LEU:HB2	1:80:A:ILE:HG12	4	0.26	0.16	0.2
(1,630)	1:75:B:LEU:HB2	1:80:B:ILE:HG12	4	0.26	0.16	0.2
(1,657)	1:82:B:GLU:HB2	1:86:B:LYS:HD2	4	0.24	0.02	0.24
(1,657)	1:82:A:GLU:HB2	1:86:A:LYS:HD2	4	0.24	0.02	0.24
(1,639)	1:57:B:LEU:HD22	1:84:B:THR:HG22	4	0.22	0.09	0.22
(1,639)	1:57:B:LEU:HD23	1:84:B:THR:HG22	4	0.22	0.09	0.22
(1,639)	1:57:B:LEU:HD21	1:84:B:THR:HG23	4	0.22	0.09	0.22
(1,931)	1:72:B:HIS:N	1:68:B:ASP:O	4	0.16	0.06	0.14
(1,931)	1:72:A:HIS:N	1:68:A:ASP:O	4	0.16	0.06	0.14
(1,523)	1:66:A:LYS:HB3	1:67:A:LYS:H	4	0.14	0.03	0.13
(1,523)	1:66:A:LYS:HB2	1:67:A:LYS:H	4	0.14	0.03	0.13
(1,582)	1:76:B:GLU:HB3	1:79:B:ASP:HB3	3	0.91	0.04	0.91
(1,582)	1:76:A:GLU:HB3	1:79:A:ASP:HB3	3	0.91	0.04	0.91
(1,705)	1:72:B:HIS:HA	1:75:B:LEU:HD13	3	0.63	0.16	0.53
(1,705)	1:72:A:HIS:HA	1:75:A:LEU:HD12	3	0.63	0.16	0.53
(1,933)	1:73:A:SER:N	1:69:A:SER:O	3	0.46	0.17	0.46
(1,920)	1:94:B:ALA:HB2	1:95:B:GLN:HG2	3	0.42	0.13	0.46
(1,920)	1:94:B:ALA:HB1	1:95:B:GLN:HG2	3	0.42	0.13	0.46
(1,663)	1:54:B:LEU:HD12	1:77:B:LYS:HE3	3	0.4	0.12	0.33
(1,663)	1:54:B:LEU:HD11	1:77:B:LYS:HE2	3	0.4	0.12	0.33
(1,663)	1:54:B:LEU:HD13	1:77:B:LYS:HE2	3	0.4	0.12	0.33
(1,619)	1:77:B:LYS:HG3	1:77:B:LYS:HE2	3	0.32	0.09	0.37
(1,619)	1:77:A:LYS:HG3	1:77:A:LYS:HE2	3	0.32	0.09	0.37
(1,683)	1:71:A:ARG:HD3	1:75:A:LEU:HD13	3	0.32	0.21	0.21
(1,683)	1:71:A:ARG:HD3	1:75:A:LEU:HD11	3	0.32	0.21	0.21
(1,456)	1:77:B:LYS:HA	1:77:B:LYS:HE2	3	0.24	0.08	0.28
(1,349)	1:86:B:LYS:H	1:89:B:ARG:HD3	3	0.24	0.08	0.29
(1,349)	1:86:A:LYS:H	1:89:A:ARG:HD3	3	0.24	0.08	0.29
(1,202)	1:86:B:LYS:H	1:86:B:LYS:HE2	3	0.19	0.03	0.19
(1,202)	1:86:B:LYS:H	1:86:B:LYS:HE3	3	0.19	0.03	0.19
(1,202)	1:86:A:LYS:H	1:86:A:LYS:HE2	3	0.19	0.03	0.19
(1,661)	1:74:A:LYS:HG3	1:76:A:GLU:HG2	3	0.16	0.02	0.18
(1,661)	1:74:B:LYS:HG2	1:76:B:GLU:HG2	3	0.16	0.02	0.18
(1,696)	1:89:A:ARG:HB2	1:90:A:ASN:HA	3	0.14	0.02	0.14
(1,696)	1:89:B:ARG:HB3	1:90:B:ASN:HA	3	0.14	0.02	0.14

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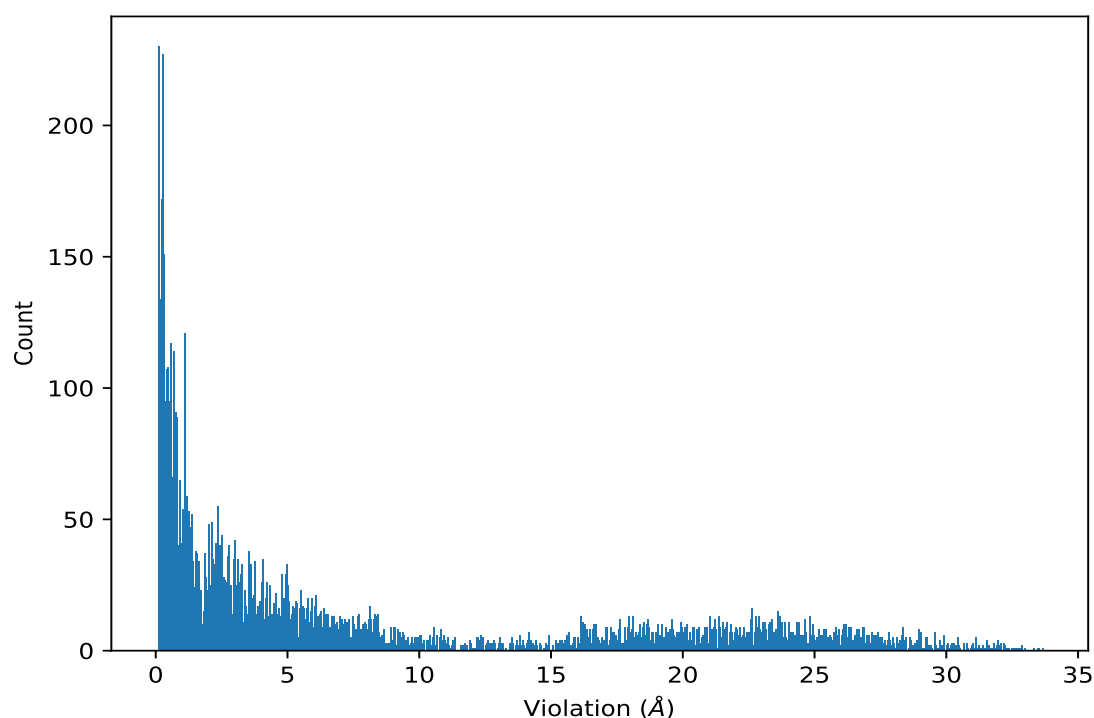
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,30)	1:85:B:VAL:H	1:88:B:LEU:HB2	2	1.01	0.71	1.01
(1,30)	1:85:A:VAL:H	1:88:A:LEU:HB2	2	1.01	0.71	1.01
(1,918)	1:88:A:LEU:HD12	1:92:A:GLN:HE22	2	0.36	0.12	0.36
(1,918)	1:88:B:LEU:HD21	1:92:B:GLN:HE22	2	0.36	0.12	0.36
(1,470)	1:71:A:ARG:HA	1:71:A:ARG:HD3	2	0.28	0.09	0.28
(1,470)	1:71:B:ARG:HA	1:71:B:ARG:HD3	2	0.28	0.09	0.28
(1,729)	1:65:B:LEU:HD13	1:87:B:HIS:HA	2	0.26	0.16	0.26
(1,729)	1:65:B:LEU:HD11	1:87:B:HIS:HA	2	0.26	0.16	0.26
(1,169)	1:94:B:ALA:HB1	1:95:B:GLN:H	2	0.24	0.03	0.24
(1,167)	1:91:A:LEU:HD22	1:94:A:ALA:H	2	0.22	0.02	0.22
(1,167)	1:91:B:LEU:HD21	1:94:B:ALA:H	2	0.22	0.02	0.22
(1,440)	1:89:A:ARG:HD2	1:92:A:GLN:HB2	2	0.21	0.01	0.21
(1,440)	1:89:B:ARG:HD2	1:92:B:GLN:HB2	2	0.21	0.01	0.21
(1,278)	1:65:B:LEU:HD13	1:90:B:ASN:HD21	2	0.2	0.08	0.2
(1,278)	1:65:B:LEU:HD11	1:90:B:ASN:HD21	2	0.2	0.08	0.2
(1,791)	1:69:B:SER:HA	1:69:B:SER:HG	2	0.2	0.05	0.2
(1,791)	1:69:A:SER:HA	1:69:A:SER:HG	2	0.2	0.05	0.2
(1,208)	1:86:A:LYS:HB3	1:90:A:ASN:HD21	2	0.18	0.01	0.18
(1,919)	1:94:B:ALA:H	1:95:B:GLN:HG3	2	0.17	0.04	0.17
(1,919)	1:94:A:ALA:H	1:95:A:GLN:HG2	2	0.17	0.04	0.17
(1,623)	1:41:B:ILE:HG13	1:44:B:LYS:HE2	2	0.16	0.05	0.16
(1,623)	1:41:B:ILE:HG13	1:44:B:LYS:HE3	2	0.16	0.05	0.16
(1,922)	1:95:B:GLN:HA	1:95:B:GLN:HG2	2	0.15	0.03	0.15

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



9.5.2 Table : All distance violations [i](#)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,410)	1:64:B:ALA:HA	1:40:A:PRO:HG3	8	33.68
(1,544)	1:64:A:ALA:HA	1:39:B:LYS:HE3	19	33.52
(1,410)	1:64:B:ALA:HA	1:40:A:PRO:HG3	19	33.45
(1,410)	1:64:A:ALA:HA	1:40:B:PRO:HG3	18	33.34
(1,410)	1:64:B:ALA:HA	1:40:A:PRO:HG3	17	32.99
(1,410)	1:64:A:ALA:HA	1:40:B:PRO:HG3	4	32.88
(1,410)	1:64:B:ALA:HA	1:40:A:PRO:HG3	9	32.85
(1,411)	1:64:B:ALA:HA	1:40:A:PRO:HG2	8	32.82
(1,544)	1:64:A:ALA:HA	1:39:B:LYS:HE3	8	32.76
(1,733)	1:64:B:ALA:HA	1:39:A:LYS:HD2	19	32.7
(1,544)	1:64:A:ALA:HA	1:39:B:LYS:HE2	3	32.66
(1,410)	1:64:A:ALA:HA	1:40:B:PRO:HG3	6	32.6
(1,411)	1:64:B:ALA:HA	1:40:A:PRO:HG2	19	32.56
(1,410)	1:64:B:ALA:HA	1:40:A:PRO:HG3	3	32.55
(1,410)	1:64:B:ALA:HA	1:40:A:PRO:HG3	15	32.47
(1,410)	1:64:B:ALA:HA	1:40:A:PRO:HG3	11	32.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,411)	1:64:B:ALA:HA	1:40:A:PRO:HG2	18	32.31
(1,410)	1:64:B:ALA:HA	1:40:A:PRO:HG3	14	32.25
(1,410)	1:64:A:ALA:HA	1:40:B:PRO:HG3	20	32.24
(1,411)	1:64:B:ALA:HA	1:40:A:PRO:HG2	12	32.23
(1,410)	1:64:A:ALA:HA	1:40:B:PRO:HG3	7	32.19
(1,410)	1:64:B:ALA:HA	1:40:A:PRO:HG3	5	32.16
(1,411)	1:64:A:ALA:HA	1:40:B:PRO:HG2	5	32.15
(1,733)	1:64:A:ALA:HA	1:39:B:LYS:HD3	8	32.09
(1,410)	1:64:A:ALA:HA	1:40:B:PRO:HG3	10	32.08
(1,544)	1:64:B:ALA:HA	1:39:A:LYS:HE2	9	32.06
(1,411)	1:64:B:ALA:HA	1:40:A:PRO:HG2	9	32.01
(1,733)	1:64:B:ALA:HA	1:39:A:LYS:HD2	9	32.0
(1,411)	1:64:A:ALA:HA	1:40:B:PRO:HG2	4	31.99
(1,733)	1:64:B:ALA:HA	1:39:A:LYS:HD2	3	31.97
(1,544)	1:64:A:ALA:HA	1:39:B:LYS:HE3	5	31.97
(1,410)	1:64:A:ALA:HA	1:40:B:PRO:HG3	16	31.96
(1,410)	1:64:A:ALA:HA	1:40:B:PRO:HG3	12	31.93
(1,733)	1:64:B:ALA:HA	1:39:A:LYS:HD2	18	31.92
(1,411)	1:64:B:ALA:HA	1:40:A:PRO:HG2	3	31.88
(1,544)	1:64:B:ALA:HA	1:39:A:LYS:HE2	13	31.84
(1,411)	1:64:B:ALA:HA	1:40:A:PRO:HG2	17	31.83
(1,544)	1:64:A:ALA:HA	1:39:B:LYS:HE3	2	31.8
(1,410)	1:64:B:ALA:HA	1:40:A:PRO:HG3	2	31.79
(1,411)	1:64:B:ALA:HA	1:40:A:PRO:HG2	6	31.73
(1,544)	1:64:B:ALA:HA	1:39:A:LYS:HE2	17	31.7
(1,411)	1:64:B:ALA:HA	1:40:A:PRO:HG2	16	31.65
(1,544)	1:64:A:ALA:HA	1:39:B:LYS:HE3	15	31.64
(1,411)	1:64:A:ALA:HA	1:40:B:PRO:HG2	11	31.54
(1,733)	1:64:A:ALA:HA	1:39:B:LYS:HD3	5	31.53
(1,410)	1:64:B:ALA:HA	1:40:A:PRO:HG3	1	31.5
(1,410)	1:64:B:ALA:HA	1:40:A:PRO:HG3	13	31.5
(1,780)	1:64:A:ALA:HB3	1:39:B:LYS:HE3	19	31.49
(1,411)	1:64:A:ALA:HA	1:40:B:PRO:HG2	10	31.45
(1,411)	1:64:A:ALA:HA	1:40:B:PRO:HG2	7	31.35
(1,411)	1:64:B:ALA:HA	1:40:A:PRO:HG2	15	31.35
(1,544)	1:64:A:ALA:HA	1:39:B:LYS:HE3	4	31.34
(1,411)	1:64:B:ALA:HA	1:40:A:PRO:HG2	2	31.27
(1,733)	1:64:A:ALA:HA	1:39:B:LYS:HD3	16	31.24
(1,411)	1:64:B:ALA:HA	1:40:A:PRO:HG2	14	31.22
(1,544)	1:64:B:ALA:HA	1:39:A:LYS:HE2	11	31.2
(1,544)	1:64:A:ALA:HA	1:39:B:LYS:HE3	16	31.15
(1,544)	1:64:A:ALA:HA	1:39:B:LYS:HE2	20	31.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,411)	1:64:A:ALA:HA	1:40:B:PRO:HG2	20	31.13
(1,733)	1:64:B:ALA:HA	1:39:A:LYS:HD2	17	31.1
(1,411)	1:64:B:ALA:HA	1:40:A:PRO:HG2	13	31.1
(1,733)	1:64:B:ALA:HA	1:39:A:LYS:HD2	12	31.07
(1,733)	1:64:B:ALA:HA	1:39:A:LYS:HD2	2	31.04
(1,733)	1:64:B:ALA:HA	1:39:A:LYS:HD2	13	31.02
(1,544)	1:64:B:ALA:HA	1:39:A:LYS:HE2	12	31.02
(1,780)	1:64:B:ALA:HB2	1:39:A:LYS:HE2	8	30.99
(1,733)	1:64:A:ALA:HA	1:39:B:LYS:HD2	4	30.99
(1,780)	1:64:A:ALA:HB3	1:39:B:LYS:HE2	3	30.94
(1,411)	1:64:B:ALA:HA	1:40:A:PRO:HG2	1	30.84
(1,733)	1:64:A:ALA:HA	1:39:B:LYS:HD3	11	30.79
(1,544)	1:64:B:ALA:HA	1:39:A:LYS:HE2	14	30.78
(1,732)	1:64:B:ALA:HA	1:39:A:LYS:HG2	19	30.77
(1,732)	1:64:A:ALA:HA	1:39:B:LYS:HG2	8	30.69
(1,526)	1:40:B:PRO:HG3	1:66:A:LYS:H	8	30.69
(1,733)	1:64:B:ALA:HA	1:39:A:LYS:HD2	15	30.66
(1,526)	1:40:A:PRO:HG3	1:66:B:LYS:H	19	30.5
(1,632)	1:66:B:LYS:HG2	1:41:A:ILE:HG13	13	30.47
(1,544)	1:64:A:ALA:HA	1:39:B:LYS:HE3	7	30.46
(1,632)	1:66:A:LYS:HG2	1:41:B:ILE:HG13	4	30.45
(1,632)	1:66:B:LYS:HG2	1:41:A:ILE:HG13	19	30.45
(1,733)	1:64:A:ALA:HA	1:39:B:LYS:HD2	7	30.44
(1,780)	1:64:B:ALA:HB3	1:39:A:LYS:HE2	13	30.41
(1,544)	1:64:A:ALA:HA	1:39:B:LYS:HE3	10	30.41
(1,732)	1:64:B:ALA:HA	1:39:A:LYS:HG2	18	30.38
(1,733)	1:64:A:ALA:HA	1:39:B:LYS:HD3	20	30.36
(1,526)	1:40:A:PRO:HG3	1:66:B:LYS:H	9	30.28
(1,733)	1:64:A:ALA:HA	1:39:B:LYS:HD2	10	30.27
(1,632)	1:66:A:LYS:HG2	1:41:B:ILE:HG13	12	30.27
(1,779)	1:64:A:ALA:HB3	1:39:B:LYS:HG2	8	30.23
(1,632)	1:66:A:LYS:HG2	1:41:B:ILE:HG13	8	30.23
(1,732)	1:64:B:ALA:HA	1:39:A:LYS:HG2	9	30.21
(1,632)	1:66:A:LYS:HG2	1:41:B:ILE:HG13	16	30.17
(1,544)	1:64:B:ALA:HA	1:39:A:LYS:HE2	1	30.16
(1,779)	1:64:B:ALA:HB3	1:39:A:LYS:HG2	19	30.15
(1,733)	1:64:B:ALA:HA	1:39:A:LYS:HD2	14	30.07
(1,544)	1:64:B:ALA:HA	1:39:A:LYS:HE2	18	30.07
(1,734)	1:64:B:ALA:HA	1:39:A:LYS:HG3	19	30.06
(1,780)	1:64:A:ALA:HB3	1:39:B:LYS:HE3	2	30.04
(1,604)	1:61:B:ILE:HD11	1:36:A:LYS:HE2	8	30.02
(1,780)	1:64:B:ALA:HB1	1:39:A:LYS:HE2	9	29.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,526)	1:40:B:PRO:HG3	1:66:A:LYS:H	4	29.94
(1,780)	1:64:A:ALA:HB1	1:39:B:LYS:HE2	5	29.93
(1,526)	1:40:A:PRO:HG3	1:66:B:LYS:H	18	29.93
(1,732)	1:64:A:ALA:HA	1:39:B:LYS:HG2	5	29.91
(1,632)	1:66:B:LYS:HG2	1:41:A:ILE:HG13	2	29.91
(1,780)	1:64:B:ALA:HB1	1:39:A:LYS:HE2	17	29.88
(1,733)	1:64:B:ALA:HA	1:39:A:LYS:HD2	1	29.86
(1,780)	1:64:A:ALA:HB2	1:39:B:LYS:HE3	15	29.84
(1,21)	1:64:A:ALA:H	1:39:B:LYS:HE3	19	29.8
(1,632)	1:66:B:LYS:HG2	1:41:A:ILE:HG13	7	29.77
(1,288)	1:40:B:PRO:HG2	1:66:A:LYS:H	8	29.76
(1,732)	1:64:B:ALA:HA	1:39:A:LYS:HG2	3	29.75
(1,632)	1:66:A:LYS:HG2	1:41:B:ILE:HG13	5	29.75
(1,786)	1:39:A:LYS:HE2	1:65:B:LEU:HG	19	29.71
(1,632)	1:66:A:LYS:HG2	1:41:B:ILE:HG13	3	29.66
(1,780)	1:64:A:ALA:HB3	1:39:B:LYS:HE3	4	29.63
(1,780)	1:64:A:ALA:HB1	1:39:B:LYS:HE3	16	29.61
(1,732)	1:64:B:ALA:HA	1:39:A:LYS:HG2	17	29.59
(1,632)	1:66:A:LYS:HG2	1:41:B:ILE:HG13	9	29.59
(1,526)	1:40:A:PRO:HG3	1:66:B:LYS:H	3	29.59
(1,632)	1:66:B:LYS:HG2	1:41:A:ILE:HG13	1	29.58
(1,632)	1:66:A:LYS:HG2	1:41:B:ILE:HG13	10	29.57
(1,734)	1:64:A:ALA:HA	1:39:B:LYS:HG3	8	29.56
(1,288)	1:40:A:PRO:HG2	1:66:B:LYS:H	19	29.55
(1,786)	1:39:B:LYS:HE3	1:65:A:LEU:HG	8	29.48
(1,780)	1:64:A:ALA:HB3	1:39:B:LYS:HE2	11	29.44
(1,779)	1:64:B:ALA:HB2	1:39:A:LYS:HG2	18	29.44
(1,288)	1:40:A:PRO:HG2	1:66:B:LYS:H	9	29.37
(1,526)	1:40:A:PRO:HG3	1:66:B:LYS:H	17	29.34
(1,526)	1:40:B:PRO:HG3	1:66:A:LYS:H	11	29.32
(1,526)	1:40:A:PRO:HG3	1:66:B:LYS:H	7	29.28
(1,734)	1:64:B:ALA:HA	1:39:A:LYS:HG3	9	29.27
(1,526)	1:40:B:PRO:HG3	1:66:A:LYS:H	6	29.27
(1,780)	1:64:A:ALA:HB1	1:39:B:LYS:HE2	20	29.26
(1,780)	1:64:B:ALA:HB3	1:39:A:LYS:HE2	12	29.25
(1,779)	1:64:B:ALA:HB1	1:39:A:LYS:HG2	9	29.24
(1,734)	1:64:B:ALA:HA	1:39:A:LYS:HG3	3	29.24
(1,288)	1:40:A:PRO:HG2	1:66:B:LYS:H	6	29.24
(1,732)	1:64:B:ALA:HA	1:39:A:LYS:HG2	16	29.23
(1,732)	1:64:A:ALA:HA	1:39:B:LYS:HG2	20	29.23
(1,734)	1:64:B:ALA:HA	1:39:A:LYS:HG3	18	29.18
(1,732)	1:64:B:ALA:HA	1:39:A:LYS:HG2	2	29.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,526)	1:40:B:PRO:HG3	1:66:A:LYS:H	20	29.09
(1,632)	1:66:A:LYS:HG2	1:41:B:ILE:HG13	11	29.04
(1,732)	1:64:B:ALA:HA	1:39:A:LYS:HG2	11	29.03
(1,288)	1:40:A:PRO:HG2	1:66:B:LYS:H	12	29.01
(1,21)	1:64:A:ALA:H	1:39:B:LYS:HE3	8	29.01
(1,780)	1:64:B:ALA:HB3	1:39:A:LYS:HE2	14	29.0
(1,526)	1:40:A:PRO:HG3	1:66:B:LYS:H	14	29.0
(1,288)	1:40:B:PRO:HG2	1:66:A:LYS:H	4	29.0
(1,734)	1:64:A:ALA:HA	1:39:B:LYS:HG3	5	28.99
(1,732)	1:64:B:ALA:HA	1:39:A:LYS:HG2	15	28.99
(1,779)	1:64:A:ALA:HB1	1:39:B:LYS:HG2	5	28.98
(1,632)	1:66:B:LYS:HG2	1:41:A:ILE:HG13	18	28.98
(1,732)	1:64:A:ALA:HA	1:39:B:LYS:HG2	4	28.97
(1,527)	1:39:B:LYS:HE3	1:66:A:LYS:H	19	28.96
(1,526)	1:40:A:PRO:HG3	1:66:B:LYS:H	5	28.96
(1,526)	1:40:A:PRO:HG3	1:66:B:LYS:H	16	28.96
(1,779)	1:64:B:ALA:HB3	1:39:A:LYS:HG2	3	28.95
(1,779)	1:64:B:ALA:HB1	1:39:A:LYS:HG2	17	28.9
(1,288)	1:40:A:PRO:HG2	1:66:B:LYS:H	3	28.89
(1,604)	1:61:A:ILE:HD11	1:36:B:LYS:HE3	6	28.87
(1,526)	1:40:A:PRO:HG3	1:66:B:LYS:H	15	28.86
(1,288)	1:40:A:PRO:HG2	1:66:B:LYS:H	18	28.83
(1,21)	1:64:A:ALA:H	1:39:B:LYS:HE2	3	28.83
(1,465)	1:61:B:ILE:HA	1:36:A:LYS:HE2	8	28.81
(1,732)	1:64:B:ALA:HA	1:39:A:LYS:HG2	12	28.79
(1,734)	1:64:B:ALA:HA	1:39:A:LYS:HG3	16	28.76
(1,780)	1:64:A:ALA:HB2	1:39:B:LYS:HE3	7	28.74
(1,632)	1:66:B:LYS:HG2	1:41:A:ILE:HG13	14	28.72
(1,732)	1:64:B:ALA:HA	1:39:A:LYS:HG2	13	28.68
(1,786)	1:39:B:LYS:HE2	1:65:A:LEU:HG	3	28.67
(1,780)	1:64:B:ALA:HB3	1:39:A:LYS:HE2	1	28.67
(1,632)	1:66:B:LYS:HG2	1:41:A:ILE:HG13	15	28.66
(1,571)	1:39:B:LYS:HE3	1:65:A:LEU:HD11	19	28.65
(1,734)	1:64:B:ALA:HA	1:39:A:LYS:HG3	12	28.64
(1,526)	1:40:B:PRO:HG3	1:66:A:LYS:H	12	28.62
(1,632)	1:66:A:LYS:HG2	1:41:B:ILE:HG13	6	28.6
(1,527)	1:39:B:LYS:HE3	1:66:A:LYS:H	8	28.6
(1,288)	1:40:B:PRO:HG2	1:66:A:LYS:H	5	28.59
(1,779)	1:64:A:ALA:HB1	1:39:B:LYS:HG2	20	28.49
(1,734)	1:64:B:ALA:HA	1:39:A:LYS:HG3	17	28.49
(1,732)	1:64:A:ALA:HA	1:39:B:LYS:HG2	7	28.49
(1,779)	1:64:A:ALA:HB3	1:39:B:LYS:HG2	11	28.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,732)	1:64:B:ALA:HA	1:39:A:LYS:HG2	14	28.47
(1,526)	1:40:A:PRO:HG3	1:66:B:LYS:H	13	28.45
(1,780)	1:64:A:ALA:HB1	1:39:B:LYS:HE3	10	28.44
(1,779)	1:64:B:ALA:HB1	1:39:A:LYS:HG2	16	28.44
(1,526)	1:40:B:PRO:HG3	1:66:A:LYS:H	10	28.42
(1,526)	1:40:A:PRO:HG3	1:66:B:LYS:H	1	28.4
(1,317)	1:64:B:ALA:H	1:39:A:LYS:HG2	19	28.4
(1,779)	1:64:B:ALA:HB1	1:39:A:LYS:HG2	2	28.39
(1,779)	1:64:A:ALA:HB3	1:39:B:LYS:HG2	4	28.39
(1,526)	1:40:A:PRO:HG3	1:66:B:LYS:H	2	28.39
(1,779)	1:64:B:ALA:HB3	1:39:A:LYS:HG2	15	28.38
(1,288)	1:40:A:PRO:HG2	1:66:B:LYS:H	16	28.38
(1,305)	1:39:A:LYS:HD2	1:66:B:LYS:H	19	28.36
(1,786)	1:39:A:LYS:HE2	1:65:B:LEU:HG	9	28.35
(1,779)	1:64:B:ALA:HB3	1:39:A:LYS:HG2	13	28.34
(1,734)	1:64:A:ALA:HA	1:39:B:LYS:HG3	4	28.34
(1,288)	1:40:A:PRO:HG2	1:66:B:LYS:H	7	28.34
(1,734)	1:64:B:ALA:HA	1:39:A:LYS:HG3	13	28.32
(1,21)	1:64:A:ALA:H	1:39:B:LYS:HE3	5	28.32
(1,21)	1:64:B:ALA:H	1:39:A:LYS:HE2	9	28.32
(1,632)	1:66:A:LYS:HG2	1:41:B:ILE:HG13	20	28.29
(1,734)	1:64:B:ALA:HA	1:39:A:LYS:HG3	2	28.27
(1,572)	1:39:A:LYS:HE2	1:65:B:LEU:HD23	13	28.26
(1,734)	1:64:A:ALA:HA	1:39:B:LYS:HG3	11	28.25
(1,527)	1:39:A:LYS:HE2	1:66:B:LYS:H	9	28.24
(1,317)	1:64:A:ALA:H	1:39:B:LYS:HG2	8	28.23
(1,301)	1:64:B:ALA:H	1:39:A:LYS:HD2	19	28.23
(1,703)	1:66:A:LYS:HA	1:41:B:ILE:HG13	4	28.21
(1,572)	1:39:A:LYS:HE2	1:65:B:LEU:HD22	15	28.2
(1,21)	1:64:B:ALA:H	1:39:A:LYS:HE2	13	28.2
(1,288)	1:40:A:PRO:HG2	1:66:B:LYS:H	17	28.16
(1,288)	1:40:B:PRO:HG2	1:66:A:LYS:H	11	28.15
(1,21)	1:64:A:ALA:H	1:39:B:LYS:HE3	2	28.15
(1,571)	1:39:A:LYS:HE2	1:65:B:LEU:HD12	8	28.14
(1,527)	1:39:B:LYS:HE3	1:66:A:LYS:H	3	28.13
(1,779)	1:64:B:ALA:HB3	1:39:A:LYS:HG2	12	28.1
(1,734)	1:64:B:ALA:HA	1:39:A:LYS:HG3	15	28.06
(1,632)	1:66:B:LYS:HG2	1:41:A:ILE:HG13	17	28.03
(1,734)	1:64:A:ALA:HA	1:39:B:LYS:HG3	20	28.02
(1,732)	1:64:A:ALA:HA	1:39:B:LYS:HG2	10	28.02
(1,732)	1:64:B:ALA:HA	1:39:A:LYS:HG2	1	27.99
(1,21)	1:64:B:ALA:H	1:39:A:LYS:HE2	17	27.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,780)	1:64:B:ALA:HB2	1:39:A:LYS:HE2	18	27.98
(1,703)	1:66:B:LYS:HA	1:41:A:ILE:HG13	13	27.98
(1,288)	1:40:A:PRO:HG2	1:66:B:LYS:H	13	27.98
(1,317)	1:64:B:ALA:H	1:39:A:LYS:HG2	18	27.94
(1,288)	1:40:A:PRO:HG2	1:66:B:LYS:H	14	27.93
(1,305)	1:39:A:LYS:HD2	1:66:B:LYS:H	9	27.89
(1,288)	1:40:B:PRO:HG2	1:66:A:LYS:H	20	27.89
(1,21)	1:64:A:ALA:H	1:39:B:LYS:HE3	15	27.88
(1,288)	1:40:A:PRO:HG2	1:66:B:LYS:H	2	27.86
(1,734)	1:64:A:ALA:HA	1:39:B:LYS:HG3	10	27.84
(1,792)	1:69:A:SER:HG	1:44:B:LYS:HE2	9	27.82
(1,734)	1:64:B:ALA:HA	1:39:A:LYS:HG3	6	27.82
(1,734)	1:64:A:ALA:HA	1:39:B:LYS:HG3	7	27.82
(1,703)	1:66:B:LYS:HA	1:41:A:ILE:HG13	19	27.82
(1,779)	1:64:B:ALA:HB3	1:39:A:LYS:HG2	14	27.81
(1,572)	1:39:A:LYS:HE2	1:65:B:LEU:HD22	12	27.8
(1,779)	1:64:A:ALA:HB2	1:39:B:LYS:HG2	7	27.77
(1,565)	1:66:A:LYS:HA	1:44:B:LYS:HE3	9	27.75
(1,317)	1:64:B:ALA:H	1:39:A:LYS:HG2	9	27.75
(1,288)	1:40:B:PRO:HG2	1:66:A:LYS:H	10	27.75
(1,305)	1:39:B:LYS:HD2	1:66:A:LYS:H	8	27.74
(1,288)	1:40:A:PRO:HG2	1:66:B:LYS:H	15	27.72
(1,572)	1:39:B:LYS:HE3	1:65:A:LEU:HD22	4	27.69
(1,565)	1:66:A:LYS:HA	1:44:B:LYS:HE3	8	27.69
(1,288)	1:40:A:PRO:HG2	1:66:B:LYS:H	1	27.69
(1,703)	1:66:A:LYS:HA	1:41:B:ILE:HG13	12	27.68
(1,21)	1:64:A:ALA:H	1:39:B:LYS:HE3	4	27.65
(1,779)	1:64:B:ALA:HB3	1:39:A:LYS:HG2	1	27.64
(1,703)	1:66:B:LYS:HA	1:41:A:ILE:HG13	16	27.62
(1,305)	1:39:B:LYS:HD3	1:66:A:LYS:H	3	27.57
(1,792)	1:69:A:SER:HG	1:44:B:LYS:HE3	15	27.56
(1,317)	1:64:A:ALA:H	1:39:B:LYS:HG2	5	27.56
(1,703)	1:66:A:LYS:HA	1:41:B:ILE:HG13	8	27.55
(1,703)	1:66:A:LYS:HA	1:41:B:ILE:HG13	9	27.55
(1,732)	1:64:B:ALA:HA	1:39:A:LYS:HG2	6	27.54
(1,21)	1:64:A:ALA:H	1:39:B:LYS:HE3	16	27.54
(1,547)	1:65:A:LEU:HA	1:43:B:GLU:HG3	8	27.52
(1,301)	1:64:A:ALA:H	1:39:B:LYS:HD3	8	27.52
(1,734)	1:64:B:ALA:HA	1:39:A:LYS:HG3	14	27.51
(1,565)	1:66:A:LYS:HA	1:44:B:LYS:HE3	18	27.49
(1,527)	1:39:A:LYS:HE2	1:66:B:LYS:H	13	27.48
(1,301)	1:64:B:ALA:H	1:39:A:LYS:HD2	3	27.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,572)	1:39:A:LYS:HE2	1:65:B:LEU:HD21	19	27.46
(1,21)	1:64:B:ALA:H	1:39:A:LYS:HE2	11	27.46
(1,792)	1:69:A:SER:HG	1:44:A:LYS:HE2	2	27.44
(1,301)	1:64:B:ALA:H	1:39:A:LYS:HD2	9	27.44
(1,24)	1:64:B:ALA:H	1:39:A:LYS:HG3	19	27.44
(1,724)	1:39:B:LYS:HD2	1:65:A:LEU:HD21	12	27.43
(1,786)	1:39:B:LYS:HE3	1:65:A:LEU:HG	2	27.42
(1,527)	1:39:B:LYS:HE3	1:66:A:LYS:H	2	27.42
(1,465)	1:61:A:ILE:HA	1:36:B:LYS:HE3	6	27.42
(1,21)	1:64:A:ALA:H	1:39:B:LYS:HE2	20	27.4
(1,317)	1:64:B:ALA:H	1:39:A:LYS:HG2	3	27.38
(1,571)	1:39:B:LYS:HE2	1:65:A:LEU:HD12	3	27.36
(1,571)	1:39:A:LYS:HE2	1:65:B:LEU:HD11	9	27.36
(1,301)	1:64:B:ALA:H	1:39:A:LYS:HD2	18	27.36
(1,792)	1:69:A:SER:HG	1:44:B:LYS:HE3	8	27.35
(1,565)	1:66:B:LYS:HA	1:44:A:LYS:HE2	14	27.34
(1,565)	1:66:B:LYS:HA	1:44:A:LYS:HE2	2	27.33
(1,792)	1:69:B:SER:HG	1:44:A:LYS:HE2	16	27.31
(1,572)	1:39:B:LYS:HE3	1:65:A:LEU:HD23	8	27.31
(1,733)	1:64:B:ALA:HA	1:39:A:LYS:HD2	6	27.3
(1,792)	1:69:B:SER:HG	1:44:B:LYS:HE3	17	27.29
(1,565)	1:66:A:LYS:HA	1:44:B:LYS:HE3	15	27.29
(1,305)	1:39:A:LYS:HD2	1:66:B:LYS:H	18	27.29
(1,572)	1:39:A:LYS:HE2	1:65:B:LEU:HD21	17	27.28
(1,786)	1:39:B:LYS:HE2	1:65:A:LEU:HG	17	27.27
(1,724)	1:39:B:LYS:HD2	1:65:A:LEU:HD21	13	27.25
(1,527)	1:39:B:LYS:HE3	1:66:A:LYS:H	4	27.24
(1,565)	1:66:A:LYS:HA	1:44:B:LYS:HE3	19	27.23
(1,734)	1:64:B:ALA:HA	1:39:A:LYS:HG3	1	27.22
(1,703)	1:66:A:LYS:HA	1:41:B:ILE:HG13	1	27.22
(1,21)	1:64:B:ALA:H	1:39:A:LYS:HE2	12	27.22
(1,565)	1:66:A:LYS:HA	1:44:B:LYS:HE3	5	27.21
(1,703)	1:66:B:LYS:HA	1:41:A:ILE:HG13	2	27.19
(1,317)	1:64:B:ALA:H	1:39:A:LYS:HG2	17	27.18
(1,21)	1:64:B:ALA:H	1:39:A:LYS:HE2	14	27.18
(1,792)	1:69:A:SER:HG	1:44:B:LYS:HE2	18	27.17
(1,786)	1:39:A:LYS:HE2	1:65:B:LEU:HG	7	27.17
(1,786)	1:39:B:LYS:HE2	1:65:A:LEU:HG	20	27.17
(1,724)	1:39:B:LYS:HD3	1:65:A:LEU:HD22	4	27.17
(1,792)	1:69:B:SER:HG	1:44:A:LYS:HE2	14	27.13
(1,779)	1:64:A:ALA:HB1	1:39:B:LYS:HG2	10	27.12
(1,527)	1:39:B:LYS:HE3	1:66:A:LYS:H	5	27.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,527)	1:39:B:LYS:HE3	1:66:A:LYS:H	15	27.09
(1,786)	1:39:B:LYS:HE2	1:65:A:LEU:HG	11	27.08
(1,301)	1:64:A:ALA:H	1:39:B:LYS:HD3	5	27.08
(1,527)	1:39:B:LYS:HE3	1:66:A:LYS:H	16	27.07
(1,547)	1:65:B:LEU:HA	1:43:A:GLU:HG2	9	27.06
(1,786)	1:39:A:LYS:HE2	1:65:B:LEU:HG	5	27.05
(1,786)	1:39:B:LYS:HE3	1:65:A:LEU:HG	16	27.04
(1,703)	1:66:A:LYS:HA	1:41:B:ILE:HG13	3	27.04
(1,571)	1:39:B:LYS:HE3	1:65:A:LEU:HD13	2	27.03
(1,565)	1:66:B:LYS:HA	1:44:A:LYS:HE2	4	27.03
(1,703)	1:66:A:LYS:HA	1:41:B:ILE:HG13	5	27.01
(1,613)	1:61:B:ILE:HG21	1:36:A:LYS:HE2	8	26.99
(1,792)	1:69:B:SER:HG	1:44:A:LYS:HE2	6	26.98
(1,599)	1:69:A:SER:HB2	1:44:B:LYS:HE2	9	26.97
(1,547)	1:65:B:LEU:HA	1:43:A:GLU:HG2	17	26.97
(1,786)	1:39:B:LYS:HE3	1:65:A:LEU:HG	10	26.96
(1,572)	1:39:B:LYS:HE2	1:65:A:LEU:HD22	5	26.96
(1,547)	1:65:B:LEU:HA	1:43:A:GLU:HG2	19	26.95
(1,604)	1:61:B:ILE:HD13	1:36:A:LYS:HE2	9	26.92
(1,565)	1:66:B:LYS:HA	1:44:A:LYS:HE2	16	26.91
(1,527)	1:39:A:LYS:HE2	1:66:B:LYS:H	17	26.89
(1,599)	1:69:A:SER:HB3	1:44:B:LYS:HE3	5	26.88
(1,527)	1:39:B:LYS:HE2	1:66:A:LYS:H	20	26.88
(1,434)	1:63:B:ASP:HB2	1:39:A:LYS:HG2	19	26.88
(1,792)	1:69:A:SER:HG	1:44:B:LYS:HE3	5	26.86
(1,565)	1:66:A:LYS:HA	1:44:B:LYS:HE3	6	26.86
(1,703)	1:66:A:LYS:HA	1:41:B:ILE:HG13	10	26.85
(1,317)	1:64:B:ALA:H	1:39:A:LYS:HG2	16	26.85
(1,24)	1:64:A:ALA:H	1:39:B:LYS:HG3	8	26.85
(1,792)	1:69:A:SER:HG	1:44:B:LYS:HE2	10	26.83
(1,686)	1:66:B:LYS:HG2	1:45:A:ARG:HD2	2	26.83
(1,565)	1:66:A:LYS:HA	1:44:B:LYS:HE2	10	26.83
(1,579)	1:61:B:ILE:HB	1:36:A:LYS:HE2	8	26.82
(1,547)	1:65:B:LEU:HA	1:43:A:GLU:HG2	5	26.81
(1,317)	1:64:B:ALA:H	1:39:A:LYS:HG2	2	26.81
(1,301)	1:64:A:ALA:H	1:39:B:LYS:HD3	16	26.81
(1,779)	1:64:B:ALA:HB2	1:39:A:LYS:HG2	6	26.8
(1,724)	1:39:A:LYS:HD2	1:65:B:LEU:HD22	15	26.8
(1,21)	1:64:A:ALA:H	1:39:B:LYS:HE3	10	26.79
(1,305)	1:39:A:LYS:HD2	1:66:B:LYS:H	16	26.78
(1,786)	1:39:A:LYS:HE2	1:65:B:LEU:HG	14	26.77
(1,317)	1:64:A:ALA:H	1:39:B:LYS:HG2	20	26.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,317)	1:64:B:ALA:H	1:39:A:LYS:HG2	15	26.75
(1,565)	1:66:A:LYS:HA	1:44:B:LYS:HE3	11	26.73
(1,21)	1:64:A:ALA:H	1:39:B:LYS:HE3	7	26.73
(1,527)	1:39:B:LYS:HE3	1:66:A:LYS:H	11	26.71
(1,547)	1:65:B:LEU:HA	1:43:A:GLU:HG2	6	26.7
(1,599)	1:69:A:SER:HB3	1:44:B:LYS:HE3	8	26.69
(1,544)	1:64:B:ALA:HA	1:39:A:LYS:HE2	6	26.69
(1,305)	1:39:B:LYS:HD3	1:66:A:LYS:H	5	26.69
(1,792)	1:69:A:SER:HG	1:44:B:LYS:HE3	3	26.68
(1,527)	1:39:A:LYS:HE2	1:66:B:LYS:H	12	26.67
(1,301)	1:64:B:ALA:H	1:39:A:LYS:HD2	2	26.67
(1,565)	1:66:A:LYS:HA	1:44:B:LYS:HE3	17	26.66
(1,703)	1:66:A:LYS:HA	1:41:B:ILE:HG13	7	26.64
(1,572)	1:39:A:LYS:HE2	1:65:B:LEU:HD21	3	26.64
(1,305)	1:39:B:LYS:HD2	1:66:A:LYS:H	4	26.64
(1,317)	1:64:B:ALA:H	1:39:A:LYS:HG2	11	26.62
(1,24)	1:64:B:ALA:H	1:39:A:LYS:HG3	3	26.62
(1,547)	1:65:B:LEU:HA	1:43:A:GLU:HG2	3	26.61
(1,301)	1:64:B:ALA:H	1:39:A:LYS:HD2	17	26.61
(1,317)	1:64:A:ALA:H	1:39:B:LYS:HG2	4	26.6
(1,434)	1:63:A:ASP:HB2	1:39:B:LYS:HG2	9	26.58
(1,301)	1:64:B:ALA:H	1:39:A:LYS:HD2	13	26.58
(1,599)	1:69:A:SER:HB3	1:44:B:LYS:HE2	11	26.57
(1,434)	1:63:B:ASP:HB2	1:39:A:LYS:HG2	18	26.57
(1,24)	1:64:B:ALA:H	1:39:A:LYS:HG3	9	26.56
(1,547)	1:65:A:LEU:HA	1:43:B:GLU:HG3	4	26.53
(1,301)	1:64:A:ALA:H	1:39:B:LYS:HD2	4	26.53
(1,792)	1:69:A:SER:HG	1:44:B:LYS:HE2	13	26.52
(1,792)	1:69:A:SER:HG	1:44:A:LYS:HE2	11	26.51
(1,305)	1:39:A:LYS:HD2	1:66:B:LYS:H	13	26.51
(1,21)	1:64:B:ALA:H	1:39:A:LYS:HE2	1	26.5
(1,301)	1:64:B:ALA:H	1:39:A:LYS:HD2	12	26.49
(1,24)	1:64:B:ALA:H	1:39:A:LYS:HG3	18	26.49
(1,305)	1:39:A:LYS:HD2	1:66:B:LYS:H	12	26.47
(1,21)	1:64:B:ALA:H	1:39:A:LYS:HE2	18	26.46
(1,599)	1:69:A:SER:HB3	1:44:B:LYS:HE2	18	26.44
(1,724)	1:39:A:LYS:HD2	1:65:B:LEU:HD21	17	26.41
(1,702)	1:66:A:LYS:HA	1:41:B:ILE:HG12	4	26.4
(1,24)	1:64:A:ALA:H	1:39:B:LYS:HG3	5	26.4
(1,547)	1:65:A:LEU:HA	1:43:B:GLU:HG3	11	26.39
(1,301)	1:64:A:ALA:H	1:39:B:LYS:HD3	11	26.38
(1,599)	1:69:A:SER:HB2	1:44:B:LYS:HE2	10	26.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	1:65:A:LEU:HA	1:43:B:GLU:HG3	18	26.37
(1,527)	1:39:A:LYS:HE2	1:66:B:LYS:H	14	26.37
(1,301)	1:64:B:ALA:H	1:39:A:LYS:HD2	15	26.36
(1,317)	1:64:B:ALA:H	1:39:A:LYS:HG2	13	26.35
(1,724)	1:39:B:LYS:HD3	1:65:A:LEU:HD23	8	26.34
(1,565)	1:66:A:LYS:HA	1:44:B:LYS:HE2	1	26.33
(1,703)	1:66:A:LYS:HA	1:41:B:ILE:HG13	11	26.32
(1,317)	1:64:B:ALA:H	1:39:A:LYS:HG2	12	26.32
(1,547)	1:65:B:LEU:HA	1:43:A:GLU:HG2	7	26.31
(1,302)	1:39:A:LYS:HD2	1:67:B:LYS:H	19	26.31
(1,599)	1:69:A:SER:HB3	1:44:B:LYS:HE2	17	26.3
(1,547)	1:65:A:LEU:HA	1:43:B:GLU:HG3	12	26.3
(1,434)	1:63:A:ASP:HB2	1:39:B:LYS:HG2	5	26.3
(1,527)	1:39:B:LYS:HE3	1:66:A:LYS:H	7	26.28
(1,786)	1:39:A:LYS:HE2	1:65:B:LEU:HG	13	26.27
(1,571)	1:39:B:LYS:HE3	1:65:A:LEU:HD13	16	26.27
(1,434)	1:63:A:ASP:HB2	1:39:B:LYS:HG2	8	26.27
(1,305)	1:39:A:LYS:HD2	1:66:B:LYS:H	2	26.26
(1,599)	1:69:B:SER:HB3	1:44:A:LYS:HE2	4	26.21
(1,702)	1:66:B:LYS:HA	1:41:A:ILE:HG12	13	26.2
(1,547)	1:65:A:LEU:HA	1:43:B:GLU:HG2	20	26.2
(1,792)	1:69:A:SER:HG	1:44:B:LYS:HE2	12	26.19
(1,703)	1:66:B:LYS:HA	1:41:A:ILE:HG13	18	26.19
(1,565)	1:66:B:LYS:HA	1:44:A:LYS:HE2	3	26.19
(1,434)	1:63:B:ASP:HB2	1:39:A:LYS:HG2	3	26.18
(1,786)	1:39:A:LYS:HE2	1:65:B:LEU:HG	15	26.17
(1,702)	1:66:B:LYS:HA	1:41:A:ILE:HG12	19	26.17
(1,724)	1:39:A:LYS:HD2	1:65:B:LEU:HD21	19	26.16
(1,317)	1:64:B:ALA:H	1:39:A:LYS:HG2	14	26.16
(1,24)	1:64:B:ALA:H	1:39:A:LYS:HG3	16	26.15
(1,786)	1:39:A:LYS:HE2	1:65:B:LEU:HG	18	26.14
(1,703)	1:66:A:LYS:HA	1:41:B:ILE:HG13	6	26.14
(1,571)	1:39:A:LYS:HE2	1:65:B:LEU:HD12	5	26.14
(1,565)	1:66:A:LYS:HA	1:44:B:LYS:HE2	12	26.12
(1,724)	1:39:B:LYS:HD3	1:65:A:LEU:HD22	5	26.11
(1,572)	1:39:A:LYS:HE2	1:65:B:LEU:HD21	9	26.11
(1,305)	1:39:B:LYS:HD2	1:66:A:LYS:H	7	26.11
(1,703)	1:66:B:LYS:HA	1:41:A:ILE:HG13	14	26.1
(1,613)	1:61:A:ILE:HG13	1:36:B:LYS:HE3	6	26.1
(1,786)	1:39:A:LYS:HE2	1:65:B:LEU:HG	1	26.08
(1,305)	1:39:B:LYS:HD2	1:66:A:LYS:H	11	26.08
(1,305)	1:39:A:LYS:HD2	1:66:B:LYS:H	17	26.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,686)	1:66:B:LYS:HG2	1:45:A:ARG:HD2	19	26.06
(1,571)	1:39:A:LYS:HE2	1:65:B:LEU:HD12	14	26.06
(1,317)	1:64:A:ALA:H	1:39:B:LYS:HG2	7	26.06
(1,565)	1:66:B:LYS:HA	1:44:A:LYS:HE2	13	26.05
(1,547)	1:65:B:LEU:HA	1:43:A:GLU:HG2	10	26.05
(1,792)	1:69:A:SER:HG	1:44:B:LYS:HE2	1	26.04
(1,792)	1:69:B:SER:HG	1:44:A:LYS:HE2	19	26.02
(1,599)	1:69:A:SER:HB3	1:44:B:LYS:HE3	19	26.02
(1,328)	1:69:A:SER:H	1:44:B:LYS:HE2	9	26.01
(1,434)	1:63:A:ASP:HB2	1:39:B:LYS:HG2	4	26.0
(1,434)	1:63:B:ASP:HB2	1:39:A:LYS:HG2	17	26.0
(1,686)	1:66:B:LYS:HG2	1:45:A:ARG:HD2	13	25.98
(1,702)	1:66:A:LYS:HA	1:41:B:ILE:HG12	9	25.96
(1,599)	1:69:B:SER:HB3	1:44:A:LYS:HE2	3	25.95
(1,599)	1:69:B:SER:HB2	1:44:B:LYS:HE3	2	25.94
(1,305)	1:39:B:LYS:HD3	1:66:A:LYS:H	20	25.93
(1,599)	1:69:A:SER:HB3	1:44:B:LYS:HE2	1	25.92
(1,24)	1:64:B:ALA:H	1:39:A:LYS:HG3	12	25.92
(1,702)	1:66:B:LYS:HA	1:41:A:ILE:HG12	16	25.91
(1,547)	1:65:B:LEU:HA	1:43:A:GLU:HG2	14	25.91
(1,301)	1:64:A:ALA:H	1:39:B:LYS:HD2	7	25.91
(1,571)	1:39:A:LYS:HE2	1:65:B:LEU:HD12	11	25.89
(1,301)	1:64:A:ALA:H	1:39:B:LYS:HD2	10	25.89
(1,571)	1:39:B:LYS:HE3	1:65:A:LEU:HD13	7	25.88
(1,527)	1:39:A:LYS:HE2	1:66:B:LYS:H	1	25.88
(1,571)	1:39:B:LYS:HE2	1:65:A:LEU:HD13	20	25.87
(1,702)	1:66:A:LYS:HA	1:41:B:ILE:HG12	12	25.85
(1,515)	1:36:A:LYS:HE2	1:62:B:LEU:H	8	25.83
(1,302)	1:39:A:LYS:HD2	1:67:B:LYS:H	9	25.83
(1,24)	1:64:B:ALA:H	1:39:A:LYS:HG3	17	25.83
(1,703)	1:66:B:LYS:HA	1:41:A:ILE:HG13	15	25.82
(1,599)	1:69:B:SER:HB3	1:44:A:LYS:HE2	16	25.82
(1,702)	1:66:A:LYS:HA	1:41:B:ILE:HG12	8	25.81
(1,301)	1:64:A:ALA:H	1:39:B:LYS:HD3	20	25.81
(1,724)	1:39:A:LYS:HD2	1:65:B:LEU:HD21	9	25.8
(1,328)	1:69:B:SER:H	1:44:A:LYS:HE2	2	25.8
(1,786)	1:39:B:LYS:HE3	1:65:A:LEU:HG	4	25.76
(1,24)	1:64:B:ALA:H	1:39:A:LYS:HG3	2	25.75
(1,599)	1:69:A:SER:HB2	1:44:B:LYS:HE3	15	25.74
(1,317)	1:64:A:ALA:H	1:39:B:LYS:HG2	10	25.74
(1,24)	1:64:B:ALA:H	1:39:A:LYS:HG3	13	25.74
(1,571)	1:39:A:LYS:HE2	1:65:B:LEU:HD12	17	25.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,305)	1:39:A:LYS:HD2	1:66:B:LYS:H	15	25.73
(1,24)	1:64:A:ALA:H	1:39:B:LYS:HG3	4	25.73
(1,45)	1:69:A:SER:H	1:44:B:LYS:HG3	12	25.71
(1,301)	1:64:B:ALA:H	1:39:A:LYS:HD2	14	25.7
(1,24)	1:64:A:ALA:H	1:39:B:LYS:HG3	11	25.69
(1,434)	1:63:B:ASP:HB2	1:39:A:LYS:HG2	13	25.67
(1,317)	1:64:B:ALA:H	1:39:A:LYS:HG2	1	25.66
(1,786)	1:39:A:LYS:HE2	1:65:B:LEU:HG	12	25.64
(1,434)	1:63:B:ASP:HB2	1:39:A:LYS:HG2	2	25.63
(1,429)	1:69:A:SER:HA	1:44:B:LYS:HD2	8	25.62
(1,547)	1:65:A:LEU:HA	1:43:B:GLU:HG3	16	25.6
(1,24)	1:64:B:ALA:H	1:39:A:LYS:HG3	15	25.6
(1,686)	1:66:A:LYS:HG2	1:45:B:ARG:HD3	9	25.59
(1,686)	1:66:A:LYS:HG2	1:45:B:ARG:HD3	12	25.59
(1,302)	1:39:B:LYS:HD2	1:67:A:LYS:H	8	25.58
(1,686)	1:66:A:LYS:HG2	1:45:B:ARG:HD3	4	25.57
(1,434)	1:63:B:ASP:HB2	1:39:A:LYS:HG2	16	25.56
(1,434)	1:63:A:ASP:HB2	1:39:B:LYS:HG2	15	25.55
(1,527)	1:39:B:LYS:HE3	1:66:A:LYS:H	10	25.54
(1,604)	1:61:B:ILE:HD13	1:36:A:LYS:HE2	10	25.52
(1,599)	1:69:B:SER:HB3	1:44:A:LYS:HE2	6	25.51
(1,605)	1:39:A:LYS:HD2	1:67:B:LYS:HG2	19	25.5
(1,328)	1:69:A:SER:H	1:44:B:LYS:HE3	8	25.5
(1,703)	1:66:A:LYS:HA	1:41:B:ILE:HG13	20	25.49
(1,571)	1:39:B:LYS:HE3	1:65:A:LEU:HD13	10	25.49
(1,724)	1:39:A:LYS:HD2	1:65:B:LEU:HD21	3	25.48
(1,571)	1:39:A:LYS:HE2	1:65:B:LEU:HD12	1	25.48
(1,301)	1:64:B:ALA:H	1:39:A:LYS:HD2	1	25.45
(1,702)	1:66:A:LYS:HA	1:41:B:ILE:HG12	1	25.43
(1,599)	1:69:B:SER:HB2	1:44:A:LYS:HE2	13	25.43
(1,547)	1:65:B:LEU:HA	1:43:A:GLU:HG2	1	25.43
(1,305)	1:39:A:LYS:HD2	1:66:B:LYS:H	14	25.43
(1,571)	1:39:A:LYS:HE2	1:65:B:LEU:HD12	13	25.42
(1,328)	1:69:A:SER:H	1:44:B:LYS:HE2	18	25.42
(1,45)	1:69:A:SER:H	1:44:B:LYS:HG3	4	25.42
(1,792)	1:69:A:SER:HG	1:44:B:LYS:HE2	7	25.39
(1,547)	1:65:B:LEU:HA	1:43:A:GLU:HG2	15	25.39
(1,702)	1:66:B:LYS:HA	1:41:A:ILE:HG12	2	25.38
(1,527)	1:39:A:LYS:HE2	1:66:B:LYS:H	18	25.37
(1,565)	1:66:A:LYS:HA	1:44:B:LYS:HE2	7	25.36
(1,305)	1:39:A:LYS:HD2	1:66:B:LYS:H	1	25.36
(1,32)	1:66:A:LYS:H	1:41:B:ILE:HG12	8	25.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,703)	1:66:B:LYS:HA	1:41:A:ILE:HG13	17	25.35
(1,579)	1:61:A:ILE:HB	1:36:B:LYS:HE3	6	25.34
(1,429)	1:69:A:SER:HA	1:44:B:LYS:HD2	10	25.34
(1,24)	1:64:A:ALA:H	1:39:B:LYS:HG3	10	25.34
(1,599)	1:69:B:SER:HB2	1:44:B:LYS:HE3	12	25.31
(1,24)	1:64:A:ALA:H	1:39:B:LYS:HG3	20	25.3
(1,702)	1:66:A:LYS:HA	1:41:B:ILE:HG12	3	25.28
(1,429)	1:69:A:SER:HA	1:44:A:LYS:HD2	5	25.28
(1,434)	1:63:A:ASP:HB2	1:39:B:LYS:HG2	20	25.26
(1,32)	1:66:B:LYS:H	1:41:A:ILE:HG12	19	25.26
(1,686)	1:66:A:LYS:HG2	1:45:B:ARG:HD3	8	25.25
(1,328)	1:69:B:SER:H	1:44:A:LYS:HE2	6	25.25
(1,429)	1:69:B:SER:HA	1:44:A:LYS:HD2	16	25.23
(1,328)	1:69:A:SER:H	1:44:B:LYS:HE3	5	25.23
(1,606)	1:39:A:LYS:HD2	1:67:B:LYS:HG3	19	25.22
(1,302)	1:39:B:LYS:HD3	1:67:A:LYS:H	3	25.22
(1,722)	1:39:A:LYS:HG2	1:65:B:LEU:HD22	12	25.21
(1,571)	1:39:A:LYS:HE2	1:65:B:LEU:HD11	15	25.21
(1,328)	1:69:A:SER:H	1:44:B:LYS:HE3	19	25.19
(1,305)	1:39:B:LYS:HD2	1:66:A:LYS:H	10	25.18
(1,32)	1:66:B:LYS:H	1:41:A:ILE:HG12	9	25.18
(1,702)	1:66:A:LYS:HA	1:41:B:ILE:HG12	5	25.17
(1,686)	1:66:B:LYS:HG2	1:45:A:ARG:HD2	18	25.17
(1,572)	1:39:B:LYS:HE3	1:65:A:LEU:HD23	2	25.17
(1,724)	1:39:B:LYS:HD3	1:65:A:LEU:HD22	18	25.16
(1,32)	1:66:A:LYS:H	1:41:B:ILE:HG12	12	25.16
(1,686)	1:66:A:LYS:HG2	1:45:B:ARG:HD3	16	25.15
(1,572)	1:39:B:LYS:HE3	1:65:A:LEU:HD23	10	25.15
(1,302)	1:39:A:LYS:HD2	1:67:B:LYS:H	18	25.15
(1,24)	1:64:A:ALA:H	1:39:B:LYS:HG3	7	25.14
(1,722)	1:39:B:LYS:HG2	1:65:A:LEU:HD23	8	25.1
(1,722)	1:39:B:LYS:HG2	1:65:A:LEU:HD22	4	25.09
(1,429)	1:69:B:SER:HA	1:44:A:LYS:HD2	17	25.08
(1,317)	1:64:B:ALA:H	1:39:A:LYS:HG2	6	25.07
(1,572)	1:39:B:LYS:HE2	1:65:A:LEU:HD22	20	25.05
(1,32)	1:66:B:LYS:H	1:41:A:ILE:HG12	13	25.05
(1,780)	1:64:B:ALA:HB2	1:39:A:LYS:HE2	6	25.03
(1,24)	1:64:B:ALA:H	1:39:A:LYS:HG3	6	25.02
(1,547)	1:65:A:LEU:HA	1:43:B:GLU:HG3	2	25.01
(1,32)	1:66:A:LYS:H	1:41:B:ILE:HG12	4	25.01
(1,702)	1:66:A:LYS:HA	1:41:B:ILE:HG12	10	24.98
(1,750)	1:69:A:SER:H	1:44:B:LYS:HG2	19	24.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,686)	1:66:A:LYS:HG2	1:45:B:ARG:HD3	3	24.97
(1,465)	1:61:B:ILE:HA	1:36:A:LYS:HE2	9	24.97
(1,24)	1:64:B:ALA:H	1:39:A:LYS:HG3	14	24.97
(1,45)	1:69:B:SER:H	1:44:A:LYS:HG3	2	24.96
(1,722)	1:39:A:LYS:HG2	1:65:B:LEU:HD21	17	24.95
(1,686)	1:66:A:LYS:HG2	1:45:B:ARG:HD3	5	24.94
(1,599)	1:69:B:SER:HB3	1:44:A:LYS:HE2	14	24.94
(1,750)	1:69:A:SER:H	1:44:B:LYS:HG2	6	24.93
(1,722)	1:39:A:LYS:HG2	1:65:B:LEU:HD22	15	24.93
(1,328)	1:69:A:SER:H	1:44:B:LYS:HE2	11	24.92
(1,686)	1:66:A:LYS:HG2	1:45:B:ARG:HD3	1	24.91
(1,571)	1:39:A:LYS:HE2	1:65:B:LEU:HD13	12	24.91
(1,328)	1:69:B:SER:H	1:44:A:LYS:HE2	4	24.91
(1,328)	1:69:B:SER:H	1:44:A:LYS:HE2	16	24.91
(1,686)	1:66:A:LYS:HG2	1:45:B:ARG:HD3	14	24.9
(1,572)	1:39:A:LYS:HE2	1:65:B:LEU:HD23	7	24.9
(1,547)	1:65:B:LEU:HA	1:43:A:GLU:HG2	13	24.9
(1,723)	1:39:A:LYS:HG3	1:65:B:LEU:HD22	12	24.87
(1,571)	1:39:B:LYS:HE3	1:65:A:LEU:HD12	4	24.87
(1,32)	1:66:A:LYS:H	1:41:B:ILE:HG12	16	24.85
(1,605)	1:39:B:LYS:HD3	1:67:A:LYS:HG2	8	24.84
(1,434)	1:63:B:ASP:HB2	1:39:A:LYS:HG2	14	24.84
(1,45)	1:69:B:SER:H	1:44:A:LYS:HG3	1	24.84
(1,45)	1:69:B:SER:H	1:44:A:LYS:HG3	13	24.84
(1,773)	1:63:B:ASP:H	1:39:A:LYS:HG2	19	24.83
(1,722)	1:39:A:LYS:HG2	1:65:B:LEU:HD23	13	24.83
(1,702)	1:66:A:LYS:HA	1:41:B:ILE:HG12	7	24.83
(1,328)	1:69:A:SER:H	1:44:B:LYS:HE2	17	24.83
(1,750)	1:69:A:SER:H	1:44:B:LYS:HG2	12	24.82
(1,572)	1:39:B:LYS:HE2	1:65:A:LEU:HD22	11	24.82
(1,328)	1:69:A:SER:H	1:44:B:LYS:HE3	15	24.82
(1,328)	1:69:A:SER:H	1:44:B:LYS:HE2	12	24.81
(1,32)	1:66:A:LYS:H	1:41:B:ILE:HG12	3	24.81
(1,572)	1:39:B:LYS:HE3	1:65:A:LEU:HD21	16	24.78
(1,750)	1:69:A:SER:H	1:44:B:LYS:HG2	4	24.77
(1,434)	1:63:B:ASP:HB2	1:39:A:LYS:HG2	12	24.76
(1,434)	1:63:B:ASP:HB2	1:39:A:LYS:HG2	11	24.74
(1,429)	1:69:B:SER:HA	1:44:B:LYS:HD2	18	24.74
(1,302)	1:39:B:LYS:HD2	1:67:A:LYS:H	4	24.74
(1,686)	1:66:A:LYS:HG2	1:45:B:ARG:HD3	10	24.7
(1,604)	1:61:A:ILE:HD11	1:36:B:LYS:HE3	20	24.7
(1,599)	1:69:A:SER:HB3	1:44:B:LYS:HE2	20	24.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,686)	1:66:A:LYS:HG2	1:45:B:ARG:HD3	15	24.69
(1,302)	1:39:A:LYS:HD2	1:67:B:LYS:H	16	24.69
(1,571)	1:39:A:LYS:HE2	1:65:B:LEU:HD11	18	24.68
(1,328)	1:69:B:SER:H	1:44:A:LYS:HE2	3	24.66
(1,724)	1:39:B:LYS:HD2	1:65:A:LEU:HD23	10	24.65
(1,24)	1:64:B:ALA:H	1:39:A:LYS:HG3	1	24.65
(1,750)	1:69:B:SER:H	1:44:A:LYS:HG2	3	24.64
(1,606)	1:39:A:LYS:HD2	1:67:B:LYS:HG3	9	24.64
(1,722)	1:39:B:LYS:HG2	1:65:A:LEU:HD22	5	24.63
(1,434)	1:63:A:ASP:HB2	1:39:B:LYS:HG2	10	24.63
(1,792)	1:69:A:SER:HG	1:44:B:LYS:HE2	20	24.62
(1,686)	1:66:A:LYS:HG2	1:45:B:ARG:HD3	7	24.61
(1,45)	1:69:A:SER:H	1:44:B:LYS:HG3	20	24.61
(1,605)	1:39:A:LYS:HD2	1:67:B:LYS:HG2	18	24.6
(1,604)	1:61:B:ILE:HD13	1:36:A:LYS:HE2	15	24.6
(1,434)	1:63:B:ASP:HB2	1:39:A:LYS:HG2	6	24.6
(1,702)	1:66:A:LYS:HA	1:41:B:ILE:HG12	11	24.59
(1,32)	1:66:B:LYS:H	1:41:A:ILE:HG12	2	24.59
(1,605)	1:39:A:LYS:HD2	1:67:B:LYS:HG2	9	24.58
(1,429)	1:69:B:SER:HA	1:44:B:LYS:HD2	9	24.56
(1,328)	1:69:A:SER:H	1:44:B:LYS:HE2	10	24.56
(1,328)	1:69:A:SER:H	1:44:B:LYS:HE2	1	24.55
(1,773)	1:63:B:ASP:H	1:39:A:LYS:HG2	9	24.54
(1,773)	1:63:B:ASP:H	1:39:A:LYS:HG2	18	24.52
(1,572)	1:39:A:LYS:HE2	1:65:B:LEU:HD23	14	24.52
(1,302)	1:39:B:LYS:HD2	1:67:A:LYS:H	5	24.52
(1,686)	1:66:A:LYS:HG2	1:45:B:ARG:HD3	17	24.51
(1,434)	1:63:A:ASP:HB2	1:39:B:LYS:HG2	7	24.5
(1,724)	1:39:B:LYS:HD3	1:65:A:LEU:HD21	16	24.49
(1,45)	1:69:A:SER:H	1:44:B:LYS:HG3	3	24.48
(1,515)	1:36:B:LYS:HE3	1:62:A:LEU:H	6	24.47
(1,45)	1:69:A:SER:H	1:44:B:LYS:HG3	6	24.47
(1,441)	1:68:A:ASP:HA	1:43:B:GLU:HG3	8	24.46
(1,328)	1:69:B:SER:H	1:44:A:LYS:HE2	14	24.46
(1,773)	1:63:A:ASP:H	1:39:B:LYS:HG2	8	24.45
(1,750)	1:69:B:SER:H	1:44:A:LYS:HG2	8	24.45
(1,323)	1:41:B:ILE:HG13	1:67:A:LYS:H	9	24.45
(1,792)	1:69:A:SER:HG	1:44:A:LYS:HE2	4	24.43
(1,702)	1:66:B:LYS:HA	1:41:A:ILE:HG12	18	24.43
(1,693)	1:41:A:ILE:HG12	1:67:B:LYS:HA	19	24.43
(1,323)	1:41:A:ILE:HG13	1:67:B:LYS:H	19	24.43
(1,302)	1:39:A:LYS:HD2	1:67:B:LYS:H	13	24.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:39:A:LYS:HD2	1:67:B:LYS:H	12	24.42
(1,45)	1:69:A:SER:H	1:44:B:LYS:HG3	8	24.42
(1,32)	1:66:A:LYS:H	1:41:B:ILE:HG12	5	24.42
(1,724)	1:39:A:LYS:HD2	1:65:B:LEU:HD23	7	24.39
(1,465)	1:61:A:ILE:HA	1:36:B:LYS:HE3	10	24.39
(1,686)	1:66:A:LYS:HG2	1:45:B:ARG:HD3	11	24.36
(1,429)	1:69:A:SER:HA	1:44:B:LYS:HD3	15	24.36
(1,45)	1:69:A:SER:H	1:44:B:LYS:HG3	9	24.36
(1,323)	1:41:B:ILE:HG13	1:67:A:LYS:H	4	24.34
(1,723)	1:39:B:LYS:HG3	1:65:A:LEU:HD22	4	24.33
(1,323)	1:41:B:ILE:HG13	1:67:A:LYS:H	12	24.33
(1,323)	1:41:A:ILE:HG13	1:67:B:LYS:H	13	24.33
(1,323)	1:41:B:ILE:HG13	1:67:A:LYS:H	8	24.32
(1,723)	1:39:A:LYS:HG3	1:65:B:LEU:HD23	13	24.31
(1,441)	1:68:A:ASP:HA	1:43:B:GLU:HG2	4	24.31
(1,434)	1:63:B:ASP:HB2	1:39:A:LYS:HG2	1	24.31
(1,336)	1:66:A:LYS:H	1:43:B:GLU:HG3	8	24.31
(1,606)	1:39:A:LYS:HD2	1:67:B:LYS:HG3	18	24.3
(1,605)	1:39:A:LYS:HD2	1:67:B:LYS:HG2	3	24.3
(1,32)	1:66:A:LYS:H	1:41:B:ILE:HG12	10	24.29
(1,750)	1:69:A:SER:H	1:44:B:LYS:HG2	5	24.28
(1,336)	1:66:A:LYS:H	1:43:B:GLU:HG3	4	24.28
(1,702)	1:66:B:LYS:HA	1:41:A:ILE:HG12	14	24.27
(1,702)	1:66:A:LYS:HA	1:41:B:ILE:HG12	6	24.26
(1,773)	1:63:A:ASP:H	1:39:B:LYS:HG2	5	24.25
(1,724)	1:39:A:LYS:HD2	1:65:B:LEU:HD23	2	24.24
(1,32)	1:66:B:LYS:H	1:41:A:ILE:HG12	1	24.23
(1,750)	1:69:A:SER:H	1:44:B:LYS:HG2	20	24.22
(1,722)	1:39:A:LYS:HG2	1:65:B:LEU:HD21	19	24.21
(1,302)	1:39:A:LYS:HD2	1:67:B:LYS:H	17	24.19
(1,323)	1:41:B:ILE:HG13	1:67:A:LYS:H	16	24.18
(1,525)	1:44:B:LYS:HE2	1:70:A:SER:H	9	24.17
(1,302)	1:39:B:LYS:HD2	1:67:A:LYS:H	7	24.17
(1,702)	1:66:B:LYS:HA	1:41:A:ILE:HG12	15	24.16
(1,429)	1:69:B:SER:HA	1:44:A:LYS:HD2	14	24.16
(1,32)	1:66:A:LYS:H	1:41:B:ILE:HG12	7	24.16
(1,750)	1:69:A:SER:H	1:44:B:LYS:HG2	9	24.15
(1,441)	1:68:B:ASP:HA	1:43:A:GLU:HG2	18	24.15
(1,441)	1:68:B:ASP:HA	1:43:A:GLU:HG2	6	24.14
(1,572)	1:39:A:LYS:HE2	1:65:B:LEU:HD22	18	24.13
(1,457)	1:69:B:SER:HA	1:44:A:LYS:HE2	2	24.13
(1,773)	1:63:B:ASP:H	1:39:A:LYS:HG2	3	24.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:69:A:SER:H	1:44:B:LYS:HG3	7	24.11
(1,694)	1:41:A:ILE:HG13	1:67:B:LYS:HA	19	24.08
(1,45)	1:69:B:SER:H	1:44:A:LYS:HG3	18	24.07
(1,750)	1:69:B:SER:H	1:44:A:LYS:HG2	2	24.05
(1,693)	1:41:B:ILE:HG12	1:67:A:LYS:HA	9	24.05
(1,336)	1:66:A:LYS:H	1:43:B:GLU:HG3	19	24.03
(1,750)	1:69:B:SER:H	1:44:A:LYS:HG2	13	24.02
(1,310)	1:41:A:ILE:HG12	1:67:B:LYS:H	19	24.02
(1,45)	1:69:A:SER:H	1:44:B:LYS:HG3	11	24.02
(1,605)	1:39:A:LYS:HD2	1:67:B:LYS:HG2	17	24.01
(1,302)	1:39:A:LYS:HD2	1:67:B:LYS:H	2	24.01
(1,45)	1:69:B:SER:H	1:44:A:LYS:HG3	16	24.01
(1,693)	1:41:B:ILE:HG12	1:67:A:LYS:HA	12	24.0
(1,565)	1:66:A:LYS:HA	1:44:B:LYS:HE2	20	24.0
(1,310)	1:41:A:ILE:HG12	1:67:B:LYS:H	9	24.0
(1,302)	1:39:B:LYS:HD3	1:67:A:LYS:H	20	24.0
(1,722)	1:39:A:LYS:HG2	1:65:B:LEU:HD21	9	23.99
(1,724)	1:39:B:LYS:HD3	1:65:A:LEU:HD22	20	23.98
(1,336)	1:66:A:LYS:H	1:43:B:GLU:HG3	9	23.98
(1,22)	1:64:B:ALA:H	1:43:A:GLU:HG2	17	23.96
(1,336)	1:66:A:LYS:H	1:43:B:GLU:HG3	18	23.95
(1,750)	1:69:B:SER:H	1:44:A:LYS:HG2	1	23.93
(1,302)	1:39:B:LYS:HD2	1:67:A:LYS:H	11	23.93
(1,723)	1:39:A:LYS:HG3	1:65:B:LEU:HD22	15	23.92
(1,693)	1:41:A:ILE:HG12	1:67:B:LYS:HA	13	23.92
(1,441)	1:68:A:ASP:HA	1:43:B:GLU:HG2	19	23.9
(1,22)	1:64:B:ALA:H	1:43:A:GLU:HG2	19	23.9
(1,693)	1:41:B:ILE:HG12	1:67:A:LYS:HA	4	23.87
(1,457)	1:69:A:SER:HA	1:44:B:LYS:HE2	9	23.87
(1,336)	1:66:B:LYS:H	1:43:A:GLU:HG2	6	23.87
(1,724)	1:39:B:LYS:HD3	1:65:A:LEU:HD22	11	23.86
(1,694)	1:41:B:ILE:HG13	1:67:A:LYS:HA	12	23.86
(1,310)	1:41:B:ILE:HG12	1:67:A:LYS:H	8	23.86
(1,457)	1:69:A:SER:HA	1:44:B:LYS:HE3	8	23.85
(1,323)	1:41:A:ILE:HG13	1:67:B:LYS:H	2	23.85
(1,45)	1:69:A:SER:H	1:44:B:LYS:HG3	5	23.85
(1,773)	1:63:B:ASP:H	1:39:A:LYS:HG2	17	23.84
(1,572)	1:39:A:LYS:HE2	1:65:B:LEU:HD22	1	23.84
(1,328)	1:69:B:SER:H	1:44:A:LYS:HE2	13	23.82
(1,305)	1:39:A:LYS:HD2	1:66:B:LYS:H	6	23.82
(1,32)	1:66:B:LYS:H	1:41:A:ILE:HG12	18	23.81
(1,723)	1:39:B:LYS:HG3	1:65:A:LEU:HD23	8	23.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,599)	1:69:A:SER:HB3	1:44:B:LYS:HE2	7	23.79
(1,310)	1:41:B:ILE:HG12	1:67:A:LYS:H	4	23.79
(1,310)	1:41:A:ILE:HG12	1:67:B:LYS:H	13	23.79
(1,605)	1:39:B:LYS:HD3	1:67:A:LYS:HG2	16	23.78
(1,525)	1:44:A:LYS:HE2	1:70:B:SER:H	2	23.78
(1,45)	1:69:B:SER:H	1:44:A:LYS:HG3	17	23.78
(1,686)	1:66:A:LYS:HG2	1:45:B:ARG:HD3	6	23.77
(1,605)	1:39:B:LYS:HD2	1:67:A:LYS:HG2	4	23.77
(1,336)	1:66:B:LYS:H	1:43:A:GLU:HG2	17	23.76
(1,22)	1:64:A:ALA:H	1:43:B:GLU:HG3	8	23.75
(1,694)	1:41:A:ILE:HG13	1:67:B:LYS:HA	13	23.73
(1,310)	1:41:B:ILE:HG12	1:67:A:LYS:H	12	23.73
(1,750)	1:69:A:SER:H	1:44:B:LYS:HG2	10	23.69
(1,702)	1:66:A:LYS:HA	1:41:B:ILE:HG12	20	23.69
(1,702)	1:66:B:LYS:HA	1:41:A:ILE:HG12	17	23.68
(1,429)	1:69:B:SER:HA	1:44:A:LYS:HD2	11	23.68
(1,323)	1:41:B:ILE:HG13	1:67:A:LYS:H	3	23.68
(1,32)	1:66:A:LYS:H	1:41:B:ILE:HG12	6	23.68
(1,724)	1:39:A:LYS:HD2	1:65:B:LEU:HD23	14	23.67
(1,694)	1:41:B:ILE:HG13	1:67:A:LYS:HA	4	23.67
(1,457)	1:69:A:SER:HA	1:44:B:LYS:HE2	18	23.67
(1,336)	1:66:B:LYS:H	1:43:A:GLU:HG2	3	23.67
(1,750)	1:69:B:SER:H	1:44:A:LYS:HG2	16	23.66
(1,722)	1:39:B:LYS:HG2	1:65:A:LEU:HD22	18	23.66
(1,693)	1:41:A:ILE:HG12	1:67:B:LYS:HA	2	23.66
(1,617)	1:39:A:LYS:HG2	1:67:B:LYS:HG3	19	23.65
(1,32)	1:66:A:LYS:H	1:41:B:ILE:HG12	11	23.65
(1,457)	1:69:A:SER:HA	1:44:B:LYS:HE3	5	23.64
(1,441)	1:68:A:ASP:HA	1:43:B:GLU:HG2	5	23.64
(1,22)	1:64:A:ALA:H	1:43:B:GLU:HG3	4	23.64
(1,723)	1:39:A:LYS:HG3	1:65:B:LEU:HD21	17	23.63
(1,694)	1:41:B:ILE:HG13	1:67:A:LYS:HA	9	23.63
(1,32)	1:66:B:LYS:H	1:41:A:ILE:HG12	14	23.63
(1,693)	1:41:B:ILE:HG12	1:67:A:LYS:HA	8	23.62
(1,613)	1:61:B:ILE:HG22	1:36:A:LYS:HE2	9	23.62
(1,310)	1:41:B:ILE:HG12	1:67:A:LYS:H	16	23.61
(1,457)	1:69:A:SER:HA	1:44:B:LYS:HE2	10	23.6
(1,441)	1:68:A:ASP:HA	1:43:B:GLU:HG2	9	23.6
(1,441)	1:68:A:ASP:HA	1:43:B:GLU:HG2	20	23.6
(1,323)	1:41:B:ILE:HG13	1:67:A:LYS:H	5	23.6
(1,22)	1:64:A:ALA:H	1:43:B:GLU:HG3	18	23.58
(1,786)	1:39:A:LYS:HE2	1:65:B:LEU:HG	6	23.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,672)	1:39:A:LYS:HG2	1:67:B:LYS:HG2	19	23.55
(1,773)	1:63:B:ASP:H	1:39:A:LYS:HG2	16	23.54
(1,773)	1:63:B:ASP:H	1:39:A:LYS:HG2	15	23.52
(1,336)	1:66:A:LYS:H	1:43:B:GLU:HG3	5	23.52
(1,45)	1:69:A:SER:H	1:44:B:LYS:HG3	15	23.52
(1,694)	1:41:A:ILE:HG13	1:67:B:LYS:HA	2	23.51
(1,605)	1:39:B:LYS:HD2	1:67:A:LYS:HG2	5	23.51
(1,429)	1:69:A:SER:HA	1:44:B:LYS:HD2	12	23.51
(1,323)	1:41:B:ILE:HG13	1:67:A:LYS:H	1	23.5
(1,750)	1:69:A:SER:H	1:44:B:LYS:HG2	11	23.49
(1,441)	1:68:B:ASP:HA	1:43:A:GLU:HG2	3	23.49
(1,22)	1:64:A:ALA:H	1:43:B:GLU:HG3	5	23.49
(1,773)	1:63:B:ASP:H	1:39:A:LYS:HG2	2	23.48
(1,723)	1:39:B:LYS:HG3	1:65:A:LEU:HD22	5	23.47
(1,606)	1:39:B:LYS:HD2	1:67:A:LYS:HG3	4	23.47
(1,606)	1:39:B:LYS:HD3	1:67:A:LYS:HG3	5	23.46
(1,605)	1:39:A:LYS:HD2	1:67:B:LYS:HG2	13	23.42
(1,606)	1:39:A:LYS:HD2	1:67:B:LYS:HG3	13	23.41
(1,441)	1:68:B:ASP:HA	1:43:A:GLU:HG2	17	23.41
(1,32)	1:66:B:LYS:H	1:41:A:ILE:HG12	15	23.39
(1,750)	1:69:A:SER:H	1:44:B:LYS:HG2	7	23.38
(1,750)	1:69:B:SER:H	1:44:A:LYS:HG2	14	23.38
(1,724)	1:39:A:LYS:HD2	1:65:B:LEU:HD22	1	23.38
(1,336)	1:66:A:LYS:H	1:43:B:GLU:HG2	20	23.38
(1,773)	1:63:A:ASP:H	1:39:B:LYS:HG2	20	23.37
(1,606)	1:39:B:LYS:HD2	1:67:A:LYS:HG3	12	23.36
(1,686)	1:66:A:LYS:HG2	1:45:B:ARG:HD3	20	23.35
(1,323)	1:41:B:ILE:HG13	1:67:A:LYS:H	7	23.35
(1,302)	1:39:A:LYS:HD2	1:67:B:LYS:H	15	23.35
(1,45)	1:69:A:SER:H	1:44:B:LYS:HG3	10	23.35
(1,45)	1:69:B:SER:H	1:44:A:LYS:HG3	19	23.35
(1,605)	1:39:B:LYS:HD2	1:67:A:LYS:HG2	12	23.34
(1,336)	1:66:B:LYS:H	1:43:A:GLU:HG2	11	23.34
(1,22)	1:64:B:ALA:H	1:43:A:GLU:HG2	3	23.33
(1,693)	1:41:B:ILE:HG12	1:67:A:LYS:HA	5	23.32
(1,525)	1:44:B:LYS:HE3	1:70:A:SER:H	5	23.32
(1,477)	1:66:B:LYS:HA	1:45:A:ARG:HD2	2	23.32
(1,22)	1:64:A:ALA:H	1:43:B:GLU:HG3	9	23.32
(1,441)	1:68:B:ASP:HA	1:43:A:GLU:HG2	11	23.31
(1,42)	1:43:B:GLU:HG2	1:69:A:SER:H	4	23.31
(1,723)	1:39:A:LYS:HG3	1:65:B:LEU:HD21	19	23.3
(1,525)	1:44:B:LYS:HE3	1:70:A:SER:H	8	23.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,694)	1:41:B:ILE:HG13	1:67:A:LYS:HA	8	23.29
(1,773)	1:63:A:ASP:H	1:39:B:LYS:HG2	4	23.28
(1,525)	1:44:B:LYS:HE2	1:70:A:SER:H	18	23.28
(1,323)	1:41:A:ILE:HG13	1:67:B:LYS:H	10	23.27
(1,310)	1:41:A:ILE:HG12	1:67:B:LYS:H	2	23.27
(1,750)	1:69:A:SER:H	1:44:B:LYS:HG2	15	23.26
(1,672)	1:39:B:LYS:HG2	1:67:A:LYS:HG2	8	23.26
(1,606)	1:39:A:LYS:HD2	1:67:B:LYS:HG3	17	23.26
(1,336)	1:66:A:LYS:H	1:43:B:GLU:HG3	7	23.26
(1,302)	1:39:A:LYS:HD2	1:67:B:LYS:H	1	23.25
(1,336)	1:66:A:LYS:H	1:43:B:GLU:HG3	12	23.23
(1,605)	1:39:A:LYS:HD2	1:67:B:LYS:HG2	7	23.22
(1,617)	1:39:A:LYS:HG2	1:67:B:LYS:HG3	9	23.21
(1,525)	1:44:B:LYS:HE3	1:70:A:SER:H	6	23.21
(1,750)	1:69:B:SER:H	1:44:A:LYS:HG2	18	23.2
(1,722)	1:39:A:LYS:HG2	1:65:B:LEU:HD21	3	23.2
(1,302)	1:39:B:LYS:HD2	1:67:A:LYS:H	10	23.2
(1,22)	1:64:A:ALA:H	1:43:B:GLU:HG2	20	23.2
(1,457)	1:69:A:SER:HA	1:44:B:LYS:HE3	19	23.19
(1,310)	1:41:B:ILE:HG12	1:67:A:LYS:H	3	23.18
(1,302)	1:39:A:LYS:HD2	1:67:B:LYS:H	14	23.17
(1,527)	1:39:A:LYS:HE2	1:66:B:LYS:H	6	23.16
(1,694)	1:41:B:ILE:HG13	1:67:A:LYS:HA	5	23.15
(1,611)	1:39:A:LYS:HG3	1:67:B:LYS:HG2	19	23.15
(1,457)	1:69:A:SER:HA	1:44:B:LYS:HE2	11	23.14
(1,525)	1:44:B:LYS:HE3	1:70:A:SER:H	19	23.13
(1,457)	1:69:A:SER:HA	1:44:B:LYS:HE2	12	23.13
(1,429)	1:69:B:SER:HA	1:44:A:LYS:HD2	19	23.12
(1,605)	1:39:A:LYS:HD2	1:67:B:LYS:HG2	2	23.11
(1,465)	1:61:A:ILE:HA	1:36:B:LYS:HE3	15	23.11
(1,429)	1:69:B:SER:HA	1:44:A:LYS:HD2	3	23.11
(1,677)	1:39:A:LYS:HG3	1:67:B:LYS:HG3	19	23.1
(1,457)	1:69:A:SER:HA	1:44:B:LYS:HE2	17	23.1
(1,693)	1:41:B:ILE:HG12	1:67:A:LYS:HA	6	23.09
(1,525)	1:44:B:LYS:HE2	1:70:A:SER:H	12	23.09
(1,22)	1:64:A:ALA:H	1:43:B:GLU:HG3	15	23.08
(1,42)	1:43:A:GLU:HG2	1:69:B:SER:H	8	23.06
(1,722)	1:39:B:LYS:HG2	1:65:A:LEU:HD22	20	23.05
(1,336)	1:66:B:LYS:H	1:43:A:GLU:HG2	14	23.05
(1,605)	1:39:B:LYS:HD2	1:67:A:LYS:HG2	10	23.04
(1,32)	1:66:B:LYS:H	1:41:A:ILE:HG12	17	23.04
(1,750)	1:69:B:SER:H	1:44:A:LYS:HG2	17	23.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,604)	1:61:A:ILE:HD12	1:36:B:LYS:HE3	11	23.02
(1,773)	1:63:B:ASP:H	1:39:A:LYS:HG2	11	23.01
(1,441)	1:68:A:ASP:HA	1:43:B:GLU:HG2	15	23.01
(1,310)	1:41:B:ILE:HG12	1:67:A:LYS:H	5	23.01
(1,579)	1:61:B:ILE:HB	1:36:A:LYS:HE2	9	23.0
(1,429)	1:69:B:SER:HA	1:44:A:LYS:HD2	2	23.0
(1,429)	1:69:B:SER:HA	1:44:A:LYS:HD2	6	23.0
(1,22)	1:64:B:ALA:H	1:43:A:GLU:HG2	14	23.0
(1,693)	1:41:B:ILE:HG12	1:67:A:LYS:HA	16	22.98
(1,617)	1:39:A:LYS:HG2	1:67:B:LYS:HG3	18	22.98
(1,310)	1:41:B:ILE:HG12	1:67:A:LYS:H	1	22.98
(1,613)	1:61:B:ILE:HG21	1:36:A:LYS:HE2	10	22.97
(1,465)	1:61:A:ILE:HA	1:36:B:LYS:HE3	20	22.97
(1,22)	1:64:A:ALA:H	1:43:B:GLU:HG3	12	22.97
(1,605)	1:39:B:LYS:HD3	1:67:A:LYS:HG2	20	22.96
(1,773)	1:63:B:ASP:H	1:39:A:LYS:HG2	13	22.95
(1,457)	1:69:B:SER:HA	1:44:A:LYS:HE2	16	22.95
(1,606)	1:39:B:LYS:HD3	1:67:A:LYS:HG3	8	22.94
(1,323)	1:41:B:ILE:HG13	1:67:A:LYS:H	6	22.94
(1,22)	1:64:B:ALA:H	1:43:A:GLU:HG2	6	22.94
(1,606)	1:39:A:LYS:HD2	1:67:B:LYS:HG3	7	22.93
(1,525)	1:44:B:LYS:HE2	1:70:A:SER:H	1	22.93
(1,323)	1:41:B:ILE:HG13	1:67:A:LYS:H	11	22.92
(1,525)	1:44:A:LYS:HE2	1:70:B:SER:H	16	22.9
(1,441)	1:68:A:ASP:HA	1:43:B:GLU:HG2	12	22.9
(1,606)	1:39:B:LYS:HD3	1:67:A:LYS:HG3	20	22.89
(1,429)	1:69:B:SER:HA	1:44:A:LYS:HD2	13	22.89
(1,42)	1:43:A:GLU:HG2	1:69:B:SER:H	18	22.89
(1,694)	1:41:B:ILE:HG13	1:67:A:LYS:HA	6	22.88
(1,672)	1:39:A:LYS:HG2	1:67:B:LYS:HG2	18	22.88
(1,525)	1:44:B:LYS:HE2	1:70:A:SER:H	17	22.88
(1,457)	1:69:B:SER:HA	1:44:A:LYS:HE2	3	22.87
(1,723)	1:39:A:LYS:HG3	1:65:B:LEU:HD21	9	22.86
(1,336)	1:66:B:LYS:H	1:43:A:GLU:HG2	16	22.86
(1,457)	1:69:A:SER:HA	1:44:B:LYS:HE3	15	22.85
(1,21)	1:64:B:ALA:H	1:39:A:LYS:HE2	6	22.85
(1,336)	1:66:B:LYS:H	1:43:A:GLU:HG2	15	22.83
(1,606)	1:39:B:LYS:HD2	1:67:A:LYS:HG3	11	22.82
(1,589)	1:68:B:ASP:HB3	1:43:A:GLU:HG2	6	22.82
(1,525)	1:44:A:LYS:HE2	1:70:B:SER:H	4	22.82
(1,310)	1:41:B:ILE:HG12	1:67:A:LYS:H	7	22.82
(1,694)	1:41:B:ILE:HG13	1:67:A:LYS:HA	16	22.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,477)	1:66:A:LYS:HA	1:45:B:ARG:HD3	9	22.81
(1,525)	1:44:B:LYS:HE3	1:70:A:SER:H	15	22.8
(1,45)	1:69:B:SER:H	1:44:A:LYS:HG3	14	22.8
(1,672)	1:39:A:LYS:HG2	1:67:B:LYS:HG2	9	22.79
(1,323)	1:41:A:ILE:HG13	1:67:B:LYS:H	18	22.79
(1,693)	1:41:B:ILE:HG12	1:67:A:LYS:HA	1	22.78
(1,604)	1:61:B:ILE:HD12	1:36:A:LYS:HE2	18	22.78
(1,525)	1:44:B:LYS:HE2	1:70:A:SER:H	11	22.78
(1,477)	1:66:B:LYS:HA	1:45:A:ARG:HD2	13	22.78
(1,773)	1:63:B:ASP:H	1:39:A:LYS:HG2	14	22.77
(1,32)	1:66:A:LYS:H	1:41:B:ILE:HG12	20	22.77
(1,22)	1:64:A:ALA:H	1:43:B:GLU:HG3	10	22.77
(1,457)	1:69:B:SER:HA	1:44:A:LYS:HE2	6	22.76
(1,773)	1:63:B:ASP:H	1:39:A:LYS:HG2	12	22.75
(1,605)	1:39:B:LYS:HD2	1:67:A:LYS:HG2	11	22.75
(1,323)	1:41:A:ILE:HG13	1:67:B:LYS:H	14	22.75
(1,693)	1:41:B:ILE:HG12	1:67:A:LYS:HA	3	22.73
(1,606)	1:39:B:LYS:HD3	1:67:A:LYS:HG3	3	22.73
(1,518)	1:68:A:ASP:H	1:43:B:GLU:HG3	8	22.73
(1,441)	1:68:B:ASP:HA	1:43:A:GLU:HG2	14	22.73
(1,525)	1:44:A:LYS:HE2	1:70:B:SER:H	3	22.72
(1,477)	1:66:B:LYS:HA	1:45:A:ARG:HD2	19	22.72
(1,429)	1:69:A:SER:HA	1:44:B:LYS:HD2	1	22.72
(1,441)	1:68:B:ASP:HA	1:43:A:GLU:HG2	16	22.7
(1,17)	1:95:A:GLN:H	1:71:B:ARG:H	15	22.66
(1,693)	1:41:B:ILE:HG12	1:67:A:LYS:HA	7	22.65
(1,693)	1:41:B:ILE:HG12	1:67:A:LYS:HA	11	22.65
(1,310)	1:41:A:ILE:HG12	1:67:B:LYS:H	10	22.65
(1,42)	1:43:B:GLU:HG2	1:69:A:SER:H	9	22.65
(1,589)	1:68:A:ASP:HB3	1:43:B:GLU:HG3	8	22.64
(1,336)	1:66:B:LYS:H	1:43:A:GLU:HG2	1	22.64
(1,42)	1:43:A:GLU:HG2	1:69:B:SER:H	6	22.64
(1,723)	1:39:B:LYS:HG3	1:65:A:LEU:HD22	18	22.63
(1,301)	1:64:B:ALA:H	1:39:A:LYS:HD2	6	22.63
(1,693)	1:41:A:ILE:HG12	1:67:B:LYS:HA	18	22.62
(1,457)	1:69:B:SER:HA	1:44:A:LYS:HE2	4	22.62
(1,22)	1:64:B:ALA:H	1:43:A:GLU:HG2	11	22.62
(1,604)	1:61:A:ILE:HD11	1:36:B:LYS:HE3	13	22.61
(1,336)	1:66:A:LYS:H	1:43:B:GLU:HG3	10	22.61
(1,477)	1:66:A:LYS:HA	1:45:B:ARG:HD3	4	22.6
(1,441)	1:68:B:ASP:HA	1:43:A:GLU:HG2	1	22.6
(1,42)	1:43:B:GLU:HG2	1:69:A:SER:H	20	22.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,611)	1:39:B:LYS:HG3	1:67:A:LYS:HG2	8	22.58
(1,606)	1:39:A:LYS:HD2	1:67:B:LYS:HG3	14	22.58
(1,457)	1:69:A:SER:HA	1:44:B:LYS:HE2	1	22.58
(1,42)	1:43:B:GLU:HG2	1:69:A:SER:H	5	22.58
(1,328)	1:69:A:SER:H	1:44:B:LYS:HE2	7	22.57
(1,773)	1:63:A:ASP:H	1:39:B:LYS:HG2	7	22.56
(1,694)	1:41:B:ILE:HG13	1:67:A:LYS:HA	1	22.56
(1,518)	1:68:A:ASP:H	1:43:B:GLU:HG2	4	22.56
(1,457)	1:69:B:SER:HA	1:44:A:LYS:HE2	14	22.56
(1,441)	1:68:A:ASP:HA	1:43:B:GLU:HG2	7	22.56
(1,328)	1:69:A:SER:H	1:44:B:LYS:HE2	20	22.56
(1,518)	1:68:A:ASP:H	1:43:B:GLU:HG3	18	22.54
(1,42)	1:43:B:GLU:HG2	1:69:A:SER:H	19	22.54
(1,773)	1:63:A:ASP:H	1:39:B:LYS:HG2	10	22.53
(1,672)	1:39:A:LYS:HG2	1:67:B:LYS:HG2	17	22.53
(1,863)	1:95:B:GLN:HB2	1:71:A:ARG:H	10	22.51
(1,722)	1:39:B:LYS:HG2	1:65:A:LEU:HD22	11	22.5
(1,22)	1:64:A:ALA:H	1:43:B:GLU:HG3	7	22.5
(1,722)	1:39:A:LYS:HG2	1:65:B:LEU:HD23	7	22.49
(1,429)	1:69:A:SER:HA	1:44:A:LYS:HD2	4	22.49
(1,722)	1:39:A:LYS:HG2	1:65:B:LEU:HD22	16	22.48
(1,579)	1:61:A:ILE:HB	1:36:B:LYS:HE3	10	22.48
(1,42)	1:43:A:GLU:HG2	1:69:B:SER:H	3	22.47
(1,677)	1:39:A:LYS:HG3	1:67:B:LYS:HG3	9	22.46
(1,723)	1:39:A:LYS:HG3	1:65:B:LEU:HD21	3	22.45
(1,605)	1:39:A:LYS:HD2	1:67:B:LYS:HG2	14	22.45
(1,310)	1:41:B:ILE:HG12	1:67:A:LYS:H	11	22.43
(1,694)	1:41:B:ILE:HG13	1:67:A:LYS:HA	3	22.42
(1,694)	1:41:B:ILE:HG13	1:67:A:LYS:HA	7	22.42
(1,525)	1:44:B:LYS:HE2	1:70:A:SER:H	10	22.42
(1,22)	1:64:A:ALA:H	1:43:B:GLU:HG3	16	22.42
(1,22)	1:64:B:ALA:H	1:43:A:GLU:HG2	1	22.39
(1,694)	1:41:B:ILE:HG13	1:67:A:LYS:HA	11	22.38
(1,693)	1:41:A:ILE:HG12	1:67:B:LYS:HA	17	22.38
(1,589)	1:68:A:ASP:HB3	1:43:B:GLU:HG2	4	22.38
(1,457)	1:69:B:SER:HA	1:44:A:LYS:HE2	13	22.38
(1,518)	1:68:A:ASP:H	1:43:B:GLU:HG2	19	22.34
(1,310)	1:41:B:ILE:HG12	1:67:A:LYS:H	6	22.34
(1,606)	1:39:A:LYS:HD2	1:67:B:LYS:HG3	1	22.33
(1,42)	1:43:A:GLU:HG2	1:69:B:SER:H	17	22.33
(1,863)	1:95:B:GLN:HB2	1:71:A:ARG:H	16	22.32
(1,694)	1:41:A:ILE:HG13	1:67:B:LYS:HA	18	22.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,336)	1:66:A:LYS:H	1:43:B:GLU:HG3	2	22.31
(1,722)	1:39:B:LYS:HG2	1:65:A:LEU:HD23	10	22.3
(1,310)	1:41:A:ILE:HG12	1:67:B:LYS:H	18	22.3
(1,518)	1:68:B:ASP:H	1:43:A:GLU:HG2	6	22.29
(1,429)	1:69:A:SER:HA	1:44:B:LYS:HD2	20	22.29
(1,17)	1:95:A:GLN:H	1:71:B:ARG:H	16	22.28
(1,773)	1:63:A:ASP:H	1:39:B:LYS:HG2	1	22.27
(1,17)	1:95:A:GLN:H	1:71:A:ARG:H	18	22.27
(1,477)	1:66:A:LYS:HA	1:45:B:ARG:HD3	12	22.25
(1,722)	1:39:A:LYS:HG2	1:65:B:LEU:HD23	2	22.24
(1,323)	1:41:A:ILE:HG13	1:67:B:LYS:H	15	22.24
(1,571)	1:39:A:LYS:HE2	1:65:B:LEU:HD11	6	22.22
(1,336)	1:66:B:LYS:H	1:43:A:GLU:HG2	13	22.22
(1,17)	1:95:B:GLN:H	1:71:B:ARG:H	2	22.22
(1,693)	1:41:A:ILE:HG12	1:67:B:LYS:HA	10	22.2
(1,693)	1:41:A:ILE:HG12	1:67:B:LYS:HA	14	22.19
(1,617)	1:39:B:LYS:HG2	1:67:A:LYS:HG3	20	22.19
(1,611)	1:39:A:LYS:HG3	1:67:B:LYS:HG2	9	22.18
(1,606)	1:39:B:LYS:HD2	1:67:A:LYS:HG3	2	22.17
(1,310)	1:41:A:ILE:HG12	1:67:B:LYS:H	14	22.17
(1,22)	1:64:A:ALA:H	1:43:B:GLU:HG3	2	22.17
(1,297)	1:70:B:SER:H	1:45:A:ARG:HG3	12	22.16
(1,17)	1:95:B:GLN:H	1:71:A:ARG:H	14	22.16
(1,525)	1:44:A:LYS:HE2	1:70:B:SER:H	14	22.15
(1,323)	1:41:A:ILE:HG13	1:67:B:LYS:H	17	22.15
(1,617)	1:39:A:LYS:HG2	1:67:B:LYS:HG3	17	22.14
(1,589)	1:68:B:ASP:HB3	1:43:A:GLU:HG2	18	22.13
(1,17)	1:95:A:GLN:H	1:71:A:ARG:H	12	22.11
(1,302)	1:39:A:LYS:HD2	1:67:B:LYS:H	6	22.1
(1,604)	1:61:A:ILE:HD13	1:36:B:LYS:HE2	4	22.09
(1,589)	1:68:A:ASP:HB3	1:43:B:GLU:HG2	19	22.08
(1,518)	1:68:B:ASP:H	1:43:A:GLU:HG2	9	22.08
(1,617)	1:39:B:LYS:HG2	1:67:A:LYS:HG3	5	22.07
(1,518)	1:68:B:ASP:H	1:43:A:GLU:HG2	17	22.07
(1,441)	1:68:B:ASP:HA	1:43:A:GLU:HG2	2	22.06
(1,297)	1:70:A:SER:H	1:45:B:ARG:HG3	9	22.06
(1,323)	1:41:B:ILE:HG13	1:67:A:LYS:H	20	22.05
(1,604)	1:61:A:ILE:HD11	1:36:B:LYS:HE3	16	22.04
(1,477)	1:66:A:LYS:HA	1:45:B:ARG:HD3	16	22.04
(1,694)	1:41:A:ILE:HG13	1:67:B:LYS:HA	10	22.03
(1,22)	1:64:B:ALA:H	1:43:A:GLU:HG2	13	22.03
(1,42)	1:43:A:GLU:HG2	1:69:B:SER:H	11	22.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:95:A:GLN:H	1:71:B:ARG:H	20	22.01
(1,722)	1:39:A:LYS:HG2	1:65:B:LEU:HD23	14	22.0
(1,611)	1:39:A:LYS:HG3	1:67:B:LYS:HG2	18	22.0
(1,477)	1:66:B:LYS:HA	1:45:A:ARG:HD2	14	22.0
(1,589)	1:68:A:ASP:HB2	1:43:B:GLU:HG2	5	21.99
(1,17)	1:95:B:GLN:H	1:71:A:ARG:H	6	21.99
(1,518)	1:68:A:ASP:H	1:43:B:GLU:HG3	5	21.98
(1,694)	1:41:A:ILE:HG13	1:67:B:LYS:HA	14	21.97
(1,518)	1:68:A:ASP:H	1:43:B:GLU:HG2	20	21.97
(1,694)	1:41:A:ILE:HG13	1:67:B:LYS:HA	17	21.96
(1,441)	1:68:A:ASP:HA	1:43:B:GLU:HG2	10	21.96
(1,677)	1:39:A:LYS:HG3	1:67:B:LYS:HG3	18	21.95
(1,672)	1:39:A:LYS:HG2	1:67:B:LYS:HG2	3	21.95
(1,672)	1:39:B:LYS:HG2	1:67:A:LYS:HG2	20	21.93
(1,297)	1:70:A:SER:H	1:45:B:ARG:HG3	4	21.93
(1,617)	1:39:B:LYS:HG2	1:67:A:LYS:HG3	8	21.9
(1,518)	1:68:B:ASP:H	1:43:A:GLU:HG2	3	21.9
(1,723)	1:39:A:LYS:HG3	1:65:B:LEU:HD22	6	21.88
(1,474)	1:67:A:LYS:HA	1:45:B:ARG:HD3	2	21.88
(1,605)	1:39:A:LYS:HD2	1:67:B:LYS:HG2	15	21.87
(1,606)	1:39:B:LYS:HD3	1:67:A:LYS:HG3	16	21.86
(1,477)	1:66:A:LYS:HA	1:45:B:ARG:HD3	8	21.86
(1,773)	1:63:B:ASP:H	1:39:A:LYS:HG2	6	21.83
(1,723)	1:39:B:LYS:HG3	1:65:A:LEU:HD23	10	21.83
(1,617)	1:39:B:LYS:HG2	1:67:A:LYS:HG3	4	21.83
(1,611)	1:39:A:LYS:HG3	1:67:B:LYS:HG2	3	21.83
(1,525)	1:44:A:LYS:HE2	1:70:B:SER:H	13	21.83
(1,310)	1:41:A:ILE:HG12	1:67:B:LYS:H	15	21.83
(1,17)	1:95:A:GLN:H	1:71:A:ARG:H	1	21.83
(1,605)	1:39:B:LYS:HD2	1:67:A:LYS:HG2	1	21.82
(1,17)	1:95:B:GLN:H	1:71:A:ARG:H	7	21.82
(1,42)	1:43:B:GLU:HG2	1:69:A:SER:H	15	21.8
(1,611)	1:39:A:LYS:HG3	1:67:B:LYS:HG2	17	21.79
(1,613)	1:61:A:ILE:HG23	1:36:B:LYS:HE3	20	21.78
(1,310)	1:41:A:ILE:HG12	1:67:B:LYS:H	17	21.78
(1,723)	1:39:B:LYS:HG3	1:65:A:LEU:HD21	16	21.77
(1,672)	1:39:B:LYS:HG2	1:67:A:LYS:HG2	4	21.77
(1,589)	1:68:A:ASP:HB3	1:43:B:GLU:HG2	9	21.76
(1,672)	1:39:B:LYS:HG2	1:67:A:LYS:HG2	5	21.75
(1,863)	1:95:B:GLN:HB3	1:71:A:ARG:H	13	21.74
(1,441)	1:68:B:ASP:HA	1:43:A:GLU:HG2	13	21.74
(1,863)	1:95:A:GLN:HB2	1:71:B:ARG:H	18	21.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,477)	1:66:A:LYS:HA	1:45:B:ARG:HD3	1	21.7
(1,723)	1:39:B:LYS:HG3	1:65:A:LEU:HD22	20	21.69
(1,697)	1:70:A:SER:HA	1:45:B:ARG:HG2	9	21.69
(1,617)	1:39:B:LYS:HG2	1:67:A:LYS:HG3	11	21.69
(1,606)	1:39:A:LYS:HD2	1:67:B:LYS:HG3	15	21.69
(1,515)	1:36:A:LYS:HE2	1:62:B:LEU:H	9	21.68
(1,677)	1:39:A:LYS:HG3	1:67:B:LYS:HG3	6	21.67
(1,604)	1:61:B:ILE:HD12	1:36:A:LYS:HE2	3	21.67
(1,518)	1:68:B:ASP:H	1:43:A:GLU:HG2	11	21.67
(1,42)	1:43:B:GLU:HG2	1:69:A:SER:H	12	21.67
(1,863)	1:95:B:GLN:HB3	1:71:A:ARG:H	1	21.65
(1,697)	1:70:B:SER:HA	1:45:A:ARG:HG2	12	21.65
(1,477)	1:66:B:LYS:HA	1:45:A:ARG:HD2	18	21.65
(1,477)	1:66:A:LYS:HA	1:45:B:ARG:HD3	3	21.64
(1,17)	1:95:B:GLN:H	1:71:A:ARG:H	3	21.63
(1,863)	1:95:B:GLN:HB3	1:71:A:ARG:H	12	21.62
(1,693)	1:41:A:ILE:HG12	1:67:B:LYS:HA	15	21.62
(1,518)	1:68:A:ASP:H	1:43:B:GLU:HG2	15	21.62
(1,604)	1:61:B:ILE:HD13	1:36:A:LYS:HE2	12	21.61
(1,617)	1:39:A:LYS:HG2	1:67:B:LYS:HG3	12	21.59
(1,595)	1:39:A:LYS:HG3	1:67:B:LYS:HB2	19	21.59
(1,17)	1:95:B:GLN:H	1:71:A:ARG:H	10	21.59
(1,426)	1:70:A:SER:HA	1:45:B:ARG:HG3	9	21.58
(1,589)	1:68:B:ASP:HB3	1:43:A:GLU:HG2	11	21.57
(1,589)	1:68:B:ASP:HB3	1:43:A:GLU:HG2	17	21.57
(1,589)	1:68:A:ASP:HB3	1:43:B:GLU:HG2	20	21.57
(1,613)	1:61:A:ILE:HG21	1:36:B:LYS:HE2	15	21.55
(1,612)	1:41:A:ILE:HG12	1:67:B:LYS:HG2	19	21.54
(1,677)	1:39:B:LYS:HG3	1:67:A:LYS:HG3	12	21.53
(1,612)	1:41:B:ILE:HG12	1:67:A:LYS:HG2	8	21.53
(1,589)	1:68:B:ASP:HB3	1:43:A:GLU:HG2	3	21.53
(1,611)	1:39:A:LYS:HG3	1:67:B:LYS:HG2	6	21.52
(1,426)	1:70:A:SER:HA	1:45:B:ARG:HG3	12	21.52
(1,724)	1:39:A:LYS:HD2	1:65:B:LEU:HD22	6	21.51
(1,693)	1:41:B:ILE:HG12	1:67:A:LYS:HA	20	21.51
(1,672)	1:39:A:LYS:HG2	1:67:B:LYS:HG2	12	21.51
(1,310)	1:41:B:ILE:HG12	1:67:A:LYS:H	20	21.51
(1,297)	1:70:B:SER:H	1:45:A:ARG:HG3	19	21.51
(1,477)	1:66:A:LYS:HA	1:45:B:ARG:HD3	5	21.48
(1,429)	1:69:A:SER:HA	1:44:B:LYS:HD2	7	21.48
(1,42)	1:43:A:GLU:HG2	1:69:B:SER:H	16	21.48
(1,303)	1:70:A:SER:H	1:45:B:ARG:HG2	9	21.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:95:A:GLN:H	1:71:B:ARG:H	17	21.46
(1,617)	1:39:B:LYS:HG2	1:67:A:LYS:HG3	3	21.45
(1,572)	1:39:A:LYS:HE2	1:65:B:LEU:HD22	6	21.44
(1,40)	1:69:B:SER:H	1:45:A:ARG:HD2	2	21.44
(1,723)	1:39:A:LYS:HG3	1:65:B:LEU:HD23	7	21.43
(1,617)	1:39:A:LYS:HG2	1:67:B:LYS:HG3	7	21.43
(1,722)	1:39:A:LYS:HG2	1:65:B:LEU:HD22	1	21.42
(1,672)	1:39:B:LYS:HG2	1:67:A:LYS:HG2	16	21.42
(1,474)	1:67:A:LYS:HA	1:45:B:ARG:HD3	19	21.42
(1,611)	1:39:B:LYS:HG3	1:67:A:LYS:HG2	4	21.41
(1,863)	1:95:B:GLN:HB2	1:71:A:ARG:H	17	21.4
(1,474)	1:67:A:LYS:HA	1:45:B:ARG:HD3	9	21.4
(1,303)	1:70:A:SER:H	1:45:B:ARG:HG2	4	21.4
(1,604)	1:61:A:ILE:HD12	1:36:B:LYS:HE3	17	21.39
(1,617)	1:39:A:LYS:HG2	1:67:B:LYS:HG3	13	21.37
(1,617)	1:39:A:LYS:HG2	1:67:B:LYS:HG3	14	21.37
(1,611)	1:39:A:LYS:HG3	1:67:B:LYS:HG2	16	21.36
(1,606)	1:39:A:LYS:HD2	1:67:B:LYS:HG3	10	21.36
(1,303)	1:70:B:SER:H	1:45:A:ARG:HG2	12	21.36
(1,863)	1:95:A:GLN:HB2	1:71:B:ARG:H	15	21.35
(1,677)	1:39:B:LYS:HG3	1:67:A:LYS:HG3	4	21.35
(1,677)	1:39:B:LYS:HG3	1:67:A:LYS:HG3	5	21.35
(1,17)	1:95:B:GLN:H	1:71:A:ARG:H	5	21.35
(1,17)	1:95:B:GLN:H	1:71:A:ARG:H	19	21.3
(1,672)	1:39:B:LYS:HG2	1:67:A:LYS:HG2	7	21.29
(1,42)	1:43:B:GLU:HG2	1:69:A:SER:H	7	21.29
(1,465)	1:61:A:ILE:HA	1:36:B:LYS:HE3	11	21.28
(1,297)	1:70:B:SER:H	1:45:A:ARG:HG3	2	21.28
(1,672)	1:39:B:LYS:HG2	1:67:A:LYS:HG2	11	21.27
(1,477)	1:66:A:LYS:HA	1:45:B:ARG:HD3	15	21.26
(1,694)	1:41:A:ILE:HG13	1:67:B:LYS:HA	15	21.25
(1,42)	1:43:A:GLU:HG2	1:69:B:SER:H	1	21.25
(1,723)	1:39:B:LYS:HG3	1:65:A:LEU:HD22	11	21.24
(1,677)	1:39:A:LYS:HG3	1:67:B:LYS:HG3	17	21.24
(1,611)	1:39:B:LYS:HG3	1:67:A:LYS:HG2	12	21.24
(1,589)	1:68:A:ASP:HB3	1:43:B:GLU:HG2	15	21.23
(1,477)	1:66:A:LYS:HA	1:45:B:ARG:HD3	10	21.23
(1,347)	1:67:B:LYS:H	1:45:A:ARG:HD2	2	21.23
(1,330)	1:93:A:ARG:HB3	1:71:B:ARG:H	9	21.23
(1,297)	1:70:B:SER:H	1:45:A:ARG:HG3	13	21.23
(1,723)	1:39:A:LYS:HG3	1:65:B:LEU:HD23	2	21.22
(1,722)	1:39:A:LYS:HG2	1:65:B:LEU:HD22	6	21.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,697)	1:70:B:SER:HA	1:45:A:ARG:HG2	2	21.21
(1,694)	1:41:B:ILE:HG13	1:67:A:LYS:HA	20	21.21
(1,863)	1:95:A:GLN:HB2	1:71:B:ARG:H	20	21.2
(1,17)	1:95:B:GLN:H	1:71:A:ARG:H	4	21.2
(1,611)	1:39:B:LYS:HG3	1:67:A:LYS:HG2	5	21.18
(1,677)	1:39:A:LYS:HG3	1:67:B:LYS:HG3	13	21.17
(1,605)	1:39:A:LYS:HD2	1:67:B:LYS:HG2	6	21.17
(1,457)	1:69:A:SER:HA	1:44:B:LYS:HE2	20	21.17
(1,42)	1:43:A:GLU:HG2	1:69:B:SER:H	14	21.17
(1,589)	1:68:B:ASP:HB3	1:43:A:GLU:HG2	14	21.16
(1,42)	1:43:B:GLU:HG2	1:69:A:SER:H	10	21.16
(1,518)	1:68:A:ASP:H	1:43:B:GLU:HG3	7	21.15
(1,303)	1:70:B:SER:H	1:45:A:ARG:HG2	2	21.15
(1,677)	1:39:B:LYS:HG3	1:67:A:LYS:HG3	20	21.14
(1,465)	1:61:A:ILE:HA	1:36:B:LYS:HE3	13	21.14
(1,579)	1:61:A:ILE:HB	1:36:B:LYS:HE3	15	21.13
(1,465)	1:61:A:ILE:HA	1:36:B:LYS:HE2	4	21.13
(1,330)	1:93:B:ARG:HB3	1:71:A:ARG:H	12	21.13
(1,518)	1:68:B:ASP:H	1:43:A:GLU:HG2	16	21.1
(1,672)	1:39:A:LYS:HG2	1:67:B:LYS:HG2	2	21.09
(1,697)	1:70:B:SER:HA	1:45:A:ARG:HG2	4	21.07
(1,589)	1:68:A:ASP:HB3	1:43:B:GLU:HG2	12	21.07
(1,518)	1:68:B:ASP:H	1:43:A:GLU:HG2	14	21.07
(1,612)	1:41:A:ILE:HG12	1:67:B:LYS:HG2	9	21.05
(1,612)	1:41:B:ILE:HG12	1:67:A:LYS:HG2	4	21.04
(1,612)	1:41:B:ILE:HG12	1:67:A:LYS:HG2	3	21.03
(1,595)	1:39:A:LYS:HG3	1:67:B:LYS:HB2	9	21.03
(1,465)	1:61:B:ILE:HA	1:36:A:LYS:HE2	18	21.03
(1,297)	1:70:A:SER:H	1:45:B:ARG:HG3	16	21.03
(1,42)	1:43:A:GLU:HG2	1:69:B:SER:H	2	21.03
(1,611)	1:39:B:LYS:HG3	1:67:A:LYS:HG2	20	21.02
(1,347)	1:67:A:LYS:H	1:45:B:ARG:HD3	9	21.02
(1,330)	1:93:A:ARG:HB3	1:71:A:ARG:H	5	21.02
(1,297)	1:70:A:SER:H	1:45:B:ARG:HG3	5	21.02
(1,672)	1:39:A:LYS:HG2	1:67:B:LYS:HG2	13	21.0
(1,518)	1:68:A:ASP:H	1:43:B:GLU:HG2	12	21.0
(1,474)	1:67:B:LYS:HA	1:45:A:ARG:HD2	13	21.0
(1,677)	1:39:B:LYS:HG3	1:67:A:LYS:HG3	8	20.98
(1,606)	1:39:A:LYS:HD2	1:67:B:LYS:HG3	6	20.96
(1,47)	1:43:B:GLU:HG2	1:70:A:SER:H	4	20.96
(1,612)	1:41:A:ILE:HG12	1:67:B:LYS:HG2	13	20.95
(1,595)	1:39:B:LYS:HG3	1:67:A:LYS:HB2	8	20.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,297)	1:70:A:SER:H	1:45:B:ARG:HG3	3	20.95
(1,589)	1:68:A:ASP:HB3	1:43:B:GLU:HG2	7	20.94
(1,579)	1:61:A:ILE:HB	1:36:B:LYS:HE3	20	20.94
(1,477)	1:66:A:LYS:HA	1:45:B:ARG:HD3	17	20.93
(1,611)	1:39:A:LYS:HG3	1:67:B:LYS:HG2	13	20.92
(1,477)	1:66:A:LYS:HA	1:45:B:ARG:HD3	11	20.91
(1,474)	1:67:A:LYS:HA	1:45:B:ARG:HD3	12	20.91
(1,672)	1:39:A:LYS:HG2	1:67:B:LYS:HG2	14	20.9
(1,515)	1:36:B:LYS:HE3	1:62:A:LEU:H	10	20.89
(1,863)	1:95:A:GLN:HB2	1:71:B:ARG:H	2	20.88
(1,612)	1:41:B:ILE:HG12	1:67:A:LYS:HG2	12	20.88
(1,518)	1:68:B:ASP:H	1:43:A:GLU:HG2	1	20.87
(1,518)	1:68:A:ASP:H	1:43:B:GLU:HG2	10	20.87
(1,723)	1:39:A:LYS:HG3	1:65:B:LEU:HD23	14	20.85
(1,617)	1:39:A:LYS:HG2	1:67:B:LYS:HG3	1	20.85
(1,611)	1:39:A:LYS:HG3	1:67:B:LYS:HG2	7	20.84
(1,863)	1:95:A:GLN:HB2	1:71:B:ARG:H	6	20.83
(1,303)	1:70:A:SER:H	1:45:B:ARG:HG2	13	20.83
(1,17)	1:95:B:GLN:H	1:71:B:ARG:H	8	20.82
(1,677)	1:39:B:LYS:HG3	1:67:A:LYS:HG3	11	20.81
(1,589)	1:68:B:ASP:HB3	1:43:A:GLU:HG2	16	20.81
(1,500)	1:70:B:SER:H	1:45:A:ARG:HD2	2	20.81
(1,617)	1:39:A:LYS:HG2	1:67:B:LYS:HG3	6	20.8
(1,457)	1:69:A:SER:HA	1:44:B:LYS:HE2	7	20.8
(1,863)	1:95:A:GLN:HB2	1:71:B:ARG:H	14	20.79
(1,426)	1:70:B:SER:HA	1:45:A:ARG:HG3	4	20.79
(1,677)	1:39:A:LYS:HG3	1:67:B:LYS:HG3	7	20.77
(1,612)	1:41:A:ILE:HG12	1:67:B:LYS:HG2	2	20.77
(1,330)	1:93:B:ARG:HB3	1:71:B:ARG:H	1	20.77
(1,677)	1:39:B:LYS:HG3	1:67:A:LYS:HG3	3	20.75
(1,672)	1:39:B:LYS:HG2	1:67:A:LYS:HG2	10	20.73
(1,612)	1:41:B:ILE:HG12	1:67:A:LYS:HG2	16	20.73
(1,611)	1:39:A:LYS:HG3	1:67:B:LYS:HG2	10	20.73
(1,40)	1:69:A:SER:H	1:45:B:ARG:HD3	9	20.72
(1,465)	1:61:A:ILE:HA	1:36:B:LYS:HE3	16	20.71
(1,330)	1:93:B:ARG:HB3	1:71:A:ARG:H	2	20.69
(1,589)	1:68:B:ASP:HB3	1:43:A:GLU:HG2	1	20.68
(1,17)	1:95:A:GLN:H	1:71:B:ARG:H	11	20.66
(1,347)	1:67:B:LYS:H	1:45:A:ARG:HD2	19	20.65
(1,863)	1:95:B:GLN:HB3	1:71:A:ARG:H	7	20.64
(1,426)	1:70:B:SER:HA	1:45:A:ARG:HG3	2	20.64
(1,47)	1:43:A:GLU:HG2	1:70:B:SER:H	8	20.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,611)	1:39:A:LYS:HG3	1:67:B:LYS:HG2	2	20.63
(1,474)	1:67:A:LYS:HA	1:45:B:ARG:HD3	4	20.63
(1,477)	1:66:A:LYS:HA	1:45:B:ARG:HD3	6	20.61
(1,303)	1:70:B:SER:H	1:45:A:ARG:HG2	19	20.61
(1,47)	1:43:A:GLU:HG2	1:70:B:SER:H	6	20.61
(1,677)	1:39:A:LYS:HG3	1:67:B:LYS:HG3	14	20.59
(1,297)	1:70:A:SER:H	1:45:B:ARG:HG3	8	20.57
(1,611)	1:39:B:LYS:HG3	1:67:A:LYS:HG2	11	20.54
(1,465)	1:61:B:ILE:HA	1:36:A:LYS:HE2	12	20.54
(1,297)	1:70:B:SER:H	1:45:A:ARG:HG3	1	20.54
(1,42)	1:43:A:GLU:HG2	1:69:B:SER:H	13	20.54
(1,17)	1:95:A:GLN:H	1:71:A:ARG:H	13	20.53
(1,863)	1:95:B:GLN:HB2	1:71:A:ARG:H	5	20.52
(1,595)	1:39:B:LYS:HG3	1:67:A:LYS:HB2	3	20.5
(1,303)	1:70:B:SER:H	1:45:A:ARG:HG2	1	20.5
(1,303)	1:70:A:SER:H	1:45:B:ARG:HG2	16	20.48
(1,40)	1:69:A:SER:H	1:45:B:ARG:HD3	12	20.48
(1,477)	1:66:A:LYS:HA	1:45:B:ARG:HD3	7	20.45
(1,723)	1:39:A:LYS:HG3	1:65:B:LEU:HD22	1	20.44
(1,426)	1:70:B:SER:HA	1:45:A:ARG:HG3	19	20.44
(1,297)	1:70:A:SER:H	1:45:B:ARG:HG3	11	20.44
(1,525)	1:44:B:LYS:HE2	1:70:A:SER:H	20	20.43
(1,347)	1:67:B:LYS:H	1:45:A:ARG:HD2	13	20.42
(1,518)	1:68:B:ASP:H	1:43:A:GLU:HG2	2	20.41
(1,330)	1:93:B:ARG:HB3	1:71:B:ARG:H	7	20.41
(1,330)	1:93:B:ARG:HB3	1:71:B:ARG:H	16	20.41
(1,426)	1:70:B:SER:HA	1:45:A:ARG:HG3	13	20.39
(1,47)	1:43:B:GLU:HG2	1:70:A:SER:H	9	20.39
(1,612)	1:41:B:ILE:HG12	1:67:A:LYS:HG2	5	20.37
(1,525)	1:44:B:LYS:HE2	1:70:A:SER:H	7	20.36
(1,297)	1:70:A:SER:H	1:45:B:ARG:HG3	10	20.36
(1,697)	1:70:A:SER:HA	1:45:B:ARG:HG2	13	20.35
(1,672)	1:39:A:LYS:HG2	1:67:B:LYS:HG2	6	20.35
(1,47)	1:43:A:GLU:HG2	1:70:B:SER:H	18	20.35
(1,40)	1:69:B:SER:H	1:45:A:ARG:HD2	19	20.35
(1,617)	1:39:A:LYS:HG2	1:67:B:LYS:HG3	15	20.34
(1,303)	1:70:A:SER:H	1:45:B:ARG:HG2	5	20.33
(1,297)	1:70:A:SER:H	1:45:B:ARG:HG3	6	20.32
(1,47)	1:43:B:GLU:HG2	1:70:A:SER:H	5	20.3
(1,422)	1:70:B:SER:HB3	1:45:A:ARG:HD2	2	20.29
(1,330)	1:93:A:ARG:HB3	1:71:B:ARG:H	20	20.29
(1,303)	1:70:A:SER:H	1:45:B:ARG:HG2	3	20.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,612)	1:41:B:ILE:HG12	1:67:A:LYS:HG2	6	20.27
(1,697)	1:70:A:SER:HA	1:45:B:ARG:HG2	16	20.26
(1,611)	1:39:A:LYS:HG3	1:67:B:LYS:HG2	14	20.25
(1,500)	1:70:A:SER:H	1:45:B:ARG:HD3	9	20.25
(1,677)	1:39:A:LYS:HG3	1:67:B:LYS:HG3	1	20.24
(1,697)	1:70:B:SER:HA	1:45:A:ARG:HG2	19	20.23
(1,474)	1:67:A:LYS:HA	1:45:B:ARG:HD3	8	20.21
(1,474)	1:67:B:LYS:HA	1:45:A:ARG:HD2	18	20.21
(1,595)	1:39:A:LYS:HG3	1:67:B:LYS:HB2	18	20.2
(1,518)	1:68:B:ASP:H	1:43:A:GLU:HG2	13	20.2
(1,474)	1:67:A:LYS:HA	1:45:B:ARG:HD3	5	20.2
(1,672)	1:39:A:LYS:HG2	1:67:B:LYS:HG2	15	20.19
(1,347)	1:67:A:LYS:H	1:45:B:ARG:HD3	12	20.19
(1,595)	1:39:A:LYS:HG3	1:67:B:LYS:HB2	6	20.18
(1,330)	1:93:A:ARG:HB3	1:71:A:ARG:H	13	20.18
(1,297)	1:70:A:SER:H	1:45:B:ARG:HG3	15	20.18
(1,672)	1:39:B:LYS:HG2	1:67:A:LYS:HG2	1	20.16
(1,40)	1:69:A:SER:H	1:45:B:ARG:HD3	4	20.16
(1,612)	1:41:A:ILE:HG12	1:67:B:LYS:HG2	10	20.13
(1,330)	1:93:A:ARG:HB3	1:71:A:ARG:H	15	20.12
(1,500)	1:70:A:SER:H	1:45:B:ARG:HD3	12	20.11
(1,595)	1:39:A:LYS:HG3	1:67:B:LYS:HB2	12	20.1
(1,426)	1:70:A:SER:HA	1:45:B:ARG:HG3	16	20.1
(1,40)	1:69:B:SER:H	1:45:A:ARG:HD2	13	20.1
(1,589)	1:68:B:ASP:HB2	1:43:A:GLU:HG2	2	20.09
(1,47)	1:43:B:GLU:HG2	1:70:A:SER:H	19	20.09
(1,612)	1:41:B:ILE:HG12	1:67:A:LYS:HG2	7	20.08
(1,303)	1:70:B:SER:H	1:45:A:ARG:HG2	10	20.08
(1,474)	1:67:A:LYS:HA	1:45:B:ARG:HD3	6	20.07
(1,330)	1:93:A:ARG:HB3	1:71:A:ARG:H	6	20.07
(1,697)	1:70:B:SER:HA	1:45:A:ARG:HG2	1	20.05
(1,617)	1:39:B:LYS:HG2	1:67:A:LYS:HG3	2	20.05
(1,347)	1:67:A:LYS:H	1:45:B:ARG:HD3	4	20.05
(1,604)	1:61:B:ILE:HD13	1:36:A:LYS:HE2	1	20.04
(1,47)	1:43:A:GLU:HG2	1:70:B:SER:H	3	20.03
(1,47)	1:43:B:GLU:HG2	1:70:A:SER:H	20	20.03
(1,863)	1:95:B:GLN:HB2	1:71:A:ARG:H	3	20.02
(1,330)	1:93:A:ARG:HB3	1:71:A:ARG:H	10	20.02
(1,617)	1:39:B:LYS:HG2	1:67:A:LYS:HG3	16	20.01
(1,330)	1:93:A:ARG:HB3	1:71:A:ARG:H	17	20.0
(1,697)	1:70:A:SER:HA	1:45:B:ARG:HG2	3	19.99
(1,613)	1:61:B:ILE:HG13	1:36:A:LYS:HE2	18	19.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	1:70:A:SER:H	1:45:B:ARG:HG2	11	19.99
(1,347)	1:67:A:LYS:H	1:45:B:ARG:HD3	8	19.98
(1,330)	1:93:B:ARG:HB3	1:71:A:ARG:H	14	19.98
(1,677)	1:39:B:LYS:HG3	1:67:A:LYS:HG3	2	19.96
(1,613)	1:61:A:ILE:HG22	1:36:B:LYS:HE3	11	19.96
(1,595)	1:39:A:LYS:HG3	1:67:B:LYS:HB2	16	19.96
(1,426)	1:70:A:SER:HA	1:45:B:ARG:HG3	3	19.96
(1,612)	1:41:A:ILE:HG12	1:67:B:LYS:HG2	17	19.95
(1,595)	1:39:B:LYS:HG3	1:67:A:LYS:HB2	4	19.95
(1,697)	1:70:A:SER:HA	1:45:B:ARG:HG2	5	19.94
(1,697)	1:70:B:SER:HA	1:45:A:ARG:HG2	10	19.94
(1,515)	1:36:B:LYS:HE3	1:62:A:LEU:H	15	19.94
(1,426)	1:70:A:SER:HA	1:45:B:ARG:HG3	5	19.94
(1,330)	1:93:A:ARG:HB3	1:71:A:ARG:H	3	19.94
(1,863)	1:95:B:GLN:HB2	1:71:A:ARG:H	8	19.93
(1,670)	1:93:B:ARG:HB3	1:71:B:ARG:HB2	12	19.93
(1,303)	1:70:A:SER:H	1:45:B:ARG:HG2	15	19.92
(1,453)	1:67:A:LYS:HG2	1:45:B:ARG:HD3	9	19.91
(1,863)	1:95:B:GLN:HB2	1:71:A:ARG:H	19	19.9
(1,515)	1:36:B:LYS:HE3	1:62:A:LEU:H	20	19.88
(1,477)	1:66:A:LYS:HA	1:45:B:ARG:HD3	20	19.87
(1,330)	1:93:B:ARG:HB3	1:71:B:ARG:H	4	19.87
(1,612)	1:41:A:ILE:HG12	1:67:B:LYS:HG2	18	19.86
(1,589)	1:68:A:ASP:HB2	1:43:B:GLU:HG2	10	19.86
(1,303)	1:70:A:SER:H	1:45:B:ARG:HG2	8	19.86
(1,468)	1:70:B:SER:HA	1:45:A:ARG:HD2	2	19.83
(1,465)	1:61:A:ILE:HA	1:36:B:LYS:HE3	17	19.83
(1,40)	1:69:A:SER:H	1:45:B:ARG:HD3	16	19.83
(1,697)	1:70:A:SER:HA	1:45:B:ARG:HG2	15	19.8
(1,422)	1:70:A:SER:HB3	1:45:B:ARG:HD3	9	19.8
(1,589)	1:68:B:ASP:HB2	1:43:A:GLU:HG2	13	19.78
(1,47)	1:43:A:GLU:HG2	1:70:B:SER:H	17	19.78
(1,697)	1:70:A:SER:HA	1:45:B:ARG:HG2	11	19.76
(1,595)	1:39:B:LYS:HG3	1:67:A:LYS:HB2	5	19.76
(1,860)	1:94:B:ALA:HA	1:72:B:HIS:HB2	2	19.75
(1,677)	1:39:B:LYS:HG3	1:67:A:LYS:HG3	16	19.75
(1,347)	1:67:A:LYS:H	1:45:B:ARG:HD3	16	19.75
(1,617)	1:39:A:LYS:HG2	1:67:B:LYS:HG3	10	19.73
(1,604)	1:61:A:ILE:HD12	1:36:B:LYS:HE3	2	19.73
(1,727)	1:93:A:ARG:HA	1:71:A:ARG:HG2	9	19.72
(1,453)	1:67:B:LYS:HG2	1:45:A:ARG:HD2	2	19.72
(1,347)	1:67:A:LYS:H	1:45:B:ARG:HD3	14	19.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,670)	1:93:A:ARG:HB3	1:71:A:ARG:HB2	9	19.7
(1,330)	1:93:A:ARG:HB3	1:71:A:ARG:H	18	19.7
(1,330)	1:93:B:ARG:HB3	1:71:B:ARG:H	11	19.69
(1,330)	1:93:B:ARG:HB3	1:71:B:ARG:H	8	19.67
(1,297)	1:70:B:SER:H	1:45:A:ARG:HG3	18	19.67
(1,109)	1:95:A:GLN:H	1:71:A:ARG:HG2	15	19.67
(1,474)	1:67:A:LYS:HA	1:45:B:ARG:HD3	3	19.64
(1,677)	1:39:A:LYS:HG3	1:67:B:LYS:HG3	15	19.63
(1,595)	1:39:A:LYS:HG3	1:67:B:LYS:HB2	13	19.63
(1,474)	1:67:A:LYS:HA	1:45:B:ARG:HD3	17	19.61
(1,347)	1:67:A:LYS:H	1:45:B:ARG:HD3	3	19.61
(1,611)	1:39:A:LYS:HG3	1:67:B:LYS:HG2	15	19.6
(1,500)	1:70:A:SER:H	1:45:B:ARG:HD3	4	19.6
(1,465)	1:61:B:ILE:HA	1:36:A:LYS:HE2	3	19.6
(1,595)	1:39:A:LYS:HG3	1:67:B:LYS:HB2	17	19.59
(1,474)	1:67:B:LYS:HA	1:45:A:ARG:HD2	10	19.58
(1,426)	1:70:A:SER:HA	1:45:B:ARG:HG3	10	19.58
(1,611)	1:39:B:LYS:HG3	1:67:A:LYS:HG2	1	19.57
(1,595)	1:39:B:LYS:HG3	1:67:A:LYS:HB2	20	19.57
(1,474)	1:67:A:LYS:HA	1:45:B:ARG:HD3	1	19.57
(1,474)	1:67:A:LYS:HA	1:45:B:ARG:HD3	16	19.57
(1,612)	1:41:B:ILE:HG12	1:67:A:LYS:HG2	1	19.56
(1,613)	1:61:A:ILE:HG21	1:36:B:LYS:HE3	13	19.55
(1,500)	1:70:B:SER:H	1:45:A:ARG:HD2	19	19.55
(1,426)	1:70:A:SER:HA	1:45:B:ARG:HG3	8	19.55
(1,40)	1:69:A:SER:H	1:45:B:ARG:HD3	1	19.55
(1,612)	1:41:B:ILE:HG12	1:67:A:LYS:HG2	11	19.54
(1,347)	1:67:B:LYS:H	1:45:A:ARG:HD2	18	19.54
(1,697)	1:70:A:SER:HA	1:45:B:ARG:HG2	8	19.53
(1,474)	1:67:A:LYS:HA	1:45:B:ARG:HD3	11	19.52
(1,474)	1:67:B:LYS:HA	1:45:A:ARG:HD2	15	19.52
(1,422)	1:70:A:SER:HB2	1:45:B:ARG:HD3	12	19.52
(1,474)	1:67:A:LYS:HA	1:45:B:ARG:HD3	14	19.5
(1,426)	1:70:A:SER:HA	1:45:B:ARG:HG3	11	19.5
(1,727)	1:93:B:ARG:HA	1:71:A:ARG:HG3	12	19.49
(1,612)	1:41:A:ILE:HG12	1:67:B:LYS:HG2	14	19.49
(1,613)	1:61:A:ILE:HG21	1:36:B:LYS:HE2	4	19.45
(1,500)	1:70:B:SER:H	1:45:A:ARG:HD2	13	19.45
(1,426)	1:70:A:SER:HA	1:45:B:ARG:HG3	6	19.44
(1,297)	1:70:B:SER:H	1:45:A:ARG:HG3	17	19.44
(1,352)	1:93:A:ARG:HA	1:72:B:HIS:H	15	19.41
(1,303)	1:70:A:SER:H	1:45:B:ARG:HG2	6	19.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:43:B:GLU:HG2	1:70:A:SER:H	15	19.41
(1,604)	1:61:A:ILE:HD12	1:36:B:LYS:HE3	7	19.4
(1,863)	1:95:B:GLN:HB2	1:71:A:ARG:H	4	19.39
(1,426)	1:70:B:SER:HA	1:45:A:ARG:HG3	1	19.39
(1,347)	1:67:A:LYS:H	1:45:B:ARG:HD3	5	19.39
(1,47)	1:43:B:GLU:HG2	1:70:A:SER:H	12	19.39
(1,297)	1:70:A:SER:H	1:45:B:ARG:HG3	7	19.36
(1,670)	1:93:A:ARG:HB3	1:71:A:ARG:HB2	2	19.35
(1,595)	1:39:B:LYS:HG3	1:67:A:LYS:HB2	11	19.35
(1,426)	1:70:A:SER:HA	1:45:B:ARG:HG3	15	19.35
(1,595)	1:39:B:LYS:HG3	1:67:A:LYS:HB2	7	19.33
(1,47)	1:43:A:GLU:HG2	1:70:B:SER:H	11	19.33
(1,40)	1:69:A:SER:H	1:45:B:ARG:HD3	5	19.32
(1,40)	1:69:A:SER:H	1:45:B:ARG:HD3	3	19.31
(1,347)	1:67:A:LYS:H	1:45:B:ARG:HD3	1	19.28
(1,109)	1:95:B:GLN:H	1:71:A:ARG:HG3	6	19.28
(1,500)	1:70:A:SER:H	1:45:B:ARG:HD3	1	19.27
(1,468)	1:70:A:SER:HA	1:45:B:ARG:HD3	9	19.26
(1,860)	1:94:A:ALA:HA	1:72:A:HIS:HB2	15	19.25
(1,347)	1:67:A:LYS:H	1:45:B:ARG:HD3	10	19.24
(1,297)	1:70:B:SER:H	1:45:A:ARG:HG3	14	19.24
(1,109)	1:95:B:GLN:H	1:71:B:ARG:HG3	2	19.24
(1,297)	1:70:A:SER:H	1:45:B:ARG:HG3	20	19.23
(1,697)	1:70:A:SER:HA	1:45:B:ARG:HG2	6	19.22
(1,109)	1:95:A:GLN:H	1:71:A:ARG:HG2	1	19.22
(1,697)	1:70:B:SER:HA	1:45:A:ARG:HG2	17	19.21
(1,595)	1:39:A:LYS:HG3	1:67:B:LYS:HB2	2	19.21
(1,579)	1:61:A:ILE:HB	1:36:B:LYS:HE3	11	19.21
(1,453)	1:67:A:LYS:HG2	1:45:B:ARG:HD3	19	19.21
(1,579)	1:61:A:ILE:HB	1:36:B:LYS:HE3	16	19.17
(1,109)	1:95:A:GLN:H	1:71:A:ARG:HG2	12	19.17
(1,40)	1:69:B:SER:H	1:45:A:ARG:HD2	14	19.16
(1,677)	1:39:A:LYS:HG3	1:67:B:LYS:HG3	10	19.15
(1,47)	1:43:A:GLU:HG2	1:70:B:SER:H	16	19.14
(1,775)	1:67:A:LYS:HG3	1:45:B:ARG:HD3	9	19.13
(1,17)	1:95:A:GLN:H	1:71:A:ARG:H	9	19.13
(1,347)	1:67:A:LYS:H	1:45:B:ARG:HD3	15	19.12
(1,422)	1:70:A:SER:HB3	1:45:B:ARG:HD3	1	19.1
(1,579)	1:61:A:ILE:HB	1:36:B:LYS:HE2	4	19.09
(1,393)	1:93:A:ARG:H	1:71:A:ARG:H	2	19.09
(1,330)	1:93:B:ARG:HB3	1:71:B:ARG:H	19	19.09
(1,40)	1:69:A:SER:H	1:45:B:ARG:HD3	8	19.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,614)	1:93:A:ARG:HB2	1:71:A:ARG:HG2	9	19.08
(1,579)	1:61:A:ILE:HB	1:36:B:LYS:HE3	13	19.08
(1,727)	1:93:A:ARG:HA	1:71:B:ARG:HG3	2	19.05
(1,727)	1:93:B:ARG:HA	1:71:A:ARG:HG3	6	19.05
(1,303)	1:70:B:SER:H	1:45:A:ARG:HG2	17	19.05
(1,40)	1:69:B:SER:H	1:45:A:ARG:HD2	18	19.05
(1,614)	1:93:B:ARG:HB2	1:71:B:ARG:HG2	12	19.03
(1,468)	1:70:A:SER:HA	1:45:B:ARG:HD3	12	19.01
(1,863)	1:95:A:GLN:HB2	1:71:B:ARG:H	11	19.0
(1,604)	1:61:A:ILE:HD11	1:36:B:LYS:HE2	14	19.0
(1,109)	1:95:B:GLN:H	1:71:B:ARG:HG2	16	19.0
(1,579)	1:61:B:ILE:HB	1:36:A:LYS:HE2	18	18.99
(1,109)	1:95:B:GLN:H	1:71:A:ARG:HG3	7	18.99
(1,500)	1:70:A:SER:H	1:45:B:ARG:HD3	16	18.98
(1,352)	1:93:A:ARG:HA	1:72:B:HIS:H	9	18.97
(1,393)	1:93:A:ARG:H	1:71:A:ARG:H	9	18.96
(1,860)	1:94:A:ALA:HA	1:72:A:HIS:HB2	1	18.95
(1,670)	1:93:A:ARG:HB3	1:71:A:ARG:HB2	5	18.95
(1,860)	1:94:A:ALA:HA	1:72:A:HIS:HB2	3	18.92
(1,453)	1:67:A:LYS:HG2	1:45:B:ARG:HD3	8	18.91
(1,109)	1:95:A:GLN:H	1:71:B:ARG:HG3	17	18.91
(1,727)	1:93:A:ARG:HA	1:71:A:ARG:HG2	15	18.89
(1,422)	1:70:A:SER:HB2	1:45:B:ARG:HD3	4	18.89
(1,426)	1:70:B:SER:HA	1:45:A:ARG:HG3	17	18.87
(1,422)	1:70:B:SER:HB3	1:45:A:ARG:HD2	19	18.87
(1,352)	1:93:A:ARG:HA	1:72:B:HIS:H	1	18.87
(1,109)	1:95:B:GLN:H	1:71:B:ARG:HG2	14	18.86
(1,500)	1:70:A:SER:H	1:45:B:ARG:HD3	5	18.85
(1,40)	1:69:A:SER:H	1:45:B:ARG:HD3	10	18.84
(1,347)	1:67:A:LYS:H	1:45:B:ARG:HD3	11	18.83
(1,860)	1:94:B:ALA:HA	1:72:B:HIS:HB2	13	18.82
(1,40)	1:69:A:SER:H	1:45:B:ARG:HD3	11	18.81
(1,668)	1:93:B:ARG:HB3	1:71:B:ARG:HG2	12	18.8
(1,595)	1:39:A:LYS:HG3	1:67:B:LYS:HB2	14	18.8
(1,465)	1:61:B:ILE:HA	1:36:A:LYS:HE2	1	18.8
(1,347)	1:67:A:LYS:H	1:45:B:ARG:HD3	6	18.77
(1,303)	1:70:B:SER:H	1:45:A:ARG:HG2	14	18.77
(1,352)	1:93:A:ARG:HA	1:72:B:HIS:H	3	18.76
(1,453)	1:67:B:LYS:HG2	1:45:A:ARG:HD2	13	18.75
(1,47)	1:43:B:GLU:HG2	1:70:A:SER:H	7	18.74
(1,727)	1:93:B:ARG:HA	1:71:B:ARG:HG3	4	18.73
(1,347)	1:67:A:LYS:H	1:45:B:ARG:HD3	17	18.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,515)	1:36:B:LYS:HE2	1:62:A:LEU:H	4	18.72
(1,47)	1:43:A:GLU:HG2	1:70:B:SER:H	1	18.72
(1,860)	1:94:B:ALA:HA	1:72:B:HIS:HB2	20	18.71
(1,595)	1:39:B:LYS:HG3	1:67:A:LYS:HB2	10	18.71
(1,426)	1:70:B:SER:HA	1:45:A:ARG:HG3	18	18.7
(1,47)	1:43:A:GLU:HG2	1:70:B:SER:H	14	18.7
(1,109)	1:95:B:GLN:H	1:71:A:ARG:HG3	4	18.69
(1,40)	1:69:A:SER:H	1:45:B:ARG:HD3	17	18.69
(1,613)	1:61:B:ILE:HG21	1:36:A:LYS:HE2	12	18.68
(1,595)	1:39:A:LYS:HG3	1:67:B:LYS:HB2	1	18.68
(1,453)	1:67:A:LYS:HG2	1:45:B:ARG:HD3	3	18.68
(1,352)	1:93:B:ARG:HA	1:72:A:HIS:H	16	18.68
(1,613)	1:61:A:ILE:HG22	1:36:B:LYS:HE3	16	18.67
(1,612)	1:41:B:ILE:HG12	1:67:A:LYS:HG2	20	18.67
(1,393)	1:93:A:ARG:H	1:71:A:ARG:H	12	18.67
(1,109)	1:95:A:GLN:H	1:71:A:ARG:HG2	18	18.67
(1,727)	1:93:B:ARG:HA	1:71:B:ARG:HG2	1	18.66
(1,595)	1:39:A:LYS:HG3	1:67:B:LYS:HB2	15	18.66
(1,670)	1:93:A:ARG:HB3	1:71:A:ARG:HB2	20	18.65
(1,352)	1:93:A:ARG:HA	1:72:B:HIS:H	8	18.64
(1,303)	1:70:B:SER:H	1:45:A:ARG:HG2	18	18.64
(1,40)	1:69:A:SER:H	1:45:B:ARG:HD3	6	18.64
(1,727)	1:93:B:ARG:HA	1:71:B:ARG:HG2	16	18.63
(1,468)	1:70:A:SER:HA	1:45:B:ARG:HD3	4	18.62
(1,426)	1:70:A:SER:HA	1:45:B:ARG:HG3	7	18.62
(1,47)	1:43:B:GLU:HG2	1:70:A:SER:H	10	18.62
(1,474)	1:67:A:LYS:HA	1:45:B:ARG:HD3	7	18.61
(1,352)	1:93:A:ARG:HA	1:72:B:HIS:H	2	18.61
(1,614)	1:93:A:ARG:HB2	1:71:A:ARG:HG2	2	18.59
(1,860)	1:94:A:ALA:HA	1:72:A:HIS:HB2	18	18.58
(1,352)	1:93:B:ARG:HA	1:72:A:HIS:H	12	18.58
(1,500)	1:70:A:SER:H	1:45:B:ARG:HD3	3	18.56
(1,860)	1:94:A:ALA:HA	1:72:A:HIS:HB2	4	18.55
(1,109)	1:95:B:GLN:H	1:71:B:ARG:HG2	20	18.55
(1,860)	1:94:B:ALA:HA	1:72:B:HIS:HB2	11	18.54
(1,453)	1:67:A:LYS:HG2	1:45:B:ARG:HD3	4	18.54
(1,303)	1:70:A:SER:H	1:45:B:ARG:HG2	7	18.54
(1,40)	1:69:A:SER:H	1:45:B:ARG:HD3	15	18.54
(1,47)	1:43:A:GLU:HG2	1:70:B:SER:H	2	18.53
(1,697)	1:70:A:SER:HA	1:45:B:ARG:HG2	7	18.52
(1,453)	1:67:A:LYS:HG2	1:45:B:ARG:HD3	12	18.52
(1,579)	1:61:B:ILE:HB	1:36:A:LYS:HE2	12	18.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:93:A:ARG:H	1:71:A:ARG:H	14	18.51
(1,468)	1:70:B:SER:HA	1:45:A:ARG:HD2	1	18.5
(1,393)	1:93:A:ARG:H	1:71:A:ARG:H	15	18.5
(1,515)	1:36:B:LYS:HE3	1:62:A:LEU:H	13	18.49
(1,352)	1:93:A:ARG:HA	1:72:B:HIS:H	18	18.49
(1,860)	1:94:B:ALA:HA	1:72:B:HIS:HB2	16	18.46
(1,612)	1:41:A:ILE:HG12	1:67:B:LYS:HG2	15	18.46
(1,393)	1:93:A:ARG:H	1:71:A:ARG:H	6	18.46
(1,109)	1:95:A:GLN:H	1:71:A:ARG:HG2	19	18.46
(1,668)	1:93:A:ARG:HB3	1:71:A:ARG:HG2	9	18.45
(1,426)	1:70:A:SER:HA	1:45:B:ARG:HG3	20	18.45
(1,352)	1:93:B:ARG:HA	1:72:A:HIS:H	17	18.45
(1,860)	1:94:A:ALA:HA	1:72:A:HIS:HB2	8	18.44
(1,352)	1:93:B:ARG:HA	1:72:A:HIS:H	6	18.44
(1,727)	1:93:A:ARG:HA	1:71:A:ARG:HG2	5	18.41
(1,727)	1:93:B:ARG:HA	1:71:A:ARG:HG3	7	18.41
(1,668)	1:93:A:ARG:HB3	1:71:A:ARG:HG2	2	18.41
(1,727)	1:93:A:ARG:HA	1:71:A:ARG:HG2	17	18.4
(1,393)	1:93:B:ARG:H	1:71:B:ARG:H	1	18.4
(1,393)	1:93:B:ARG:H	1:71:B:ARG:H	20	18.4
(1,613)	1:61:A:ILE:HG21	1:36:B:LYS:HE3	17	18.39
(1,103)	1:93:A:ARG:H	1:72:A:HIS:H	9	18.39
(1,860)	1:94:B:ALA:HA	1:72:B:HIS:HB2	14	18.38
(1,347)	1:67:A:LYS:H	1:45:B:ARG:HD3	7	18.38
(1,860)	1:94:B:ALA:HA	1:72:B:HIS:HB2	6	18.37
(1,697)	1:70:B:SER:HA	1:45:A:ARG:HG2	18	18.37
(1,109)	1:95:A:GLN:H	1:71:A:ARG:HG2	5	18.35
(1,860)	1:94:B:ALA:HA	1:72:B:HIS:HB2	17	18.34
(1,515)	1:36:B:LYS:HE3	1:62:A:LEU:H	11	18.34
(1,474)	1:67:A:LYS:HA	1:45:B:ARG:HD3	20	18.34
(1,393)	1:93:B:ARG:H	1:71:B:ARG:H	4	18.34
(1,860)	1:94:A:ALA:HA	1:72:A:HIS:HB2	7	18.32
(1,775)	1:67:A:LYS:HG3	1:45:B:ARG:HD3	19	18.31
(1,352)	1:93:B:ARG:HA	1:72:A:HIS:H	5	18.31
(1,465)	1:61:A:ILE:HA	1:36:B:LYS:HE3	7	18.29
(1,352)	1:93:B:ARG:HA	1:72:A:HIS:H	4	18.28
(1,453)	1:67:B:LYS:HG2	1:45:A:ARG:HD2	10	18.27
(1,393)	1:93:B:ARG:H	1:71:B:ARG:H	16	18.27
(1,303)	1:70:A:SER:H	1:45:B:ARG:HG2	20	18.27
(1,465)	1:61:A:ILE:HA	1:36:B:LYS:HE2	14	18.25
(1,500)	1:70:B:SER:H	1:45:A:ARG:HD2	14	18.24
(1,500)	1:70:B:SER:H	1:45:A:ARG:HD2	18	18.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,500)	1:70:A:SER:H	1:45:B:ARG:HD3	8	18.23
(1,670)	1:93:B:ARG:HB3	1:71:B:ARG:HB2	1	18.22
(1,500)	1:70:A:SER:H	1:45:B:ARG:HD3	10	18.22
(1,697)	1:70:A:SER:HA	1:45:B:ARG:HG2	20	18.21
(1,453)	1:67:B:LYS:HG2	1:45:A:ARG:HD2	18	18.21
(1,670)	1:93:B:ARG:HB3	1:71:B:ARG:HB2	16	18.19
(1,352)	1:93:B:ARG:HA	1:72:A:HIS:H	10	18.18
(1,500)	1:70:A:SER:H	1:45:B:ARG:HD3	17	18.17
(1,422)	1:70:B:SER:HB3	1:45:A:ARG:HD2	13	18.17
(1,109)	1:95:A:GLN:H	1:71:A:ARG:HG2	3	18.17
(1,697)	1:70:B:SER:HA	1:45:A:ARG:HG2	14	18.15
(1,103)	1:93:B:ARG:H	1:72:B:HIS:H	16	18.15
(1,775)	1:67:B:LYS:HG3	1:45:A:ARG:HD2	13	18.14
(1,393)	1:93:A:ARG:H	1:71:A:ARG:H	7	18.14
(1,393)	1:93:A:ARG:H	1:71:A:ARG:H	18	18.14
(1,468)	1:70:A:SER:HA	1:45:B:ARG:HD3	13	18.13
(1,103)	1:93:B:ARG:H	1:72:B:HIS:H	1	18.13
(1,670)	1:93:B:ARG:HB3	1:71:B:ARG:HB2	7	18.12
(1,614)	1:93:A:ARG:HB2	1:71:A:ARG:HG2	6	18.12
(1,515)	1:36:A:LYS:HE2	1:62:B:LEU:H	12	18.11
(1,393)	1:93:A:ARG:H	1:71:A:ARG:H	5	18.11
(1,727)	1:93:A:ARG:HA	1:71:A:ARG:HG2	18	18.1
(1,453)	1:67:A:LYS:HG2	1:45:B:ARG:HD3	16	18.1
(1,579)	1:61:B:ILE:HB	1:36:A:LYS:HE2	3	18.09
(1,500)	1:70:A:SER:H	1:45:B:ARG:HD3	11	18.09
(1,393)	1:93:B:ARG:H	1:71:B:ARG:H	17	18.09
(1,727)	1:93:A:ARG:HA	1:71:B:ARG:HG3	11	18.08
(1,103)	1:93:A:ARG:H	1:72:B:HIS:H	2	18.07
(1,727)	1:93:B:ARG:HA	1:71:A:ARG:HG3	14	18.05
(1,103)	1:93:A:ARG:H	1:72:A:HIS:H	12	18.05
(1,47)	1:43:A:GLU:HG2	1:70:B:SER:H	13	18.05
(1,860)	1:94:B:ALA:HA	1:72:B:HIS:HB2	19	18.04
(1,352)	1:93:B:ARG:HA	1:72:A:HIS:H	7	18.03
(1,352)	1:93:B:ARG:HA	1:72:A:HIS:H	14	18.02
(1,727)	1:93:A:ARG:HA	1:71:B:ARG:HG3	20	18.01
(1,109)	1:95:A:GLN:H	1:71:B:ARG:HG3	11	18.01
(1,614)	1:93:A:ARG:HB2	1:71:A:ARG:HG2	13	18.0
(1,453)	1:67:A:LYS:HG2	1:45:B:ARG:HD3	5	18.0
(1,670)	1:93:A:ARG:HB3	1:71:A:ARG:HB2	17	17.99
(1,670)	1:93:A:ARG:HB3	1:71:A:ARG:HB2	14	17.98
(1,453)	1:67:A:LYS:HG2	1:45:B:ARG:HD3	6	17.98
(1,109)	1:95:B:GLN:H	1:71:B:ARG:HG2	10	17.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,103)	1:93:A:ARG:H	1:72:B:HIS:H	20	17.97
(1,515)	1:36:B:LYS:HE3	1:62:A:LEU:H	16	17.96
(1,422)	1:70:A:SER:HB3	1:45:B:ARG:HD3	16	17.96
(1,670)	1:93:A:ARG:HB3	1:71:A:ARG:HB2	15	17.95
(1,604)	1:61:A:ILE:HD12	1:36:B:LYS:HE2	5	17.95
(1,393)	1:93:B:ARG:H	1:71:B:ARG:H	11	17.95
(1,352)	1:93:A:ARG:HA	1:72:B:HIS:H	20	17.95
(1,103)	1:93:A:ARG:H	1:72:A:HIS:H	3	17.95
(1,103)	1:93:A:ARG:H	1:72:A:HIS:H	15	17.95
(1,727)	1:93:A:ARG:HA	1:71:B:ARG:HG3	19	17.94
(1,613)	1:61:B:ILE:HG22	1:36:A:LYS:HE2	3	17.94
(1,468)	1:70:B:SER:HA	1:45:A:ARG:HD2	19	17.94
(1,614)	1:93:B:ARG:HB2	1:71:B:ARG:HG3	4	17.93
(1,426)	1:70:B:SER:HA	1:45:A:ARG:HG3	14	17.93
(1,103)	1:93:A:ARG:H	1:72:A:HIS:H	18	17.93
(1,515)	1:36:A:LYS:HE2	1:62:B:LEU:H	18	17.92
(1,500)	1:70:A:SER:H	1:45:B:ARG:HD3	6	17.92
(1,500)	1:70:A:SER:H	1:45:B:ARG:HD3	15	17.92
(1,861)	1:94:B:ALA:HB2	1:72:B:HIS:HB2	9	17.87
(1,775)	1:67:A:LYS:HG3	1:45:B:ARG:HD3	12	17.87
(1,727)	1:93:B:ARG:HA	1:71:A:ARG:HG3	13	17.87
(1,614)	1:93:A:ARG:HB2	1:71:A:ARG:HG2	14	17.87
(1,614)	1:93:A:ARG:HB2	1:71:A:ARG:HG2	15	17.84
(1,727)	1:93:B:ARG:HA	1:71:B:ARG:HG2	10	17.83
(1,614)	1:93:B:ARG:HB2	1:71:B:ARG:HG2	1	17.83
(1,393)	1:93:A:ARG:H	1:71:A:ARG:H	3	17.83
(1,860)	1:94:A:ALA:HA	1:72:A:HIS:HB2	12	17.82
(1,670)	1:93:A:ARG:HB3	1:71:A:ARG:HB2	6	17.82
(1,614)	1:93:A:ARG:HB2	1:71:A:ARG:HG2	5	17.81
(1,668)	1:93:A:ARG:HB3	1:71:A:ARG:HG2	5	17.8
(1,614)	1:93:B:ARG:HB2	1:71:B:ARG:HG2	20	17.8
(1,347)	1:67:A:LYS:H	1:45:B:ARG:HD3	20	17.78
(1,614)	1:93:B:ARG:HB2	1:71:B:ARG:HG2	16	17.76
(1,579)	1:61:A:ILE:HB	1:36:B:LYS:HE3	17	17.75
(1,109)	1:95:A:GLN:H	1:71:A:ARG:HG2	13	17.74
(1,352)	1:93:A:ARG:HA	1:72:B:HIS:H	11	17.71
(1,670)	1:93:A:ARG:HB3	1:71:A:ARG:HB2	10	17.69
(1,668)	1:93:B:ARG:HB3	1:71:B:ARG:HG2	20	17.66
(1,453)	1:67:A:LYS:HG2	1:45:B:ARG:HD3	17	17.66
(1,422)	1:70:A:SER:HB3	1:45:B:ARG:HD3	5	17.64
(1,393)	1:93:A:ARG:H	1:71:A:ARG:H	10	17.64
(1,103)	1:93:B:ARG:H	1:72:B:HIS:H	8	17.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,103)	1:93:B:ARG:H	1:72:A:HIS:H	14	17.64
(1,668)	1:93:A:ARG:HB3	1:71:A:ARG:HG2	13	17.63
(1,393)	1:93:A:ARG:H	1:71:A:ARG:H	13	17.63
(1,860)	1:94:A:ALA:HA	1:72:A:HIS:HB2	9	17.62
(1,775)	1:67:A:LYS:HG3	1:45:B:ARG:HD3	4	17.62
(1,465)	1:61:A:ILE:HA	1:36:B:LYS:HE3	2	17.61
(1,393)	1:93:B:ARG:H	1:71:B:ARG:H	19	17.61
(1,40)	1:69:A:SER:H	1:45:B:ARG:HD3	20	17.61
(1,727)	1:93:A:ARG:HA	1:71:A:ARG:HG2	8	17.6
(1,468)	1:70:A:SER:HA	1:45:B:ARG:HD3	16	17.58
(1,393)	1:93:A:ARG:H	1:71:A:ARG:H	8	17.58
(1,727)	1:93:A:ARG:HA	1:71:A:ARG:HG2	3	17.57
(1,103)	1:93:A:ARG:H	1:72:A:HIS:H	5	17.57
(1,103)	1:93:B:ARG:H	1:72:B:HIS:H	11	17.56
(1,775)	1:67:B:LYS:HG3	1:45:A:ARG:HD2	18	17.55
(1,668)	1:93:A:ARG:HB3	1:71:A:ARG:HG3	6	17.55
(1,352)	1:93:A:ARG:HA	1:72:B:HIS:H	19	17.55
(1,614)	1:93:B:ARG:HB2	1:71:B:ARG:HG2	7	17.54
(1,578)	1:43:B:GLU:HG3	1:72:A:HIS:HD2	5	17.54
(1,670)	1:93:A:ARG:HB3	1:71:A:ARG:HB2	13	17.52
(1,103)	1:93:B:ARG:H	1:72:B:HIS:H	17	17.52
(1,422)	1:70:A:SER:HB3	1:45:B:ARG:HD3	6	17.49
(1,103)	1:93:A:ARG:H	1:72:A:HIS:H	6	17.49
(1,860)	1:94:A:ALA:HA	1:72:A:HIS:HB2	10	17.46
(1,670)	1:93:A:ARG:HB3	1:71:A:ARG:HB2	3	17.46
(1,668)	1:93:B:ARG:HB3	1:71:B:ARG:HG2	1	17.46
(1,422)	1:70:A:SER:HB2	1:45:B:ARG:HD3	17	17.45
(1,772)	1:94:A:ALA:H	1:71:A:ARG:HG2	9	17.44
(1,578)	1:43:A:GLU:HG2	1:72:B:HIS:HD2	4	17.44
(1,578)	1:43:A:GLU:HG2	1:72:B:HIS:HD2	17	17.44
(1,465)	1:61:A:ILE:HA	1:36:B:LYS:HE2	5	17.42
(1,422)	1:70:A:SER:HB3	1:45:B:ARG:HD3	11	17.42
(1,772)	1:94:A:ALA:H	1:71:A:ARG:HG3	6	17.4
(1,614)	1:93:A:ARG:HB2	1:71:A:ARG:HG2	17	17.39
(1,103)	1:93:B:ARG:H	1:72:B:HIS:H	4	17.39
(1,40)	1:69:A:SER:H	1:45:B:ARG:HD3	7	17.39
(1,352)	1:93:B:ARG:HA	1:72:A:HIS:H	13	17.38
(1,856)	1:93:A:ARG:HA	1:72:B:HIS:HB2	15	17.36
(1,775)	1:67:A:LYS:HG3	1:45:B:ARG:HD3	14	17.35
(1,313)	1:93:A:ARG:H	1:71:A:ARG:HG2	9	17.33
(1,109)	1:95:B:GLN:H	1:71:B:ARG:HG2	8	17.33
(1,51)	1:43:B:GLU:HG2	1:72:A:HIS:H	4	17.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,103)	1:93:A:ARG:H	1:72:A:HIS:H	7	17.32
(1,775)	1:67:A:LYS:HG3	1:45:B:ARG:HD3	2	17.31
(1,775)	1:67:A:LYS:HG3	1:45:B:ARG:HD3	5	17.31
(1,313)	1:93:A:ARG:H	1:71:A:ARG:HG2	2	17.31
(1,422)	1:70:B:SER:HB3	1:45:A:ARG:HD2	18	17.28
(1,468)	1:70:A:SER:HA	1:45:B:ARG:HD3	5	17.27
(1,454)	1:93:A:ARG:HB2	1:71:A:ARG:HD2	9	17.27
(1,422)	1:70:A:SER:HB3	1:45:B:ARG:HD3	3	17.27
(1,775)	1:67:A:LYS:HG3	1:45:B:ARG:HD3	1	17.26
(1,668)	1:93:B:ARG:HB3	1:71:B:ARG:HG2	16	17.26
(1,604)	1:61:B:ILE:HD11	1:36:A:LYS:HE2	19	17.26
(1,772)	1:94:A:ALA:H	1:71:A:ARG:HG2	15	17.25
(1,454)	1:93:B:ARG:HB2	1:71:B:ARG:HD2	12	17.25
(1,468)	1:70:A:SER:HA	1:45:B:ARG:HD3	17	17.24
(1,668)	1:93:A:ARG:HB3	1:71:A:ARG:HG2	14	17.22
(1,453)	1:67:A:LYS:HG2	1:45:B:ARG:HD3	11	17.2
(1,422)	1:70:A:SER:HB3	1:45:B:ARG:HD3	15	17.2
(1,860)	1:94:A:ALA:HA	1:72:A:HIS:HB2	5	17.18
(1,670)	1:93:B:ARG:HB3	1:71:B:ARG:HB2	4	17.16
(1,856)	1:93:B:ARG:HA	1:72:A:HIS:HB2	9	17.14
(1,103)	1:93:B:ARG:H	1:72:A:HIS:H	13	17.14
(1,614)	1:93:B:ARG:HB2	1:71:B:ARG:HG2	11	17.13
(1,422)	1:70:A:SER:HB3	1:45:B:ARG:HD3	8	17.12
(1,772)	1:94:A:ALA:H	1:71:A:ARG:HG2	12	17.11
(1,670)	1:93:A:ARG:HB3	1:71:A:ARG:HB2	18	17.11
(1,453)	1:67:B:LYS:HG2	1:45:A:ARG:HD2	15	17.11
(1,772)	1:94:B:ALA:H	1:71:B:ARG:HG3	2	17.1
(1,51)	1:43:A:GLU:HG2	1:72:B:HIS:H	8	17.1
(1,670)	1:93:B:ARG:HB3	1:71:B:ARG:HB2	11	17.09
(1,668)	1:93:A:ARG:HB3	1:71:A:ARG:HG2	15	17.09
(1,453)	1:67:A:LYS:HG2	1:45:B:ARG:HD3	1	17.09
(1,313)	1:93:A:ARG:H	1:71:A:ARG:HG2	12	17.09
(1,668)	1:93:B:ARG:HB3	1:71:B:ARG:HG3	4	17.07
(1,578)	1:43:B:GLU:HG3	1:72:A:HIS:HD2	8	17.07
(1,613)	1:61:B:ILE:HG21	1:36:A:LYS:HE2	1	17.05
(1,468)	1:70:A:SER:HA	1:45:B:ARG:HD3	3	17.05
(1,468)	1:70:A:SER:HA	1:45:B:ARG:HD3	10	17.05
(1,614)	1:93:B:ARG:HB2	1:71:B:ARG:HG3	19	17.04
(1,422)	1:70:A:SER:HB3	1:45:B:ARG:HD3	10	17.04
(1,668)	1:93:B:ARG:HB3	1:71:B:ARG:HG2	7	17.02
(1,453)	1:67:A:LYS:HG2	1:45:B:ARG:HD3	14	17.01
(1,772)	1:94:A:ALA:H	1:71:A:ARG:HG2	4	16.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,614)	1:93:B:ARG:HB2	1:71:B:ARG:HG2	10	16.98
(1,614)	1:93:A:ARG:HB2	1:71:A:ARG:HG2	18	16.98
(1,856)	1:93:A:ARG:HA	1:72:B:HIS:HB2	2	16.93
(1,578)	1:43:B:GLU:HG2	1:72:A:HIS:HD2	20	16.92
(1,103)	1:93:A:ARG:H	1:72:A:HIS:H	10	16.92
(1,51)	1:43:B:GLU:HG2	1:72:A:HIS:H	18	16.92
(1,578)	1:43:B:GLU:HG2	1:72:A:HIS:HD2	7	16.91
(1,454)	1:93:A:ARG:HB2	1:71:A:ARG:HD2	2	16.89
(1,861)	1:94:B:ALA:HB2	1:72:B:HIS:HB2	2	16.87
(1,468)	1:70:B:SER:HA	1:45:A:ARG:HD2	18	16.86
(1,670)	1:93:B:ARG:HB3	1:71:B:ARG:HB2	8	16.84
(1,313)	1:93:A:ARG:H	1:71:A:ARG:HG3	6	16.84
(1,515)	1:36:B:LYS:HE3	1:62:A:LEU:H	17	16.83
(1,856)	1:93:A:ARG:HA	1:72:B:HIS:HB2	1	16.82
(1,422)	1:70:B:SER:HB3	1:45:A:ARG:HD2	14	16.78
(1,578)	1:43:A:GLU:HG2	1:72:B:HIS:HD2	11	16.77
(1,775)	1:67:A:LYS:HG3	1:45:B:ARG:HD3	6	16.76
(1,772)	1:94:A:ALA:H	1:71:A:ARG:HG2	17	16.75
(1,500)	1:70:A:SER:H	1:45:B:ARG:HD3	20	16.75
(1,579)	1:61:B:ILE:HB	1:36:A:LYS:HE2	1	16.74
(1,772)	1:94:B:ALA:H	1:71:B:ARG:HG2	16	16.73
(1,856)	1:93:B:ARG:HA	1:72:A:HIS:HB2	16	16.72
(1,668)	1:93:A:ARG:HB3	1:71:A:ARG:HG2	17	16.72
(1,453)	1:67:A:LYS:HG2	1:45:B:ARG:HD3	7	16.72
(1,51)	1:43:B:GLU:HG2	1:72:A:HIS:H	5	16.72
(1,861)	1:94:A:ALA:HB2	1:72:A:HIS:HB2	15	16.71
(1,772)	1:94:B:ALA:H	1:71:B:ARG:HG2	14	16.7
(1,614)	1:93:A:ARG:HB2	1:71:A:ARG:HG2	3	16.7
(1,468)	1:70:A:SER:HA	1:45:B:ARG:HD3	11	16.7
(1,614)	1:93:A:ARG:HB2	1:71:A:ARG:HG2	8	16.68
(1,468)	1:70:A:SER:HA	1:45:B:ARG:HD3	8	16.67
(1,468)	1:70:A:SER:HA	1:45:B:ARG:HD3	15	16.67
(1,51)	1:43:B:GLU:HG2	1:72:A:HIS:H	9	16.65
(1,103)	1:93:B:ARG:H	1:72:B:HIS:H	19	16.64
(1,51)	1:43:A:GLU:HG2	1:72:B:HIS:H	6	16.64
(1,313)	1:93:A:ARG:H	1:71:A:ARG:HG2	15	16.63
(1,51)	1:43:B:GLU:HG2	1:72:A:HIS:H	20	16.63
(1,670)	1:93:B:ARG:HB3	1:71:B:ARG:HB2	19	16.62
(1,613)	1:61:A:ILE:HG22	1:36:B:LYS:HE3	7	16.62
(1,861)	1:94:A:ALA:HB3	1:72:A:HIS:HB2	3	16.61
(1,772)	1:94:B:ALA:H	1:71:B:ARG:HG2	11	16.61
(1,452)	1:93:B:ARG:HB3	1:71:B:ARG:HD2	12	16.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,861)	1:94:B:ALA:HB3	1:72:B:HIS:HB2	14	16.59
(1,775)	1:67:B:LYS:HG3	1:45:A:ARG:HD2	15	16.59
(1,772)	1:94:B:ALA:H	1:71:B:ARG:HG2	1	16.59
(1,775)	1:67:A:LYS:HG3	1:45:B:ARG:HD3	11	16.58
(1,500)	1:70:A:SER:H	1:45:B:ARG:HD3	7	16.57
(1,772)	1:94:A:ALA:H	1:71:A:ARG:HG3	7	16.56
(1,51)	1:43:B:GLU:HG2	1:72:A:HIS:H	19	16.56
(1,856)	1:93:A:ARG:HA	1:72:B:HIS:HB2	3	16.55
(1,578)	1:43:A:GLU:HG2	1:72:B:HIS:HD2	10	16.53
(1,775)	1:67:A:LYS:HG3	1:45:B:ARG:HD3	17	16.52
(1,668)	1:93:B:ARG:HB3	1:71:B:ARG:HG2	11	16.52
(1,856)	1:93:A:ARG:HA	1:72:B:HIS:HB2	17	16.49
(1,856)	1:93:B:ARG:HA	1:72:A:HIS:HB2	12	16.48
(1,468)	1:70:A:SER:HA	1:45:B:ARG:HD3	6	16.48
(1,468)	1:70:B:SER:HA	1:45:A:ARG:HD2	14	16.48
(1,863)	1:95:A:GLN:HB3	1:71:A:ARG:H	9	16.46
(1,51)	1:43:A:GLU:HG2	1:72:B:HIS:H	17	16.46
(1,668)	1:93:B:ARG:HB3	1:71:B:ARG:HG2	10	16.45
(1,578)	1:43:A:GLU:HG2	1:72:B:HIS:HD2	3	16.45
(1,861)	1:94:A:ALA:HB3	1:72:A:HIS:HB3	6	16.44
(1,856)	1:93:A:ARG:HA	1:72:B:HIS:HB2	8	16.42
(1,313)	1:93:A:ARG:H	1:71:A:ARG:HG2	14	16.42
(1,454)	1:93:B:ARG:HB2	1:71:B:ARG:HD2	20	16.41
(1,313)	1:93:B:ARG:H	1:71:B:ARG:HG3	4	16.41
(1,861)	1:94:A:ALA:HB2	1:72:A:HIS:HB2	8	16.4
(1,51)	1:43:A:GLU:HG2	1:72:B:HIS:H	3	16.4
(1,856)	1:93:B:ARG:HA	1:72:A:HIS:HB2	10	16.38
(1,668)	1:93:A:ARG:HB3	1:71:A:ARG:HG2	18	16.38
(1,515)	1:36:B:LYS:HE2	1:62:A:LEU:H	14	16.38
(1,578)	1:43:A:GLU:HG2	1:72:B:HIS:HD2	19	16.37
(1,668)	1:93:B:ARG:HB3	1:71:B:ARG:HG2	8	16.35
(1,454)	1:93:A:ARG:HB2	1:71:A:ARG:HD2	14	16.35
(1,313)	1:93:B:ARG:H	1:71:B:ARG:HG2	7	16.33
(1,454)	1:93:B:ARG:HB2	1:71:B:ARG:HD2	1	16.32
(1,579)	1:61:A:ILE:HB	1:36:B:LYS:HE2	14	16.3
(1,578)	1:43:A:GLU:HG2	1:72:B:HIS:HD1	12	16.3
(1,856)	1:93:A:ARG:HA	1:72:B:HIS:HB2	18	16.29
(1,775)	1:67:A:LYS:HG3	1:45:B:ARG:HD3	8	16.29
(1,668)	1:93:B:ARG:HB3	1:71:B:ARG:HG3	19	16.29
(1,515)	1:36:A:LYS:HE2	1:62:B:LEU:H	3	16.29
(1,454)	1:93:B:ARG:HB2	1:71:B:ARG:HD2	16	16.29
(1,856)	1:93:B:ARG:HA	1:72:A:HIS:HB3	6	16.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,313)	1:93:B:ARG:H	1:71:B:ARG:HG2	16	16.28
(1,772)	1:94:A:ALA:H	1:71:A:ARG:HG2	5	16.27
(1,772)	1:94:B:ALA:H	1:71:B:ARG:HG2	20	16.27
(1,452)	1:93:A:ARG:HB3	1:71:A:ARG:HD2	2	16.25
(1,772)	1:94:A:ALA:H	1:71:A:ARG:HG2	18	16.24
(1,668)	1:93:A:ARG:HB3	1:71:A:ARG:HG2	3	16.24
(1,453)	1:67:A:LYS:HG2	1:45:B:ARG:HD3	20	16.24
(1,454)	1:93:A:ARG:HB2	1:71:A:ARG:HD2	7	16.23
(1,454)	1:93:A:ARG:HB2	1:71:A:ARG:HD2	17	16.23
(1,578)	1:43:A:GLU:HG2	1:72:B:HIS:HD2	9	16.22
(1,313)	1:93:B:ARG:H	1:71:B:ARG:HG2	1	16.22
(1,579)	1:61:A:ILE:HB	1:36:B:LYS:HE3	7	16.21
(1,452)	1:93:A:ARG:HB3	1:71:A:ARG:HD2	9	16.21
(1,613)	1:61:A:ILE:HG22	1:36:B:LYS:HE2	14	16.2
(1,578)	1:43:B:GLU:HG3	1:72:A:HIS:HD2	18	16.2
(1,861)	1:94:B:ALA:HB3	1:72:B:HIS:HB2	16	16.19
(1,861)	1:94:A:ALA:HB2	1:72:A:HIS:HB2	18	16.18
(1,861)	1:94:A:ALA:HB1	1:72:A:HIS:HB2	20	16.18
(1,856)	1:93:B:ARG:HA	1:72:A:HIS:HB2	5	16.15
(1,109)	1:95:A:GLN:H	1:71:A:ARG:HG2	9	16.15
(1,861)	1:94:B:ALA:HB1	1:72:B:HIS:HB2	11	16.14
(1,775)	1:67:A:LYS:HG3	1:45:B:ARG:HD3	3	16.14
(1,856)	1:93:B:ARG:HA	1:72:A:HIS:HB2	7	16.13
(1,454)	1:93:A:ARG:HB2	1:71:A:ARG:HD2	5	16.12
(1,775)	1:67:A:LYS:HG3	1:45:B:ARG:HD3	7	16.11
(1,515)	1:36:A:LYS:HE2	1:62:B:LEU:H	1	16.11
(1,454)	1:93:A:ARG:HB2	1:71:A:ARG:HD2	15	16.11
(1,313)	1:93:A:ARG:H	1:71:A:ARG:HG2	13	16.11
(1,313)	1:93:A:ARG:H	1:71:A:ARG:HG2	17	16.11
(1,856)	1:93:B:ARG:HA	1:72:A:HIS:HB2	4	16.1
(1,772)	1:94:A:ALA:H	1:71:A:ARG:HG2	13	16.1
(1,613)	1:61:A:ILE:HG21	1:36:B:LYS:HE3	2	16.06
(1,772)	1:94:A:ALA:H	1:71:A:ARG:HG2	19	16.05
(1,313)	1:93:B:ARG:H	1:71:B:ARG:HG2	20	16.05
(1,861)	1:94:A:ALA:HB2	1:72:A:HIS:HB2	4	16.03
(1,51)	1:43:A:GLU:HG2	1:72:B:HIS:H	11	16.03
(1,578)	1:43:A:GLU:HG2	1:72:B:HIS:HD2	13	16.02
(1,313)	1:93:A:ARG:H	1:71:A:ARG:HG2	5	16.02
(1,861)	1:94:A:ALA:HB3	1:72:A:HIS:HB2	1	16.0
(1,856)	1:93:A:ARG:HA	1:72:B:HIS:HB2	20	15.99
(1,422)	1:70:A:SER:HB3	1:45:B:ARG:HD3	20	15.95
(1,454)	1:93:A:ARG:HB2	1:71:A:ARG:HD2	13	15.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,313)	1:93:B:ARG:H	1:71:B:ARG:HG2	11	15.93
(1,313)	1:93:A:ARG:H	1:71:A:ARG:HG2	18	15.91
(1,51)	1:43:B:GLU:HG2	1:72:A:HIS:H	15	15.9
(1,454)	1:93:A:ARG:HB2	1:71:A:ARG:HD2	6	15.89
(1,856)	1:93:B:ARG:HA	1:72:A:HIS:HB2	14	15.88
(1,454)	1:93:A:ARG:HB2	1:71:A:ARG:HD2	3	15.87
(1,579)	1:61:A:ILE:HB	1:36:B:LYS:HE3	2	15.86
(1,454)	1:93:B:ARG:HB2	1:71:B:ARG:HD2	4	15.86
(1,452)	1:93:B:ARG:HB3	1:71:B:ARG:HD2	20	15.83
(1,861)	1:94:B:ALA:HB1	1:72:B:HIS:HB2	17	15.81
(1,579)	1:61:A:ILE:HB	1:36:B:LYS:HE2	5	15.81
(1,861)	1:94:A:ALA:HB1	1:72:A:HIS:HB2	7	15.78
(1,772)	1:94:B:ALA:H	1:71:B:ARG:HG2	8	15.78
(1,856)	1:93:A:ARG:HA	1:72:B:HIS:HB2	19	15.71
(1,861)	1:94:A:ALA:HB3	1:72:A:HIS:HB2	13	15.7
(1,515)	1:36:B:LYS:HE3	1:62:A:LEU:H	7	15.7
(1,465)	1:61:B:ILE:HA	1:36:A:LYS:HE2	19	15.69
(1,454)	1:93:A:ARG:HB2	1:71:A:ARG:HD2	18	15.68
(1,422)	1:70:A:SER:HB3	1:45:B:ARG:HD3	7	15.68
(1,313)	1:93:B:ARG:H	1:71:B:ARG:HG3	19	15.68
(1,452)	1:93:A:ARG:HB3	1:71:A:ARG:HD2	5	15.67
(1,775)	1:67:A:LYS:HG3	1:45:B:ARG:HD3	20	15.64
(1,578)	1:43:A:GLU:HG2	1:72:B:HIS:HD1	6	15.64
(1,775)	1:67:B:LYS:HG3	1:45:A:ARG:HD2	10	15.63
(1,454)	1:93:A:ARG:HB2	1:71:A:ARG:HD2	8	15.63
(1,51)	1:43:B:GLU:HG2	1:72:A:HIS:H	12	15.63
(1,772)	1:94:B:ALA:H	1:71:B:ARG:HG2	10	15.61
(1,775)	1:67:A:LYS:HG3	1:45:B:ARG:HD3	16	15.59
(1,772)	1:94:A:ALA:H	1:71:A:ARG:HG2	3	15.59
(1,578)	1:43:B:GLU:HG3	1:72:A:HIS:HD2	15	15.57
(1,452)	1:93:B:ARG:HB3	1:71:B:ARG:HD2	1	15.54
(1,51)	1:43:A:GLU:HG2	1:72:B:HIS:H	16	15.54
(1,468)	1:70:A:SER:HA	1:45:B:ARG:HD3	7	15.52
(1,454)	1:93:B:ARG:HB2	1:71:B:ARG:HD2	11	15.5
(1,454)	1:93:A:ARG:HB2	1:71:A:ARG:HD2	10	15.48
(1,51)	1:43:B:GLU:HG2	1:72:A:HIS:H	10	15.48
(1,856)	1:93:B:ARG:HA	1:72:A:HIS:HB2	13	15.47
(1,861)	1:94:B:ALA:HB3	1:72:B:HIS:HB2	19	15.45
(1,468)	1:70:A:SER:HA	1:45:B:ARG:HD3	20	15.42
(1,51)	1:43:A:GLU:HG2	1:72:B:HIS:H	1	15.42
(1,861)	1:94:A:ALA:HB1	1:72:A:HIS:HB2	12	15.41
(1,313)	1:93:B:ARG:H	1:71:B:ARG:HG2	10	15.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,856)	1:93:A:ARG:HA	1:72:B:HIS:HB2	11	15.38
(1,452)	1:93:B:ARG:HB3	1:71:B:ARG:HD2	7	15.36
(1,51)	1:43:B:GLU:HG2	1:72:A:HIS:H	7	15.35
(1,452)	1:93:B:ARG:HB3	1:71:B:ARG:HD2	16	15.34
(1,515)	1:36:B:LYS:HE2	1:62:A:LEU:H	5	15.32
(1,861)	1:94:A:ALA:HB2	1:72:A:HIS:HB2	10	15.31
(1,578)	1:43:A:GLU:HG2	1:72:B:HIS:HD2	16	15.29
(1,452)	1:93:A:ARG:HB3	1:71:A:ARG:HD2	14	15.28
(1,51)	1:43:A:GLU:HG2	1:72:B:HIS:H	14	15.28
(1,313)	1:93:A:ARG:H	1:71:A:ARG:HG2	8	15.24
(1,578)	1:43:A:GLU:HG2	1:72:B:HIS:HD2	14	15.2
(1,313)	1:93:A:ARG:H	1:71:A:ARG:HG2	3	15.2
(1,452)	1:93:A:ARG:HB3	1:71:A:ARG:HD2	13	15.19
(1,452)	1:93:A:ARG:HB3	1:71:A:ARG:HD2	17	15.16
(1,219)	1:72:B:HIS:HB2	1:51:B:ASN:HD21	8	15.07
(1,51)	1:43:A:GLU:HG2	1:72:B:HIS:H	2	15.05
(1,452)	1:93:A:ARG:HB3	1:71:A:ARG:HD2	3	14.94
(1,454)	1:93:B:ARG:HB2	1:71:B:ARG:HD2	19	14.93
(1,452)	1:93:A:ARG:HB3	1:71:A:ARG:HD2	6	14.93
(1,452)	1:93:A:ARG:HB3	1:71:A:ARG:HD2	10	14.92
(1,452)	1:93:A:ARG:HB3	1:71:A:ARG:HD2	15	14.92
(1,542)	1:72:B:HIS:HB2	1:51:B:ASN:HD22	8	14.9
(1,613)	1:61:A:ILE:HG22	1:36:B:LYS:HE2	5	14.88
(1,861)	1:94:A:ALA:HB2	1:72:A:HIS:HB2	5	14.86
(1,452)	1:93:B:ARG:HB3	1:71:B:ARG:HD2	8	14.85
(1,56)	1:73:A:SER:H	1:51:A:ASN:HD22	6	14.85
(1,578)	1:43:A:GLU:HG2	1:72:B:HIS:HD2	1	14.8
(1,452)	1:93:B:ARG:HB3	1:71:B:ARG:HD2	4	14.78
(1,51)	1:43:A:GLU:HG2	1:72:B:HIS:H	13	14.74
(1,220)	1:73:A:SER:HB3	1:51:A:ASN:HD21	6	14.63
(1,578)	1:43:B:GLU:HG3	1:72:A:HIS:HD2	2	14.62
(1,452)	1:93:A:ARG:HB3	1:71:A:ARG:HD2	18	14.6
(1,220)	1:73:A:SER:HB3	1:51:A:ASN:HD21	8	14.59
(1,219)	1:72:A:HIS:HB3	1:51:A:ASN:HD21	20	14.56
(1,452)	1:93:B:ARG:HB3	1:71:B:ARG:HD2	11	14.47
(1,220)	1:73:A:SER:HB3	1:51:A:ASN:HD21	15	14.46
(1,542)	1:72:A:HIS:HB3	1:51:A:ASN:HD22	15	14.43
(1,220)	1:73:A:SER:HB3	1:51:A:ASN:HD21	20	14.43
(1,219)	1:72:A:HIS:HB3	1:51:A:ASN:HD21	11	14.43
(1,542)	1:72:A:HIS:HB3	1:51:A:ASN:HD22	1	14.42
(1,542)	1:72:A:HIS:HB3	1:51:A:ASN:HD22	12	14.38
(1,542)	1:72:A:HIS:HB3	1:51:A:ASN:HD22	20	14.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,542)	1:72:B:HIS:HB3	1:51:B:ASN:HD22	3	14.32
(1,515)	1:36:B:LYS:HE3	1:62:A:LEU:H	2	14.32
(1,56)	1:73:B:SER:H	1:51:B:ASN:HD22	15	14.32
(1,219)	1:72:B:HIS:HB3	1:51:B:ASN:HD21	3	14.28
(1,220)	1:73:A:SER:HB3	1:51:A:ASN:HD21	19	14.27
(1,219)	1:72:A:HIS:HB3	1:51:A:ASN:HD21	12	14.24
(1,220)	1:73:B:SER:HB3	1:51:B:ASN:HD21	3	14.23
(1,220)	1:73:B:SER:HB3	1:51:B:ASN:HD21	10	14.23
(1,219)	1:72:A:HIS:HB3	1:51:A:ASN:HD21	1	14.22
(1,219)	1:72:A:HIS:HB3	1:51:A:ASN:HD21	19	14.2
(1,542)	1:72:A:HIS:HB2	1:51:A:ASN:HD22	7	14.18
(1,542)	1:72:A:HIS:HB2	1:51:A:ASN:HD22	17	14.18
(1,219)	1:72:A:HIS:HB3	1:51:A:ASN:HD21	15	14.18
(1,219)	1:72:B:HIS:HB3	1:51:B:ASN:HD21	18	14.18
(1,56)	1:73:A:SER:H	1:51:A:ASN:HD22	1	14.17
(1,219)	1:72:A:HIS:HB2	1:51:A:ASN:HD21	7	14.16
(1,542)	1:72:A:HIS:HB3	1:51:A:ASN:HD22	11	14.14
(1,542)	1:72:B:HIS:HB3	1:51:B:ASN:HD22	18	14.14
(1,56)	1:73:A:SER:H	1:51:A:ASN:HD22	12	14.13
(1,220)	1:73:A:SER:HB3	1:51:A:ASN:HD21	11	14.12
(1,219)	1:72:B:HIS:HB3	1:51:B:ASN:HD21	13	14.08
(1,220)	1:73:B:SER:HB2	1:51:B:ASN:HD21	13	14.06
(1,219)	1:72:A:HIS:HB3	1:51:A:ASN:HD21	10	14.06
(1,219)	1:72:A:HIS:HB2	1:51:A:ASN:HD21	17	14.02
(1,542)	1:72:A:HIS:HB3	1:51:A:ASN:HD22	5	13.98
(1,542)	1:72:B:HIS:HB3	1:51:B:ASN:HD22	13	13.96
(1,542)	1:72:A:HIS:HB3	1:51:A:ASN:HD22	19	13.95
(1,452)	1:93:B:ARG:HB3	1:71:B:ARG:HD2	19	13.95
(1,613)	1:61:B:ILE:HG21	1:36:A:LYS:HE2	19	13.94
(1,56)	1:73:A:SER:H	1:51:A:ASN:HD22	19	13.91
(1,56)	1:73:B:SER:H	1:51:B:ASN:HD22	3	13.87
(1,220)	1:73:A:SER:HB2	1:51:A:ASN:HD21	14	13.86
(1,220)	1:73:A:SER:HB3	1:51:A:ASN:HD21	16	13.85
(1,219)	1:72:A:HIS:HB3	1:51:A:ASN:HD21	16	13.84
(1,56)	1:73:A:SER:H	1:51:A:ASN:HD22	20	13.84
(1,542)	1:72:A:HIS:HB3	1:51:A:ASN:HD22	10	13.82
(1,219)	1:72:A:HIS:HB3	1:51:A:ASN:HD21	5	13.82
(1,229)	1:73:A:SER:HB3	1:51:A:ASN:HD22	6	13.8
(1,56)	1:73:A:SER:H	1:51:A:ASN:HD22	11	13.78
(1,542)	1:72:B:HIS:HB3	1:51:B:ASN:HD22	2	13.76
(1,542)	1:72:A:HIS:HB3	1:51:A:ASN:HD22	6	13.74
(1,56)	1:73:A:SER:H	1:51:A:ASN:HD22	5	13.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:61:B:ILE:HB	1:36:A:LYS:HE2	19	13.71
(1,56)	1:73:A:SER:H	1:51:A:ASN:HD22	7	13.71
(1,220)	1:73:A:SER:HB2	1:51:A:ASN:HD21	1	13.67
(1,219)	1:72:A:HIS:HB3	1:51:A:ASN:HD21	6	13.65
(1,220)	1:73:A:SER:HB3	1:51:A:ASN:HD21	7	13.6
(1,542)	1:72:A:HIS:HB3	1:51:A:ASN:HD22	16	13.58
(1,56)	1:73:B:SER:H	1:51:B:ASN:HD22	18	13.57
(1,219)	1:72:B:HIS:HB3	1:51:B:ASN:HD21	2	13.54
(1,219)	1:72:A:HIS:HB3	1:51:A:ASN:HD21	14	13.53
(1,220)	1:73:A:SER:HB3	1:51:A:ASN:HD21	12	13.51
(1,219)	1:72:B:HIS:HB3	1:51:B:ASN:HD21	9	13.5
(1,56)	1:73:A:SER:H	1:51:A:ASN:HD22	16	13.5
(1,220)	1:73:B:SER:HB3	1:51:B:ASN:HD21	18	13.49
(1,217)	1:73:A:SER:HA	1:51:A:ASN:HD21	6	13.46
(1,542)	1:72:A:HIS:HB3	1:51:A:ASN:HD22	14	13.43
(1,227)	1:73:A:SER:HA	1:51:A:ASN:HD22	6	13.43
(1,220)	1:73:A:SER:HB3	1:51:A:ASN:HD21	5	13.41
(1,56)	1:73:B:SER:H	1:51:B:ASN:HD22	13	13.26
(1,229)	1:73:B:SER:HB3	1:51:B:ASN:HD22	15	13.18
(1,229)	1:73:A:SER:HB3	1:51:A:ASN:HD22	8	13.17
(1,56)	1:73:A:SER:H	1:51:A:ASN:HD22	14	13.17
(1,56)	1:73:A:SER:H	1:51:A:ASN:HD22	10	13.14
(1,217)	1:73:A:SER:HA	1:51:A:ASN:HD21	8	13.13
(1,217)	1:73:A:SER:HA	1:51:A:ASN:HD21	15	13.11
(1,494)	1:72:B:HIS:HD2	1:51:B:ASN:HD22	6	13.09
(1,494)	1:72:A:HIS:HD2	1:51:A:ASN:HD22	7	13.07
(1,229)	1:73:B:SER:HB3	1:51:B:ASN:HD22	3	13.07
(1,542)	1:72:B:HIS:HB3	1:51:B:ASN:HD22	9	13.06
(1,217)	1:73:A:SER:HA	1:51:A:ASN:HD21	19	13.06
(1,542)	1:72:A:HIS:HB3	1:51:A:ASN:HD22	4	13.03
(1,229)	1:73:A:SER:HB3	1:51:A:ASN:HD22	20	13.02
(1,217)	1:73:A:SER:HA	1:51:A:ASN:HD21	20	13.01
(1,494)	1:72:B:HIS:HD2	1:51:B:ASN:HD22	8	12.98
(1,229)	1:73:B:SER:HB2	1:51:B:ASN:HD22	13	12.89
(1,217)	1:73:A:SER:HA	1:51:A:ASN:HD21	11	12.89
(1,217)	1:73:B:SER:HA	1:51:B:ASN:HD21	3	12.86
(1,229)	1:73:A:SER:HB3	1:51:A:ASN:HD22	19	12.85
(1,227)	1:73:B:SER:HA	1:51:B:ASN:HD22	15	12.81
(1,494)	1:72:A:HIS:HD2	1:51:A:ASN:HD22	11	12.8
(1,229)	1:73:A:SER:HB2	1:51:A:ASN:HD22	1	12.8
(1,515)	1:36:A:LYS:HE2	1:62:B:LEU:H	19	12.77
(1,229)	1:73:B:SER:HB3	1:51:B:ASN:HD22	10	12.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,219)	1:72:A:HIS:HB3	1:51:A:ASN:HD21	4	12.76
(1,217)	1:73:A:SER:HA	1:51:A:ASN:HD21	12	12.73
(1,229)	1:73:A:SER:HB3	1:51:A:ASN:HD22	7	12.7
(1,494)	1:72:B:HIS:HD1	1:51:B:ASN:HD22	12	12.68
(1,217)	1:73:A:SER:HA	1:51:A:ASN:HD21	1	12.65
(1,227)	1:73:A:SER:HA	1:51:A:ASN:HD22	1	12.63
(1,217)	1:73:A:SER:HA	1:51:A:ASN:HD21	16	12.63
(1,227)	1:73:B:SER:HA	1:51:B:ASN:HD22	3	12.61
(1,227)	1:73:A:SER:HA	1:51:A:ASN:HD22	8	12.61
(1,229)	1:73:A:SER:HB2	1:51:A:ASN:HD22	14	12.6
(1,229)	1:73:A:SER:HB3	1:51:A:ASN:HD22	11	12.55
(1,227)	1:73:A:SER:HA	1:51:A:ASN:HD22	12	12.55
(1,229)	1:73:A:SER:HB3	1:51:A:ASN:HD22	12	12.54
(1,227)	1:73:A:SER:HA	1:51:A:ASN:HD22	20	12.5
(1,217)	1:73:A:SER:HA	1:51:A:ASN:HD21	7	12.43
(1,217)	1:73:A:SER:HA	1:51:A:ASN:HD21	10	12.43
(1,227)	1:73:A:SER:HA	1:51:A:ASN:HD22	19	12.41
(1,56)	1:73:B:SER:H	1:51:B:ASN:HD22	9	12.41
(1,494)	1:72:A:HIS:HD2	1:51:A:ASN:HD22	10	12.4
(1,217)	1:73:B:SER:HA	1:51:B:ASN:HD21	18	12.34
(1,494)	1:72:A:HIS:HD2	1:51:A:ASN:HD22	5	12.33
(1,494)	1:72:B:HIS:HD2	1:51:B:ASN:HD22	13	12.33
(1,56)	1:73:A:SER:H	1:51:A:ASN:HD22	8	12.32
(1,494)	1:72:B:HIS:HD2	1:51:B:ASN:HD22	15	12.31
(1,229)	1:73:A:SER:HB3	1:51:A:ASN:HD22	16	12.3
(1,217)	1:73:A:SER:HA	1:51:A:ASN:HD21	5	12.27
(1,229)	1:73:B:SER:HB3	1:51:B:ASN:HD22	18	12.26
(1,494)	1:72:A:HIS:HD2	1:51:A:ASN:HD22	17	12.25
(1,229)	1:73:B:SER:HB3	1:51:B:ASN:HD22	5	12.25
(1,438)	1:92:B:GLN:HG3	1:71:A:ARG:HD2	15	12.24
(1,494)	1:72:A:HIS:HD2	1:51:A:ASN:HD22	19	12.23
(1,227)	1:73:A:SER:HA	1:51:A:ASN:HD22	11	12.23
(1,217)	1:73:B:SER:HA	1:51:B:ASN:HD21	13	12.21
(1,56)	1:73:A:SER:H	1:51:A:ASN:HD22	4	12.21
(1,494)	1:72:B:HIS:HD2	1:51:B:ASN:HD22	3	12.2
(1,227)	1:73:A:SER:HA	1:51:A:ASN:HD22	7	12.2
(1,494)	1:72:A:HIS:HD2	1:51:A:ASN:HD22	14	12.18
(1,217)	1:73:A:SER:HA	1:51:A:ASN:HD21	14	12.18
(1,227)	1:73:B:SER:HA	1:51:B:ASN:HD22	5	12.16
(1,494)	1:72:A:HIS:HD2	1:51:A:ASN:HD22	20	12.11
(1,218)	1:72:B:HIS:HD2	1:51:B:ASN:HD21	6	12.07
(1,494)	1:72:B:HIS:HD2	1:51:B:ASN:HD22	1	12.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:73:B:SER:HA	1:51:B:ASN:HD22	18	11.99
(1,227)	1:73:A:SER:HA	1:51:A:ASN:HD22	16	11.98
(1,220)	1:73:B:SER:HB3	1:51:B:ASN:HD21	9	11.97
(1,494)	1:72:A:HIS:HD2	1:51:A:ASN:HD22	4	11.95
(1,438)	1:92:A:GLN:HG3	1:71:B:ARG:HD2	9	11.94
(1,218)	1:72:B:HIS:HD2	1:51:B:ASN:HD21	8	11.93
(1,227)	1:73:A:SER:HA	1:51:A:ASN:HD22	10	11.91
(1,220)	1:73:A:SER:HB3	1:51:A:ASN:HD21	17	11.83
(1,438)	1:92:B:GLN:HG3	1:71:A:ARG:HD2	12	11.8
(1,227)	1:73:B:SER:HA	1:51:B:ASN:HD22	13	11.79
(1,218)	1:72:A:HIS:HD2	1:51:A:ASN:HD21	7	11.73
(1,218)	1:72:A:HIS:HD2	1:51:A:ASN:HD21	11	11.72
(1,438)	1:92:A:GLN:HG3	1:71:B:ARG:HD2	6	11.71
(1,594)	1:73:A:SER:HB3	1:77:A:LYS:HG3	20	11.7
(1,227)	1:73:A:SER:HA	1:51:A:ASN:HD22	14	11.69
(1,494)	1:72:B:HIS:HD2	1:51:B:ASN:HD22	18	11.56
(1,309)	1:92:B:GLN:H	1:67:B:LYS:HD2	2	11.56
(1,494)	1:72:B:HIS:HD2	1:51:B:ASN:HD22	2	11.39
(1,217)	1:73:B:SER:HA	1:51:B:ASN:HD21	9	11.39
(1,594)	1:73:B:SER:HB3	1:77:B:LYS:HG3	3	11.37
(1,309)	1:92:A:GLN:H	1:67:A:LYS:HD2	6	11.37
(1,218)	1:72:A:HIS:HD2	1:51:A:ASN:HD21	12	11.36
(1,438)	1:92:A:GLN:HG3	1:71:B:ARG:HD2	2	11.35
(1,218)	1:72:B:HIS:HD2	1:51:B:ASN:HD21	15	11.32
(1,438)	1:92:B:GLN:HG3	1:71:A:ARG:HD2	4	11.31
(1,309)	1:92:B:GLN:H	1:67:B:LYS:HD2	16	11.3
(1,218)	1:72:A:HIS:HD2	1:51:A:ASN:HD21	19	11.29
(1,594)	1:73:A:SER:HB3	1:77:A:LYS:HG3	6	11.27
(1,594)	1:73:B:SER:HB3	1:77:B:LYS:HG3	10	11.25
(1,218)	1:72:A:HIS:HD2	1:51:A:ASN:HD21	10	11.25
(1,594)	1:73:A:SER:HB3	1:77:A:LYS:HG3	7	11.23
(1,438)	1:92:B:GLN:HG3	1:71:A:ARG:HD2	17	11.22
(1,494)	1:72:A:HIS:HD2	1:51:A:ASN:HD22	16	11.17
(1,594)	1:73:A:SER:HB2	1:77:A:LYS:HG3	14	11.13
(1,218)	1:72:B:HIS:HD2	1:51:B:ASN:HD21	1	11.12
(1,218)	1:72:B:HIS:HD2	1:51:B:ASN:HD21	13	11.1
(1,438)	1:92:A:GLN:HG3	1:71:B:ARG:HD2	1	11.08
(1,220)	1:73:A:SER:HB3	1:51:A:ASN:HD21	4	11.08
(1,839)	1:87:B:HIS:HD1	1:72:B:HIS:H	1	11.07
(1,401)	1:75:B:LEU:HB3	1:51:B:ASN:HD22	8	11.05
(1,594)	1:73:A:SER:HB3	1:77:A:LYS:HG3	15	11.02
(1,438)	1:92:B:GLN:HG3	1:71:A:ARG:HD2	5	11.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	1:72:A:HIS:HD2	1:51:A:ASN:HD21	20	11.01
(1,217)	1:73:A:SER:HA	1:51:A:ASN:HD21	17	10.99
(1,839)	1:87:B:HIS:HD1	1:72:B:HIS:H	2	10.98
(1,401)	1:75:A:LEU:HB3	1:51:A:ASN:HD22	6	10.97
(1,309)	1:92:B:GLN:H	1:67:B:LYS:HD2	18	10.96
(1,594)	1:73:B:SER:HB3	1:77:B:LYS:HG3	18	10.94
(1,218)	1:72:B:HIS:HD2	1:51:B:ASN:HD21	3	10.94
(1,839)	1:87:A:HIS:HD1	1:72:A:HIS:H	9	10.93
(1,218)	1:72:A:HIS:HD2	1:51:A:ASN:HD21	14	10.93
(1,229)	1:73:A:SER:HB3	1:51:A:ASN:HD22	17	10.91
(1,218)	1:72:A:HIS:HD2	1:51:A:ASN:HD21	17	10.9
(1,839)	1:87:A:HIS:HD1	1:72:A:HIS:H	16	10.89
(1,218)	1:72:A:HIS:HD2	1:51:A:ASN:HD21	5	10.88
(1,309)	1:92:A:GLN:H	1:67:A:LYS:HD2	5	10.87
(1,309)	1:92:A:GLN:H	1:67:A:LYS:HD2	12	10.86
(1,494)	1:72:B:HIS:HD2	1:51:B:ASN:HD22	9	10.84
(1,309)	1:92:B:GLN:H	1:67:B:LYS:HD2	11	10.83
(1,227)	1:73:A:SER:HA	1:51:A:ASN:HD22	17	10.82
(1,438)	1:92:B:GLN:HG3	1:71:A:ARG:HD2	7	10.81
(1,309)	1:92:A:GLN:H	1:67:A:LYS:HD2	15	10.81
(1,283)	1:87:A:HIS:HD2	1:72:A:HIS:H	9	10.81
(1,438)	1:92:A:GLN:HG3	1:71:B:ARG:HD2	18	10.8
(1,309)	1:92:A:GLN:H	1:67:B:LYS:HD2	20	10.8
(1,594)	1:73:A:SER:HB2	1:77:A:LYS:HG3	1	10.78
(1,594)	1:73:A:SER:HB3	1:77:A:LYS:HG3	5	10.77
(1,401)	1:75:B:LEU:HB3	1:51:B:ASN:HD22	1	10.77
(1,56)	1:73:A:SER:H	1:51:A:ASN:HD22	17	10.77
(1,438)	1:92:B:GLN:HG3	1:71:A:ARG:HD2	10	10.75
(1,327)	1:90:B:ASN:H	1:66:B:LYS:HE3	1	10.69
(1,283)	1:87:A:HIS:HD2	1:72:A:HIS:H	15	10.69
(1,594)	1:73:A:SER:HB3	1:77:A:LYS:HG3	16	10.67
(1,401)	1:75:B:LEU:HB3	1:51:B:ASN:HD22	3	10.66
(1,401)	1:75:B:LEU:HB3	1:51:B:ASN:HD22	19	10.66
(1,839)	1:87:A:HIS:HD1	1:72:A:HIS:H	6	10.65
(1,839)	1:87:A:HIS:HD1	1:72:A:HIS:H	15	10.61
(1,839)	1:87:B:HIS:HD2	1:72:B:HIS:H	18	10.61
(1,594)	1:73:A:SER:HB3	1:77:A:LYS:HG3	11	10.6
(1,227)	1:73:B:SER:HA	1:51:B:ASN:HD22	9	10.6
(1,327)	1:90:A:ASN:H	1:66:B:LYS:HE2	9	10.59
(1,283)	1:87:B:HIS:HD2	1:72:B:HIS:H	16	10.59
(1,594)	1:73:A:SER:HB2	1:77:A:LYS:HG3	13	10.58
(1,438)	1:92:A:GLN:HG3	1:71:B:ARG:HD2	8	10.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,309)	1:92:A:GLN:H	1:67:A:LYS:HD2	1	10.57
(1,438)	1:92:B:GLN:HG3	1:71:A:ARG:HD2	3	10.55
(1,401)	1:75:B:LEU:HB3	1:51:B:ASN:HD22	2	10.55
(1,839)	1:87:B:HIS:HD1	1:72:B:HIS:H	8	10.54
(1,218)	1:72:A:HIS:HD2	1:51:A:ASN:HD21	4	10.54
(1,438)	1:92:A:GLN:HG3	1:71:B:ARG:HD2	11	10.52
(1,438)	1:92:B:GLN:HG3	1:71:A:ARG:HD2	16	10.51
(1,401)	1:75:B:LEU:HB3	1:51:B:ASN:HD22	11	10.5
(1,438)	1:92:A:GLN:HG3	1:71:B:ARG:HD2	20	10.48
(1,283)	1:87:B:HIS:HD2	1:72:B:HIS:H	1	10.48
(1,309)	1:92:B:GLN:H	1:67:B:LYS:HD2	4	10.45
(1,309)	1:92:B:GLN:H	1:67:B:LYS:HD2	19	10.45
(1,283)	1:87:A:HIS:HD2	1:72:A:HIS:H	6	10.45
(1,229)	1:73:B:SER:HB3	1:51:B:ASN:HD22	9	10.42
(1,227)	1:73:A:SER:HA	1:51:A:ASN:HD22	4	10.42
(1,217)	1:73:A:SER:HA	1:51:A:ASN:HD21	4	10.42
(1,841)	1:87:B:HIS:HD2	1:72:B:HIS:HB2	2	10.38
(1,594)	1:73:A:SER:HB2	1:77:A:LYS:HG3	19	10.38
(1,218)	1:72:B:HIS:HD2	1:51:B:ASN:HD21	18	10.37
(1,401)	1:75:B:LEU:HB3	1:51:B:ASN:HD22	12	10.36
(1,401)	1:75:A:LEU:HB3	1:51:A:ASN:HD22	7	10.32
(1,839)	1:87:B:HIS:HD1	1:72:B:HIS:H	4	10.3
(1,839)	1:87:B:HIS:HD2	1:72:B:HIS:H	17	10.3
(1,309)	1:92:B:GLN:H	1:67:B:LYS:HD2	17	10.28
(1,560)	1:91:B:LEU:HA	1:66:B:LYS:HE3	1	10.25
(1,229)	1:73:A:SER:HB3	1:51:A:ASN:HD22	4	10.25
(1,218)	1:72:A:HIS:HD2	1:51:A:ASN:HD21	16	10.25
(1,755)	1:87:B:HIS:HD1	1:72:B:HIS:H	18	10.2
(1,594)	1:73:A:SER:HB3	1:77:A:LYS:HG3	4	10.17
(1,438)	1:92:B:GLN:HG3	1:71:A:ARG:HD2	19	10.16
(1,839)	1:87:B:HIS:HD1	1:72:B:HIS:H	11	10.15
(1,755)	1:87:B:HIS:HD1	1:72:B:HIS:H	1	10.12
(1,283)	1:87:B:HIS:HD2	1:72:B:HIS:H	2	10.12
(1,401)	1:75:B:LEU:HB3	1:51:B:ASN:HD22	17	10.11
(1,438)	1:92:B:GLN:HG3	1:71:A:ARG:HD2	14	10.1
(1,401)	1:75:A:LEU:HB3	1:51:A:ASN:HD22	14	10.09
(1,309)	1:92:A:GLN:H	1:67:A:LYS:HD2	7	10.09
(1,56)	1:73:B:SER:H	1:51:B:ASN:HD22	2	10.07
(1,283)	1:87:B:HIS:HD2	1:72:B:HIS:H	11	10.06
(1,594)	1:73:A:SER:HB3	1:77:A:LYS:HG3	8	10.05
(1,218)	1:72:B:HIS:HD2	1:51:B:ASN:HD21	9	10.04
(1,839)	1:87:A:HIS:HD1	1:72:A:HIS:H	10	10.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	1:87:B:HIS:HD1	1:72:B:HIS:H	2	10.03
(1,401)	1:75:A:LEU:HB3	1:51:A:ASN:HD22	16	10.01
(1,560)	1:91:B:LEU:HA	1:66:B:LYS:HE2	9	10.0
(1,283)	1:87:B:HIS:HD2	1:72:B:HIS:H	8	10.0
(1,841)	1:87:A:HIS:HD1	1:72:A:HIS:HB2	9	9.99
(1,309)	1:92:B:GLN:H	1:67:B:LYS:HD3	14	9.99
(1,755)	1:87:A:HIS:HD1	1:72:A:HIS:H	9	9.98
(1,841)	1:87:A:HIS:HD1	1:72:A:HIS:HB2	16	9.97
(1,839)	1:87:A:HIS:HD1	1:72:A:HIS:H	7	9.97
(1,755)	1:87:A:HIS:HD1	1:72:A:HIS:H	16	9.94
(1,438)	1:92:B:GLN:HG3	1:71:A:ARG:HD2	13	9.93
(1,218)	1:72:B:HIS:HD2	1:51:B:ASN:HD21	2	9.93
(1,327)	1:90:B:ASN:H	1:66:A:LYS:HE2	13	9.91
(1,401)	1:75:B:LEU:HB3	1:51:B:ASN:HD22	5	9.9
(1,536)	1:89:A:ARG:H	1:66:B:LYS:HE3	1	9.89
(1,537)	1:91:B:LEU:H	1:66:B:LYS:HE3	1	9.84
(1,594)	1:73:A:SER:HB3	1:77:A:LYS:HG3	17	9.83
(1,841)	1:87:A:HIS:HD2	1:72:A:HIS:HB2	1	9.8
(1,327)	1:90:A:ASN:H	1:66:A:LYS:HE2	6	9.8
(1,327)	1:90:B:ASN:H	1:66:B:LYS:HE2	8	9.8
(1,401)	1:75:B:LEU:HB3	1:51:B:ASN:HD22	13	9.77
(1,283)	1:87:A:HIS:HD2	1:72:A:HIS:H	4	9.77
(1,283)	1:87:A:HIS:HD2	1:72:A:HIS:H	10	9.76
(1,537)	1:91:B:LEU:H	1:66:B:LYS:HE2	9	9.74
(1,309)	1:92:B:GLN:H	1:67:B:LYS:HD3	10	9.73
(1,283)	1:87:A:HIS:HD2	1:72:A:HIS:H	7	9.73
(1,401)	1:75:B:LEU:HB3	1:51:B:ASN:HD22	18	9.72
(1,401)	1:75:A:LEU:HB3	1:51:A:ASN:HD22	20	9.72
(1,755)	1:87:A:HIS:HD1	1:72:A:HIS:H	6	9.7
(1,755)	1:87:A:HIS:HD1	1:72:A:HIS:H	15	9.66
(1,283)	1:87:B:HIS:HD2	1:72:B:HIS:H	18	9.66
(1,536)	1:89:A:ARG:H	1:66:B:LYS:HE2	17	9.64
(1,401)	1:75:A:LEU:HB3	1:51:A:ASN:HD22	9	9.64
(1,755)	1:87:B:HIS:HD1	1:72:B:HIS:H	8	9.59
(1,309)	1:92:A:GLN:H	1:67:A:LYS:HD2	3	9.59
(1,536)	1:89:A:ARG:H	1:66:B:LYS:HE2	4	9.58
(1,755)	1:87:B:HIS:HD1	1:72:B:HIS:H	17	9.56
(1,401)	1:75:A:LEU:HB3	1:51:A:ASN:HD22	4	9.56
(1,755)	1:87:B:HIS:HD1	1:72:B:HIS:H	20	9.54
(1,546)	1:88:A:LEU:HA	1:66:B:LYS:HE3	1	9.54
(1,327)	1:90:A:ASN:H	1:66:A:LYS:HE2	10	9.54
(1,841)	1:87:A:HIS:HD1	1:72:A:HIS:HB2	10	9.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	1:87:A:HIS:HD1	1:72:A:HIS:H	14	9.49
(1,309)	1:92:A:GLN:H	1:67:A:LYS:HD2	8	9.49
(1,217)	1:73:B:SER:HA	1:51:B:ASN:HD21	2	9.49
(1,594)	1:73:A:SER:HB3	1:77:A:LYS:HG3	12	9.48
(1,664)	1:86:A:LYS:HG2	1:92:A:GLN:HE21	8	9.45
(1,401)	1:75:B:LEU:HB3	1:51:B:ASN:HD22	15	9.44
(1,327)	1:90:B:ASN:H	1:66:B:LYS:HE2	4	9.43
(1,536)	1:89:B:ARG:H	1:66:A:LYS:HE2	5	9.42
(1,327)	1:90:B:ASN:H	1:66:B:LYS:HE2	14	9.42
(1,227)	1:73:B:SER:HA	1:51:B:ASN:HD22	2	9.4
(1,594)	1:73:B:SER:HB2	1:77:B:LYS:HG3	9	9.39
(1,841)	1:87:B:HIS:HD2	1:72:B:HIS:HB2	18	9.38
(1,309)	1:92:A:GLN:H	1:67:A:LYS:HD2	9	9.38
(1,327)	1:90:A:ASN:H	1:66:A:LYS:HE2	17	9.37
(1,327)	1:90:A:ASN:H	1:66:A:LYS:HE2	5	9.36
(1,755)	1:87:B:HIS:HD1	1:72:B:HIS:H	4	9.35
(1,283)	1:87:B:HIS:HD2	1:72:B:HIS:H	17	9.35
(1,401)	1:75:A:LEU:HB3	1:51:A:ASN:HD22	10	9.34
(1,546)	1:88:A:LEU:HA	1:66:B:LYS:HE2	9	9.31
(1,327)	1:90:B:ASN:H	1:66:B:LYS:HE2	12	9.31
(1,664)	1:86:A:LYS:HG2	1:92:B:GLN:HE21	13	9.3
(1,536)	1:89:B:ARG:H	1:66:A:LYS:HE2	10	9.3
(1,755)	1:87:A:HIS:HD1	1:72:A:HIS:H	12	9.28
(1,536)	1:89:B:ARG:H	1:66:A:LYS:HE2	15	9.28
(1,327)	1:90:B:ASN:H	1:66:B:LYS:HE2	3	9.27
(1,327)	1:90:B:ASN:H	1:66:B:LYS:HE2	7	9.27
(1,664)	1:86:B:LYS:HG2	1:92:B:GLN:HE21	20	9.26
(1,841)	1:87:B:HIS:HD1	1:72:B:HIS:HB2	4	9.25
(1,220)	1:73:B:SER:HB3	1:51:B:ASN:HD21	2	9.25
(1,327)	1:90:A:ASN:H	1:66:A:LYS:HE2	11	9.23
(1,755)	1:87:B:HIS:HD1	1:72:B:HIS:H	11	9.2
(1,327)	1:90:B:ASN:H	1:66:B:LYS:HE2	16	9.2
(1,546)	1:88:B:LEU:HA	1:66:A:LYS:HE2	17	9.19
(1,327)	1:90:B:ASN:H	1:66:B:LYS:HE2	2	9.18
(1,664)	1:86:A:LYS:HG2	1:92:A:GLN:HE21	5	9.17
(1,841)	1:87:B:HIS:HD1	1:72:B:HIS:HB2	11	9.15
(1,546)	1:88:A:LEU:HA	1:66:B:LYS:HE2	4	9.15
(1,354)	1:76:B:GLU:HA	1:51:A:ASN:HD21	2	9.15
(1,615)	1:91:B:LEU:HG	1:66:B:LYS:HE3	1	9.13
(1,841)	1:87:A:HIS:HD1	1:72:A:HIS:HB2	15	9.1
(1,840)	1:87:B:HIS:HD2	1:72:B:HIS:HA	2	9.09
(1,664)	1:86:B:LYS:HG2	1:92:B:GLN:HE21	15	9.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	1:87:A:HIS:HD1	1:72:A:HIS:H	3	9.08
(1,755)	1:87:A:HIS:HD1	1:72:A:HIS:H	10	9.08
(1,841)	1:87:B:HIS:HD1	1:72:B:HIS:HB2	17	9.07
(1,841)	1:87:A:HIS:HD1	1:72:A:HIS:HB2	7	9.06
(1,615)	1:91:B:LEU:HG	1:66:B:LYS:HE2	9	9.05
(1,536)	1:89:A:ARG:H	1:66:B:LYS:HE2	16	9.05
(1,327)	1:90:B:ASN:H	1:66:B:LYS:HE2	15	9.05
(1,841)	1:87:B:HIS:HD1	1:72:B:HIS:HB2	8	9.04
(1,664)	1:86:A:LYS:HG2	1:92:A:GLN:HE21	4	9.03
(1,664)	1:86:A:LYS:HG2	1:92:A:GLN:HE21	7	9.03
(1,536)	1:89:A:ARG:H	1:66:B:LYS:HE2	3	9.03
(1,327)	1:90:A:ASN:H	1:66:A:LYS:HE2	20	9.03
(1,755)	1:87:A:HIS:HD1	1:72:A:HIS:H	7	9.02
(1,536)	1:89:A:ARG:H	1:66:B:LYS:HE2	9	9.02
(1,664)	1:86:A:LYS:HG2	1:92:A:GLN:HE21	11	9.01
(1,327)	1:90:A:ASN:H	1:66:B:LYS:HE2	19	9.01
(1,664)	1:86:B:LYS:HG2	1:92:B:GLN:HE21	19	8.99
(1,536)	1:89:A:ARG:H	1:66:B:LYS:HE2	7	8.98
(1,536)	1:89:A:ARG:H	1:66:B:LYS:HE3	6	8.97
(1,841)	1:87:A:HIS:HD1	1:72:A:HIS:HB3	6	8.96
(1,664)	1:86:B:LYS:HG2	1:92:B:GLN:HE21	12	8.95
(1,664)	1:86:A:LYS:HG2	1:92:A:GLN:HE21	18	8.95
(1,840)	1:87:B:HIS:HD2	1:72:B:HIS:HA	1	8.94
(1,536)	1:89:A:ARG:H	1:66:B:LYS:HE2	8	8.92
(1,840)	1:87:A:HIS:HD1	1:72:A:HIS:HA	6	8.91
(1,557)	1:89:A:ARG:HA	1:66:B:LYS:HE3	1	8.91
(1,536)	1:89:B:ARG:H	1:66:A:LYS:HE2	12	8.91
(1,664)	1:86:A:LYS:HG2	1:92:B:GLN:HE21	2	8.9
(1,546)	1:88:B:LEU:HA	1:66:A:LYS:HE2	6	8.9
(1,536)	1:89:B:ARG:H	1:66:A:LYS:HE2	11	8.88
(1,57)	1:73:A:SER:H	1:77:A:LYS:HG3	20	8.88
(1,57)	1:73:A:SER:H	1:77:A:LYS:HG3	10	8.86
(1,536)	1:89:B:ARG:H	1:66:A:LYS:HE2	14	8.84
(1,839)	1:87:B:HIS:HD2	1:72:B:HIS:H	20	8.83
(1,536)	1:89:B:ARG:H	1:66:A:LYS:HE2	18	8.81
(1,537)	1:91:B:LEU:H	1:66:B:LYS:HE2	8	8.78
(1,537)	1:91:A:LEU:H	1:66:A:LYS:HE2	6	8.77
(1,536)	1:89:B:ARG:H	1:66:A:LYS:HE2	2	8.72
(1,842)	1:87:B:HIS:HD1	1:75:B:LEU:HD13	9	8.71
(1,216)	1:76:B:GLU:HB3	1:51:A:ASN:HD21	2	8.71
(1,560)	1:91:B:LEU:HA	1:66:B:LYS:HE2	8	8.7
(1,537)	1:91:A:LEU:H	1:66:A:LYS:HE2	13	8.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,57)	1:73:B:SER:H	1:77:B:LYS:HG3	6	8.69
(1,664)	1:86:B:LYS:HG2	1:92:B:GLN:HE21	3	8.67
(1,664)	1:86:A:LYS:HG2	1:92:B:GLN:HE21	10	8.67
(1,560)	1:91:A:LEU:HA	1:66:A:LYS:HE2	13	8.67
(1,536)	1:89:B:ARG:H	1:66:A:LYS:HE2	13	8.66
(1,57)	1:73:A:SER:H	1:77:A:LYS:HG3	16	8.65
(1,57)	1:73:A:SER:H	1:77:A:LYS:HG3	7	8.62
(1,546)	1:88:A:LEU:HA	1:66:B:LYS:HE2	16	8.61
(1,560)	1:91:B:LEU:HA	1:66:B:LYS:HE2	14	8.6
(1,557)	1:89:B:ARG:HA	1:66:A:LYS:HE2	10	8.6
(1,546)	1:88:B:LEU:HA	1:66:A:LYS:HE2	14	8.59
(1,57)	1:73:A:SER:H	1:77:A:LYS:HG3	4	8.59
(1,228)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	4	8.57
(1,840)	1:87:B:HIS:HD2	1:72:B:HIS:HA	10	8.56
(1,537)	1:91:A:LEU:H	1:66:A:LYS:HE2	10	8.56
(1,283)	1:87:A:HIS:HD2	1:72:A:HIS:H	19	8.56
(1,842)	1:87:B:HIS:HD1	1:75:B:LEU:HD11	17	8.54
(1,840)	1:87:B:HIS:HD1	1:72:B:HIS:HA	9	8.54
(1,546)	1:88:A:LEU:HA	1:66:B:LYS:HE2	3	8.54
(1,560)	1:91:A:LEU:HA	1:66:A:LYS:HE2	10	8.52
(1,57)	1:73:B:SER:H	1:77:B:LYS:HG3	1	8.52
(1,560)	1:91:A:LEU:HA	1:66:A:LYS:HE2	6	8.49
(1,546)	1:88:B:LEU:HA	1:66:A:LYS:HE2	5	8.49
(1,546)	1:88:B:LEU:HA	1:66:A:LYS:HE2	15	8.49
(1,664)	1:86:A:LYS:HG2	1:92:A:GLN:HE21	16	8.48
(1,560)	1:91:B:LEU:HA	1:66:B:LYS:HE2	4	8.48
(1,228)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	5	8.48
(1,537)	1:91:B:LEU:H	1:66:B:LYS:HE2	14	8.46
(1,327)	1:90:A:ASN:H	1:66:A:LYS:HE2	18	8.45
(1,229)	1:73:B:SER:HB3	1:51:B:ASN:HD22	2	8.45
(1,839)	1:87:A:HIS:HD1	1:72:A:HIS:H	19	8.44
(1,537)	1:91:B:LEU:H	1:66:B:LYS:HE2	4	8.44
(1,842)	1:87:A:HIS:HD1	1:75:A:LEU:HD11	16	8.43
(1,839)	1:87:A:HIS:HD2	1:72:A:HIS:H	12	8.43
(1,560)	1:91:A:LEU:HA	1:66:A:LYS:HE2	12	8.43
(1,57)	1:73:A:SER:H	1:77:A:LYS:HG3	15	8.43
(1,842)	1:87:A:HIS:HD2	1:75:A:LEU:HD12	11	8.42
(1,664)	1:86:B:LYS:HG2	1:92:B:GLN:HE21	1	8.42
(1,557)	1:89:A:ARG:HA	1:66:B:LYS:HE2	17	8.42
(1,842)	1:87:A:HIS:HD2	1:75:A:LEU:HD23	1	8.41
(1,354)	1:76:A:GLU:HA	1:51:A:ASN:HD21	4	8.41
(1,309)	1:92:A:GLN:H	1:67:A:LYS:HD2	13	8.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,840)	1:87:A:HIS:HD1	1:72:A:HIS:HA	15	8.39
(1,560)	1:91:B:LEU:HA	1:66:B:LYS:HE2	3	8.39
(1,537)	1:91:A:LEU:H	1:66:A:LYS:HE2	17	8.39
(1,57)	1:73:A:SER:H	1:77:A:LYS:HG3	18	8.39
(1,560)	1:91:A:LEU:HA	1:66:A:LYS:HE2	11	8.38
(1,557)	1:89:A:ARG:HA	1:66:B:LYS:HE2	15	8.38
(1,839)	1:87:A:HIS:HD2	1:72:A:HIS:H	3	8.37
(1,537)	1:91:B:LEU:H	1:66:B:LYS:HE2	12	8.37
(1,537)	1:91:B:LEU:H	1:66:B:LYS:HE2	3	8.36
(1,354)	1:76:A:GLU:HA	1:51:B:ASN:HD21	10	8.36
(1,560)	1:91:A:LEU:HA	1:66:A:LYS:HE2	15	8.35
(1,546)	1:88:A:LEU:HA	1:66:B:LYS:HE2	8	8.35
(1,354)	1:76:B:GLU:HA	1:51:A:ASN:HD21	19	8.35
(1,725)	1:75:A:LEU:HA	1:50:B:ILE:HG21	20	8.34
(1,560)	1:91:B:LEU:HA	1:66:B:LYS:HE2	7	8.34
(1,557)	1:89:B:ARG:HA	1:66:A:LYS:HE2	5	8.34
(1,536)	1:89:B:ARG:H	1:66:A:LYS:HE2	20	8.34
(1,57)	1:73:A:SER:H	1:77:A:LYS:HG3	5	8.34
(1,664)	1:86:A:LYS:HG2	1:92:A:GLN:HE21	17	8.32
(1,57)	1:73:A:SER:H	1:77:A:LYS:HG3	11	8.32
(1,840)	1:87:A:HIS:HD1	1:72:A:HIS:HA	16	8.31
(1,560)	1:91:A:LEU:HA	1:66:A:LYS:HE2	17	8.31
(1,557)	1:89:A:ARG:HA	1:66:B:LYS:HE2	4	8.31
(1,546)	1:88:B:LEU:HA	1:66:A:LYS:HE2	11	8.31
(1,228)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	18	8.31
(1,725)	1:75:A:LEU:HA	1:50:B:ILE:HG21	18	8.3
(1,546)	1:88:B:LEU:HA	1:66:A:LYS:HE2	12	8.3
(1,557)	1:89:A:ARG:HA	1:66:B:LYS:HE3	6	8.29
(1,228)	1:76:B:GLU:HB3	1:51:A:ASN:HD22	13	8.29
(1,216)	1:76:A:GLU:HB3	1:51:B:ASN:HD21	4	8.29
(1,841)	1:87:A:HIS:HD2	1:72:A:HIS:HB2	3	8.28
(1,840)	1:87:B:HIS:HD1	1:72:B:HIS:HA	8	8.28
(1,840)	1:87:B:HIS:HD1	1:72:B:HIS:HA	17	8.27
(1,560)	1:91:B:LEU:HA	1:66:B:LYS:HE2	2	8.26
(1,537)	1:91:B:LEU:H	1:66:B:LYS:HE2	7	8.26
(1,537)	1:91:A:LEU:H	1:66:A:LYS:HE2	11	8.26
(1,283)	1:87:A:HIS:HD2	1:72:A:HIS:H	5	8.26
(1,57)	1:73:B:SER:H	1:77:B:LYS:HG3	3	8.26
(1,537)	1:91:B:LEU:H	1:66:B:LYS:HE2	15	8.25
(1,57)	1:73:A:SER:H	1:77:A:LYS:HG3	14	8.24
(1,228)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	9	8.23
(1,228)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	10	8.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,57)	1:73:A:SER:H	1:77:A:LYS:HG3	13	8.23
(1,546)	1:88:B:LEU:HA	1:66:A:LYS:HE2	7	8.22
(1,354)	1:76:A:GLU:HA	1:51:B:ASN:HD21	15	8.22
(1,228)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	19	8.21
(1,840)	1:87:B:HIS:HD1	1:72:B:HIS:HA	11	8.2
(1,839)	1:87:A:HIS:HD2	1:72:A:HIS:H	14	8.2
(1,725)	1:75:A:LEU:HA	1:50:B:ILE:HG21	6	8.19
(1,354)	1:76:A:GLU:HA	1:51:B:ASN:HD21	13	8.19
(1,228)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	20	8.19
(1,546)	1:88:B:LEU:HA	1:66:A:LYS:HE2	13	8.18
(1,354)	1:76:B:GLU:HA	1:51:A:ASN:HD21	14	8.18
(1,99)	1:66:B:LYS:HE3	1:92:A:GLN:H	1	8.18
(1,228)	1:76:B:GLU:HB3	1:51:A:ASN:HD22	2	8.17
(1,725)	1:75:A:LEU:HA	1:50:B:ILE:HG21	8	8.16
(1,354)	1:76:B:GLU:HA	1:51:A:ASN:HD21	20	8.16
(1,546)	1:88:B:LEU:HA	1:66:A:LYS:HE2	10	8.15
(1,842)	1:87:A:HIS:HD1	1:75:A:LEU:HD11	7	8.14
(1,664)	1:86:A:LYS:HG2	1:92:A:GLN:HE21	6	8.14
(1,664)	1:86:B:LYS:HG2	1:92:B:GLN:HE21	9	8.14
(1,560)	1:91:B:LEU:HA	1:66:B:LYS:HE2	16	8.14
(1,354)	1:76:A:GLU:HA	1:51:B:ASN:HD21	18	8.14
(1,228)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	15	8.14
(1,840)	1:87:A:HIS:HD1	1:72:A:HIS:HA	7	8.13
(1,840)	1:87:B:HIS:HD2	1:72:B:HIS:HA	18	8.13
(1,841)	1:87:A:HIS:HD1	1:72:A:HIS:HB2	19	8.12
(1,840)	1:87:A:HIS:HD2	1:72:A:HIS:HA	4	8.12
(1,228)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	1	8.12
(1,228)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	17	8.12
(1,725)	1:75:A:LEU:HA	1:50:B:ILE:HG23	10	8.11
(1,546)	1:88:A:LEU:HA	1:66:B:LYS:HE2	18	8.11
(1,537)	1:91:B:LEU:H	1:66:B:LYS:HE2	16	8.11
(1,838)	1:87:A:HIS:HD1	1:71:A:ARG:HD2	15	8.1
(1,664)	1:86:A:LYS:HG2	1:92:A:GLN:HE21	14	8.1
(1,725)	1:75:A:LEU:HA	1:50:B:ILE:HG23	7	8.09
(1,354)	1:76:A:GLU:HA	1:51:B:ASN:HD21	5	8.09
(1,354)	1:76:A:GLU:HA	1:51:B:ASN:HD21	7	8.09
(1,537)	1:91:A:LEU:H	1:66:A:LYS:HE2	5	8.08
(1,725)	1:75:A:LEU:HA	1:50:B:ILE:HG22	17	8.07
(1,57)	1:73:A:SER:H	1:77:A:LYS:HG3	19	8.07
(1,842)	1:87:B:HIS:HD2	1:75:B:LEU:HD23	2	8.06
(1,228)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	7	8.06
(1,228)	1:76:B:GLU:HB3	1:51:A:ASN:HD22	14	8.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,725)	1:75:A:LEU:HA	1:50:B:ILE:HG22	4	8.05
(1,615)	1:91:B:LEU:HG	1:66:B:LYS:HE2	8	8.05
(1,557)	1:89:A:ARG:HA	1:66:B:LYS:HE2	16	8.05
(1,537)	1:91:B:LEU:H	1:66:B:LYS:HE2	2	8.04
(1,841)	1:87:B:HIS:HD2	1:72:B:HIS:HB2	20	8.03
(1,725)	1:75:A:LEU:HA	1:50:B:ILE:HG23	1	8.03
(1,228)	1:76:B:GLU:HB3	1:51:A:ASN:HD22	8	8.03
(1,841)	1:87:A:HIS:HD2	1:72:A:HIS:HB2	12	8.02
(1,725)	1:75:A:LEU:HA	1:50:B:ILE:HG21	5	8.02
(1,842)	1:87:A:HIS:HD2	1:75:A:LEU:HD23	8	8.0
(1,399)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	4	8.0
(1,650)	1:79:B:ASP:HB2	1:54:B:LEU:HD11	3	7.99
(1,354)	1:76:A:GLU:HA	1:51:B:ASN:HD21	8	7.99
(1,725)	1:75:A:LEU:HA	1:50:B:ILE:HG21	9	7.98
(1,615)	1:91:A:LEU:HG	1:66:A:LYS:HE2	6	7.98
(1,354)	1:76:A:GLU:HA	1:51:B:ASN:HD21	11	7.98
(1,354)	1:76:A:GLU:HA	1:51:B:ASN:HD21	6	7.97
(1,57)	1:73:B:SER:H	1:77:B:LYS:HG3	9	7.97
(1,842)	1:87:A:HIS:HD1	1:75:A:LEU:HD22	6	7.95
(1,725)	1:75:B:LEU:HA	1:50:A:ILE:HG21	14	7.95
(1,691)	1:87:B:HIS:HD2	1:71:B:ARG:HD2	2	7.95
(1,725)	1:75:A:LEU:HA	1:50:B:ILE:HG23	2	7.94
(1,354)	1:76:A:GLU:HA	1:51:B:ASN:HD21	17	7.94
(1,842)	1:87:A:HIS:HD1	1:75:A:LEU:HD21	18	7.93
(1,839)	1:87:A:HIS:HD1	1:72:A:HIS:H	5	7.93
(1,228)	1:76:B:GLU:HB3	1:51:A:ASN:HD22	3	7.93
(1,725)	1:75:A:LEU:HA	1:50:B:ILE:HG21	15	7.92
(1,560)	1:91:A:LEU:HA	1:66:A:LYS:HE2	20	7.92
(1,216)	1:76:B:GLU:HB3	1:51:A:ASN:HD21	13	7.92
(1,399)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	5	7.91
(1,228)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	6	7.91
(1,216)	1:76:A:GLU:HB3	1:51:B:ASN:HD21	5	7.9
(1,842)	1:87:A:HIS:HD1	1:75:A:LEU:HD23	15	7.89
(1,283)	1:87:B:HIS:HD2	1:72:B:HIS:H	20	7.88
(1,838)	1:87:B:HIS:HD1	1:71:B:ARG:HD2	6	7.87
(1,725)	1:75:A:LEU:HA	1:50:B:ILE:HG21	11	7.87
(1,691)	1:87:B:HIS:HD2	1:71:B:ARG:HD2	9	7.87
(1,537)	1:91:B:LEU:H	1:66:B:LYS:HE2	19	7.87
(1,354)	1:76:A:GLU:HA	1:51:B:ASN:HD21	3	7.87
(1,354)	1:76:B:GLU:HA	1:51:A:ASN:HD21	16	7.87
(1,842)	1:87:B:HIS:HD2	1:75:B:LEU:HD12	10	7.86
(1,228)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	11	7.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,838)	1:87:B:HIS:HD1	1:71:B:ARG:HD2	2	7.85
(1,537)	1:91:A:LEU:H	1:66:A:LYS:HE2	20	7.84
(1,216)	1:76:A:GLU:HB3	1:51:B:ASN:HD21	10	7.84
(1,615)	1:91:B:LEU:HG	1:66:B:LYS:HE2	14	7.82
(1,546)	1:88:A:LEU:HA	1:66:B:LYS:HE2	2	7.81
(1,354)	1:76:A:GLU:HA	1:51:B:ASN:HD21	9	7.81
(1,557)	1:89:A:ARG:HA	1:66:B:LYS:HE2	9	7.8
(1,615)	1:91:A:LEU:HG	1:66:A:LYS:HE2	10	7.79
(1,560)	1:91:A:LEU:HA	1:66:A:LYS:HE2	5	7.79
(1,725)	1:75:A:LEU:HA	1:50:B:ILE:HG21	3	7.78
(1,615)	1:91:A:LEU:HG	1:66:A:LYS:HE2	13	7.78
(1,725)	1:75:B:LEU:HA	1:50:A:ILE:HG21	13	7.77
(1,354)	1:76:A:GLU:HA	1:51:B:ASN:HD21	1	7.76
(1,838)	1:87:A:HIS:HD1	1:71:A:ARG:HD2	9	7.75
(1,557)	1:89:A:ARG:HA	1:66:B:LYS:HE2	3	7.74
(1,399)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	18	7.74
(1,57)	1:73:A:SER:H	1:77:A:LYS:HG3	12	7.74
(1,725)	1:75:B:LEU:HA	1:50:A:ILE:HG21	16	7.73
(1,354)	1:76:A:GLU:HA	1:51:B:ASN:HD21	12	7.73
(1,216)	1:76:A:GLU:HB3	1:51:B:ASN:HD21	18	7.73
(1,691)	1:87:A:HIS:HD2	1:71:A:ARG:HD2	6	7.72
(1,557)	1:89:B:ARG:HA	1:66:A:LYS:HE2	18	7.72
(1,399)	1:76:B:GLU:HB3	1:51:A:ASN:HD22	13	7.72
(1,228)	1:76:B:GLU:HB3	1:51:A:ASN:HD22	16	7.72
(1,838)	1:87:B:HIS:HD2	1:71:B:ARG:HD2	4	7.71
(1,755)	1:87:A:HIS:HD1	1:72:A:HIS:H	13	7.7
(1,725)	1:75:A:LEU:HA	1:50:B:ILE:HG23	19	7.7
(1,216)	1:76:B:GLU:HB3	1:51:A:ASN:HD21	19	7.7
(1,594)	1:73:B:SER:HB3	1:77:B:LYS:HG3	2	7.69
(1,557)	1:89:A:ARG:HA	1:66:B:LYS:HE2	7	7.69
(1,557)	1:89:A:ARG:HA	1:66:B:LYS:HE2	12	7.68
(1,725)	1:75:A:LEU:HA	1:50:B:ILE:HG23	12	7.67
(1,679)	1:92:A:GLN:HG3	1:83:B:MET:HG2	15	7.67
(1,615)	1:91:B:LEU:HG	1:66:B:LYS:HE2	17	7.67
(1,216)	1:76:A:GLU:HB3	1:51:B:ASN:HD21	17	7.67
(1,557)	1:89:B:ARG:HA	1:66:A:LYS:HE2	11	7.66
(1,399)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	9	7.66
(1,399)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	10	7.66
(1,642)	1:79:B:ASP:HB3	1:54:B:LEU:HD12	6	7.65
(1,615)	1:91:B:LEU:HG	1:66:B:LYS:HE2	4	7.65
(1,557)	1:89:B:ARG:HA	1:66:A:LYS:HE2	14	7.65
(1,615)	1:91:B:LEU:HG	1:66:B:LYS:HE2	15	7.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,399)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	19	7.64
(1,228)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	12	7.64
(1,536)	1:89:A:ARG:H	1:66:B:LYS:HE2	19	7.63
(1,691)	1:87:B:HIS:HD2	1:71:B:ARG:HD2	1	7.62
(1,399)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	20	7.62
(1,216)	1:76:A:GLU:HB3	1:51:B:ASN:HD21	7	7.62
(1,216)	1:76:B:GLU:HB3	1:51:A:ASN:HD21	20	7.61
(1,399)	1:76:B:GLU:HB3	1:51:A:ASN:HD22	2	7.6
(1,842)	1:87:A:HIS:HD2	1:75:A:LEU:HD23	4	7.59
(1,557)	1:89:A:ARG:HA	1:66:B:LYS:HE2	8	7.59
(1,537)	1:91:A:LEU:H	1:66:A:LYS:HE2	18	7.58
(1,216)	1:76:A:GLU:HB3	1:51:B:ASN:HD21	15	7.58
(1,399)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	15	7.57
(1,216)	1:76:B:GLU:HB3	1:51:A:ASN:HD21	14	7.57
(1,615)	1:91:B:LEU:HG	1:66:B:LYS:HE2	3	7.56
(1,399)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	1	7.55
(1,399)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	17	7.55
(1,640)	1:86:B:LYS:HD3	1:84:B:THR:HG23	20	7.54
(1,615)	1:91:A:LEU:HG	1:66:A:LYS:HE2	11	7.54
(1,216)	1:76:B:GLU:HB3	1:51:A:ASN:HD21	3	7.53
(1,216)	1:76:A:GLU:HB3	1:51:B:ASN:HD21	8	7.53
(1,925)	1:69:B:SER:H	1:65:B:LEU:O	11	7.52
(1,691)	1:87:A:HIS:HD2	1:71:A:ARG:HD2	15	7.52
(1,560)	1:91:B:LEU:HA	1:66:B:LYS:HE2	19	7.51
(1,615)	1:91:A:LEU:HG	1:66:A:LYS:HE2	12	7.5
(1,755)	1:87:A:HIS:HD1	1:72:A:HIS:H	19	7.49
(1,650)	1:79:B:ASP:HB2	1:54:B:LEU:HD13	17	7.49
(1,399)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	7	7.49
(1,399)	1:76:B:GLU:HB3	1:51:A:ASN:HD22	14	7.49
(1,838)	1:87:B:HIS:HD1	1:71:B:ARG:HD2	16	7.48
(1,283)	1:87:A:HIS:HD2	1:72:A:HIS:H	12	7.48
(1,216)	1:76:A:GLU:HB3	1:51:B:ASN:HD21	9	7.48
(1,216)	1:76:A:GLU:HB3	1:51:B:ASN:HD21	11	7.48
(1,838)	1:87:A:HIS:HD2	1:71:A:ARG:HD2	7	7.47
(1,399)	1:76:B:GLU:HB3	1:51:A:ASN:HD22	8	7.46
(1,216)	1:76:A:GLU:HB3	1:51:B:ASN:HD21	1	7.46
(1,650)	1:79:B:ASP:HB2	1:54:B:LEU:HD13	12	7.45
(1,99)	1:66:B:LYS:HE2	1:92:A:GLN:H	9	7.45
(1,560)	1:91:A:LEU:HA	1:66:A:LYS:HE2	18	7.43
(1,546)	1:88:B:LEU:HA	1:66:A:LYS:HE2	20	7.42
(1,283)	1:87:A:HIS:HD2	1:72:A:HIS:H	3	7.42
(1,650)	1:79:A:ASP:HB2	1:54:A:LEU:HD11	1	7.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,615)	1:91:B:LEU:HG	1:66:B:LYS:HE2	16	7.4
(1,216)	1:76:A:GLU:HB3	1:51:B:ASN:HD21	6	7.38
(1,687)	1:87:A:HIS:HD1	1:71:A:ARG:HD2	15	7.36
(1,399)	1:76:B:GLU:HB3	1:51:A:ASN:HD22	3	7.36
(1,925)	1:69:B:SER:H	1:65:B:LEU:O	20	7.35
(1,650)	1:79:B:ASP:HB2	1:54:B:LEU:HD12	15	7.35
(1,557)	1:89:B:ARG:HA	1:66:A:LYS:HE2	13	7.35
(1,925)	1:69:A:SER:H	1:65:A:LEU:O	14	7.34
(1,925)	1:69:B:SER:H	1:65:B:LEU:O	16	7.34
(1,838)	1:87:B:HIS:HD1	1:71:B:ARG:HD2	18	7.34
(1,691)	1:87:B:HIS:HD2	1:71:B:ARG:HD2	11	7.34
(1,399)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	6	7.34
(1,615)	1:91:A:LEU:HG	1:66:A:LYS:HE2	7	7.33
(1,503)	1:65:B:LEU:HA	1:69:B:SER:H	20	7.33
(1,557)	1:89:B:ARG:HA	1:66:A:LYS:HE2	20	7.32
(1,640)	1:86:B:LYS:HD3	1:84:B:THR:HG21	6	7.31
(1,687)	1:87:B:HIS:HD1	1:71:B:ARG:HD2	4	7.3
(1,615)	1:91:B:LEU:HG	1:66:B:LYS:HE2	2	7.29
(1,399)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	11	7.29
(1,216)	1:76:B:GLU:HB3	1:51:A:ASN:HD21	16	7.28
(1,650)	1:79:A:ASP:HB2	1:54:A:LEU:HD11	7	7.27
(1,503)	1:65:B:LEU:HA	1:69:B:SER:H	11	7.27
(1,216)	1:76:A:GLU:HB3	1:51:B:ASN:HD21	12	7.27
(1,925)	1:69:A:SER:H	1:65:A:LEU:O	13	7.26
(1,642)	1:79:A:ASP:HB3	1:54:A:LEU:HD11	14	7.25
(1,283)	1:87:A:HIS:HD2	1:72:A:HIS:H	14	7.25
(1,23)	1:64:A:ALA:H	1:68:A:ASP:HB2	5	7.25
(1,841)	1:87:A:HIS:HD2	1:72:A:HIS:HB2	14	7.24
(1,640)	1:86:A:LYS:HD3	1:84:A:THR:HG21	7	7.24
(1,925)	1:69:A:SER:H	1:65:A:LEU:O	2	7.23
(1,557)	1:89:B:ARG:HA	1:66:A:LYS:HE2	2	7.22
(1,838)	1:87:B:HIS:HD1	1:71:B:ARG:HD2	1	7.21
(1,691)	1:87:B:HIS:HD2	1:71:B:ARG:HD2	10	7.21
(1,503)	1:65:A:LEU:HA	1:69:A:SER:H	14	7.21
(1,99)	1:66:A:LYS:HE2	1:92:B:GLN:H	17	7.21
(1,925)	1:69:A:SER:H	1:65:A:LEU:O	3	7.2
(1,838)	1:87:B:HIS:HD2	1:71:B:ARG:HD2	8	7.2
(1,99)	1:66:A:LYS:HE2	1:92:B:GLN:H	10	7.2
(1,640)	1:86:A:LYS:HD3	1:84:A:THR:HG23	9	7.19
(1,503)	1:65:B:LEU:HA	1:69:B:SER:H	3	7.19
(1,99)	1:66:B:LYS:HE2	1:92:A:GLN:H	4	7.19
(1,640)	1:86:B:LYS:HD3	1:84:B:THR:HG21	14	7.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,446)	1:77:A:LYS:HA	1:56:B:GLN:HG2	1	7.18
(1,446)	1:77:B:LYS:HA	1:56:A:GLN:HG2	5	7.18
(1,925)	1:69:A:SER:H	1:65:A:LEU:O	19	7.17
(1,642)	1:79:B:ASP:HB3	1:54:B:LEU:HD11	2	7.16
(1,848)	1:90:B:ASN:HD21	1:66:B:LYS:HE2	9	7.15
(1,679)	1:92:A:GLN:HG3	1:83:B:MET:HG2	1	7.15
(1,640)	1:86:A:LYS:HD3	1:84:A:THR:HG23	12	7.15
(1,399)	1:76:B:GLU:HB3	1:51:A:ASN:HD22	16	7.15
(1,503)	1:65:A:LEU:HA	1:69:A:SER:H	13	7.14
(1,23)	1:64:B:ALA:H	1:68:B:ASP:HB2	19	7.14
(1,687)	1:87:B:HIS:HD1	1:71:B:ARG:HD2	6	7.13
(1,640)	1:86:B:LYS:HD3	1:84:B:THR:HG22	19	7.13
(1,99)	1:66:A:LYS:HE2	1:92:B:GLN:H	15	7.12
(1,925)	1:69:A:SER:H	1:65:A:LEU:O	18	7.11
(1,838)	1:87:B:HIS:HD2	1:71:B:ARG:HD2	17	7.11
(1,687)	1:87:B:HIS:HD1	1:71:B:ARG:HD2	2	7.11
(1,642)	1:79:A:ASP:HB3	1:54:A:LEU:HD11	8	7.11
(1,503)	1:65:B:LEU:HA	1:69:B:SER:H	2	7.11
(1,640)	1:86:B:LYS:HD3	1:84:B:THR:HG21	1	7.1
(1,640)	1:86:B:LYS:HD3	1:84:B:THR:HG22	2	7.1
(1,23)	1:64:B:ALA:H	1:68:B:ASP:HB2	2	7.1
(1,650)	1:79:B:ASP:HB2	1:54:B:LEU:HD12	11	7.09
(1,640)	1:86:B:LYS:HD3	1:84:B:THR:HG22	17	7.09
(1,640)	1:86:A:LYS:HD3	1:84:A:THR:HG23	18	7.09
(1,640)	1:86:B:LYS:HD3	1:84:B:THR:HG21	3	7.08
(1,615)	1:91:A:LEU:HG	1:66:A:LYS:HE2	20	7.08
(1,503)	1:65:A:LEU:HA	1:69:A:SER:H	19	7.08
(1,399)	1:76:A:GLU:HB3	1:51:B:ASN:HD22	12	7.07
(1,23)	1:64:A:ALA:H	1:68:A:ASP:HB2	18	7.07
(1,503)	1:65:B:LEU:HA	1:69:B:SER:H	16	7.06
(1,848)	1:90:B:ASN:HD21	1:66:B:LYS:HE2	1	7.04
(1,839)	1:87:A:HIS:HD2	1:72:A:HIS:H	13	7.04
(1,650)	1:79:B:ASP:HB2	1:54:B:LEU:HD12	18	7.04
(1,615)	1:91:A:LEU:HG	1:66:A:LYS:HE2	5	7.04
(1,925)	1:69:A:SER:H	1:65:A:LEU:O	4	7.03
(1,640)	1:86:B:LYS:HD3	1:84:B:THR:HG23	5	7.03
(1,640)	1:86:B:LYS:HD3	1:84:B:THR:HG22	11	7.02
(1,640)	1:86:B:LYS:HD3	1:84:B:THR:HG21	16	7.02
(1,687)	1:87:A:HIS:HD1	1:71:A:ARG:HD2	9	7.01
(1,679)	1:92:A:GLN:HG2	1:83:B:MET:HG2	12	7.01
(1,925)	1:69:B:SER:H	1:65:B:LEU:O	12	7.0
(1,640)	1:86:B:LYS:HD3	1:84:B:THR:HG21	13	6.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	1:87:A:HIS:HD1	1:72:A:HIS:H	5	6.98
(1,687)	1:87:A:HIS:HD1	1:71:A:ARG:HD2	17	6.98
(1,642)	1:79:B:ASP:HB3	1:54:B:LEU:HD13	13	6.98
(1,640)	1:86:A:LYS:HD3	1:84:A:THR:HG22	15	6.98
(1,503)	1:65:A:LEU:HA	1:69:A:SER:H	18	6.98
(1,99)	1:66:A:LYS:HE2	1:92:B:GLN:H	6	6.98
(1,691)	1:87:B:HIS:HD2	1:71:B:ARG:HD2	4	6.97
(1,650)	1:79:B:ASP:HB2	1:54:B:LEU:HD11	14	6.97
(1,642)	1:79:B:ASP:HB3	1:54:B:LEU:HD11	19	6.97
(1,642)	1:79:A:ASP:HB3	1:54:A:LEU:HD11	5	6.96
(1,503)	1:65:A:LEU:HA	1:69:A:SER:H	8	6.96
(1,446)	1:77:B:LYS:HA	1:56:A:GLN:HG2	16	6.96
(1,671)	1:92:A:GLN:HG2	1:83:B:MET:HG3	5	6.94
(1,446)	1:77:B:LYS:HA	1:56:A:GLN:HG2	8	6.92
(1,23)	1:64:B:ALA:H	1:68:B:ASP:HB3	12	6.92
(1,925)	1:69:A:SER:H	1:65:A:LEU:O	9	6.91
(1,640)	1:86:A:LYS:HD3	1:84:A:THR:HG23	4	6.91
(1,446)	1:77:B:LYS:HA	1:56:A:GLN:HG2	17	6.91
(1,925)	1:69:B:SER:H	1:65:B:LEU:O	5	6.9
(1,546)	1:88:B:LEU:HA	1:66:A:LYS:HE2	19	6.9
(1,640)	1:86:B:LYS:HD3	1:84:B:THR:HG22	8	6.89
(1,687)	1:87:A:HIS:HD1	1:71:A:ARG:HD2	7	6.88
(1,642)	1:79:A:ASP:HB3	1:54:A:LEU:HD11	9	6.88
(1,446)	1:77:A:LYS:HA	1:56:A:GLN:HG2	6	6.88
(1,99)	1:66:A:LYS:HE2	1:92:B:GLN:H	14	6.88
(1,23)	1:64:A:ALA:H	1:68:A:ASP:HB2	20	6.88
(1,925)	1:69:A:SER:H	1:65:A:LEU:O	15	6.87
(1,615)	1:91:B:LEU:HG	1:66:B:LYS:HE2	19	6.87
(1,925)	1:69:A:SER:H	1:65:A:LEU:O	8	6.86
(1,503)	1:65:B:LEU:HA	1:69:B:SER:H	12	6.86
(1,99)	1:66:B:LYS:HE2	1:92:A:GLN:H	16	6.86
(1,503)	1:65:B:LEU:HA	1:69:B:SER:H	5	6.85
(1,446)	1:77:A:LYS:HA	1:56:A:GLN:HG2	7	6.85
(1,642)	1:79:A:ASP:HB3	1:54:A:LEU:HD11	16	6.84
(1,446)	1:77:A:LYS:HA	1:56:A:GLN:HG2	15	6.84
(1,23)	1:64:B:ALA:H	1:68:B:ASP:HB3	4	6.83
(1,925)	1:69:A:SER:H	1:65:A:LEU:O	7	6.82
(1,650)	1:79:B:ASP:HB2	1:54:B:LEU:HD13	8	6.82
(1,615)	1:91:A:LEU:HG	1:66:A:LYS:HE2	18	6.82
(1,99)	1:66:B:LYS:HE2	1:92:A:GLN:H	3	6.82
(1,23)	1:64:B:ALA:H	1:68:B:ASP:HB2	6	6.81
(1,23)	1:64:B:ALA:H	1:68:B:ASP:HB3	3	6.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:64:A:ALA:H	1:68:A:ASP:HB2	10	6.8
(1,23)	1:64:A:ALA:H	1:68:A:ASP:HB3	15	6.8
(1,841)	1:87:A:HIS:HD1	1:72:A:HIS:HB2	5	6.79
(1,691)	1:87:B:HIS:HD2	1:71:B:ARG:HD2	18	6.79
(1,503)	1:65:A:LEU:HA	1:69:A:SER:H	7	6.78
(1,23)	1:64:B:ALA:H	1:68:B:ASP:HB2	11	6.78
(1,925)	1:69:A:SER:H	1:65:A:LEU:O	6	6.77
(1,691)	1:87:A:HIS:HD2	1:71:A:ARG:HD2	16	6.77
(1,503)	1:65:A:LEU:HA	1:69:A:SER:H	15	6.77
(1,635)	1:89:B:ARG:HB2	1:65:B:LEU:HG	15	6.76
(1,23)	1:64:B:ALA:H	1:68:B:ASP:HB3	17	6.76
(1,432)	1:90:A:ASN:HA	1:65:A:LEU:HG	12	6.75
(1,687)	1:87:B:HIS:HD1	1:71:B:ARG:HD2	16	6.74
(1,503)	1:65:A:LEU:HA	1:69:A:SER:H	9	6.74
(1,99)	1:66:A:LYS:HE2	1:92:B:GLN:H	5	6.74
(1,838)	1:87:A:HIS:HD1	1:71:A:ARG:HD2	10	6.73
(1,691)	1:87:A:HIS:HD2	1:71:A:ARG:HD2	7	6.73
(1,679)	1:92:A:GLN:HG3	1:83:B:MET:HG2	11	6.73
(1,635)	1:89:B:ARG:HB2	1:65:B:LEU:HG	13	6.73
(1,561)	1:92:B:GLN:HE21	1:83:A:MET:HA	15	6.73
(1,503)	1:65:A:LEU:HA	1:69:A:SER:H	6	6.73
(1,925)	1:69:A:SER:H	1:65:A:LEU:O	1	6.72
(1,503)	1:65:A:LEU:HA	1:69:A:SER:H	4	6.71
(1,446)	1:77:B:LYS:HA	1:56:A:GLN:HG2	3	6.7
(1,642)	1:79:A:ASP:HB3	1:54:A:LEU:HD11	10	6.69
(1,446)	1:77:B:LYS:HA	1:56:A:GLN:HG2	12	6.69
(1,23)	1:64:B:ALA:H	1:68:B:ASP:HB2	9	6.69
(1,446)	1:77:A:LYS:HA	1:56:A:GLN:HG2	10	6.68
(1,940)	1:78:A:ALA:H	1:74:A:LYS:O	20	6.67
(1,679)	1:92:B:GLN:HG3	1:83:A:MET:HG2	2	6.67
(1,635)	1:89:B:ARG:HB2	1:65:B:LEU:HG	12	6.67
(1,524)	1:78:A:ALA:H	1:56:B:GLN:HG2	10	6.67
(1,687)	1:87:A:HIS:HD1	1:71:A:ARG:HD2	8	6.66
(1,650)	1:79:B:ASP:HB2	1:54:B:LEU:HD12	6	6.66
(1,679)	1:92:B:GLN:HG3	1:83:A:MET:HG2	14	6.65
(1,446)	1:77:B:LYS:HA	1:56:B:GLN:HG2	18	6.65
(1,23)	1:64:A:ALA:H	1:68:A:ASP:HB2	13	6.65
(1,23)	1:64:A:ALA:H	1:68:A:ASP:HB2	14	6.64
(1,23)	1:64:A:ALA:H	1:68:A:ASP:HB2	16	6.64
(1,939)	1:77:A:LYS:N	1:73:A:SER:O	20	6.63
(1,446)	1:77:B:LYS:HA	1:56:B:GLN:HG2	14	6.62
(1,23)	1:64:B:ALA:H	1:68:B:ASP:HB3	8	6.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:80:A:ILE:H	1:56:B:GLN:HG2	19	6.62
(1,925)	1:69:A:SER:H	1:65:A:LEU:O	10	6.61
(1,671)	1:92:B:GLN:HG2	1:83:A:MET:HG3	15	6.61
(1,446)	1:77:A:LYS:HA	1:56:A:GLN:HG2	20	6.61
(1,687)	1:87:B:HIS:HD1	1:71:B:ARG:HD2	18	6.6
(1,524)	1:78:B:ALA:H	1:56:A:GLN:HG2	16	6.6
(1,99)	1:66:B:LYS:HE2	1:92:A:GLN:H	8	6.6
(1,927)	1:70:B:SER:H	1:66:B:LYS:O	11	6.59
(1,524)	1:78:B:ALA:H	1:56:A:GLN:HG2	5	6.58
(1,503)	1:65:A:LEU:HA	1:69:A:SER:H	10	6.58
(1,446)	1:77:B:LYS:HA	1:56:B:GLN:HG2	13	6.58
(1,642)	1:79:B:ASP:HB3	1:54:B:LEU:HD11	3	6.56
(1,524)	1:78:B:ALA:H	1:56:A:GLN:HG2	14	6.56
(1,524)	1:78:A:ALA:H	1:56:B:GLN:HG2	11	6.55
(1,939)	1:77:A:LYS:N	1:73:A:SER:O	3	6.54
(1,524)	1:78:A:ALA:H	1:56:B:GLN:HG2	19	6.54
(1,99)	1:66:A:LYS:HE2	1:92:B:GLN:H	11	6.54
(1,23)	1:64:A:ALA:H	1:68:A:ASP:HB3	7	6.54
(1,927)	1:70:A:SER:H	1:66:A:LYS:O	16	6.53
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD21	12	6.53
(1,99)	1:66:A:LYS:HE2	1:92:B:GLN:H	12	6.53
(1,650)	1:79:B:ASP:HB2	1:54:B:LEU:HD12	20	6.52
(1,524)	1:78:A:ALA:H	1:56:B:GLN:HG2	4	6.52
(1,23)	1:64:A:ALA:H	1:68:A:ASP:HB3	1	6.52
(1,650)	1:79:B:ASP:HB2	1:54:B:LEU:HD13	5	6.51
(1,557)	1:89:A:ARG:HA	1:66:B:LYS:HE2	19	6.51
(1,503)	1:65:A:LEU:HA	1:69:A:SER:H	1	6.51
(1,446)	1:77:B:LYS:HA	1:56:B:GLN:HG2	4	6.49
(1,446)	1:77:B:LYS:HA	1:56:B:GLN:HG2	19	6.49
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD23	16	6.48
(1,635)	1:89:A:ARG:HB2	1:65:A:LEU:HG	5	6.48
(1,840)	1:87:B:HIS:HD2	1:72:B:HIS:HA	20	6.47
(1,687)	1:87:B:HIS:HD1	1:71:B:ARG:HD2	1	6.47
(1,1)	1:80:A:ILE:H	1:56:B:GLN:HG2	11	6.47
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD21	7	6.46
(1,691)	1:87:B:HIS:HD2	1:71:B:ARG:HD2	8	6.46
(1,524)	1:78:B:ALA:H	1:56:A:GLN:HG2	7	6.46
(1,446)	1:77:B:LYS:HA	1:56:B:GLN:HG2	11	6.46
(1,99)	1:66:B:LYS:HE2	1:92:A:GLN:H	7	6.46
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD22	20	6.45
(1,524)	1:78:B:ALA:H	1:56:A:GLN:HG2	17	6.45
(1,927)	1:70:A:SER:H	1:66:A:LYS:O	13	6.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,925)	1:69:B:SER:H	1:65:B:LEU:O	17	6.44
(1,503)	1:65:B:LEU:HA	1:69:B:SER:H	17	6.44
(1,524)	1:78:A:ALA:H	1:56:B:GLN:HG2	1	6.43
(1,1)	1:80:B:ILE:H	1:56:A:GLN:HG2	16	6.43
(1,671)	1:92:A:GLN:HG3	1:83:B:MET:HG3	13	6.42
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD22	15	6.41
(1,671)	1:92:A:GLN:HG2	1:83:B:MET:HG3	4	6.41
(1,524)	1:78:A:ALA:H	1:56:B:GLN:HG2	18	6.41
(1,939)	1:77:A:LYS:N	1:73:A:SER:O	5	6.4
(1,642)	1:79:B:ASP:HB3	1:54:B:LEU:HD13	12	6.4
(1,432)	1:90:A:ASN:HA	1:65:A:LEU:HG	15	6.4
(1,99)	1:66:A:LYS:HE2	1:92:B:GLN:H	2	6.39
(1,927)	1:70:B:SER:H	1:66:B:LYS:O	12	6.38
(1,927)	1:70:B:SER:H	1:66:B:LYS:O	20	6.38
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD21	12	6.38
(1,642)	1:79:B:ASP:HB3	1:54:B:LEU:HD13	17	6.38
(1,524)	1:78:A:ALA:H	1:56:B:GLN:HG2	6	6.38
(1,1)	1:80:A:ILE:H	1:56:B:GLN:HG2	10	6.38
(1,838)	1:87:B:HIS:HD1	1:71:B:ARG:HD2	11	6.37
(1,691)	1:87:B:HIS:HD2	1:71:B:ARG:HD2	17	6.37
(1,524)	1:78:A:ALA:H	1:56:B:GLN:HG2	13	6.37
(1,926)	1:69:A:SER:N	1:65:A:LEU:O	11	6.36
(1,841)	1:87:A:HIS:HD2	1:72:A:HIS:HB2	13	6.36
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD22	20	6.36
(1,650)	1:79:B:ASP:HB2	1:54:B:LEU:HD13	16	6.36
(1,446)	1:77:B:LYS:HA	1:56:B:GLN:HG2	2	6.36
(1,1)	1:80:A:ILE:H	1:56:B:GLN:HG2	4	6.36
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD22	6	6.35
(1,524)	1:78:B:ALA:H	1:56:A:GLN:HG2	12	6.35
(1,1)	1:80:B:ILE:H	1:56:A:GLN:HG2	5	6.35
(1,635)	1:89:B:ARG:HB2	1:65:B:LEU:HG	4	6.34
(1,840)	1:87:A:HIS:HD1	1:72:A:HIS:HA	19	6.32
(1,99)	1:66:A:LYS:HE2	1:92:B:GLN:H	18	6.32
(1,939)	1:77:B:LYS:N	1:73:B:SER:O	6	6.31
(1,561)	1:92:A:GLN:HE21	1:83:B:MET:HA	8	6.31
(1,446)	1:77:A:LYS:HA	1:56:A:GLN:HG2	9	6.31
(1,940)	1:78:A:ALA:H	1:74:A:LYS:O	17	6.3
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD23	1	6.3
(1,650)	1:79:B:ASP:HB2	1:54:B:LEU:HD11	9	6.3
(1,1)	1:80:B:ILE:H	1:56:A:GLN:HG2	7	6.3
(1,1)	1:80:B:ILE:H	1:56:A:GLN:HG2	17	6.3
(1,927)	1:70:A:SER:H	1:66:A:LYS:O	2	6.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,635)	1:89:A:ARG:HB2	1:65:A:LEU:HG	8	6.29
(1,671)	1:92:A:GLN:HG3	1:83:B:MET:HG3	17	6.28
(1,635)	1:89:B:ARG:HB2	1:65:B:LEU:HG	17	6.28
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD21	10	6.27
(1,926)	1:69:A:SER:N	1:65:A:LEU:O	14	6.26
(1,926)	1:69:B:SER:N	1:65:B:LEU:O	20	6.25
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD22	15	6.25
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD23	16	6.25
(1,561)	1:92:B:GLN:HE21	1:83:A:MET:HA	4	6.25
(1,939)	1:77:B:LYS:N	1:73:B:SER:O	10	6.24
(1,848)	1:90:A:ASN:HD21	1:66:A:LYS:HE2	13	6.24
(1,642)	1:79:B:ASP:HB3	1:54:B:LEU:HD11	7	6.24
(1,524)	1:78:A:ALA:H	1:56:B:GLN:HG2	2	6.23
(1,1)	1:80:A:ILE:H	1:56:B:GLN:HG2	18	6.23
(1,928)	1:70:B:SER:N	1:66:B:LYS:O	11	6.22
(1,926)	1:69:B:SER:N	1:65:B:LEU:O	16	6.22
(1,524)	1:78:B:ALA:H	1:56:A:GLN:HG2	15	6.22
(1,939)	1:77:A:LYS:N	1:73:A:SER:O	13	6.21
(1,927)	1:70:A:SER:H	1:66:A:LYS:O	14	6.21
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD22	19	6.21
(1,445)	1:65:B:LEU:HA	1:68:B:ASP:HB2	13	6.21
(1,1)	1:80:A:ILE:H	1:56:B:GLN:HG2	14	6.21
(1,679)	1:92:B:GLN:HG3	1:83:A:MET:HG2	9	6.2
(1,927)	1:70:A:SER:H	1:66:A:LYS:O	3	6.19
(1,524)	1:78:B:ALA:H	1:56:A:GLN:HG2	20	6.19
(1,445)	1:65:A:LEU:HA	1:68:A:ASP:HB2	9	6.19
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD21	7	6.18
(1,687)	1:87:A:HIS:HD1	1:71:A:ARG:HD2	12	6.18
(1,927)	1:70:A:SER:H	1:66:A:LYS:O	9	6.17
(1,642)	1:79:A:ASP:HB3	1:54:A:LEU:HD11	1	6.17
(1,524)	1:78:A:ALA:H	1:56:B:GLN:HG2	9	6.17
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD22	18	6.16
(1,927)	1:70:B:SER:H	1:66:B:LYS:O	5	6.15
(1,926)	1:69:A:SER:N	1:65:A:LEU:O	13	6.15
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD21	4	6.15
(1,561)	1:92:A:GLN:HE21	1:83:B:MET:HA	6	6.15
(1,928)	1:70:A:SER:N	1:66:A:LYS:O	16	6.13
(1,671)	1:92:B:GLN:HG2	1:83:A:MET:HG3	10	6.13
(1,642)	1:79:B:ASP:HB3	1:54:B:LEU:HD12	11	6.13
(1,561)	1:92:A:GLN:HE21	1:83:B:MET:HA	9	6.13
(1,99)	1:66:A:LYS:HE2	1:92:B:GLN:H	13	6.13
(1,848)	1:90:A:ASN:HD21	1:66:A:LYS:HE2	6	6.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD23	1	6.12
(1,99)	1:66:B:LYS:HE2	1:92:A:GLN:H	20	6.12
(1,1)	1:80:A:ILE:H	1:56:B:GLN:HG2	1	6.12
(1,650)	1:79:B:ASP:HB2	1:54:B:LEU:HD11	2	6.11
(1,1)	1:80:A:ILE:H	1:56:B:GLN:HG2	13	6.11
(1,1)	1:80:A:ILE:H	1:56:B:GLN:HG2	15	6.11
(1,939)	1:77:A:LYS:N	1:73:A:SER:O	1	6.1
(1,939)	1:77:A:LYS:N	1:73:A:SER:O	15	6.1
(1,926)	1:69:A:SER:N	1:65:A:LEU:O	2	6.1
(1,926)	1:69:A:SER:N	1:65:A:LEU:O	3	6.1
(1,840)	1:87:A:HIS:HD2	1:72:A:HIS:HA	3	6.1
(1,928)	1:70:A:SER:N	1:66:A:LYS:O	13	6.09
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD22	6	6.09
(1,650)	1:79:B:ASP:HB2	1:54:B:LEU:HD12	10	6.09
(1,561)	1:92:A:GLN:HE21	1:83:B:MET:HA	3	6.09
(1,283)	1:87:A:HIS:HD2	1:72:A:HIS:H	13	6.09
(1,940)	1:78:A:ALA:H	1:74:A:LYS:O	8	6.08
(1,926)	1:69:A:SER:N	1:65:A:LEU:O	19	6.08
(1,671)	1:92:B:GLN:HG3	1:83:A:MET:HG3	7	6.08
(1,642)	1:79:B:ASP:HB3	1:54:B:LEU:HD12	15	6.08
(1,635)	1:89:B:ARG:HB2	1:65:B:LEU:HG	3	6.08
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD21	4	6.07
(1,1)	1:80:A:ILE:H	1:56:B:GLN:HG2	2	6.07
(1,927)	1:70:A:SER:H	1:66:A:LYS:O	19	6.06
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD21	14	6.06
(1,524)	1:78:B:ALA:H	1:56:A:GLN:HG2	8	6.06
(1,1)	1:80:A:ILE:H	1:56:B:GLN:HG2	6	6.06
(1,928)	1:70:B:SER:N	1:66:B:LYS:O	20	6.05
(1,679)	1:92:B:GLN:HG2	1:83:A:MET:HG2	17	6.05
(1,679)	1:92:A:GLN:HG3	1:83:B:MET:HG2	18	6.05
(1,460)	1:73:A:SER:HA	1:76:A:GLU:HB2	20	6.05
(1,940)	1:78:A:ALA:H	1:74:A:LYS:O	3	6.04
(1,928)	1:70:B:SER:N	1:66:B:LYS:O	12	6.04
(1,926)	1:69:A:SER:N	1:65:A:LEU:O	9	6.04
(1,57)	1:73:A:SER:H	1:77:A:LYS:HG3	8	6.04
(1,1)	1:80:B:ILE:H	1:56:A:GLN:HG2	8	6.03
(1,842)	1:87:A:HIS:HD1	1:75:A:LEU:HD11	5	6.02
(1,840)	1:87:A:HIS:HD2	1:72:A:HIS:HA	14	6.02
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD21	14	6.02
(1,939)	1:77:B:LYS:N	1:73:B:SER:O	7	6.01
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD21	8	6.01
(1,561)	1:92:A:GLN:HE21	1:83:B:MET:HA	16	6.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:80:B:ILE:H	1:56:A:GLN:HG2	12	6.01
(1,939)	1:77:A:LYS:N	1:73:A:SER:O	18	6.0
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD21	8	5.99
(1,687)	1:87:A:HIS:HD1	1:71:A:ARG:HD2	10	5.99
(1,524)	1:78:A:ALA:H	1:56:B:GLN:HG2	3	5.99
(1,927)	1:70:A:SER:H	1:66:A:LYS:O	6	5.97
(1,840)	1:87:A:HIS:HD2	1:72:A:HIS:HA	12	5.97
(1,926)	1:69:A:SER:N	1:65:A:LEU:O	18	5.96
(1,679)	1:92:A:GLN:HG2	1:83:B:MET:HG2	10	5.96
(1,679)	1:92:A:GLN:HG2	1:83:B:MET:HG2	16	5.96
(1,1)	1:80:B:ILE:H	1:56:A:GLN:HG2	20	5.95
(1,928)	1:70:A:SER:N	1:66:A:LYS:O	2	5.94
(1,561)	1:92:B:GLN:HE21	1:83:A:MET:HA	17	5.94
(1,671)	1:92:A:GLN:HG2	1:83:B:MET:HG3	1	5.93
(1,460)	1:73:B:SER:HA	1:76:B:GLU:HB2	1	5.93
(1,460)	1:73:A:SER:HA	1:76:A:GLU:HB2	6	5.93
(1,927)	1:70:A:SER:H	1:66:A:LYS:O	4	5.92
(1,926)	1:69:A:SER:N	1:65:A:LEU:O	4	5.92
(1,561)	1:92:A:GLN:HE21	1:83:B:MET:HA	1	5.92
(1,561)	1:92:B:GLN:HE21	1:83:A:MET:HA	10	5.92
(1,1)	1:80:A:ILE:H	1:56:B:GLN:HG2	9	5.92
(1,928)	1:70:A:SER:N	1:66:A:LYS:O	14	5.91
(1,926)	1:69:B:SER:N	1:65:B:LEU:O	12	5.91
(1,650)	1:79:B:ASP:HB2	1:54:B:LEU:HD11	4	5.91
(1,640)	1:86:A:LYS:HD3	1:84:B:THR:HG22	10	5.91
(1,941)	1:78:A:ALA:N	1:74:A:LYS:O	20	5.9
(1,939)	1:77:A:LYS:N	1:73:A:SER:O	17	5.9
(1,650)	1:79:B:ASP:HB2	1:54:B:LEU:HD11	19	5.9
(1,642)	1:79:A:ASP:HB3	1:54:A:LEU:HD11	20	5.9
(1,460)	1:73:A:SER:HA	1:76:A:GLU:HB2	7	5.9
(1,445)	1:65:B:LEU:HA	1:68:B:ASP:HB2	12	5.9
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD21	10	5.89
(1,460)	1:73:B:SER:HA	1:76:B:GLU:HB2	18	5.89
(1,445)	1:65:B:LEU:HA	1:68:B:ASP:HB2	5	5.89
(1,445)	1:65:B:LEU:HA	1:68:B:ASP:HB2	10	5.89
(1,940)	1:78:B:ALA:H	1:74:B:LYS:O	12	5.88
(1,928)	1:70:A:SER:N	1:66:A:LYS:O	9	5.88
(1,927)	1:70:A:SER:H	1:66:A:LYS:O	18	5.88
(1,848)	1:90:B:ASN:HD21	1:66:B:LYS:HE2	8	5.88
(1,842)	1:87:B:HIS:HD2	1:75:B:LEU:HD12	20	5.88
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD23	2	5.88
(1,650)	1:79:B:ASP:HB2	1:54:B:LEU:HD13	13	5.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD22	19	5.87
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD21	10	5.87
(1,679)	1:92:B:GLN:HG3	1:83:A:MET:HG2	4	5.87
(1,927)	1:70:A:SER:H	1:66:A:LYS:O	15	5.86
(1,460)	1:73:A:SER:HA	1:76:A:GLU:HB2	3	5.85
(1,940)	1:78:A:ALA:H	1:74:A:LYS:O	9	5.84
(1,445)	1:65:A:LEU:HA	1:68:A:ASP:HB2	19	5.84
(1,926)	1:69:A:SER:N	1:65:A:LEU:O	7	5.83
(1,460)	1:73:A:SER:HA	1:76:A:GLU:HB2	5	5.83
(1,939)	1:77:A:LYS:N	1:73:A:SER:O	16	5.82
(1,928)	1:70:A:SER:N	1:66:A:LYS:O	3	5.82
(1,445)	1:65:B:LEU:HA	1:68:B:ASP:HB2	11	5.82
(1,671)	1:92:A:GLN:HG3	1:83:B:MET:HG3	6	5.81
(1,635)	1:89:B:ARG:HB2	1:65:B:LEU:HG	9	5.81
(1,445)	1:65:B:LEU:HA	1:68:B:ASP:HB2	20	5.81
(1,926)	1:69:B:SER:N	1:65:B:LEU:O	5	5.8
(1,1)	1:80:A:ILE:H	1:56:B:GLN:HG2	3	5.8
(1,940)	1:78:A:ALA:H	1:74:A:LYS:O	6	5.79
(1,927)	1:70:A:SER:H	1:66:A:LYS:O	8	5.79
(1,926)	1:69:A:SER:N	1:65:A:LEU:O	8	5.79
(1,642)	1:79:B:ASP:HB3	1:54:B:LEU:HD12	18	5.79
(1,940)	1:78:B:ALA:H	1:74:B:LYS:O	1	5.78
(1,926)	1:69:A:SER:N	1:65:A:LEU:O	15	5.78
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD22	18	5.78
(1,561)	1:92:B:GLN:HE21	1:83:A:MET:HA	2	5.78
(1,635)	1:89:A:ARG:HB2	1:65:A:LEU:HG	16	5.77
(1,561)	1:92:A:GLN:HE21	1:83:B:MET:HA	11	5.77
(1,561)	1:92:B:GLN:HE21	1:83:A:MET:HA	18	5.77
(1,926)	1:69:A:SER:N	1:65:A:LEU:O	1	5.76
(1,561)	1:92:A:GLN:HE21	1:83:B:MET:HA	5	5.76
(1,561)	1:92:B:GLN:HE21	1:83:A:MET:HA	13	5.76
(1,940)	1:78:A:ALA:H	1:74:A:LYS:O	5	5.75
(1,928)	1:70:A:SER:N	1:66:A:LYS:O	5	5.75
(1,928)	1:70:A:SER:N	1:66:A:LYS:O	19	5.75
(1,840)	1:87:A:HIS:HD1	1:72:A:HIS:HA	5	5.75
(1,561)	1:92:A:GLN:HE21	1:83:B:MET:HA	7	5.74
(1,679)	1:92:A:GLN:HG3	1:83:B:MET:HG2	8	5.73
(1,445)	1:65:B:LEU:HA	1:68:B:ASP:HB2	1	5.73
(1,445)	1:65:A:LEU:HA	1:68:A:ASP:HB2	7	5.73
(1,940)	1:78:B:ALA:H	1:74:B:LYS:O	7	5.72
(1,939)	1:77:A:LYS:N	1:73:A:SER:O	12	5.72
(1,927)	1:70:A:SER:H	1:66:A:LYS:O	1	5.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,671)	1:92:B:GLN:HG3	1:83:A:MET:HG3	8	5.72
(1,603)	1:64:B:ALA:HB2	1:67:B:LYS:HG2	5	5.72
(1,561)	1:92:A:GLN:HE21	1:83:B:MET:HA	19	5.72
(1,926)	1:69:A:SER:N	1:65:A:LEU:O	6	5.71
(1,561)	1:92:A:GLN:HE21	1:83:B:MET:HA	12	5.71
(1,445)	1:65:A:LEU:HA	1:68:A:ASP:HB2	2	5.71
(1,445)	1:65:A:LEU:HA	1:68:A:ASP:HB2	16	5.71
(1,57)	1:73:A:SER:H	1:77:A:LYS:HG3	17	5.71
(1,679)	1:92:B:GLN:HG3	1:83:A:MET:HG2	19	5.7
(1,940)	1:78:A:ALA:H	1:74:A:LYS:O	15	5.69
(1,848)	1:90:B:ASN:HD21	1:66:B:LYS:HE2	4	5.69
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD22	19	5.69
(1,679)	1:92:A:GLN:HG3	1:83:B:MET:HG2	7	5.69
(1,561)	1:92:B:GLN:HE21	1:83:A:MET:HA	14	5.69
(1,445)	1:65:A:LEU:HA	1:68:A:ASP:HB2	3	5.69
(1,940)	1:78:B:ALA:H	1:74:B:LYS:O	18	5.68
(1,445)	1:65:B:LEU:HA	1:68:B:ASP:HB2	14	5.67
(1,940)	1:78:B:ALA:H	1:74:B:LYS:O	16	5.66
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD23	2	5.66
(1,671)	1:92:B:GLN:HG2	1:83:A:MET:HG3	18	5.66
(1,635)	1:89:B:ARG:HB2	1:65:B:LEU:HG	6	5.66
(1,927)	1:70:A:SER:H	1:66:A:LYS:O	7	5.64
(1,848)	1:90:A:ASN:HD21	1:66:A:LYS:HE2	5	5.64
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD21	12	5.64
(1,603)	1:64:B:ALA:HB2	1:67:B:LYS:HG2	20	5.64
(1,940)	1:78:B:ALA:H	1:74:B:LYS:O	4	5.63
(1,928)	1:70:A:SER:N	1:66:A:LYS:O	4	5.63
(1,820)	1:86:B:LYS:HG2	1:87:B:HIS:HD2	4	5.63
(1,820)	1:86:B:LYS:HG2	1:87:B:HIS:HD1	11	5.63
(1,784)	1:64:B:ALA:HB3	1:67:B:LYS:HB2	12	5.63
(1,687)	1:87:B:HIS:HD1	1:71:B:ARG:HD2	11	5.63
(1,671)	1:92:B:GLN:HG3	1:83:A:MET:HG3	16	5.63
(1,940)	1:78:A:ALA:H	1:74:A:LYS:O	11	5.62
(1,928)	1:70:A:SER:N	1:66:A:LYS:O	6	5.62
(1,820)	1:86:A:LYS:HG2	1:87:A:HIS:HD1	1	5.62
(1,820)	1:86:B:LYS:HG2	1:87:B:HIS:HD2	17	5.62
(1,432)	1:90:B:ASN:HA	1:65:B:LEU:HG	17	5.62
(1,927)	1:70:A:SER:H	1:66:A:LYS:O	10	5.6
(1,820)	1:86:B:LYS:HG2	1:87:B:HIS:HD2	9	5.6
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD22	15	5.6
(1,671)	1:92:A:GLN:HG3	1:83:B:MET:HG3	9	5.6
(1,635)	1:89:A:ARG:HB2	1:65:A:LEU:HG	20	5.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,460)	1:73:A:SER:HA	1:76:A:GLU:HB2	15	5.6
(1,460)	1:73:A:SER:HA	1:76:A:GLU:HB2	16	5.6
(1,445)	1:65:A:LEU:HA	1:68:A:ASP:HB2	15	5.6
(1,784)	1:64:B:ALA:HB1	1:67:B:LYS:HB2	2	5.59
(1,939)	1:77:A:LYS:N	1:73:A:SER:O	11	5.58
(1,848)	1:90:A:ASN:HD21	1:66:A:LYS:HE2	10	5.58
(1,820)	1:86:A:LYS:HG2	1:87:A:HIS:HD2	6	5.58
(1,561)	1:92:A:GLN:HE21	1:83:B:MET:HA	20	5.58
(1,460)	1:73:B:SER:HA	1:76:B:GLU:HB2	13	5.58
(1,820)	1:86:B:LYS:HG2	1:87:B:HIS:HD1	18	5.57
(1,601)	1:64:A:ALA:HB1	1:67:A:LYS:HG2	19	5.57
(1,635)	1:89:A:ARG:HB2	1:65:A:LEU:HG	11	5.56
(1,941)	1:78:A:ALA:N	1:74:A:LYS:O	17	5.55
(1,784)	1:64:A:ALA:HB1	1:67:A:LYS:HB2	5	5.55
(1,460)	1:73:A:SER:HA	1:76:A:GLU:HB2	12	5.55
(1,928)	1:70:A:SER:N	1:66:A:LYS:O	15	5.54
(1,820)	1:86:A:LYS:HG2	1:87:A:HIS:HD2	7	5.54
(1,784)	1:64:B:ALA:HB3	1:67:B:LYS:HB2	19	5.54
(1,848)	1:90:B:ASN:HD21	1:66:B:LYS:HE2	17	5.53
(1,842)	1:87:A:HIS:HD2	1:75:A:LEU:HD21	14	5.53
(1,679)	1:92:B:GLN:HG3	1:83:A:MET:HG2	3	5.53
(1,671)	1:92:A:GLN:HG3	1:83:B:MET:HG3	3	5.53
(1,928)	1:70:A:SER:N	1:66:A:LYS:O	18	5.52
(1,820)	1:86:A:LYS:HG2	1:87:A:HIS:HD1	8	5.52
(1,687)	1:87:A:HIS:HD1	1:71:A:ARG:HD2	14	5.52
(1,460)	1:73:A:SER:HA	1:76:A:GLU:HB2	8	5.52
(1,940)	1:78:B:ALA:H	1:74:B:LYS:O	2	5.51
(1,812)	1:84:B:THR:HG22	1:60:B:LEU:HD22	19	5.51
(1,671)	1:92:B:GLN:HG2	1:83:A:MET:HG3	14	5.51
(1,460)	1:73:B:SER:HA	1:76:B:GLU:HB2	10	5.51
(1,445)	1:65:A:LEU:HA	1:68:A:ASP:HB2	4	5.51
(1,820)	1:86:A:LYS:HG2	1:87:A:HIS:HD2	2	5.5
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD23	16	5.5
(1,671)	1:92:A:GLN:HG3	1:83:B:MET:HG3	11	5.5
(1,333)	1:81:B:LEU:H	1:56:A:GLN:HG3	10	5.5
(1,941)	1:78:A:ALA:N	1:74:A:LYS:O	8	5.49
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD22	20	5.49
(1,679)	1:92:A:GLN:HG2	1:83:B:MET:HG2	5	5.49
(1,601)	1:64:A:ALA:HB1	1:67:A:LYS:HG2	12	5.49
(1,926)	1:69:A:SER:N	1:65:A:LEU:O	10	5.48
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD23	1	5.48
(1,784)	1:64:B:ALA:HB1	1:67:B:LYS:HB2	17	5.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,445)	1:65:A:LEU:HA	1:68:A:ASP:HB2	18	5.47
(1,939)	1:77:A:LYS:N	1:73:A:SER:O	4	5.46
(1,820)	1:86:A:LYS:HG2	1:87:A:HIS:HD2	16	5.46
(1,603)	1:64:A:ALA:HB2	1:67:A:LYS:HG2	13	5.46
(1,460)	1:73:A:SER:HA	1:76:A:GLU:HB2	11	5.46
(1,928)	1:70:A:SER:N	1:66:A:LYS:O	1	5.45
(1,848)	1:90:B:ASN:HD21	1:66:B:LYS:HE2	14	5.45
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD22	6	5.45
(1,226)	1:81:B:LEU:H	1:56:A:GLN:HE21	5	5.45
(1,928)	1:70:A:SER:N	1:66:A:LYS:O	8	5.44
(1,671)	1:92:A:GLN:HG2	1:83:B:MET:HG3	12	5.44
(1,940)	1:78:B:ALA:H	1:74:B:LYS:O	13	5.43
(1,445)	1:65:A:LEU:HA	1:68:A:ASP:HB2	6	5.43
(1,820)	1:86:B:LYS:HG2	1:87:B:HIS:HD2	15	5.42
(1,940)	1:78:B:ALA:H	1:74:B:LYS:O	10	5.39
(1,842)	1:87:A:HIS:HD2	1:75:A:LEU:HD13	13	5.39
(1,671)	1:92:B:GLN:HG3	1:83:A:MET:HG3	2	5.39
(1,635)	1:89:B:ARG:HB2	1:65:B:LEU:HG	2	5.39
(1,445)	1:65:B:LEU:HA	1:68:B:ASP:HB2	17	5.39
(1,812)	1:84:B:THR:HG23	1:60:B:LEU:HD21	10	5.38
(1,784)	1:64:B:ALA:HB2	1:67:B:LYS:HB2	10	5.38
(1,642)	1:79:A:ASP:HB3	1:54:A:LEU:HD11	4	5.38
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD23	2	5.37
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD22	18	5.37
(1,784)	1:64:A:ALA:HB2	1:67:A:LYS:HB2	15	5.37
(1,226)	1:81:A:LEU:H	1:56:B:GLN:HE21	10	5.37
(1,939)	1:77:B:LYS:N	1:73:B:SER:O	9	5.36
(1,939)	1:77:A:LYS:N	1:73:A:SER:O	14	5.36
(1,939)	1:77:A:LYS:N	1:73:A:SER:O	19	5.36
(1,848)	1:90:B:ASN:HD21	1:66:B:LYS:HE2	12	5.36
(1,823)	1:86:A:LYS:HG3	1:84:A:THR:HG23	20	5.36
(1,99)	1:66:B:LYS:HE2	1:92:A:GLN:H	19	5.36
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD21	7	5.35
(1,784)	1:64:B:ALA:HB1	1:67:B:LYS:HB2	20	5.35
(1,62)	1:81:A:LEU:H	1:56:B:GLN:HG2	10	5.35
(1,940)	1:78:B:ALA:H	1:74:B:LYS:O	14	5.34
(1,926)	1:69:B:SER:N	1:65:B:LEU:O	17	5.34
(1,848)	1:90:B:ASN:HD21	1:66:B:LYS:HE3	3	5.34
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD21	4	5.34
(1,679)	1:92:B:GLN:HG3	1:83:A:MET:HG2	20	5.34
(1,928)	1:70:A:SER:N	1:66:A:LYS:O	7	5.33
(1,848)	1:90:B:ASN:HD21	1:66:B:LYS:HE3	19	5.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,635)	1:89:B:ARG:HB2	1:65:B:LEU:HG	7	5.33
(1,603)	1:64:B:ALA:HB2	1:67:B:LYS:HG2	1	5.33
(1,838)	1:87:B:HIS:HD2	1:71:B:ARG:HD2	20	5.32
(1,784)	1:64:B:ALA:HB2	1:67:B:LYS:HB2	11	5.32
(1,601)	1:64:B:ALA:HB1	1:67:B:LYS:HG2	11	5.32
(1,333)	1:81:B:LEU:H	1:56:A:GLN:HG3	16	5.32
(1,635)	1:89:B:ARG:HB2	1:65:B:LEU:HG	14	5.31
(1,445)	1:65:A:LEU:HA	1:68:A:ASP:HB2	8	5.31
(1,62)	1:81:B:LEU:H	1:56:A:GLN:HG2	5	5.31
(1,714)	1:86:B:LYS:HD3	1:84:B:THR:HA	6	5.3
(1,848)	1:90:A:ASN:HD21	1:66:A:LYS:HE2	11	5.29
(1,635)	1:89:B:ARG:HB2	1:65:B:LEU:HG	1	5.29
(1,226)	1:81:B:LEU:H	1:56:A:GLN:HE21	7	5.29
(1,848)	1:90:B:ASN:HD21	1:66:B:LYS:HE2	16	5.28
(1,784)	1:64:B:ALA:HB2	1:67:B:LYS:HB2	6	5.28
(1,333)	1:81:A:LEU:H	1:56:B:GLN:HG3	5	5.28
(1,226)	1:81:B:LEU:H	1:56:A:GLN:HE21	11	5.28
(1,848)	1:90:A:ASN:HD21	1:66:A:LYS:HE2	20	5.27
(1,679)	1:92:B:GLN:HG2	1:83:A:MET:HG2	6	5.27
(1,671)	1:92:A:GLN:HG3	1:83:B:MET:HG3	19	5.27
(1,460)	1:73:B:SER:HA	1:76:B:GLU:HB2	4	5.27
(1,941)	1:78:B:ALA:N	1:74:B:LYS:O	12	5.26
(1,927)	1:70:B:SER:H	1:66:B:LYS:O	17	5.26
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD21	8	5.25
(1,784)	1:64:A:ALA:HB3	1:67:A:LYS:HB2	3	5.25
(1,635)	1:89:B:ARG:HB2	1:65:B:LEU:HG	19	5.24
(1,226)	1:81:A:LEU:H	1:56:B:GLN:HE21	4	5.24
(1,840)	1:87:A:HIS:HD2	1:72:A:HIS:HA	13	5.23
(1,687)	1:87:B:HIS:HD1	1:71:B:ARG:HD2	20	5.22
(1,460)	1:73:A:SER:HA	1:76:A:GLU:HB2	17	5.22
(1,432)	1:90:A:ASN:HA	1:65:A:LEU:HG	13	5.22
(1,226)	1:81:B:LEU:H	1:56:A:GLN:HE21	16	5.22
(1,941)	1:78:A:ALA:N	1:74:A:LYS:O	3	5.21
(1,848)	1:90:B:ASN:HD21	1:66:B:LYS:HE3	7	5.21
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD21	14	5.21
(1,635)	1:89:A:ARG:HB2	1:65:A:LEU:HG	18	5.21
(1,308)	1:90:B:ASN:H	1:65:B:LEU:HG	12	5.21
(1,226)	1:81:A:LEU:H	1:56:B:GLN:HE21	20	5.21
(1,62)	1:81:B:LEU:H	1:56:A:GLN:HG2	16	5.21
(1,848)	1:90:B:ASN:HD21	1:66:B:LYS:HE2	2	5.2
(1,714)	1:86:B:LYS:HD3	1:84:B:THR:HA	3	5.2
(1,333)	1:81:A:LEU:H	1:56:B:GLN:HG3	11	5.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,460)	1:73:B:SER:HA	1:76:B:GLU:HB2	9	5.19
(1,62)	1:81:A:LEU:H	1:56:B:GLN:HG2	4	5.19
(1,941)	1:78:A:ALA:N	1:74:A:LYS:O	9	5.18
(1,714)	1:86:A:LYS:HD3	1:84:A:THR:HA	11	5.18
(1,714)	1:86:B:LYS:HD3	1:84:B:THR:HA	20	5.18
(1,62)	1:81:A:LEU:H	1:56:B:GLN:HG2	11	5.18
(1,928)	1:70:A:SER:N	1:66:A:LYS:O	10	5.17
(1,739)	1:50:B:ILE:HG21	1:76:A:GLU:HA	5	5.17
(1,333)	1:81:A:LEU:H	1:56:B:GLN:HG3	4	5.17
(1,62)	1:81:A:LEU:H	1:56:B:GLN:HG2	19	5.17
(1,835)	1:87:B:HIS:HD1	1:67:B:LYS:HD2	16	5.16
(1,714)	1:86:B:LYS:HD3	1:84:B:THR:HA	4	5.16
(1,679)	1:92:B:GLN:HG3	1:83:A:MET:HG2	13	5.16
(1,601)	1:64:A:ALA:HB1	1:67:A:LYS:HG2	14	5.15
(1,941)	1:78:A:ALA:N	1:74:A:LYS:O	6	5.14
(1,784)	1:64:B:ALA:HB1	1:67:B:LYS:HB2	4	5.14
(1,603)	1:64:A:ALA:HB2	1:67:A:LYS:HG2	4	5.14
(1,333)	1:81:A:LEU:H	1:56:B:GLN:HG3	13	5.14
(1,62)	1:81:B:LEU:H	1:56:A:GLN:HG2	7	5.14
(1,940)	1:78:A:ALA:H	1:74:A:LYS:O	19	5.12
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD11	9	5.12
(1,784)	1:64:A:ALA:HB1	1:67:A:LYS:HB2	16	5.12
(1,714)	1:86:A:LYS:HD3	1:84:A:THR:HA	7	5.12
(1,739)	1:50:B:ILE:HG22	1:76:A:GLU:HA	4	5.11
(1,333)	1:81:A:LEU:H	1:56:B:GLN:HG3	15	5.11
(1,226)	1:81:B:LEU:H	1:56:A:GLN:HE21	17	5.11
(1,835)	1:87:B:HIS:HD1	1:67:B:LYS:HD2	2	5.1
(1,835)	1:87:A:HIS:HD2	1:67:A:LYS:HD2	15	5.1
(1,823)	1:86:B:LYS:HG3	1:84:B:THR:HG22	19	5.1
(1,812)	1:84:B:THR:HG23	1:60:B:LEU:HD21	12	5.1
(1,714)	1:86:A:LYS:HD3	1:84:A:THR:HA	9	5.1
(1,671)	1:92:A:GLN:HG3	1:83:B:MET:HG3	20	5.1
(1,838)	1:87:A:HIS:HD2	1:71:A:ARG:HD2	12	5.09
(1,784)	1:64:B:ALA:HB1	1:67:B:LYS:HB2	9	5.09
(1,409)	1:64:B:ALA:HA	1:67:B:LYS:HB2	5	5.09
(1,510)	1:79:A:ASP:H	1:54:A:LEU:HG	14	5.08
(1,226)	1:81:A:LEU:H	1:56:B:GLN:HE21	6	5.08
(1,941)	1:78:B:ALA:N	1:74:B:LYS:O	1	5.07
(1,941)	1:78:A:ALA:N	1:74:A:LYS:O	5	5.07
(1,333)	1:81:A:LEU:H	1:56:B:GLN:HG3	18	5.07
(1,823)	1:86:B:LYS:HG3	1:84:B:THR:HG21	14	5.06
(1,812)	1:84:B:THR:HG23	1:60:B:LEU:HD22	20	5.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,739)	1:50:B:ILE:HG23	1:76:A:GLU:HA	14	5.06
(1,333)	1:81:B:LEU:H	1:56:A:GLN:HG3	17	5.06
(1,62)	1:81:B:LEU:H	1:56:A:GLN:HG2	17	5.06
(1,941)	1:78:B:ALA:N	1:74:B:LYS:O	18	5.05
(1,823)	1:86:A:LYS:HG3	1:84:A:THR:HG23	9	5.05
(1,823)	1:86:B:LYS:HG3	1:84:B:THR:HG23	10	5.05
(1,812)	1:84:B:THR:HG21	1:60:B:LEU:HD21	8	5.05
(1,812)	1:84:B:THR:HG23	1:60:B:LEU:HD22	18	5.05
(1,784)	1:64:B:ALA:HB2	1:67:B:LYS:HB2	8	5.05
(1,784)	1:64:A:ALA:HB2	1:67:A:LYS:HB2	18	5.05
(1,714)	1:86:A:LYS:HD3	1:84:A:THR:HA	1	5.05
(1,62)	1:81:A:LEU:H	1:56:B:GLN:HG2	1	5.05
(1,823)	1:86:B:LYS:HG3	1:84:B:THR:HG23	7	5.04
(1,714)	1:86:A:LYS:HD3	1:84:A:THR:HA	5	5.04
(1,714)	1:86:B:LYS:HD3	1:84:B:THR:HA	16	5.04
(1,603)	1:64:A:ALA:HB2	1:67:A:LYS:HG2	19	5.04
(1,823)	1:86:B:LYS:HG3	1:84:B:THR:HG22	17	5.02
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD13	3	5.02
(1,739)	1:50:B:ILE:HG21	1:76:A:GLU:HA	20	5.02
(1,601)	1:64:A:ALA:HB1	1:67:A:LYS:HG2	15	5.02
(1,432)	1:90:B:ASN:HA	1:65:B:LEU:HG	8	5.02
(1,333)	1:81:A:LEU:H	1:56:B:GLN:HG3	1	5.02
(1,941)	1:78:A:ALA:N	1:74:A:LYS:O	15	5.01
(1,835)	1:87:B:HIS:HD1	1:67:B:LYS:HD2	6	5.01
(1,823)	1:86:A:LYS:HG3	1:84:A:THR:HG21	6	5.01
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD13	13	5.01
(1,432)	1:90:B:ASN:HA	1:65:B:LEU:HG	3	5.01
(1,246)	1:81:B:LEU:H	1:56:A:GLN:HE22	5	5.0
(1,812)	1:84:B:THR:HG22	1:60:B:LEU:HD22	15	4.99
(1,714)	1:86:B:LYS:HD3	1:84:B:THR:HA	12	4.99
(1,714)	1:86:A:LYS:HD3	1:84:A:THR:HA	15	4.99
(1,687)	1:87:A:HIS:HD1	1:71:A:ARG:HD2	3	4.99
(1,460)	1:73:A:SER:HA	1:76:A:GLU:HB2	19	4.99
(1,941)	1:78:B:ALA:N	1:74:B:LYS:O	16	4.98
(1,823)	1:86:A:LYS:HG3	1:84:A:THR:HG23	12	4.98
(1,823)	1:86:B:LYS:HG3	1:84:B:THR:HG21	13	4.98
(1,812)	1:84:B:THR:HG22	1:60:B:LEU:HD21	7	4.98
(1,739)	1:50:B:ILE:HG23	1:76:A:GLU:HA	7	4.98
(1,460)	1:73:B:SER:HA	1:76:B:GLU:HB2	14	4.98
(1,62)	1:81:A:LEU:H	1:56:B:GLN:HG2	6	4.98
(1,941)	1:78:B:ALA:N	1:74:B:LYS:O	7	4.97
(1,849)	1:90:B:ASN:HD21	1:92:A:GLN:HG2	4	4.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	1:86:B:LYS:HD3	1:84:B:THR:HA	2	4.97
(1,333)	1:81:B:LEU:H	1:56:A:GLN:HG3	2	4.97
(1,333)	1:81:B:LEU:H	1:56:A:GLN:HG3	7	4.97
(1,308)	1:90:A:ASN:H	1:65:A:LEU:HG	15	4.97
(1,246)	1:81:A:LEU:H	1:56:B:GLN:HE22	10	4.97
(1,812)	1:84:B:THR:HG23	1:60:B:LEU:HD23	16	4.96
(1,714)	1:86:B:LYS:HD3	1:84:B:THR:HA	19	4.96
(1,510)	1:79:A:ASP:H	1:54:A:LEU:HG	17	4.96
(1,409)	1:64:A:ALA:HA	1:67:A:LYS:HB2	17	4.96
(1,333)	1:81:B:LEU:H	1:56:A:GLN:HG3	8	4.96
(1,333)	1:81:A:LEU:H	1:56:B:GLN:HG3	9	4.96
(1,941)	1:78:B:ALA:N	1:74:B:LYS:O	4	4.95
(1,838)	1:87:A:HIS:HD1	1:71:A:ARG:HD2	5	4.95
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD21	12	4.95
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD13	3	4.95
(1,802)	1:81:B:LEU:HB3	1:60:A:LEU:HD11	5	4.95
(1,739)	1:50:A:ILE:HG21	1:76:B:GLU:HA	2	4.95
(1,739)	1:50:B:ILE:HG23	1:76:A:GLU:HA	13	4.95
(1,333)	1:81:A:LEU:H	1:56:B:GLN:HG3	6	4.95
(1,941)	1:78:A:ALA:N	1:74:A:LYS:O	2	4.94
(1,784)	1:64:A:ALA:HB1	1:67:A:LYS:HB2	13	4.94
(1,714)	1:86:B:LYS:HD3	1:84:B:THR:HA	14	4.94
(1,62)	1:81:A:LEU:H	1:56:B:GLN:HG2	15	4.94
(1,941)	1:78:B:ALA:N	1:74:B:LYS:O	11	4.93
(1,823)	1:86:B:LYS:HG3	1:84:B:THR:HG22	2	4.93
(1,823)	1:86:B:LYS:HG3	1:84:B:THR:HG21	3	4.93
(1,739)	1:50:B:ILE:HG21	1:76:A:GLU:HA	6	4.93
(1,739)	1:50:B:ILE:HG21	1:76:A:GLU:HA	15	4.93
(1,714)	1:86:B:LYS:HD3	1:84:B:THR:HA	17	4.93
(1,739)	1:50:B:ILE:HG23	1:76:A:GLU:HA	19	4.92
(1,226)	1:81:A:LEU:H	1:56:B:GLN:HE21	18	4.92
(1,62)	1:81:A:LEU:H	1:56:B:GLN:HG2	13	4.92
(1,928)	1:70:B:SER:N	1:66:B:LYS:O	17	4.91
(1,823)	1:86:B:LYS:HG3	1:84:B:THR:HG21	18	4.91
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD13	13	4.91
(1,802)	1:81:B:LEU:HB3	1:60:A:LEU:HD11	11	4.91
(1,603)	1:64:A:ALA:HB2	1:67:A:LYS:HG2	14	4.91
(1,226)	1:81:A:LEU:H	1:56:B:GLN:HE21	3	4.91
(1,226)	1:81:B:LEU:H	1:56:A:GLN:HE21	8	4.91
(1,823)	1:86:B:LYS:HG3	1:84:B:THR:HG21	1	4.9
(1,823)	1:86:B:LYS:HG3	1:84:B:THR:HG23	5	4.9
(1,823)	1:86:B:LYS:HG3	1:84:B:THR:HG22	11	4.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD23	16	4.9
(1,510)	1:79:A:ASP:H	1:54:A:LEU:HG	3	4.9
(1,415)	1:86:A:LYS:HD3	1:84:A:THR:HB	20	4.9
(1,333)	1:81:B:LEU:H	1:56:A:GLN:HG3	20	4.9
(1,62)	1:81:A:LEU:H	1:56:B:GLN:HG2	2	4.9
(1,62)	1:81:A:LEU:H	1:56:B:GLN:HG2	18	4.9
(1,835)	1:87:B:HIS:HD1	1:67:B:LYS:HD2	18	4.89
(1,823)	1:86:B:LYS:HG3	1:84:B:THR:HG21	16	4.89
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD22	20	4.89
(1,811)	1:84:B:THR:HB	1:60:A:LEU:HD11	5	4.89
(1,811)	1:84:A:THR:HB	1:60:B:LEU:HD11	11	4.89
(1,784)	1:64:A:ALA:HB1	1:67:A:LYS:HB2	1	4.89
(1,714)	1:86:A:LYS:HD3	1:84:A:THR:HA	8	4.89
(1,409)	1:64:B:ALA:HA	1:67:B:LYS:HB2	12	4.89
(1,333)	1:81:B:LEU:H	1:56:A:GLN:HG3	12	4.89
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD22	15	4.88
(1,432)	1:90:A:ASN:HA	1:65:A:LEU:HG	2	4.88
(1,333)	1:81:A:LEU:H	1:56:B:GLN:HG3	19	4.88
(1,62)	1:81:B:LEU:H	1:56:A:GLN:HG2	8	4.88
(1,62)	1:81:A:LEU:H	1:56:B:GLN:HG2	14	4.88
(1,941)	1:78:B:ALA:N	1:74:B:LYS:O	13	4.87
(1,739)	1:50:B:ILE:HG21	1:76:A:GLU:HA	8	4.87
(1,432)	1:90:A:ASN:HA	1:65:A:LEU:HG	9	4.87
(1,739)	1:50:B:ILE:HG23	1:76:A:GLU:HA	10	4.86
(1,333)	1:81:A:LEU:H	1:56:B:GLN:HG3	3	4.86
(1,333)	1:81:A:LEU:H	1:56:B:GLN:HG3	14	4.86
(1,849)	1:90:A:ASN:HD21	1:92:B:GLN:HG2	18	4.85
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD21	7	4.85
(1,739)	1:50:B:ILE:HG22	1:76:A:GLU:HA	17	4.85
(1,739)	1:50:B:ILE:HG21	1:76:A:GLU:HA	18	4.85
(1,226)	1:81:A:LEU:H	1:56:B:GLN:HE21	15	4.85
(1,849)	1:90:A:ASN:HD21	1:92:B:GLN:HG2	1	4.84
(1,849)	1:90:A:ASN:HD21	1:92:B:GLN:HG2	14	4.84
(1,691)	1:87:A:HIS:HD2	1:71:A:ARG:HD2	19	4.84
(1,603)	1:64:A:ALA:HB2	1:67:A:LYS:HG2	17	4.84
(1,510)	1:79:B:ASP:H	1:54:B:LEU:HG	15	4.84
(1,432)	1:90:B:ASN:HA	1:65:B:LEU:HG	4	4.84
(1,812)	1:84:B:THR:HG21	1:60:B:LEU:HD23	2	4.83
(1,432)	1:90:B:ASN:HA	1:65:B:LEU:HG	6	4.83
(1,432)	1:90:B:ASN:HA	1:65:B:LEU:HG	14	4.83
(1,432)	1:90:A:ASN:HA	1:65:A:LEU:HG	20	4.83
(1,409)	1:64:A:ALA:HA	1:67:A:LYS:HB2	2	4.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:90:B:ASN:HD21	1:66:B:LYS:HE3	15	4.82
(1,823)	1:86:A:LYS:HG3	1:84:A:THR:HG22	15	4.82
(1,510)	1:79:B:ASP:H	1:54:B:LEU:HG	5	4.82
(1,842)	1:87:A:HIS:HD1	1:75:A:LEU:HD11	19	4.81
(1,838)	1:87:A:HIS:HD1	1:71:A:ARG:HD2	19	4.8
(1,739)	1:50:B:ILE:HG21	1:76:A:GLU:HA	11	4.8
(1,415)	1:86:B:LYS:HD3	1:84:B:THR:HB	6	4.8
(1,226)	1:81:A:LEU:H	1:56:B:GLN:HE21	14	4.8
(1,812)	1:84:B:THR:HG23	1:60:B:LEU:HD11	6	4.79
(1,802)	1:81:A:LEU:HB3	1:60:B:LEU:HD11	9	4.79
(1,739)	1:50:B:ILE:HG21	1:76:A:GLU:HA	3	4.79
(1,684)	1:86:A:LYS:HD3	1:87:A:HIS:HB3	4	4.79
(1,510)	1:79:B:ASP:H	1:54:B:LEU:HG	12	4.79
(1,415)	1:86:A:LYS:HD3	1:84:A:THR:HB	9	4.79
(1,62)	1:81:A:LEU:H	1:56:B:GLN:HG2	3	4.79
(1,820)	1:86:B:LYS:HG2	1:87:B:HIS:HD2	10	4.78
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD21	10	4.78
(1,62)	1:81:B:LEU:H	1:56:A:GLN:HG2	12	4.78
(1,849)	1:90:B:ASN:HD21	1:92:A:GLN:HG2	3	4.77
(1,812)	1:84:B:THR:HG23	1:60:B:LEU:HD23	1	4.77
(1,415)	1:86:B:LYS:HD3	1:84:B:THR:HB	14	4.77
(1,226)	1:81:A:LEU:H	1:56:B:GLN:HE21	2	4.77
(1,849)	1:90:B:ASN:HD21	1:92:A:GLN:HG2	6	4.76
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD23	1	4.76
(1,739)	1:50:B:ILE:HG23	1:76:A:GLU:HA	1	4.76
(1,510)	1:79:B:ASP:H	1:54:B:LEU:HG	8	4.76
(1,432)	1:90:B:ASN:HA	1:65:B:LEU:HG	11	4.76
(1,226)	1:81:A:LEU:H	1:56:B:GLN:HE21	13	4.76
(1,848)	1:90:A:ASN:HD21	1:66:A:LYS:HE2	18	4.75
(1,823)	1:86:B:LYS:HG3	1:84:B:THR:HG23	4	4.75
(1,823)	1:86:B:LYS:HG3	1:84:B:THR:HG22	8	4.75
(1,812)	1:84:B:THR:HG23	1:60:B:LEU:HD21	14	4.75
(1,409)	1:64:A:ALA:HA	1:67:A:LYS:HB2	15	4.75
(1,62)	1:81:A:LEU:H	1:56:B:GLN:HG2	9	4.74
(1,849)	1:90:A:ASN:HD21	1:92:B:GLN:HG2	16	4.73
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD22	6	4.73
(1,601)	1:64:A:ALA:HB1	1:67:A:LYS:HG2	18	4.73
(1,510)	1:79:B:ASP:H	1:54:B:LEU:HG	16	4.73
(1,226)	1:81:B:LEU:H	1:56:A:GLN:HE21	12	4.73
(1,739)	1:50:B:ILE:HG21	1:76:A:GLU:HA	9	4.72
(1,415)	1:86:B:LYS:HD3	1:84:B:THR:HB	7	4.71
(1,811)	1:84:B:THR:HB	1:60:A:LEU:HD11	17	4.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	1:86:A:LYS:HD3	1:84:A:THR:HA	18	4.7
(1,409)	1:64:B:ALA:HA	1:67:B:LYS:HB2	19	4.7
(1,62)	1:81:B:LEU:H	1:56:A:GLN:HG2	20	4.7
(1,57)	1:73:B:SER:H	1:77:B:LYS:HG3	2	4.7
(1,812)	1:84:B:THR:HG22	1:60:B:LEU:HD21	4	4.69
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD13	3	4.69
(1,684)	1:86:A:LYS:HD3	1:87:A:HIS:HB3	11	4.69
(1,510)	1:79:A:ASP:H	1:54:A:LEU:HG	1	4.69
(1,246)	1:81:B:LEU:H	1:56:A:GLN:HE22	16	4.69
(1,739)	1:50:A:ILE:HG21	1:76:B:GLU:HA	16	4.68
(1,684)	1:86:B:LYS:HD3	1:87:B:HIS:HB3	3	4.68
(1,714)	1:86:B:LYS:HD3	1:84:B:THR:HA	13	4.67
(1,246)	1:81:A:LEU:H	1:56:B:GLN:HE22	11	4.67
(1,809)	1:84:B:THR:H	1:60:A:LEU:HD11	5	4.66
(1,802)	1:81:B:LEU:HB3	1:60:A:LEU:HD11	17	4.66
(1,432)	1:90:B:ASN:HA	1:65:B:LEU:HG	1	4.66
(1,432)	1:90:B:ASN:HA	1:65:B:LEU:HG	7	4.66
(1,226)	1:81:A:LEU:H	1:56:B:GLN:HE21	9	4.66
(1,849)	1:90:B:ASN:HD21	1:92:B:GLN:HG2	10	4.65
(1,602)	1:64:B:ALA:HB2	1:67:B:LYS:HG3	2	4.65
(1,510)	1:79:A:ASP:H	1:54:A:LEU:HG	10	4.64
(1,415)	1:86:B:LYS:HD3	1:84:B:THR:HB	17	4.64
(1,941)	1:78:B:ALA:N	1:74:B:LYS:O	14	4.63
(1,849)	1:90:B:ASN:HD21	1:92:A:GLN:HG2	5	4.63
(1,510)	1:79:A:ASP:H	1:54:A:LEU:HG	6	4.63
(1,246)	1:81:A:LEU:H	1:56:B:GLN:HE22	20	4.63
(1,941)	1:78:B:ALA:N	1:74:B:LYS:O	10	4.62
(1,510)	1:79:B:ASP:H	1:54:B:LEU:HG	7	4.62
(1,849)	1:90:A:ASN:HD21	1:92:B:GLN:HG2	2	4.61
(1,849)	1:90:B:ASN:HD21	1:92:A:GLN:HG2	9	4.61
(1,849)	1:90:A:ASN:HD21	1:92:B:GLN:HG2	11	4.61
(1,838)	1:87:A:HIS:HD2	1:71:A:ARG:HD2	14	4.61
(1,739)	1:50:B:ILE:HG23	1:76:A:GLU:HA	12	4.61
(1,432)	1:90:A:ASN:HA	1:65:A:LEU:HG	5	4.61
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD13	13	4.6
(1,510)	1:79:B:ASP:H	1:54:B:LEU:HG	2	4.6
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD11	11	4.59
(1,432)	1:90:B:ASN:HA	1:65:B:LEU:HG	16	4.59
(1,308)	1:90:A:ASN:H	1:65:A:LEU:HG	13	4.59
(1,941)	1:78:A:ALA:N	1:74:A:LYS:O	19	4.58
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD22	19	4.58
(1,691)	1:87:B:HIS:HD2	1:71:B:ARG:HD2	20	4.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,602)	1:64:B:ALA:HB2	1:67:B:LYS:HG3	16	4.58
(1,564)	1:66:B:LYS:HA	1:69:B:SER:HB2	16	4.58
(1,510)	1:79:A:ASP:H	1:54:A:LEU:HG	9	4.58
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD21	4	4.57
(1,784)	1:64:A:ALA:HB2	1:67:A:LYS:HB2	7	4.56
(1,684)	1:86:A:LYS:HD3	1:87:A:HIS:HB3	5	4.56
(1,601)	1:64:A:ALA:HB1	1:67:A:LYS:HG2	1	4.56
(1,842)	1:87:A:HIS:HD2	1:75:A:LEU:HD12	3	4.55
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD21	8	4.55
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD22	18	4.55
(1,784)	1:64:A:ALA:HB3	1:67:A:LYS:HB2	14	4.55
(1,684)	1:86:A:LYS:HD3	1:87:A:HIS:HB3	15	4.55
(1,603)	1:64:B:ALA:HB2	1:67:B:LYS:HG2	6	4.55
(1,409)	1:64:B:ALA:HA	1:67:B:LYS:HB2	13	4.55
(1,849)	1:90:B:ASN:HD21	1:92:A:GLN:HG2	17	4.54
(1,409)	1:64:B:ALA:HA	1:67:B:LYS:HB2	3	4.54
(1,602)	1:64:A:ALA:HB2	1:67:A:LYS:HG3	5	4.53
(1,415)	1:86:B:LYS:HD3	1:84:B:THR:HB	19	4.53
(1,809)	1:84:A:THR:H	1:60:B:LEU:HD11	9	4.52
(1,409)	1:64:B:ALA:HA	1:67:B:LYS:HB2	9	4.52
(1,939)	1:77:A:LYS:N	1:73:A:SER:O	8	4.5
(1,510)	1:79:A:ASP:H	1:54:A:LEU:HG	20	4.5
(1,432)	1:90:A:ASN:HA	1:65:A:LEU:HG	18	4.5
(1,415)	1:86:B:LYS:HD3	1:84:B:THR:HB	13	4.5
(1,601)	1:64:A:ALA:HB1	1:67:A:LYS:HG2	2	4.49
(1,246)	1:81:A:LEU:H	1:56:B:GLN:HE22	4	4.49
(1,789)	1:66:B:LYS:HA	1:69:B:SER:HG	13	4.48
(1,308)	1:90:B:ASN:H	1:65:B:LEU:HG	17	4.48
(1,849)	1:90:B:ASN:HD21	1:92:A:GLN:HG2	8	4.47
(1,510)	1:79:B:ASP:H	1:54:B:LEU:HG	13	4.47
(1,409)	1:64:B:ALA:HA	1:67:B:LYS:HB2	10	4.47
(1,246)	1:81:B:LEU:H	1:56:A:GLN:HE22	1	4.47
(1,835)	1:87:A:HIS:HD1	1:67:A:LYS:HD2	10	4.46
(1,585)	1:64:A:ALA:HB1	1:67:A:LYS:HG3	19	4.46
(1,510)	1:79:B:ASP:H	1:54:B:LEU:HG	11	4.46
(1,409)	1:64:A:ALA:HA	1:67:A:LYS:HB2	18	4.46
(1,409)	1:64:B:ALA:HA	1:67:B:LYS:HB2	20	4.46
(1,308)	1:90:A:ASN:H	1:65:A:LEU:HG	5	4.46
(1,835)	1:87:B:HIS:HD2	1:67:B:LYS:HD2	4	4.45
(1,635)	1:89:B:ARG:HB2	1:65:B:LEU:HG	10	4.45
(1,603)	1:64:A:ALA:HB2	1:67:A:LYS:HG2	12	4.45
(1,214)	1:81:A:LEU:HB2	1:56:B:GLN:HE22	10	4.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,357)	1:67:A:LYS:HA	1:70:A:SER:H	15	4.44
(1,246)	1:81:B:LEU:H	1:56:A:GLN:HE22	17	4.43
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD21	14	4.42
(1,460)	1:73:B:SER:HA	1:76:B:GLU:HB2	2	4.42
(1,357)	1:67:A:LYS:HA	1:70:A:SER:H	12	4.42
(1,684)	1:86:A:LYS:HD3	1:87:A:HIS:HB3	16	4.41
(1,409)	1:64:A:ALA:HA	1:67:A:LYS:HB2	8	4.41
(1,357)	1:67:A:LYS:HA	1:70:A:SER:H	13	4.41
(1,357)	1:67:A:LYS:HA	1:70:A:SER:H	18	4.41
(1,849)	1:90:B:ASN:HD21	1:92:A:GLN:HG2	7	4.4
(1,849)	1:90:B:ASN:HD21	1:92:A:GLN:HG2	20	4.4
(1,585)	1:64:A:ALA:HB1	1:67:A:LYS:HG3	12	4.4
(1,357)	1:67:B:LYS:HA	1:70:B:SER:H	10	4.4
(1,246)	1:81:B:LEU:H	1:56:A:GLN:HE22	7	4.4
(1,688)	1:86:A:LYS:HD3	1:87:A:HIS:HB2	19	4.39
(1,684)	1:86:B:LYS:HD3	1:87:B:HIS:HB3	19	4.39
(1,357)	1:67:B:LYS:HA	1:70:B:SER:H	5	4.39
(1,246)	1:81:A:LEU:H	1:56:B:GLN:HE22	6	4.39
(1,226)	1:81:B:LEU:H	1:56:A:GLN:HE21	1	4.39
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD23	2	4.38
(1,409)	1:64:A:ALA:HA	1:67:A:LYS:HB2	4	4.38
(1,357)	1:67:B:LYS:HA	1:70:B:SER:H	9	4.38
(1,849)	1:90:A:ASN:HD21	1:92:B:GLN:HG2	13	4.37
(1,809)	1:84:B:THR:H	1:60:A:LEU:HD11	17	4.37
(1,510)	1:79:B:ASP:H	1:54:B:LEU:HG	18	4.37
(1,409)	1:64:B:ALA:HA	1:67:B:LYS:HB2	6	4.37
(1,357)	1:67:A:LYS:HA	1:70:A:SER:H	8	4.36
(1,246)	1:81:A:LEU:H	1:56:B:GLN:HE22	18	4.36
(1,691)	1:87:A:HIS:HD2	1:71:A:ARG:HD2	5	4.35
(1,691)	1:87:A:HIS:HD2	1:71:A:ARG:HD2	12	4.35
(1,357)	1:67:B:LYS:HA	1:70:B:SER:H	4	4.35
(1,355)	1:65:B:LEU:HA	1:68:B:ASP:H	9	4.35
(1,357)	1:67:B:LYS:HA	1:70:B:SER:H	1	4.34
(1,357)	1:67:A:LYS:HA	1:70:A:SER:H	2	4.34
(1,602)	1:64:B:ALA:HB2	1:67:B:LYS:HG3	13	4.33
(1,564)	1:66:A:LYS:HA	1:69:A:SER:HB3	6	4.33
(1,76)	1:86:A:LYS:H	1:61:B:ILE:HG12	18	4.33
(1,849)	1:90:B:ASN:HD21	1:92:A:GLN:HG2	19	4.32
(1,812)	1:84:A:THR:HG21	1:60:A:LEU:HD11	5	4.32
(1,688)	1:86:B:LYS:HD3	1:87:B:HIS:HB2	4	4.32
(1,626)	1:83:B:MET:HE1	1:84:B:THR:HG23	12	4.32
(1,357)	1:67:B:LYS:HA	1:70:B:SER:H	20	4.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,246)	1:81:A:LEU:H	1:56:B:GLN:HE22	3	4.32
(1,626)	1:83:B:MET:HE3	1:84:B:THR:HG21	11	4.31
(1,564)	1:66:A:LYS:HA	1:69:A:SER:HB2	7	4.31
(1,357)	1:67:B:LYS:HA	1:70:B:SER:H	3	4.31
(1,835)	1:87:A:HIS:HD1	1:67:A:LYS:HD2	1	4.3
(1,585)	1:64:B:ALA:HB1	1:67:B:LYS:HG3	3	4.3
(1,357)	1:67:B:LYS:HA	1:70:B:SER:H	11	4.3
(1,357)	1:67:B:LYS:HA	1:70:B:SER:H	16	4.3
(1,357)	1:67:A:LYS:HA	1:70:A:SER:H	19	4.3
(1,237)	1:79:B:ASP:H	1:54:B:LEU:HD11	14	4.3
(1,76)	1:86:A:LYS:H	1:61:B:ILE:HG12	3	4.3
(1,246)	1:81:B:LEU:H	1:56:A:GLN:HE22	8	4.29
(1,246)	1:81:A:LEU:H	1:56:B:GLN:HE22	15	4.29
(1,603)	1:64:B:ALA:HB2	1:67:B:LYS:HG2	11	4.28
(1,838)	1:87:A:HIS:HD2	1:71:A:ARG:HD2	13	4.27
(1,510)	1:79:A:ASP:H	1:54:A:LEU:HG	4	4.27
(1,626)	1:83:A:MET:HE1	1:84:A:THR:HG22	4	4.26
(1,357)	1:67:B:LYS:HA	1:70:B:SER:H	7	4.26
(1,308)	1:90:B:ASN:H	1:65:B:LEU:HG	8	4.26
(1,687)	1:87:A:HIS:HD1	1:71:A:ARG:HD2	13	4.25
(1,684)	1:86:A:LYS:HD3	1:87:A:HIS:HB3	20	4.25
(1,626)	1:83:A:MET:HE3	1:84:A:THR:HG23	1	4.25
(1,76)	1:86:A:LYS:H	1:61:A:ILE:HG12	2	4.25
(1,76)	1:86:A:LYS:H	1:61:B:ILE:HG12	11	4.25
(1,812)	1:84:B:THR:HG21	1:60:B:LEU:HD11	9	4.24
(1,603)	1:64:A:ALA:HB2	1:67:A:LYS:HG2	9	4.24
(1,601)	1:64:B:ALA:HB1	1:67:B:LYS:HG2	7	4.24
(1,510)	1:79:B:ASP:H	1:54:B:LEU:HG	19	4.24
(1,76)	1:86:A:LYS:H	1:61:A:ILE:HG12	7	4.24
(1,76)	1:86:B:LYS:H	1:61:B:ILE:HG12	16	4.24
(1,849)	1:90:B:ASN:HD21	1:92:A:GLN:HG2	15	4.23
(1,415)	1:86:B:LYS:HD3	1:84:B:THR:HB	2	4.23
(1,357)	1:67:B:LYS:HA	1:70:B:SER:H	6	4.23
(1,237)	1:79:B:ASP:H	1:54:B:LEU:HD11	3	4.23
(1,214)	1:81:B:LEU:HB3	1:56:A:GLN:HE22	11	4.23
(1,633)	1:90:B:ASN:HB2	1:92:B:GLN:HG2	5	4.22
(1,409)	1:64:A:ALA:HA	1:67:A:LYS:HB2	7	4.22
(1,308)	1:90:B:ASN:H	1:65:B:LEU:HG	4	4.22
(1,76)	1:86:A:LYS:H	1:61:A:ILE:HG12	9	4.22
(1,849)	1:90:B:ASN:HD21	1:92:A:GLN:HG2	12	4.21
(1,687)	1:87:A:HIS:HD1	1:71:A:ARG:HD2	5	4.21
(1,684)	1:86:A:LYS:HD3	1:87:A:HIS:HB3	2	4.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,684)	1:86:B:LYS:HD3	1:87:B:HIS:HB3	6	4.21
(1,684)	1:86:B:LYS:HD3	1:87:B:HIS:HB3	14	4.21
(1,601)	1:64:B:ALA:HB1	1:67:B:LYS:HG2	4	4.21
(1,76)	1:86:B:LYS:H	1:61:B:ILE:HG12	5	4.21
(1,812)	1:84:B:THR:HG23	1:60:B:LEU:HD13	3	4.2
(1,626)	1:83:A:MET:HE2	1:84:A:THR:HG23	13	4.2
(1,601)	1:64:B:ALA:HB1	1:67:B:LYS:HG2	5	4.2
(1,76)	1:86:B:LYS:H	1:61:B:ILE:HG12	14	4.2
(1,835)	1:87:B:HIS:HD2	1:67:B:LYS:HD2	17	4.19
(1,633)	1:90:B:ASN:HB2	1:92:B:GLN:HG2	4	4.19
(1,602)	1:64:A:ALA:HB2	1:67:A:LYS:HG3	19	4.19
(1,688)	1:86:B:LYS:HD3	1:87:B:HIS:HB2	11	4.18
(1,415)	1:86:A:LYS:HD3	1:84:A:THR:HB	12	4.18
(1,214)	1:81:B:LEU:HB2	1:56:A:GLN:HE22	1	4.18
(1,76)	1:86:A:LYS:H	1:61:B:ILE:HG12	10	4.18
(1,929)	1:71:B:ARG:N	1:67:B:LYS:O	13	4.17
(1,626)	1:83:A:MET:HE1	1:84:A:THR:HG22	2	4.17
(1,601)	1:64:B:ALA:HB1	1:67:B:LYS:HG2	20	4.17
(1,415)	1:86:B:LYS:HD3	1:84:B:THR:HB	3	4.17
(1,355)	1:65:B:LEU:HA	1:68:B:ASP:H	14	4.17
(1,76)	1:86:A:LYS:H	1:61:A:ILE:HG12	15	4.17
(1,409)	1:64:B:ALA:HA	1:67:B:LYS:HB2	11	4.16
(1,835)	1:87:A:HIS:HD2	1:67:A:LYS:HD2	7	4.15
(1,602)	1:64:B:ALA:HB2	1:67:B:LYS:HG3	20	4.15
(1,408)	1:64:B:ALA:HA	1:67:B:LYS:HG2	13	4.15
(1,357)	1:67:A:LYS:HA	1:70:A:SER:H	14	4.15
(1,214)	1:81:A:LEU:HB2	1:56:B:GLN:HE22	20	4.15
(1,76)	1:86:B:LYS:H	1:61:B:ILE:HG12	12	4.15
(1,633)	1:90:B:ASN:HB2	1:92:B:GLN:HG2	12	4.14
(1,603)	1:64:A:ALA:HB2	1:67:A:LYS:HG2	2	4.14
(1,602)	1:64:B:ALA:HB2	1:67:B:LYS:HG3	10	4.14
(1,684)	1:86:B:LYS:HD3	1:87:B:HIS:HB3	7	4.13
(1,76)	1:86:A:LYS:H	1:61:A:ILE:HG12	8	4.13
(1,714)	1:86:A:LYS:HD3	1:84:A:THR:HA	10	4.12
(1,415)	1:86:B:LYS:HD3	1:84:B:THR:HB	18	4.12
(1,408)	1:64:B:ALA:HA	1:67:B:LYS:HG2	12	4.12
(1,355)	1:65:A:LEU:HA	1:68:A:ASP:H	3	4.12
(1,415)	1:86:B:LYS:HD3	1:84:B:THR:HB	1	4.11
(1,415)	1:86:A:LYS:HD3	1:84:A:THR:HB	15	4.11
(1,76)	1:86:B:LYS:H	1:61:B:ILE:HG12	13	4.11
(1,633)	1:90:B:ASN:HB2	1:92:B:GLN:HG3	8	4.1
(1,603)	1:64:A:ALA:HB2	1:67:A:LYS:HG2	15	4.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,602)	1:64:B:ALA:HB2	1:67:B:LYS:HG3	1	4.1
(1,355)	1:65:A:LEU:HA	1:68:A:ASP:H	11	4.1
(1,929)	1:71:A:ARG:N	1:67:A:LYS:O	12	4.09
(1,633)	1:90:B:ASN:HB2	1:92:B:GLN:HG2	7	4.09
(1,585)	1:64:B:ALA:HB1	1:67:B:LYS:HG3	11	4.09
(1,355)	1:65:B:LEU:HA	1:68:B:ASP:H	2	4.09
(1,76)	1:86:B:LYS:H	1:61:B:ILE:HG12	4	4.09
(1,633)	1:90:A:ASN:HB2	1:92:A:GLN:HG2	11	4.08
(1,415)	1:86:B:LYS:HD3	1:84:B:THR:HB	16	4.08
(1,409)	1:64:A:ALA:HA	1:67:A:LYS:HB2	14	4.08
(1,355)	1:65:B:LEU:HA	1:68:B:ASP:H	19	4.08
(1,246)	1:81:A:LEU:H	1:56:B:GLN:HE22	13	4.08
(1,214)	1:81:B:LEU:HB3	1:56:A:GLN:HE22	5	4.08
(1,633)	1:90:A:ASN:HB2	1:92:A:GLN:HG2	1	4.07
(1,602)	1:64:B:ALA:HB2	1:67:B:LYS:HG3	3	4.07
(1,602)	1:64:A:ALA:HB2	1:67:A:LYS:HG3	4	4.07
(1,602)	1:64:A:ALA:HB2	1:67:A:LYS:HG3	17	4.07
(1,408)	1:64:A:ALA:HA	1:67:A:LYS:HG2	19	4.07
(1,357)	1:67:A:LYS:HA	1:70:A:SER:H	17	4.07
(1,76)	1:86:B:LYS:H	1:61:B:ILE:HG12	17	4.07
(1,76)	1:86:A:LYS:H	1:61:B:ILE:HG12	19	4.07
(1,687)	1:87:A:HIS:HD1	1:71:A:ARG:HD2	19	4.06
(1,409)	1:64:A:ALA:HA	1:67:A:LYS:HB2	1	4.06
(1,214)	1:81:B:LEU:HB3	1:56:A:GLN:HE22	18	4.06
(1,812)	1:84:A:THR:HG21	1:60:A:LEU:HD11	11	4.05
(1,684)	1:86:A:LYS:HD3	1:87:A:HIS:HB3	9	4.05
(1,633)	1:90:A:ASN:HB2	1:92:A:GLN:HG3	15	4.05
(1,633)	1:90:B:ASN:HB2	1:92:B:GLN:HG2	20	4.05
(1,415)	1:86:B:LYS:HD3	1:84:B:THR:HB	5	4.05
(1,408)	1:64:A:ALA:HA	1:67:A:LYS:HG2	20	4.05
(1,355)	1:65:A:LEU:HA	1:68:A:ASP:H	20	4.05
(1,246)	1:81:A:LEU:H	1:56:B:GLN:HE22	14	4.05
(1,76)	1:86:A:LYS:H	1:61:A:ILE:HG12	1	4.05
(1,835)	1:87:B:HIS:HD1	1:67:B:LYS:HD2	11	4.04
(1,834)	1:87:B:HIS:HD1	1:92:A:GLN:HB2	5	4.04
(1,246)	1:81:B:LEU:H	1:56:A:GLN:HE22	12	4.04
(1,684)	1:86:B:LYS:HD3	1:87:B:HIS:HB3	12	4.03
(1,649)	1:71:A:ARG:HG2	1:75:A:LEU:HD11	5	4.03
(1,415)	1:86:B:LYS:HD3	1:84:B:THR:HB	11	4.03
(1,214)	1:81:B:LEU:HB2	1:56:A:GLN:HE22	17	4.03
(1,76)	1:86:B:LYS:H	1:61:B:ILE:HG12	6	4.03
(1,785)	1:64:B:ALA:HB1	1:67:B:LYS:HG3	2	4.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,684)	1:86:B:LYS:HD3	1:87:B:HIS:HB3	17	4.02
(1,451)	1:81:B:LEU:HA	1:56:A:GLN:HG3	10	4.02
(1,409)	1:64:A:ALA:HA	1:67:A:LYS:HB2	16	4.02
(1,408)	1:64:B:ALA:HA	1:67:B:LYS:HG2	5	4.02
(1,308)	1:90:B:ASN:H	1:65:B:LEU:HG	3	4.02
(1,237)	1:79:B:ASP:H	1:54:B:LEU:HD13	8	4.02
(1,838)	1:87:A:HIS:HD2	1:71:A:ARG:HD2	3	4.01
(1,688)	1:86:B:LYS:HD3	1:87:B:HIS:HB2	15	4.01
(1,633)	1:90:A:ASN:HB2	1:92:A:GLN:HG2	13	4.01
(1,633)	1:90:B:ASN:HB2	1:92:B:GLN:HG2	18	4.01
(1,415)	1:86:B:LYS:HD3	1:84:B:THR:HB	8	4.01
(1,237)	1:79:B:ASP:H	1:54:B:LEU:HD13	17	4.01
(1,842)	1:87:A:HIS:HD2	1:75:A:LEU:HD23	12	4.0
(1,837)	1:87:B:HIS:HD1	1:93:B:ARG:H	14	4.0
(1,785)	1:64:A:ALA:HB1	1:67:A:LYS:HG3	13	4.0
(1,633)	1:90:B:ASN:HB2	1:92:B:GLN:HG2	9	4.0
(1,355)	1:65:B:LEU:HA	1:68:B:ASP:H	1	4.0
(1,415)	1:86:A:LYS:HD3	1:84:A:THR:HB	4	3.99
(1,246)	1:81:A:LEU:H	1:56:B:GLN:HE22	9	3.99
(1,684)	1:86:A:LYS:HD3	1:87:A:HIS:HB3	1	3.98
(1,355)	1:65:B:LEU:HA	1:68:B:ASP:H	16	3.98
(1,929)	1:71:A:ARG:N	1:67:A:LYS:O	17	3.97
(1,688)	1:86:B:LYS:HD3	1:87:B:HIS:HB2	3	3.97
(1,585)	1:64:A:ALA:HB1	1:67:A:LYS:HG3	15	3.97
(1,408)	1:64:B:ALA:HA	1:67:B:LYS:HG2	1	3.97
(1,355)	1:65:B:LEU:HA	1:68:B:ASP:H	12	3.97
(1,929)	1:71:A:ARG:N	1:67:A:LYS:O	9	3.96
(1,789)	1:66:A:LYS:HA	1:69:A:SER:HG	2	3.96
(1,633)	1:90:B:ASN:HB2	1:92:B:GLN:HG2	2	3.96
(1,408)	1:64:A:ALA:HA	1:67:A:LYS:HG2	15	3.96
(1,226)	1:81:A:LEU:H	1:56:B:GLN:HE21	19	3.96
(1,929)	1:71:A:ARG:N	1:67:A:LYS:O	4	3.95
(1,603)	1:64:A:ALA:HB2	1:67:A:LYS:HG2	16	3.95
(1,355)	1:65:B:LEU:HA	1:68:B:ASP:H	5	3.95
(1,246)	1:81:A:LEU:H	1:56:B:GLN:HE22	2	3.95
(1,224)	1:81:B:LEU:HB3	1:56:A:GLN:HE21	10	3.95
(1,633)	1:90:B:ASN:HB2	1:92:B:GLN:HG2	3	3.94
(1,447)	1:81:B:LEU:HA	1:56:A:GLN:HG2	10	3.94
(1,837)	1:87:B:HIS:HD1	1:93:B:ARG:H	11	3.93
(1,447)	1:81:A:LEU:HA	1:56:B:GLN:HG2	1	3.93
(1,237)	1:79:B:ASP:H	1:54:B:LEU:HD12	6	3.93
(1,237)	1:79:B:ASP:H	1:54:B:LEU:HD13	12	3.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,633)	1:90:A:ASN:HB2	1:92:A:GLN:HG2	6	3.92
(1,601)	1:64:A:ALA:HB1	1:67:A:LYS:HG2	6	3.92
(1,355)	1:65:B:LEU:HA	1:68:B:ASP:H	13	3.92
(1,785)	1:64:B:ALA:HB1	1:67:B:LYS:HG3	16	3.91
(1,633)	1:90:A:ASN:HB2	1:92:A:GLN:HG2	14	3.91
(1,633)	1:90:A:ASN:HB2	1:92:A:GLN:HG2	16	3.91
(1,237)	1:79:B:ASP:H	1:54:B:LEU:HD13	5	3.91
(1,214)	1:81:A:LEU:HB3	1:56:B:GLN:HE22	6	3.91
(1,214)	1:81:A:LEU:HB2	1:56:B:GLN:HE22	15	3.91
(1,214)	1:81:B:LEU:HB3	1:56:A:GLN:HE22	16	3.91
(1,684)	1:86:A:LYS:HD3	1:87:A:HIS:HB3	8	3.9
(1,447)	1:81:A:LEU:HA	1:56:B:GLN:HG2	5	3.9
(1,785)	1:64:B:ALA:HB3	1:67:B:LYS:HG3	12	3.89
(1,684)	1:86:A:LYS:HD3	1:87:A:HIS:HB3	18	3.89
(1,432)	1:90:B:ASN:HA	1:65:B:LEU:HG	19	3.89
(1,684)	1:86:B:LYS:HD3	1:87:B:HIS:HB3	13	3.88
(1,447)	1:81:B:LEU:HA	1:56:A:GLN:HG2	7	3.88
(1,355)	1:65:A:LEU:HA	1:68:A:ASP:H	7	3.88
(1,785)	1:64:A:ALA:HB1	1:67:A:LYS:HG3	6	3.87
(1,691)	1:87:A:HIS:HD2	1:71:A:ARG:HD2	14	3.87
(1,451)	1:81:A:LEU:HA	1:56:B:GLN:HG3	11	3.87
(1,76)	1:86:B:LYS:H	1:61:A:ILE:HG12	20	3.87
(1,633)	1:90:B:ASN:HB2	1:92:B:GLN:HG2	17	3.86
(1,308)	1:90:B:ASN:H	1:65:B:LEU:HG	9	3.86
(1,214)	1:81:B:LEU:HB3	1:56:A:GLN:HE22	3	3.86
(1,834)	1:87:B:HIS:HD1	1:92:A:GLN:HB2	13	3.85
(1,246)	1:81:A:LEU:H	1:56:B:GLN:HE22	19	3.85
(1,408)	1:64:B:ALA:HA	1:67:B:LYS:HG2	11	3.84
(1,929)	1:71:B:ARG:N	1:67:B:LYS:O	6	3.83
(1,633)	1:90:B:ASN:HB2	1:92:B:GLN:HG2	19	3.83
(1,447)	1:81:B:LEU:HA	1:56:A:GLN:HG2	11	3.83
(1,432)	1:90:B:ASN:HA	1:65:B:LEU:HG	10	3.83
(1,355)	1:65:B:LEU:HA	1:68:B:ASP:H	8	3.83
(1,237)	1:79:B:ASP:H	1:54:B:LEU:HD13	16	3.83
(1,929)	1:71:A:ARG:N	1:67:A:LYS:O	19	3.82
(1,603)	1:64:A:ALA:HB2	1:67:A:LYS:HG2	18	3.82
(1,564)	1:66:B:LYS:HA	1:69:B:SER:HB2	19	3.82
(1,408)	1:64:B:ALA:HA	1:67:B:LYS:HG2	14	3.82
(1,224)	1:81:B:LEU:HB3	1:56:A:GLN:HE21	17	3.82
(1,214)	1:81:B:LEU:HB3	1:56:A:GLN:HE22	7	3.82
(1,308)	1:90:B:ASN:H	1:65:B:LEU:HG	14	3.81
(1,939)	1:77:B:LYS:N	1:73:B:SER:O	2	3.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,785)	1:64:A:ALA:HB1	1:67:A:LYS:HG3	5	3.8
(1,451)	1:81:A:LEU:HA	1:56:B:GLN:HG3	13	3.8
(1,447)	1:81:B:LEU:HA	1:56:A:GLN:HG2	17	3.8
(1,408)	1:64:A:ALA:HA	1:67:A:LYS:HG2	4	3.8
(1,308)	1:90:A:ASN:H	1:65:A:LEU:HG	20	3.8
(1,785)	1:64:A:ALA:HB1	1:67:A:LYS:HG3	1	3.79
(1,684)	1:86:A:LYS:HD3	1:87:A:HIS:HB3	10	3.79
(1,627)	1:66:B:LYS:HG2	1:67:B:LYS:HG2	18	3.79
(1,601)	1:64:A:ALA:HB1	1:67:A:LYS:HG2	13	3.79
(1,447)	1:81:B:LEU:HA	1:56:A:GLN:HG2	16	3.79
(1,929)	1:71:A:ARG:N	1:67:A:LYS:O	5	3.78
(1,858)	1:93:B:ARG:HB3	1:95:B:GLN:HB3	5	3.78
(1,821)	1:86:A:LYS:HG2	1:83:A:MET:HG3	9	3.78
(1,785)	1:64:B:ALA:HB2	1:67:B:LYS:HG3	11	3.78
(1,785)	1:64:A:ALA:HB3	1:67:A:LYS:HG3	19	3.78
(1,688)	1:86:A:LYS:HD3	1:87:A:HIS:HB2	5	3.78
(1,627)	1:66:B:LYS:HG2	1:67:B:LYS:HG2	15	3.78
(1,451)	1:81:B:LEU:HA	1:56:A:GLN:HG3	16	3.78
(1,308)	1:90:A:ASN:H	1:65:A:LEU:HG	11	3.78
(1,237)	1:79:A:ASP:H	1:54:A:LEU:HD11	1	3.78
(1,601)	1:64:A:ALA:HB1	1:67:A:LYS:HG2	10	3.77
(1,408)	1:64:A:ALA:HA	1:67:A:LYS:HG2	7	3.77
(1,214)	1:81:A:LEU:HB2	1:56:B:GLN:HE22	12	3.77
(1,929)	1:71:B:ARG:N	1:67:B:LYS:O	7	3.76
(1,451)	1:81:A:LEU:HA	1:56:B:GLN:HG3	1	3.76
(1,408)	1:64:A:ALA:HA	1:67:A:LYS:HG2	6	3.76
(1,408)	1:64:A:ALA:HA	1:67:A:LYS:HG2	18	3.76
(1,237)	1:79:B:ASP:H	1:54:B:LEU:HD11	7	3.76
(1,237)	1:79:B:ASP:H	1:54:B:LEU:HD12	15	3.76
(1,837)	1:87:B:HIS:HD2	1:93:B:ARG:H	12	3.75
(1,812)	1:84:B:THR:HG23	1:60:B:LEU:HD13	13	3.75
(1,447)	1:81:A:LEU:HA	1:56:B:GLN:HG2	6	3.75
(1,224)	1:81:A:LEU:HB3	1:56:B:GLN:HE21	20	3.75
(1,451)	1:81:A:LEU:HA	1:56:B:GLN:HG3	15	3.74
(1,785)	1:64:B:ALA:HB3	1:67:B:LYS:HG3	3	3.73
(1,649)	1:71:B:ARG:HG2	1:75:B:LEU:HD12	16	3.73
(1,633)	1:90:A:ASN:HB2	1:92:A:GLN:HG2	10	3.73
(1,447)	1:81:A:LEU:HA	1:56:B:GLN:HG2	4	3.73
(1,447)	1:81:A:LEU:HA	1:56:B:GLN:HG2	18	3.73
(1,355)	1:65:A:LEU:HA	1:68:A:ASP:H	6	3.73
(1,355)	1:65:A:LEU:HA	1:68:A:ASP:H	15	3.73
(1,308)	1:90:B:ASN:H	1:65:B:LEU:HG	6	3.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,929)	1:71:A:ARG:N	1:67:A:LYS:O	8	3.72
(1,821)	1:86:A:LYS:HG2	1:83:A:MET:HG3	6	3.72
(1,224)	1:81:B:LEU:HB3	1:56:A:GLN:HE21	11	3.72
(1,929)	1:71:B:ARG:N	1:67:B:LYS:O	20	3.71
(1,817)	1:60:B:LEU:HD22	1:88:A:LEU:HB2	15	3.71
(1,447)	1:81:B:LEU:HA	1:56:A:GLN:HG2	19	3.71
(1,355)	1:65:A:LEU:HA	1:68:A:ASP:H	18	3.71
(1,214)	1:81:B:LEU:HB3	1:56:A:GLN:HE22	8	3.71
(1,929)	1:71:A:ARG:N	1:67:A:LYS:O	18	3.7
(1,837)	1:87:A:HIS:HD1	1:93:A:ARG:H	17	3.7
(1,308)	1:90:A:ASN:H	1:65:A:LEU:HG	2	3.7
(1,224)	1:81:B:LEU:HB3	1:56:A:GLN:HE21	18	3.7
(1,929)	1:71:B:ARG:N	1:67:B:LYS:O	11	3.69
(1,785)	1:64:A:ALA:HB2	1:67:A:LYS:HG3	15	3.69
(1,451)	1:81:A:LEU:HA	1:56:B:GLN:HG3	5	3.69
(1,224)	1:81:B:LEU:HB3	1:56:A:GLN:HE21	7	3.69
(1,214)	1:81:A:LEU:HB2	1:56:B:GLN:HE22	19	3.69
(1,834)	1:87:A:HIS:HD2	1:92:B:GLN:HB2	10	3.68
(1,834)	1:87:B:HIS:HD2	1:92:A:GLN:HB2	14	3.68
(1,821)	1:86:A:LYS:HG2	1:83:A:MET:HG3	17	3.68
(1,688)	1:86:A:LYS:HD3	1:87:A:HIS:HB2	10	3.68
(1,627)	1:66:B:LYS:HG2	1:67:B:LYS:HG2	7	3.68
(1,627)	1:66:A:LYS:HG2	1:67:A:LYS:HG2	12	3.68
(1,564)	1:66:A:LYS:HA	1:69:A:SER:HB3	14	3.68
(1,451)	1:81:B:LEU:HA	1:56:A:GLN:HG3	18	3.68
(1,834)	1:87:A:HIS:HD1	1:92:B:GLN:HB2	6	3.67
(1,834)	1:87:A:HIS:HD1	1:92:B:GLN:HB2	18	3.67
(1,447)	1:81:B:LEU:HA	1:56:A:GLN:HG2	8	3.67
(1,447)	1:81:A:LEU:HA	1:56:B:GLN:HG2	13	3.67
(1,439)	1:86:B:LYS:HA	1:84:A:THR:HG21	19	3.67
(1,585)	1:64:B:ALA:HB1	1:67:B:LYS:HG3	8	3.66
(1,447)	1:81:A:LEU:HA	1:56:B:GLN:HG2	3	3.66
(1,938)	1:76:A:GLU:N	1:72:A:HIS:O	20	3.65
(1,929)	1:71:B:ARG:N	1:67:B:LYS:O	1	3.65
(1,929)	1:71:A:ARG:N	1:67:A:LYS:O	2	3.65
(1,834)	1:87:B:HIS:HD2	1:92:A:GLN:HB2	16	3.65
(1,564)	1:66:A:LYS:HA	1:69:A:SER:HB2	3	3.65
(1,451)	1:81:B:LEU:HA	1:56:A:GLN:HG3	17	3.65
(1,237)	1:79:B:ASP:H	1:54:B:LEU:HD12	10	3.65
(1,214)	1:81:A:LEU:HB3	1:56:B:GLN:HE22	4	3.65
(1,214)	1:81:A:LEU:HB2	1:56:B:GLN:HE22	13	3.65
(1,447)	1:81:B:LEU:HA	1:56:A:GLN:HG2	15	3.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,834)	1:87:B:HIS:HD1	1:92:A:GLN:HB2	7	3.63
(1,785)	1:64:B:ALA:HB1	1:67:B:LYS:HG3	20	3.63
(1,601)	1:64:A:ALA:HB1	1:67:A:LYS:HG2	3	3.63
(1,451)	1:81:B:LEU:HA	1:56:A:GLN:HG3	8	3.63
(1,439)	1:86:B:LYS:HA	1:84:B:THR:HG21	10	3.63
(1,308)	1:90:B:ASN:H	1:65:B:LEU:HG	16	3.63
(1,929)	1:71:A:ARG:N	1:67:A:LYS:O	14	3.62
(1,834)	1:87:A:HIS:HD2	1:92:B:GLN:HB2	8	3.62
(1,627)	1:66:A:LYS:HG2	1:67:A:LYS:HG2	20	3.62
(1,585)	1:64:A:ALA:HB1	1:67:A:LYS:HG3	14	3.62
(1,451)	1:81:A:LEU:HA	1:56:B:GLN:HG3	19	3.62
(1,834)	1:87:A:HIS:HD2	1:92:B:GLN:HB2	4	3.61
(1,451)	1:81:A:LEU:HA	1:56:B:GLN:HG3	4	3.61
(1,355)	1:65:A:LEU:HA	1:68:A:ASP:H	4	3.61
(1,355)	1:65:A:LEU:HA	1:68:A:ASP:H	10	3.61
(1,224)	1:81:A:LEU:HB3	1:56:B:GLN:HE21	6	3.61
(1,837)	1:87:B:HIS:HD2	1:93:B:ARG:H	3	3.6
(1,821)	1:86:A:LYS:HG2	1:83:A:MET:HG3	11	3.6
(1,821)	1:86:A:LYS:HG2	1:83:A:MET:HG3	20	3.6
(1,817)	1:60:B:LEU:HD21	1:88:A:LEU:HB2	8	3.6
(1,237)	1:79:B:ASP:H	1:54:B:LEU:HD12	11	3.6
(1,224)	1:81:B:LEU:HB3	1:56:A:GLN:HE21	5	3.6
(1,224)	1:81:A:LEU:HB2	1:56:B:GLN:HE21	15	3.6
(1,837)	1:87:A:HIS:HD1	1:93:A:ARG:H	1	3.59
(1,785)	1:64:B:ALA:HB1	1:67:B:LYS:HG3	4	3.59
(1,785)	1:64:A:ALA:HB1	1:67:A:LYS:HG3	10	3.59
(1,761)	1:86:A:LYS:HD3	1:84:A:THR:H	20	3.59
(1,585)	1:64:A:ALA:HB1	1:67:A:LYS:HG3	18	3.59
(1,451)	1:81:B:LEU:HA	1:56:A:GLN:HG3	2	3.59
(1,451)	1:81:B:LEU:HA	1:56:A:GLN:HG3	7	3.59
(1,447)	1:81:A:LEU:HA	1:56:B:GLN:HG2	2	3.59
(1,938)	1:76:B:GLU:N	1:72:B:HIS:O	17	3.58
(1,488)	1:64:A:ALA:HA	1:65:A:LEU:HD13	15	3.58
(1,451)	1:81:A:LEU:HA	1:56:B:GLN:HG3	3	3.58
(1,628)	1:66:A:LYS:HG2	1:67:A:LYS:HB2	17	3.57
(1,564)	1:66:B:LYS:HA	1:69:B:SER:HB3	17	3.57
(1,447)	1:81:B:LEU:HA	1:56:A:GLN:HG2	12	3.57
(1,224)	1:81:B:LEU:HB2	1:56:A:GLN:HE21	12	3.57
(1,837)	1:87:B:HIS:HD1	1:93:B:ARG:H	18	3.56
(1,603)	1:64:A:ALA:HB2	1:67:A:LYS:HG2	7	3.56
(1,857)	1:93:B:ARG:HB2	1:95:B:GLN:HB3	5	3.55
(1,821)	1:86:A:LYS:HG2	1:83:A:MET:HG3	12	3.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:86:A:LYS:HB2	1:84:A:THR:HG23	20	3.55
(1,626)	1:83:A:MET:HE1	1:84:A:THR:HG22	9	3.55
(1,564)	1:66:A:LYS:HA	1:69:A:SER:HB2	20	3.55
(1,451)	1:81:B:LEU:HA	1:56:A:GLN:HG3	20	3.55
(1,835)	1:87:A:HIS:HD1	1:67:A:LYS:HD2	8	3.54
(1,821)	1:86:B:LYS:HG2	1:83:B:MET:HG3	7	3.54
(1,785)	1:64:B:ALA:HB1	1:67:B:LYS:HG3	17	3.54
(1,627)	1:66:B:LYS:HG2	1:67:B:LYS:HG2	19	3.54
(1,601)	1:64:B:ALA:HB1	1:67:B:LYS:HG2	17	3.54
(1,564)	1:66:A:LYS:HA	1:69:A:SER:HB2	11	3.54
(1,308)	1:90:B:ASN:H	1:65:B:LEU:HG	7	3.54
(1,929)	1:71:A:ARG:N	1:67:A:LYS:O	16	3.53
(1,837)	1:87:A:HIS:HD2	1:93:A:ARG:H	2	3.53
(1,834)	1:87:B:HIS:HD2	1:92:A:GLN:HB2	1	3.53
(1,691)	1:87:A:HIS:HD2	1:71:A:ARG:HD2	13	3.53
(1,688)	1:86:B:LYS:HD3	1:87:B:HIS:HB2	6	3.53
(1,688)	1:86:A:LYS:HD3	1:87:A:HIS:HB2	16	3.53
(1,603)	1:64:A:ALA:HB2	1:67:A:LYS:HG2	3	3.53
(1,564)	1:66:A:LYS:HA	1:69:A:SER:HB2	1	3.53
(1,451)	1:81:A:LEU:HA	1:56:B:GLN:HG3	6	3.53
(1,451)	1:81:B:LEU:HA	1:56:A:GLN:HG3	12	3.53
(1,447)	1:81:B:LEU:HA	1:56:A:GLN:HG2	20	3.53
(1,408)	1:64:B:ALA:HA	1:67:B:LYS:HG2	17	3.53
(1,834)	1:87:B:HIS:HD1	1:92:A:GLN:HB2	3	3.52
(1,308)	1:90:B:ASN:H	1:65:B:LEU:HG	1	3.52
(1,214)	1:81:B:LEU:HB3	1:56:A:GLN:HE22	14	3.52
(1,938)	1:76:B:GLU:N	1:72:B:HIS:O	8	3.51
(1,834)	1:87:B:HIS:HD1	1:92:A:GLN:HB2	9	3.51
(1,812)	1:84:A:THR:HG21	1:60:A:LEU:HD11	17	3.51
(1,602)	1:64:A:ALA:HB2	1:67:A:LYS:HG3	14	3.51
(1,237)	1:79:B:ASP:H	1:54:B:LEU:HD13	13	3.51
(1,821)	1:86:B:LYS:HG2	1:83:B:MET:HG3	1	3.5
(1,821)	1:86:B:LYS:HG2	1:83:B:MET:HG3	14	3.5
(1,654)	1:86:B:LYS:HB2	1:84:B:THR:HG22	11	3.5
(1,601)	1:64:A:ALA:HB1	1:67:A:LYS:HG2	8	3.5
(1,308)	1:90:A:ASN:H	1:65:A:LEU:HG	18	3.5
(1,938)	1:76:A:GLU:N	1:72:A:HIS:O	3	3.49
(1,602)	1:64:A:ALA:HB2	1:67:A:LYS:HG3	9	3.49
(1,451)	1:81:A:LEU:HA	1:56:B:GLN:HG3	9	3.49
(1,627)	1:66:B:LYS:HG2	1:67:B:LYS:HG2	5	3.48
(1,627)	1:66:A:LYS:HG2	1:67:A:LYS:HG2	17	3.48
(1,929)	1:71:B:ARG:N	1:67:B:LYS:O	15	3.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:81:B:LEU:HB3	1:56:A:GLN:HE21	16	3.47
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD21	12	3.46
(1,237)	1:79:B:ASP:H	1:54:B:LEU:HD11	9	3.46
(1,929)	1:71:B:ARG:N	1:67:B:LYS:O	10	3.45
(1,837)	1:87:A:HIS:HD2	1:93:A:ARG:H	20	3.45
(1,821)	1:86:A:LYS:HG2	1:83:A:MET:HG3	13	3.45
(1,789)	1:66:B:LYS:HA	1:69:B:SER:HG	20	3.45
(1,355)	1:65:B:LEU:HA	1:68:B:ASP:H	17	3.45
(1,834)	1:87:B:HIS:HD1	1:92:A:GLN:HB2	12	3.44
(1,834)	1:87:B:HIS:HD1	1:92:A:GLN:HB2	15	3.44
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD21	7	3.44
(1,789)	1:66:A:LYS:HA	1:69:A:SER:HG	4	3.44
(1,628)	1:66:B:LYS:HG2	1:67:B:LYS:HB2	18	3.44
(1,834)	1:87:B:HIS:HD2	1:92:A:GLN:HB2	11	3.43
(1,237)	1:79:B:ASP:H	1:54:B:LEU:HD12	18	3.43
(1,237)	1:79:A:ASP:H	1:54:A:LEU:HD11	20	3.43
(1,833)	1:87:B:HIS:HD2	1:92:A:GLN:H	14	3.42
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD23	16	3.42
(1,688)	1:86:B:LYS:HD3	1:87:B:HIS:HB2	14	3.42
(1,649)	1:71:A:ARG:HG2	1:75:A:LEU:HD12	20	3.42
(1,447)	1:81:A:LEU:HA	1:56:B:GLN:HG2	14	3.42
(1,224)	1:81:A:LEU:HB3	1:56:B:GLN:HE21	4	3.42
(1,837)	1:87:B:HIS:HD2	1:93:B:ARG:H	9	3.41
(1,834)	1:87:A:HIS:HD2	1:92:B:GLN:HB2	17	3.41
(1,833)	1:87:B:HIS:HD2	1:92:B:GLN:H	3	3.41
(1,761)	1:86:B:LYS:HD3	1:84:B:THR:H	6	3.4
(1,761)	1:86:A:LYS:HD3	1:84:A:THR:H	9	3.4
(1,837)	1:87:A:HIS:HD2	1:93:A:ARG:H	16	3.39
(1,821)	1:86:B:LYS:HG2	1:83:B:MET:HG3	19	3.39
(1,654)	1:86:B:LYS:HB2	1:84:B:THR:HG21	3	3.39
(1,649)	1:71:A:ARG:HG2	1:75:A:LEU:HD11	11	3.39
(1,237)	1:79:B:ASP:H	1:54:B:LEU:HD11	2	3.39
(1,817)	1:60:B:LEU:HD23	1:88:A:LEU:HB2	1	3.38
(1,688)	1:86:A:LYS:HD3	1:87:A:HIS:HB2	2	3.38
(1,654)	1:86:B:LYS:HB2	1:84:B:THR:HG21	6	3.38
(1,447)	1:81:A:LEU:HA	1:56:B:GLN:HG2	9	3.38
(1,224)	1:81:B:LEU:HB3	1:56:A:GLN:HE21	3	3.38
(1,834)	1:87:A:HIS:HD1	1:92:B:GLN:HB2	2	3.37
(1,564)	1:66:B:LYS:HA	1:69:B:SER:HB3	8	3.37
(1,224)	1:81:B:LEU:HB3	1:56:A:GLN:HE21	13	3.37
(1,942)	1:79:B:ASP:H	1:75:B:LEU:O	7	3.36
(1,834)	1:87:B:HIS:HD1	1:92:A:GLN:HB2	19	3.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,747)	1:87:A:HIS:HD2	1:92:A:GLN:H	19	3.36
(1,785)	1:64:A:ALA:HB2	1:67:A:LYS:HG3	18	3.35
(1,688)	1:86:B:LYS:HD3	1:87:B:HIS:HB2	12	3.35
(1,564)	1:66:A:LYS:HA	1:69:A:SER:HB2	5	3.35
(1,214)	1:81:A:LEU:HB3	1:56:B:GLN:HE22	2	3.35
(1,176)	1:75:A:LEU:HA	1:78:A:ALA:H	9	3.35
(1,821)	1:86:A:LYS:HG2	1:83:A:MET:HG3	3	3.33
(1,654)	1:86:A:LYS:HB2	1:84:A:THR:HG22	5	3.32
(1,628)	1:66:B:LYS:HG2	1:67:B:LYS:HB2	13	3.32
(1,627)	1:66:B:LYS:HG2	1:67:B:LYS:HG2	6	3.32
(1,564)	1:66:B:LYS:HA	1:69:B:SER:HB3	13	3.32
(1,224)	1:81:B:LEU:HB3	1:56:A:GLN:HE21	8	3.32
(1,214)	1:81:A:LEU:HB3	1:56:B:GLN:HE22	9	3.32
(1,821)	1:86:B:LYS:HG2	1:83:B:MET:HG2	15	3.31
(1,439)	1:86:B:LYS:HA	1:84:B:THR:HG22	2	3.31
(1,439)	1:86:A:LYS:HA	1:84:A:THR:HG23	20	3.31
(1,237)	1:79:B:ASP:H	1:54:B:LEU:HD11	19	3.31
(1,834)	1:87:A:HIS:HD1	1:92:B:GLN:HB2	20	3.3
(1,761)	1:86:B:LYS:HD3	1:84:B:THR:H	7	3.3
(1,688)	1:86:A:LYS:HD3	1:87:A:HIS:HB2	7	3.3
(1,626)	1:83:B:MET:HE2	1:84:B:THR:HG23	20	3.3
(1,439)	1:86:B:LYS:HA	1:84:B:THR:HG21	3	3.3
(1,942)	1:79:B:ASP:H	1:75:B:LEU:O	13	3.29
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD22	15	3.29
(1,654)	1:86:A:LYS:HB2	1:84:A:THR:HG23	4	3.29
(1,439)	1:86:B:LYS:HA	1:84:B:THR:HG21	18	3.29
(1,783)	1:64:A:ALA:HB2	1:67:A:LYS:H	12	3.28
(1,628)	1:66:B:LYS:HG2	1:67:B:LYS:HB2	6	3.28
(1,942)	1:79:A:ASP:H	1:75:A:LEU:O	20	3.27
(1,833)	1:87:B:HIS:HD2	1:92:A:GLN:H	11	3.27
(1,833)	1:87:A:HIS:HD2	1:92:A:GLN:H	20	3.27
(1,789)	1:66:B:LYS:HA	1:69:B:SER:HG	14	3.27
(1,691)	1:87:A:HIS:HD2	1:71:A:ARG:HD2	3	3.27
(1,783)	1:64:B:ALA:HB2	1:67:B:LYS:H	11	3.26
(1,688)	1:86:A:LYS:HD3	1:87:A:HIS:HB2	20	3.26
(1,654)	1:86:A:LYS:HB2	1:84:A:THR:HG21	7	3.26
(1,654)	1:86:A:LYS:HB2	1:84:A:THR:HG23	9	3.26
(1,654)	1:86:B:LYS:HB2	1:84:B:THR:HG21	12	3.26
(1,654)	1:86:B:LYS:HB2	1:84:B:THR:HG21	16	3.26
(1,626)	1:83:B:MET:HE2	1:84:B:THR:HG23	14	3.26
(1,451)	1:81:A:LEU:HA	1:56:B:GLN:HG3	14	3.26
(1,439)	1:86:B:LYS:HA	1:84:B:THR:HG22	11	3.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,942)	1:79:B:ASP:H	1:75:B:LEU:O	9	3.25
(1,942)	1:79:A:ASP:H	1:75:A:LEU:O	11	3.25
(1,929)	1:71:A:ARG:N	1:67:A:LYS:O	3	3.25
(1,833)	1:87:A:HIS:HD1	1:92:A:GLN:H	17	3.25
(1,816)	1:60:B:LEU:HD21	1:86:A:LYS:H	10	3.25
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD22	20	3.25
(1,628)	1:66:B:LYS:HG2	1:67:B:LYS:HB2	7	3.25
(1,628)	1:66:B:LYS:HG2	1:67:B:LYS:HB2	10	3.25
(1,837)	1:87:A:HIS:HD2	1:93:A:ARG:H	7	3.24
(1,761)	1:86:B:LYS:HD3	1:84:B:THR:H	14	3.24
(1,688)	1:86:A:LYS:HD3	1:87:A:HIS:HB2	9	3.24
(1,680)	1:66:B:LYS:HG2	1:67:B:LYS:HG3	15	3.24
(1,628)	1:66:B:LYS:HG2	1:67:B:LYS:HB2	15	3.24
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD22	6	3.23
(1,783)	1:64:A:ALA:HB3	1:67:A:LYS:H	2	3.23
(1,654)	1:86:A:LYS:HB2	1:84:A:THR:HG21	1	3.23
(1,603)	1:64:B:ALA:HB2	1:67:B:LYS:HG2	8	3.23
(1,439)	1:86:B:LYS:HA	1:84:B:THR:HG21	12	3.23
(1,224)	1:81:B:LEU:HB3	1:56:A:GLN:HE21	1	3.23
(1,628)	1:66:B:LYS:HG2	1:67:B:LYS:HB2	19	3.22
(1,564)	1:66:B:LYS:HA	1:69:B:SER:HB3	18	3.22
(1,308)	1:90:B:ASN:H	1:65:B:LEU:HG	19	3.22
(1,837)	1:87:B:HIS:HD2	1:93:B:ARG:H	13	3.21
(1,833)	1:87:B:HIS:HD2	1:92:B:GLN:H	9	3.21
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD22	18	3.21
(1,746)	1:87:B:HIS:HD1	1:92:A:GLN:H	5	3.21
(1,654)	1:86:B:LYS:HB2	1:84:B:THR:HG22	19	3.21
(1,439)	1:86:B:LYS:HA	1:84:B:THR:HG21	16	3.21
(1,176)	1:75:B:LEU:HA	1:78:B:ALA:H	3	3.21
(1,942)	1:79:A:ASP:H	1:75:A:LEU:O	4	3.2
(1,821)	1:86:A:LYS:HG2	1:83:A:MET:HG3	4	3.2
(1,817)	1:60:A:LEU:HD11	1:88:B:LEU:HB2	12	3.2
(1,816)	1:60:B:LEU:HD23	1:86:A:LYS:H	16	3.2
(1,813)	1:85:B:VAL:H	1:60:A:LEU:HD11	5	3.2
(1,654)	1:86:A:LYS:HB2	1:84:A:THR:HG22	15	3.2
(1,649)	1:71:A:ARG:HG2	1:75:A:LEU:HD13	8	3.2
(1,602)	1:64:A:ALA:HB2	1:67:A:LYS:HG3	12	3.2
(1,943)	1:79:B:ASP:N	1:75:B:LEU:O	7	3.19
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD23	1	3.19
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD21	4	3.19
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD11	11	3.19
(1,627)	1:66:B:LYS:HG2	1:67:B:LYS:HG2	13	3.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,176)	1:75:A:LEU:HA	1:78:A:ALA:H	7	3.19
(1,942)	1:79:B:ASP:H	1:75:B:LEU:O	3	3.18
(1,837)	1:87:A:HIS:HD1	1:93:A:ARG:H	8	3.18
(1,821)	1:86:A:LYS:HG2	1:83:A:MET:HG3	18	3.18
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD13	3	3.18
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD11	9	3.18
(1,688)	1:86:A:LYS:HD3	1:87:A:HIS:HB2	1	3.18
(1,585)	1:64:B:ALA:HB1	1:67:B:LYS:HG3	2	3.18
(1,439)	1:86:A:LYS:HA	1:84:A:THR:HG22	5	3.18
(1,813)	1:85:A:VAL:H	1:60:B:LEU:HD13	13	3.17
(1,688)	1:86:B:LYS:HD3	1:87:B:HIS:HB2	17	3.17
(1,688)	1:86:A:LYS:HD3	1:87:A:HIS:HB2	18	3.17
(1,647)	1:90:A:ASN:HB2	1:65:A:LEU:HD11	13	3.17
(1,439)	1:86:B:LYS:HA	1:84:B:THR:HG21	13	3.17
(1,833)	1:87:B:HIS:HD2	1:92:A:GLN:H	1	3.16
(1,816)	1:60:B:LEU:HD22	1:86:A:LYS:H	15	3.16
(1,816)	1:60:B:LEU:HD22	1:86:A:LYS:H	20	3.16
(1,628)	1:66:B:LYS:HG2	1:67:B:LYS:HB2	4	3.16
(1,585)	1:64:A:ALA:HB1	1:67:A:LYS:HG3	13	3.16
(1,439)	1:86:A:LYS:HA	1:84:A:THR:HG22	15	3.16
(1,176)	1:75:A:LEU:HA	1:78:A:ALA:H	6	3.16
(1,942)	1:79:A:ASP:H	1:75:A:LEU:O	16	3.15
(1,942)	1:79:B:ASP:H	1:75:B:LEU:O	17	3.15
(1,176)	1:75:B:LEU:HA	1:78:B:ALA:H	18	3.15
(1,785)	1:64:B:ALA:HB2	1:67:B:LYS:HG3	8	3.14
(1,774)	1:86:A:LYS:HD3	1:88:A:LEU:H	19	3.14
(1,680)	1:66:B:LYS:HG2	1:67:B:LYS:HG3	7	3.14
(1,224)	1:81:B:LEU:HB3	1:56:A:GLN:HE21	14	3.14
(1,942)	1:79:B:ASP:H	1:75:B:LEU:O	10	3.13
(1,942)	1:79:B:ASP:H	1:75:B:LEU:O	14	3.13
(1,833)	1:87:B:HIS:HD1	1:92:A:GLN:H	12	3.13
(1,816)	1:60:B:LEU:HD21	1:86:A:LYS:H	7	3.13
(1,783)	1:64:B:ALA:HB2	1:67:B:LYS:H	6	3.13
(1,761)	1:86:B:LYS:HD3	1:84:B:THR:H	17	3.13
(1,654)	1:86:A:LYS:HB2	1:84:A:THR:HG23	2	3.13
(1,654)	1:86:B:LYS:HB2	1:84:B:THR:HG22	17	3.13
(1,627)	1:66:B:LYS:HG2	1:67:B:LYS:HG2	1	3.13
(1,627)	1:66:B:LYS:HG2	1:67:B:LYS:HG2	11	3.13
(1,817)	1:60:B:LEU:HD23	1:88:A:LEU:HB2	2	3.12
(1,680)	1:66:A:LYS:HG2	1:67:A:LYS:HG3	17	3.12
(1,649)	1:71:B:ARG:HG2	1:75:B:LEU:HD13	14	3.12
(1,628)	1:66:B:LYS:HG2	1:67:B:LYS:HB2	11	3.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:86:B:LYS:HA	1:84:B:THR:HG22	8	3.12
(1,942)	1:79:A:ASP:H	1:75:A:LEU:O	15	3.11
(1,837)	1:87:B:HIS:HD1	1:93:B:ARG:H	10	3.11
(1,833)	1:87:B:HIS:HD1	1:92:B:GLN:H	18	3.11
(1,585)	1:64:B:ALA:HB1	1:67:B:LYS:HG3	7	3.11
(1,439)	1:86:A:LYS:HA	1:84:A:THR:HG21	1	3.11
(1,439)	1:86:A:LYS:HA	1:84:A:THR:HG21	7	3.11
(1,224)	1:81:A:LEU:HB3	1:56:B:GLN:HE21	2	3.11
(1,176)	1:75:B:LEU:HA	1:78:B:ALA:H	1	3.11
(1,942)	1:79:A:ASP:H	1:75:A:LEU:O	5	3.1
(1,688)	1:86:A:LYS:HD3	1:87:A:HIS:HB2	8	3.1
(1,439)	1:86:A:LYS:HA	1:84:A:THR:HG23	4	3.1
(1,176)	1:75:B:LEU:HA	1:78:B:ALA:H	8	3.1
(1,176)	1:75:B:LEU:HA	1:78:B:ALA:H	17	3.1
(1,942)	1:79:A:ASP:H	1:75:A:LEU:O	18	3.09
(1,817)	1:60:A:LEU:HD11	1:88:B:LEU:HB2	18	3.09
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD21	8	3.09
(1,654)	1:86:B:LYS:HB2	1:84:B:THR:HG21	13	3.09
(1,654)	1:86:B:LYS:HB2	1:84:B:THR:HG21	14	3.09
(1,654)	1:86:A:LYS:HB2	1:84:A:THR:HG23	18	3.09
(1,628)	1:66:A:LYS:HG2	1:67:A:LYS:HB2	12	3.09
(1,176)	1:75:A:LEU:HA	1:78:A:ALA:H	12	3.09
(1,176)	1:75:A:LEU:HA	1:78:A:ALA:H	15	3.09
(1,943)	1:79:A:ASP:N	1:75:A:LEU:O	20	3.08
(1,837)	1:87:B:HIS:HD2	1:93:B:ARG:H	4	3.08
(1,821)	1:86:A:LYS:HG2	1:83:A:MET:HG3	8	3.08
(1,654)	1:86:A:LYS:HB2	1:84:A:THR:HG23	10	3.08
(1,821)	1:86:B:LYS:HG2	1:83:B:MET:HG3	5	3.07
(1,817)	1:60:B:LEU:HD12	1:88:A:LEU:HB2	19	3.07
(1,783)	1:64:A:ALA:HB1	1:67:A:LYS:H	5	3.07
(1,680)	1:66:B:LYS:HG2	1:67:B:LYS:HG3	3	3.07
(1,585)	1:64:B:ALA:HB1	1:67:B:LYS:HG3	16	3.07
(1,408)	1:64:A:ALA:HA	1:67:A:LYS:HG2	9	3.07
(1,176)	1:75:B:LEU:HA	1:78:B:ALA:H	20	3.07
(1,943)	1:79:B:ASP:N	1:75:B:LEU:O	13	3.06
(1,816)	1:60:B:LEU:HD23	1:86:A:LYS:H	1	3.06
(1,680)	1:66:B:LYS:HG2	1:67:B:LYS:HG3	18	3.06
(1,439)	1:86:A:LYS:HA	1:84:A:THR:HG22	17	3.06
(1,415)	1:86:A:LYS:HD3	1:84:A:THR:HB	10	3.06
(1,943)	1:79:B:ASP:N	1:75:B:LEU:O	3	3.05
(1,943)	1:79:B:ASP:N	1:75:B:LEU:O	9	3.05
(1,942)	1:79:A:ASP:H	1:75:A:LEU:O	8	3.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,813)	1:85:B:VAL:H	1:60:A:LEU:HD11	17	3.05
(1,785)	1:64:A:ALA:HB2	1:67:A:LYS:HG3	7	3.05
(1,785)	1:64:A:ALA:HB1	1:67:A:LYS:HG3	9	3.05
(1,654)	1:86:A:LYS:HB2	1:84:A:THR:HG23	8	3.05
(1,628)	1:66:B:LYS:HG2	1:67:B:LYS:HB2	5	3.05
(1,602)	1:64:B:ALA:HB2	1:67:B:LYS:HG3	6	3.05
(1,439)	1:86:B:LYS:HA	1:84:B:THR:HG21	14	3.05
(1,237)	1:79:A:ASP:H	1:54:A:LEU:HD11	4	3.05
(1,833)	1:87:A:HIS:HD2	1:92:A:GLN:H	16	3.04
(1,680)	1:66:A:LYS:HG2	1:67:A:LYS:HG3	10	3.04
(1,439)	1:86:A:LYS:HA	1:84:A:THR:HG23	9	3.04
(1,404)	1:64:B:ALA:HA	1:67:B:LYS:H	5	3.04
(1,176)	1:75:A:LEU:HA	1:78:A:ALA:H	5	3.04
(1,176)	1:75:A:LEU:HA	1:78:A:ALA:H	11	3.04
(1,943)	1:79:A:ASP:N	1:75:A:LEU:O	11	3.03
(1,942)	1:79:A:ASP:H	1:75:A:LEU:O	19	3.03
(1,837)	1:87:B:HIS:HD1	1:93:B:ARG:H	19	3.03
(1,816)	1:60:B:LEU:HD21	1:86:A:LYS:H	12	3.03
(1,783)	1:64:A:ALA:HB3	1:67:A:LYS:H	19	3.03
(1,774)	1:86:A:LYS:HD3	1:88:A:LEU:H	3	3.03
(1,774)	1:86:B:LYS:HD3	1:88:B:LEU:H	4	3.03
(1,680)	1:66:B:LYS:HG2	1:67:B:LYS:HG3	16	3.03
(1,628)	1:66:A:LYS:HG2	1:67:A:LYS:HB2	1	3.03
(1,585)	1:64:A:ALA:HB1	1:67:A:LYS:HG3	6	3.03
(1,564)	1:66:B:LYS:HA	1:69:B:SER:HB3	2	3.03
(1,821)	1:86:B:LYS:HG2	1:83:B:MET:HG3	16	3.02
(1,785)	1:64:A:ALA:HB3	1:67:A:LYS:HG3	14	3.02
(1,649)	1:71:A:ARG:HG2	1:75:A:LEU:HD11	18	3.02
(1,628)	1:66:A:LYS:HG2	1:67:A:LYS:HB2	2	3.02
(1,783)	1:64:A:ALA:HB3	1:67:A:LYS:H	3	3.01
(1,783)	1:64:A:ALA:HB1	1:67:A:LYS:H	9	3.01
(1,783)	1:64:A:ALA:HB2	1:67:A:LYS:H	15	3.01
(1,783)	1:64:A:ALA:HB1	1:67:A:LYS:H	16	3.01
(1,783)	1:64:B:ALA:HB1	1:67:B:LYS:H	20	3.01
(1,574)	1:64:B:ALA:HB2	1:65:B:LEU:HD23	16	3.01
(1,176)	1:75:B:LEU:HA	1:78:B:ALA:H	4	3.01
(1,176)	1:75:A:LEU:HA	1:78:A:ALA:H	16	3.01
(1,938)	1:76:B:GLU:N	1:72:B:HIS:O	6	3.0
(1,267)	1:86:B:LYS:H	1:61:B:ILE:HG13	19	3.0
(1,942)	1:79:A:ASP:H	1:75:A:LEU:O	12	2.99
(1,821)	1:86:A:LYS:HG2	1:83:A:MET:HG3	2	2.99
(1,774)	1:86:B:LYS:HD3	1:88:B:LEU:H	15	2.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,761)	1:86:B:LYS:HD3	1:84:B:THR:H	13	2.99
(1,628)	1:66:A:LYS:HG2	1:67:A:LYS:HB2	16	2.99
(1,627)	1:66:A:LYS:HG2	1:67:A:LYS:HG2	14	2.99
(1,439)	1:86:A:LYS:HA	1:84:A:THR:HG21	6	2.99
(1,431)	1:71:A:ARG:HG2	1:75:A:LEU:HA	6	2.99
(1,267)	1:86:A:LYS:H	1:61:A:ILE:HG13	20	2.99
(1,176)	1:75:A:LEU:HA	1:78:A:ALA:H	2	2.99
(1,943)	1:79:A:ASP:N	1:75:A:LEU:O	16	2.98
(1,943)	1:79:A:ASP:N	1:75:A:LEU:O	17	2.98
(1,938)	1:76:B:GLU:N	1:72:B:HIS:O	7	2.98
(1,789)	1:66:B:LYS:HA	1:69:B:SER:HG	9	2.98
(1,783)	1:64:A:ALA:HB1	1:67:A:LYS:H	10	2.98
(1,628)	1:66:A:LYS:HG2	1:67:A:LYS:HB2	8	2.98
(1,574)	1:64:B:ALA:HB2	1:65:B:LEU:HD23	20	2.98
(1,833)	1:87:A:HIS:HD2	1:92:A:GLN:H	2	2.97
(1,680)	1:66:B:LYS:HG2	1:67:B:LYS:HG3	8	2.97
(1,224)	1:81:A:LEU:HB3	1:56:B:GLN:HE21	9	2.97
(1,176)	1:75:B:LEU:HA	1:78:B:ALA:H	10	2.97
(1,176)	1:75:B:LEU:HA	1:78:B:ALA:H	13	2.97
(1,942)	1:79:A:ASP:H	1:75:A:LEU:O	1	2.96
(1,833)	1:87:B:HIS:HD2	1:92:B:GLN:H	13	2.96
(1,816)	1:60:B:LEU:HD21	1:86:A:LYS:H	8	2.96
(1,783)	1:64:B:ALA:HB1	1:67:B:LYS:H	4	2.96
(1,774)	1:86:B:LYS:HD3	1:88:B:LEU:H	11	2.96
(1,680)	1:66:B:LYS:HG2	1:67:B:LYS:HG3	19	2.96
(1,627)	1:66:A:LYS:HG2	1:67:A:LYS:HG2	4	2.96
(1,585)	1:64:A:ALA:HB1	1:67:A:LYS:HG3	5	2.96
(1,943)	1:79:A:ASP:N	1:75:A:LEU:O	4	2.95
(1,942)	1:79:B:ASP:H	1:75:B:LEU:O	2	2.95
(1,688)	1:86:B:LYS:HD3	1:87:B:HIS:HB2	13	2.95
(1,680)	1:66:A:LYS:HG2	1:67:A:LYS:HG3	12	2.95
(1,585)	1:64:A:ALA:HB1	1:67:A:LYS:HG3	1	2.95
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD21	10	2.94
(1,680)	1:66:B:LYS:HG2	1:67:B:LYS:HG3	2	2.94
(1,602)	1:64:B:ALA:HB2	1:67:B:LYS:HG3	11	2.94
(1,943)	1:79:A:ASP:N	1:75:A:LEU:O	5	2.93
(1,938)	1:76:A:GLU:N	1:72:A:HIS:O	5	2.93
(1,817)	1:60:A:LEU:HD11	1:88:B:LEU:HB2	7	2.93
(1,647)	1:90:A:ASN:HB2	1:65:A:LEU:HD11	12	2.93
(1,404)	1:64:A:ALA:HA	1:67:A:LYS:H	12	2.93
(1,943)	1:79:A:ASP:N	1:75:A:LEU:O	18	2.92
(1,942)	1:79:B:ASP:H	1:75:B:LEU:O	6	2.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,943)	1:79:B:ASP:N	1:75:B:LEU:O	14	2.91
(1,816)	1:60:B:LEU:HD22	1:86:A:LYS:H	6	2.91
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD22	19	2.91
(1,259)	1:56:A:GLN:HG3	1:82:B:GLU:H	10	2.91
(1,943)	1:79:B:ASP:N	1:75:B:LEU:O	10	2.9
(1,833)	1:87:B:HIS:HD2	1:92:B:GLN:H	4	2.9
(1,833)	1:87:A:HIS:HD2	1:92:A:GLN:H	7	2.9
(1,816)	1:60:B:LEU:HD22	1:86:A:LYS:H	18	2.9
(1,700)	1:87:B:HIS:HD1	1:91:B:LEU:HA	5	2.9
(1,564)	1:66:A:LYS:HA	1:69:A:SER:HB2	4	2.9
(1,267)	1:86:A:LYS:H	1:61:A:ILE:HG13	18	2.9
(1,224)	1:81:A:LEU:HB2	1:56:B:GLN:HE21	19	2.9
(1,783)	1:64:B:ALA:HB1	1:67:B:LYS:H	17	2.89
(1,569)	1:87:B:HIS:HA	1:92:A:GLN:HE21	3	2.89
(1,943)	1:79:A:ASP:N	1:75:A:LEU:O	8	2.88
(1,943)	1:79:A:ASP:N	1:75:A:LEU:O	15	2.88
(1,649)	1:71:A:ARG:HG2	1:75:A:LEU:HD13	7	2.88
(1,626)	1:83:A:MET:HE1	1:84:A:THR:HG21	17	2.88
(1,408)	1:64:A:ALA:HA	1:67:A:LYS:HG2	2	2.88
(1,816)	1:60:B:LEU:HD21	1:86:A:LYS:H	4	2.87
(1,783)	1:64:A:ALA:HB1	1:67:A:LYS:H	13	2.87
(1,176)	1:75:B:LEU:HA	1:78:B:ALA:H	14	2.87
(1,761)	1:86:B:LYS:HD3	1:84:B:THR:H	3	2.86
(1,746)	1:87:B:HIS:HD1	1:92:A:GLN:H	3	2.86
(1,835)	1:87:A:HIS:HD1	1:67:A:LYS:HD2	5	2.85
(1,761)	1:86:B:LYS:HD3	1:84:B:THR:H	8	2.85
(1,628)	1:66:A:LYS:HG2	1:67:A:LYS:HB2	3	2.85
(1,602)	1:64:A:ALA:HB2	1:67:A:LYS:HG3	15	2.85
(1,176)	1:75:B:LEU:HA	1:78:B:ALA:H	19	2.85
(1,837)	1:87:B:HIS:HD2	1:93:B:ARG:H	15	2.84
(1,669)	1:88:B:LEU:HB3	1:91:B:LEU:HG	19	2.84
(1,817)	1:60:B:LEU:HD13	1:88:A:LEU:HB2	10	2.83
(1,789)	1:66:B:LYS:HA	1:69:B:SER:HG	10	2.83
(1,761)	1:86:B:LYS:HD3	1:84:B:THR:H	18	2.83
(1,649)	1:71:B:ARG:HG2	1:75:B:LEU:HD13	6	2.83
(1,647)	1:90:A:ASN:HB2	1:65:A:LEU:HD11	15	2.83
(1,938)	1:76:A:GLU:N	1:72:A:HIS:O	15	2.82
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD21	14	2.82
(1,647)	1:90:B:ASN:HB2	1:65:B:LEU:HD11	11	2.82
(1,404)	1:64:B:ALA:HA	1:67:B:LYS:H	17	2.82
(1,943)	1:79:A:ASP:N	1:75:A:LEU:O	19	2.81
(1,817)	1:60:A:LEU:HD11	1:88:B:LEU:HB2	4	2.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,628)	1:66:A:LYS:HG2	1:67:A:LYS:HB2	14	2.81
(1,603)	1:64:B:ALA:HB2	1:67:B:LYS:HG2	10	2.81
(1,938)	1:76:B:GLU:N	1:72:B:HIS:O	13	2.8
(1,837)	1:87:A:HIS:HD2	1:93:A:ARG:H	6	2.8
(1,833)	1:87:A:HIS:HD1	1:92:A:GLN:H	8	2.8
(1,832)	1:87:B:HIS:HD1	1:91:B:LEU:HA	14	2.8
(1,761)	1:86:B:LYS:HD3	1:84:B:THR:H	1	2.8
(1,761)	1:86:A:LYS:HD3	1:84:A:THR:H	12	2.8
(1,404)	1:64:B:ALA:HA	1:67:B:LYS:H	9	2.8
(1,267)	1:86:A:LYS:H	1:61:A:ILE:HG13	2	2.8
(1,267)	1:86:B:LYS:H	1:61:B:ILE:HG13	3	2.8
(1,41)	1:67:B:LYS:HG3	1:69:B:SER:H	11	2.8
(1,943)	1:79:A:ASP:N	1:75:A:LEU:O	1	2.79
(1,938)	1:76:A:GLU:N	1:72:A:HIS:O	9	2.79
(1,858)	1:93:A:ARG:HB3	1:95:A:GLN:HB2	14	2.79
(1,835)	1:87:A:HIS:HD1	1:67:A:LYS:HD2	19	2.79
(1,761)	1:86:B:LYS:HD3	1:84:B:THR:H	4	2.79
(1,761)	1:86:A:LYS:HD3	1:84:A:THR:H	11	2.79
(1,731)	1:86:A:LYS:HD3	1:87:A:HIS:HA	4	2.79
(1,731)	1:86:B:LYS:HD3	1:87:B:HIS:HA	11	2.79
(1,700)	1:87:B:HIS:HD1	1:91:B:LEU:HA	13	2.79
(1,628)	1:66:B:LYS:HG2	1:67:B:LYS:HB2	20	2.79
(1,585)	1:64:B:ALA:HB1	1:67:B:LYS:HG3	20	2.79
(1,308)	1:90:B:ASN:H	1:65:B:LEU:HG	10	2.79
(1,943)	1:79:A:ASP:N	1:75:A:LEU:O	12	2.78
(1,783)	1:64:A:ALA:HB2	1:67:A:LYS:H	18	2.78
(1,569)	1:87:B:HIS:HA	1:92:A:GLN:HE21	9	2.78
(1,404)	1:64:A:ALA:HA	1:67:A:LYS:H	2	2.78
(1,943)	1:79:B:ASP:N	1:75:B:LEU:O	2	2.77
(1,938)	1:76:B:GLU:N	1:72:B:HIS:O	10	2.77
(1,783)	1:64:A:ALA:HB1	1:67:A:LYS:H	1	2.77
(1,680)	1:66:B:LYS:HG2	1:67:B:LYS:HG3	20	2.77
(1,569)	1:87:A:HIS:HA	1:92:B:GLN:HE21	15	2.77
(1,259)	1:56:B:GLN:HG3	1:82:A:GLU:H	5	2.77
(1,404)	1:64:A:ALA:HA	1:67:A:LYS:H	15	2.76
(1,41)	1:67:B:LYS:HG3	1:69:B:SER:H	13	2.76
(1,943)	1:79:B:ASP:N	1:75:B:LEU:O	6	2.75
(1,858)	1:93:A:ARG:HB3	1:95:A:GLN:HB2	11	2.75
(1,816)	1:60:B:LEU:HD22	1:86:A:LYS:H	19	2.75
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD23	2	2.75
(1,585)	1:64:B:ALA:HB1	1:67:B:LYS:HG3	4	2.75
(1,585)	1:64:A:ALA:HB1	1:67:A:LYS:HG3	10	2.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,938)	1:76:B:GLU:N	1:72:B:HIS:O	1	2.74
(1,938)	1:76:A:GLU:N	1:72:A:HIS:O	12	2.74
(1,833)	1:87:A:HIS:HD2	1:92:A:GLN:H	15	2.74
(1,816)	1:60:B:LEU:HD23	1:86:A:LYS:H	2	2.74
(1,789)	1:66:B:LYS:HA	1:69:B:SER:HG	12	2.74
(1,746)	1:87:B:HIS:HD1	1:92:A:GLN:H	13	2.74
(1,680)	1:66:B:LYS:HG2	1:67:B:LYS:HG3	5	2.74
(1,601)	1:64:A:ALA:HB1	1:67:A:LYS:HG2	9	2.74
(1,404)	1:64:B:ALA:HA	1:67:B:LYS:H	3	2.74
(1,267)	1:86:A:LYS:H	1:61:A:ILE:HG13	9	2.74
(1,41)	1:67:B:LYS:HG3	1:69:B:SER:H	4	2.74
(1,41)	1:67:A:LYS:HG3	1:69:A:SER:H	18	2.74
(1,783)	1:64:A:ALA:HB3	1:67:A:LYS:H	8	2.73
(1,558)	1:81:B:LEU:HA	1:83:B:MET:HE3	4	2.73
(1,267)	1:86:A:LYS:H	1:61:A:ILE:HG13	10	2.73
(1,857)	1:93:A:ARG:HB2	1:95:A:GLN:HB2	14	2.72
(1,817)	1:60:B:LEU:HD11	1:88:A:LEU:HB2	20	2.72
(1,761)	1:86:B:LYS:HD3	1:84:B:THR:H	5	2.72
(1,647)	1:90:B:ASN:HB2	1:65:B:LEU:HD11	2	2.72
(1,647)	1:90:B:ASN:HB2	1:65:B:LEU:HD13	18	2.72
(1,404)	1:64:B:ALA:HA	1:67:B:LYS:H	19	2.72
(1,41)	1:67:B:LYS:HG3	1:69:B:SER:H	20	2.72
(1,832)	1:87:A:HIS:HD1	1:91:A:LEU:HA	11	2.71
(1,649)	1:71:B:ARG:HG2	1:75:B:LEU:HD12	9	2.71
(1,573)	1:64:A:ALA:HB1	1:65:A:LEU:HD21	14	2.71
(1,569)	1:87:B:HIS:HA	1:92:A:GLN:HE21	6	2.71
(1,267)	1:86:B:LYS:H	1:61:B:ILE:HG13	14	2.71
(1,857)	1:93:B:ARG:HB2	1:95:B:GLN:HB2	4	2.7
(1,817)	1:60:B:LEU:HD13	1:88:A:LEU:HB2	14	2.7
(1,761)	1:86:B:LYS:HD3	1:84:B:THR:H	19	2.7
(1,647)	1:90:B:ASN:HB2	1:65:B:LEU:HD13	6	2.7
(1,585)	1:64:B:ALA:HB1	1:67:B:LYS:HG3	17	2.7
(1,564)	1:66:A:LYS:HA	1:69:A:SER:HB3	10	2.7
(1,564)	1:66:A:LYS:HA	1:69:A:SER:HB3	15	2.7
(1,558)	1:81:B:LEU:HA	1:83:B:MET:HE2	17	2.7
(1,41)	1:67:B:LYS:HG3	1:69:B:SER:H	7	2.7
(1,850)	1:90:B:ASN:HD22	1:83:B:MET:HG3	7	2.69
(1,816)	1:60:B:LEU:HD21	1:86:A:LYS:H	14	2.69
(1,649)	1:71:A:ARG:HG2	1:75:A:LEU:HD13	17	2.69
(1,267)	1:86:B:LYS:H	1:61:B:ILE:HG13	7	2.69
(1,41)	1:67:B:LYS:HG3	1:69:B:SER:H	3	2.69
(1,41)	1:67:A:LYS:HG3	1:69:A:SER:H	15	2.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:67:B:LYS:HG3	1:69:B:SER:H	16	2.69
(1,858)	1:93:A:ARG:HB3	1:95:A:GLN:HB2	6	2.68
(1,789)	1:66:B:LYS:HA	1:69:B:SER:HG	3	2.68
(1,761)	1:86:B:LYS:HD3	1:84:B:THR:H	2	2.68
(1,761)	1:86:A:LYS:HD3	1:84:A:THR:H	15	2.68
(1,761)	1:86:B:LYS:HD3	1:84:B:THR:H	16	2.68
(1,746)	1:87:B:HIS:HD1	1:92:B:GLN:H	14	2.68
(1,649)	1:71:B:ARG:HG2	1:75:B:LEU:HD11	4	2.68
(1,404)	1:64:B:ALA:HA	1:67:B:LYS:H	13	2.68
(1,259)	1:56:A:GLN:HG3	1:82:B:GLU:H	16	2.68
(1,850)	1:90:A:ASN:HD22	1:83:A:MET:HG3	17	2.67
(1,837)	1:87:B:HIS:HD2	1:93:B:ARG:H	5	2.67
(1,731)	1:86:A:LYS:HD3	1:87:A:HIS:HA	19	2.67
(1,408)	1:64:B:ALA:HA	1:67:B:LYS:HG2	10	2.67
(1,649)	1:71:B:ARG:HG2	1:75:B:LEU:HD12	13	2.66
(1,488)	1:64:A:ALA:HA	1:65:A:LEU:HD12	12	2.66
(1,394)	1:67:B:LYS:H	1:69:B:SER:H	8	2.66
(1,267)	1:86:B:LYS:H	1:61:B:ILE:HG13	11	2.66
(1,267)	1:86:B:LYS:H	1:61:B:ILE:HG13	12	2.66
(1,41)	1:67:B:LYS:HG3	1:69:B:SER:H	2	2.66
(1,938)	1:76:B:GLU:N	1:72:B:HIS:O	16	2.65
(1,857)	1:93:A:ARG:HB2	1:95:A:GLN:HB2	6	2.65
(1,746)	1:87:A:HIS:HD1	1:92:A:GLN:H	11	2.65
(1,731)	1:86:B:LYS:HD3	1:87:B:HIS:HA	15	2.65
(1,649)	1:71:A:ARG:HG2	1:75:A:LEU:HD13	1	2.65
(1,649)	1:71:B:ARG:HG2	1:75:B:LEU:HD13	3	2.65
(1,267)	1:86:B:LYS:H	1:61:B:ILE:HG13	16	2.65
(1,858)	1:93:B:ARG:HB3	1:95:B:GLN:HB2	17	2.64
(1,850)	1:90:A:ASN:HD21	1:83:A:MET:HG2	20	2.64
(1,774)	1:86:A:LYS:HD3	1:88:A:LEU:H	16	2.64
(1,746)	1:87:B:HIS:HD1	1:92:B:GLN:H	6	2.64
(1,573)	1:64:A:ALA:HB1	1:65:A:LEU:HD23	19	2.64
(1,41)	1:67:B:LYS:HG3	1:69:B:SER:H	5	2.64
(1,769)	1:50:B:ILE:HG21	1:79:A:ASP:H	5	2.63
(1,601)	1:64:A:ALA:HB1	1:67:A:LYS:HG2	16	2.63
(1,394)	1:67:B:LYS:H	1:69:B:SER:H	14	2.63
(1,259)	1:56:A:GLN:HG3	1:82:B:GLU:H	17	2.63
(1,41)	1:67:B:LYS:HG3	1:69:B:SER:H	12	2.63
(1,41)	1:67:A:LYS:HG3	1:69:A:SER:H	19	2.63
(1,746)	1:87:A:HIS:HD1	1:92:B:GLN:H	20	2.62
(1,41)	1:67:A:LYS:HG3	1:69:A:SER:H	14	2.62
(1,669)	1:88:A:LEU:HB3	1:91:A:LEU:HG	10	2.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:93:B:ARG:HB3	1:95:B:GLN:HB2	4	2.6
(1,649)	1:71:A:ARG:HG2	1:75:A:LEU:HD11	10	2.6
(1,649)	1:71:B:ARG:HG2	1:75:B:LEU:HD13	19	2.6
(1,583)	1:76:B:GLU:HB2	1:77:B:LYS:HG2	2	2.6
(1,267)	1:86:A:LYS:H	1:61:A:ILE:HG13	15	2.6
(1,938)	1:76:A:GLU:N	1:72:A:HIS:O	11	2.59
(1,820)	1:86:A:LYS:HG2	1:87:A:HIS:HD2	3	2.59
(1,431)	1:71:A:ARG:HG2	1:75:A:LEU:HA	11	2.59
(1,404)	1:64:B:ALA:HA	1:67:B:LYS:H	10	2.59
(1,404)	1:64:B:ALA:HA	1:67:B:LYS:H	20	2.59
(1,394)	1:67:A:LYS:H	1:69:A:SER:H	4	2.59
(1,370)	1:66:A:LYS:HA	1:69:A:SER:H	14	2.59
(1,259)	1:56:B:GLN:HG3	1:82:A:GLU:H	11	2.59
(1,65)	1:56:B:GLN:HG2	1:82:A:GLU:H	5	2.59
(1,858)	1:93:A:ARG:HB3	1:95:A:GLN:HB2	18	2.58
(1,774)	1:86:A:LYS:HD3	1:88:A:LEU:H	2	2.58
(1,774)	1:86:B:LYS:HD3	1:88:B:LEU:H	7	2.58
(1,774)	1:86:A:LYS:HD3	1:88:A:LEU:H	17	2.58
(1,769)	1:50:B:ILE:HG21	1:79:A:ASP:H	20	2.58
(1,700)	1:87:A:HIS:HD1	1:91:A:LEU:HA	7	2.58
(1,573)	1:64:B:ALA:HB1	1:65:B:LEU:HD23	11	2.58
(1,370)	1:66:B:LYS:HA	1:69:B:SER:H	8	2.58
(1,769)	1:50:B:ILE:HG21	1:79:A:ASP:H	18	2.57
(1,747)	1:87:B:HIS:HD2	1:92:A:GLN:H	14	2.57
(1,731)	1:86:A:LYS:HD3	1:87:A:HIS:HA	3	2.57
(1,370)	1:66:B:LYS:HA	1:69:B:SER:H	11	2.57
(1,370)	1:66:A:LYS:HA	1:69:A:SER:H	20	2.57
(1,267)	1:86:B:LYS:H	1:61:B:ILE:HG13	5	2.57
(1,747)	1:87:B:HIS:HD2	1:92:B:GLN:H	3	2.56
(1,649)	1:71:A:ARG:HG2	1:75:A:LEU:HD11	12	2.56
(1,628)	1:66:A:LYS:HG2	1:67:A:LYS:HB2	9	2.56
(1,394)	1:67:B:LYS:H	1:69:B:SER:H	19	2.56
(1,41)	1:67:A:LYS:HG3	1:69:A:SER:H	1	2.56
(1,938)	1:76:A:GLU:N	1:72:A:HIS:O	18	2.55
(1,858)	1:93:B:ARG:HB3	1:95:B:GLN:HB2	15	2.55
(1,583)	1:76:B:GLU:HB2	1:77:B:LYS:HG2	1	2.55
(1,259)	1:56:B:GLN:HG3	1:82:A:GLU:H	15	2.55
(1,41)	1:67:B:LYS:HG3	1:69:B:SER:H	8	2.55
(1,833)	1:87:A:HIS:HD2	1:92:A:GLN:H	6	2.54
(1,820)	1:86:A:LYS:HG2	1:87:A:HIS:HD1	14	2.54
(1,746)	1:87:A:HIS:HD1	1:92:B:GLN:H	2	2.54
(1,746)	1:87:B:HIS:HD1	1:92:A:GLN:H	9	2.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,267)	1:86:B:LYS:H	1:61:B:ILE:HG13	6	2.54
(1,267)	1:86:B:LYS:H	1:61:B:ILE:HG13	13	2.54
(1,259)	1:56:B:GLN:HG3	1:82:A:GLU:H	4	2.54
(1,857)	1:93:A:ARG:HB2	1:95:A:GLN:HB2	11	2.53
(1,820)	1:86:A:LYS:HG2	1:87:A:HIS:HD1	13	2.53
(1,747)	1:87:A:HIS:HD2	1:92:B:GLN:H	17	2.53
(1,577)	1:68:B:ASP:HB3	1:72:B:HIS:HD2	17	2.53
(1,404)	1:64:B:ALA:HA	1:67:B:LYS:H	6	2.53
(1,404)	1:64:A:ALA:HA	1:67:A:LYS:H	18	2.53
(1,41)	1:67:A:LYS:HG3	1:69:A:SER:H	6	2.53
(1,850)	1:90:B:ASN:HD22	1:83:B:MET:HG3	16	2.52
(1,774)	1:86:A:LYS:HD3	1:88:A:LEU:H	6	2.52
(1,769)	1:50:B:ILE:HG21	1:79:A:ASP:H	6	2.52
(1,558)	1:81:A:LEU:HA	1:83:A:MET:HE2	12	2.52
(1,394)	1:67:A:LYS:H	1:69:A:SER:H	15	2.52
(1,259)	1:56:B:GLN:HG3	1:82:A:GLU:H	13	2.52
(1,938)	1:76:A:GLU:N	1:72:A:HIS:O	2	2.51
(1,858)	1:93:A:ARG:HB3	1:95:A:GLN:HB2	10	2.51
(1,850)	1:90:A:ASN:HD21	1:83:A:MET:HG3	15	2.51
(1,832)	1:87:B:HIS:HD2	1:91:B:LEU:HA	3	2.51
(1,769)	1:50:B:ILE:HG23	1:79:A:ASP:H	14	2.51
(1,744)	1:66:A:LYS:HD3	1:67:A:LYS:H	17	2.51
(1,647)	1:90:B:ASN:HB2	1:65:B:LEU:HD11	14	2.51
(1,602)	1:64:A:ALA:HB2	1:67:A:LYS:HG3	18	2.51
(1,358)	1:67:B:LYS:HA	1:69:B:SER:H	8	2.51
(1,358)	1:67:B:LYS:HA	1:69:B:SER:H	18	2.51
(1,65)	1:56:B:GLN:HG2	1:82:A:GLU:H	10	2.51
(1,850)	1:90:B:ASN:HD21	1:83:B:MET:HG3	3	2.5
(1,774)	1:86:A:LYS:HD3	1:88:A:LEU:H	18	2.5
(1,744)	1:66:B:LYS:HD3	1:67:B:LYS:H	18	2.5
(1,680)	1:66:A:LYS:HG2	1:67:A:LYS:HG3	4	2.5
(1,627)	1:66:A:LYS:HG2	1:67:A:LYS:HG2	2	2.5
(1,583)	1:76:B:GLU:HB2	1:77:B:LYS:HG2	19	2.5
(1,370)	1:66:B:LYS:HA	1:69:B:SER:H	18	2.5
(1,358)	1:67:B:LYS:HA	1:69:B:SER:H	20	2.5
(1,858)	1:93:A:ARG:HB3	1:95:A:GLN:HB2	8	2.49
(1,850)	1:90:B:ASN:HD21	1:83:B:MET:HG3	1	2.49
(1,817)	1:60:B:LEU:HD12	1:88:A:LEU:HB2	13	2.49
(1,746)	1:87:B:HIS:HD1	1:92:A:GLN:H	15	2.49
(1,744)	1:66:B:LYS:HD3	1:67:B:LYS:H	15	2.49
(1,680)	1:66:B:LYS:HG2	1:67:B:LYS:HG3	6	2.49
(1,647)	1:90:A:ASN:HB2	1:65:A:LEU:HD11	9	2.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,267)	1:86:B:LYS:H	1:61:B:ILE:HG13	4	2.49
(1,267)	1:86:B:LYS:H	1:61:B:ILE:HG13	17	2.49
(1,938)	1:76:A:GLU:N	1:72:A:HIS:O	19	2.48
(1,850)	1:90:A:ASN:HD22	1:83:A:MET:HG3	4	2.48
(1,774)	1:86:A:LYS:HD3	1:88:A:LEU:H	20	2.48
(1,626)	1:83:A:MET:HE2	1:84:A:THR:HG22	16	2.48
(1,858)	1:93:B:ARG:HB3	1:95:B:GLN:HB2	16	2.47
(1,820)	1:86:A:LYS:HG2	1:87:A:HIS:HD2	5	2.47
(1,769)	1:50:B:ILE:HG23	1:79:A:ASP:H	2	2.47
(1,746)	1:87:B:HIS:HD1	1:92:B:GLN:H	1	2.47
(1,680)	1:66:B:LYS:HG2	1:67:B:LYS:HG3	13	2.47
(1,647)	1:90:B:ASN:HB2	1:65:B:LEU:HD13	3	2.47
(1,358)	1:67:A:LYS:HA	1:69:A:SER:H	19	2.47
(1,41)	1:67:A:LYS:HG3	1:69:A:SER:H	10	2.47
(1,850)	1:90:A:ASN:HD22	1:83:A:MET:HG3	5	2.46
(1,820)	1:86:A:LYS:HG2	1:87:A:HIS:HD2	12	2.46
(1,774)	1:86:A:LYS:HD3	1:88:A:LEU:H	8	2.46
(1,774)	1:86:B:LYS:HD3	1:88:B:LEU:H	12	2.46
(1,647)	1:90:B:ASN:HB2	1:65:B:LEU:HD11	1	2.46
(1,647)	1:90:B:ASN:HB2	1:65:B:LEU:HD11	7	2.46
(1,583)	1:76:A:GLU:HB2	1:77:A:LYS:HG2	3	2.46
(1,583)	1:76:A:GLU:HB2	1:77:A:LYS:HG2	20	2.46
(1,431)	1:71:A:ARG:HG2	1:75:A:LEU:HA	16	2.46
(1,370)	1:66:A:LYS:HA	1:69:A:SER:H	13	2.46
(1,358)	1:67:B:LYS:HA	1:69:B:SER:H	11	2.46
(1,358)	1:67:A:LYS:HA	1:69:A:SER:H	14	2.46
(1,850)	1:90:B:ASN:HD22	1:83:B:MET:HG3	8	2.45
(1,850)	1:90:B:ASN:HD22	1:83:B:MET:HG3	9	2.45
(1,844)	1:89:A:ARG:HB2	1:90:A:ASN:HD22	8	2.45
(1,769)	1:50:B:ILE:HG22	1:79:A:ASP:H	4	2.45
(1,574)	1:64:A:ALA:HB2	1:65:A:LEU:HD23	9	2.45
(1,267)	1:86:A:LYS:H	1:61:A:ILE:HG13	8	2.45
(1,938)	1:76:B:GLU:N	1:72:B:HIS:O	4	2.44
(1,783)	1:64:A:ALA:HB3	1:67:A:LYS:H	14	2.44
(1,769)	1:50:B:ILE:HG23	1:79:A:ASP:H	10	2.44
(1,404)	1:64:A:ALA:HA	1:67:A:LYS:H	8	2.44
(1,858)	1:93:A:ARG:HB3	1:95:A:GLN:HB2	20	2.43
(1,850)	1:90:B:ASN:HD21	1:83:B:MET:HG3	11	2.43
(1,835)	1:87:B:HIS:HD2	1:67:B:LYS:HD2	20	2.43
(1,832)	1:87:A:HIS:HD2	1:91:A:LEU:HA	20	2.43
(1,774)	1:86:A:LYS:HD3	1:88:A:LEU:H	1	2.43
(1,769)	1:50:B:ILE:HG23	1:79:A:ASP:H	7	2.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,747)	1:87:A:HIS:HD2	1:92:A:GLN:H	18	2.43
(1,583)	1:76:A:GLU:HB2	1:77:A:LYS:HG2	12	2.43
(1,583)	1:76:B:GLU:HB2	1:77:B:LYS:HG2	18	2.43
(1,404)	1:64:A:ALA:HA	1:67:A:LYS:H	4	2.43
(1,394)	1:67:B:LYS:H	1:69:B:SER:H	18	2.43
(1,850)	1:90:A:ASN:HD21	1:83:A:MET:HG3	12	2.42
(1,747)	1:87:B:HIS:HD2	1:92:A:GLN:H	11	2.42
(1,747)	1:87:B:HIS:HD2	1:92:B:GLN:H	12	2.42
(1,747)	1:87:A:HIS:HD2	1:92:A:GLN:H	20	2.42
(1,746)	1:87:B:HIS:HD1	1:92:B:GLN:H	16	2.42
(1,700)	1:87:B:HIS:HD1	1:91:B:LEU:HA	15	2.42
(1,394)	1:67:A:LYS:H	1:69:A:SER:H	1	2.42
(1,394)	1:67:A:LYS:H	1:69:A:SER:H	6	2.42
(1,394)	1:67:B:LYS:H	1:69:B:SER:H	10	2.42
(1,394)	1:67:B:LYS:H	1:69:B:SER:H	11	2.42
(1,358)	1:67:B:LYS:HA	1:69:B:SER:H	16	2.42
(1,850)	1:90:A:ASN:HD21	1:83:A:MET:HG3	14	2.41
(1,783)	1:64:A:ALA:HB2	1:67:A:LYS:H	7	2.41
(1,774)	1:86:A:LYS:HD3	1:88:A:LEU:H	9	2.41
(1,774)	1:86:B:LYS:HD3	1:88:B:LEU:H	14	2.41
(1,769)	1:50:B:ILE:HG21	1:79:A:ASP:H	11	2.41
(1,627)	1:66:A:LYS:HG2	1:67:A:LYS:HG2	9	2.41
(1,583)	1:76:A:GLU:HB2	1:77:A:LYS:HG2	5	2.41
(1,583)	1:76:A:GLU:HB2	1:77:A:LYS:HG2	16	2.41
(1,404)	1:64:A:ALA:HA	1:67:A:LYS:H	1	2.41
(1,394)	1:67:A:LYS:H	1:69:A:SER:H	20	2.41
(1,358)	1:67:B:LYS:HA	1:69:B:SER:H	3	2.41
(1,267)	1:86:A:LYS:H	1:61:A:ILE:HG13	1	2.41
(1,259)	1:56:B:GLN:HG3	1:82:A:GLU:H	18	2.41
(1,41)	1:67:A:LYS:HG3	1:69:A:SER:H	17	2.41
(1,746)	1:87:A:HIS:HD1	1:92:A:GLN:H	17	2.4
(1,431)	1:71:A:ARG:HG2	1:75:A:LEU:HA	8	2.4
(1,404)	1:64:B:ALA:HA	1:67:B:LYS:H	11	2.4
(1,370)	1:66:B:LYS:HA	1:69:B:SER:H	3	2.4
(1,358)	1:67:A:LYS:HA	1:69:A:SER:H	4	2.4
(1,259)	1:56:B:GLN:HG3	1:82:A:GLU:H	14	2.4
(1,817)	1:60:B:LEU:HD11	1:88:A:LEU:HB2	9	2.39
(1,817)	1:60:B:LEU:HD11	1:88:A:LEU:HB2	16	2.39
(1,746)	1:87:B:HIS:HD1	1:92:A:GLN:H	7	2.39
(1,583)	1:76:B:GLU:HB2	1:77:B:LYS:HG2	13	2.39
(1,564)	1:66:B:LYS:HA	1:69:B:SER:HB3	12	2.39
(1,431)	1:71:A:ARG:HG2	1:75:A:LEU:HA	20	2.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,394)	1:67:B:LYS:H	1:69:B:SER:H	13	2.39
(1,370)	1:66:A:LYS:HA	1:69:A:SER:H	19	2.39
(1,65)	1:56:B:GLN:HG2	1:82:A:GLU:H	11	2.39
(1,850)	1:90:B:ASN:HD22	1:83:B:MET:HG3	10	2.38
(1,844)	1:89:B:ARG:HB2	1:90:B:ASN:HD22	9	2.38
(1,832)	1:87:A:HIS:HD1	1:91:A:LEU:HA	1	2.38
(1,774)	1:86:A:LYS:HD3	1:88:A:LEU:H	5	2.38
(1,774)	1:86:B:LYS:HD3	1:88:B:LEU:H	13	2.38
(1,769)	1:50:B:ILE:HG23	1:79:A:ASP:H	19	2.38
(1,744)	1:66:A:LYS:HD3	1:67:A:LYS:H	2	2.38
(1,394)	1:67:B:LYS:H	1:69:B:SER:H	7	2.38
(1,761)	1:86:A:LYS:HD3	1:84:A:THR:H	10	2.37
(1,583)	1:76:B:GLU:HB2	1:77:B:LYS:HG2	10	2.37
(1,431)	1:71:B:ARG:HG2	1:75:B:LEU:HA	19	2.37
(1,408)	1:64:A:ALA:HA	1:67:A:LYS:HG2	3	2.37
(1,370)	1:66:B:LYS:HA	1:69:B:SER:H	2	2.37
(1,259)	1:56:B:GLN:HG3	1:82:A:GLU:H	1	2.37
(1,65)	1:56:B:GLN:HG2	1:82:A:GLU:H	17	2.37
(1,857)	1:93:A:ARG:HB2	1:95:A:GLN:HB2	18	2.36
(1,844)	1:89:A:ARG:HB2	1:90:A:ASN:HD22	4	2.36
(1,835)	1:87:A:HIS:HD1	1:67:A:LYS:HD2	9	2.36
(1,832)	1:87:A:HIS:HD2	1:91:A:LEU:HA	18	2.36
(1,747)	1:87:B:HIS:HD2	1:92:B:GLN:H	9	2.36
(1,744)	1:66:A:LYS:HD3	1:67:A:LYS:H	12	2.36
(1,744)	1:66:B:LYS:HD3	1:67:B:LYS:H	19	2.36
(1,647)	1:90:B:ASN:HB2	1:65:B:LEU:HD11	17	2.36
(1,488)	1:64:B:ALA:HA	1:65:B:LEU:HD13	17	2.36
(1,431)	1:71:A:ARG:HG2	1:75:A:LEU:HA	4	2.36
(1,431)	1:71:B:ARG:HG2	1:75:B:LEU:HA	5	2.36
(1,420)	1:87:B:HIS:HD2	1:91:B:LEU:HA	14	2.36
(1,358)	1:67:B:LYS:HA	1:69:B:SER:H	5	2.36
(1,358)	1:67:A:LYS:HA	1:69:A:SER:H	7	2.36
(1,858)	1:93:B:ARG:HB3	1:95:B:GLN:HB2	3	2.35
(1,844)	1:89:A:ARG:HB2	1:90:A:ASN:HD22	11	2.35
(1,844)	1:89:B:ARG:HB2	1:90:B:ASN:HD22	15	2.35
(1,844)	1:89:A:ARG:HB2	1:90:A:ASN:HD22	16	2.35
(1,832)	1:87:A:HIS:HD2	1:91:A:LEU:HA	16	2.35
(1,769)	1:50:A:ILE:HG21	1:79:B:ASP:H	13	2.35
(1,680)	1:66:B:LYS:HG2	1:67:B:LYS:HG3	11	2.35
(1,569)	1:87:B:HIS:HA	1:92:A:GLN:HE21	8	2.35
(1,564)	1:66:A:LYS:HA	1:69:A:SER:HB3	9	2.35
(1,394)	1:67:B:LYS:H	1:69:B:SER:H	3	2.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,358)	1:67:A:LYS:HA	1:69:A:SER:H	15	2.35
(1,936)	1:75:B:LEU:H	1:71:B:ARG:O	20	2.34
(1,820)	1:86:A:LYS:HG2	1:87:A:HIS:HD1	19	2.34
(1,769)	1:50:B:ILE:HG23	1:79:A:ASP:H	1	2.34
(1,649)	1:71:A:ARG:HG2	1:75:A:LEU:HD12	15	2.34
(1,583)	1:76:A:GLU:HB2	1:77:A:LYS:HG2	17	2.34
(1,408)	1:64:A:ALA:HA	1:67:A:LYS:HG2	16	2.34
(1,394)	1:67:B:LYS:H	1:69:B:SER:H	2	2.34
(1,259)	1:56:A:GLN:HG3	1:82:B:GLU:H	12	2.34
(1,938)	1:76:B:GLU:N	1:72:B:HIS:O	14	2.33
(1,833)	1:87:B:HIS:HD2	1:92:B:GLN:H	5	2.33
(1,832)	1:87:B:HIS:HD2	1:91:B:LEU:HA	9	2.33
(1,820)	1:86:B:LYS:HG2	1:87:B:HIS:HD1	20	2.33
(1,769)	1:50:B:ILE:HG22	1:79:A:ASP:H	17	2.33
(1,764)	1:86:B:LYS:HG2	1:90:B:ASN:H	10	2.33
(1,583)	1:76:B:GLU:HB2	1:77:B:LYS:HG2	4	2.33
(1,358)	1:67:A:LYS:HA	1:69:A:SER:H	6	2.33
(1,358)	1:67:A:LYS:HA	1:69:A:SER:H	13	2.33
(1,259)	1:56:A:GLN:HG3	1:82:B:GLU:H	7	2.33
(1,850)	1:90:A:ASN:HD22	1:83:A:MET:HG3	2	2.32
(1,558)	1:81:B:LEU:HA	1:83:B:MET:HE3	11	2.32
(1,404)	1:64:A:ALA:HA	1:67:A:LYS:H	7	2.32
(1,370)	1:66:B:LYS:HA	1:69:B:SER:H	16	2.32
(1,65)	1:56:B:GLN:HG2	1:82:A:GLU:H	4	2.32
(1,65)	1:56:A:GLN:HG2	1:82:B:GLU:H	16	2.32
(1,832)	1:87:B:HIS:HD2	1:91:B:LEU:HA	12	2.31
(1,803)	1:57:B:LEU:HD11	1:83:B:MET:H	10	2.31
(1,769)	1:50:B:ILE:HG21	1:79:A:ASP:H	8	2.31
(1,764)	1:86:B:LYS:HG2	1:90:B:ASN:H	11	2.31
(1,747)	1:87:B:HIS:HD2	1:92:A:GLN:H	1	2.31
(1,744)	1:66:A:LYS:HD3	1:67:A:LYS:H	8	2.31
(1,680)	1:66:B:LYS:HG2	1:67:B:LYS:HG3	1	2.31
(1,370)	1:66:A:LYS:HA	1:69:A:SER:H	7	2.31
(1,744)	1:66:B:LYS:HD3	1:67:B:LYS:H	5	2.3
(1,744)	1:66:B:LYS:HD3	1:67:B:LYS:H	20	2.3
(1,602)	1:64:B:ALA:HB2	1:67:B:LYS:HG3	8	2.3
(1,437)	1:90:B:ASN:HA	1:92:B:GLN:HG2	5	2.3
(1,431)	1:71:B:ARG:HG2	1:75:B:LEU:HA	1	2.3
(1,394)	1:67:B:LYS:H	1:69:B:SER:H	16	2.3
(1,259)	1:56:A:GLN:HG3	1:82:B:GLU:H	20	2.3
(1,627)	1:66:A:LYS:HG2	1:67:A:LYS:HG2	8	2.29
(1,583)	1:76:B:GLU:HB2	1:77:B:LYS:HG2	9	2.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,583)	1:76:B:GLU:HB2	1:77:B:LYS:HG2	11	2.29
(1,404)	1:64:A:ALA:HA	1:67:A:LYS:H	14	2.29
(1,394)	1:67:B:LYS:H	1:69:B:SER:H	5	2.29
(1,358)	1:67:B:LYS:HA	1:69:B:SER:H	2	2.29
(1,358)	1:67:B:LYS:HA	1:69:B:SER:H	12	2.29
(1,746)	1:87:B:HIS:HD1	1:92:A:GLN:H	12	2.28
(1,669)	1:88:A:LEU:HB3	1:91:A:LEU:HG	15	2.28
(1,583)	1:76:A:GLU:HB2	1:77:A:LYS:HG2	6	2.28
(1,574)	1:64:B:ALA:HB2	1:65:B:LEU:HD23	1	2.28
(1,450)	1:56:A:GLN:HG3	1:84:B:THR:HB	10	2.28
(1,420)	1:87:B:HIS:HD2	1:91:B:LEU:HA	1	2.28
(1,259)	1:56:B:GLN:HG3	1:82:A:GLU:H	9	2.28
(1,844)	1:89:B:ARG:HB2	1:90:B:ASN:HD22	6	2.27
(1,769)	1:50:B:ILE:HG21	1:79:A:ASP:H	9	2.27
(1,647)	1:90:B:ASN:HB2	1:65:B:LEU:HD11	20	2.27
(1,583)	1:76:B:GLU:HB2	1:77:B:LYS:HG2	8	2.27
(1,558)	1:81:B:LEU:HA	1:83:B:MET:HE2	16	2.27
(1,404)	1:64:A:ALA:HA	1:67:A:LYS:H	16	2.27
(1,844)	1:89:A:ARG:HB2	1:90:A:ASN:HD22	2	2.26
(1,832)	1:87:A:HIS:HD1	1:91:A:LEU:HA	17	2.26
(1,789)	1:66:A:LYS:HA	1:69:A:SER:HG	19	2.26
(1,769)	1:50:B:ILE:HG21	1:79:A:ASP:H	3	2.26
(1,746)	1:87:B:HIS:HD1	1:92:B:GLN:H	18	2.26
(1,450)	1:56:A:GLN:HG3	1:84:B:THR:HB	16	2.26
(1,358)	1:67:A:LYS:HA	1:69:A:SER:H	1	2.26
(1,844)	1:89:A:ARG:HB2	1:90:A:ASN:HD22	17	2.25
(1,769)	1:50:B:ILE:HG21	1:79:A:ASP:H	15	2.25
(1,450)	1:56:B:GLN:HG3	1:84:A:THR:HB	5	2.25
(1,437)	1:90:B:ASN:HA	1:92:B:GLN:HG2	20	2.25
(1,431)	1:71:A:ARG:HG2	1:75:A:LEU:HA	15	2.25
(1,259)	1:56:B:GLN:HG3	1:82:A:GLU:H	6	2.25
(1,65)	1:56:B:GLN:HG2	1:82:A:GLU:H	19	2.25
(1,858)	1:93:B:ARG:HB3	1:95:B:GLN:HB2	7	2.24
(1,803)	1:57:B:LEU:HD13	1:83:B:MET:H	14	2.24
(1,583)	1:76:B:GLU:HB2	1:77:B:LYS:HG2	14	2.24
(1,577)	1:68:A:ASP:HB3	1:72:A:HIS:HD2	8	2.24
(1,270)	1:79:B:ASP:H	1:54:B:LEU:HD21	14	2.24
(1,259)	1:56:A:GLN:HG3	1:82:B:GLU:H	2	2.24
(1,65)	1:56:A:GLN:HG2	1:82:B:GLU:H	7	2.24
(1,843)	1:89:B:ARG:H	1:90:B:ASN:HD21	19	2.23
(1,764)	1:86:A:LYS:HG2	1:90:A:ASN:H	8	2.23
(1,744)	1:66:A:LYS:HD3	1:67:A:LYS:H	3	2.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:88:A:LEU:HB3	1:91:A:LEU:HG	20	2.23
(1,450)	1:56:B:GLN:HG3	1:84:A:THR:HB	11	2.23
(1,936)	1:75:A:LEU:H	1:71:A:ARG:O	8	2.22
(1,832)	1:87:B:HIS:HD2	1:91:B:LEU:HA	13	2.22
(1,747)	1:87:A:HIS:HD2	1:92:B:GLN:H	10	2.22
(1,577)	1:68:A:ASP:HB3	1:72:A:HIS:HD2	11	2.22
(1,450)	1:56:B:GLN:HG3	1:84:A:THR:HB	13	2.22
(1,358)	1:67:A:LYS:HA	1:69:A:SER:H	9	2.22
(1,259)	1:56:B:GLN:HG3	1:82:A:GLU:H	8	2.22
(1,857)	1:93:B:ARG:HB2	1:95:B:GLN:HB2	3	2.21
(1,844)	1:89:B:ARG:HB2	1:90:B:ASN:HD22	5	2.21
(1,817)	1:60:B:LEU:HD13	1:88:A:LEU:HB2	3	2.21
(1,769)	1:50:A:ILE:HG21	1:79:B:ASP:H	16	2.21
(1,649)	1:71:B:ARG:HG2	1:75:B:LEU:HD11	2	2.21
(1,602)	1:64:A:ALA:HB2	1:67:A:LYS:HG3	7	2.21
(1,585)	1:64:A:ALA:HB1	1:67:A:LYS:HG3	9	2.21
(1,569)	1:87:A:HIS:HA	1:92:B:GLN:HE21	14	2.21
(1,437)	1:90:A:ASN:HA	1:92:A:GLN:HG2	4	2.21
(1,420)	1:87:A:HIS:HD2	1:91:A:LEU:HA	10	2.21
(1,270)	1:79:B:ASP:H	1:54:B:LEU:HD21	3	2.21
(1,431)	1:71:A:ARG:HG2	1:75:A:LEU:HA	18	2.2
(1,370)	1:66:A:LYS:HA	1:69:A:SER:H	4	2.2
(1,259)	1:56:B:GLN:HG3	1:82:A:GLU:H	19	2.2
(1,850)	1:90:A:ASN:HD22	1:83:A:MET:HG3	13	2.19
(1,747)	1:87:A:HIS:HD2	1:92:A:GLN:H	16	2.19
(1,450)	1:56:B:GLN:HG3	1:84:A:THR:HB	1	2.19
(1,857)	1:93:A:ARG:HB2	1:95:A:GLN:HB2	10	2.18
(1,844)	1:89:A:ARG:HB2	1:90:A:ASN:HD22	3	2.18
(1,803)	1:57:B:LEU:HD13	1:83:B:MET:H	5	2.18
(1,647)	1:90:B:ASN:HB2	1:65:B:LEU:HD11	16	2.18
(1,574)	1:64:A:ALA:HB2	1:65:A:LEU:HD21	2	2.18
(1,394)	1:67:B:LYS:H	1:69:B:SER:H	12	2.18
(1,358)	1:67:A:LYS:HA	1:69:A:SER:H	10	2.18
(1,65)	1:56:B:GLN:HG2	1:82:A:GLU:H	15	2.18
(1,764)	1:86:B:LYS:HG2	1:90:B:ASN:H	15	2.17
(1,583)	1:76:B:GLU:HB2	1:77:B:LYS:HG2	7	2.17
(1,577)	1:68:B:ASP:HB3	1:72:B:HIS:HD1	14	2.17
(1,450)	1:56:B:GLN:HG3	1:84:A:THR:HB	4	2.17
(1,259)	1:56:B:GLN:HG3	1:82:A:GLU:H	3	2.17
(1,65)	1:56:B:GLN:HG2	1:82:A:GLU:H	1	2.17
(1,857)	1:93:A:ARG:HB2	1:95:A:GLN:HB3	9	2.16
(1,844)	1:89:B:ARG:HB2	1:90:B:ASN:HD22	20	2.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,835)	1:87:A:HIS:HD2	1:67:A:LYS:HD2	12	2.16
(1,764)	1:86:A:LYS:HG2	1:90:A:ASN:H	5	2.16
(1,669)	1:88:A:LEU:HB3	1:91:A:LEU:HG	4	2.16
(1,450)	1:56:A:GLN:HG3	1:84:B:THR:HB	20	2.16
(1,437)	1:90:B:ASN:HA	1:92:B:GLN:HG2	11	2.16
(1,437)	1:90:A:ASN:HA	1:92:A:GLN:HG2	12	2.16
(1,370)	1:66:A:LYS:HA	1:69:A:SER:H	15	2.16
(1,857)	1:93:A:ARG:HB2	1:95:A:GLN:HB2	8	2.15
(1,843)	1:89:B:ARG:H	1:90:B:ASN:HD21	14	2.15
(1,803)	1:57:B:LEU:HD21	1:83:B:MET:H	17	2.15
(1,764)	1:86:B:LYS:HG2	1:90:B:ASN:H	3	2.15
(1,764)	1:86:A:LYS:HG2	1:90:A:ASN:H	16	2.15
(1,647)	1:90:B:ASN:HB2	1:65:B:LEU:HD11	8	2.15
(1,450)	1:56:A:GLN:HG3	1:84:B:THR:HB	9	2.15
(1,450)	1:56:A:GLN:HG3	1:84:B:THR:HB	17	2.15
(1,450)	1:56:B:GLN:HG3	1:84:A:THR:HB	18	2.15
(1,858)	1:93:B:ARG:HB3	1:95:B:GLN:HB2	9	2.14
(1,843)	1:89:A:ARG:H	1:90:A:ASN:HD21	16	2.14
(1,803)	1:57:B:LEU:HD22	1:83:B:MET:H	3	2.14
(1,803)	1:57:B:LEU:HD23	1:83:B:MET:H	9	2.14
(1,769)	1:50:B:ILE:HG23	1:79:A:ASP:H	12	2.14
(1,669)	1:88:B:LEU:HB3	1:91:B:LEU:HG	14	2.14
(1,577)	1:68:B:ASP:HB3	1:72:B:HIS:HD1	15	2.14
(1,408)	1:64:A:ALA:HA	1:67:A:LYS:HG2	8	2.14
(1,843)	1:89:B:ARG:H	1:90:B:ASN:HD21	15	2.13
(1,781)	1:64:A:ALA:HB3	1:65:A:LEU:HD23	11	2.13
(1,781)	1:64:B:ALA:HB1	1:65:B:LEU:HD23	20	2.13
(1,764)	1:86:B:LYS:HG2	1:90:B:ASN:H	13	2.13
(1,747)	1:87:B:HIS:HD2	1:92:B:GLN:H	8	2.13
(1,746)	1:87:A:HIS:HD1	1:92:A:GLN:H	4	2.13
(1,573)	1:64:B:ALA:HB1	1:65:B:LEU:HD22	8	2.13
(1,370)	1:66:A:LYS:HA	1:69:A:SER:H	6	2.13
(1,65)	1:56:B:GLN:HG2	1:82:A:GLU:H	13	2.13
(1,65)	1:56:B:GLN:HG2	1:82:A:GLU:H	14	2.13
(1,844)	1:89:A:ARG:HB2	1:90:A:ASN:HD22	19	2.12
(1,843)	1:89:B:ARG:H	1:90:B:ASN:HD21	20	2.12
(1,832)	1:87:B:HIS:HD1	1:91:B:LEU:HA	19	2.12
(1,803)	1:57:B:LEU:HD22	1:83:B:MET:H	2	2.12
(1,803)	1:57:B:LEU:HD23	1:83:B:MET:H	16	2.12
(1,747)	1:87:A:HIS:HD2	1:92:A:GLN:H	2	2.12
(1,669)	1:88:B:LEU:HB3	1:91:B:LEU:HG	3	2.12
(1,669)	1:88:B:LEU:HB3	1:91:B:LEU:HG	5	2.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:88:B:LEU:HB3	1:91:B:LEU:HG	6	2.12
(1,669)	1:88:A:LEU:HB3	1:91:A:LEU:HG	11	2.12
(1,583)	1:76:A:GLU:HB2	1:77:A:LYS:HG2	15	2.12
(1,569)	1:87:A:HIS:HA	1:92:B:GLN:HE21	4	2.12
(1,569)	1:87:B:HIS:HA	1:92:A:GLN:HE21	20	2.12
(1,437)	1:90:A:ASN:HA	1:92:A:GLN:HG2	7	2.12
(1,431)	1:71:B:ARG:HG2	1:75:B:LEU:HA	3	2.12
(1,270)	1:79:B:ASP:H	1:54:B:LEU:HD22	8	2.12
(1,858)	1:93:B:ARG:HB3	1:95:B:GLN:HB2	1	2.11
(1,844)	1:89:A:ARG:HB2	1:90:A:ASN:HD22	18	2.11
(1,803)	1:57:B:LEU:HD22	1:83:B:MET:H	6	2.11
(1,803)	1:57:B:LEU:HD23	1:83:B:MET:H	13	2.11
(1,803)	1:57:B:LEU:HD21	1:83:B:MET:H	19	2.11
(1,781)	1:64:A:ALA:HB3	1:65:A:LEU:HD21	2	2.11
(1,781)	1:64:A:ALA:HB3	1:65:A:LEU:HD21	8	2.11
(1,781)	1:64:B:ALA:HB1	1:65:B:LEU:HD23	16	2.11
(1,747)	1:87:B:HIS:HD2	1:92:B:GLN:H	13	2.11
(1,700)	1:87:A:HIS:HD1	1:91:A:LEU:HA	20	2.11
(1,270)	1:79:B:ASP:H	1:54:B:LEU:HD22	17	2.11
(1,844)	1:89:B:ARG:HB2	1:90:B:ASN:HD22	12	2.1
(1,821)	1:86:A:LYS:HG2	1:83:A:MET:HG3	10	2.1
(1,558)	1:81:A:LEU:HA	1:83:A:MET:HE1	14	2.1
(1,437)	1:90:B:ASN:HA	1:92:B:GLN:HG2	19	2.1
(1,844)	1:89:A:ARG:HB2	1:90:A:ASN:HD22	7	2.09
(1,843)	1:89:A:ARG:H	1:90:A:ASN:HD21	8	2.09
(1,764)	1:86:A:LYS:HG2	1:90:A:ASN:H	1	2.09
(1,627)	1:66:A:LYS:HG2	1:67:A:LYS:HG2	3	2.09
(1,450)	1:56:B:GLN:HG3	1:84:A:THR:HB	3	2.09
(1,431)	1:71:B:ARG:HG2	1:75:B:LEU:HA	12	2.09
(1,370)	1:66:B:LYS:HA	1:69:B:SER:H	12	2.09
(1,577)	1:68:B:ASP:HB3	1:72:B:HIS:HD1	3	2.08
(1,496)	1:64:A:ALA:H	1:65:A:LEU:HD22	20	2.08
(1,857)	1:93:A:ARG:HB2	1:95:A:GLN:HB2	2	2.07
(1,857)	1:93:B:ARG:HB2	1:95:B:GLN:HB2	17	2.07
(1,843)	1:89:B:ARG:H	1:90:B:ASN:HD21	4	2.07
(1,803)	1:57:B:LEU:HD21	1:83:B:MET:H	4	2.07
(1,803)	1:57:B:LEU:HD23	1:83:B:MET:H	18	2.07
(1,764)	1:86:B:LYS:HG2	1:90:B:ASN:H	7	2.07
(1,764)	1:86:A:LYS:HG2	1:90:A:ASN:H	14	2.07
(1,577)	1:68:B:ASP:HB3	1:72:B:HIS:HD1	20	2.07
(1,450)	1:56:B:GLN:HG3	1:84:A:THR:HB	2	2.07
(1,431)	1:71:B:ARG:HG2	1:75:B:LEU:HA	13	2.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,358)	1:67:A:LYS:HA	1:69:A:SER:H	17	2.07
(1,832)	1:87:A:HIS:HD1	1:91:A:LEU:HA	4	2.06
(1,832)	1:87:A:HIS:HD2	1:91:A:LEU:HA	7	2.06
(1,647)	1:90:B:ASN:HB2	1:65:B:LEU:HD12	10	2.06
(1,558)	1:81:B:LEU:HA	1:83:B:MET:HE2	2	2.06
(1,431)	1:71:A:ARG:HG2	1:75:A:LEU:HA	7	2.06
(1,843)	1:89:B:ARG:H	1:90:B:ASN:HD21	6	2.05
(1,803)	1:57:B:LEU:HD21	1:83:B:MET:H	7	2.05
(1,747)	1:87:B:HIS:HD2	1:92:B:GLN:H	4	2.05
(1,747)	1:87:A:HIS:HD2	1:92:A:GLN:H	7	2.05
(1,569)	1:87:A:HIS:HA	1:92:B:GLN:HE21	10	2.05
(1,569)	1:87:B:HIS:HA	1:92:A:GLN:HE21	19	2.05
(1,850)	1:90:A:ASN:HD21	1:83:A:MET:HG3	18	2.04
(1,844)	1:89:B:ARG:HB2	1:90:B:ASN:HD22	1	2.04
(1,764)	1:86:A:LYS:HG2	1:90:A:ASN:H	20	2.04
(1,577)	1:68:A:ASP:HB3	1:72:A:HIS:HD2	1	2.04
(1,569)	1:87:A:HIS:HA	1:92:B:GLN:HE21	11	2.04
(1,450)	1:56:A:GLN:HG3	1:84:B:THR:HB	7	2.04
(1,437)	1:90:B:ASN:HA	1:92:B:GLN:HG3	8	2.04
(1,437)	1:90:A:ASN:HA	1:92:A:GLN:HG2	14	2.04
(1,843)	1:89:A:ARG:H	1:90:A:ASN:HD21	5	2.03
(1,843)	1:89:B:ARG:H	1:90:B:ASN:HD21	11	2.03
(1,577)	1:68:B:ASP:HB3	1:72:B:HIS:HD1	5	2.03
(1,370)	1:66:B:LYS:HA	1:69:B:SER:H	5	2.03
(1,270)	1:79:B:ASP:H	1:54:B:LEU:HD22	12	2.03
(1,65)	1:56:B:GLN:HG2	1:82:A:GLU:H	18	2.03
(1,844)	1:89:B:ARG:HB2	1:90:B:ASN:HD22	10	2.02
(1,843)	1:89:A:ARG:H	1:90:A:ASN:HD21	9	2.02
(1,843)	1:89:B:ARG:H	1:90:B:ASN:HD21	10	2.02
(1,803)	1:57:B:LEU:HD23	1:83:B:MET:H	11	2.02
(1,764)	1:86:B:LYS:HG2	1:90:B:ASN:H	12	2.02
(1,627)	1:66:B:LYS:HG2	1:67:B:LYS:HG2	10	2.02
(1,577)	1:68:A:ASP:HB2	1:72:A:HIS:HD1	13	2.02
(1,558)	1:81:B:LEU:HA	1:83:B:MET:HE1	13	2.02
(1,394)	1:67:A:LYS:H	1:69:A:SER:H	17	2.02
(1,270)	1:79:B:ASP:H	1:54:B:LEU:HD22	5	2.02
(1,857)	1:93:B:ARG:HB2	1:95:B:GLN:HB2	7	2.01
(1,850)	1:90:A:ASN:HD22	1:83:A:MET:HG3	6	2.01
(1,844)	1:89:B:ARG:HB2	1:90:B:ASN:HD22	14	2.01
(1,832)	1:87:A:HIS:HD1	1:91:A:LEU:HA	8	2.01
(1,803)	1:57:B:LEU:HD22	1:83:B:MET:H	1	2.01
(1,803)	1:57:B:LEU:HD23	1:83:B:MET:H	12	2.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:88:A:LEU:HB3	1:91:A:LEU:HG	1	2.01
(1,569)	1:87:B:HIS:HA	1:92:A:GLN:HE21	1	2.01
(1,569)	1:87:B:HIS:HA	1:92:A:GLN:HE21	16	2.01
(1,450)	1:56:A:GLN:HG3	1:84:B:THR:HB	8	2.01
(1,437)	1:90:B:ASN:HA	1:92:B:GLN:HG2	2	2.01
(1,437)	1:90:B:ASN:HA	1:92:B:GLN:HG2	9	2.01
(1,65)	1:56:B:GLN:HG2	1:82:A:GLU:H	8	2.01
(1,858)	1:93:A:ARG:HB3	1:95:A:GLN:HB2	2	2.0
(1,857)	1:93:B:ARG:HB2	1:95:B:GLN:HB2	16	2.0
(1,577)	1:68:B:ASP:HB3	1:72:B:HIS:HD1	7	2.0
(1,437)	1:90:A:ASN:HA	1:92:A:GLN:HG2	16	2.0
(1,65)	1:56:A:GLN:HG2	1:82:B:GLU:H	12	2.0
(1,843)	1:89:B:ARG:H	1:90:B:ASN:HD21	2	1.99
(1,843)	1:89:B:ARG:H	1:90:B:ASN:HD21	13	1.99
(1,832)	1:87:A:HIS:HD2	1:91:A:LEU:HA	2	1.99
(1,764)	1:86:A:LYS:HG2	1:90:A:ASN:H	4	1.99
(1,764)	1:86:B:LYS:HG2	1:90:B:ASN:H	9	1.99
(1,764)	1:86:A:LYS:HG2	1:90:A:ASN:H	18	1.99
(1,700)	1:87:A:HIS:HD1	1:91:A:LEU:HA	3	1.99
(1,569)	1:87:B:HIS:HA	1:92:A:GLN:HE21	5	1.99
(1,431)	1:71:A:ARG:HG2	1:75:A:LEU:HA	14	1.99
(1,270)	1:79:A:ASP:H	1:54:A:LEU:HD21	1	1.99
(1,558)	1:81:A:LEU:HA	1:83:A:MET:HE3	1	1.98
(1,558)	1:81:B:LEU:HA	1:83:B:MET:HE2	20	1.98
(1,437)	1:90:A:ASN:HA	1:92:A:GLN:HG2	17	1.98
(1,65)	1:56:B:GLN:HG2	1:82:A:GLU:H	2	1.98
(1,450)	1:56:A:GLN:HG3	1:84:B:THR:HB	15	1.97
(1,437)	1:90:B:ASN:HA	1:92:B:GLN:HG2	3	1.97
(1,437)	1:90:A:ASN:HA	1:92:A:GLN:HG3	13	1.97
(1,370)	1:66:B:LYS:HA	1:69:B:SER:H	17	1.97
(1,270)	1:79:B:ASP:H	1:54:B:LEU:HD23	7	1.97
(1,764)	1:86:A:LYS:HG2	1:90:A:ASN:H	6	1.96
(1,731)	1:86:A:LYS:HD3	1:87:A:HIS:HA	10	1.96
(1,437)	1:90:A:ASN:HA	1:92:A:GLN:HG2	1	1.96
(1,65)	1:56:B:GLN:HG2	1:82:A:GLU:H	6	1.96
(1,858)	1:93:B:ARG:HB3	1:95:B:GLN:HB2	13	1.95
(1,857)	1:93:A:ARG:HB2	1:95:A:GLN:HB2	20	1.95
(1,835)	1:87:A:HIS:HD2	1:67:A:LYS:HD2	14	1.95
(1,832)	1:87:B:HIS:HD1	1:91:B:LEU:HA	10	1.95
(1,746)	1:87:A:HIS:HD1	1:92:A:GLN:H	8	1.95
(1,437)	1:90:A:ASN:HA	1:92:A:GLN:HG3	15	1.95
(1,437)	1:90:B:ASN:HA	1:92:B:GLN:HG2	18	1.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:79:B:ASP:H	1:54:B:LEU:HD22	16	1.95
(1,843)	1:89:A:ARG:H	1:90:A:ASN:HD21	3	1.94
(1,843)	1:89:A:ARG:H	1:90:A:ASN:HD21	12	1.94
(1,843)	1:89:A:ARG:H	1:90:A:ASN:HD21	18	1.94
(1,835)	1:87:A:HIS:HD1	1:67:A:LYS:HD2	3	1.94
(1,450)	1:56:B:GLN:HG3	1:84:A:THR:HB	6	1.94
(1,437)	1:90:A:ASN:HA	1:92:A:GLN:HG2	6	1.94
(1,496)	1:64:A:ALA:H	1:65:A:LEU:HD22	18	1.93
(1,450)	1:56:A:GLN:HG3	1:84:B:THR:HB	19	1.93
(1,789)	1:66:A:LYS:HA	1:69:A:SER:HG	18	1.92
(1,647)	1:90:B:ASN:HB2	1:65:B:LEU:HD11	4	1.92
(1,577)	1:68:B:ASP:HB3	1:72:B:HIS:HD1	4	1.92
(1,577)	1:68:A:ASP:HB3	1:72:A:HIS:HD1	19	1.92
(1,569)	1:87:A:HIS:HA	1:92:B:GLN:HE21	13	1.92
(1,450)	1:56:B:GLN:HG3	1:84:A:THR:HB	14	1.92
(1,843)	1:89:A:ARG:H	1:90:A:ASN:HD21	17	1.91
(1,817)	1:60:A:LEU:HD11	1:88:B:LEU:HB2	11	1.91
(1,781)	1:64:A:ALA:HB3	1:65:A:LEU:HD23	19	1.91
(1,569)	1:87:A:HIS:HA	1:92:B:GLN:HE21	17	1.91
(1,458)	1:76:A:GLU:HB3	1:80:A:ILE:HB	9	1.91
(1,370)	1:66:A:LYS:HA	1:69:A:SER:H	10	1.91
(1,844)	1:89:B:ARG:HB2	1:90:B:ASN:HD22	13	1.9
(1,764)	1:86:A:LYS:HG2	1:90:A:ASN:H	2	1.9
(1,627)	1:66:A:LYS:HG2	1:67:A:LYS:HG2	16	1.9
(1,496)	1:64:A:ALA:H	1:65:A:LEU:HD22	11	1.9
(1,431)	1:71:A:ARG:HG2	1:75:A:LEU:HA	9	1.9
(1,789)	1:66:B:LYS:HA	1:69:B:SER:HG	11	1.89
(1,747)	1:87:A:HIS:HD2	1:92:A:GLN:H	15	1.89
(1,669)	1:88:A:LEU:HB3	1:91:B:LEU:HG	7	1.89
(1,496)	1:64:B:ALA:H	1:65:B:LEU:HD23	7	1.89
(1,437)	1:90:A:ASN:HA	1:92:A:GLN:HG2	10	1.89
(1,370)	1:66:A:LYS:HA	1:69:A:SER:H	9	1.89
(1,857)	1:93:B:ARG:HB2	1:95:B:GLN:HB2	15	1.88
(1,843)	1:89:B:ARG:H	1:90:B:ASN:HD21	7	1.88
(1,781)	1:64:A:ALA:HB2	1:65:A:LEU:HD23	7	1.88
(1,781)	1:64:A:ALA:HB3	1:65:A:LEU:HD23	14	1.88
(1,781)	1:64:B:ALA:HB2	1:65:B:LEU:HD23	18	1.88
(1,458)	1:76:A:GLU:HB3	1:80:A:ILE:HB	5	1.88
(1,458)	1:76:A:GLU:HB3	1:80:A:ILE:HB	10	1.88
(1,450)	1:56:A:GLN:HG3	1:84:B:THR:HB	12	1.88
(1,420)	1:87:B:HIS:HD2	1:91:B:LEU:HA	11	1.88
(1,394)	1:67:A:LYS:H	1:69:A:SER:H	9	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:93:A:ARG:HB3	1:95:A:GLN:HB2	19	1.87
(1,781)	1:64:B:ALA:HB2	1:65:B:LEU:HD22	10	1.87
(1,764)	1:86:B:LYS:HG2	1:90:B:ASN:H	19	1.87
(1,496)	1:64:B:ALA:H	1:65:B:LEU:HD23	14	1.87
(1,65)	1:56:B:GLN:HG2	1:82:A:GLU:H	3	1.87
(1,843)	1:89:B:ARG:H	1:90:B:ASN:HD21	1	1.86
(1,803)	1:57:B:LEU:HD22	1:83:B:MET:H	20	1.86
(1,764)	1:86:A:LYS:HG2	1:90:A:ASN:H	17	1.86
(1,577)	1:68:B:ASP:HB3	1:72:B:HIS:HD1	10	1.86
(1,496)	1:64:A:ALA:H	1:65:A:LEU:HD23	8	1.86
(1,270)	1:79:A:ASP:H	1:54:A:LEU:HD21	6	1.86
(1,65)	1:56:B:GLN:HG2	1:82:A:GLU:H	9	1.86
(1,65)	1:56:A:GLN:HG2	1:82:B:GLU:H	20	1.86
(1,673)	1:56:B:GLN:HG2	1:82:A:GLU:HB2	10	1.85
(1,520)	1:68:B:ASP:H	1:69:B:SER:HB2	16	1.85
(1,420)	1:87:A:HIS:HD2	1:91:A:LEU:HA	19	1.85
(1,680)	1:66:A:LYS:HG2	1:67:A:LYS:HG3	14	1.84
(1,577)	1:68:B:ASP:HB3	1:72:B:HIS:HD1	16	1.84
(1,277)	1:54:B:LEU:HD21	1:80:B:ILE:H	14	1.84
(1,69)	1:83:B:MET:H	1:80:B:ILE:HG23	19	1.84
(1,69)	1:83:A:MET:H	1:80:A:ILE:HG23	6	1.83
(1,817)	1:60:A:LEU:HD11	1:88:B:LEU:HB2	17	1.82
(1,803)	1:57:A:LEU:HD11	1:83:A:MET:H	8	1.82
(1,803)	1:57:B:LEU:HD23	1:83:B:MET:H	15	1.82
(1,850)	1:90:B:ASN:HD21	1:83:B:MET:HG3	19	1.81
(1,744)	1:66:A:LYS:HD3	1:67:A:LYS:H	7	1.81
(1,669)	1:88:B:LEU:HB3	1:91:B:LEU:HG	8	1.8
(1,647)	1:90:B:ASN:HB2	1:65:B:LEU:HD12	19	1.8
(1,520)	1:68:B:ASP:H	1:69:B:SER:HB2	6	1.8
(1,520)	1:68:B:ASP:H	1:69:B:SER:HB2	17	1.8
(1,270)	1:79:B:ASP:H	1:54:B:LEU:HD21	9	1.8
(1,487)	1:88:A:LEU:HA	1:91:A:LEU:HA	10	1.79
(1,69)	1:83:A:MET:H	1:80:A:ILE:HG22	7	1.79
(1,69)	1:83:B:MET:H	1:80:B:ILE:HG23	14	1.79
(1,41)	1:67:A:LYS:HG3	1:69:A:SER:H	9	1.79
(1,781)	1:64:A:ALA:HB1	1:65:A:LEU:HD21	1	1.78
(1,520)	1:68:A:ASP:H	1:69:A:SER:HB2	7	1.78
(1,458)	1:76:B:GLU:HB3	1:80:B:ILE:HB	1	1.78
(1,69)	1:83:A:MET:H	1:80:A:ILE:HG21	13	1.76
(1,370)	1:66:A:LYS:HA	1:69:A:SER:H	1	1.75
(1,69)	1:83:A:MET:H	1:80:A:ILE:HG23	3	1.75
(1,934)	1:74:B:LYS:H	1:70:B:SER:O	2	1.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,832)	1:87:A:HIS:HD2	1:91:A:LEU:HA	15	1.74
(1,824)	1:86:B:LYS:HG3	1:87:B:HIS:HB2	6	1.74
(1,824)	1:86:A:LYS:HG3	1:87:A:HIS:HB2	9	1.74
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD11	9	1.74
(1,577)	1:68:B:ASP:HB3	1:72:B:HIS:HD2	12	1.74
(1,270)	1:79:B:ASP:H	1:54:B:LEU:HD22	15	1.74
(1,700)	1:87:A:HIS:HD1	1:91:A:LEU:HA	9	1.73
(1,676)	1:88:B:LEU:HB2	1:89:B:ARG:HB2	14	1.73
(1,558)	1:81:A:LEU:HA	1:83:A:MET:HE1	9	1.73
(1,487)	1:88:A:LEU:HA	1:91:A:LEU:HA	19	1.73
(1,431)	1:71:A:ARG:HG2	1:75:A:LEU:HA	17	1.73
(1,69)	1:83:A:MET:H	1:80:A:ILE:HG21	8	1.73
(1,69)	1:83:B:MET:H	1:80:B:ILE:HG22	18	1.73
(1,458)	1:76:B:GLU:HB3	1:80:B:ILE:HB	3	1.72
(1,270)	1:79:B:ASP:H	1:54:B:LEU:HD23	13	1.72
(1,69)	1:83:B:MET:H	1:80:B:ILE:HG21	11	1.72
(1,30)	1:85:B:VAL:H	1:88:B:LEU:HB2	17	1.72
(1,745)	1:72:A:HIS:H	1:75:A:LEU:HD12	20	1.71
(1,674)	1:88:A:LEU:HB2	1:91:A:LEU:HG	19	1.71
(1,496)	1:64:B:ALA:H	1:65:B:LEU:HD21	19	1.71
(1,458)	1:76:A:GLU:HB3	1:80:A:ILE:HB	2	1.71
(1,458)	1:76:A:GLU:HB3	1:80:A:ILE:HB	11	1.71
(1,824)	1:86:B:LYS:HG3	1:87:B:HIS:HB2	14	1.7
(1,669)	1:88:B:LEU:HB3	1:91:B:LEU:HG	18	1.7
(1,577)	1:68:B:ASP:HB3	1:72:B:HIS:HD1	9	1.7
(1,69)	1:83:A:MET:H	1:80:A:ILE:HG21	16	1.7
(1,747)	1:87:A:HIS:HD2	1:92:A:GLN:H	6	1.69
(1,669)	1:88:A:LEU:HB3	1:91:A:LEU:HG	9	1.69
(1,458)	1:76:B:GLU:HB3	1:80:B:ILE:HB	16	1.69
(1,270)	1:79:A:ASP:H	1:54:A:LEU:HD21	10	1.69
(1,69)	1:83:B:MET:H	1:80:B:ILE:HG22	1	1.69
(1,69)	1:83:B:MET:H	1:80:B:ILE:HG23	5	1.69
(1,754)	1:86:B:LYS:HD3	1:87:B:HIS:H	4	1.68
(1,458)	1:76:B:GLU:HB3	1:80:B:ILE:HB	17	1.68
(1,760)	1:86:B:LYS:HG2	1:87:B:HIS:H	17	1.67
(1,458)	1:76:A:GLU:HB3	1:80:A:ILE:HB	6	1.67
(1,69)	1:83:A:MET:H	1:80:A:ILE:HG22	9	1.67
(1,69)	1:83:B:MET:H	1:80:B:ILE:HG21	15	1.67
(1,760)	1:86:B:LYS:HG2	1:87:B:HIS:H	9	1.66
(1,496)	1:64:A:ALA:H	1:65:A:LEU:HD23	2	1.66
(1,496)	1:64:A:ALA:H	1:65:A:LEU:HD21	16	1.66
(1,467)	1:68:B:ASP:HA	1:71:B:ARG:HD2	9	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,458)	1:76:B:GLU:HB3	1:80:B:ILE:HB	4	1.66
(1,69)	1:83:A:MET:H	1:80:A:ILE:HG23	12	1.66
(1,857)	1:93:B:ARG:HB2	1:95:B:GLN:HB2	1	1.65
(1,833)	1:87:B:HIS:HD1	1:92:B:GLN:H	10	1.65
(1,824)	1:86:A:LYS:HG3	1:87:A:HIS:HB2	7	1.65
(1,824)	1:86:B:LYS:HG3	1:87:B:HIS:HB2	17	1.65
(1,760)	1:86:B:LYS:HG2	1:87:B:HIS:H	13	1.65
(1,760)	1:86:B:LYS:HG2	1:87:B:HIS:H	20	1.65
(1,669)	1:88:A:LEU:HB3	1:91:A:LEU:HG	13	1.65
(1,577)	1:68:B:ASP:HB2	1:72:B:HIS:HD1	2	1.65
(1,577)	1:68:B:ASP:HB3	1:72:B:HIS:HD1	18	1.65
(1,569)	1:87:B:HIS:HA	1:92:A:GLN:HE21	12	1.65
(1,551)	1:67:B:LYS:HA	1:67:B:LYS:HE2	5	1.65
(1,467)	1:68:B:ASP:HA	1:71:B:ARG:HD3	5	1.65
(1,69)	1:83:A:MET:H	1:80:A:ILE:HG21	2	1.65
(1,824)	1:86:A:LYS:HG3	1:87:A:HIS:HB2	20	1.64
(1,817)	1:60:B:LEU:HD11	1:88:A:LEU:HB2	6	1.64
(1,760)	1:86:A:LYS:HG2	1:87:A:HIS:H	7	1.64
(1,573)	1:64:B:ALA:HB1	1:65:B:LEU:HD23	18	1.64
(1,69)	1:83:B:MET:H	1:80:B:ILE:HG23	10	1.64
(1,69)	1:83:A:MET:H	1:80:A:ILE:HG21	20	1.64
(1,789)	1:66:B:LYS:HA	1:69:B:SER:HG	16	1.63
(1,760)	1:86:B:LYS:HG2	1:87:B:HIS:H	14	1.63
(1,467)	1:68:A:ASP:HA	1:71:A:ARG:HD2	20	1.62
(1,458)	1:76:A:GLU:HB3	1:80:A:ILE:HB	8	1.62
(1,458)	1:76:B:GLU:HB3	1:80:B:ILE:HB	13	1.62
(1,458)	1:76:A:GLU:HB3	1:80:A:ILE:HB	14	1.62
(1,277)	1:54:B:LEU:HD21	1:80:B:ILE:H	3	1.62
(1,69)	1:83:B:MET:H	1:80:B:ILE:HG21	4	1.62
(1,833)	1:87:B:HIS:HD1	1:92:B:GLN:H	19	1.61
(1,760)	1:86:B:LYS:HG2	1:87:B:HIS:H	4	1.61
(1,487)	1:88:A:LEU:HA	1:91:A:LEU:HA	20	1.61
(1,270)	1:79:B:ASP:H	1:54:B:LEU:HD23	19	1.61
(1,760)	1:86:B:LYS:HG2	1:87:B:HIS:H	18	1.6
(1,731)	1:86:B:LYS:HD3	1:87:B:HIS:HA	6	1.6
(1,609)	1:92:B:GLN:HB2	1:93:B:ARG:HB2	19	1.6
(1,760)	1:86:A:LYS:HG2	1:87:A:HIS:H	6	1.59
(1,754)	1:86:A:LYS:HD3	1:87:A:HIS:H	19	1.59
(1,609)	1:92:A:GLN:HB3	1:93:A:ARG:HB2	3	1.59
(1,609)	1:92:A:GLN:HB3	1:93:A:ARG:HB2	8	1.59
(1,487)	1:88:A:LEU:HA	1:91:A:LEU:HA	14	1.59
(1,483)	1:76:B:GLU:HA	1:80:B:ILE:HB	1	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,789)	1:66:A:LYS:HA	1:69:A:SER:HG	6	1.58
(1,760)	1:86:B:LYS:HG2	1:87:B:HIS:H	5	1.58
(1,760)	1:86:A:LYS:HG2	1:87:A:HIS:H	19	1.58
(1,520)	1:68:A:ASP:H	1:69:A:SER:HB2	5	1.58
(1,458)	1:76:B:GLU:HB3	1:80:B:ILE:HB	7	1.58
(1,431)	1:71:A:ARG:HG2	1:75:A:LEU:HA	10	1.58
(1,69)	1:83:A:MET:H	1:80:A:ILE:HG22	17	1.58
(1,832)	1:87:A:HIS:HD2	1:91:A:LEU:HA	6	1.57
(1,824)	1:86:B:LYS:HG3	1:87:B:HIS:HB2	13	1.57
(1,760)	1:86:B:LYS:HG2	1:87:B:HIS:H	1	1.57
(1,760)	1:86:B:LYS:HG2	1:87:B:HIS:H	16	1.57
(1,731)	1:86:A:LYS:HD3	1:87:A:HIS:HA	2	1.57
(1,676)	1:88:B:LEU:HB2	1:89:B:ARG:HB2	7	1.57
(1,551)	1:67:A:LYS:HA	1:67:A:LYS:HE2	12	1.57
(1,487)	1:88:B:LEU:HA	1:91:B:LEU:HA	6	1.57
(1,487)	1:88:A:LEU:HA	1:91:A:LEU:HA	11	1.57
(1,467)	1:68:A:ASP:HA	1:71:A:ARG:HD2	15	1.57
(1,270)	1:79:B:ASP:H	1:54:B:LEU:HD22	2	1.57
(1,270)	1:79:B:ASP:H	1:54:B:LEU:HD23	18	1.57
(1,270)	1:79:A:ASP:H	1:54:A:LEU:HD21	20	1.57
(1,754)	1:86:B:LYS:HD3	1:87:B:HIS:H	11	1.56
(1,680)	1:66:A:LYS:HG2	1:67:A:LYS:HG3	9	1.56
(1,669)	1:88:A:LEU:HB3	1:91:A:LEU:HG	12	1.56
(1,609)	1:92:B:GLN:HB2	1:93:B:ARG:HB2	9	1.56
(1,569)	1:87:B:HIS:HA	1:92:A:GLN:HE21	7	1.56
(1,431)	1:71:B:ARG:HG2	1:75:B:LEU:HA	2	1.56
(1,277)	1:54:B:LEU:HD22	1:80:B:ILE:H	8	1.56
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD11	11	1.55
(1,745)	1:72:B:HIS:H	1:75:B:LEU:HD13	14	1.55
(1,700)	1:87:A:HIS:HD1	1:91:A:LEU:HA	12	1.55
(1,673)	1:56:B:GLN:HG2	1:82:A:GLU:HB2	5	1.55
(1,824)	1:86:B:LYS:HG3	1:87:B:HIS:HB2	4	1.54
(1,817)	1:60:A:LEU:HD11	1:88:B:LEU:HB2	5	1.54
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD13	3	1.54
(1,781)	1:64:A:ALA:HB1	1:65:A:LEU:HD23	9	1.54
(1,551)	1:67:B:LYS:HA	1:67:B:LYS:HE2	19	1.54
(1,531)	1:87:A:HIS:H	1:88:A:LEU:HB2	17	1.54
(1,467)	1:68:A:ASP:HA	1:71:A:ARG:HD2	12	1.54
(1,789)	1:66:A:LYS:HA	1:69:A:SER:HG	7	1.53
(1,760)	1:86:B:LYS:HG2	1:87:B:HIS:H	11	1.53
(1,760)	1:86:A:LYS:HG2	1:87:A:HIS:H	15	1.53
(1,731)	1:86:B:LYS:HD3	1:87:B:HIS:HA	14	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,731)	1:86:A:LYS:HD3	1:87:A:HIS:HA	16	1.53
(1,669)	1:88:A:LEU:HB3	1:91:A:LEU:HG	16	1.53
(1,609)	1:92:A:GLN:HB2	1:93:A:ARG:HB2	6	1.53
(1,574)	1:64:B:ALA:HB2	1:65:B:LEU:HD23	11	1.53
(1,487)	1:88:A:LEU:HA	1:91:A:LEU:HA	4	1.53
(1,458)	1:76:B:GLU:HB3	1:80:B:ILE:HB	20	1.53
(1,270)	1:79:B:ASP:H	1:54:B:LEU:HD23	11	1.53
(1,268)	1:86:B:LYS:H	1:84:B:THR:HG23	19	1.53
(1,824)	1:86:B:LYS:HG3	1:87:B:HIS:HB2	16	1.52
(1,760)	1:86:A:LYS:HG2	1:87:A:HIS:H	12	1.52
(1,673)	1:56:B:GLN:HG2	1:82:A:GLU:HB2	11	1.52
(1,609)	1:92:A:GLN:HB2	1:93:A:ARG:HB2	15	1.52
(1,569)	1:87:A:HIS:HA	1:92:B:GLN:HE21	18	1.52
(1,496)	1:64:B:ALA:H	1:65:B:LEU:HD21	9	1.52
(1,487)	1:88:B:LEU:HA	1:91:B:LEU:HA	15	1.52
(1,467)	1:68:A:ASP:HA	1:71:A:ARG:HD2	16	1.52
(1,458)	1:76:A:GLU:HB3	1:80:A:ILE:HB	18	1.52
(1,35)	1:66:A:LYS:HG2	1:67:A:LYS:H	17	1.52
(1,824)	1:86:B:LYS:HG3	1:87:B:HIS:HB2	1	1.51
(1,609)	1:92:A:GLN:HB3	1:93:A:ARG:HB2	20	1.51
(1,731)	1:86:B:LYS:HD3	1:87:B:HIS:HA	12	1.5
(1,609)	1:92:A:GLN:HB3	1:93:A:ARG:HB2	11	1.5
(1,520)	1:68:A:ASP:H	1:69:A:SER:HB3	10	1.5
(1,487)	1:88:A:LEU:HA	1:91:A:LEU:HA	1	1.5
(1,487)	1:88:A:LEU:HA	1:91:A:LEU:HA	5	1.5
(1,467)	1:68:B:ASP:HA	1:71:B:ARG:HD2	17	1.5
(1,458)	1:76:A:GLU:HB3	1:80:A:ILE:HB	15	1.5
(1,858)	1:93:A:ARG:HB3	1:95:A:GLN:HB2	12	1.49
(1,832)	1:87:B:HIS:HD2	1:91:B:LEU:HA	5	1.49
(1,496)	1:64:B:ALA:H	1:65:B:LEU:HD22	1	1.49
(1,467)	1:68:B:ASP:HA	1:71:B:ARG:HD2	11	1.49
(1,35)	1:66:B:LYS:HG2	1:67:B:LYS:H	18	1.49
(1,760)	1:86:A:LYS:HG2	1:87:A:HIS:H	3	1.48
(1,747)	1:87:B:HIS:HD2	1:92:B:GLN:H	5	1.48
(1,836)	1:87:B:HIS:HD2	1:92:A:GLN:HE21	13	1.47
(1,788)	1:65:B:LEU:HG	1:66:B:LYS:H	2	1.47
(1,676)	1:88:A:LEU:HB2	1:89:A:ARG:HB2	13	1.47
(1,673)	1:56:B:GLN:HG2	1:82:A:GLU:HB2	15	1.47
(1,487)	1:88:B:LEU:HA	1:91:B:LEU:HA	3	1.47
(1,467)	1:68:B:ASP:HA	1:71:B:ARG:HD2	3	1.47
(1,467)	1:68:B:ASP:HA	1:71:B:ARG:HD2	6	1.47
(1,824)	1:86:B:LYS:HG3	1:87:B:HIS:HB2	18	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,754)	1:86:A:LYS:HD3	1:87:A:HIS:H	15	1.46
(1,676)	1:88:A:LEU:HB2	1:89:A:ARG:HB2	16	1.46
(1,676)	1:88:B:LEU:HB2	1:89:B:ARG:HB2	17	1.46
(1,673)	1:56:B:GLN:HG2	1:82:A:GLU:HB2	16	1.46
(1,609)	1:92:A:GLN:HB3	1:93:A:ARG:HB2	7	1.46
(1,609)	1:92:B:GLN:HB2	1:93:B:ARG:HB2	10	1.46
(1,487)	1:88:A:LEU:HA	1:91:A:LEU:HA	9	1.46
(1,483)	1:76:B:GLU:HA	1:80:B:ILE:HB	17	1.46
(1,458)	1:76:B:GLU:HB3	1:80:B:ILE:HB	12	1.46
(1,936)	1:75:B:LEU:H	1:71:B:ARG:O	16	1.45
(1,788)	1:65:A:LEU:HG	1:66:A:LYS:H	14	1.45
(1,760)	1:86:A:LYS:HG2	1:87:A:HIS:H	8	1.45
(1,713)	1:87:B:HIS:HA	1:87:B:HIS:HD2	1	1.45
(1,674)	1:88:A:LEU:HB2	1:91:A:LEU:HG	10	1.45
(1,569)	1:87:A:HIS:HA	1:92:B:GLN:HE21	2	1.45
(1,551)	1:67:B:LYS:HA	1:67:B:LYS:HE2	11	1.45
(1,824)	1:86:B:LYS:HG3	1:87:B:HIS:HB2	5	1.44
(1,745)	1:72:B:HIS:H	1:75:B:LEU:HD13	3	1.44
(1,609)	1:92:A:GLN:HB2	1:93:A:ARG:HB2	16	1.44
(1,574)	1:64:A:ALA:HB2	1:65:A:LEU:HD21	14	1.44
(1,520)	1:68:B:ASP:H	1:69:B:SER:HB2	19	1.44
(1,35)	1:66:B:LYS:HG2	1:67:B:LYS:H	15	1.44
(1,934)	1:74:B:LYS:H	1:70:B:SER:O	12	1.43
(1,824)	1:86:B:LYS:HG3	1:87:B:HIS:HB2	11	1.43
(1,815)	1:85:B:VAL:HA	1:60:A:LEU:HD11	5	1.43
(1,805)	1:57:B:LEU:HD13	1:86:A:LYS:H	6	1.43
(1,805)	1:57:B:LEU:HD13	1:86:A:LYS:H	15	1.43
(1,467)	1:68:B:ASP:HA	1:71:B:ARG:HD2	1	1.43
(1,754)	1:86:A:LYS:HD3	1:87:A:HIS:H	3	1.42
(1,713)	1:87:A:HIS:HA	1:87:A:HIS:HD2	10	1.42
(1,324)	1:83:B:MET:H	1:84:B:THR:HG21	9	1.42
(1,824)	1:86:B:LYS:HG3	1:87:B:HIS:HB3	19	1.41
(1,805)	1:57:B:LEU:HD11	1:86:A:LYS:H	19	1.41
(1,788)	1:65:A:LEU:HG	1:66:A:LYS:H	16	1.41
(1,760)	1:86:A:LYS:HG2	1:87:A:HIS:H	2	1.41
(1,745)	1:72:B:HIS:H	1:75:B:LEU:HD13	18	1.41
(1,731)	1:86:A:LYS:HD3	1:87:A:HIS:HA	8	1.41
(1,676)	1:88:B:LEU:HB2	1:89:B:ARG:HB2	5	1.41
(1,551)	1:67:B:LYS:HA	1:67:B:LYS:HE2	6	1.41
(1,483)	1:76:B:GLU:HA	1:80:B:ILE:HB	5	1.41
(1,483)	1:76:A:GLU:HA	1:80:A:ILE:HB	7	1.41
(1,324)	1:83:B:MET:H	1:84:B:THR:HG22	4	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,268)	1:86:A:LYS:H	1:84:A:THR:HG21	10	1.41
(1,487)	1:88:A:LEU:HA	1:91:A:LEU:HA	13	1.4
(1,731)	1:86:A:LYS:HD3	1:87:A:HIS:HA	7	1.39
(1,710)	1:87:A:HIS:HA	1:87:A:HIS:HD1	7	1.39
(1,710)	1:87:B:HIS:HA	1:87:B:HIS:HD1	15	1.39
(1,676)	1:88:B:LEU:HB2	1:89:B:ARG:HB2	12	1.39
(1,483)	1:76:B:GLU:HA	1:80:B:ILE:HB	9	1.39
(1,324)	1:83:A:MET:H	1:84:A:THR:HG23	7	1.39
(1,324)	1:83:B:MET:H	1:84:B:THR:HG21	17	1.39
(1,277)	1:54:B:LEU:HD22	1:80:B:ILE:H	12	1.39
(1,277)	1:54:B:LEU:HD22	1:80:B:ILE:H	17	1.39
(1,35)	1:66:B:LYS:HG2	1:67:B:LYS:H	7	1.39
(1,35)	1:66:A:LYS:HG2	1:67:A:LYS:H	8	1.39
(1,731)	1:86:A:LYS:HD3	1:87:A:HIS:HA	1	1.38
(1,731)	1:86:A:LYS:HD3	1:87:A:HIS:HA	9	1.38
(1,676)	1:88:B:LEU:HB2	1:89:B:ARG:HB2	9	1.38
(1,626)	1:83:B:MET:HE1	1:84:B:THR:HG22	7	1.38
(1,520)	1:68:B:ASP:H	1:69:B:SER:HB3	13	1.38
(1,487)	1:88:B:LEU:HA	1:91:B:LEU:HA	8	1.38
(1,483)	1:76:A:GLU:HA	1:80:A:ILE:HB	18	1.38
(1,467)	1:68:A:ASP:HA	1:71:A:ARG:HD2	18	1.38
(1,421)	1:79:A:ASP:HB3	1:80:A:ILE:HB	2	1.38
(1,936)	1:75:B:LEU:H	1:71:B:ARG:O	1	1.37
(1,935)	1:74:A:LYS:N	1:70:A:SER:O	2	1.37
(1,815)	1:85:A:VAL:HA	1:60:B:LEU:HD13	13	1.37
(1,789)	1:66:B:LYS:HA	1:69:B:SER:HG	5	1.37
(1,788)	1:65:B:LEU:HG	1:66:B:LYS:H	8	1.37
(1,669)	1:88:B:LEU:HB3	1:91:B:LEU:HG	2	1.37
(1,609)	1:92:B:GLN:HB3	1:93:B:ARG:HB2	14	1.37
(1,573)	1:64:B:ALA:HB1	1:65:B:LEU:HD21	7	1.37
(1,551)	1:67:B:LYS:HA	1:67:B:LYS:HE3	20	1.37
(1,407)	1:93:B:ARG:HA	1:94:B:ALA:HB1	11	1.37
(1,324)	1:83:A:MET:H	1:84:A:THR:HG23	3	1.37
(1,324)	1:83:B:MET:H	1:84:B:THR:HG23	6	1.37
(1,322)	1:90:A:ASN:H	1:92:A:GLN:HG2	5	1.37
(1,270)	1:79:A:ASP:H	1:54:A:LEU:HD21	4	1.37
(1,936)	1:75:A:LEU:H	1:71:A:ARG:O	6	1.36
(1,824)	1:86:B:LYS:HG3	1:87:B:HIS:HB2	15	1.36
(1,744)	1:66:A:LYS:HD3	1:67:A:LYS:H	4	1.36
(1,676)	1:88:B:LEU:HB2	1:89:B:ARG:HB2	8	1.36
(1,673)	1:56:B:GLN:HG2	1:82:A:GLU:HB2	17	1.36
(1,574)	1:64:B:ALA:HB2	1:65:B:LEU:HD22	8	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,483)	1:76:A:GLU:HA	1:80:A:ILE:HB	10	1.36
(1,458)	1:76:B:GLU:HB3	1:80:B:ILE:HB	19	1.36
(1,324)	1:83:B:MET:H	1:84:B:THR:HG23	13	1.36
(1,324)	1:83:B:MET:H	1:84:B:THR:HG23	14	1.36
(1,324)	1:83:A:MET:H	1:84:A:THR:HG22	16	1.36
(1,277)	1:54:B:LEU:HD23	1:80:B:ILE:H	7	1.36
(1,824)	1:86:B:LYS:HG3	1:87:B:HIS:HB3	10	1.35
(1,731)	1:86:B:LYS:HD3	1:87:B:HIS:HA	20	1.35
(1,626)	1:83:A:MET:HE1	1:84:A:THR:HG21	5	1.35
(1,483)	1:76:A:GLU:HA	1:80:A:ILE:HB	8	1.35
(1,483)	1:76:B:GLU:HA	1:80:B:ILE:HB	12	1.35
(1,709)	1:86:B:LYS:HA	1:86:B:LYS:HD3	3	1.34
(1,709)	1:86:A:LYS:HA	1:86:A:LYS:HD3	15	1.34
(1,676)	1:88:B:LEU:HB2	1:89:B:ARG:HB2	18	1.34
(1,574)	1:64:A:ALA:HB2	1:65:A:LEU:HD23	19	1.34
(1,324)	1:83:A:MET:H	1:84:A:THR:HG21	11	1.34
(1,816)	1:60:A:LEU:HD11	1:86:B:LYS:H	5	1.33
(1,709)	1:86:B:LYS:HA	1:86:B:LYS:HD3	19	1.33
(1,676)	1:88:A:LEU:HB2	1:89:A:ARG:HB2	2	1.33
(1,467)	1:68:B:ASP:HA	1:71:B:ARG:HD2	19	1.33
(1,324)	1:83:B:MET:H	1:84:B:THR:HG23	12	1.33
(1,826)	1:87:A:HIS:H	1:87:A:HIS:HD1	4	1.32
(1,609)	1:92:A:GLN:HB3	1:93:A:ARG:HB2	5	1.32
(1,483)	1:76:B:GLU:HA	1:80:B:ILE:HB	6	1.32
(1,482)	1:81:B:LEU:HA	1:84:B:THR:HB	10	1.32
(1,324)	1:83:B:MET:H	1:84:B:THR:HG23	1	1.32
(1,324)	1:83:B:MET:H	1:84:B:THR:HG22	5	1.32
(1,324)	1:83:A:MET:H	1:84:A:THR:HG22	18	1.32
(1,805)	1:57:B:LEU:HD13	1:86:A:LYS:H	1	1.31
(1,805)	1:57:B:LEU:HD13	1:86:A:LYS:H	12	1.31
(1,788)	1:65:A:LEU:HG	1:66:A:LYS:H	20	1.31
(1,731)	1:86:B:LYS:HD3	1:87:B:HIS:HA	17	1.31
(1,731)	1:86:A:LYS:HD3	1:87:A:HIS:HA	18	1.31
(1,676)	1:88:B:LEU:HB2	1:89:B:ARG:HB2	3	1.31
(1,676)	1:88:A:LEU:HB2	1:89:A:ARG:HB2	20	1.31
(1,598)	1:66:B:LYS:HB2	1:67:B:LYS:HG2	12	1.31
(1,573)	1:64:B:ALA:HB1	1:65:B:LEU:HD21	2	1.31
(1,520)	1:68:B:ASP:H	1:69:B:SER:HB2	1	1.31
(1,483)	1:76:B:GLU:HA	1:80:B:ILE:HB	3	1.31
(1,421)	1:79:B:ASP:HB3	1:80:B:ILE:HB	19	1.31
(1,407)	1:93:B:ARG:HA	1:94:B:ALA:HB1	7	1.31
(1,324)	1:83:A:MET:H	1:84:A:THR:HG22	8	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,277)	1:54:A:LEU:HD21	1:80:A:ILE:H	6	1.31
(1,936)	1:75:B:LEU:H	1:71:B:ARG:O	14	1.3
(1,816)	1:60:B:LEU:HD11	1:86:A:LYS:H	11	1.3
(1,805)	1:57:B:LEU:HD12	1:86:A:LYS:H	8	1.3
(1,789)	1:66:A:LYS:HA	1:69:A:SER:HG	8	1.3
(1,788)	1:65:A:LEU:HG	1:66:A:LYS:H	10	1.3
(1,709)	1:86:B:LYS:HA	1:86:B:LYS:HD3	11	1.3
(1,609)	1:92:A:GLN:HB2	1:93:A:ARG:HB2	13	1.3
(1,609)	1:92:A:GLN:HB2	1:93:A:ARG:HB2	18	1.3
(1,573)	1:64:B:ALA:HB1	1:65:B:LEU:HD23	20	1.3
(1,551)	1:67:B:LYS:HA	1:67:B:LYS:HE3	4	1.3
(1,551)	1:67:B:LYS:HA	1:67:B:LYS:HE2	17	1.3
(1,467)	1:68:A:ASP:HA	1:71:A:ARG:HD2	10	1.3
(1,322)	1:90:B:ASN:H	1:92:B:GLN:HG2	20	1.3
(1,35)	1:66:B:LYS:HG2	1:67:B:LYS:H	13	1.3
(1,35)	1:66:A:LYS:HG2	1:67:A:LYS:H	20	1.3
(1,826)	1:87:B:HIS:H	1:87:B:HIS:HD2	17	1.29
(1,788)	1:65:A:LEU:HG	1:66:A:LYS:H	7	1.29
(1,774)	1:86:A:LYS:HD3	1:88:A:LEU:H	10	1.29
(1,745)	1:72:A:HIS:H	1:75:A:LEU:HD13	11	1.29
(1,713)	1:87:B:HIS:HA	1:87:B:HIS:HD2	11	1.29
(1,709)	1:86:B:LYS:HA	1:86:B:LYS:HD3	4	1.29
(1,609)	1:92:A:GLN:HB3	1:93:A:ARG:HB2	4	1.29
(1,421)	1:79:A:ASP:HB3	1:80:A:ILE:HB	6	1.29
(1,407)	1:93:A:ARG:HA	1:94:A:ALA:HB2	3	1.29
(1,35)	1:66:A:LYS:HG2	1:67:A:LYS:H	2	1.29
(1,35)	1:66:B:LYS:HG2	1:67:B:LYS:H	6	1.29
(1,857)	1:93:A:ARG:HB2	1:95:A:GLN:HB2	19	1.28
(1,826)	1:87:B:HIS:H	1:87:B:HIS:HD1	9	1.28
(1,826)	1:87:B:HIS:H	1:87:B:HIS:HD1	11	1.28
(1,673)	1:56:B:GLN:HG2	1:82:A:GLU:HB2	13	1.28
(1,573)	1:64:B:ALA:HB1	1:65:B:LEU:HD23	16	1.28
(1,552)	1:93:B:ARG:HB3	1:94:B:ALA:HA	5	1.28
(1,551)	1:67:B:LYS:HA	1:67:B:LYS:HE2	15	1.28
(1,483)	1:76:B:GLU:HA	1:80:B:ILE:HB	16	1.28
(1,936)	1:75:A:LEU:H	1:71:A:ARG:O	3	1.27
(1,824)	1:86:A:LYS:HG3	1:87:A:HIS:HB2	8	1.27
(1,788)	1:65:A:LEU:HG	1:66:A:LYS:H	1	1.27
(1,731)	1:86:A:LYS:HD3	1:87:A:HIS:HA	5	1.27
(1,713)	1:87:A:HIS:HA	1:87:A:HIS:HD2	14	1.27
(1,700)	1:87:B:HIS:HD1	1:91:B:LEU:HA	14	1.27
(1,676)	1:88:A:LEU:HB2	1:89:A:ARG:HB2	1	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,676)	1:88:A:LEU:HB2	1:89:A:ARG:HB2	10	1.27
(1,673)	1:56:A:GLN:HG2	1:82:B:GLU:HB2	14	1.27
(1,598)	1:66:B:LYS:HB2	1:67:B:LYS:HG2	5	1.27
(1,496)	1:64:B:ALA:H	1:65:B:LEU:HD22	10	1.27
(1,35)	1:66:B:LYS:HG2	1:67:B:LYS:H	1	1.27
(1,35)	1:66:A:LYS:HG2	1:67:A:LYS:H	4	1.27
(1,35)	1:66:A:LYS:HG2	1:67:A:LYS:H	12	1.27
(1,35)	1:66:B:LYS:HG2	1:67:B:LYS:H	19	1.27
(1,826)	1:87:A:HIS:H	1:87:A:HIS:HD1	8	1.26
(1,805)	1:57:B:LEU:HD11	1:86:A:LYS:H	7	1.26
(1,805)	1:57:B:LEU:HD11	1:86:A:LYS:H	17	1.26
(1,789)	1:66:B:LYS:HA	1:69:B:SER:HG	15	1.26
(1,598)	1:66:A:LYS:HB2	1:67:A:LYS:HG2	7	1.26
(1,520)	1:68:A:ASP:H	1:69:A:SER:HB2	11	1.26
(1,520)	1:68:A:ASP:H	1:69:A:SER:HB2	20	1.26
(1,483)	1:76:B:GLU:HA	1:80:B:ILE:HB	2	1.26
(1,379)	1:65:B:LEU:HD21	1:66:B:LYS:H	8	1.26
(1,277)	1:54:B:LEU:HD22	1:80:B:ILE:H	5	1.26
(1,35)	1:66:B:LYS:HG2	1:67:B:LYS:H	10	1.26
(1,826)	1:87:B:HIS:H	1:87:B:HIS:HD1	6	1.25
(1,815)	1:85:B:VAL:HA	1:60:A:LEU:HD11	17	1.25
(1,731)	1:86:B:LYS:HD3	1:87:B:HIS:HA	13	1.25
(1,647)	1:90:A:ASN:HB2	1:65:A:LEU:HD11	5	1.25
(1,573)	1:64:A:ALA:HB1	1:65:A:LEU:HD22	3	1.25
(1,482)	1:81:B:LEU:HA	1:84:B:THR:HB	19	1.25
(1,322)	1:90:B:ASN:H	1:92:B:GLN:HG2	4	1.25
(1,277)	1:54:A:LEU:HD21	1:80:A:ILE:H	1	1.25
(1,934)	1:74:B:LYS:H	1:70:B:SER:O	6	1.24
(1,824)	1:86:A:LYS:HG3	1:87:A:HIS:HB2	3	1.24
(1,745)	1:72:B:HIS:H	1:75:B:LEU:HD13	8	1.24
(1,700)	1:87:B:HIS:HD1	1:91:B:LEU:HA	6	1.24
(1,609)	1:92:A:GLN:HB3	1:93:A:ARG:HB2	1	1.24
(1,520)	1:68:A:ASP:H	1:69:A:SER:HB2	2	1.24
(1,498)	1:65:B:LEU:HD23	1:67:B:LYS:H	12	1.24
(1,487)	1:88:B:LEU:HA	1:91:B:LEU:HA	18	1.24
(1,407)	1:93:A:ARG:HA	1:94:A:ALA:HB1	16	1.24
(1,857)	1:93:B:ARG:HB2	1:95:B:GLN:HB2	13	1.23
(1,826)	1:87:B:HIS:H	1:87:B:HIS:HD2	15	1.23
(1,788)	1:65:B:LEU:HG	1:66:B:LYS:H	18	1.23
(1,745)	1:72:A:HIS:H	1:75:A:LEU:HD11	5	1.23
(1,552)	1:93:B:ARG:HB3	1:94:B:ALA:HA	9	1.23
(1,483)	1:76:A:GLU:HA	1:80:A:ILE:HB	11	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,379)	1:65:A:LEU:HD22	1:66:A:LYS:H	20	1.23
(1,324)	1:83:A:MET:H	1:84:A:THR:HG22	2	1.23
(1,322)	1:90:B:ASN:H	1:92:B:GLN:HG2	12	1.23
(1,277)	1:54:B:LEU:HD21	1:80:B:ILE:H	9	1.23
(1,96)	1:90:B:ASN:HB2	1:92:B:GLN:H	1	1.23
(1,96)	1:90:B:ASN:HB2	1:92:B:GLN:H	4	1.23
(1,836)	1:87:B:HIS:HD1	1:92:A:GLN:HE21	19	1.22
(1,826)	1:87:B:HIS:H	1:87:B:HIS:HD1	1	1.22
(1,826)	1:87:A:HIS:H	1:87:A:HIS:HD2	2	1.22
(1,826)	1:87:A:HIS:H	1:87:A:HIS:HD1	18	1.22
(1,754)	1:86:A:LYS:HD3	1:87:A:HIS:H	16	1.22
(1,710)	1:87:A:HIS:HA	1:87:A:HIS:HD1	5	1.22
(1,626)	1:83:A:MET:HE1	1:84:A:THR:HG23	6	1.22
(1,552)	1:93:A:ARG:HB3	1:94:A:ALA:HA	7	1.22
(1,407)	1:93:B:ARG:HA	1:94:B:ALA:HB2	1	1.22
(1,96)	1:90:A:ASN:HB2	1:92:A:GLN:H	9	1.22
(1,805)	1:57:B:LEU:HD11	1:86:A:LYS:H	9	1.21
(1,552)	1:93:B:ARG:HB3	1:94:B:ALA:HA	12	1.21
(1,520)	1:68:B:ASP:H	1:69:B:SER:HB3	18	1.21
(1,407)	1:93:B:ARG:HA	1:94:B:ALA:HB3	17	1.21
(1,379)	1:65:B:LEU:HD21	1:66:B:LYS:H	19	1.21
(1,277)	1:54:A:LEU:HD21	1:80:A:ILE:H	16	1.21
(1,96)	1:90:A:ASN:HB2	1:92:A:GLN:H	3	1.21
(1,816)	1:60:A:LEU:HD11	1:86:B:LYS:H	17	1.2
(1,782)	1:64:A:ALA:HB3	1:66:A:LYS:H	11	1.2
(1,782)	1:64:B:ALA:HB3	1:66:B:LYS:H	15	1.2
(1,782)	1:64:A:ALA:HB3	1:66:A:LYS:H	17	1.2
(1,676)	1:88:B:LEU:HB2	1:89:B:ARG:HB2	11	1.2
(1,598)	1:66:A:LYS:HB2	1:67:A:LYS:HG2	20	1.2
(1,276)	1:75:B:LEU:H	1:75:B:LEU:HD12	8	1.2
(1,181)	1:83:B:MET:H	1:84:B:THR:HG21	9	1.2
(1,826)	1:87:B:HIS:H	1:87:B:HIS:HD1	16	1.19
(1,788)	1:65:A:LEU:HG	1:66:A:LYS:H	19	1.19
(1,487)	1:88:A:LEU:HA	1:91:A:LEU:HA	16	1.19
(1,483)	1:76:B:GLU:HA	1:80:B:ILE:HB	20	1.19
(1,407)	1:93:A:ARG:HA	1:94:A:ALA:HB1	10	1.19
(1,379)	1:65:B:LEU:HD23	1:66:B:LYS:H	14	1.19
(1,181)	1:83:B:MET:H	1:84:B:THR:HG22	4	1.19
(1,936)	1:75:A:LEU:H	1:71:A:ARG:O	5	1.18
(1,846)	1:90:A:ASN:HA	1:90:A:ASN:HD21	2	1.18
(1,846)	1:90:B:ASN:HA	1:90:B:ASN:HD21	14	1.18
(1,700)	1:87:B:HIS:HD1	1:91:B:LEU:HA	2	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,700)	1:87:A:HIS:HD1	1:91:A:LEU:HA	11	1.18
(1,673)	1:56:A:GLN:HG2	1:82:B:GLU:HB2	7	1.18
(1,598)	1:66:B:LYS:HB2	1:67:B:LYS:HG2	6	1.18
(1,598)	1:66:B:LYS:HB2	1:67:B:LYS:HG2	14	1.18
(1,552)	1:93:A:ARG:HB3	1:94:A:ALA:HA	6	1.18
(1,552)	1:93:A:ARG:HB3	1:94:A:ALA:HA	20	1.18
(1,551)	1:67:B:LYS:HA	1:67:B:LYS:HE2	7	1.18
(1,407)	1:93:B:ARG:HA	1:94:B:ALA:HB2	15	1.18
(1,96)	1:90:B:ASN:HB2	1:92:B:GLN:H	15	1.18
(1,35)	1:66:B:LYS:HG2	1:67:B:LYS:H	11	1.18
(1,934)	1:74:A:LYS:H	1:70:A:SER:O	9	1.17
(1,846)	1:90:B:ASN:HA	1:90:B:ASN:HD21	15	1.17
(1,805)	1:57:B:LEU:HD13	1:86:A:LYS:H	16	1.17
(1,598)	1:66:B:LYS:HB2	1:67:B:LYS:HG2	11	1.17
(1,598)	1:66:A:LYS:HB2	1:67:A:LYS:HG2	15	1.17
(1,552)	1:93:B:ARG:HB3	1:94:B:ALA:HA	4	1.17
(1,552)	1:93:B:ARG:HB3	1:94:B:ALA:HA	19	1.17
(1,407)	1:93:A:ARG:HA	1:94:A:ALA:HB3	2	1.17
(1,407)	1:93:B:ARG:HA	1:94:B:ALA:HB1	18	1.17
(1,181)	1:83:A:MET:H	1:84:A:THR:HG23	7	1.17
(1,181)	1:83:B:MET:H	1:84:B:THR:HG21	17	1.17
(1,96)	1:90:B:ASN:HB2	1:92:B:GLN:H	7	1.17
(1,35)	1:66:A:LYS:HG2	1:67:A:LYS:H	3	1.17
(1,35)	1:66:B:LYS:HG2	1:67:B:LYS:H	5	1.17
(1,934)	1:74:A:LYS:H	1:70:A:SER:O	7	1.16
(1,846)	1:90:B:ASN:HA	1:90:B:ASN:HD21	6	1.16
(1,846)	1:90:B:ASN:HA	1:90:B:ASN:HD21	7	1.16
(1,846)	1:90:B:ASN:HA	1:90:B:ASN:HD21	13	1.16
(1,846)	1:90:B:ASN:HA	1:90:B:ASN:HD21	16	1.16
(1,824)	1:86:A:LYS:HG3	1:87:A:HIS:HB2	12	1.16
(1,816)	1:60:B:LEU:HD13	1:86:A:LYS:H	13	1.16
(1,805)	1:57:B:LEU:HD11	1:86:A:LYS:H	2	1.16
(1,745)	1:72:A:HIS:H	1:75:A:LEU:HD13	16	1.16
(1,743)	1:61:A:ILE:HD11	1:62:A:LEU:H	18	1.16
(1,552)	1:93:A:ARG:HB3	1:94:A:ALA:HA	1	1.16
(1,552)	1:93:B:ARG:HB3	1:94:B:ALA:HA	10	1.16
(1,484)	1:91:B:LEU:HA	1:93:B:ARG:HA	17	1.16
(1,407)	1:93:A:ARG:HA	1:94:A:ALA:HB1	4	1.16
(1,96)	1:90:B:ASN:HB2	1:92:B:GLN:H	19	1.16
(1,50)	1:68:A:ASP:HA	1:71:A:ARG:H	6	1.16
(1,846)	1:90:A:ASN:HA	1:90:A:ASN:HD21	3	1.15
(1,846)	1:90:A:ASN:HA	1:90:A:ASN:HD21	8	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,846)	1:90:B:ASN:HA	1:90:B:ASN:HD21	11	1.15
(1,846)	1:90:A:ASN:HA	1:90:A:ASN:HD21	12	1.15
(1,846)	1:90:A:ASN:HA	1:90:A:ASN:HD21	17	1.15
(1,782)	1:64:A:ALA:HB1	1:66:A:LYS:H	5	1.15
(1,782)	1:64:B:ALA:HB2	1:66:B:LYS:H	6	1.15
(1,782)	1:64:A:ALA:HB1	1:66:A:LYS:H	9	1.15
(1,676)	1:88:B:LEU:HB2	1:89:B:ARG:HB2	19	1.15
(1,673)	1:56:A:GLN:HG2	1:82:B:GLU:HB2	18	1.15
(1,552)	1:93:B:ARG:HB3	1:94:B:ALA:HA	3	1.15
(1,520)	1:68:A:ASP:H	1:69:A:SER:HB2	3	1.15
(1,487)	1:88:A:LEU:HA	1:91:A:LEU:HA	7	1.15
(1,407)	1:93:B:ARG:HA	1:94:B:ALA:HB2	6	1.15
(1,379)	1:65:B:LEU:HD22	1:66:B:LYS:H	1	1.15
(1,379)	1:65:B:LEU:HD22	1:66:B:LYS:H	18	1.15
(1,277)	1:54:B:LEU:HD23	1:80:B:ILE:H	19	1.15
(1,274)	1:86:B:LYS:HG2	1:89:B:ARG:H	3	1.15
(1,268)	1:86:A:LYS:H	1:84:A:THR:HG23	2	1.15
(1,268)	1:86:A:LYS:H	1:84:A:THR:HG23	20	1.15
(1,181)	1:83:A:MET:H	1:84:A:THR:HG23	3	1.15
(1,181)	1:83:B:MET:H	1:84:B:THR:HG23	6	1.15
(1,96)	1:90:B:ASN:HB2	1:92:B:GLN:H	8	1.15
(1,96)	1:90:A:ASN:HB2	1:92:A:GLN:H	11	1.15
(1,96)	1:90:B:ASN:HB2	1:92:B:GLN:H	18	1.15
(1,886)	1:76:A:GLU:HG3	1:80:A:ILE:HD13	15	1.14
(1,846)	1:90:B:ASN:HA	1:90:B:ASN:HD21	9	1.14
(1,846)	1:90:A:ASN:HA	1:90:A:ASN:HD21	18	1.14
(1,805)	1:57:A:LEU:HD11	1:86:B:LYS:H	4	1.14
(1,743)	1:61:B:ILE:HD11	1:62:B:LEU:H	12	1.14
(1,743)	1:61:B:ILE:HD13	1:62:B:LEU:H	19	1.14
(1,743)	1:61:B:ILE:HD12	1:62:B:LEU:H	20	1.14
(1,676)	1:88:A:LEU:HB2	1:89:A:ARG:HB2	6	1.14
(1,552)	1:93:A:ARG:HB3	1:94:A:ALA:HA	13	1.14
(1,552)	1:93:A:ARG:HB3	1:94:A:ALA:HA	14	1.14
(1,551)	1:67:A:LYS:HA	1:67:A:LYS:HE3	1	1.14
(1,551)	1:67:A:LYS:HA	1:67:A:LYS:HE2	18	1.14
(1,407)	1:93:A:ARG:HA	1:94:A:ALA:HB1	13	1.14
(1,322)	1:90:A:ASN:H	1:92:A:GLN:HG2	7	1.14
(1,322)	1:90:B:ASN:H	1:92:B:GLN:HG2	11	1.14
(1,277)	1:54:B:LEU:HD22	1:80:B:ILE:H	2	1.14
(1,181)	1:83:B:MET:H	1:84:B:THR:HG23	13	1.14
(1,181)	1:83:B:MET:H	1:84:B:THR:HG23	14	1.14
(1,181)	1:83:A:MET:H	1:84:A:THR:HG22	16	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,96)	1:90:B:ASN:HB2	1:92:B:GLN:H	6	1.14
(1,52)	1:71:A:ARG:HB3	1:72:A:HIS:H	14	1.14
(1,846)	1:90:A:ASN:HA	1:90:A:ASN:HD21	1	1.13
(1,846)	1:90:B:ASN:HA	1:90:B:ASN:HD21	4	1.13
(1,846)	1:90:A:ASN:HA	1:90:A:ASN:HD21	20	1.13
(1,782)	1:64:A:ALA:HB1	1:66:A:LYS:H	1	1.13
(1,743)	1:61:B:ILE:HD12	1:62:B:LEU:H	2	1.13
(1,743)	1:61:B:ILE:HD13	1:62:B:LEU:H	11	1.13
(1,743)	1:61:B:ILE:HD13	1:62:B:LEU:H	16	1.13
(1,673)	1:56:B:GLN:HG2	1:82:A:GLU:HB2	2	1.13
(1,551)	1:67:A:LYS:HA	1:67:A:LYS:HE2	13	1.13
(1,487)	1:88:B:LEU:HA	1:91:B:LEU:HA	2	1.13
(1,483)	1:76:B:GLU:HA	1:80:B:ILE:HB	14	1.13
(1,407)	1:93:A:ARG:HA	1:94:A:ALA:HB1	8	1.13
(1,379)	1:65:A:LEU:HD23	1:66:A:LYS:H	2	1.13
(1,96)	1:90:B:ASN:HB2	1:92:B:GLN:H	14	1.13
(1,846)	1:90:B:ASN:HA	1:90:B:ASN:HD21	19	1.12
(1,826)	1:87:B:HIS:H	1:87:B:HIS:HD1	7	1.12
(1,824)	1:86:A:LYS:HG3	1:87:A:HIS:HB2	2	1.12
(1,805)	1:57:B:LEU:HD12	1:86:A:LYS:H	3	1.12
(1,805)	1:57:B:LEU:HD11	1:86:A:LYS:H	11	1.12
(1,743)	1:61:A:ILE:HD13	1:62:A:LEU:H	6	1.12
(1,743)	1:61:A:ILE:HD11	1:62:A:LEU:H	7	1.12
(1,673)	1:56:B:GLN:HG2	1:82:A:GLU:HB2	19	1.12
(1,669)	1:88:A:LEU:HB3	1:91:A:LEU:HG	17	1.12
(1,598)	1:66:A:LYS:HB2	1:67:A:LYS:HG2	18	1.12
(1,573)	1:64:A:ALA:HB1	1:65:A:LEU:HD21	10	1.12
(1,552)	1:93:A:ARG:HB3	1:94:A:ALA:HA	15	1.12
(1,552)	1:93:B:ARG:HB3	1:94:B:ALA:HA	16	1.12
(1,552)	1:93:A:ARG:HB3	1:94:A:ALA:HA	18	1.12
(1,407)	1:93:B:ARG:HA	1:94:B:ALA:HB2	20	1.12
(1,268)	1:86:B:LYS:H	1:84:B:THR:HG21	3	1.12
(1,181)	1:83:A:MET:H	1:84:A:THR:HG21	11	1.12
(1,52)	1:71:A:ARG:HB2	1:72:A:HIS:H	12	1.12
(1,52)	1:71:A:ARG:HB3	1:72:A:HIS:H	16	1.12
(1,846)	1:90:B:ASN:HA	1:90:B:ASN:HD21	5	1.11
(1,805)	1:57:B:LEU:HD11	1:86:A:LYS:H	13	1.11
(1,788)	1:65:A:LEU:HG	1:66:A:LYS:H	9	1.11
(1,782)	1:64:B:ALA:HB1	1:66:B:LYS:H	4	1.11
(1,782)	1:64:A:ALA:HB2	1:66:A:LYS:H	7	1.11
(1,674)	1:88:B:LEU:HB2	1:91:B:LEU:HG	15	1.11
(1,609)	1:92:A:GLN:HB3	1:93:A:ARG:HB2	12	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,467)	1:68:A:ASP:HA	1:71:A:ARG:HD2	7	1.11
(1,467)	1:68:B:ASP:HA	1:71:B:ARG:HD2	14	1.11
(1,420)	1:87:B:HIS:HD2	1:91:B:LEU:HA	17	1.11
(1,407)	1:93:A:ARG:HA	1:94:A:ALA:HB1	5	1.11
(1,322)	1:90:A:ASN:H	1:92:A:GLN:HG2	2	1.11
(1,268)	1:86:A:LYS:H	1:84:A:THR:HG23	18	1.11
(1,181)	1:83:B:MET:H	1:84:B:THR:HG23	12	1.11
(1,96)	1:90:A:ASN:HB2	1:92:A:GLN:H	5	1.11
(1,96)	1:90:A:ASN:HB2	1:92:A:GLN:H	13	1.11
(1,888)	1:77:A:LYS:HE3	1:81:A:LEU:HD23	9	1.1
(1,846)	1:90:B:ASN:HA	1:90:B:ASN:HD21	10	1.1
(1,816)	1:60:B:LEU:HD13	1:86:A:LYS:H	3	1.1
(1,782)	1:64:A:ALA:HB1	1:66:A:LYS:H	16	1.1
(1,782)	1:64:B:ALA:HB2	1:66:B:LYS:H	18	1.1
(1,782)	1:64:B:ALA:HB1	1:66:B:LYS:H	20	1.1
(1,743)	1:61:A:ILE:HD13	1:62:A:LEU:H	3	1.1
(1,743)	1:61:B:ILE:HD12	1:62:B:LEU:H	13	1.1
(1,743)	1:61:B:ILE:HD11	1:62:B:LEU:H	14	1.1
(1,598)	1:66:B:LYS:HB2	1:67:B:LYS:HG2	19	1.1
(1,552)	1:93:A:ARG:HB3	1:94:A:ALA:HA	17	1.1
(1,551)	1:67:B:LYS:HA	1:67:B:LYS:HE2	14	1.1
(1,520)	1:68:A:ASP:H	1:69:A:SER:HB3	14	1.1
(1,487)	1:88:A:LEU:HA	1:91:A:LEU:HA	12	1.1
(1,467)	1:68:B:ASP:HA	1:71:B:ARG:HD2	2	1.1
(1,407)	1:93:A:ARG:HA	1:94:A:ALA:HB1	19	1.1
(1,379)	1:65:A:LEU:HD22	1:66:A:LYS:H	11	1.1
(1,322)	1:90:A:ASN:H	1:92:A:GLN:HG2	1	1.1
(1,274)	1:86:A:LYS:HG2	1:89:A:ARG:H	2	1.1
(1,274)	1:86:B:LYS:HG2	1:89:B:ARG:H	10	1.1
(1,181)	1:83:B:MET:H	1:84:B:THR:HG23	1	1.1
(1,181)	1:83:B:MET:H	1:84:B:THR:HG22	5	1.1
(1,181)	1:83:A:MET:H	1:84:A:THR:HG22	18	1.1
(1,96)	1:90:A:ASN:HB2	1:92:A:GLN:H	12	1.1
(1,52)	1:71:A:ARG:HB2	1:72:A:HIS:H	15	1.1
(1,35)	1:66:A:LYS:HG2	1:67:A:LYS:H	16	1.1
(1,782)	1:64:B:ALA:HB2	1:66:B:LYS:H	10	1.09
(1,467)	1:68:B:ASP:HA	1:71:B:ARG:HD2	4	1.09
(1,277)	1:54:B:LEU:HD22	1:80:B:ILE:H	15	1.09
(1,181)	1:83:A:MET:H	1:84:A:THR:HG22	8	1.09
(1,96)	1:90:A:ASN:HB2	1:92:A:GLN:H	16	1.09
(1,52)	1:71:A:ARG:HB2	1:72:A:HIS:H	9	1.09
(1,52)	1:71:A:ARG:HB3	1:72:A:HIS:H	20	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,831)	1:87:B:HIS:HD1	1:91:B:LEU:H	14	1.08
(1,754)	1:86:B:LYS:HD3	1:87:B:HIS:H	6	1.08
(1,743)	1:61:B:ILE:HD13	1:62:B:LEU:H	5	1.08
(1,743)	1:61:B:ILE:HD12	1:62:B:LEU:H	10	1.08
(1,558)	1:81:A:LEU:HA	1:83:A:MET:HE2	5	1.08
(1,275)	1:86:A:LYS:HG2	1:88:A:LEU:H	18	1.08
(1,52)	1:71:B:ARG:HB3	1:72:B:HIS:H	1	1.08
(1,788)	1:65:B:LEU:HG	1:66:B:LYS:H	11	1.07
(1,754)	1:86:A:LYS:HD3	1:87:A:HIS:H	7	1.07
(1,754)	1:86:B:LYS:HD3	1:87:B:HIS:H	14	1.07
(1,743)	1:61:A:ILE:HD13	1:62:A:LEU:H	9	1.07
(1,673)	1:56:B:GLN:HG2	1:82:A:GLU:HB2	1	1.07
(1,379)	1:65:B:LEU:HD22	1:66:B:LYS:H	16	1.07
(1,277)	1:54:B:LEU:HD23	1:80:B:ILE:H	13	1.07
(1,276)	1:75:B:LEU:H	1:75:B:LEU:HD13	20	1.07
(1,268)	1:86:B:LYS:H	1:84:B:THR:HG21	16	1.07
(1,52)	1:71:A:ARG:HB3	1:72:A:HIS:H	5	1.07
(1,831)	1:87:A:HIS:HD1	1:91:A:LEU:H	11	1.06
(1,816)	1:60:B:LEU:HD11	1:86:A:LYS:H	9	1.06
(1,782)	1:64:A:ALA:HB2	1:66:A:LYS:H	12	1.06
(1,743)	1:61:A:ILE:HD11	1:62:A:LEU:H	1	1.06
(1,743)	1:61:A:ILE:HD11	1:62:A:LEU:H	4	1.06
(1,743)	1:61:A:ILE:HD12	1:62:A:LEU:H	15	1.06
(1,675)	1:84:A:THR:HG21	1:88:B:LEU:HB2	17	1.06
(1,626)	1:83:B:MET:HE2	1:84:B:THR:HG21	8	1.06
(1,625)	1:88:B:LEU:HB3	1:89:B:ARG:HB2	17	1.06
(1,520)	1:68:B:ASP:H	1:69:B:SER:HB3	8	1.06
(1,483)	1:76:B:GLU:HA	1:80:B:ILE:HB	4	1.06
(1,277)	1:54:B:LEU:HD23	1:80:B:ILE:H	11	1.06
(1,275)	1:86:A:LYS:HG2	1:88:A:LEU:H	17	1.06
(1,274)	1:86:B:LYS:HG2	1:89:B:ARG:H	8	1.06
(1,782)	1:64:A:ALA:HB3	1:66:A:LYS:H	14	1.05
(1,782)	1:64:B:ALA:HB3	1:66:B:LYS:H	19	1.05
(1,673)	1:56:A:GLN:HG2	1:82:B:GLU:HB2	12	1.05
(1,574)	1:64:A:ALA:HB2	1:65:A:LEU:HD23	7	1.05
(1,574)	1:64:B:ALA:HB2	1:65:B:LEU:HD23	18	1.05
(1,484)	1:91:A:LEU:HA	1:93:A:ARG:HA	3	1.05
(1,483)	1:76:A:GLU:HA	1:80:A:ILE:HB	15	1.05
(1,268)	1:86:B:LYS:H	1:84:B:THR:HG22	11	1.05
(1,96)	1:90:B:ASN:HB2	1:92:B:GLN:H	20	1.05
(1,886)	1:76:A:GLU:HG2	1:80:A:ILE:HD12	11	1.04
(1,782)	1:64:A:ALA:HB3	1:66:A:LYS:H	8	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	1:56:A:GLN:HG2	1:82:B:GLU:HB2	20	1.04
(1,574)	1:64:B:ALA:HB2	1:65:B:LEU:HD22	10	1.04
(1,520)	1:68:B:ASP:H	1:69:B:SER:HB2	4	1.04
(1,520)	1:68:A:ASP:H	1:69:A:SER:HB3	15	1.04
(1,496)	1:64:A:ALA:H	1:65:A:LEU:HD23	3	1.04
(1,484)	1:91:B:LEU:HA	1:93:B:ARG:HA	11	1.04
(1,96)	1:90:B:ASN:HB2	1:92:B:GLN:H	10	1.04
(1,52)	1:71:A:ARG:HB3	1:72:A:HIS:H	8	1.04
(1,52)	1:71:B:ARG:HB3	1:72:B:HIS:H	18	1.04
(1,934)	1:74:B:LYS:H	1:70:B:SER:O	17	1.03
(1,886)	1:76:B:GLU:HG2	1:80:B:ILE:HD11	3	1.03
(1,805)	1:57:B:LEU:HD13	1:86:A:LYS:H	18	1.03
(1,805)	1:57:A:LEU:HD11	1:86:B:LYS:H	20	1.03
(1,782)	1:64:A:ALA:HB3	1:66:A:LYS:H	2	1.03
(1,743)	1:61:A:ILE:HD12	1:62:A:LEU:H	8	1.03
(1,743)	1:61:B:ILE:HD12	1:62:B:LEU:H	17	1.03
(1,598)	1:66:B:LYS:HB2	1:67:B:LYS:HG2	13	1.03
(1,322)	1:90:B:ASN:H	1:92:B:GLN:HG2	18	1.03
(1,276)	1:75:B:LEU:H	1:75:B:LEU:HD13	14	1.03
(1,275)	1:86:B:LYS:HG2	1:88:B:LEU:H	19	1.03
(1,268)	1:86:A:LYS:H	1:84:A:THR:HG22	15	1.03
(1,886)	1:76:A:GLU:HG2	1:80:A:ILE:HD12	1	1.02
(1,782)	1:64:A:ALA:HB1	1:66:A:LYS:H	13	1.02
(1,744)	1:66:A:LYS:HD3	1:67:A:LYS:H	16	1.02
(1,674)	1:88:A:LEU:HB2	1:91:A:LEU:HG	4	1.02
(1,483)	1:76:B:GLU:HA	1:80:B:ILE:HB	13	1.02
(1,483)	1:76:B:GLU:HA	1:80:B:ILE:HB	19	1.02
(1,277)	1:54:B:LEU:HD23	1:80:B:ILE:H	18	1.02
(1,50)	1:68:A:ASP:HA	1:71:A:ARG:H	11	1.02
(1,886)	1:76:A:GLU:HG2	1:80:A:ILE:HD11	6	1.01
(1,674)	1:88:A:LEU:HB2	1:91:A:LEU:HG	20	1.01
(1,673)	1:56:A:GLN:HG2	1:82:B:GLU:HB2	4	1.01
(1,379)	1:65:B:LEU:HD22	1:66:B:LYS:H	10	1.01
(1,274)	1:86:B:LYS:HG2	1:89:B:ARG:H	13	1.01
(1,268)	1:86:B:LYS:H	1:84:B:THR:HG23	5	1.01
(1,268)	1:86:B:LYS:H	1:84:B:THR:HG21	12	1.01
(1,181)	1:83:A:MET:H	1:84:A:THR:HG22	2	1.01
(1,50)	1:68:B:ASP:HA	1:71:B:ARG:H	13	1.01
(1,936)	1:75:A:LEU:H	1:71:A:ARG:O	17	1.0
(1,886)	1:76:A:GLU:HG2	1:80:A:ILE:HD12	18	1.0
(1,886)	1:76:A:GLU:HG2	1:80:A:ILE:HD13	20	1.0
(1,754)	1:86:B:LYS:HD3	1:87:B:HIS:H	12	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,558)	1:81:B:LEU:HA	1:83:B:MET:HE2	10	1.0
(1,552)	1:93:B:ARG:HB3	1:94:B:ALA:HA	2	1.0
(1,552)	1:93:B:ARG:HB3	1:94:B:ALA:HA	8	1.0
(1,552)	1:93:A:ARG:HB3	1:94:A:ALA:HA	11	1.0
(1,484)	1:91:B:LEU:HA	1:93:B:ARG:HA	18	1.0
(1,379)	1:65:B:LEU:HD23	1:66:B:LYS:H	7	1.0
(1,322)	1:90:B:ASN:H	1:92:B:GLN:HG2	9	1.0
(1,322)	1:90:B:ASN:H	1:92:B:GLN:HG2	19	1.0
(1,276)	1:75:A:LEU:H	1:75:A:LEU:HD13	3	1.0
(1,275)	1:86:B:LYS:HG2	1:88:B:LEU:H	3	1.0
(1,886)	1:76:B:GLU:HG3	1:80:B:ILE:HD11	13	0.99
(1,805)	1:57:B:LEU:HD21	1:86:A:LYS:H	14	0.99
(1,754)	1:86:A:LYS:HD3	1:87:A:HIS:H	2	0.99
(1,674)	1:88:B:LEU:HB2	1:91:B:LEU:HG	3	0.99
(1,467)	1:68:B:ASP:HA	1:71:B:ARG:HD2	8	0.99
(1,277)	1:54:A:LEU:HD21	1:80:A:ILE:H	10	0.99
(1,275)	1:86:B:LYS:HG2	1:88:B:LEU:H	7	0.99
(1,274)	1:86:B:LYS:HG2	1:89:B:ARG:H	11	0.99
(1,805)	1:57:B:LEU:HD21	1:86:A:LYS:H	5	0.98
(1,598)	1:66:B:LYS:HB2	1:67:B:LYS:HG2	1	0.98
(1,487)	1:88:A:LEU:HA	1:91:A:LEU:HA	17	0.98
(1,420)	1:87:B:HIS:HD2	1:91:B:LEU:HA	3	0.98
(1,322)	1:90:A:ASN:H	1:92:A:GLN:HG2	16	0.98
(1,275)	1:86:A:LYS:HG2	1:88:A:LEU:H	2	0.98
(1,189)	1:75:B:LEU:HA	1:79:B:ASP:H	9	0.98
(1,886)	1:76:A:GLU:HG2	1:80:A:ILE:HD13	8	0.97
(1,754)	1:86:A:LYS:HD3	1:87:A:HIS:H	1	0.97
(1,754)	1:86:A:LYS:HD3	1:87:A:HIS:H	9	0.97
(1,652)	1:85:A:VAL:HG13	1:86:A:LYS:HB2	10	0.97
(1,652)	1:85:A:VAL:HG13	1:86:A:LYS:HB3	11	0.97
(1,609)	1:92:B:GLN:HB3	1:93:B:ARG:HB2	2	0.97
(1,407)	1:93:A:ARG:HA	1:94:A:ALA:HB3	12	0.97
(1,322)	1:90:A:ASN:H	1:92:A:GLN:HG2	14	0.97
(1,316)	1:90:A:ASN:H	1:91:A:LEU:HG	10	0.97
(1,277)	1:54:A:LEU:HD21	1:80:A:ILE:H	20	0.97
(1,275)	1:86:B:LYS:HG2	1:88:B:LEU:H	13	0.97
(1,275)	1:86:A:LYS:HG2	1:88:A:LEU:H	16	0.97
(1,275)	1:86:A:LYS:HG2	1:88:A:LEU:H	20	0.97
(1,268)	1:86:B:LYS:H	1:84:B:THR:HG21	13	0.97
(1,50)	1:68:A:ASP:HA	1:71:A:ARG:H	18	0.97
(1,886)	1:76:B:GLU:HG3	1:80:B:ILE:HD13	14	0.96
(1,886)	1:76:A:GLU:HG3	1:80:A:ILE:HD13	17	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,782)	1:64:A:ALA:HB3	1:66:A:LYS:H	3	0.96
(1,674)	1:88:B:LEU:HB2	1:91:B:LEU:HG	6	0.96
(1,674)	1:88:A:LEU:HB2	1:91:A:LEU:HG	11	0.96
(1,652)	1:85:A:VAL:HG11	1:86:A:LYS:HB2	4	0.96
(1,598)	1:66:A:LYS:HB2	1:67:A:LYS:HG2	9	0.96
(1,582)	1:76:B:GLU:HB3	1:79:B:ASP:HB3	19	0.96
(1,414)	1:88:A:LEU:HA	1:89:A:ARG:HB2	1	0.96
(1,414)	1:88:A:LEU:HA	1:89:A:ARG:HB2	8	0.96
(1,324)	1:83:B:MET:H	1:84:B:THR:HG23	10	0.96
(1,886)	1:76:B:GLU:HG2	1:80:B:ILE:HD13	5	0.95
(1,831)	1:87:B:HIS:HD2	1:91:B:LEU:H	3	0.95
(1,674)	1:88:B:LEU:HB2	1:91:B:LEU:HG	14	0.95
(1,673)	1:56:B:GLN:HG2	1:82:A:GLU:HB2	6	0.95
(1,573)	1:64:A:ALA:HB1	1:65:A:LEU:HD21	1	0.95
(1,414)	1:88:B:LEU:HA	1:89:B:ARG:HB2	3	0.95
(1,414)	1:88:A:LEU:HA	1:89:A:ARG:HB2	9	0.95
(1,268)	1:86:A:LYS:H	1:84:A:THR:HG21	1	0.95
(1,96)	1:90:B:ASN:HB2	1:92:B:GLN:H	2	0.95
(1,50)	1:68:B:ASP:HA	1:71:B:ARG:H	12	0.95
(1,886)	1:76:A:GLU:HG2	1:80:A:ILE:HD12	16	0.94
(1,886)	1:76:B:GLU:HG3	1:80:B:ILE:HD11	19	0.94
(1,754)	1:86:B:LYS:HD3	1:87:B:HIS:H	20	0.94
(1,674)	1:88:B:LEU:HB2	1:91:B:LEU:HG	5	0.94
(1,488)	1:64:B:ALA:HA	1:65:B:LEU:HD13	4	0.94
(1,379)	1:65:A:LEU:HD23	1:66:A:LYS:H	3	0.94
(1,324)	1:83:B:MET:H	1:84:B:THR:HG22	15	0.94
(1,322)	1:90:A:ASN:H	1:92:A:GLN:HG2	17	0.94
(1,275)	1:86:B:LYS:HG2	1:88:B:LEU:H	15	0.94
(1,274)	1:86:B:LYS:HG2	1:89:B:ARG:H	15	0.94
(1,274)	1:86:A:LYS:HG2	1:89:A:ARG:H	18	0.94
(1,268)	1:86:B:LYS:H	1:84:B:THR:HG23	7	0.94
(1,50)	1:68:A:ASP:HA	1:71:A:ARG:H	4	0.94
(1,936)	1:75:A:LEU:H	1:71:A:ARG:O	11	0.93
(1,744)	1:66:B:LYS:HD3	1:67:B:LYS:H	1	0.93
(1,674)	1:88:A:LEU:HB2	1:91:A:LEU:HG	1	0.93
(1,268)	1:86:B:LYS:H	1:84:B:THR:HG23	4	0.93
(1,52)	1:71:B:ARG:HB2	1:72:B:HIS:H	3	0.93
(1,52)	1:71:A:ARG:HB3	1:72:A:HIS:H	11	0.93
(1,50)	1:68:A:ASP:HA	1:71:A:ARG:H	8	0.93
(1,886)	1:76:A:GLU:HG2	1:80:A:ILE:HD12	7	0.92
(1,886)	1:76:A:GLU:HG2	1:80:A:ILE:HD13	9	0.92
(1,877)	1:75:B:LEU:HD21	1:79:B:ASP:HA	6	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,744)	1:66:B:LYS:HD3	1:67:B:LYS:H	10	0.92
(1,652)	1:85:B:VAL:HG13	1:86:B:LYS:HB2	16	0.92
(1,520)	1:68:B:ASP:H	1:69:B:SER:HB3	12	0.92
(1,484)	1:91:A:LEU:HA	1:93:A:ARG:HA	1	0.92
(1,275)	1:86:B:LYS:HG2	1:88:B:LEU:H	8	0.92
(1,268)	1:86:A:LYS:H	1:84:A:THR:HG23	8	0.92
(1,268)	1:86:A:LYS:H	1:84:A:THR:HG23	9	0.92
(1,754)	1:86:B:LYS:HD3	1:87:B:HIS:H	17	0.91
(1,738)	1:76:A:GLU:HA	1:79:A:ASP:HB2	3	0.91
(1,673)	1:56:B:GLN:HG2	1:82:A:GLU:HB2	3	0.91
(1,582)	1:76:B:GLU:HB3	1:79:B:ASP:HB3	2	0.91
(1,484)	1:91:A:LEU:HA	1:93:A:ARG:HA	4	0.91
(1,484)	1:91:A:LEU:HA	1:93:A:ARG:HA	16	0.91
(1,414)	1:88:B:LEU:HA	1:89:B:ARG:HB2	14	0.91
(1,324)	1:83:A:MET:H	1:84:A:THR:HG23	19	0.91
(1,299)	1:82:A:GLU:HB3	1:84:A:THR:H	20	0.91
(1,275)	1:86:B:LYS:HG2	1:88:B:LEU:H	12	0.91
(1,96)	1:90:B:ASN:HB2	1:92:B:GLN:H	17	0.91
(1,894)	1:79:A:ASP:HB2	1:80:A:ILE:HD11	7	0.9
(1,894)	1:79:A:ASP:HB3	1:80:A:ILE:HD13	17	0.9
(1,762)	1:87:A:HIS:HD1	1:88:A:LEU:H	11	0.9
(1,744)	1:66:B:LYS:HD3	1:67:B:LYS:H	11	0.9
(1,676)	1:88:B:LEU:HB2	1:89:B:ARG:HB2	4	0.9
(1,676)	1:88:A:LEU:HB2	1:89:A:ARG:HB2	15	0.9
(1,626)	1:83:A:MET:HE2	1:84:A:THR:HG23	3	0.9
(1,467)	1:68:B:ASP:HA	1:71:B:ARG:HD2	13	0.9
(1,420)	1:87:A:HIS:HD2	1:91:A:LEU:HA	20	0.9
(1,322)	1:90:B:ASN:H	1:92:B:GLN:HG2	3	0.9
(1,275)	1:86:A:LYS:HG2	1:88:A:LEU:H	4	0.9
(1,274)	1:86:B:LYS:HG2	1:89:B:ARG:H	7	0.9
(1,268)	1:86:B:LYS:H	1:84:B:THR:HG21	14	0.9
(1,50)	1:68:A:ASP:HA	1:71:A:ARG:H	20	0.9
(1,888)	1:77:A:LYS:HE2	1:81:A:LEU:HD11	4	0.89
(1,414)	1:88:B:LEU:HA	1:89:B:ARG:HB2	12	0.89
(1,274)	1:86:A:LYS:HG2	1:89:A:ARG:H	4	0.89
(1,268)	1:86:B:LYS:H	1:84:B:THR:HG22	17	0.89
(1,888)	1:77:A:LYS:HE3	1:81:A:LEU:HD23	14	0.88
(1,738)	1:76:B:GLU:HA	1:79:B:ASP:HB2	12	0.88
(1,738)	1:76:B:GLU:HA	1:79:B:ASP:HB2	15	0.88
(1,700)	1:87:B:HIS:HD1	1:91:B:LEU:HA	18	0.88
(1,558)	1:81:A:LEU:HA	1:83:A:MET:HE2	6	0.88
(1,484)	1:91:A:LEU:HA	1:93:A:ARG:HA	2	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:91:A:LEU:HA	1:93:A:ARG:HA	7	0.88
(1,363)	1:68:A:ASP:HA	1:72:A:HIS:H	8	0.88
(1,274)	1:86:B:LYS:HG2	1:89:B:ARG:H	19	0.88
(1,268)	1:86:A:LYS:H	1:84:A:THR:HG21	6	0.88
(1,52)	1:71:B:ARG:HB2	1:72:B:HIS:H	17	0.88
(1,744)	1:66:B:LYS:HD3	1:67:B:LYS:H	6	0.87
(1,700)	1:87:B:HIS:HD1	1:91:B:LEU:HA	16	0.87
(1,652)	1:85:A:VAL:HG11	1:86:A:LYS:HB3	8	0.87
(1,652)	1:85:A:VAL:HG13	1:86:A:LYS:HB3	15	0.87
(1,609)	1:92:B:GLN:HB3	1:93:B:ARG:HB2	17	0.87
(1,407)	1:93:B:ARG:HA	1:94:B:ALA:HB2	14	0.87
(1,363)	1:68:B:ASP:HA	1:72:B:HIS:H	14	0.87
(1,363)	1:68:B:ASP:HA	1:72:B:HIS:H	16	0.87
(1,363)	1:68:B:ASP:HA	1:72:B:HIS:H	20	0.87
(1,299)	1:82:B:GLU:HB3	1:84:B:THR:H	1	0.87
(1,274)	1:86:B:LYS:HG2	1:89:B:ARG:H	5	0.87
(1,274)	1:86:B:LYS:HG2	1:89:B:ARG:H	12	0.87
(1,274)	1:86:A:LYS:HG2	1:89:A:ARG:H	16	0.87
(1,274)	1:86:A:LYS:HG2	1:89:A:ARG:H	20	0.87
(1,50)	1:68:A:ASP:HA	1:71:A:ARG:H	19	0.87
(1,935)	1:74:A:LYS:N	1:70:A:SER:O	6	0.86
(1,754)	1:86:A:LYS:HD3	1:87:A:HIS:H	8	0.86
(1,745)	1:72:A:HIS:H	1:75:A:LEU:HD12	12	0.86
(1,705)	1:72:B:HIS:HA	1:75:B:LEU:HD13	3	0.86
(1,582)	1:76:A:GLU:HB3	1:79:A:ASP:HB3	6	0.86
(1,558)	1:81:B:LEU:HA	1:83:B:MET:HE2	7	0.86
(1,484)	1:91:B:LEU:HA	1:93:B:ARG:HA	13	0.86
(1,322)	1:90:B:ASN:H	1:92:B:GLN:HG2	10	0.86
(1,275)	1:86:B:LYS:HG2	1:88:B:LEU:H	5	0.86
(1,50)	1:68:B:ASP:HA	1:71:B:ARG:H	2	0.86
(1,700)	1:87:A:HIS:HD1	1:91:A:LEU:HA	1	0.85
(1,652)	1:85:A:VAL:HG12	1:86:A:LYS:HB2	6	0.85
(1,363)	1:68:A:ASP:HA	1:72:A:HIS:H	4	0.85
(1,316)	1:90:B:ASN:H	1:91:B:LEU:HG	19	0.85
(1,275)	1:86:B:LYS:HG2	1:88:B:LEU:H	11	0.85
(1,106)	1:92:B:GLN:HG2	1:93:B:ARG:H	11	0.85
(1,106)	1:92:B:GLN:HG2	1:93:B:ARG:H	20	0.85
(1,50)	1:68:A:ASP:HA	1:71:A:ARG:H	3	0.85
(1,50)	1:68:B:ASP:HA	1:71:B:ARG:H	7	0.85
(1,50)	1:68:A:ASP:HA	1:71:A:ARG:H	14	0.85
(1,886)	1:76:A:GLU:HG2	1:80:A:ILE:HD11	4	0.84
(1,886)	1:76:A:GLU:HG2	1:80:A:ILE:HD12	10	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,745)	1:72:A:HIS:H	1:75:A:LEU:HD13	17	0.84
(1,566)	1:56:B:GLN:HG2	1:82:A:GLU:HA	5	0.84
(1,558)	1:81:B:LEU:HA	1:83:B:MET:HE1	15	0.84
(1,363)	1:68:A:ASP:HA	1:72:A:HIS:H	3	0.84
(1,363)	1:68:B:ASP:HA	1:72:B:HIS:H	12	0.84
(1,324)	1:83:B:MET:H	1:84:B:THR:HG23	20	0.84
(1,299)	1:82:B:GLU:HB3	1:84:B:THR:H	4	0.84
(1,106)	1:92:B:GLN:HG2	1:93:B:ARG:H	15	0.84
(1,50)	1:68:B:ASP:HA	1:71:B:ARG:H	1	0.84
(1,932)	1:73:A:SER:H	1:69:A:SER:O	2	0.83
(1,894)	1:79:B:ASP:HB3	1:80:B:ILE:HD13	18	0.83
(1,888)	1:77:A:LYS:HE2	1:81:A:LEU:HD22	3	0.83
(1,857)	1:93:A:ARG:HB2	1:95:A:GLN:HB2	12	0.83
(1,756)	1:84:B:THR:HG22	1:85:A:VAL:H	10	0.83
(1,745)	1:72:A:HIS:H	1:75:A:LEU:HD11	10	0.83
(1,738)	1:76:B:GLU:HA	1:79:B:ASP:HB2	1	0.83
(1,652)	1:85:B:VAL:HG11	1:86:B:LYS:HB2	7	0.83
(1,652)	1:85:B:VAL:HG12	1:86:B:LYS:HB2	9	0.83
(1,652)	1:85:A:VAL:HG13	1:86:A:LYS:HB2	18	0.83
(1,463)	1:88:A:LEU:HB3	1:89:A:ARG:HA	17	0.83
(1,420)	1:87:A:HIS:HD2	1:91:A:LEU:HA	18	0.83
(1,414)	1:88:B:LEU:HA	1:89:B:ARG:HB2	13	0.83
(1,363)	1:68:A:ASP:HA	1:72:A:HIS:H	1	0.83
(1,363)	1:68:B:ASP:HA	1:72:B:HIS:H	18	0.83
(1,322)	1:90:A:ASN:H	1:92:A:GLN:HG2	6	0.83
(1,299)	1:82:A:GLU:HB3	1:84:A:THR:H	9	0.83
(1,276)	1:75:A:LEU:H	1:75:A:LEU:HD13	5	0.83
(1,275)	1:86:B:LYS:HG2	1:88:B:LEU:H	1	0.83
(1,274)	1:86:A:LYS:HG2	1:89:A:ARG:H	17	0.83
(1,106)	1:92:A:GLN:HG2	1:93:A:ARG:H	8	0.83
(1,934)	1:74:B:LYS:H	1:70:B:SER:O	3	0.82
(1,894)	1:79:B:ASP:HB2	1:80:B:ILE:HD11	8	0.82
(1,871)	1:75:B:LEU:H	1:75:B:LEU:HD13	14	0.82
(1,754)	1:86:A:LYS:HD3	1:87:A:HIS:H	5	0.82
(1,745)	1:72:A:HIS:H	1:75:A:LEU:HD13	7	0.82
(1,673)	1:56:B:GLN:HG2	1:82:A:GLU:HB2	9	0.82
(1,626)	1:83:B:MET:HE1	1:84:B:THR:HG22	15	0.82
(1,484)	1:91:B:LEU:HA	1:93:B:ARG:HA	10	0.82
(1,484)	1:91:A:LEU:HA	1:93:A:ARG:HA	19	0.82
(1,420)	1:87:A:HIS:HD2	1:91:A:LEU:HA	16	0.82
(1,414)	1:88:A:LEU:HA	1:89:A:ARG:HB2	15	0.82
(1,316)	1:90:A:ASN:H	1:91:A:LEU:HG	16	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:82:B:GLU:HB3	1:84:B:THR:H	3	0.82
(1,276)	1:75:A:LEU:H	1:75:A:LEU:HD12	15	0.82
(1,274)	1:86:B:LYS:HG2	1:89:B:ARG:H	1	0.82
(1,189)	1:75:A:LEU:HA	1:79:A:ASP:H	6	0.82
(1,935)	1:74:A:LYS:N	1:70:A:SER:O	12	0.81
(1,894)	1:79:B:ASP:HB3	1:80:B:ILE:HD11	3	0.81
(1,894)	1:79:A:ASP:HB3	1:80:A:ILE:HD11	5	0.81
(1,864)	1:71:B:ARG:HA	1:75:B:LEU:HD21	16	0.81
(1,768)	1:86:B:LYS:H	1:86:B:LYS:HD3	6	0.81
(1,754)	1:86:A:LYS:HD3	1:87:A:HIS:H	18	0.81
(1,414)	1:88:B:LEU:HA	1:89:B:ARG:HB2	2	0.81
(1,363)	1:68:A:ASP:HA	1:72:A:HIS:H	13	0.81
(1,363)	1:68:A:ASP:HA	1:72:A:HIS:H	19	0.81
(1,329)	1:92:B:GLN:H	1:92:B:GLN:HE21	19	0.81
(1,316)	1:90:B:ASN:H	1:91:B:LEU:HG	2	0.81
(1,299)	1:82:B:GLU:HB3	1:84:B:THR:H	14	0.81
(1,276)	1:75:B:LEU:H	1:75:B:LEU:HD13	11	0.81
(1,275)	1:86:B:LYS:HG2	1:88:B:LEU:H	9	0.81
(1,937)	1:75:A:LEU:N	1:71:A:ARG:O	8	0.8
(1,900)	1:81:B:LEU:HD22	1:83:B:MET:H	10	0.8
(1,894)	1:79:B:ASP:HB2	1:80:B:ILE:HD12	10	0.8
(1,831)	1:87:A:HIS:HD1	1:91:A:LEU:H	1	0.8
(1,768)	1:86:A:LYS:H	1:86:A:LYS:HD3	14	0.8
(1,754)	1:86:B:LYS:HD3	1:87:B:HIS:H	13	0.8
(1,746)	1:87:B:HIS:HD1	1:92:B:GLN:H	10	0.8
(1,736)	1:84:B:THR:HB	1:85:B:VAL:HG13	2	0.8
(1,652)	1:85:B:VAL:HG13	1:86:B:LYS:HB2	3	0.8
(1,598)	1:66:A:LYS:HB2	1:67:A:LYS:HG2	17	0.8
(1,498)	1:65:A:LEU:HD23	1:67:A:LYS:H	15	0.8
(1,484)	1:91:A:LEU:HA	1:93:A:ARG:HA	8	0.8
(1,420)	1:87:B:HIS:HD2	1:91:B:LEU:HA	9	0.8
(1,379)	1:65:A:LEU:HD22	1:66:A:LYS:H	9	0.8
(1,276)	1:75:A:LEU:H	1:75:A:LEU:HD12	7	0.8
(1,106)	1:92:A:GLN:HG2	1:93:A:ARG:H	4	0.8
(1,35)	1:66:A:LYS:HG2	1:67:A:LYS:H	14	0.8
(1,936)	1:75:A:LEU:H	1:71:A:ARG:O	10	0.79
(1,934)	1:74:A:LYS:H	1:70:A:SER:O	5	0.79
(1,934)	1:74:B:LYS:H	1:70:B:SER:O	8	0.79
(1,934)	1:74:A:LYS:H	1:70:A:SER:O	15	0.79
(1,894)	1:79:A:ASP:HB2	1:80:A:ILE:HD11	11	0.79
(1,894)	1:79:B:ASP:HB3	1:80:B:ILE:HD11	15	0.79
(1,756)	1:84:A:THR:HG22	1:85:B:VAL:H	19	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,736)	1:84:B:THR:HB	1:85:B:VAL:HG12	12	0.79
(1,736)	1:84:A:THR:HB	1:85:A:VAL:HG11	13	0.79
(1,736)	1:84:A:THR:HB	1:85:A:VAL:HG11	14	0.79
(1,652)	1:85:A:VAL:HG13	1:86:A:LYS:HB2	1	0.79
(1,652)	1:85:A:VAL:HG12	1:86:A:LYS:HB2	5	0.79
(1,652)	1:85:B:VAL:HG12	1:86:B:LYS:HB2	17	0.79
(1,499)	1:65:B:LEU:HA	1:67:B:LYS:H	9	0.79
(1,414)	1:88:A:LEU:HA	1:89:A:ARG:HB2	10	0.79
(1,363)	1:68:A:ASP:HA	1:72:A:HIS:H	6	0.79
(1,316)	1:90:A:ASN:H	1:91:A:LEU:HG	4	0.79
(1,276)	1:75:A:LEU:H	1:75:A:LEU:HD12	17	0.79
(1,106)	1:92:A:GLN:HG2	1:93:A:ARG:H	7	0.79
(1,106)	1:92:B:GLN:HG2	1:93:B:ARG:H	9	0.79
(1,50)	1:68:B:ASP:HA	1:71:B:ARG:H	15	0.79
(1,934)	1:74:B:LYS:H	1:70:B:SER:O	4	0.78
(1,900)	1:81:A:LEU:HD22	1:83:A:MET:H	11	0.78
(1,894)	1:79:A:ASP:HB3	1:80:A:ILE:HD13	9	0.78
(1,888)	1:77:A:LYS:HE2	1:81:A:LEU:HD12	8	0.78
(1,855)	1:93:B:ARG:HA	1:95:B:GLN:HB3	5	0.78
(1,789)	1:66:A:LYS:HA	1:69:A:SER:HG	1	0.78
(1,598)	1:66:A:LYS:HB2	1:67:A:LYS:HG2	4	0.78
(1,580)	1:75:B:LEU:HB3	1:76:B:GLU:HB2	14	0.78
(1,558)	1:81:A:LEU:HA	1:83:A:MET:HE3	3	0.78
(1,484)	1:91:B:LEU:HA	1:93:B:ARG:HA	20	0.78
(1,420)	1:87:B:HIS:HD2	1:91:B:LEU:HA	12	0.78
(1,414)	1:88:A:LEU:HA	1:89:A:ARG:HB2	7	0.78
(1,414)	1:88:B:LEU:HA	1:89:B:ARG:HB2	11	0.78
(1,414)	1:88:B:LEU:HA	1:89:B:ARG:HB2	19	0.78
(1,316)	1:90:B:ASN:H	1:91:B:LEU:HG	3	0.78
(1,316)	1:90:B:ASN:H	1:91:B:LEU:HG	5	0.78
(1,284)	1:87:A:HIS:HD2	1:88:A:LEU:H	20	0.78
(1,50)	1:68:A:ASP:HA	1:71:A:ARG:H	9	0.78
(1,900)	1:81:A:LEU:HD21	1:83:A:MET:H	17	0.77
(1,894)	1:79:A:ASP:HB3	1:80:A:ILE:HD12	16	0.77
(1,888)	1:77:A:LYS:HE3	1:81:A:LEU:HD13	5	0.77
(1,888)	1:77:B:LYS:HE2	1:81:B:LEU:HD22	17	0.77
(1,798)	1:77:B:LYS:HB3	1:81:B:LEU:H	8	0.77
(1,745)	1:72:B:HIS:H	1:75:B:LEU:HD12	13	0.77
(1,736)	1:84:B:THR:HB	1:85:B:VAL:HG13	7	0.77
(1,652)	1:85:B:VAL:HG13	1:86:B:LYS:HB2	20	0.77
(1,484)	1:91:B:LEU:HA	1:93:B:ARG:HA	6	0.77
(1,484)	1:91:B:LEU:HA	1:93:B:ARG:HA	15	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:68:A:ASP:HA	1:72:A:HIS:H	7	0.77
(1,316)	1:90:B:ASN:H	1:91:B:LEU:HG	20	0.77
(1,299)	1:82:A:GLU:HB3	1:84:A:THR:H	11	0.77
(1,299)	1:82:B:GLU:HB3	1:84:B:THR:H	13	0.77
(1,106)	1:92:A:GLN:HG2	1:93:A:ARG:H	1	0.77
(1,106)	1:92:A:GLN:HG2	1:93:A:ARG:H	12	0.77
(1,900)	1:81:A:LEU:HD21	1:83:A:MET:H	15	0.76
(1,888)	1:77:A:LYS:HE2	1:81:A:LEU:HD11	6	0.76
(1,871)	1:75:B:LEU:H	1:75:B:LEU:HD22	8	0.76
(1,864)	1:71:B:ARG:HA	1:75:B:LEU:HD23	11	0.76
(1,831)	1:87:B:HIS:HD2	1:91:B:LEU:H	12	0.76
(1,831)	1:87:A:HIS:HD2	1:91:A:LEU:H	20	0.76
(1,768)	1:86:B:LYS:H	1:86:B:LYS:HD3	17	0.76
(1,746)	1:87:B:HIS:HD1	1:92:B:GLN:H	19	0.76
(1,414)	1:88:B:LEU:HA	1:89:B:ARG:HB2	5	0.76
(1,414)	1:88:B:LEU:HA	1:89:B:ARG:HB2	6	0.76
(1,363)	1:68:A:ASP:HA	1:72:A:HIS:H	11	0.76
(1,322)	1:90:B:ASN:H	1:92:B:GLN:HG3	8	0.76
(1,299)	1:82:B:GLU:HB3	1:84:B:THR:H	19	0.76
(1,276)	1:75:B:LEU:H	1:75:B:LEU:HD11	16	0.76
(1,274)	1:86:B:LYS:HG2	1:89:B:ARG:H	9	0.76
(1,106)	1:92:A:GLN:HG2	1:93:A:ARG:H	2	0.76
(1,106)	1:92:A:GLN:HG2	1:93:A:ARG:H	13	0.76
(1,936)	1:75:A:LEU:H	1:71:A:ARG:O	15	0.75
(1,900)	1:81:A:LEU:HD13	1:83:A:MET:H	4	0.75
(1,894)	1:79:A:ASP:HB3	1:80:A:ILE:HD12	1	0.75
(1,894)	1:79:A:ASP:HB3	1:80:A:ILE:HD11	14	0.75
(1,894)	1:79:B:ASP:HB2	1:80:B:ILE:HD11	20	0.75
(1,888)	1:77:B:LYS:HE2	1:81:B:LEU:HD21	10	0.75
(1,867)	1:72:A:HIS:H	1:75:A:LEU:HD13	11	0.75
(1,768)	1:86:A:LYS:H	1:86:A:LYS:HD3	7	0.75
(1,768)	1:86:A:LYS:H	1:86:A:LYS:HD3	9	0.75
(1,760)	1:86:A:LYS:HG2	1:87:A:HIS:H	10	0.75
(1,652)	1:85:A:VAL:HG12	1:86:A:LYS:HB2	13	0.75
(1,488)	1:64:B:ALA:HA	1:65:B:LEU:HD11	19	0.75
(1,329)	1:92:B:GLN:H	1:92:B:GLN:HE21	9	0.75
(1,316)	1:90:A:ASN:H	1:91:A:LEU:HG	13	0.75
(1,275)	1:86:A:LYS:HG2	1:88:A:LEU:H	14	0.75
(1,189)	1:75:A:LEU:HA	1:79:A:ASP:H	3	0.75
(1,189)	1:75:B:LEU:HA	1:79:B:ASP:H	7	0.75
(1,106)	1:92:A:GLN:HG2	1:93:A:ARG:H	5	0.75
(1,106)	1:92:A:GLN:HG2	1:93:A:ARG:H	17	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,894)	1:79:B:ASP:HB2	1:80:B:ILE:HD13	4	0.74
(1,888)	1:77:B:LYS:HE3	1:81:B:LEU:HD11	18	0.74
(1,864)	1:71:B:ARG:HA	1:75:B:LEU:HD21	17	0.74
(1,831)	1:87:A:HIS:HD1	1:91:A:LEU:H	17	0.74
(1,745)	1:72:B:HIS:H	1:75:B:LEU:HD13	19	0.74
(1,736)	1:84:A:THR:HB	1:85:A:VAL:HG11	3	0.74
(1,736)	1:84:B:THR:HB	1:85:B:VAL:HG11	17	0.74
(1,711)	1:71:A:ARG:HA	1:71:A:ARG:HG2	5	0.74
(1,711)	1:71:A:ARG:HA	1:71:A:ARG:HG2	16	0.74
(1,711)	1:71:A:ARG:HA	1:71:A:ARG:HG2	20	0.74
(1,652)	1:85:A:VAL:HG13	1:86:A:LYS:HB2	12	0.74
(1,363)	1:68:A:ASP:HA	1:72:A:HIS:H	9	0.74
(1,363)	1:68:A:ASP:HA	1:72:A:HIS:H	15	0.74
(1,329)	1:92:B:GLN:H	1:92:B:GLN:HE21	3	0.74
(1,316)	1:90:A:ASN:H	1:91:A:LEU:HG	18	0.74
(1,299)	1:82:B:GLU:HB3	1:84:B:THR:H	16	0.74
(1,181)	1:83:B:MET:H	1:84:B:THR:HG23	10	0.74
(1,106)	1:92:B:GLN:HG2	1:93:B:ARG:H	3	0.74
(1,106)	1:92:A:GLN:HG2	1:93:A:ARG:H	14	0.74
(1,937)	1:75:A:LEU:N	1:71:A:ARG:O	20	0.73
(1,888)	1:77:B:LYS:HE2	1:81:B:LEU:HD22	15	0.73
(1,877)	1:75:B:LEU:HD23	1:79:B:ASP:HA	18	0.73
(1,801)	1:54:B:LEU:HD23	1:81:B:LEU:HD11	19	0.73
(1,798)	1:77:A:LYS:HB3	1:81:A:LEU:H	5	0.73
(1,736)	1:84:B:THR:HB	1:85:B:VAL:HG11	9	0.73
(1,711)	1:71:B:ARG:HA	1:71:B:ARG:HG2	1	0.73
(1,711)	1:71:A:ARG:HA	1:71:A:ARG:HG2	9	0.73
(1,711)	1:71:A:ARG:HA	1:71:A:ARG:HG2	18	0.73
(1,709)	1:86:B:LYS:HA	1:86:B:LYS:HD3	12	0.73
(1,700)	1:87:A:HIS:HD1	1:91:A:LEU:HA	17	0.73
(1,667)	1:90:B:ASN:HB2	1:91:B:LEU:HD13	9	0.73
(1,652)	1:85:B:VAL:HG11	1:86:B:LYS:HB2	2	0.73
(1,652)	1:85:A:VAL:HG11	1:86:A:LYS:HB3	19	0.73
(1,598)	1:66:A:LYS:HB2	1:67:A:LYS:HG2	2	0.73
(1,566)	1:56:B:GLN:HG2	1:82:A:GLU:HA	17	0.73
(1,488)	1:64:B:ALA:HA	1:65:B:LEU:HD13	7	0.73
(1,363)	1:68:A:ASP:HA	1:72:A:HIS:H	2	0.73
(1,299)	1:82:A:GLU:HB3	1:84:A:THR:H	10	0.73
(1,299)	1:82:B:GLU:HB3	1:84:B:THR:H	12	0.73
(1,277)	1:54:A:LEU:HD21	1:80:A:ILE:H	4	0.73
(1,275)	1:86:A:LYS:HG2	1:88:A:LEU:H	6	0.73
(1,189)	1:75:B:LEU:HA	1:79:B:ASP:H	1	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,900)	1:81:B:LEU:HD21	1:83:B:MET:H	20	0.72
(1,888)	1:77:A:LYS:HE2	1:81:A:LEU:HD23	1	0.72
(1,801)	1:54:B:LEU:HD21	1:81:B:LEU:HD11	14	0.72
(1,768)	1:86:B:LYS:H	1:86:B:LYS:HD3	20	0.72
(1,709)	1:86:A:LYS:HA	1:86:A:LYS:HD3	8	0.72
(1,414)	1:88:B:LEU:HA	1:89:B:ARG:HB2	4	0.72
(1,299)	1:82:B:GLU:HB3	1:84:B:THR:H	2	0.72
(1,299)	1:82:B:GLU:HB3	1:84:B:THR:H	7	0.72
(1,299)	1:82:B:GLU:HB3	1:84:B:THR:H	8	0.72
(1,189)	1:75:B:LEU:HA	1:79:B:ASP:H	8	0.72
(1,181)	1:83:B:MET:H	1:84:B:THR:HG22	15	0.72
(1,50)	1:68:B:ASP:HA	1:71:B:ARG:H	16	0.72
(1,894)	1:79:B:ASP:HB2	1:80:B:ILE:HD13	19	0.71
(1,881)	1:75:B:LEU:HD21	1:83:B:MET:H	11	0.71
(1,881)	1:75:B:LEU:HD23	1:83:B:MET:H	18	0.71
(1,745)	1:72:A:HIS:H	1:75:A:LEU:HD12	1	0.71
(1,738)	1:76:A:GLU:HA	1:79:A:ASP:HB2	17	0.71
(1,736)	1:84:B:THR:HB	1:85:B:VAL:HG12	18	0.71
(1,711)	1:71:A:ARG:HA	1:71:A:ARG:HG2	12	0.71
(1,709)	1:86:A:LYS:HA	1:86:A:LYS:HD3	1	0.71
(1,709)	1:86:A:LYS:HA	1:86:A:LYS:HD3	13	0.71
(1,621)	1:82:B:GLU:HG3	1:85:B:VAL:HG11	14	0.71
(1,573)	1:64:A:ALA:HB1	1:65:A:LEU:HD23	9	0.71
(1,498)	1:65:A:LEU:HD22	1:67:A:LYS:H	5	0.71
(1,488)	1:64:B:ALA:HA	1:65:B:LEU:HD13	2	0.71
(1,414)	1:88:A:LEU:HA	1:89:A:ARG:HB2	20	0.71
(1,316)	1:90:A:ASN:H	1:91:A:LEU:HG	15	0.71
(1,316)	1:90:A:ASN:H	1:91:A:LEU:HG	17	0.71
(1,299)	1:82:B:GLU:HB3	1:84:B:THR:H	5	0.71
(1,274)	1:86:A:LYS:HG2	1:89:A:ARG:H	14	0.71
(1,900)	1:81:B:LEU:HD12	1:83:B:MET:H	16	0.7
(1,881)	1:75:A:LEU:HD12	1:83:A:MET:H	8	0.7
(1,864)	1:71:B:ARG:HA	1:75:B:LEU:HD22	13	0.7
(1,762)	1:87:B:HIS:HD1	1:88:B:LEU:H	1	0.7
(1,736)	1:84:B:THR:HB	1:85:B:VAL:HG13	5	0.7
(1,736)	1:84:B:THR:HB	1:85:B:VAL:HG12	11	0.7
(1,736)	1:84:A:THR:HB	1:85:A:VAL:HG13	16	0.7
(1,711)	1:71:A:ARG:HA	1:71:A:ARG:HG2	8	0.7
(1,711)	1:71:A:ARG:HA	1:71:A:ARG:HG2	11	0.7
(1,711)	1:71:B:ARG:HA	1:71:B:ARG:HG2	14	0.7
(1,709)	1:86:A:LYS:HA	1:86:A:LYS:HD3	2	0.7
(1,709)	1:86:A:LYS:HA	1:86:A:LYS:HD3	5	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,709)	1:86:A:LYS:HA	1:86:A:LYS:HD3	18	0.7
(1,709)	1:86:A:LYS:HA	1:86:A:LYS:HD3	20	0.7
(1,488)	1:64:A:ALA:HA	1:65:A:LEU:HD12	11	0.7
(1,488)	1:64:A:ALA:HA	1:65:A:LEU:HD11	18	0.7
(1,316)	1:90:A:ASN:H	1:91:A:LEU:HG	14	0.7
(1,189)	1:75:A:LEU:HA	1:79:A:ASP:H	15	0.7
(1,934)	1:74:B:LYS:H	1:70:B:SER:O	10	0.69
(1,900)	1:81:A:LEU:HD23	1:83:A:MET:H	12	0.69
(1,900)	1:81:A:LEU:HD21	1:83:A:MET:H	14	0.69
(1,888)	1:77:A:LYS:HE3	1:81:A:LEU:HD11	19	0.69
(1,888)	1:77:B:LYS:HE3	1:81:B:LEU:HD12	20	0.69
(1,876)	1:75:A:LEU:HD23	1:79:A:ASP:H	6	0.69
(1,801)	1:54:B:LEU:HD22	1:81:B:LEU:HD22	12	0.69
(1,798)	1:77:B:LYS:HB3	1:81:B:LEU:H	7	0.69
(1,798)	1:77:B:LYS:HB3	1:81:B:LEU:H	13	0.69
(1,711)	1:71:A:ARG:HA	1:71:A:ARG:HG2	15	0.69
(1,709)	1:86:A:LYS:HA	1:86:A:LYS:HD3	7	0.69
(1,598)	1:66:A:LYS:HB2	1:67:A:LYS:HG2	8	0.69
(1,488)	1:64:B:ALA:HA	1:65:B:LEU:HD12	3	0.69
(1,420)	1:87:B:HIS:HD2	1:91:B:LEU:HA	13	0.69
(1,363)	1:68:A:ASP:HA	1:72:A:HIS:H	5	0.69
(1,316)	1:90:A:ASN:H	1:91:A:LEU:HG	1	0.69
(1,316)	1:90:A:ASN:H	1:91:A:LEU:HG	11	0.69
(1,299)	1:82:A:GLU:HB3	1:84:A:THR:H	18	0.69
(1,189)	1:75:B:LEU:HA	1:79:B:ASP:H	18	0.69
(1,181)	1:83:A:MET:H	1:84:A:THR:HG23	19	0.69
(1,106)	1:92:A:GLN:HG2	1:93:A:ARG:H	6	0.69
(1,106)	1:92:B:GLN:HG2	1:93:B:ARG:H	19	0.69
(1,900)	1:81:A:LEU:HD13	1:83:A:MET:H	6	0.68
(1,888)	1:77:A:LYS:HE2	1:81:A:LEU:HD21	16	0.68
(1,881)	1:75:A:LEU:HD23	1:83:A:MET:H	16	0.68
(1,801)	1:54:B:LEU:HD23	1:81:B:LEU:HD11	13	0.68
(1,738)	1:76:B:GLU:HA	1:79:B:ASP:HB2	16	0.68
(1,736)	1:84:A:THR:HB	1:85:A:VAL:HG13	8	0.68
(1,711)	1:71:B:ARG:HA	1:71:B:ARG:HG2	3	0.68
(1,709)	1:86:B:LYS:HA	1:86:B:LYS:HD3	9	0.68
(1,673)	1:56:B:GLN:HG2	1:82:A:GLU:HB2	8	0.68
(1,558)	1:81:B:LEU:HA	1:83:B:MET:HE3	8	0.68
(1,499)	1:65:B:LEU:HA	1:67:B:LYS:H	3	0.68
(1,488)	1:64:A:ALA:HA	1:65:A:LEU:HD12	8	0.68
(1,276)	1:75:A:LEU:H	1:75:A:LEU:HD12	13	0.68
(1,933)	1:73:A:SER:N	1:69:A:SER:O	2	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,867)	1:72:A:HIS:H	1:75:A:LEU:HD23	18	0.67
(1,864)	1:71:A:ARG:HA	1:75:A:LEU:HD21	10	0.67
(1,831)	1:87:B:HIS:HD2	1:91:B:LEU:H	9	0.67
(1,768)	1:86:B:LYS:H	1:86:B:LYS:HD3	13	0.67
(1,738)	1:76:B:GLU:HA	1:79:B:ASP:HB2	8	0.67
(1,738)	1:76:B:GLU:HA	1:79:B:ASP:HB2	9	0.67
(1,709)	1:86:B:LYS:HA	1:86:B:LYS:HD3	14	0.67
(1,709)	1:86:A:LYS:HA	1:86:A:LYS:HD3	17	0.67
(1,667)	1:90:B:ASN:HB2	1:91:B:LEU:HD12	1	0.67
(1,414)	1:88:A:LEU:HA	1:89:A:ARG:HB2	16	0.67
(1,325)	1:85:B:VAL:H	1:85:B:VAL:HG11	7	0.67
(1,325)	1:85:A:VAL:H	1:85:A:VAL:HG13	9	0.67
(1,299)	1:82:B:GLU:HB3	1:84:B:THR:H	6	0.67
(1,242)	1:88:B:LEU:H	1:89:B:ARG:HB2	14	0.67
(1,189)	1:75:B:LEU:HA	1:79:B:ASP:H	20	0.67
(1,936)	1:75:B:LEU:H	1:71:B:ARG:O	9	0.66
(1,936)	1:75:A:LEU:H	1:71:A:ARG:O	12	0.66
(1,910)	1:88:A:LEU:HD21	1:89:A:ARG:H	5	0.66
(1,900)	1:81:B:LEU:HD13	1:83:B:MET:H	7	0.66
(1,900)	1:81:A:LEU:HD23	1:83:A:MET:H	13	0.66
(1,891)	1:79:A:ASP:H	1:81:A:LEU:HD13	1	0.66
(1,877)	1:75:A:LEU:HD11	1:79:A:ASP:HA	3	0.66
(1,744)	1:66:B:LYS:HD3	1:67:B:LYS:H	13	0.66
(1,709)	1:86:A:LYS:HA	1:86:A:LYS:HD3	16	0.66
(1,674)	1:88:B:LEU:HB2	1:91:B:LEU:HG	8	0.66
(1,420)	1:87:B:HIS:HD2	1:91:B:LEU:HA	4	0.66
(1,363)	1:68:A:ASP:HA	1:72:A:HIS:H	17	0.66
(1,325)	1:85:B:VAL:H	1:85:B:VAL:HG13	3	0.66
(1,325)	1:85:A:VAL:H	1:85:A:VAL:HG13	11	0.66
(1,325)	1:85:B:VAL:H	1:85:B:VAL:HG13	16	0.66
(1,299)	1:82:B:GLU:HB3	1:84:B:THR:H	17	0.66
(1,284)	1:87:A:HIS:HD2	1:88:A:LEU:H	12	0.66
(1,284)	1:87:B:HIS:HD2	1:88:B:LEU:H	13	0.66
(1,276)	1:75:A:LEU:H	1:75:A:LEU:HD13	6	0.66
(1,274)	1:86:A:LYS:HG2	1:89:A:ARG:H	6	0.66
(1,189)	1:75:B:LEU:HA	1:79:B:ASP:H	17	0.66
(1,106)	1:92:B:GLN:HG2	1:93:B:ARG:H	10	0.66
(1,50)	1:68:A:ASP:HA	1:71:A:ARG:H	5	0.66
(1,936)	1:75:B:LEU:H	1:71:B:ARG:O	4	0.65
(1,900)	1:81:B:LEU:HD23	1:83:B:MET:H	1	0.65
(1,894)	1:79:B:ASP:HB2	1:80:B:ILE:HD13	2	0.65
(1,877)	1:75:B:LEU:HD21	1:79:B:ASP:HA	10	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,867)	1:72:A:HIS:H	1:75:A:LEU:HD22	8	0.65
(1,845)	1:90:A:ASN:H	1:90:A:ASN:HD21	14	0.65
(1,801)	1:54:B:LEU:HD23	1:81:B:LEU:HD23	1	0.65
(1,801)	1:54:B:LEU:HD22	1:81:B:LEU:HD12	5	0.65
(1,798)	1:77:A:LYS:HB3	1:81:A:LEU:H	4	0.65
(1,738)	1:76:A:GLU:HA	1:79:A:ASP:HB2	11	0.65
(1,738)	1:76:A:GLU:HA	1:79:A:ASP:HB2	18	0.65
(1,736)	1:84:B:THR:HB	1:85:B:VAL:HG11	4	0.65
(1,709)	1:86:A:LYS:HA	1:86:A:LYS:HD3	6	0.65
(1,566)	1:56:A:GLN:HG2	1:82:B:GLU:HA	11	0.65
(1,551)	1:67:A:LYS:HA	1:67:A:LYS:HE2	2	0.65
(1,551)	1:67:B:LYS:HA	1:67:B:LYS:HE2	10	0.65
(1,325)	1:85:B:VAL:H	1:85:B:VAL:HG13	1	0.65
(1,325)	1:85:B:VAL:H	1:85:B:VAL:HG13	13	0.65
(1,325)	1:85:A:VAL:H	1:85:A:VAL:HG13	18	0.65
(1,325)	1:85:A:VAL:H	1:85:A:VAL:HG13	20	0.65
(1,299)	1:82:A:GLU:HB3	1:84:A:THR:H	15	0.65
(1,46)	1:73:A:SER:HB3	1:75:A:LEU:H	20	0.65
(1,900)	1:81:B:LEU:HD13	1:83:B:MET:H	3	0.64
(1,900)	1:81:B:LEU:HD13	1:83:B:MET:H	18	0.64
(1,900)	1:81:B:LEU:HD12	1:83:B:MET:H	19	0.64
(1,877)	1:75:B:LEU:HD22	1:79:B:ASP:HA	9	0.64
(1,845)	1:90:B:ASN:H	1:90:B:ASN:HD21	2	0.64
(1,845)	1:90:B:ASN:H	1:90:B:ASN:HD21	9	0.64
(1,836)	1:87:A:HIS:HD1	1:92:B:GLN:HE21	15	0.64
(1,745)	1:72:A:HIS:H	1:75:A:LEU:HD12	6	0.64
(1,667)	1:90:B:ASN:HB2	1:91:B:LEU:HD13	6	0.64
(1,566)	1:56:B:GLN:HG2	1:82:A:GLU:HA	10	0.64
(1,563)	1:56:A:GLN:HG3	1:82:B:GLU:HA	10	0.64
(1,520)	1:68:A:ASP:H	1:69:A:SER:HB3	9	0.64
(1,488)	1:64:A:ALA:HA	1:65:A:LEU:HD11	16	0.64
(1,325)	1:85:A:VAL:H	1:85:A:VAL:HG12	5	0.64
(1,325)	1:85:B:VAL:H	1:85:B:VAL:HG11	6	0.64
(1,106)	1:92:A:GLN:HG2	1:93:A:ARG:H	16	0.64
(1,106)	1:92:B:GLN:HG2	1:93:B:ARG:H	18	0.64
(1,910)	1:88:B:LEU:HD21	1:89:B:ARG:H	11	0.63
(1,900)	1:81:A:LEU:HD12	1:83:A:MET:H	9	0.63
(1,886)	1:76:B:GLU:HG2	1:80:B:ILE:HD13	2	0.63
(1,867)	1:72:B:HIS:H	1:75:B:LEU:HD23	20	0.63
(1,796)	1:76:B:GLU:HB2	1:77:B:LYS:HB3	1	0.63
(1,738)	1:76:A:GLU:HA	1:79:A:ASP:HB2	7	0.63
(1,738)	1:76:B:GLU:HA	1:79:B:ASP:HB2	19	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,736)	1:84:B:THR:HB	1:85:B:VAL:HG13	1	0.63
(1,667)	1:90:B:ASN:HB2	1:91:B:LEU:HD13	4	0.63
(1,667)	1:90:B:ASN:HB2	1:91:B:LEU:HD12	11	0.63
(1,667)	1:90:A:ASN:HB2	1:91:A:LEU:HD13	14	0.63
(1,499)	1:65:A:LEU:HA	1:67:A:LYS:H	11	0.63
(1,484)	1:91:A:LEU:HA	1:93:A:ARG:HA	12	0.63
(1,414)	1:88:B:LEU:HA	1:89:B:ARG:HB2	17	0.63
(1,325)	1:85:B:VAL:H	1:85:B:VAL:HG11	4	0.63
(1,189)	1:75:A:LEU:HA	1:79:A:ASP:H	12	0.63
(1,35)	1:66:A:LYS:HG2	1:67:A:LYS:H	9	0.63
(1,910)	1:88:B:LEU:HD13	1:89:B:ARG:H	8	0.62
(1,888)	1:77:A:LYS:HE2	1:81:A:LEU:HD12	2	0.62
(1,888)	1:77:A:LYS:HE3	1:81:A:LEU:HD11	12	0.62
(1,881)	1:75:B:LEU:HD11	1:83:B:MET:H	20	0.62
(1,867)	1:72:A:HIS:H	1:75:A:LEU:HD13	16	0.62
(1,845)	1:90:A:ASN:H	1:90:A:ASN:HD21	8	0.62
(1,738)	1:76:B:GLU:HA	1:79:B:ASP:HB2	6	0.62
(1,683)	1:71:A:ARG:HD3	1:75:A:LEU:HD13	7	0.62
(1,598)	1:66:B:LYS:HB2	1:67:B:LYS:HG2	10	0.62
(1,598)	1:66:A:LYS:HB2	1:67:A:LYS:HG2	16	0.62
(1,551)	1:67:A:LYS:HA	1:67:A:LYS:HE2	16	0.62
(1,484)	1:91:B:LEU:HA	1:93:B:ARG:HA	14	0.62
(1,325)	1:85:B:VAL:H	1:85:B:VAL:HG13	12	0.62
(1,325)	1:85:B:VAL:H	1:85:B:VAL:HG13	19	0.62
(1,322)	1:90:A:ASN:H	1:92:A:GLN:HG3	13	0.62
(1,322)	1:90:A:ASN:H	1:92:A:GLN:HG3	15	0.62
(1,316)	1:90:A:ASN:H	1:91:A:LEU:HG	6	0.62
(1,181)	1:83:B:MET:H	1:84:B:THR:HG23	20	0.62
(1,12)	1:61:A:ILE:HA	1:62:A:LEU:H	1	0.62
(1,936)	1:75:B:LEU:H	1:71:B:ARG:O	18	0.61
(1,831)	1:87:B:HIS:HD1	1:91:B:LEU:H	18	0.61
(1,798)	1:77:B:LYS:HB3	1:81:B:LEU:H	1	0.61
(1,798)	1:77:B:LYS:HB3	1:81:B:LEU:H	15	0.61
(1,484)	1:91:A:LEU:HA	1:93:A:ARG:HA	9	0.61
(1,420)	1:87:B:HIS:HD2	1:91:B:LEU:HA	8	0.61
(1,325)	1:85:B:VAL:H	1:85:B:VAL:HG12	17	0.61
(1,284)	1:87:A:HIS:HD2	1:88:A:LEU:H	7	0.61
(1,276)	1:75:A:LEU:H	1:75:A:LEU:HD13	10	0.61
(1,52)	1:71:A:ARG:HB2	1:72:A:HIS:H	6	0.61
(1,12)	1:61:A:ILE:HA	1:62:A:LEU:H	10	0.61
(1,12)	1:61:B:ILE:HA	1:62:B:LEU:H	16	0.61
(1,12)	1:61:B:ILE:HA	1:62:B:LEU:H	17	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,932)	1:73:A:SER:H	1:69:A:SER:O	12	0.6
(1,910)	1:88:B:LEU:HD23	1:89:B:ARG:H	20	0.6
(1,900)	1:81:A:LEU:HD11	1:83:A:MET:H	5	0.6
(1,796)	1:76:B:GLU:HB2	1:77:B:LYS:HB3	18	0.6
(1,754)	1:86:A:LYS:HD3	1:87:A:HIS:H	10	0.6
(1,741)	1:50:B:ILE:HG21	1:51:B:ASN:HD22	2	0.6
(1,622)	1:82:A:GLU:HB2	1:85:A:VAL:HG11	11	0.6
(1,498)	1:65:B:LEU:HD21	1:67:B:LYS:H	3	0.6
(1,488)	1:64:B:ALA:HA	1:65:B:LEU:HD12	6	0.6
(1,325)	1:85:A:VAL:H	1:85:A:VAL:HG13	2	0.6
(1,325)	1:85:A:VAL:H	1:85:A:VAL:HG12	10	0.6
(1,325)	1:85:A:VAL:H	1:85:A:VAL:HG12	14	0.6
(1,316)	1:90:B:ASN:H	1:91:B:LEU:HG	12	0.6
(1,242)	1:88:B:LEU:H	1:89:B:ARG:HB2	8	0.6
(1,242)	1:88:A:LEU:H	1:89:A:ARG:HB2	10	0.6
(1,189)	1:75:A:LEU:HA	1:79:A:ASP:H	5	0.6
(1,50)	1:68:B:ASP:HA	1:71:B:ARG:H	10	0.6
(1,12)	1:61:A:ILE:HA	1:62:A:LEU:H	2	0.6
(1,12)	1:61:A:ILE:HA	1:62:A:LEU:H	4	0.6
(1,12)	1:61:B:ILE:HA	1:62:B:LEU:H	5	0.6
(1,12)	1:61:B:ILE:HA	1:62:B:LEU:H	7	0.6
(1,12)	1:61:A:ILE:HA	1:62:A:LEU:H	9	0.6
(1,12)	1:61:A:ILE:HA	1:62:A:LEU:H	11	0.6
(1,12)	1:61:B:ILE:HA	1:62:B:LEU:H	12	0.6
(1,12)	1:61:A:ILE:HA	1:62:A:LEU:H	15	0.6
(1,936)	1:75:A:LEU:H	1:71:A:ARG:O	7	0.59
(1,935)	1:74:A:LYS:N	1:70:A:SER:O	9	0.59
(1,900)	1:81:A:LEU:HD11	1:83:A:MET:H	8	0.59
(1,881)	1:75:B:LEU:HD23	1:83:B:MET:H	9	0.59
(1,881)	1:75:B:LEU:HD21	1:83:B:MET:H	10	0.59
(1,864)	1:71:B:ARG:HA	1:75:B:LEU:HD13	6	0.59
(1,864)	1:71:A:ARG:HA	1:75:A:LEU:HD13	8	0.59
(1,798)	1:77:B:LYS:HB3	1:81:B:LEU:H	17	0.59
(1,738)	1:76:A:GLU:HA	1:79:A:ASP:HB2	2	0.59
(1,700)	1:87:B:HIS:HD1	1:91:B:LEU:HA	19	0.59
(1,667)	1:90:B:ASN:HB2	1:91:B:LEU:HD11	18	0.59
(1,622)	1:82:B:GLU:HB2	1:85:B:VAL:HG12	6	0.59
(1,622)	1:82:A:GLU:HB2	1:85:A:VAL:HG11	15	0.59
(1,559)	1:85:B:VAL:HA	1:88:B:LEU:HB2	17	0.59
(1,488)	1:64:B:ALA:HA	1:65:B:LEU:HD13	1	0.59
(1,421)	1:79:A:ASP:HB3	1:80:A:ILE:HB	16	0.59
(1,325)	1:85:A:VAL:H	1:85:A:VAL:HG11	8	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,325)	1:85:B:VAL:H	1:85:B:VAL:HG11	15	0.59
(1,52)	1:71:B:ARG:HB2	1:72:B:HIS:H	2	0.59
(1,50)	1:68:A:ASP:HA	1:71:A:ARG:H	17	0.59
(1,12)	1:61:B:ILE:HA	1:62:B:LEU:H	3	0.59
(1,12)	1:61:A:ILE:HA	1:62:A:LEU:H	6	0.59
(1,12)	1:61:A:ILE:HA	1:62:A:LEU:H	8	0.59
(1,12)	1:61:B:ILE:HA	1:62:B:LEU:H	20	0.59
(1,934)	1:74:B:LYS:H	1:70:B:SER:O	1	0.58
(1,877)	1:75:B:LEU:HD22	1:79:B:ASP:HA	17	0.58
(1,871)	1:75:A:LEU:H	1:75:A:LEU:HD12	17	0.58
(1,864)	1:71:B:ARG:HA	1:75:B:LEU:HD21	5	0.58
(1,864)	1:71:B:ARG:HA	1:75:B:LEU:HD13	14	0.58
(1,845)	1:90:B:ASN:H	1:90:B:ASN:HD21	15	0.58
(1,845)	1:90:A:ASN:H	1:90:A:ASN:HD21	16	0.58
(1,845)	1:90:B:ASN:H	1:90:B:ASN:HD21	19	0.58
(1,801)	1:54:A:LEU:HD21	1:81:A:LEU:HD23	20	0.58
(1,798)	1:77:B:LYS:HB3	1:81:B:LEU:H	14	0.58
(1,798)	1:77:A:LYS:HB3	1:81:A:LEU:H	18	0.58
(1,798)	1:77:B:LYS:HB3	1:81:B:LEU:H	20	0.58
(1,738)	1:76:B:GLU:HA	1:79:B:ASP:HB2	4	0.58
(1,738)	1:76:B:GLU:HA	1:79:B:ASP:HB2	5	0.58
(1,736)	1:84:B:THR:HB	1:85:B:VAL:HG13	6	0.58
(1,711)	1:71:B:ARG:HA	1:71:B:ARG:HG2	17	0.58
(1,622)	1:82:B:GLU:HB2	1:85:B:VAL:HG11	12	0.58
(1,622)	1:82:A:GLU:HB2	1:85:A:VAL:HG12	16	0.58
(1,499)	1:65:B:LEU:HA	1:67:B:LYS:H	16	0.58
(1,498)	1:65:A:LEU:HD22	1:67:A:LYS:H	20	0.58
(1,484)	1:91:A:LEU:HA	1:93:A:ARG:HA	5	0.58
(1,421)	1:79:A:ASP:HB3	1:80:A:ILE:HB	10	0.58
(1,316)	1:90:B:ASN:H	1:91:B:LEU:HG	7	0.58
(1,39)	1:68:B:ASP:H	1:69:B:SER:H	13	0.58
(1,12)	1:61:A:ILE:HA	1:62:A:LEU:H	13	0.58
(1,12)	1:61:A:ILE:HA	1:62:A:LEU:H	18	0.58
(1,12)	1:61:A:ILE:HA	1:62:A:LEU:H	19	0.58
(1,934)	1:74:B:LYS:H	1:70:B:SER:O	13	0.57
(1,910)	1:88:B:LEU:HD12	1:89:B:ARG:H	3	0.57
(1,894)	1:79:B:ASP:HB2	1:80:B:ILE:HD11	6	0.57
(1,881)	1:75:B:LEU:HD22	1:83:B:MET:H	17	0.57
(1,867)	1:72:B:HIS:H	1:75:B:LEU:HD23	5	0.57
(1,864)	1:71:B:ARG:HA	1:75:B:LEU:HD21	20	0.57
(1,845)	1:90:B:ASN:H	1:90:B:ASN:HD21	13	0.57
(1,765)	1:84:B:THR:H	1:84:B:THR:HG21	17	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,663)	1:54:B:LEU:HD13	1:77:B:LYS:HE2	12	0.57
(1,626)	1:83:B:MET:HE1	1:84:B:THR:HG23	10	0.57
(1,566)	1:56:A:GLN:HG2	1:82:B:GLU:HA	4	0.57
(1,499)	1:65:A:LEU:HA	1:67:A:LYS:H	2	0.57
(1,189)	1:75:B:LEU:HA	1:79:B:ASP:H	4	0.57
(1,189)	1:75:A:LEU:HA	1:79:A:ASP:H	16	0.57
(1,52)	1:71:B:ARG:HB2	1:72:B:HIS:H	13	0.57
(1,932)	1:73:A:SER:H	1:69:A:SER:O	9	0.56
(1,891)	1:79:B:ASP:H	1:81:B:LEU:HD13	12	0.56
(1,888)	1:77:B:LYS:HE2	1:81:B:LEU:HD11	7	0.56
(1,845)	1:90:A:ASN:H	1:90:A:ASN:HD21	20	0.56
(1,801)	1:54:B:LEU:HD23	1:81:B:LEU:HD13	7	0.56
(1,798)	1:77:B:LYS:HB3	1:81:B:LEU:H	2	0.56
(1,796)	1:76:A:GLU:HB2	1:77:A:LYS:HB3	3	0.56
(1,770)	1:80:B:ILE:HG23	1:83:B:MET:H	19	0.56
(1,768)	1:86:B:LYS:H	1:86:B:LYS:HD3	1	0.56
(1,756)	1:84:B:THR:HG21	1:85:B:VAL:H	18	0.56
(1,499)	1:65:B:LEU:HA	1:67:B:LYS:H	12	0.56
(1,488)	1:64:B:ALA:HA	1:65:B:LEU:HD13	20	0.56
(1,48)	1:69:B:SER:HB2	1:70:B:SER:H	9	0.56
(1,920)	1:94:B:ALA:HB2	1:95:B:GLN:HG2	1	0.55
(1,886)	1:76:A:GLU:HG3	1:80:A:ILE:HD12	12	0.55
(1,845)	1:90:A:ASN:H	1:90:A:ASN:HD21	3	0.55
(1,845)	1:90:B:ASN:H	1:90:B:ASN:HD21	12	0.55
(1,801)	1:54:B:LEU:HD22	1:81:B:LEU:HD23	17	0.55
(1,798)	1:77:B:LYS:HB3	1:81:B:LEU:H	16	0.55
(1,796)	1:76:B:GLU:HB2	1:77:B:LYS:HB3	20	0.55
(1,770)	1:80:A:ILE:HG23	1:83:A:MET:H	6	0.55
(1,738)	1:76:B:GLU:HA	1:79:B:ASP:HB2	13	0.55
(1,622)	1:82:B:GLU:HB2	1:85:B:VAL:HG11	18	0.55
(1,414)	1:88:B:LEU:HA	1:89:B:ARG:HB2	18	0.55
(1,242)	1:88:B:LEU:H	1:89:B:ARG:HB2	6	0.55
(1,52)	1:71:A:ARG:HB2	1:72:A:HIS:H	10	0.55
(1,910)	1:88:A:LEU:HD12	1:89:A:ARG:H	4	0.54
(1,831)	1:87:A:HIS:HD2	1:91:A:LEU:H	2	0.54
(1,801)	1:54:B:LEU:HD22	1:81:B:LEU:HD23	15	0.54
(1,798)	1:77:B:LYS:HB3	1:81:B:LEU:H	12	0.54
(1,798)	1:77:A:LYS:HB3	1:81:A:LEU:H	19	0.54
(1,765)	1:84:B:THR:H	1:84:B:THR:HG23	6	0.54
(1,756)	1:84:B:THR:HG22	1:85:B:VAL:H	2	0.54
(1,745)	1:72:A:HIS:H	1:75:A:LEU:HD11	2	0.54
(1,667)	1:90:A:ASN:HB2	1:91:A:LEU:HD12	8	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:90:B:ASN:HB2	1:91:B:LEU:HD11	15	0.54
(1,566)	1:56:A:GLN:HG2	1:82:B:GLU:HA	7	0.54
(1,488)	1:64:B:ALA:HA	1:65:B:LEU:HD11	10	0.54
(1,284)	1:87:B:HIS:HD2	1:88:B:LEU:H	15	0.54
(1,242)	1:88:A:LEU:H	1:89:A:ARG:HB2	9	0.54
(1,242)	1:88:B:LEU:H	1:89:B:ARG:HB2	19	0.54
(1,52)	1:71:B:ARG:HB2	1:72:B:HIS:H	19	0.54
(1,12)	1:61:A:ILE:HA	1:62:A:LEU:H	14	0.54
(1,879)	1:75:A:LEU:HD13	1:80:A:ILE:H	19	0.53
(1,864)	1:71:B:ARG:HA	1:75:B:LEU:HD22	7	0.53
(1,864)	1:71:A:ARG:HA	1:75:A:LEU:HD11	18	0.53
(1,831)	1:87:A:HIS:HD2	1:91:A:LEU:H	16	0.53
(1,768)	1:86:B:LYS:H	1:86:B:LYS:HD3	2	0.53
(1,768)	1:86:B:LYS:H	1:86:B:LYS:HD3	5	0.53
(1,765)	1:84:B:THR:H	1:84:B:THR:HG21	9	0.53
(1,736)	1:84:B:THR:HB	1:85:B:VAL:HG12	20	0.53
(1,705)	1:72:A:HIS:HA	1:75:A:LEU:HD12	20	0.53
(1,700)	1:87:A:HIS:HD1	1:91:A:LEU:HA	4	0.53
(1,667)	1:90:B:ASN:HB2	1:91:B:LEU:HD13	2	0.53
(1,667)	1:90:A:ASN:HB2	1:91:A:LEU:HD11	16	0.53
(1,622)	1:82:B:GLU:HB2	1:85:B:VAL:HG12	14	0.53
(1,563)	1:56:B:GLN:HG3	1:82:A:GLU:HA	5	0.53
(1,498)	1:65:B:LEU:HD21	1:67:B:LYS:H	19	0.53
(1,420)	1:87:A:HIS:HD2	1:91:A:LEU:HA	7	0.53
(1,363)	1:68:B:ASP:HA	1:72:B:HIS:H	10	0.53
(1,221)	1:50:B:ILE:HG21	1:51:B:ASN:HD21	2	0.53
(1,189)	1:75:A:LEU:HA	1:79:A:ASP:H	2	0.53
(1,894)	1:79:B:ASP:HB2	1:80:B:ILE:HD11	13	0.52
(1,888)	1:77:A:LYS:HE3	1:81:A:LEU:HD11	11	0.52
(1,845)	1:90:A:ASN:H	1:90:A:ASN:HD21	18	0.52
(1,798)	1:77:B:LYS:HB3	1:81:B:LEU:H	9	0.52
(1,781)	1:64:A:ALA:HB3	1:65:A:LEU:HD22	3	0.52
(1,768)	1:86:B:LYS:H	1:86:B:LYS:HD3	18	0.52
(1,765)	1:84:A:THR:H	1:84:A:THR:HG23	7	0.52
(1,756)	1:84:A:THR:HG22	1:85:A:VAL:H	15	0.52
(1,741)	1:50:B:ILE:HG21	1:51:B:ASN:HD22	1	0.52
(1,652)	1:85:A:VAL:HG12	1:86:A:LYS:HB3	14	0.52
(1,566)	1:56:B:GLN:HG2	1:82:A:GLU:HA	1	0.52
(1,499)	1:65:B:LEU:HA	1:67:B:LYS:H	13	0.52
(1,461)	1:76:A:GLU:HB2	1:77:A:LYS:HA	16	0.52
(1,242)	1:88:A:LEU:H	1:89:A:ARG:HB2	1	0.52
(1,242)	1:88:B:LEU:H	1:89:B:ARG:HB2	5	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,189)	1:75:B:LEU:HA	1:79:B:ASP:H	11	0.52
(1,52)	1:71:B:ARG:HB2	1:72:B:HIS:H	4	0.52
(1,52)	1:71:A:ARG:HB2	1:72:A:HIS:H	7	0.52
(1,900)	1:81:A:LEU:HD11	1:83:A:MET:H	2	0.51
(1,889)	1:78:A:ALA:H	1:81:A:LEU:HD13	1	0.51
(1,881)	1:75:A:LEU:HD11	1:83:A:MET:H	3	0.51
(1,770)	1:80:A:ILE:HG22	1:83:A:MET:H	7	0.51
(1,770)	1:80:B:ILE:HG23	1:83:B:MET:H	14	0.51
(1,768)	1:86:B:LYS:H	1:86:B:LYS:HD3	8	0.51
(1,768)	1:86:A:LYS:H	1:86:A:LYS:HD3	11	0.51
(1,705)	1:72:B:HIS:HA	1:75:B:LEU:HD13	14	0.51
(1,667)	1:90:A:ASN:HB2	1:91:A:LEU:HD13	3	0.51
(1,667)	1:90:A:ASN:HB2	1:91:A:LEU:HD13	7	0.51
(1,630)	1:75:B:LEU:HB2	1:80:B:ILE:HG12	14	0.51
(1,566)	1:56:A:GLN:HG2	1:82:B:GLU:HA	16	0.51
(1,499)	1:65:B:LEU:HA	1:67:B:LYS:H	20	0.51
(1,461)	1:76:A:GLU:HB2	1:77:A:LYS:HA	2	0.51
(1,421)	1:79:A:ASP:HB3	1:80:A:ILE:HB	13	0.51
(1,316)	1:90:A:ASN:H	1:91:A:LEU:HG	9	0.51
(1,242)	1:88:A:LEU:H	1:89:A:ARG:HB2	7	0.51
(1,934)	1:74:A:LYS:H	1:70:A:SER:O	19	0.5
(1,882)	1:75:B:LEU:HD12	1:83:B:MET:HG3	5	0.5
(1,877)	1:75:A:LEU:HD23	1:79:A:ASP:HA	7	0.5
(1,845)	1:90:B:ASN:H	1:90:B:ASN:HD21	4	0.5
(1,845)	1:90:B:ASN:H	1:90:B:ASN:HD21	11	0.5
(1,806)	1:57:B:LEU:HD13	1:84:B:THR:H	14	0.5
(1,798)	1:77:A:LYS:HB3	1:81:A:LEU:H	11	0.5
(1,796)	1:76:A:GLU:HB2	1:77:A:LYS:HB3	7	0.5
(1,768)	1:86:A:LYS:H	1:86:A:LYS:HD3	3	0.5
(1,768)	1:86:A:LYS:H	1:86:A:LYS:HD3	4	0.5
(1,768)	1:86:A:LYS:H	1:86:A:LYS:HD3	19	0.5
(1,756)	1:84:B:THR:HG21	1:85:B:VAL:H	12	0.5
(1,756)	1:84:A:THR:HG23	1:85:A:VAL:H	20	0.5
(1,744)	1:66:A:LYS:HD3	1:67:A:LYS:H	14	0.5
(1,736)	1:84:B:THR:HB	1:85:B:VAL:HG12	10	0.5
(1,736)	1:84:B:THR:HB	1:85:B:VAL:HG13	19	0.5
(1,674)	1:88:A:LEU:HB2	1:91:A:LEU:HG	9	0.5
(1,622)	1:82:A:GLU:HB2	1:85:A:VAL:HG11	10	0.5
(1,598)	1:66:A:LYS:HB2	1:67:A:LYS:HG2	3	0.5
(1,421)	1:79:B:ASP:HB3	1:80:B:ILE:HB	1	0.5
(1,421)	1:79:A:ASP:HB3	1:80:A:ILE:HB	20	0.5
(1,348)	1:71:A:ARG:H	1:71:A:ARG:HD2	6	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,276)	1:75:B:LEU:H	1:75:B:LEU:HD12	18	0.5
(1,13)	1:88:A:LEU:H	1:89:A:ARG:HD2	5	0.5
(1,930)	1:72:B:HIS:H	1:68:B:ASP:O	8	0.49
(1,877)	1:75:B:LEU:HD23	1:79:B:ASP:HA	8	0.49
(1,864)	1:71:B:ARG:HA	1:75:B:LEU:HD13	19	0.49
(1,845)	1:90:B:ASN:H	1:90:B:ASN:HD21	1	0.49
(1,845)	1:90:B:ASN:H	1:90:B:ASN:HD21	6	0.49
(1,845)	1:90:B:ASN:H	1:90:B:ASN:HD21	7	0.49
(1,801)	1:54:B:LEU:HD21	1:81:B:LEU:HD22	10	0.49
(1,798)	1:77:B:LYS:HB3	1:81:B:LEU:H	6	0.49
(1,788)	1:65:A:LEU:HG	1:66:A:LYS:H	3	0.49
(1,768)	1:86:A:LYS:H	1:86:A:LYS:HD3	15	0.49
(1,768)	1:86:B:LYS:H	1:86:B:LYS:HD3	16	0.49
(1,765)	1:84:B:THR:H	1:84:B:THR:HG23	13	0.49
(1,756)	1:84:B:THR:HG21	1:85:B:VAL:H	16	0.49
(1,667)	1:90:A:ASN:HB2	1:91:A:LEU:HD12	12	0.49
(1,622)	1:82:A:GLU:HB2	1:85:A:VAL:HG11	17	0.49
(1,551)	1:67:A:LYS:HA	1:67:A:LYS:HE3	9	0.49
(1,531)	1:87:A:HIS:H	1:88:A:LEU:HB2	18	0.49
(1,421)	1:79:A:ASP:HB3	1:80:A:ILE:HB	4	0.49
(1,242)	1:88:B:LEU:H	1:89:B:ARG:HB2	3	0.49
(1,242)	1:88:A:LEU:H	1:89:A:ARG:HB2	15	0.49
(1,70)	1:83:B:MET:HE3	1:84:B:THR:H	4	0.49
(1,918)	1:88:A:LEU:HD12	1:92:A:GLN:HE22	17	0.48
(1,871)	1:75:A:LEU:H	1:75:A:LEU:HD23	11	0.48
(1,845)	1:90:B:ASN:H	1:90:B:ASN:HD21	5	0.48
(1,806)	1:57:B:LEU:HD13	1:84:B:THR:H	5	0.48
(1,801)	1:54:A:LEU:HD21	1:81:A:LEU:HD22	16	0.48
(1,796)	1:76:B:GLU:HB2	1:77:B:LYS:HB3	5	0.48
(1,770)	1:80:A:ILE:HG21	1:83:A:MET:H	13	0.48
(1,768)	1:86:A:LYS:H	1:86:A:LYS:HD3	12	0.48
(1,762)	1:87:B:HIS:HD1	1:88:B:LEU:H	5	0.48
(1,741)	1:50:B:ILE:HG22	1:51:B:ASN:HD22	15	0.48
(1,738)	1:76:B:GLU:HA	1:79:B:ASP:HB2	14	0.48
(1,738)	1:76:B:GLU:HA	1:79:B:ASP:HB2	20	0.48
(1,700)	1:87:A:HIS:HD1	1:91:A:LEU:HA	8	0.48
(1,667)	1:90:A:ASN:HB2	1:91:A:LEU:HD12	19	0.48
(1,631)	1:66:B:LYS:HG2	1:66:B:LYS:HD3	1	0.48
(1,622)	1:82:A:GLU:HB2	1:85:A:VAL:HG13	3	0.48
(1,566)	1:56:B:GLN:HG2	1:82:A:GLU:HA	13	0.48
(1,566)	1:56:B:GLN:HG2	1:82:A:GLU:HA	15	0.48
(1,540)	1:89:B:ARG:HB3	1:92:B:GLN:H	1	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,540)	1:89:B:ARG:HB3	1:92:B:GLN:H	19	0.48
(1,499)	1:65:A:LEU:HA	1:67:A:LYS:H	5	0.48
(1,461)	1:76:B:GLU:HB2	1:77:B:LYS:HA	6	0.48
(1,421)	1:79:B:ASP:HB3	1:80:B:ILE:HB	7	0.48
(1,421)	1:79:A:ASP:HB3	1:80:A:ILE:HB	9	0.48
(1,329)	1:92:B:GLN:H	1:92:B:GLN:HE21	17	0.48
(1,316)	1:90:B:ASN:H	1:91:B:LEU:HG	8	0.48
(1,275)	1:86:A:LYS:HG2	1:88:A:LEU:H	10	0.48
(1,242)	1:88:B:LEU:H	1:89:B:ARG:HB2	2	0.48
(1,242)	1:88:B:LEU:H	1:89:B:ARG:HB2	11	0.48
(1,242)	1:88:B:LEU:H	1:89:B:ARG:HB2	13	0.48
(1,189)	1:75:B:LEU:HA	1:79:B:ASP:H	13	0.48
(1,108)	1:93:B:ARG:HB2	1:95:B:GLN:H	14	0.48
(1,881)	1:75:B:LEU:HD13	1:83:B:MET:H	7	0.47
(1,798)	1:77:A:LYS:HB3	1:81:A:LEU:H	10	0.47
(1,770)	1:80:A:ILE:HG23	1:83:A:MET:H	3	0.47
(1,765)	1:84:B:THR:H	1:84:B:THR:HG22	4	0.47
(1,765)	1:84:B:THR:H	1:84:B:THR:HG23	16	0.47
(1,759)	1:84:B:THR:H	1:84:B:THR:HG21	17	0.47
(1,741)	1:50:B:ILE:HG21	1:51:B:ASN:HD22	7	0.47
(1,580)	1:75:B:LEU:HB3	1:76:B:GLU:HB2	19	0.47
(1,499)	1:65:A:LEU:HA	1:67:A:LYS:H	19	0.47
(1,498)	1:65:A:LEU:HD21	1:67:A:LYS:H	13	0.47
(1,461)	1:76:B:GLU:HB2	1:77:B:LYS:HA	4	0.47
(1,421)	1:79:A:ASP:HB3	1:80:A:ILE:HB	8	0.47
(1,242)	1:88:B:LEU:H	1:89:B:ARG:HB2	12	0.47
(1,112)	1:71:B:ARG:HD3	1:72:B:HIS:H	6	0.47
(1,39)	1:68:B:ASP:H	1:69:B:SER:H	5	0.47
(1,39)	1:68:A:ASP:H	1:69:A:SER:H	18	0.47
(1,937)	1:75:B:LEU:N	1:71:B:ARG:O	16	0.46
(1,933)	1:73:A:SER:N	1:69:A:SER:O	12	0.46
(1,920)	1:94:B:ALA:HB1	1:95:B:GLN:HG2	12	0.46
(1,895)	1:80:B:ILE:HA	1:81:B:LEU:HD23	17	0.46
(1,891)	1:79:B:ASP:H	1:81:B:LEU:HD11	20	0.46
(1,881)	1:75:B:LEU:HD11	1:83:B:MET:H	5	0.46
(1,877)	1:75:B:LEU:HD11	1:79:B:ASP:HA	5	0.46
(1,877)	1:75:B:LEU:HD11	1:79:B:ASP:HA	14	0.46
(1,877)	1:75:B:LEU:HD11	1:79:B:ASP:HA	20	0.46
(1,763)	1:86:A:LYS:H	1:86:A:LYS:HD3	11	0.46
(1,741)	1:50:B:ILE:HG22	1:51:B:ASN:HD22	20	0.46
(1,540)	1:89:B:ARG:HB2	1:92:B:GLN:H	7	0.46
(1,421)	1:79:B:ASP:HB3	1:80:B:ILE:HB	17	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,420)	1:87:A:HIS:HD2	1:91:A:LEU:HA	2	0.46
(1,348)	1:71:A:ARG:H	1:71:A:ARG:HD3	19	0.46
(1,284)	1:87:A:HIS:HD2	1:88:A:LEU:H	3	0.46
(1,108)	1:93:A:ARG:HB2	1:95:A:GLN:H	6	0.46
(1,39)	1:68:A:ASP:H	1:69:A:SER:H	2	0.46
(1,39)	1:68:A:ASP:H	1:69:A:SER:H	19	0.46
(1,903)	1:84:B:THR:H	1:87:B:HIS:HB3	16	0.45
(1,891)	1:79:B:ASP:H	1:81:B:LEU:HD13	11	0.45
(1,881)	1:75:A:LEU:HD22	1:83:A:MET:H	13	0.45
(1,881)	1:75:B:LEU:HD12	1:83:B:MET:H	14	0.45
(1,877)	1:75:A:LEU:HD21	1:79:A:ASP:HA	1	0.45
(1,871)	1:75:A:LEU:H	1:75:A:LEU:HD13	6	0.45
(1,867)	1:72:A:HIS:H	1:75:A:LEU:HD23	14	0.45
(1,864)	1:71:A:ARG:HA	1:75:A:LEU:HD12	1	0.45
(1,796)	1:76:A:GLU:HB2	1:77:A:LYS:HB3	2	0.45
(1,770)	1:80:A:ILE:HG21	1:83:A:MET:H	8	0.45
(1,770)	1:80:B:ILE:HG22	1:83:B:MET:H	18	0.45
(1,765)	1:84:B:THR:H	1:84:B:THR:HG22	5	0.45
(1,763)	1:86:A:LYS:H	1:86:A:LYS:HD3	3	0.45
(1,763)	1:86:A:LYS:H	1:86:A:LYS:HD3	4	0.45
(1,763)	1:86:A:LYS:H	1:86:A:LYS:HD3	19	0.45
(1,756)	1:84:A:THR:HG21	1:85:A:VAL:H	13	0.45
(1,421)	1:79:B:ASP:HB3	1:80:B:ILE:HB	12	0.45
(1,242)	1:88:A:LEU:H	1:89:A:ARG:HB2	16	0.45
(1,242)	1:88:B:LEU:H	1:89:B:ARG:HB2	17	0.45
(1,39)	1:68:B:ASP:H	1:69:B:SER:H	4	0.45
(1,909)	1:88:A:LEU:H	1:88:A:LEU:HD12	6	0.44
(1,903)	1:84:A:THR:H	1:87:A:HIS:HB3	17	0.44
(1,895)	1:80:A:ILE:HA	1:81:A:LEU:HD22	11	0.44
(1,877)	1:75:A:LEU:HD21	1:79:A:ASP:HA	11	0.44
(1,864)	1:71:A:ARG:HA	1:75:A:LEU:HD11	2	0.44
(1,770)	1:80:B:ILE:HG21	1:83:B:MET:H	11	0.44
(1,765)	1:84:B:THR:H	1:84:B:THR:HG23	1	0.44
(1,765)	1:84:A:THR:H	1:84:A:THR:HG21	11	0.44
(1,765)	1:84:A:THR:H	1:84:A:THR:HG22	12	0.44
(1,763)	1:86:A:LYS:H	1:86:A:LYS:HD3	15	0.44
(1,759)	1:84:B:THR:H	1:84:B:THR:HG23	6	0.44
(1,756)	1:84:B:THR:HG22	1:85:B:VAL:H	11	0.44
(1,756)	1:84:A:THR:HG22	1:85:A:VAL:H	14	0.44
(1,622)	1:82:B:GLU:HB2	1:85:B:VAL:HG13	4	0.44
(1,498)	1:65:B:LEU:HD23	1:67:B:LYS:H	14	0.44
(1,416)	1:82:B:GLU:HA	1:85:B:VAL:HG12	6	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,416)	1:82:B:GLU:HA	1:85:B:VAL:HG13	9	0.44
(1,39)	1:68:B:ASP:H	1:69:B:SER:H	15	0.44
(1,39)	1:68:B:ASP:H	1:69:B:SER:H	16	0.44
(1,935)	1:74:A:LYS:N	1:70:A:SER:O	3	0.43
(1,909)	1:88:B:LEU:H	1:88:B:LEU:HD23	20	0.43
(1,877)	1:75:B:LEU:HD22	1:79:B:ASP:HA	16	0.43
(1,876)	1:75:A:LEU:HD22	1:79:A:ASP:H	13	0.43
(1,876)	1:75:A:LEU:HD13	1:79:A:ASP:H	19	0.43
(1,845)	1:90:B:ASN:H	1:90:B:ASN:HD21	17	0.43
(1,831)	1:87:A:HIS:HD1	1:91:A:LEU:H	4	0.43
(1,801)	1:54:A:LEU:HD21	1:81:A:LEU:HD21	11	0.43
(1,798)	1:77:B:LYS:HB3	1:81:B:LEU:H	3	0.43
(1,796)	1:76:B:GLU:HB2	1:77:B:LYS:HB3	16	0.43
(1,793)	1:69:A:SER:HG	1:70:A:SER:H	1	0.43
(1,759)	1:84:B:THR:H	1:84:B:THR:HG21	9	0.43
(1,756)	1:84:A:THR:HG21	1:85:A:VAL:H	1	0.43
(1,756)	1:84:B:THR:HG21	1:85:B:VAL:H	3	0.43
(1,756)	1:84:A:THR:HG22	1:85:A:VAL:H	5	0.43
(1,729)	1:65:B:LEU:HD11	1:87:B:HIS:HA	20	0.43
(1,563)	1:56:B:GLN:HG3	1:82:A:GLU:HA	17	0.43
(1,461)	1:76:B:GLU:HB2	1:77:B:LYS:HA	10	0.43
(1,461)	1:76:B:GLU:HB2	1:77:B:LYS:HA	18	0.43
(1,419)	1:75:B:LEU:HA	1:80:B:ILE:HD11	19	0.43
(1,39)	1:68:B:ASP:H	1:69:B:SER:H	10	0.43
(1,39)	1:68:B:ASP:H	1:69:B:SER:H	11	0.43
(1,39)	1:68:B:ASP:H	1:69:B:SER:H	20	0.43
(1,930)	1:72:A:HIS:H	1:68:A:ASP:O	20	0.42
(1,903)	1:84:B:THR:H	1:87:B:HIS:HB3	1	0.42
(1,903)	1:84:A:THR:H	1:87:A:HIS:HB3	4	0.42
(1,864)	1:71:A:ARG:HA	1:75:A:LEU:HD23	9	0.42
(1,831)	1:87:B:HIS:HD2	1:91:B:LEU:H	13	0.42
(1,801)	1:54:B:LEU:HD23	1:81:B:LEU:HD13	18	0.42
(1,796)	1:76:A:GLU:HB2	1:77:A:LYS:HB3	19	0.42
(1,770)	1:80:A:ILE:HG21	1:83:A:MET:H	16	0.42
(1,759)	1:84:A:THR:H	1:84:A:THR:HG23	7	0.42
(1,740)	1:79:A:ASP:H	1:80:A:ILE:HD11	2	0.42
(1,700)	1:87:B:HIS:HD1	1:91:B:LEU:HA	10	0.42
(1,667)	1:90:B:ASN:HB2	1:91:B:LEU:HD13	10	0.42
(1,566)	1:56:B:GLN:HG2	1:82:A:GLU:HA	14	0.42
(1,566)	1:56:B:GLN:HG2	1:82:A:GLU:HA	19	0.42
(1,540)	1:89:A:ARG:HB3	1:92:A:GLN:H	9	0.42
(1,540)	1:89:A:ARG:HB2	1:92:A:GLN:H	12	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:81:B:LEU:HA	1:84:B:THR:HB	11	0.42
(1,461)	1:76:B:GLU:HB2	1:77:B:LYS:HA	9	0.42
(1,461)	1:76:B:GLU:HB2	1:77:B:LYS:HA	17	0.42
(1,421)	1:79:B:ASP:HB3	1:80:B:ILE:HB	3	0.42
(1,421)	1:79:B:ASP:HB3	1:80:B:ILE:HB	18	0.42
(1,329)	1:92:A:GLN:H	1:92:A:GLN:HE21	20	0.42
(1,121)	1:73:A:SER:HB3	1:75:A:LEU:H	20	0.42
(1,39)	1:68:B:ASP:H	1:69:B:SER:H	3	0.42
(1,39)	1:68:B:ASP:H	1:69:B:SER:H	8	0.42
(1,39)	1:68:B:ASP:H	1:69:B:SER:H	12	0.42
(1,39)	1:68:B:ASP:H	1:69:B:SER:H	17	0.42
(1,13)	1:88:A:LEU:H	1:89:A:ARG:HD2	19	0.42
(1,930)	1:72:B:HIS:H	1:68:B:ASP:O	12	0.41
(1,909)	1:88:B:LEU:H	1:88:B:LEU:HD22	10	0.41
(1,865)	1:71:B:ARG:HD2	1:72:B:HIS:HB2	2	0.41
(1,864)	1:71:A:ARG:HA	1:75:A:LEU:HD12	15	0.41
(1,788)	1:65:A:LEU:HG	1:66:A:LYS:H	4	0.41
(1,770)	1:80:B:ILE:HG22	1:83:B:MET:H	1	0.41
(1,770)	1:80:B:ILE:HG23	1:83:B:MET:H	5	0.41
(1,710)	1:87:A:HIS:HA	1:87:A:HIS:HD1	19	0.41
(1,622)	1:82:B:GLU:HB2	1:85:B:VAL:HG12	7	0.41
(1,540)	1:89:A:ARG:HB3	1:92:A:GLN:H	20	0.41
(1,498)	1:65:B:LEU:HD23	1:67:B:LYS:H	2	0.41
(1,482)	1:81:A:LEU:HA	1:84:A:THR:HB	15	0.41
(1,461)	1:76:B:GLU:HB2	1:77:B:LYS:HA	1	0.41
(1,461)	1:76:B:GLU:HB2	1:77:B:LYS:HA	8	0.41
(1,461)	1:76:A:GLU:HB2	1:77:A:LYS:HA	12	0.41
(1,416)	1:82:A:GLU:HA	1:85:A:VAL:HG11	17	0.41
(1,225)	1:92:B:GLN:HB3	1:92:B:GLN:HE21	2	0.41
(1,225)	1:92:B:GLN:HB3	1:92:B:GLN:HE21	7	0.41
(1,225)	1:92:B:GLN:HB3	1:92:B:GLN:HE21	11	0.41
(1,225)	1:92:A:GLN:HB3	1:92:A:GLN:HE21	18	0.41
(1,39)	1:68:A:ASP:H	1:69:A:SER:H	7	0.41
(1,31)	1:66:A:LYS:H	1:66:A:LYS:HB2	9	0.41
(1,930)	1:72:B:HIS:H	1:68:B:ASP:O	1	0.4
(1,930)	1:72:B:HIS:H	1:68:B:ASP:O	18	0.4
(1,914)	1:88:B:LEU:HD11	1:92:B:GLN:HB2	11	0.4
(1,909)	1:88:A:LEU:H	1:88:A:LEU:HD22	14	0.4
(1,881)	1:75:B:LEU:HD22	1:83:B:MET:H	19	0.4
(1,871)	1:75:A:LEU:H	1:75:A:LEU:HD13	10	0.4
(1,845)	1:90:B:ASN:H	1:90:B:ASN:HD21	10	0.4
(1,806)	1:57:B:LEU:HD22	1:84:B:THR:H	6	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,740)	1:79:A:ASP:H	1:80:A:ILE:HD11	18	0.4
(1,621)	1:82:B:GLU:HG3	1:85:B:VAL:HG12	6	0.4
(1,558)	1:81:B:LEU:HA	1:83:B:MET:HE1	18	0.4
(1,482)	1:81:A:LEU:HA	1:84:A:THR:HB	18	0.4
(1,421)	1:79:A:ASP:HB3	1:80:A:ILE:HB	15	0.4
(1,419)	1:75:B:LEU:HA	1:80:B:ILE:HD11	6	0.4
(1,39)	1:68:A:ASP:H	1:69:A:SER:H	6	0.4
(1,909)	1:88:B:LEU:H	1:88:B:LEU:HD23	5	0.39
(1,909)	1:88:B:LEU:H	1:88:B:LEU:HD23	19	0.39
(1,877)	1:75:B:LEU:HD23	1:79:B:ASP:HA	13	0.39
(1,877)	1:75:A:LEU:HD13	1:79:A:ASP:HA	19	0.39
(1,871)	1:75:B:LEU:H	1:75:B:LEU:HD21	16	0.39
(1,796)	1:76:B:GLU:HB2	1:77:B:LYS:HB3	6	0.39
(1,770)	1:80:A:ILE:HG22	1:83:A:MET:H	9	0.39
(1,770)	1:80:B:ILE:HG21	1:83:B:MET:H	15	0.39
(1,765)	1:84:A:THR:H	1:84:A:THR:HG21	14	0.39
(1,759)	1:84:B:THR:H	1:84:B:THR:HG23	13	0.39
(1,626)	1:83:B:MET:HE3	1:84:B:THR:HG23	18	0.39
(1,622)	1:82:B:GLU:HB2	1:85:B:VAL:HG11	13	0.39
(1,619)	1:77:A:LYS:HG3	1:77:A:LYS:HE2	12	0.39
(1,482)	1:81:A:LEU:HA	1:84:A:THR:HB	14	0.39
(1,421)	1:79:B:ASP:HB3	1:80:B:ILE:HB	11	0.39
(1,242)	1:88:A:LEU:H	1:89:A:ARG:HB2	20	0.39
(1,225)	1:92:B:GLN:HB3	1:92:B:GLN:HE21	12	0.39
(1,188)	1:76:A:GLU:HA	1:79:A:ASP:H	9	0.39
(1,87)	1:88:B:LEU:HB2	1:90:B:ASN:H	5	0.39
(1,39)	1:68:A:ASP:H	1:69:A:SER:H	14	0.39
(1,935)	1:74:A:LYS:N	1:70:A:SER:O	7	0.38
(1,903)	1:84:A:THR:H	1:87:A:HIS:HB3	9	0.38
(1,889)	1:78:B:ALA:H	1:81:B:LEU:HD13	12	0.38
(1,876)	1:75:A:LEU:HD22	1:79:A:ASP:H	10	0.38
(1,865)	1:71:B:ARG:HD2	1:72:B:HIS:HB2	4	0.38
(1,801)	1:54:B:LEU:HD21	1:81:B:LEU:HD11	3	0.38
(1,770)	1:80:A:ILE:HG23	1:83:A:MET:H	12	0.38
(1,765)	1:84:A:THR:H	1:84:A:THR:HG22	2	0.38
(1,740)	1:79:B:ASP:H	1:80:B:ILE:HD13	16	0.38
(1,711)	1:71:A:ARG:HA	1:71:A:ARG:HG2	6	0.38
(1,667)	1:90:B:ASN:HB2	1:91:B:LEU:HD11	17	0.38
(1,622)	1:82:A:GLU:HB2	1:85:A:VAL:HG13	5	0.38
(1,622)	1:82:B:GLU:HB2	1:85:B:VAL:HG13	9	0.38
(1,540)	1:89:A:ARG:HB2	1:92:A:GLN:H	14	0.38
(1,531)	1:87:B:HIS:H	1:88:B:LEU:HB2	16	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,516)	1:67:A:LYS:HG2	1:68:A:ASP:H	15	0.38
(1,488)	1:64:A:ALA:HA	1:65:A:LEU:HD12	13	0.38
(1,461)	1:76:B:GLU:HB2	1:77:B:LYS:HA	11	0.38
(1,461)	1:76:B:GLU:HB2	1:77:B:LYS:HA	20	0.38
(1,419)	1:75:A:LEU:HA	1:80:A:ILE:HD12	14	0.38
(1,416)	1:82:A:GLU:HA	1:85:A:VAL:HG13	14	0.38
(1,189)	1:75:B:LEU:HA	1:79:B:ASP:H	10	0.38
(1,13)	1:88:B:LEU:H	1:89:B:ARG:HD2	9	0.38
(1,930)	1:72:A:HIS:H	1:68:A:ASP:O	16	0.37
(1,903)	1:84:A:THR:H	1:87:A:HIS:HB3	8	0.37
(1,876)	1:75:A:LEU:HD21	1:79:A:ASP:H	2	0.37
(1,806)	1:57:B:LEU:HD21	1:84:B:THR:H	17	0.37
(1,796)	1:76:A:GLU:HB2	1:77:A:LYS:HB3	12	0.37
(1,793)	1:69:B:SER:HG	1:70:B:SER:H	4	0.37
(1,771)	1:83:B:MET:H	1:86:B:LYS:HD3	4	0.37
(1,770)	1:80:A:ILE:HG21	1:83:A:MET:H	2	0.37
(1,765)	1:84:B:THR:H	1:84:B:THR:HG23	18	0.37
(1,759)	1:84:B:THR:H	1:84:B:THR:HG22	4	0.37
(1,759)	1:84:B:THR:H	1:84:B:THR:HG23	16	0.37
(1,740)	1:79:B:ASP:H	1:80:B:ILE:HD12	5	0.37
(1,740)	1:79:A:ASP:H	1:80:A:ILE:HD13	6	0.37
(1,740)	1:79:B:ASP:H	1:80:B:ILE:HD13	9	0.37
(1,740)	1:79:A:ASP:H	1:80:A:ILE:HD11	10	0.37
(1,740)	1:79:A:ASP:H	1:80:A:ILE:HD11	19	0.37
(1,638)	1:57:B:LEU:HD13	1:84:B:THR:HG21	5	0.37
(1,621)	1:82:A:GLU:HG3	1:85:A:VAL:HG12	9	0.37
(1,619)	1:77:A:LYS:HG3	1:77:A:LYS:HE2	19	0.37
(1,563)	1:56:A:GLN:HG3	1:82:B:GLU:HA	16	0.37
(1,482)	1:81:B:LEU:HA	1:84:B:THR:HB	3	0.37
(1,470)	1:71:A:ARG:HA	1:71:A:ARG:HD3	13	0.37
(1,461)	1:76:A:GLU:HB2	1:77:A:LYS:HA	19	0.37
(1,421)	1:79:A:ASP:HB3	1:80:A:ILE:HB	5	0.37
(1,329)	1:92:A:GLN:H	1:92:A:GLN:HE21	15	0.37
(1,271)	1:76:B:GLU:H	1:80:B:ILE:HD11	1	0.37
(1,225)	1:92:A:GLN:HB3	1:92:A:GLN:HE21	4	0.37
(1,930)	1:72:A:HIS:H	1:68:A:ASP:O	15	0.36
(1,914)	1:88:A:LEU:HD13	1:92:A:GLN:HB2	20	0.36
(1,903)	1:84:A:THR:H	1:87:A:HIS:HB3	2	0.36
(1,903)	1:84:A:THR:H	1:87:A:HIS:HB3	15	0.36
(1,895)	1:80:A:ILE:HA	1:81:A:LEU:HD21	15	0.36
(1,867)	1:72:A:HIS:H	1:75:A:LEU:HD21	3	0.36
(1,827)	1:87:A:HIS:HA	1:87:A:HIS:HD2	19	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,771)	1:83:B:MET:H	1:86:B:LYS:HD3	3	0.36
(1,770)	1:80:B:ILE:HG23	1:83:B:MET:H	10	0.36
(1,770)	1:80:A:ILE:HG21	1:83:A:MET:H	20	0.36
(1,745)	1:72:B:HIS:H	1:75:B:LEU:HD11	9	0.36
(1,740)	1:79:B:ASP:H	1:80:B:ILE:HD13	1	0.36
(1,738)	1:76:B:GLU:HA	1:79:B:ASP:HB2	10	0.36
(1,624)	1:84:B:THR:HG21	1:88:A:LEU:HB3	10	0.36
(1,516)	1:67:A:LYS:HG2	1:68:A:ASP:H	11	0.36
(1,498)	1:65:B:LEU:HD22	1:67:B:LYS:H	6	0.36
(1,482)	1:81:B:LEU:HA	1:84:B:THR:HB	2	0.36
(1,421)	1:79:A:ASP:HB3	1:80:A:ILE:HB	14	0.36
(1,419)	1:75:B:LEU:HA	1:80:B:ILE:HD13	2	0.36
(1,416)	1:82:A:GLU:HA	1:85:A:VAL:HG13	5	0.36
(1,416)	1:82:B:GLU:HA	1:85:B:VAL:HG11	16	0.36
(1,206)	1:93:B:ARG:HG3	1:95:B:GLN:HE21	5	0.36
(1,189)	1:75:B:LEU:HA	1:79:B:ASP:H	14	0.36
(1,87)	1:88:B:LEU:HB2	1:90:B:ASN:H	16	0.36
(1,81)	1:88:B:LEU:HB2	1:89:B:ARG:H	17	0.36
(1,930)	1:72:B:HIS:H	1:68:B:ASP:O	4	0.35
(1,930)	1:72:B:HIS:H	1:68:B:ASP:O	13	0.35
(1,914)	1:88:B:LEU:HD12	1:92:B:GLN:HB2	3	0.35
(1,903)	1:84:A:THR:H	1:87:A:HIS:HB3	6	0.35
(1,876)	1:75:B:LEU:HD22	1:79:B:ASP:H	17	0.35
(1,864)	1:71:A:ARG:HA	1:75:A:LEU:HD12	4	0.35
(1,796)	1:76:B:GLU:HB2	1:77:B:LYS:HB3	11	0.35
(1,788)	1:65:A:LEU:HG	1:66:A:LYS:H	17	0.35
(1,765)	1:84:A:THR:H	1:84:A:THR:HG23	3	0.35
(1,759)	1:84:B:THR:H	1:84:B:THR:HG22	5	0.35
(1,756)	1:84:B:THR:HG23	1:85:B:VAL:H	7	0.35
(1,740)	1:79:B:ASP:H	1:80:B:ILE:HD13	4	0.35
(1,622)	1:82:B:GLU:HB2	1:85:B:VAL:HG11	20	0.35
(1,499)	1:65:A:LEU:HA	1:67:A:LYS:H	14	0.35
(1,482)	1:81:A:LEU:HA	1:84:A:THR:HB	1	0.35
(1,461)	1:76:A:GLU:HB2	1:77:A:LYS:HA	3	0.35
(1,461)	1:76:B:GLU:HB2	1:77:B:LYS:HA	13	0.35
(1,271)	1:76:B:GLU:H	1:80:B:ILE:HD11	19	0.35
(1,201)	1:85:B:VAL:HG21	1:86:B:LYS:H	1	0.35
(1,201)	1:85:B:VAL:HG23	1:86:B:LYS:H	12	0.35
(1,201)	1:85:A:VAL:HG21	1:86:A:LYS:H	17	0.35
(1,189)	1:75:A:LEU:HA	1:79:A:ASP:H	19	0.35
(1,188)	1:76:A:GLU:HA	1:79:A:ASP:H	4	0.35
(1,112)	1:71:A:ARG:HD3	1:72:A:HIS:H	19	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:88:A:LEU:HB2	1:90:A:ASN:H	18	0.35
(1,86)	1:88:A:LEU:HB3	1:90:A:ASN:H	17	0.35
(1,31)	1:66:B:LYS:H	1:66:B:LYS:HB2	1	0.35
(1,13)	1:88:B:LEU:H	1:89:B:ARG:HD2	2	0.35
(1,930)	1:72:B:HIS:H	1:68:B:ASP:O	3	0.34
(1,909)	1:88:A:LEU:H	1:88:A:LEU:HD23	11	0.34
(1,896)	1:80:A:ILE:HB	1:81:A:LEU:HD23	12	0.34
(1,891)	1:79:A:ASP:H	1:81:A:LEU:HD11	10	0.34
(1,888)	1:77:B:LYS:HE2	1:81:B:LEU:HD12	13	0.34
(1,881)	1:75:A:LEU:HD22	1:83:A:MET:H	6	0.34
(1,877)	1:75:A:LEU:HD21	1:79:A:ASP:HA	4	0.34
(1,801)	1:54:B:LEU:HD22	1:81:B:LEU:HD13	8	0.34
(1,789)	1:66:B:LYS:HA	1:69:B:SER:HG	17	0.34
(1,788)	1:65:B:LEU:HG	1:66:B:LYS:H	5	0.34
(1,771)	1:83:A:MET:H	1:86:A:LYS:HD3	15	0.34
(1,770)	1:80:B:ILE:HG21	1:83:B:MET:H	4	0.34
(1,759)	1:84:B:THR:H	1:84:B:THR:HG23	1	0.34
(1,759)	1:84:A:THR:H	1:84:A:THR:HG21	11	0.34
(1,759)	1:84:A:THR:H	1:84:A:THR:HG22	12	0.34
(1,756)	1:84:B:THR:HG22	1:85:B:VAL:H	9	0.34
(1,756)	1:84:B:THR:HG22	1:85:B:VAL:H	17	0.34
(1,741)	1:50:B:ILE:HG22	1:51:B:ASN:HD22	18	0.34
(1,740)	1:79:A:ASP:H	1:80:A:ILE:HD11	11	0.34
(1,740)	1:79:B:ASP:H	1:80:B:ILE:HD11	17	0.34
(1,740)	1:79:B:ASP:H	1:80:B:ILE:HD11	20	0.34
(1,516)	1:67:A:LYS:HG2	1:68:A:ASP:H	18	0.34
(1,461)	1:76:B:GLU:HB2	1:77:B:LYS:HA	14	0.34
(1,416)	1:82:B:GLU:HA	1:85:B:VAL:HG12	7	0.34
(1,416)	1:82:A:GLU:HA	1:85:A:VAL:HG11	11	0.34
(1,348)	1:71:A:ARG:H	1:71:A:ARG:HD2	13	0.34
(1,329)	1:92:A:GLN:H	1:92:A:GLN:HE21	8	0.34
(1,284)	1:87:A:HIS:HD2	1:88:A:LEU:H	8	0.34
(1,242)	1:88:B:LEU:H	1:89:B:ARG:HB2	4	0.34
(1,201)	1:85:B:VAL:HG22	1:86:B:LYS:H	5	0.34
(1,201)	1:85:A:VAL:HG22	1:86:A:LYS:H	7	0.34
(1,201)	1:85:A:VAL:HG23	1:86:A:LYS:H	15	0.34
(1,934)	1:74:B:LYS:H	1:70:B:SER:O	18	0.33
(1,896)	1:80:B:ILE:HB	1:81:B:LEU:HD23	11	0.33
(1,796)	1:76:A:GLU:HB2	1:77:A:LYS:HB3	17	0.33
(1,788)	1:65:B:LEU:HG	1:66:B:LYS:H	12	0.33
(1,763)	1:86:A:LYS:H	1:86:A:LYS:HD2	16	0.33
(1,741)	1:50:B:ILE:HG22	1:51:B:ASN:HD22	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,740)	1:79:A:ASP:H	1:80:A:ILE:HD12	15	0.33
(1,663)	1:54:B:LEU:HD11	1:77:B:LYS:HE2	19	0.33
(1,616)	1:86:A:LYS:HG2	1:86:A:LYS:HE2	15	0.33
(1,566)	1:56:B:GLN:HG2	1:82:A:GLU:HA	8	0.33
(1,541)	1:77:B:LYS:HB3	1:79:B:ASP:H	12	0.33
(1,482)	1:81:B:LEU:HA	1:84:B:THR:HB	8	0.33
(1,461)	1:76:B:GLU:HB2	1:77:B:LYS:HA	7	0.33
(1,271)	1:76:B:GLU:H	1:80:B:ILE:HD11	6	0.33
(1,206)	1:93:B:ARG:HG3	1:95:B:GLN:HE21	10	0.33
(1,206)	1:93:A:ARG:HG3	1:95:A:GLN:HE21	20	0.33
(1,201)	1:85:B:VAL:HG22	1:86:B:LYS:H	11	0.33
(1,155)	1:91:B:LEU:H	1:91:B:LEU:HD13	10	0.33
(1,155)	1:91:B:LEU:H	1:91:B:LEU:HD11	16	0.33
(1,87)	1:88:A:LEU:HB2	1:90:A:ASN:H	20	0.33
(1,13)	1:88:A:LEU:H	1:89:A:ARG:HD2	4	0.33
(1,13)	1:88:A:LEU:H	1:89:A:ARG:HD2	12	0.33
(1,7)	1:74:A:LYS:H	1:74:A:LYS:HE2	19	0.33
(1,934)	1:74:A:LYS:H	1:70:A:SER:O	20	0.32
(1,914)	1:88:B:LEU:HD13	1:92:B:GLN:HB2	5	0.32
(1,914)	1:88:B:LEU:HD12	1:92:B:GLN:HB2	8	0.32
(1,903)	1:84:B:THR:H	1:87:B:HIS:HB3	11	0.32
(1,895)	1:80:B:ILE:HA	1:81:B:LEU:HD21	20	0.32
(1,881)	1:75:A:LEU:HD21	1:83:A:MET:H	2	0.32
(1,877)	1:75:A:LEU:HD21	1:79:A:ASP:HA	12	0.32
(1,876)	1:75:A:LEU:HD21	1:79:A:ASP:H	11	0.32
(1,796)	1:76:B:GLU:HB2	1:77:B:LYS:HB3	13	0.32
(1,771)	1:83:A:MET:H	1:86:A:LYS:HD3	11	0.32
(1,765)	1:84:A:THR:H	1:84:A:THR:HG22	8	0.32
(1,740)	1:79:A:ASP:H	1:80:A:ILE:HD13	3	0.32
(1,740)	1:79:B:ASP:H	1:80:B:ILE:HD11	8	0.32
(1,667)	1:90:A:ASN:HB2	1:91:A:LEU:HD12	13	0.32
(1,639)	1:57:B:LEU:HD22	1:84:B:THR:HG22	6	0.32
(1,637)	1:85:B:VAL:HG13	1:86:B:LYS:HG2	10	0.32
(1,621)	1:82:B:GLU:HG3	1:85:B:VAL:HG12	7	0.32
(1,621)	1:82:A:GLU:HG3	1:85:A:VAL:HG11	17	0.32
(1,540)	1:89:A:ARG:HB3	1:92:A:GLN:H	5	0.32
(1,486)	1:93:A:ARG:HA	1:94:A:ALA:HA	14	0.32
(1,482)	1:81:A:LEU:HA	1:84:A:THR:HB	5	0.32
(1,428)	1:86:B:LYS:HA	1:86:B:LYS:HD2	3	0.32
(1,419)	1:75:A:LEU:HA	1:80:A:ILE:HD11	4	0.32
(1,419)	1:75:A:LEU:HA	1:80:A:ILE:HD13	8	0.32
(1,371)	1:72:A:HIS:HA	1:75:A:LEU:H	20	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,329)	1:92:B:GLN:H	1:92:B:GLN:HE21	12	0.32
(1,321)	1:87:B:HIS:HB2	1:88:B:LEU:H	11	0.32
(1,271)	1:76:B:GLU:H	1:80:B:ILE:HD12	13	0.32
(1,201)	1:85:B:VAL:HG22	1:86:B:LYS:H	8	0.32
(1,155)	1:91:A:LEU:H	1:91:A:LEU:HD12	5	0.32
(1,155)	1:91:A:LEU:H	1:91:A:LEU:HD13	14	0.32
(1,31)	1:66:B:LYS:H	1:66:B:LYS:HB2	7	0.32
(1,13)	1:88:B:LEU:H	1:89:B:ARG:HD2	1	0.32
(1,13)	1:88:A:LEU:H	1:89:A:ARG:HD2	17	0.32
(1,13)	1:88:B:LEU:H	1:89:B:ARG:HD2	20	0.32
(1,930)	1:72:A:HIS:H	1:68:A:ASP:O	14	0.31
(1,903)	1:84:B:THR:H	1:87:B:HIS:HB3	7	0.31
(1,903)	1:84:A:THR:H	1:87:A:HIS:HB3	18	0.31
(1,895)	1:80:A:ILE:HA	1:81:A:LEU:HD21	1	0.31
(1,876)	1:75:A:LEU:HD21	1:79:A:ASP:H	4	0.31
(1,867)	1:72:B:HIS:H	1:75:B:LEU:HD22	12	0.31
(1,806)	1:57:B:LEU:HD23	1:84:B:THR:H	9	0.31
(1,796)	1:76:B:GLU:HB2	1:77:B:LYS:HB3	10	0.31
(1,763)	1:86:A:LYS:H	1:86:A:LYS:HD2	2	0.31
(1,756)	1:84:A:THR:HG21	1:85:A:VAL:H	6	0.31
(1,740)	1:79:A:ASP:H	1:80:A:ILE:HD11	13	0.31
(1,711)	1:71:A:ARG:HA	1:71:A:ARG:HG2	10	0.31
(1,637)	1:85:A:VAL:HG13	1:86:A:LYS:HG2	18	0.31
(1,616)	1:86:A:LYS:HG2	1:86:A:LYS:HE2	3	0.31
(1,540)	1:89:B:ARG:HB3	1:92:B:GLN:H	8	0.31
(1,499)	1:65:A:LEU:HA	1:67:A:LYS:H	8	0.31
(1,498)	1:65:B:LEU:HD21	1:67:B:LYS:H	4	0.31
(1,498)	1:65:B:LEU:HD22	1:67:B:LYS:H	11	0.31
(1,498)	1:65:B:LEU:HD22	1:67:B:LYS:H	16	0.31
(1,482)	1:81:A:LEU:HA	1:84:A:THR:HB	16	0.31
(1,456)	1:77:B:LYS:HA	1:77:B:LYS:HE2	12	0.31
(1,419)	1:75:B:LEU:HA	1:80:B:ILE:HD11	3	0.31
(1,416)	1:82:B:GLU:HA	1:85:B:VAL:HG13	4	0.31
(1,416)	1:82:B:GLU:HA	1:85:B:VAL:HG11	13	0.31
(1,329)	1:92:B:GLN:H	1:92:B:GLN:HE21	14	0.31
(1,206)	1:93:B:ARG:HG3	1:95:B:GLN:HE21	12	0.31
(1,201)	1:85:B:VAL:HG23	1:86:B:LYS:H	4	0.31
(1,201)	1:85:A:VAL:HG23	1:86:A:LYS:H	6	0.31
(1,188)	1:76:B:GLU:HA	1:79:B:ASP:H	10	0.31
(1,165)	1:93:A:ARG:HB2	1:94:A:ALA:H	16	0.31
(1,155)	1:91:A:LEU:H	1:91:A:LEU:HD12	2	0.31
(1,155)	1:91:A:LEU:H	1:91:A:LEU:HD13	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:66:B:LYS:H	1:66:B:LYS:HB2	4	0.31
(1,937)	1:75:A:LEU:N	1:71:A:ARG:O	6	0.3
(1,934)	1:74:A:LYS:H	1:70:A:SER:O	16	0.3
(1,896)	1:80:B:ILE:HB	1:81:B:LEU:HD23	15	0.3
(1,895)	1:80:A:ILE:HA	1:81:A:LEU:HD22	10	0.3
(1,895)	1:80:A:ILE:HA	1:81:A:LEU:HD23	12	0.3
(1,889)	1:78:B:ALA:H	1:81:B:LEU:HD11	20	0.3
(1,877)	1:75:A:LEU:HD21	1:79:A:ASP:HA	2	0.3
(1,867)	1:72:A:HIS:H	1:75:A:LEU:HD13	17	0.3
(1,831)	1:87:A:HIS:HD2	1:91:A:LEU:H	7	0.3
(1,806)	1:57:B:LEU:HD22	1:84:B:THR:H	3	0.3
(1,796)	1:76:B:GLU:HB2	1:77:B:LYS:HB3	8	0.3
(1,770)	1:80:A:ILE:HG22	1:83:A:MET:H	17	0.3
(1,740)	1:79:B:ASP:H	1:80:B:ILE:HD12	7	0.3
(1,740)	1:79:A:ASP:H	1:80:A:ILE:HD11	14	0.3
(1,663)	1:54:B:LEU:HD12	1:77:B:LYS:HE3	9	0.3
(1,639)	1:57:B:LEU:HD22	1:84:B:THR:HG22	1	0.3
(1,616)	1:86:A:LYS:HG2	1:86:A:LYS:HE2	11	0.3
(1,563)	1:56:B:GLN:HG3	1:82:A:GLU:HA	11	0.3
(1,563)	1:56:B:GLN:HG3	1:82:A:GLU:HA	15	0.3
(1,541)	1:77:A:LYS:HB3	1:79:A:ASP:H	19	0.3
(1,540)	1:89:B:ARG:HB3	1:92:B:GLN:H	4	0.3
(1,516)	1:67:B:LYS:HG2	1:68:B:ASP:H	6	0.3
(1,516)	1:67:A:LYS:HG2	1:68:A:ASP:H	19	0.3
(1,498)	1:65:B:LEU:HD21	1:67:B:LYS:H	9	0.3
(1,482)	1:81:A:LEU:HA	1:84:A:THR:HB	4	0.3
(1,482)	1:81:A:LEU:HA	1:84:A:THR:HB	12	0.3
(1,428)	1:86:A:LYS:HA	1:86:A:LYS:HD2	4	0.3
(1,428)	1:86:B:LYS:HA	1:86:B:LYS:HD3	12	0.3
(1,416)	1:82:B:GLU:HA	1:85:B:VAL:HG13	15	0.3
(1,349)	1:86:B:LYS:H	1:89:B:ARG:HD3	8	0.3
(1,329)	1:92:A:GLN:H	1:92:A:GLN:HE21	11	0.3
(1,321)	1:87:B:HIS:HB2	1:88:B:LEU:H	9	0.3
(1,206)	1:93:B:ARG:HG3	1:95:B:GLN:HE21	3	0.3
(1,206)	1:93:B:ARG:HG3	1:95:B:GLN:HE21	16	0.3
(1,201)	1:85:A:VAL:HG22	1:86:A:LYS:H	3	0.3
(1,201)	1:85:A:VAL:HG22	1:86:A:LYS:H	14	0.3
(1,188)	1:76:A:GLU:HA	1:79:A:ASP:H	13	0.3
(1,162)	1:93:A:ARG:H	1:94:A:ALA:HB3	6	0.3
(1,155)	1:91:B:LEU:H	1:91:B:LEU:HD12	11	0.3
(1,155)	1:91:A:LEU:H	1:91:A:LEU:HD12	19	0.3
(1,155)	1:91:B:LEU:H	1:91:B:LEU:HD11	20	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:88:A:LEU:HB2	1:90:A:ASN:H	10	0.3
(1,87)	1:88:A:LEU:HB2	1:90:A:ASN:H	17	0.3
(1,39)	1:68:A:ASP:H	1:69:A:SER:H	1	0.3
(1,31)	1:66:A:LYS:H	1:66:A:LYS:HB2	11	0.3
(1,30)	1:85:A:VAL:H	1:88:A:LEU:HB2	18	0.3
(1,13)	1:88:A:LEU:H	1:89:A:ARG:HD2	18	0.3
(1,879)	1:75:B:LEU:HD23	1:80:B:ILE:H	8	0.29
(1,867)	1:72:A:HIS:H	1:75:A:LEU:HD11	10	0.29
(1,806)	1:57:B:LEU:HD21	1:84:B:THR:H	7	0.29
(1,793)	1:69:B:SER:HG	1:70:B:SER:H	17	0.29
(1,763)	1:86:B:LYS:H	1:86:B:LYS:HD2	6	0.29
(1,762)	1:87:A:HIS:HD1	1:88:A:LEU:H	6	0.29
(1,759)	1:84:A:THR:H	1:84:A:THR:HG21	14	0.29
(1,745)	1:72:A:HIS:H	1:75:A:LEU:HD12	4	0.29
(1,616)	1:86:B:LYS:HG2	1:86:B:LYS:HE2	19	0.29
(1,566)	1:56:B:GLN:HG2	1:82:A:GLU:HA	18	0.29
(1,541)	1:77:B:LYS:HB3	1:79:B:ASP:H	2	0.29
(1,541)	1:77:B:LYS:HB3	1:79:B:ASP:H	11	0.29
(1,540)	1:89:B:ARG:HB3	1:92:B:GLN:H	6	0.29
(1,534)	1:74:A:LYS:HE3	1:75:A:LEU:H	15	0.29
(1,499)	1:65:A:LEU:HA	1:67:A:LYS:H	1	0.29
(1,428)	1:86:A:LYS:HA	1:86:A:LYS:HD3	8	0.29
(1,428)	1:86:B:LYS:HA	1:86:B:LYS:HD2	11	0.29
(1,428)	1:86:B:LYS:HA	1:86:B:LYS:HD2	15	0.29
(1,428)	1:86:B:LYS:HA	1:86:B:LYS:HD2	19	0.29
(1,419)	1:75:A:LEU:HA	1:80:A:ILE:HD13	20	0.29
(1,349)	1:86:A:LYS:H	1:89:A:ARG:HD3	3	0.29
(1,348)	1:71:B:ARG:H	1:71:B:ARG:HD3	10	0.29
(1,329)	1:92:B:GLN:H	1:92:B:GLN:HE21	4	0.29
(1,155)	1:91:A:LEU:H	1:91:A:LEU:HD12	12	0.29
(1,155)	1:91:A:LEU:H	1:91:A:LEU:HD11	15	0.29
(1,112)	1:71:A:ARG:HD3	1:72:A:HIS:H	13	0.29
(1,70)	1:83:B:MET:HE2	1:84:B:THR:H	2	0.29
(1,70)	1:83:B:MET:HE2	1:84:B:THR:H	17	0.29
(1,31)	1:66:A:LYS:H	1:66:A:LYS:HB2	10	0.29
(1,31)	1:66:A:LYS:H	1:66:A:LYS:HB2	13	0.29
(1,934)	1:74:B:LYS:H	1:70:B:SER:O	11	0.28
(1,930)	1:72:A:HIS:H	1:68:A:ASP:O	9	0.28
(1,901)	1:83:B:MET:H	1:83:B:MET:HG3	11	0.28
(1,865)	1:71:A:ARG:HD3	1:72:A:HIS:HB2	13	0.28
(1,796)	1:76:B:GLU:HB2	1:77:B:LYS:HB3	9	0.28
(1,790)	1:69:B:SER:H	1:69:B:SER:HG	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,759)	1:84:A:THR:H	1:84:A:THR:HG22	2	0.28
(1,741)	1:50:B:ILE:HG22	1:51:B:ASN:HD22	16	0.28
(1,711)	1:71:B:ARG:HA	1:71:B:ARG:HG2	19	0.28
(1,637)	1:85:A:VAL:HG12	1:86:A:LYS:HG2	13	0.28
(1,563)	1:56:B:GLN:HG3	1:82:A:GLU:HA	13	0.28
(1,541)	1:77:A:LYS:HB3	1:79:A:ASP:H	3	0.28
(1,541)	1:77:B:LYS:HB3	1:79:B:ASP:H	5	0.28
(1,541)	1:77:B:LYS:HB3	1:79:B:ASP:H	8	0.28
(1,540)	1:89:B:ARG:HB3	1:92:B:GLN:H	2	0.28
(1,540)	1:89:B:ARG:HB3	1:92:B:GLN:H	11	0.28
(1,488)	1:64:A:ALA:HA	1:65:A:LEU:HD13	5	0.28
(1,488)	1:64:B:ALA:HA	1:65:B:LEU:HD12	9	0.28
(1,456)	1:77:B:LYS:HA	1:77:B:LYS:HE2	19	0.28
(1,428)	1:86:A:LYS:HA	1:86:A:LYS:HD3	1	0.28
(1,428)	1:86:A:LYS:HA	1:86:A:LYS:HD3	13	0.28
(1,416)	1:82:B:GLU:HA	1:85:B:VAL:HG11	20	0.28
(1,329)	1:92:A:GLN:H	1:92:A:GLN:HE21	2	0.28
(1,278)	1:65:B:LEU:HD13	1:90:B:ASN:HD21	18	0.28
(1,206)	1:93:A:ARG:HG3	1:95:A:GLN:HE21	18	0.28
(1,206)	1:93:B:ARG:HG3	1:95:B:GLN:HE21	19	0.28
(1,201)	1:85:B:VAL:HG21	1:86:B:LYS:H	20	0.28
(1,188)	1:76:A:GLU:HA	1:79:A:ASP:H	8	0.28
(1,155)	1:91:A:LEU:H	1:91:A:LEU:HD12	8	0.28
(1,87)	1:88:B:LEU:HB2	1:90:B:ASN:H	13	0.28
(1,70)	1:83:B:MET:HE1	1:84:B:THR:H	12	0.28
(1,13)	1:88:B:LEU:H	1:89:B:ARG:HD2	3	0.28
(1,13)	1:88:A:LEU:H	1:89:A:ARG:HD2	7	0.28
(1,931)	1:72:B:HIS:N	1:68:B:ASP:O	13	0.27
(1,909)	1:88:A:LEU:H	1:88:A:LEU:HD12	1	0.27
(1,876)	1:75:B:LEU:HD22	1:79:B:ASP:H	16	0.27
(1,871)	1:75:B:LEU:H	1:75:B:LEU:HD22	18	0.27
(1,864)	1:71:A:ARG:HA	1:75:A:LEU:HD13	12	0.27
(1,859)	1:94:A:ALA:H	1:95:A:GLN:HB2	20	0.27
(1,831)	1:87:A:HIS:HD1	1:91:A:LEU:H	8	0.27
(1,806)	1:57:B:LEU:HD22	1:84:B:THR:H	1	0.27
(1,806)	1:57:B:LEU:HD21	1:84:B:THR:H	4	0.27
(1,806)	1:57:B:LEU:HD23	1:84:B:THR:H	12	0.27
(1,759)	1:84:B:THR:H	1:84:B:THR:HG23	18	0.27
(1,756)	1:84:A:THR:HG23	1:85:A:VAL:H	4	0.27
(1,657)	1:82:B:GLU:HB2	1:86:B:LYS:HD2	20	0.27
(1,637)	1:85:A:VAL:HG11	1:86:A:LYS:HG2	4	0.27
(1,637)	1:85:B:VAL:HG13	1:86:B:LYS:HG2	11	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,637)	1:85:B:VAL:HG13	1:86:B:LYS:HG2	12	0.27
(1,637)	1:85:B:VAL:HG12	1:86:B:LYS:HG2	15	0.27
(1,541)	1:77:A:LYS:HB3	1:79:A:ASP:H	20	0.27
(1,516)	1:67:A:LYS:HG2	1:68:A:ASP:H	5	0.27
(1,516)	1:67:B:LYS:HG2	1:68:B:ASP:H	7	0.27
(1,516)	1:67:A:LYS:HG2	1:68:A:ASP:H	12	0.27
(1,486)	1:93:B:ARG:HA	1:94:B:ALA:HA	16	0.27
(1,486)	1:93:A:ARG:HA	1:94:A:ALA:HA	20	0.27
(1,428)	1:86:A:LYS:HA	1:86:A:LYS:HD3	2	0.27
(1,428)	1:86:A:LYS:HA	1:86:A:LYS:HD3	5	0.27
(1,428)	1:86:A:LYS:HA	1:86:A:LYS:HD3	18	0.27
(1,428)	1:86:A:LYS:HA	1:86:A:LYS:HD3	20	0.27
(1,416)	1:82:A:GLU:HA	1:85:A:VAL:HG11	12	0.27
(1,416)	1:82:B:GLU:HA	1:85:B:VAL:HG11	18	0.27
(1,329)	1:92:A:GLN:H	1:92:A:GLN:HE21	7	0.27
(1,329)	1:92:A:GLN:H	1:92:A:GLN:HE21	16	0.27
(1,271)	1:76:B:GLU:H	1:80:B:ILE:HD13	14	0.27
(1,241)	1:88:A:LEU:H	1:88:A:LEU:HB2	17	0.27
(1,206)	1:93:A:ARG:HG3	1:95:A:GLN:HE21	1	0.27
(1,206)	1:93:A:ARG:HG3	1:95:A:GLN:HE21	6	0.27
(1,206)	1:93:B:ARG:HG3	1:95:B:GLN:HE21	7	0.27
(1,206)	1:93:A:ARG:HG3	1:95:A:GLN:HE21	14	0.27
(1,201)	1:85:A:VAL:HG21	1:86:A:LYS:H	16	0.27
(1,169)	1:94:B:ALA:HB1	1:95:B:GLN:H	12	0.27
(1,155)	1:91:A:LEU:H	1:91:A:LEU:HD11	18	0.27
(1,87)	1:88:B:LEU:HB2	1:90:B:ASN:H	11	0.27
(1,87)	1:88:B:LEU:HB2	1:90:B:ASN:H	19	0.27
(1,31)	1:66:A:LYS:H	1:66:A:LYS:HB2	3	0.27
(1,13)	1:88:B:LEU:H	1:89:B:ARG:HD2	8	0.27
(1,914)	1:88:A:LEU:HD11	1:92:A:GLN:HB2	16	0.26
(1,901)	1:83:A:MET:H	1:83:A:MET:HG3	12	0.26
(1,879)	1:75:A:LEU:HD11	1:80:A:ILE:H	14	0.26
(1,865)	1:71:B:ARG:HD3	1:72:B:HIS:HB2	7	0.26
(1,831)	1:87:B:HIS:HD2	1:91:B:LEU:H	15	0.26
(1,806)	1:57:B:LEU:HD23	1:84:B:THR:H	16	0.26
(1,788)	1:65:A:LEU:HG	1:66:A:LYS:H	6	0.26
(1,788)	1:65:B:LEU:HG	1:66:B:LYS:H	15	0.26
(1,763)	1:86:A:LYS:H	1:86:A:LYS:HD2	9	0.26
(1,736)	1:84:B:THR:HB	1:85:B:VAL:HG11	15	0.26
(1,711)	1:71:B:ARG:HA	1:71:B:ARG:HG2	2	0.26
(1,711)	1:71:B:ARG:HA	1:71:B:ARG:HG2	4	0.26
(1,637)	1:85:B:VAL:HG13	1:86:B:LYS:HG2	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,637)	1:85:B:VAL:HG11	1:86:B:LYS:HG2	5	0.26
(1,637)	1:85:A:VAL:HG11	1:86:A:LYS:HG2	7	0.26
(1,637)	1:85:A:VAL:HG11	1:86:A:LYS:HG2	8	0.26
(1,637)	1:85:A:VAL:HG13	1:86:A:LYS:HG2	17	0.26
(1,630)	1:75:B:LEU:HB2	1:80:B:ILE:HG13	19	0.26
(1,621)	1:82:B:GLU:HG3	1:85:B:VAL:HG11	16	0.26
(1,616)	1:86:B:LYS:HG2	1:86:B:LYS:HE2	4	0.26
(1,541)	1:77:B:LYS:HB3	1:79:B:ASP:H	1	0.26
(1,541)	1:77:B:LYS:HB3	1:79:B:ASP:H	18	0.26
(1,475)	1:71:A:ARG:HA	1:71:A:ARG:HD3	13	0.26
(1,428)	1:86:A:LYS:HA	1:86:A:LYS:HD3	7	0.26
(1,419)	1:75:A:LEU:HA	1:80:A:ILE:HD12	13	0.26
(1,419)	1:75:B:LEU:HA	1:80:B:ILE:HD11	15	0.26
(1,348)	1:71:A:ARG:H	1:71:A:ARG:HD3	4	0.26
(1,201)	1:85:B:VAL:HG21	1:86:B:LYS:H	2	0.26
(1,201)	1:85:A:VAL:HG21	1:86:A:LYS:H	9	0.26
(1,201)	1:85:A:VAL:HG21	1:86:A:LYS:H	13	0.26
(1,201)	1:85:A:VAL:HG21	1:86:A:LYS:H	19	0.26
(1,188)	1:76:B:GLU:HA	1:79:B:ASP:H	11	0.26
(1,165)	1:93:B:ARG:HB2	1:94:B:ALA:H	5	0.26
(1,162)	1:93:A:ARG:H	1:94:A:ALA:HB3	3	0.26
(1,162)	1:93:A:ARG:H	1:94:A:ALA:HB2	18	0.26
(1,155)	1:91:A:LEU:H	1:91:A:LEU:HD11	6	0.26
(1,155)	1:91:A:LEU:H	1:91:A:LEU:HD13	7	0.26
(1,112)	1:71:A:ARG:HD3	1:72:A:HIS:H	2	0.26
(1,87)	1:88:B:LEU:HB2	1:90:B:ASN:H	12	0.26
(1,87)	1:88:A:LEU:HB2	1:90:A:ASN:H	14	0.26
(1,31)	1:66:B:LYS:H	1:66:B:LYS:HB2	16	0.26
(1,31)	1:66:B:LYS:H	1:66:B:LYS:HB2	17	0.26
(1,31)	1:66:A:LYS:H	1:66:A:LYS:HB2	18	0.26
(1,25)	1:63:B:ASP:HA	1:64:B:ALA:H	12	0.26
(1,25)	1:63:A:ASP:HA	1:64:A:ALA:H	15	0.26
(1,933)	1:73:A:SER:N	1:69:A:SER:O	9	0.25
(1,918)	1:88:B:LEU:HD21	1:92:B:GLN:HE22	7	0.25
(1,914)	1:88:B:LEU:HD11	1:92:B:GLN:HB2	18	0.25
(1,896)	1:80:A:ILE:HB	1:81:A:LEU:HD21	17	0.25
(1,791)	1:69:A:SER:HA	1:69:A:SER:HG	13	0.25
(1,762)	1:87:A:HIS:HD1	1:88:A:LEU:H	16	0.25
(1,759)	1:84:A:THR:H	1:84:A:THR:HG23	3	0.25
(1,711)	1:71:A:ARG:HA	1:71:A:ARG:HG2	7	0.25
(1,692)	1:74:A:LYS:HA	1:74:A:LYS:HD3	19	0.25
(1,637)	1:85:A:VAL:HG13	1:86:A:LYS:HG2	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,637)	1:85:A:VAL:HG11	1:86:A:LYS:HG2	16	0.25
(1,621)	1:82:B:GLU:HG3	1:85:B:VAL:HG11	20	0.25
(1,566)	1:56:A:GLN:HG2	1:82:B:GLU:HA	20	0.25
(1,541)	1:77:A:LYS:HB3	1:79:A:ASP:H	6	0.25
(1,541)	1:77:B:LYS:HB3	1:79:B:ASP:H	7	0.25
(1,486)	1:93:B:ARG:HA	1:94:B:ALA:HA	3	0.25
(1,486)	1:93:A:ARG:HA	1:94:A:ALA:HA	10	0.25
(1,428)	1:86:B:LYS:HA	1:86:B:LYS:HD3	9	0.25
(1,419)	1:75:A:LEU:HA	1:80:A:ILE:HD12	7	0.25
(1,348)	1:71:B:ARG:H	1:71:B:ARG:HD3	7	0.25
(1,321)	1:87:B:HIS:HB2	1:88:B:LEU:H	1	0.25
(1,321)	1:87:B:HIS:HB2	1:88:B:LEU:H	8	0.25
(1,206)	1:93:B:ARG:HG2	1:95:B:GLN:HE21	17	0.25
(1,188)	1:76:B:GLU:HA	1:79:B:ASP:H	14	0.25
(1,155)	1:91:B:LEU:H	1:91:B:LEU:HD12	1	0.25
(1,155)	1:91:A:LEU:H	1:91:A:LEU:HD11	17	0.25
(1,80)	1:88:A:LEU:HB3	1:89:A:ARG:H	17	0.25
(1,13)	1:88:B:LEU:H	1:89:B:ARG:HD2	10	0.25
(1,935)	1:74:B:LYS:N	1:70:B:SER:O	4	0.24
(1,930)	1:72:B:HIS:H	1:68:B:ASP:O	2	0.24
(1,930)	1:72:B:HIS:H	1:68:B:ASP:O	19	0.24
(1,920)	1:94:B:ALA:HB1	1:95:B:GLN:HG2	4	0.24
(1,865)	1:71:A:ARG:HD2	1:72:A:HIS:HB2	19	0.24
(1,788)	1:65:B:LEU:HG	1:66:B:LYS:H	13	0.24
(1,763)	1:86:A:LYS:H	1:86:A:LYS:HD2	5	0.24
(1,763)	1:86:A:LYS:H	1:86:A:LYS:HD2	14	0.24
(1,763)	1:86:B:LYS:H	1:86:B:LYS:HD2	17	0.24
(1,751)	1:73:A:SER:HB2	1:74:A:LYS:H	5	0.24
(1,667)	1:90:B:ASN:HB2	1:91:B:LEU:HD11	20	0.24
(1,657)	1:82:B:GLU:HB2	1:86:B:LYS:HD2	13	0.24
(1,622)	1:82:A:GLU:HB2	1:85:A:VAL:HG12	19	0.24
(1,486)	1:93:A:ARG:HA	1:94:A:ALA:HA	6	0.24
(1,486)	1:93:B:ARG:HA	1:94:B:ALA:HA	15	0.24
(1,482)	1:81:A:LEU:HA	1:84:A:THR:HB	20	0.24
(1,461)	1:76:A:GLU:HB2	1:77:A:LYS:HA	5	0.24
(1,428)	1:86:B:LYS:HA	1:86:B:LYS:HD3	14	0.24
(1,428)	1:86:A:LYS:HA	1:86:A:LYS:HD3	17	0.24
(1,419)	1:75:B:LEU:HA	1:80:B:ILE:HD13	5	0.24
(1,419)	1:75:A:LEU:HA	1:80:A:ILE:HD13	9	0.24
(1,419)	1:75:A:LEU:HA	1:80:A:ILE:HD12	12	0.24
(1,416)	1:82:A:GLU:HA	1:85:A:VAL:HG11	1	0.24
(1,379)	1:65:A:LEU:HD23	1:66:A:LYS:H	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,379)	1:65:B:LEU:HD23	1:66:B:LYS:H	12	0.24
(1,321)	1:87:B:HIS:HB2	1:88:B:LEU:H	4	0.24
(1,271)	1:76:A:GLU:H	1:80:A:ILE:HD13	8	0.24
(1,271)	1:76:B:GLU:H	1:80:B:ILE:HD12	11	0.24
(1,271)	1:76:A:GLU:H	1:80:A:ILE:HD13	20	0.24
(1,206)	1:93:B:ARG:HG3	1:95:B:GLN:HE21	15	0.24
(1,167)	1:91:A:LEU:HD22	1:94:A:ALA:H	17	0.24
(1,155)	1:91:B:LEU:H	1:91:B:LEU:HD11	3	0.24
(1,155)	1:91:A:LEU:H	1:91:A:LEU:HD11	4	0.24
(1,87)	1:88:B:LEU:HB2	1:90:B:ASN:H	7	0.24
(1,31)	1:66:A:LYS:H	1:66:A:LYS:HB2	8	0.24
(1,932)	1:73:A:SER:H	1:69:A:SER:O	20	0.23
(1,895)	1:80:B:ILE:HA	1:81:B:LEU:HD13	14	0.23
(1,879)	1:75:B:LEU:HD22	1:80:B:ILE:H	17	0.23
(1,867)	1:72:B:HIS:H	1:75:B:LEU:HD12	13	0.23
(1,806)	1:57:B:LEU:HD22	1:84:B:THR:H	2	0.23
(1,806)	1:57:B:LEU:HD23	1:84:B:THR:H	13	0.23
(1,741)	1:50:B:ILE:HG21	1:51:B:ASN:HD22	14	0.23
(1,711)	1:71:B:ARG:HA	1:71:B:ARG:HG2	13	0.23
(1,667)	1:90:A:ASN:HB2	1:91:A:LEU:HD12	5	0.23
(1,660)	1:74:A:LYS:HG3	1:76:A:GLU:HG3	20	0.23
(1,657)	1:82:A:GLU:HB2	1:86:A:LYS:HD2	7	0.23
(1,644)	1:86:B:LYS:HB3	1:86:B:LYS:HD3	11	0.23
(1,566)	1:56:B:GLN:HG2	1:82:A:GLU:HA	9	0.23
(1,566)	1:56:A:GLN:HG2	1:82:B:GLU:HA	12	0.23
(1,563)	1:56:B:GLN:HG3	1:82:A:GLU:HA	4	0.23
(1,540)	1:89:B:ARG:HB3	1:92:B:GLN:H	18	0.23
(1,531)	1:87:A:HIS:H	1:88:A:LEU:HB2	11	0.23
(1,516)	1:67:A:LYS:HG2	1:68:A:ASP:H	1	0.23
(1,516)	1:67:A:LYS:HG2	1:68:A:ASP:H	17	0.23
(1,498)	1:65:A:LEU:HD23	1:67:A:LYS:H	1	0.23
(1,482)	1:81:A:LEU:HA	1:84:A:THR:HB	13	0.23
(1,461)	1:76:B:GLU:HB2	1:77:B:LYS:HA	15	0.23
(1,428)	1:86:A:LYS:HA	1:86:A:LYS:HD3	16	0.23
(1,276)	1:75:A:LEU:H	1:75:A:LEU:HD12	1	0.23
(1,202)	1:86:B:LYS:H	1:86:B:LYS:HE2	17	0.23
(1,165)	1:93:A:ARG:HB2	1:94:A:ALA:H	6	0.23
(1,81)	1:88:B:LEU:HB2	1:89:B:ARG:H	16	0.23
(1,31)	1:66:A:LYS:H	1:66:A:LYS:HB2	2	0.23
(1,31)	1:66:A:LYS:H	1:66:A:LYS:HB2	15	0.23
(1,930)	1:72:A:HIS:H	1:68:A:ASP:O	5	0.22
(1,930)	1:72:A:HIS:H	1:68:A:ASP:O	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,901)	1:83:A:MET:H	1:83:A:MET:HG2	1	0.22
(1,891)	1:79:A:ASP:H	1:81:A:LEU:HD13	17	0.22
(1,876)	1:75:A:LEU:HD12	1:79:A:ASP:H	18	0.22
(1,796)	1:76:B:GLU:HB2	1:77:B:LYS:HB3	4	0.22
(1,796)	1:76:B:GLU:HB2	1:77:B:LYS:HB3	14	0.22
(1,763)	1:86:B:LYS:H	1:86:B:LYS:HD2	7	0.22
(1,763)	1:86:A:LYS:H	1:86:A:LYS:HD2	8	0.22
(1,763)	1:86:B:LYS:H	1:86:B:LYS:HD2	12	0.22
(1,759)	1:84:A:THR:H	1:84:A:THR:HG22	8	0.22
(1,660)	1:74:A:LYS:HG3	1:76:A:GLU:HG3	2	0.22
(1,644)	1:86:B:LYS:HB3	1:86:B:LYS:HD3	4	0.22
(1,637)	1:85:B:VAL:HG13	1:86:B:LYS:HG2	20	0.22
(1,580)	1:75:A:LEU:HB3	1:76:A:GLU:HB2	6	0.22
(1,563)	1:56:B:GLN:HG3	1:82:A:GLU:HA	14	0.22
(1,516)	1:67:A:LYS:HG2	1:68:A:ASP:H	13	0.22
(1,499)	1:65:A:LEU:HA	1:67:A:LYS:H	6	0.22
(1,486)	1:93:A:ARG:HA	1:94:A:ALA:HA	17	0.22
(1,486)	1:93:A:ARG:HA	1:94:A:ALA:HA	19	0.22
(1,482)	1:81:A:LEU:HA	1:84:A:THR:HB	9	0.22
(1,466)	1:93:A:ARG:HA	1:93:A:ARG:HD2	8	0.22
(1,440)	1:89:B:ARG:HD2	1:92:B:GLN:HB2	5	0.22
(1,428)	1:86:A:LYS:HA	1:86:A:LYS:HD3	6	0.22
(1,379)	1:65:B:LEU:HD22	1:66:B:LYS:H	5	0.22
(1,321)	1:87:B:HIS:HB2	1:88:B:LEU:H	7	0.22
(1,321)	1:87:A:HIS:HB2	1:88:A:LEU:H	10	0.22
(1,321)	1:87:B:HIS:HB2	1:88:B:LEU:H	17	0.22
(1,276)	1:75:B:LEU:H	1:75:B:LEU:HD11	9	0.22
(1,271)	1:76:B:GLU:H	1:80:B:ILE:HD11	4	0.22
(1,271)	1:76:B:GLU:H	1:80:B:ILE:HD13	18	0.22
(1,206)	1:93:A:ARG:HG2	1:95:A:GLN:HE21	11	0.22
(1,188)	1:76:A:GLU:HA	1:79:A:ASP:H	16	0.22
(1,188)	1:76:B:GLU:HA	1:79:B:ASP:H	20	0.22
(1,169)	1:94:B:ALA:HB1	1:95:B:GLN:H	9	0.22
(1,165)	1:93:A:ARG:HB3	1:94:A:ALA:H	18	0.22
(1,70)	1:83:A:MET:HE1	1:84:A:THR:H	20	0.22
(1,31)	1:66:B:LYS:H	1:66:B:LYS:HB2	14	0.22
(1,25)	1:63:B:ASP:HA	1:64:B:ALA:H	2	0.22
(1,25)	1:63:B:ASP:HA	1:64:B:ALA:H	14	0.22
(1,919)	1:94:A:ALA:H	1:95:A:GLN:HG2	16	0.21
(1,914)	1:88:A:LEU:HD13	1:92:A:GLN:HB2	17	0.21
(1,831)	1:87:B:HIS:HD1	1:91:B:LEU:H	19	0.21
(1,771)	1:83:B:MET:H	1:86:B:LYS:HD3	19	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,757)	1:80:B:ILE:H	1:80:B:ILE:HD13	16	0.21
(1,757)	1:80:A:ILE:H	1:80:A:ILE:HD11	18	0.21
(1,683)	1:71:A:ARG:HD3	1:75:A:LEU:HD13	13	0.21
(1,660)	1:74:A:LYS:HG3	1:76:A:GLU:HG3	5	0.21
(1,660)	1:74:A:LYS:HG3	1:76:A:GLU:HG3	6	0.21
(1,657)	1:82:B:GLU:HB2	1:86:B:LYS:HD2	17	0.21
(1,644)	1:86:B:LYS:HB3	1:86:B:LYS:HD3	3	0.21
(1,644)	1:86:A:LYS:HB3	1:86:A:LYS:HD3	15	0.21
(1,623)	1:41:B:ILE:HG13	1:44:B:LYS:HE3	14	0.21
(1,622)	1:82:A:GLU:HB2	1:85:A:VAL:HG11	1	0.21
(1,540)	1:89:B:ARG:HB3	1:92:B:GLN:H	3	0.21
(1,540)	1:89:A:ARG:HB3	1:92:A:GLN:H	10	0.21
(1,534)	1:74:B:LYS:HE2	1:75:B:LEU:H	4	0.21
(1,531)	1:87:B:HIS:H	1:88:B:LEU:HB2	20	0.21
(1,516)	1:67:B:LYS:HG2	1:68:B:ASP:H	4	0.21
(1,516)	1:67:B:LYS:HG2	1:68:B:ASP:H	20	0.21
(1,486)	1:93:B:ARG:HA	1:94:B:ALA:HA	18	0.21
(1,425)	1:93:B:ARG:HA	1:93:B:ARG:HG3	13	0.21
(1,420)	1:87:A:HIS:HD2	1:91:A:LEU:HA	15	0.21
(1,348)	1:71:A:ARG:H	1:71:A:ARG:HD3	2	0.21
(1,321)	1:87:A:HIS:HB2	1:88:A:LEU:H	18	0.21
(1,284)	1:87:A:HIS:HD2	1:88:A:LEU:H	4	0.21
(1,242)	1:88:B:LEU:H	1:89:B:ARG:HB2	18	0.21
(1,165)	1:93:B:ARG:HB3	1:94:B:ALA:H	2	0.21
(1,165)	1:93:A:ARG:HB2	1:94:A:ALA:H	7	0.21
(1,165)	1:93:B:ARG:HB2	1:94:B:ALA:H	9	0.21
(1,165)	1:93:B:ARG:HB2	1:94:B:ALA:H	12	0.21
(1,165)	1:93:A:ARG:HB2	1:94:A:ALA:H	15	0.21
(1,39)	1:68:A:ASP:H	1:69:A:SER:H	9	0.21
(1,31)	1:66:B:LYS:H	1:66:B:LYS:HB2	5	0.21
(1,31)	1:66:A:LYS:H	1:66:A:LYS:HB2	6	0.21
(1,31)	1:66:A:LYS:H	1:66:A:LYS:HB2	12	0.21
(1,25)	1:63:B:ASP:HA	1:64:B:ALA:H	4	0.21
(1,25)	1:63:B:ASP:HA	1:64:B:ALA:H	11	0.21
(1,25)	1:63:B:ASP:HA	1:64:B:ALA:H	16	0.21
(1,25)	1:63:B:ASP:HA	1:64:B:ALA:H	17	0.21
(1,25)	1:63:A:ASP:HA	1:64:A:ALA:H	18	0.21
(1,19)	1:62:A:LEU:HA	1:63:A:ASP:H	14	0.21
(1,13)	1:88:A:LEU:H	1:89:A:ARG:HD3	14	0.21
(1,930)	1:72:B:HIS:H	1:68:B:ASP:O	11	0.2
(1,912)	1:88:A:LEU:HD13	1:91:A:LEU:H	17	0.2
(1,867)	1:72:B:HIS:H	1:75:B:LEU:HD22	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,867)	1:72:B:HIS:H	1:75:B:LEU:HD13	19	0.2
(1,806)	1:57:A:LEU:HD11	1:84:A:THR:H	8	0.2
(1,757)	1:80:A:ILE:H	1:80:A:ILE:HD11	2	0.2
(1,644)	1:86:B:LYS:HB3	1:86:B:LYS:HD3	19	0.2
(1,619)	1:77:B:LYS:HG3	1:77:B:LYS:HE2	9	0.2
(1,558)	1:81:A:LEU:HA	1:83:A:MET:HE2	19	0.2
(1,541)	1:77:A:LYS:HB3	1:79:A:ASP:H	15	0.2
(1,476)	1:69:A:SER:HA	1:72:A:HIS:HD2	7	0.2
(1,440)	1:89:A:ARG:HD2	1:92:A:GLN:HB2	16	0.2
(1,425)	1:93:A:ARG:HA	1:93:A:ARG:HG3	15	0.2
(1,419)	1:75:B:LEU:HA	1:80:B:ILE:HD12	11	0.2
(1,416)	1:82:A:GLU:HA	1:85:A:VAL:HG13	3	0.2
(1,329)	1:92:A:GLN:H	1:92:A:GLN:HE21	18	0.2
(1,271)	1:76:A:GLU:H	1:80:A:ILE:HD13	17	0.2
(1,201)	1:85:A:VAL:HG23	1:86:A:LYS:H	18	0.2
(1,188)	1:76:A:GLU:HA	1:79:A:ASP:H	3	0.2
(1,165)	1:93:A:ARG:HB2	1:94:A:ALA:H	13	0.2
(1,112)	1:71:B:ARG:HD3	1:72:B:HIS:H	7	0.2
(1,31)	1:66:B:LYS:H	1:66:B:LYS:HB2	19	0.2
(1,25)	1:63:B:ASP:HA	1:64:B:ALA:H	7	0.2
(1,25)	1:63:A:ASP:HA	1:64:A:ALA:H	20	0.2
(1,19)	1:62:A:LEU:HA	1:63:A:ASP:H	13	0.2
(1,935)	1:74:B:LYS:N	1:70:B:SER:O	17	0.19
(1,932)	1:73:A:SER:H	1:69:A:SER:O	15	0.19
(1,901)	1:83:A:MET:H	1:83:A:MET:HG3	2	0.19
(1,896)	1:80:A:ILE:HB	1:81:A:LEU:HD21	1	0.19
(1,879)	1:75:A:LEU:HD23	1:80:A:ILE:H	16	0.19
(1,877)	1:75:A:LEU:HD22	1:79:A:ASP:HA	15	0.19
(1,864)	1:71:B:ARG:HA	1:75:B:LEU:HD13	3	0.19
(1,796)	1:76:A:GLU:HB2	1:77:A:LYS:HB3	15	0.19
(1,763)	1:86:A:LYS:H	1:86:A:LYS:HD2	1	0.19
(1,751)	1:73:B:SER:HB2	1:74:B:LYS:H	1	0.19
(1,741)	1:50:A:ILE:HG21	1:51:A:ASN:HD22	10	0.19
(1,624)	1:84:B:THR:HG23	1:88:A:LEU:HB3	19	0.19
(1,541)	1:77:B:LYS:HB3	1:79:B:ASP:H	16	0.19
(1,531)	1:87:B:HIS:H	1:88:B:LEU:HB2	5	0.19
(1,523)	1:66:A:LYS:HB2	1:67:A:LYS:H	1	0.19
(1,486)	1:93:B:ARG:HA	1:94:B:ALA:HA	11	0.19
(1,482)	1:81:B:LEU:HA	1:84:B:THR:HB	7	0.19
(1,470)	1:71:B:ARG:HA	1:71:B:ARG:HD3	6	0.19
(1,419)	1:75:A:LEU:HA	1:80:A:ILE:HD13	17	0.19
(1,379)	1:65:A:LEU:HD23	1:66:A:LYS:H	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,271)	1:76:B:GLU:H	1:80:B:ILE:HD11	16	0.19
(1,208)	1:86:A:LYS:HB3	1:90:A:ASN:HD21	9	0.19
(1,202)	1:86:B:LYS:H	1:86:B:LYS:HE3	20	0.19
(1,188)	1:76:B:GLU:HA	1:79:B:ASP:H	19	0.19
(1,167)	1:91:B:LEU:HD21	1:94:B:ALA:H	18	0.19
(1,165)	1:93:A:ARG:HB2	1:94:A:ALA:H	20	0.19
(1,162)	1:93:B:ARG:H	1:94:B:ALA:HB3	2	0.19
(1,112)	1:71:A:ARG:HD3	1:72:A:HIS:H	4	0.19
(1,87)	1:88:A:LEU:HB2	1:90:A:ASN:H	2	0.19
(1,70)	1:83:B:MET:HE1	1:84:B:THR:H	13	0.19
(1,46)	1:73:A:SER:HB2	1:75:A:LEU:H	6	0.19
(1,25)	1:63:A:ASP:HA	1:64:A:ALA:H	10	0.19
(1,25)	1:63:A:ASP:HA	1:64:A:ALA:H	19	0.19
(1,13)	1:88:B:LEU:H	1:89:B:ARG:HD3	11	0.19
(1,937)	1:75:B:LEU:N	1:71:B:ARG:O	1	0.18
(1,932)	1:73:B:SER:H	1:69:B:SER:O	6	0.18
(1,901)	1:83:A:MET:H	1:83:A:MET:HG3	4	0.18
(1,896)	1:80:A:ILE:HB	1:81:A:LEU:HD23	20	0.18
(1,879)	1:75:A:LEU:HD21	1:80:A:ILE:H	2	0.18
(1,763)	1:86:A:LYS:H	1:86:A:LYS:HD2	18	0.18
(1,757)	1:80:B:ILE:H	1:80:B:ILE:HD13	19	0.18
(1,741)	1:50:B:ILE:HG22	1:51:B:ASN:HD22	6	0.18
(1,661)	1:74:A:LYS:HG3	1:76:A:GLU:HG2	9	0.18
(1,661)	1:74:A:LYS:HG3	1:76:A:GLU:HG2	15	0.18
(1,660)	1:74:A:LYS:HG3	1:76:A:GLU:HG3	16	0.18
(1,624)	1:84:A:THR:HG21	1:88:B:LEU:HB3	14	0.18
(1,541)	1:77:A:LYS:HB3	1:79:A:ASP:H	14	0.18
(1,540)	1:89:B:ARG:HB3	1:92:B:GLN:H	16	0.18
(1,534)	1:74:A:LYS:HE2	1:75:A:LEU:H	9	0.18
(1,486)	1:93:B:ARG:HA	1:94:B:ALA:HA	5	0.18
(1,482)	1:81:B:LEU:HA	1:84:B:THR:HB	17	0.18
(1,425)	1:93:B:ARG:HA	1:93:B:ARG:HG3	9	0.18
(1,321)	1:87:A:HIS:HB2	1:88:A:LEU:H	2	0.18
(1,321)	1:87:B:HIS:HB2	1:88:B:LEU:H	6	0.18
(1,306)	1:81:B:LEU:H	1:82:B:GLU:HB3	4	0.18
(1,271)	1:76:B:GLU:H	1:80:B:ILE:HD13	2	0.18
(1,208)	1:86:A:LYS:HB3	1:90:A:ASN:HD21	4	0.18
(1,165)	1:93:B:ARG:HB2	1:94:B:ALA:H	10	0.18
(1,159)	1:92:B:GLN:HB2	1:93:B:ARG:H	11	0.18
(1,112)	1:71:B:ARG:HD3	1:72:B:HIS:H	14	0.18
(1,112)	1:71:B:ARG:HD3	1:72:B:HIS:H	16	0.18
(1,25)	1:63:B:ASP:HA	1:64:B:ALA:H	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:63:A:ASP:HA	1:64:A:ALA:H	13	0.18
(1,19)	1:62:B:LEU:HA	1:63:B:ASP:H	4	0.18
(1,19)	1:62:B:LEU:HA	1:63:B:ASP:H	6	0.18
(1,932)	1:73:B:SER:H	1:69:B:SER:O	3	0.17
(1,930)	1:72:A:HIS:H	1:68:A:ASP:O	17	0.17
(1,922)	1:95:B:GLN:HA	1:95:B:GLN:HG2	5	0.17
(1,910)	1:88:A:LEU:HD21	1:89:A:ARG:H	1	0.17
(1,910)	1:88:B:LEU:HD23	1:89:B:ARG:H	9	0.17
(1,901)	1:83:B:MET:H	1:83:B:MET:HG3	8	0.17
(1,879)	1:75:B:LEU:HD21	1:80:B:ILE:H	10	0.17
(1,876)	1:75:A:LEU:HD21	1:79:A:ASP:H	1	0.17
(1,867)	1:72:A:HIS:H	1:75:A:LEU:HD12	1	0.17
(1,828)	1:87:A:HIS:HB3	1:87:A:HIS:HD2	10	0.17
(1,828)	1:87:B:HIS:HB3	1:87:B:HIS:HD2	14	0.17
(1,763)	1:86:B:LYS:H	1:86:B:LYS:HD2	20	0.17
(1,757)	1:80:A:ILE:H	1:80:A:ILE:HD12	15	0.17
(1,751)	1:73:A:SER:HB3	1:74:A:LYS:H	10	0.17
(1,741)	1:50:B:ILE:HG22	1:51:B:ASN:HD22	8	0.17
(1,660)	1:74:B:LYS:HG3	1:76:B:GLU:HG3	1	0.17
(1,588)	1:82:A:GLU:HB2	1:86:A:LYS:HE2	3	0.17
(1,588)	1:82:A:GLU:HB2	1:86:A:LYS:HE2	11	0.17
(1,566)	1:56:B:GLN:HG2	1:82:A:GLU:HA	2	0.17
(1,566)	1:56:B:GLN:HG2	1:82:A:GLU:HA	6	0.17
(1,541)	1:77:A:LYS:HB3	1:79:A:ASP:H	13	0.17
(1,534)	1:74:A:LYS:HE3	1:75:A:LEU:H	2	0.17
(1,534)	1:74:A:LYS:HE2	1:75:A:LEU:H	19	0.17
(1,482)	1:81:A:LEU:HA	1:84:A:THR:HB	6	0.17
(1,425)	1:93:B:ARG:HA	1:93:B:ARG:HG3	3	0.17
(1,425)	1:93:A:ARG:HA	1:93:A:ARG:HG3	6	0.17
(1,416)	1:82:A:GLU:HA	1:85:A:VAL:HG11	10	0.17
(1,348)	1:71:A:ARG:H	1:71:A:ARG:HD3	18	0.17
(1,329)	1:92:A:GLN:H	1:92:A:GLN:HE21	1	0.17
(1,321)	1:87:B:HIS:HB2	1:88:B:LEU:H	15	0.17
(1,284)	1:87:A:HIS:HD2	1:88:A:LEU:H	5	0.17
(1,284)	1:87:B:HIS:HD2	1:88:B:LEU:H	14	0.17
(1,276)	1:75:A:LEU:H	1:75:A:LEU:HD12	19	0.17
(1,215)	1:92:A:GLN:HB3	1:92:A:GLN:HE22	18	0.17
(1,165)	1:93:B:ARG:HB3	1:94:B:ALA:H	19	0.17
(1,112)	1:71:B:ARG:HD3	1:72:B:HIS:H	11	0.17
(1,81)	1:88:A:LEU:HB2	1:89:A:ARG:H	5	0.17
(1,70)	1:83:B:MET:HE3	1:84:B:THR:H	11	0.17
(1,31)	1:66:B:LYS:H	1:66:B:LYS:HB2	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:63:A:ASP:HA	1:64:A:ALA:H	1	0.17
(1,25)	1:63:B:ASP:HA	1:64:B:ALA:H	3	0.17
(1,25)	1:63:A:ASP:HA	1:64:A:ALA:H	5	0.17
(1,19)	1:62:B:LEU:HA	1:63:B:ASP:H	3	0.17
(1,935)	1:74:A:LYS:N	1:70:A:SER:O	15	0.16
(1,930)	1:72:A:HIS:H	1:68:A:ASP:O	6	0.16
(1,901)	1:83:A:MET:H	1:83:A:MET:HG3	3	0.16
(1,901)	1:83:A:MET:H	1:83:A:MET:HG3	6	0.16
(1,889)	1:78:B:ALA:H	1:81:B:LEU:HD13	11	0.16
(1,881)	1:75:A:LEU:HD21	1:83:A:MET:H	1	0.16
(1,828)	1:87:A:HIS:HB3	1:87:A:HIS:HD2	1	0.16
(1,793)	1:69:B:SER:HG	1:70:B:SER:H	11	0.16
(1,757)	1:80:A:ILE:H	1:80:A:ILE:HD13	3	0.16
(1,757)	1:80:B:ILE:H	1:80:B:ILE:HD11	17	0.16
(1,741)	1:50:B:ILE:HG23	1:51:B:ASN:HD22	4	0.16
(1,696)	1:89:A:ARG:HB2	1:90:A:ASN:HA	11	0.16
(1,656)	1:82:B:GLU:HB2	1:86:B:LYS:HG2	19	0.16
(1,588)	1:82:B:GLU:HB2	1:86:B:LYS:HE2	15	0.16
(1,425)	1:93:A:ARG:HA	1:93:A:ARG:HG3	1	0.16
(1,345)	1:93:A:ARG:HD3	1:95:A:GLN:H	6	0.16
(1,215)	1:92:B:GLN:HB3	1:92:B:GLN:HE22	7	0.16
(1,215)	1:92:A:GLN:HB3	1:92:A:GLN:HE22	11	0.16
(1,188)	1:76:B:GLU:HA	1:79:B:ASP:H	2	0.16
(1,155)	1:91:A:LEU:H	1:91:A:LEU:HD12	13	0.16
(1,112)	1:71:B:ARG:HD3	1:72:B:HIS:H	10	0.16
(1,101)	1:91:B:LEU:HA	1:92:B:GLN:H	4	0.16
(1,70)	1:83:A:MET:HE1	1:84:A:THR:H	14	0.16
(1,25)	1:63:B:ASP:HA	1:64:B:ALA:H	9	0.16
(1,19)	1:62:A:LEU:HA	1:63:A:ASP:H	9	0.16
(1,13)	1:88:A:LEU:H	1:89:A:ARG:HD3	6	0.16
(1,914)	1:88:A:LEU:HD23	1:92:A:GLN:HB2	1	0.15
(1,903)	1:84:A:THR:H	1:87:A:HIS:HB2	5	0.15
(1,903)	1:84:B:THR:H	1:87:B:HIS:HB2	20	0.15
(1,871)	1:75:B:LEU:H	1:75:B:LEU:HD23	15	0.15
(1,865)	1:71:A:ARG:HD2	1:72:A:HIS:HB2	10	0.15
(1,836)	1:87:B:HIS:HD2	1:92:A:GLN:HE21	14	0.15
(1,828)	1:87:A:HIS:HB3	1:87:A:HIS:HD2	11	0.15
(1,810)	1:84:A:THR:H	1:86:A:LYS:HG3	20	0.15
(1,791)	1:69:B:SER:HA	1:69:B:SER:HG	10	0.15
(1,762)	1:87:A:HIS:HD1	1:88:A:LEU:H	13	0.15
(1,757)	1:80:B:ILE:H	1:80:B:ILE:HD13	1	0.15
(1,757)	1:80:B:ILE:H	1:80:B:ILE:HD13	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,756)	1:84:B:THR:HG22	1:85:B:VAL:H	8	0.15
(1,751)	1:73:B:SER:HB2	1:74:B:LYS:H	12	0.15
(1,656)	1:82:A:GLU:HB2	1:86:A:LYS:HG2	12	0.15
(1,656)	1:82:B:GLU:HB2	1:86:B:LYS:HG2	18	0.15
(1,639)	1:57:B:LEU:HD23	1:84:B:THR:HG22	12	0.15
(1,637)	1:85:A:VAL:HG13	1:86:A:LYS:HG2	2	0.15
(1,630)	1:75:A:LEU:HB2	1:80:A:ILE:HG12	6	0.15
(1,563)	1:56:B:GLN:HG3	1:82:A:GLU:HA	1	0.15
(1,516)	1:67:A:LYS:HG2	1:68:A:ASP:H	14	0.15
(1,486)	1:93:A:ARG:HA	1:94:A:ALA:HA	2	0.15
(1,425)	1:93:A:ARG:HA	1:93:A:ARG:HG3	14	0.15
(1,425)	1:93:A:ARG:HA	1:93:A:ARG:HG3	19	0.15
(1,419)	1:75:B:LEU:HA	1:80:B:ILE:HD11	1	0.15
(1,413)	1:88:A:LEU:HA	1:91:A:LEU:HG	19	0.15
(1,348)	1:71:B:ARG:H	1:71:B:ARG:HD3	3	0.15
(1,348)	1:71:B:ARG:H	1:71:B:ARG:HD3	11	0.15
(1,215)	1:92:B:GLN:HB3	1:92:B:GLN:HE22	2	0.15
(1,202)	1:86:A:LYS:H	1:86:A:LYS:HE2	7	0.15
(1,165)	1:93:B:ARG:HB2	1:94:B:ALA:H	3	0.15
(1,120)	1:74:B:LYS:HA	1:75:B:LEU:H	19	0.15
(1,108)	1:93:A:ARG:HB2	1:95:A:GLN:H	18	0.15
(1,101)	1:91:A:LEU:HA	1:92:A:GLN:H	7	0.15
(1,101)	1:91:A:LEU:HA	1:92:A:GLN:H	9	0.15
(1,81)	1:88:A:LEU:HB2	1:89:A:ARG:H	18	0.15
(1,46)	1:73:B:SER:HB2	1:75:B:LEU:H	1	0.15
(1,46)	1:73:A:SER:HB3	1:75:A:LEU:H	3	0.15
(1,25)	1:63:A:ASP:HA	1:64:A:ALA:H	6	0.15
(1,13)	1:88:A:LEU:H	1:89:A:ARG:HD3	15	0.15
(1,931)	1:72:A:HIS:N	1:68:A:ASP:O	19	0.14
(1,903)	1:84:A:THR:H	1:87:A:HIS:HB2	13	0.14
(1,903)	1:84:A:THR:H	1:87:A:HIS:HB2	14	0.14
(1,901)	1:83:B:MET:H	1:83:B:MET:HG3	5	0.14
(1,835)	1:87:A:HIS:HD2	1:67:A:LYS:HD2	13	0.14
(1,806)	1:57:B:LEU:HD23	1:84:B:THR:H	11	0.14
(1,801)	1:54:A:LEU:HD21	1:81:A:LEU:HD13	4	0.14
(1,762)	1:87:B:HIS:HD1	1:88:B:LEU:H	4	0.14
(1,757)	1:80:B:ILE:H	1:80:B:ILE:HD12	7	0.14
(1,757)	1:80:A:ILE:H	1:80:A:ILE:HD11	14	0.14
(1,696)	1:89:B:ARG:HB3	1:90:B:ASN:HA	6	0.14
(1,656)	1:82:A:GLU:HB2	1:86:A:LYS:HG2	4	0.14
(1,588)	1:82:B:GLU:HB2	1:86:B:LYS:HE2	19	0.14
(1,580)	1:75:B:LEU:HB3	1:76:B:GLU:HB2	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,566)	1:56:B:GLN:HG2	1:82:A:GLU:HA	3	0.14
(1,541)	1:77:B:LYS:HB3	1:79:B:ASP:H	9	0.14
(1,540)	1:89:A:ARG:HB3	1:92:A:GLN:H	15	0.14
(1,516)	1:67:A:LYS:HG2	1:68:A:ASP:H	9	0.14
(1,486)	1:93:B:ARG:HA	1:94:B:ALA:HA	7	0.14
(1,466)	1:93:A:ARG:HA	1:93:A:ARG:HD3	17	0.14
(1,425)	1:93:A:ARG:HA	1:93:A:ARG:HG3	7	0.14
(1,425)	1:93:B:ARG:HA	1:93:B:ARG:HG3	16	0.14
(1,379)	1:65:B:LEU:HD23	1:66:B:LYS:H	15	0.14
(1,321)	1:87:B:HIS:HB2	1:88:B:LEU:H	16	0.14
(1,271)	1:76:B:GLU:H	1:80:B:ILE:HD13	7	0.14
(1,230)	1:86:A:LYS:HB3	1:90:A:ASN:HD22	4	0.14
(1,225)	1:92:B:GLN:HB3	1:92:B:GLN:HE21	1	0.14
(1,215)	1:92:A:GLN:HB3	1:92:A:GLN:HE22	4	0.14
(1,215)	1:92:A:GLN:HB3	1:92:A:GLN:HE22	12	0.14
(1,188)	1:76:B:GLU:HA	1:79:B:ASP:H	1	0.14
(1,188)	1:76:B:GLU:HA	1:79:B:ASP:H	6	0.14
(1,174)	1:78:B:ALA:H	1:79:B:ASP:HB2	19	0.14
(1,165)	1:93:B:ARG:HB2	1:94:B:ALA:H	4	0.14
(1,112)	1:71:B:ARG:HD3	1:72:B:HIS:H	15	0.14
(1,108)	1:93:B:ARG:HB2	1:95:B:GLN:H	11	0.14
(1,101)	1:91:A:LEU:HA	1:92:A:GLN:H	8	0.14
(1,101)	1:91:A:LEU:HA	1:92:A:GLN:H	12	0.14
(1,101)	1:91:B:LEU:HA	1:92:B:GLN:H	13	0.14
(1,70)	1:83:A:MET:HE1	1:84:A:THR:H	9	0.14
(1,46)	1:73:A:SER:HB2	1:75:A:LEU:H	12	0.14
(1,19)	1:62:A:LEU:HA	1:63:A:ASP:H	8	0.14
(1,935)	1:74:A:LYS:N	1:70:A:SER:O	19	0.13
(1,931)	1:72:B:HIS:N	1:68:B:ASP:O	8	0.13
(1,919)	1:94:B:ALA:H	1:95:B:GLN:HG3	8	0.13
(1,903)	1:84:A:THR:H	1:87:A:HIS:HB2	12	0.13
(1,903)	1:84:A:THR:H	1:87:A:HIS:HB2	19	0.13
(1,901)	1:83:B:MET:H	1:83:B:MET:HG3	14	0.13
(1,901)	1:83:A:MET:H	1:83:A:MET:HG3	17	0.13
(1,889)	1:78:B:ALA:H	1:81:B:LEU:HD11	19	0.13
(1,879)	1:75:A:LEU:HD23	1:80:A:ILE:H	6	0.13
(1,876)	1:75:A:LEU:HD11	1:79:A:ASP:H	3	0.13
(1,771)	1:83:B:MET:H	1:86:B:LYS:HD3	10	0.13
(1,771)	1:83:A:MET:H	1:86:A:LYS:HD2	16	0.13
(1,757)	1:80:B:ILE:H	1:80:B:ILE:HD13	4	0.13
(1,757)	1:80:B:ILE:H	1:80:B:ILE:HD12	10	0.13
(1,683)	1:71:A:ARG:HD3	1:75:A:LEU:HD11	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,674)	1:88:B:LEU:HB2	1:91:A:LEU:HG	18	0.13
(1,661)	1:74:B:LYS:HG2	1:76:B:GLU:HG2	19	0.13
(1,656)	1:82:A:GLU:HB2	1:86:A:LYS:HG2	3	0.13
(1,656)	1:82:A:GLU:HB2	1:86:A:LYS:HG2	15	0.13
(1,656)	1:82:A:GLU:HB2	1:86:A:LYS:HG2	17	0.13
(1,624)	1:84:B:THR:HG21	1:88:B:LEU:HB3	1	0.13
(1,580)	1:75:A:LEU:HB3	1:76:A:GLU:HB2	10	0.13
(1,580)	1:75:B:LEU:HB3	1:76:B:GLU:HB2	20	0.13
(1,541)	1:77:A:LYS:HB3	1:79:A:ASP:H	17	0.13
(1,534)	1:74:A:LYS:HE3	1:75:A:LEU:H	11	0.13
(1,523)	1:66:A:LYS:HB3	1:67:A:LYS:H	6	0.13
(1,523)	1:66:A:LYS:HB2	1:67:A:LYS:H	10	0.13
(1,499)	1:65:A:LEU:HA	1:67:A:LYS:H	10	0.13
(1,466)	1:93:B:ARG:HA	1:93:B:ARG:HD3	20	0.13
(1,456)	1:77:B:LYS:HA	1:77:B:LYS:HE2	9	0.13
(1,419)	1:75:A:LEU:HA	1:80:A:ILE:HD12	16	0.13
(1,278)	1:65:B:LEU:HD11	1:90:B:ASN:HD21	20	0.13
(1,215)	1:92:B:GLN:HB3	1:92:B:GLN:HE22	19	0.13
(1,165)	1:93:B:ARG:HB2	1:94:B:ALA:H	1	0.13
(1,162)	1:93:B:ARG:H	1:94:B:ALA:HB1	17	0.13
(1,108)	1:93:A:ARG:HB2	1:95:A:GLN:H	4	0.13
(1,101)	1:91:A:LEU:HA	1:92:A:GLN:H	1	0.13
(1,101)	1:91:B:LEU:HA	1:92:B:GLN:H	11	0.13
(1,101)	1:91:B:LEU:HA	1:92:B:GLN:H	15	0.13
(1,101)	1:91:B:LEU:HA	1:92:B:GLN:H	19	0.13
(1,87)	1:88:A:LEU:HB2	1:90:A:ASN:H	1	0.13
(1,81)	1:88:B:LEU:HB2	1:89:B:ARG:H	11	0.13
(1,19)	1:62:B:LEU:HA	1:63:B:ASP:H	1	0.13
(1,19)	1:62:B:LEU:HA	1:63:B:ASP:H	7	0.13
(1,19)	1:62:B:LEU:HA	1:63:B:ASP:H	16	0.13
(1,931)	1:72:B:HIS:N	1:68:B:ASP:O	7	0.12
(1,922)	1:95:B:GLN:HA	1:95:B:GLN:HG2	4	0.12
(1,895)	1:80:A:ILE:HA	1:81:A:LEU:HD12	9	0.12
(1,865)	1:71:A:ARG:HD3	1:72:A:HIS:HB2	9	0.12
(1,836)	1:87:B:HIS:HD1	1:92:A:GLN:HE21	8	0.12
(1,828)	1:87:B:HIS:HB3	1:87:B:HIS:HD1	5	0.12
(1,762)	1:87:A:HIS:HD1	1:88:A:LEU:H	2	0.12
(1,757)	1:80:B:ILE:H	1:80:B:ILE:HD12	5	0.12
(1,757)	1:80:B:ILE:H	1:80:B:ILE:HD11	8	0.12
(1,751)	1:73:A:SER:HB2	1:74:A:LYS:H	17	0.12
(1,656)	1:82:A:GLU:HB2	1:86:A:LYS:HG2	5	0.12
(1,656)	1:82:B:GLU:HB2	1:86:B:LYS:HG2	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,644)	1:86:A:LYS:HB3	1:86:A:LYS:HD3	10	0.12
(1,639)	1:57:B:LEU:HD21	1:84:B:THR:HG23	17	0.12
(1,624)	1:84:B:THR:HG23	1:88:B:LEU:HB3	5	0.12
(1,624)	1:84:B:THR:HG22	1:88:B:LEU:HB3	11	0.12
(1,588)	1:82:B:GLU:HB2	1:86:B:LYS:HE2	4	0.12
(1,541)	1:77:A:LYS:HB3	1:79:A:ASP:H	10	0.12
(1,534)	1:74:B:LYS:HE3	1:75:B:LEU:H	7	0.12
(1,486)	1:93:A:ARG:HA	1:94:A:ALA:HA	1	0.12
(1,466)	1:93:A:ARG:HA	1:93:A:ARG:HD3	12	0.12
(1,425)	1:93:A:ARG:HA	1:93:A:ARG:HG3	20	0.12
(1,419)	1:75:A:LEU:HA	1:80:A:ILE:HD12	10	0.12
(1,419)	1:75:B:LEU:HA	1:80:B:ILE:HD13	18	0.12
(1,416)	1:82:A:GLU:HA	1:85:A:VAL:HG12	19	0.12
(1,349)	1:86:A:LYS:H	1:89:A:ARG:HD3	14	0.12
(1,348)	1:71:A:ARG:H	1:71:A:ARG:HD3	1	0.12
(1,329)	1:92:B:GLN:H	1:92:B:GLN:HE21	10	0.12
(1,225)	1:92:A:GLN:HB3	1:92:A:GLN:HE21	14	0.12
(1,225)	1:92:B:GLN:HB3	1:92:B:GLN:HE21	16	0.12
(1,215)	1:92:A:GLN:HB3	1:92:A:GLN:HE22	14	0.12
(1,215)	1:92:B:GLN:HB3	1:92:B:GLN:HE22	16	0.12
(1,215)	1:92:A:GLN:HB3	1:92:A:GLN:HE22	17	0.12
(1,188)	1:76:A:GLU:HA	1:79:A:ASP:H	18	0.12
(1,165)	1:93:A:ARG:HB2	1:94:A:ALA:H	14	0.12
(1,162)	1:93:B:ARG:H	1:94:B:ALA:HB2	7	0.12
(1,101)	1:91:A:LEU:HA	1:92:A:GLN:H	3	0.12
(1,87)	1:88:B:LEU:HB2	1:90:B:ASN:H	4	0.12
(1,87)	1:88:A:LEU:HB2	1:90:A:ASN:H	6	0.12
(1,19)	1:62:A:LEU:HA	1:63:A:ASP:H	20	0.12
(1,13)	1:88:B:LEU:H	1:89:B:ARG:HD3	16	0.12
(1,935)	1:74:B:LYS:N	1:70:B:SER:O	8	0.11
(1,914)	1:88:B:LEU:HD13	1:92:B:GLN:HB2	4	0.11
(1,911)	1:88:A:LEU:HD21	1:89:A:ARG:HD2	5	0.11
(1,901)	1:83:B:MET:H	1:83:B:MET:HG3	7	0.11
(1,901)	1:83:B:MET:H	1:83:B:MET:HG3	16	0.11
(1,901)	1:83:B:MET:H	1:83:B:MET:HG3	18	0.11
(1,901)	1:83:A:MET:H	1:83:A:MET:HG3	20	0.11
(1,897)	1:80:A:ILE:HG22	1:81:A:LEU:HD22	10	0.11
(1,879)	1:75:B:LEU:HD11	1:80:B:ILE:H	20	0.11
(1,831)	1:87:A:HIS:HD2	1:91:A:LEU:H	6	0.11
(1,828)	1:87:A:HIS:HB2	1:87:A:HIS:HD1	19	0.11
(1,801)	1:54:A:LEU:HD21	1:81:A:LEU:HD13	6	0.11
(1,757)	1:80:B:ILE:H	1:80:B:ILE:HD13	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,696)	1:89:A:ARG:HB2	1:90:A:ASN:HA	3	0.11
(1,656)	1:82:A:GLU:HB2	1:86:A:LYS:HG2	7	0.11
(1,656)	1:82:A:GLU:HB2	1:86:A:LYS:HG2	13	0.11
(1,656)	1:82:B:GLU:HB2	1:86:B:LYS:HG2	16	0.11
(1,630)	1:75:A:LEU:HB2	1:80:A:ILE:HG12	15	0.11
(1,623)	1:41:B:ILE:HG13	1:44:B:LYS:HE2	20	0.11
(1,563)	1:56:A:GLN:HG3	1:82:B:GLU:HA	20	0.11
(1,540)	1:89:B:ARG:HB3	1:92:B:GLN:H	17	0.11
(1,534)	1:74:A:LYS:HE2	1:75:A:LEU:H	18	0.11
(1,466)	1:93:A:ARG:HA	1:93:A:ARG:HD3	1	0.11
(1,466)	1:93:A:ARG:HA	1:93:A:ARG:HD2	5	0.11
(1,466)	1:93:A:ARG:HA	1:93:A:ARG:HD3	9	0.11
(1,425)	1:93:B:ARG:HA	1:93:B:ARG:HG3	12	0.11
(1,379)	1:65:B:LEU:HD21	1:66:B:LYS:H	13	0.11
(1,356)	1:76:B:GLU:HA	1:78:B:ALA:H	4	0.11
(1,331)	1:67:B:LYS:H	1:67:B:LYS:HG2	13	0.11
(1,289)	1:90:B:ASN:H	1:91:B:LEU:HB2	5	0.11
(1,225)	1:92:A:GLN:HB3	1:92:A:GLN:HE21	10	0.11
(1,215)	1:92:B:GLN:HB3	1:92:B:GLN:HE22	1	0.11
(1,215)	1:92:A:GLN:HB3	1:92:A:GLN:HE22	3	0.11
(1,215)	1:92:A:GLN:HB3	1:92:A:GLN:HE22	10	0.11
(1,188)	1:76:B:GLU:HA	1:79:B:ASP:H	12	0.11
(1,188)	1:76:B:GLU:HA	1:79:B:ASP:H	17	0.11
(1,177)	1:50:B:ILE:HG21	1:51:B:ASN:H	1	0.11
(1,162)	1:93:B:ARG:H	1:94:B:ALA:HB3	14	0.11
(1,101)	1:91:B:LEU:HA	1:92:B:GLN:H	6	0.11
(1,101)	1:91:B:LEU:HA	1:92:B:GLN:H	14	0.11
(1,70)	1:83:A:MET:HE3	1:84:A:THR:H	1	0.11
(1,19)	1:62:B:LEU:HA	1:63:B:ASP:H	15	0.11
(1,19)	1:62:A:LEU:HA	1:63:A:ASP:H	19	0.11
(1,901)	1:83:A:MET:H	1:83:A:MET:HG3	13	0.1
(1,895)	1:80:A:ILE:HA	1:81:A:LEU:HD11	2	0.1
(1,891)	1:79:B:ASP:H	1:81:B:LEU:HD13	15	0.1
(1,867)	1:72:A:HIS:H	1:75:A:LEU:HD12	6	0.1
(1,751)	1:73:B:SER:HB3	1:74:B:LYS:H	13	0.1
(1,729)	1:65:B:LEU:HD13	1:87:B:HIS:HA	9	0.1
(1,656)	1:82:B:GLU:HB2	1:86:B:LYS:HG2	20	0.1
(1,541)	1:77:A:LYS:HB3	1:79:A:ASP:H	4	0.1
(1,523)	1:66:A:LYS:HB3	1:67:A:LYS:H	8	0.1
(1,486)	1:93:B:ARG:HA	1:94:B:ALA:HA	12	0.1
(1,425)	1:93:B:ARG:HA	1:93:B:ARG:HG3	18	0.1
(1,379)	1:65:A:LEU:HD23	1:66:A:LYS:H	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,286)	1:68:A:ASP:HB3	1:69:A:SER:H	8	0.1
(1,271)	1:76:A:GLU:H	1:80:A:ILE:HD11	3	0.1
(1,225)	1:92:B:GLN:HB3	1:92:B:GLN:HE21	19	0.1
(1,215)	1:92:B:GLN:HB3	1:92:B:GLN:HE22	9	0.1
(1,215)	1:92:B:GLN:HB3	1:92:B:GLN:HE22	20	0.1
(1,108)	1:93:A:ARG:HB2	1:95:A:GLN:H	16	0.1
(1,101)	1:91:A:LEU:HA	1:92:A:GLN:H	16	0.1
(1,101)	1:91:B:LEU:HA	1:92:B:GLN:H	17	0.1

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

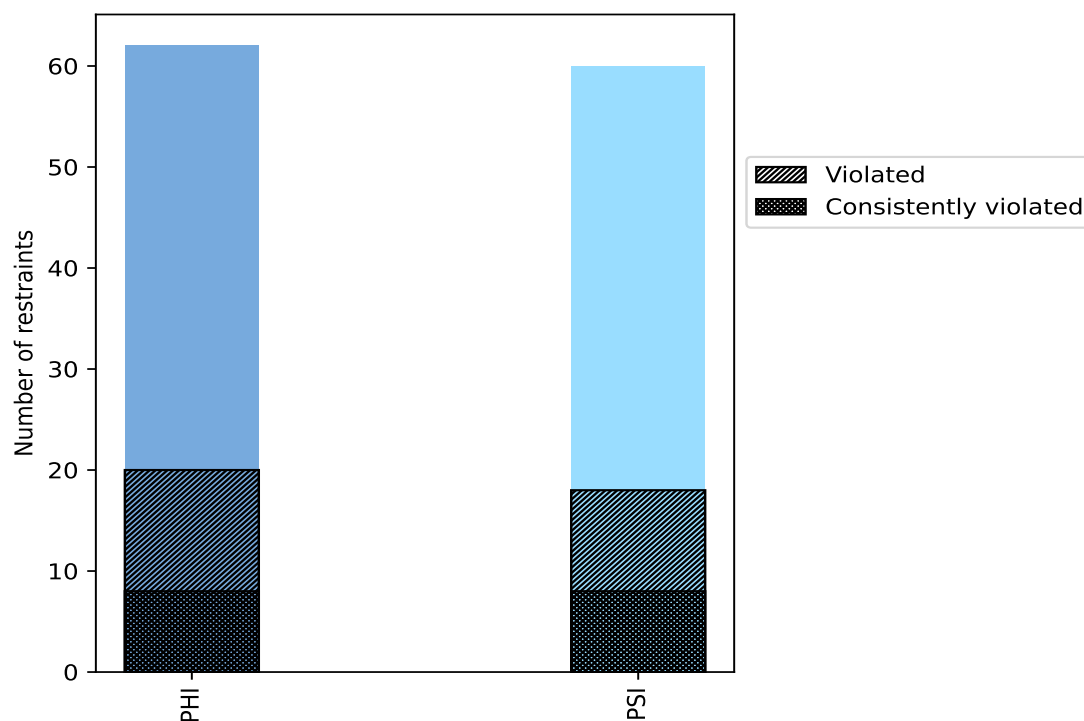
10.1 Summary of dihedral-angle violations [i](#)

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	62	50.8	20	32.3	16.4	8	12.9	6.6
PSI	60	49.2	18	30.0	14.8	8	13.3	6.6
Total	122	100.0	38	31.1	31.1	16	13.1	13.1

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](#)



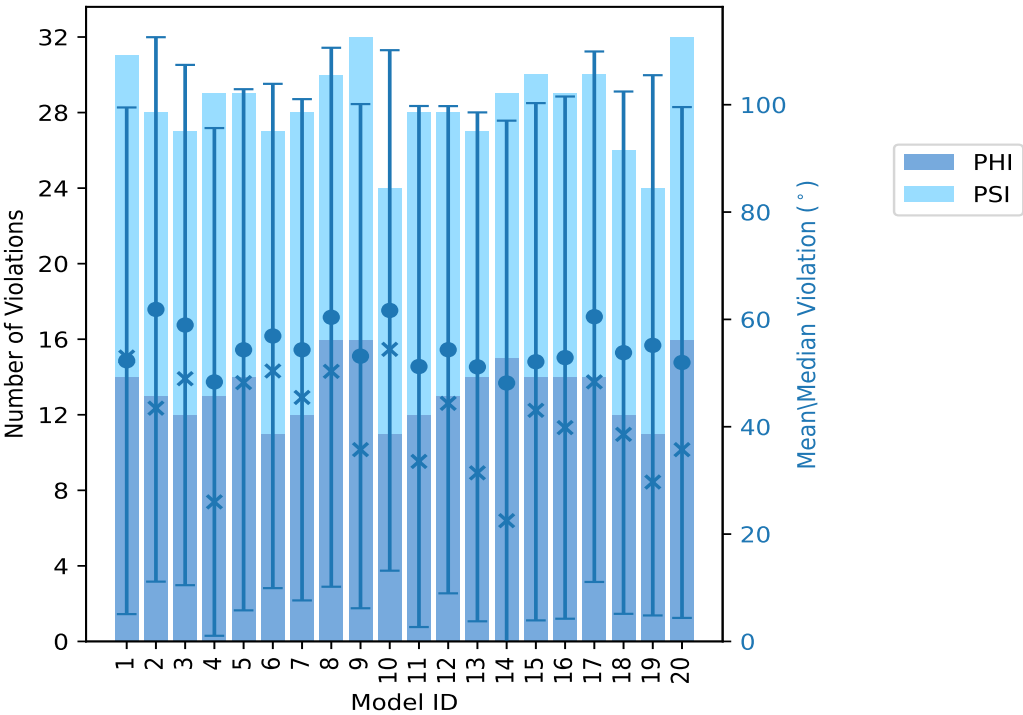
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	14	17	31	52.29	146.85	47.2	52.99
2	13	15	28	61.86	155.02	50.72	43.46
3	12	15	27	58.95	155.78	48.47	48.95
4	13	16	29	48.35	154.65	47.3	26.0
5	14	15	29	54.34	153.13	48.55	48.22
6	11	16	27	56.91	153.63	46.98	50.39
7	12	16	28	54.34	155.45	46.7	45.46
8	16	14	30	60.4	150.75	50.21	50.32
9	16	16	32	53.15	155.0	46.97	35.74
10	11	13	24	61.67	154.53	48.49	54.42
11	12	16	28	51.22	151.49	48.54	33.54
12	13	15	28	54.35	149.6	45.39	44.36
13	14	13	27	51.16	148.36	47.41	31.41
14	15	14	29	48.15	155.03	48.88	22.5
15	14	16	30	52.11	152.59	48.19	43.06
16	14	15	29	52.88	154.14	48.65	39.84
17	14	16	30	60.5	155.14	49.42	48.36
18	12	14	26	53.8	148.53	48.66	38.58
19	11	13	24	55.17	151.79	50.33	29.7
20	16	16	32	51.97	150.75	47.59	35.73

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

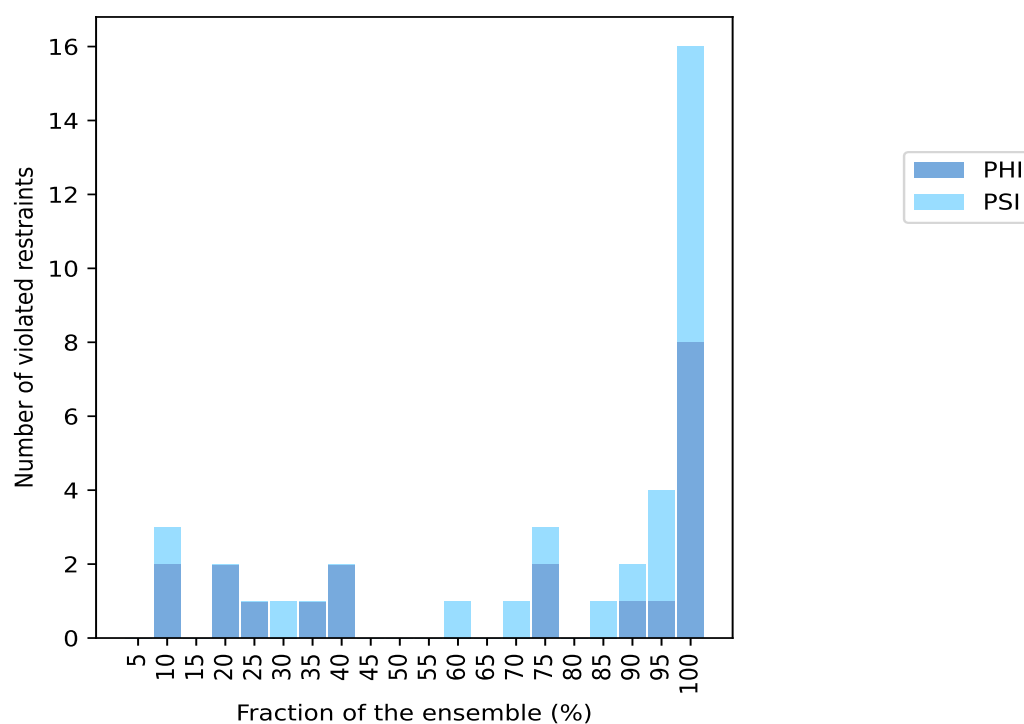
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	1	1	12	60.0
0	0	0	13	65.0
0	1	1	14	70.0
2	1	3	15	75.0
0	0	0	16	80.0
0	1	1	17	85.0
1	1	2	18	90.0
1	3	4	19	95.0
8	8	16	20	100.0

¹ Number of models with violations

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

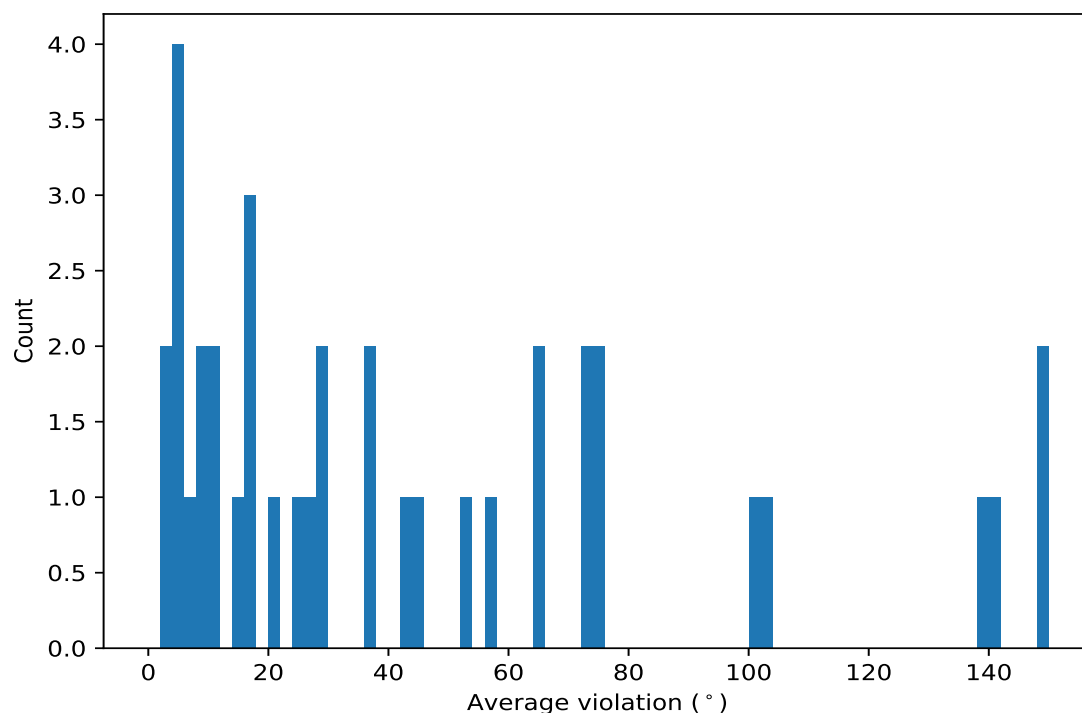


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints ⓘ

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,16)	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1:69:B:SER:N	20	149.52	4.03	150.05
(1,15)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:SER:N	20	149.44	4.09	148.91
(1,3)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:LEU:N	20	140.44	5.71	141.57
(1,4)	1:64:B:ALA:N	1:64:B:ALA:CA	1:64:B:ALA:C	1:65:B:LEU:N	20	139.5	4.25	138.85
(1,5)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	20	102.72	5.51	102.48
(1,6)	1:65:B:LEU:C	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	20	101.83	4.86	102.24
(1,14)	1:67:B:LYS:C	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	20	74.16	8.56	76.06
(1,13)	1:67:A:LYS:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	20	72.96	9.57	74.5
(1,8)	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1:67:B:LYS:N	20	72.22	6.53	73.62
(1,7)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	20	65.96	11.4	66.47
(1,38)	1:73:B:SER:C	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	20	44.67	16.51	45.8
(1,37)	1:73:A:SER:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	20	43.73	14.67	47.38
(1,109)	1:94:A:ALA:C	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	20	37.15	23.99	27.38
(1,11)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:ASP:N	20	17.5	5.83	17.26
(1,12)	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	1:68:B:ASP:N	20	16.95	6.98	17.1
(1,17)	1:68:A:ASP:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	20	8.17	3.55	8.66
(1,39)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LEU:N	19	56.57	18.63	49.69
(1,36)	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	1:74:B:LYS:N	19	29.69	8.46	30.37
(1,35)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LYS:N	19	28.35	10.93	28.35
(1,110)	1:94:B:ALA:C	1:95:B:GLN:N	1:95:B:GLN:CA	1:95:B:GLN:C	19	27.82	20.66	26.85

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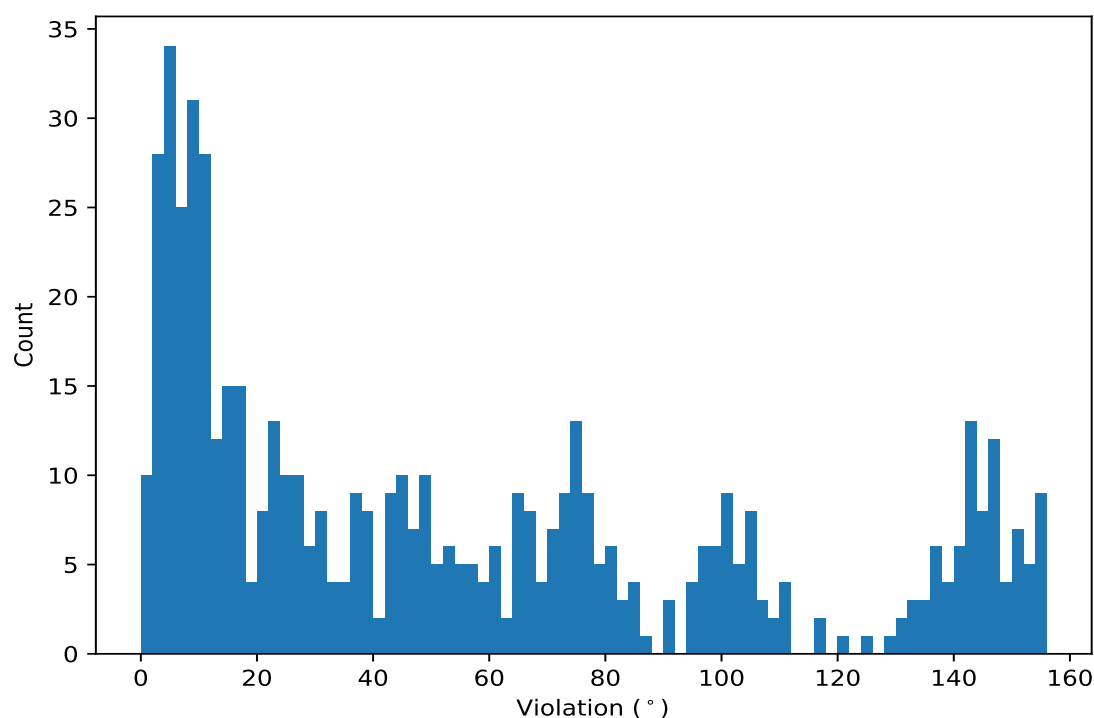
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,40)	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	1:75:B:LEU:N	18	64.71	30.63	54.37
(1,18)	1:68:B:ASP:C	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	18	10.36	2.28	11.33
(1,107)	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	1:95:A:GLN:N	17	16.74	15.8	8.95
(1,33)	1:72:A:HIS:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	15	24.46	37.94	10.82
(1,108)	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	1:95:B:GLN:N	15	21.44	15.41	15.06
(1,34)	1:72:B:HIS:C	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	15	15.84	31.18	7.99
(1,20)	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	1:70:B:SER:N	14	5.52	2.72	5.1
(1,19)	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1:70:A:SER:N	12	5.81	2.19	5.12
(1,106)	1:93:B:ARG:C	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	8	9.03	3.5	8.68
(1,26)	1:70:B:SER:C	1:71:B:ARG:N	1:71:B:ARG:CA	1:71:B:ARG:C	8	5.58	4.34	3.75
(1,25)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	7	4.64	2.48	4.55
(1,31)	1:72:A:HIS:N	1:72:A:HIS:CA	1:72:A:HIS:C	1:73:A:SER:N	6	53.2	64.37	15.52
(1,30)	1:71:B:ARG:C	1:72:B:HIS:N	1:72:B:HIS:CA	1:72:B:HIS:C	5	6.29	1.84	6.13
(1,105)	1:93:A:ARG:C	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	4	37.12	42.2	16.16
(1,29)	1:71:A:ARG:C	1:72:A:HIS:N	1:72:A:HIS:CA	1:72:A:HIS:C	4	10.47	2.22	11.49
(1,32)	1:72:B:HIS:N	1:72:B:HIS:CA	1:72:B:HIS:C	1:73:B:SER:N	2	75.2	71.05	75.2
(1,9)	1:66:A:LYS:C	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	2	2.92	0.08	2.92
(1,10)	1:66:B:LYS:C	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	2	2.38	0.59	2.38

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

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,16)	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1:69:B:SER:N	3	155.78
(1,15)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:SER:N	7	155.45
(1,31)	1:72:A:HIS:N	1:72:A:HIS:CA	1:72:A:HIS:C	1:73:A:SER:N	17	155.14
(1,15)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:SER:N	14	155.03
(1,16)	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1:69:B:SER:N	2	155.02
(1,16)	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1:69:B:SER:N	9	155.0
(1,15)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:SER:N	4	154.65
(1,15)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:SER:N	10	154.53
(1,16)	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1:69:B:SER:N	16	154.14
(1,15)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:SER:N	6	153.63
(1,15)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:SER:N	5	153.13
(1,15)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:SER:N	15	152.59
(1,16)	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1:69:B:SER:N	10	152.47
(1,16)	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1:69:B:SER:N	5	152.04
(1,15)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:SER:N	19	151.79
(1,16)	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1:69:B:SER:N	4	151.75
(1,16)	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1:69:B:SER:N	11	151.49
(1,16)	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1:69:B:SER:N	8	150.75
(1,15)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:SER:N	20	150.75
(1,15)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:SER:N	8	150.5
(1,16)	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1:69:B:SER:N	17	150.49

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,16)	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1:69:B:SER:N	12	149.6
(1,16)	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1:69:B:SER:N	18	148.53
(1,16)	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1:69:B:SER:N	7	148.51
(1,16)	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1:69:B:SER:N	13	148.36
(1,3)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:LEU:N	13	147.72
(1,3)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:LEU:N	3	147.5
(1,4)	1:64:B:ALA:N	1:64:B:ALA:CA	1:64:B:ALA:C	1:65:B:LEU:N	19	147.37
(1,15)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:SER:N	17	147.32
(1,16)	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1:69:B:SER:N	6	147.26
(1,15)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:SER:N	13	147.08
(1,3)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:LEU:N	5	147.04
(1,15)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:SER:N	12	146.91
(1,15)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:SER:N	1	146.85
(1,32)	1:72:B:HIS:N	1:72:B:HIS:CA	1:72:B:HIS:C	1:73:B:SER:N	2	146.25
(1,3)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:LEU:N	2	146.21
(1,16)	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1:69:B:SER:N	15	146.09
(1,15)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:SER:N	11	145.88
(1,15)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:SER:N	2	145.84
(1,15)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:SER:N	18	145.7
(1,3)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:LEU:N	18	145.48
(1,15)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:SER:N	16	144.77
(1,4)	1:64:B:ALA:N	1:64:B:ALA:CA	1:64:B:ALA:C	1:65:B:LEU:N	15	144.65
(1,4)	1:64:B:ALA:N	1:64:B:ALA:CA	1:64:B:ALA:C	1:65:B:LEU:N	16	144.49
(1,15)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:SER:N	3	144.17
(1,16)	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1:69:B:SER:N	1	143.99
(1,3)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:LEU:N	19	143.8
(1,16)	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1:69:B:SER:N	20	143.78
(1,4)	1:64:B:ALA:N	1:64:B:ALA:CA	1:64:B:ALA:C	1:65:B:LEU:N	2	143.69
(1,3)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:LEU:N	8	143.56
(1,4)	1:64:B:ALA:N	1:64:B:ALA:CA	1:64:B:ALA:C	1:65:B:LEU:N	10	143.36
(1,3)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:LEU:N	11	142.88
(1,16)	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1:69:B:SER:N	14	142.84
(1,4)	1:64:B:ALA:N	1:64:B:ALA:CA	1:64:B:ALA:C	1:65:B:LEU:N	8	142.76
(1,16)	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1:69:B:SER:N	19	142.49
(1,4)	1:64:B:ALA:N	1:64:B:ALA:CA	1:64:B:ALA:C	1:65:B:LEU:N	4	142.45
(1,15)	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1:69:A:SER:N	9	142.24
(1,3)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:LEU:N	1	142.17
(1,3)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:LEU:N	10	141.65
(1,3)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:LEU:N	12	141.5
(1,3)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:LEU:N	17	140.72
(1,4)	1:64:B:ALA:N	1:64:B:ALA:CA	1:64:B:ALA:C	1:65:B:LEU:N	18	140.5
(1,3)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:LEU:N	16	140.43
(1,4)	1:64:B:ALA:N	1:64:B:ALA:CA	1:64:B:ALA:C	1:65:B:LEU:N	7	140.2
(1,4)	1:64:B:ALA:N	1:64:B:ALA:CA	1:64:B:ALA:C	1:65:B:LEU:N	12	139.32
(1,4)	1:64:B:ALA:N	1:64:B:ALA:CA	1:64:B:ALA:C	1:65:B:LEU:N	6	138.39
(1,4)	1:64:B:ALA:N	1:64:B:ALA:CA	1:64:B:ALA:C	1:65:B:LEU:N	17	138.24
(1,4)	1:64:B:ALA:N	1:64:B:ALA:CA	1:64:B:ALA:C	1:65:B:LEU:N	1	138.17
(1,4)	1:64:B:ALA:N	1:64:B:ALA:CA	1:64:B:ALA:C	1:65:B:LEU:N	20	137.95
(1,3)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:LEU:N	7	137.92
(1,4)	1:64:B:ALA:N	1:64:B:ALA:CA	1:64:B:ALA:C	1:65:B:LEU:N	5	137.81
(1,3)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:LEU:N	14	137.64

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,4)	1:64:B:ALA:N	1:64:B:ALA:CA	1:64:B:ALA:C	1:65:B:LEU:N	14	136.79
(1,3)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:LEU:N	15	136.24
(1,4)	1:64:B:ALA:N	1:64:B:ALA:CA	1:64:B:ALA:C	1:65:B:LEU:N	3	135.57
(1,4)	1:64:B:ALA:N	1:64:B:ALA:CA	1:64:B:ALA:C	1:65:B:LEU:N	11	135.57
(1,3)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:LEU:N	20	135.42
(1,4)	1:64:B:ALA:N	1:64:B:ALA:CA	1:64:B:ALA:C	1:65:B:LEU:N	9	133.99
(1,3)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:LEU:N	9	133.95
(1,3)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:LEU:N	6	132.25
(1,34)	1:72:B:HIS:C	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	2	131.93
(1,31)	1:72:A:HIS:N	1:72:A:HIS:CA	1:72:A:HIS:C	1:73:A:SER:N	8	130.24
(1,4)	1:64:B:ALA:N	1:64:B:ALA:CA	1:64:B:ALA:C	1:65:B:LEU:N	13	128.75
(1,3)	1:64:A:ALA:N	1:64:A:ALA:CA	1:64:A:ALA:C	1:65:A:LEU:N	4	124.67
(1,33)	1:72:A:HIS:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	8	121.85
(1,33)	1:72:A:HIS:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	17	117.9
(1,5)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	9	116.33
(1,6)	1:65:B:LEU:C	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	9	111.01
(1,6)	1:65:B:LEU:C	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	11	110.92
(1,5)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1	110.25
(1,40)	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	1:75:B:LEU:N	15	110.17
(1,105)	1:93:A:ARG:C	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	9	109.33
(1,6)	1:65:B:LEU:C	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	13	108.1
(1,5)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	4	107.42
(1,5)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	16	106.08
(1,5)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	19	106.07
(1,5)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	20	105.86
(1,5)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	14	105.59
(1,6)	1:65:B:LEU:C	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	3	105.14
(1,6)	1:65:B:LEU:C	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	4	105.12
(1,6)	1:65:B:LEU:C	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	10	104.91
(1,6)	1:65:B:LEU:C	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	6	104.9
(1,5)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	3	104.62
(1,6)	1:65:B:LEU:C	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	18	104.43
(1,5)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	5	103.28
(1,6)	1:65:B:LEU:C	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1	103.23
(1,5)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	7	103.01
(1,6)	1:65:B:LEU:C	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	8	102.79
(1,40)	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	1:75:B:LEU:N	5	102.28
(1,5)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	11	101.96
(1,5)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	18	101.91
(1,5)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	13	101.87
(1,6)	1:65:B:LEU:C	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	7	101.69
(1,5)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	10	101.35
(1,39)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LEU:N	1	100.51
(1,6)	1:65:B:LEU:C	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	16	100.45
(1,5)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	15	100.31
(1,40)	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	1:75:B:LEU:N	8	100.1
(1,39)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LEU:N	20	99.53
(1,40)	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	1:75:B:LEU:N	6	99.3
(1,5)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	8	99.29
(1,40)	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	1:75:B:LEU:N	20	98.93
(1,6)	1:65:B:LEU:C	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	12	98.83

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,5)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	17	98.16
(1,40)	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	1:75:B:LEU:N	17	97.48
(1,6)	1:65:B:LEU:C	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	17	97.07
(1,6)	1:65:B:LEU:C	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	14	97.0
(1,6)	1:65:B:LEU:C	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	2	96.72
(1,6)	1:65:B:LEU:C	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	15	96.68
(1,6)	1:65:B:LEU:C	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	19	96.67
(1,6)	1:65:B:LEU:C	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	20	95.64
(1,6)	1:65:B:LEU:C	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	5	95.34
(1,5)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	12	95.12
(1,5)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	2	94.76
(1,40)	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	1:75:B:LEU:N	3	91.67
(1,13)	1:67:A:LYS:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	3	91.32
(1,5)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	6	91.09
(1,109)	1:94:A:ALA:C	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	9	87.64
(1,14)	1:67:B:LYS:C	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	6	85.96
(1,14)	1:67:B:LYS:C	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	15	85.46
(1,39)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LEU:N	16	84.65
(1,13)	1:67:A:LYS:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	8	84.4
(1,7)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	9	83.21
(1,14)	1:67:B:LYS:C	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	14	83.06
(1,14)	1:67:B:LYS:C	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	8	82.92
(1,14)	1:67:B:LYS:C	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	11	81.99
(1,13)	1:67:A:LYS:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	14	81.98
(1,13)	1:67:A:LYS:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	16	81.85
(1,7)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	3	81.37
(1,13)	1:67:A:LYS:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	18	80.3
(1,14)	1:67:B:LYS:C	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	20	80.17
(1,13)	1:67:A:LYS:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	2	79.22
(1,7)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	12	79.0
(1,8)	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1:67:B:LYS:N	18	78.75
(1,14)	1:67:B:LYS:C	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	19	78.19
(1,13)	1:67:A:LYS:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	20	78.08
(1,14)	1:67:B:LYS:C	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	4	77.74
(1,14)	1:67:B:LYS:C	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	3	77.62
(1,8)	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1:67:B:LYS:N	14	77.32
(1,8)	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1:67:B:LYS:N	9	77.17
(1,7)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	20	77.01
(1,8)	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1:67:B:LYS:N	7	76.94
(1,8)	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1:67:B:LYS:N	5	76.49
(1,14)	1:67:B:LYS:C	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	18	76.47
(1,13)	1:67:A:LYS:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	9	76.35
(1,8)	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1:67:B:LYS:N	15	75.91
(1,14)	1:67:B:LYS:C	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	10	75.65
(1,8)	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1:67:B:LYS:N	2	75.54
(1,7)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	2	75.38
(1,8)	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1:67:B:LYS:N	16	74.97
(1,8)	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1:67:B:LYS:N	19	74.91
(1,13)	1:67:A:LYS:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	7	74.9
(1,14)	1:67:B:LYS:C	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	5	74.89
(1,7)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	11	74.62

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,13)	1:67:A:LYS:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	11	74.52
(1,13)	1:67:A:LYS:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	19	74.48
(1,109)	1:94:A:ALA:C	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	1	74.39
(1,14)	1:67:B:LYS:C	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	16	74.21
(1,8)	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1:67:B:LYS:N	10	73.63
(1,8)	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1:67:B:LYS:N	11	73.62
(1,7)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	13	73.4
(1,8)	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1:67:B:LYS:N	12	73.28
(1,8)	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1:67:B:LYS:N	3	73.26
(1,8)	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1:67:B:LYS:N	20	72.86
(1,13)	1:67:A:LYS:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	6	72.75
(1,7)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	17	72.65
(1,14)	1:67:B:LYS:C	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	1	72.49
(1,38)	1:73:B:SER:C	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	17	71.89
(1,7)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	16	71.66
(1,13)	1:67:A:LYS:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	1	71.64
(1,37)	1:73:A:SER:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	10	71.08
(1,13)	1:67:A:LYS:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	4	70.99
(1,8)	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1:67:B:LYS:N	4	70.55
(1,13)	1:67:A:LYS:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	15	70.39
(1,39)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LEU:N	10	69.81
(1,8)	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1:67:B:LYS:N	6	69.72
(1,8)	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1:67:B:LYS:N	13	69.58
(1,14)	1:67:B:LYS:C	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	7	69.3
(1,38)	1:73:B:SER:C	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	3	67.42
(1,109)	1:94:A:ALA:C	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	7	67.26
(1,110)	1:94:B:ALA:C	1:95:B:GLN:N	1:95:B:GLN:CA	1:95:B:GLN:C	2	67.05
(1,7)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	5	66.53
(1,7)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	6	66.42
(1,109)	1:94:A:ALA:C	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	16	66.2
(1,110)	1:94:B:ALA:C	1:95:B:GLN:N	1:95:B:GLN:CA	1:95:B:GLN:C	10	66.19
(1,8)	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1:67:B:LYS:N	8	66.02
(1,7)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	8	65.97
(1,8)	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1:67:B:LYS:N	1	65.67
(1,13)	1:67:A:LYS:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	5	65.12
(1,14)	1:67:B:LYS:C	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	12	64.95
(1,14)	1:67:B:LYS:C	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	17	64.93
(1,39)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LEU:N	8	64.51
(1,13)	1:67:A:LYS:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	12	64.47
(1,109)	1:94:A:ALA:C	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	5	64.29
(1,7)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	14	64.09
(1,7)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	19	62.78
(1,40)	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	1:75:B:LEU:N	12	62.69
(1,109)	1:94:A:ALA:C	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	17	61.31
(1,39)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LEU:N	14	61.1
(1,38)	1:73:B:SER:C	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	15	60.84
(1,14)	1:67:B:LYS:C	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	13	60.75
(1,14)	1:67:B:LYS:C	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	9	60.56
(1,37)	1:73:A:SER:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1	60.09
(1,38)	1:73:B:SER:C	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	6	59.82
(1,37)	1:73:A:SER:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	7	59.58

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,38)	1:73:B:SER:C	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	20	59.18
(1,38)	1:73:B:SER:C	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	8	58.39
(1,110)	1:94:B:ALA:C	1:95:B:GLN:N	1:95:B:GLN:CA	1:95:B:GLN:C	20	57.59
(1,13)	1:67:A:LYS:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	13	56.64
(1,7)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	1	56.43
(1,38)	1:73:B:SER:C	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	1	56.39
(1,38)	1:73:B:SER:C	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	5	56.01
(1,14)	1:67:B:LYS:C	1:68:B:ASP:N	1:68:B:ASP:CA	1:68:B:ASP:C	2	55.82
(1,40)	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	1:75:B:LEU:N	1	55.78
(1,13)	1:67:A:LYS:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	17	55.44
(1,7)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	10	54.45
(1,13)	1:67:A:LYS:C	1:68:A:ASP:N	1:68:A:ASP:CA	1:68:A:ASP:C	10	54.4
(1,108)	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	1:95:B:GLN:N	1	52.99
(1,40)	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	1:75:B:LEU:N	7	52.96
(1,37)	1:73:A:SER:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	6	52.93
(1,7)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	15	52.76
(1,39)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LEU:N	3	52.64
(1,37)	1:73:A:SER:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	15	52.23
(1,38)	1:73:B:SER:C	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	12	51.21
(1,110)	1:94:B:ALA:C	1:95:B:GLN:N	1:95:B:GLN:CA	1:95:B:GLN:C	18	50.89
(1,40)	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	1:75:B:LEU:N	11	50.67
(1,39)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LEU:N	6	50.39
(1,39)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LEU:N	5	50.38
(1,39)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LEU:N	18	49.69
(1,40)	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	1:75:B:LEU:N	10	49.58
(1,37)	1:73:A:SER:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	20	49.58
(1,37)	1:73:A:SER:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	12	49.29
(1,7)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	7	49.09
(1,37)	1:73:A:SER:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	3	48.95
(1,37)	1:73:A:SER:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	17	48.52
(1,107)	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	1:95:A:GLN:N	19	48.32
(1,37)	1:73:A:SER:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	5	48.22
(1,8)	1:66:B:LYS:N	1:66:B:LYS:CA	1:66:B:LYS:C	1:67:B:LYS:N	17	48.2
(1,40)	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	1:75:B:LEU:N	14	47.42
(1,39)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LEU:N	15	47.31
(1,39)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LEU:N	17	47.18
(1,38)	1:73:B:SER:C	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	16	46.82
(1,7)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	4	46.67
(1,37)	1:73:A:SER:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	18	46.54
(1,107)	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	1:95:A:GLN:N	12	46.4
(1,37)	1:73:A:SER:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	9	45.87
(1,7)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	18	45.75
(1,37)	1:73:A:SER:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	2	45.62
(1,39)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LEU:N	7	45.53
(1,39)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LEU:N	11	45.52
(1,35)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LYS:N	7	45.4
(1,39)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LEU:N	9	45.21
(1,107)	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	1:95:A:GLN:N	9	45.14
(1,38)	1:73:B:SER:C	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	10	44.77
(1,108)	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	1:95:B:GLN:N	13	44.0
(1,108)	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	1:95:B:GLN:N	15	43.95

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,37)	1:73:A:SER:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	13	43.92
(1,39)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LEU:N	13	43.73
(1,35)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LYS:N	3	43.4
(1,36)	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	1:74:B:LYS:N	17	42.91
(1,35)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LYS:N	12	42.32
(1,109)	1:94:A:ALA:C	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	8	42.24
(1,36)	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	1:74:B:LYS:N	15	42.18
(1,40)	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	1:75:B:LEU:N	16	42.16
(1,35)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LYS:N	2	41.29
(1,110)	1:94:B:ALA:C	1:95:B:GLN:N	1:95:B:GLN:CA	1:95:B:GLN:C	8	40.56
(1,39)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LEU:N	12	39.93
(1,37)	1:73:A:SER:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	16	39.84
(1,110)	1:94:B:ALA:C	1:95:B:GLN:N	1:95:B:GLN:CA	1:95:B:GLN:C	11	39.81
(1,109)	1:94:A:ALA:C	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	2	39.42
(1,39)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LEU:N	4	39.25
(1,38)	1:73:B:SER:C	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	7	38.79
(1,109)	1:94:A:ALA:C	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	3	38.64
(1,39)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:LEU:N	2	38.03
(1,36)	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	1:74:B:LYS:N	5	37.78
(1,38)	1:73:B:SER:C	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	4	37.74
(1,35)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LYS:N	5	37.7
(1,40)	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	1:75:B:LEU:N	4	37.48
(1,36)	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	1:74:B:LYS:N	20	37.39
(1,38)	1:73:B:SER:C	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	14	37.26
(1,36)	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	1:74:B:LYS:N	1	36.81
(1,36)	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	1:74:B:LYS:N	9	36.22
(1,35)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LYS:N	6	36.22
(1,40)	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	1:75:B:LEU:N	9	35.26
(1,36)	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	1:74:B:LYS:N	10	35.0
(1,37)	1:73:A:SER:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	11	34.58
(1,107)	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	1:95:A:GLN:N	20	34.07
(1,36)	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	1:74:B:LYS:N	8	33.63
(1,38)	1:73:B:SER:C	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	11	32.5
(1,108)	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	1:95:B:GLN:N	12	32.43
(1,110)	1:94:B:ALA:C	1:95:B:GLN:N	1:95:B:GLN:CA	1:95:B:GLN:C	19	32.37
(1,37)	1:73:A:SER:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	4	31.53
(1,109)	1:94:A:ALA:C	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	18	31.42
(1,35)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LYS:N	13	31.41
(1,38)	1:73:B:SER:C	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	9	31.16
(1,36)	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	1:74:B:LYS:N	16	31.11
(1,110)	1:94:B:ALA:C	1:95:B:GLN:N	1:95:B:GLN:CA	1:95:B:GLN:C	17	30.77
(1,110)	1:94:B:ALA:C	1:95:B:GLN:N	1:95:B:GLN:CA	1:95:B:GLN:C	6	30.66
(1,36)	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	1:74:B:LYS:N	12	30.37
(1,35)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LYS:N	15	29.5
(1,12)	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	1:68:B:ASP:N	9	28.78
(1,35)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LYS:N	10	28.64
(1,36)	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	1:74:B:LYS:N	13	28.61
(1,35)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LYS:N	17	28.35
(1,31)	1:72:A:HIS:N	1:72:A:HIS:CA	1:72:A:HIS:C	1:73:A:SER:N	6	28.18
(1,108)	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	1:95:B:GLN:N	7	27.91
(1,11)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:ASP:N	14	27.78

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,36)	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	1:74:B:LYS:N	18	27.27
(1,38)	1:73:B:SER:C	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	19	27.02
(1,110)	1:94:B:ALA:C	1:95:B:GLN:N	1:95:B:GLN:CA	1:95:B:GLN:C	3	26.85
(1,35)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LYS:N	9	26.84
(1,110)	1:94:B:ALA:C	1:95:B:GLN:N	1:95:B:GLN:CA	1:95:B:GLN:C	5	26.34
(1,35)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LYS:N	16	26.06
(1,108)	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	1:95:B:GLN:N	9	26.03
(1,35)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LYS:N	4	26.0
(1,36)	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	1:74:B:LYS:N	19	25.97
(1,12)	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	1:68:B:ASP:N	20	25.74
(1,11)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:ASP:N	12	25.33
(1,11)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:ASP:N	17	25.06
(1,33)	1:72:A:HIS:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	6	24.94
(1,38)	1:73:B:SER:C	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	18	24.48
(1,36)	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	1:74:B:LYS:N	4	24.27
(1,12)	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	1:68:B:ASP:N	13	24.18
(1,38)	1:73:B:SER:C	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	13	24.16
(1,12)	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	1:68:B:ASP:N	4	24.02
(1,11)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:ASP:N	16	23.89
(1,12)	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	1:68:B:ASP:N	2	23.75
(1,105)	1:93:A:ARG:C	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	13	23.61
(1,107)	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	1:95:A:GLN:N	2	23.6
(1,109)	1:94:A:ALA:C	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	20	23.33
(1,109)	1:94:A:ALA:C	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	4	23.31
(1,12)	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	1:68:B:ASP:N	6	23.15
(1,36)	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	1:74:B:LYS:N	7	22.88
(1,36)	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	1:74:B:LYS:N	11	22.62
(1,109)	1:94:A:ALA:C	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	15	22.53
(1,36)	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	1:74:B:LYS:N	14	22.5
(1,35)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LYS:N	20	22.39
(1,11)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:ASP:N	1	22.34
(1,11)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:ASP:N	2	21.89
(1,37)	1:73:A:SER:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	14	21.8
(1,109)	1:94:A:ALA:C	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	6	21.65
(1,108)	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	1:95:B:GLN:N	3	21.37
(1,35)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LYS:N	1	21.0
(1,40)	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	1:75:B:LEU:N	2	20.7
(1,12)	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	1:68:B:ASP:N	14	20.31
(1,109)	1:94:A:ALA:C	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	10	20.24
(1,11)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:ASP:N	4	19.88
(1,12)	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	1:68:B:ASP:N	1	18.7
(1,35)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LYS:N	11	18.39
(1,11)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:ASP:N	7	18.36
(1,12)	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	1:68:B:ASP:N	7	17.99
(1,33)	1:72:A:HIS:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	20	17.79
(1,12)	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	1:68:B:ASP:N	19	17.73
(1,11)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:ASP:N	13	17.52
(1,11)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:ASP:N	19	17.44
(1,11)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:ASP:N	5	17.09
(1,36)	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	1:74:B:LYS:N	3	17.08
(1,11)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:ASP:N	18	16.73

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,33)	1:72:A:HIS:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	3	16.6
(1,12)	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	1:68:B:ASP:N	10	16.46
(1,35)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LYS:N	19	16.32
(1,11)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:ASP:N	11	16.23
(1,35)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LYS:N	18	16.19
(1,109)	1:94:A:ALA:C	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	12	16.12
(1,106)	1:93:B:ARG:C	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	9	16.08
(1,11)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:ASP:N	9	15.93
(1,109)	1:94:A:ALA:C	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	19	15.83
(1,12)	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	1:68:B:ASP:N	16	15.74
(1,12)	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	1:68:B:ASP:N	12	15.5
(1,12)	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	1:68:B:ASP:N	3	15.42
(1,37)	1:73:A:SER:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	8	15.38
(1,11)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:ASP:N	8	15.34
(1,11)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:ASP:N	15	15.09
(1,108)	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	1:95:B:GLN:N	4	15.06
(1,108)	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	1:95:B:GLN:N	2	14.77
(1,12)	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	1:68:B:ASP:N	11	14.68
(1,26)	1:70:B:SER:C	1:71:B:ARG:N	1:71:B:ARG:CA	1:71:B:ARG:C	16	14.62
(1,12)	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	1:68:B:ASP:N	8	14.58
(1,107)	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	1:95:A:GLN:N	8	14.46
(1,109)	1:94:A:ALA:C	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	14	14.14
(1,18)	1:68:B:ASP:C	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	4	12.88
(1,17)	1:68:A:ASP:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	7	12.66
(1,106)	1:93:B:ARG:C	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	4	12.63
(1,18)	1:68:B:ASP:C	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	17	12.46
(1,18)	1:68:B:ASP:C	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	5	12.4
(1,34)	1:72:B:HIS:C	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	11	12.33
(1,33)	1:72:A:HIS:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	15	12.24
(1,29)	1:71:A:ARG:C	1:72:A:HIS:N	1:72:A:HIS:CA	1:72:A:HIS:C	8	12.22
(1,18)	1:68:B:ASP:C	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	12	12.15
(1,34)	1:72:B:HIS:C	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	12	12.14
(1,17)	1:68:A:ASP:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	11	12.03
(1,17)	1:68:A:ASP:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	8	12.01
(1,18)	1:68:B:ASP:C	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	13	11.95
(1,18)	1:68:B:ASP:C	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	7	11.84
(1,17)	1:68:A:ASP:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	15	11.71
(1,18)	1:68:B:ASP:C	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	2	11.7
(1,17)	1:68:A:ASP:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	13	11.7
(1,34)	1:72:B:HIS:C	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	9	11.69
(1,17)	1:68:A:ASP:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	4	11.66
(1,29)	1:71:A:ARG:C	1:72:A:HIS:N	1:72:A:HIS:CA	1:72:A:HIS:C	18	11.6
(1,17)	1:68:A:ASP:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1	11.58
(1,18)	1:68:B:ASP:C	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	8	11.57
(1,18)	1:68:B:ASP:C	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	9	11.53
(1,29)	1:71:A:ARG:C	1:72:A:HIS:N	1:72:A:HIS:CA	1:72:A:HIS:C	20	11.38
(1,33)	1:72:A:HIS:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	5	11.29
(1,11)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:ASP:N	6	11.22
(1,18)	1:68:B:ASP:C	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	6	11.13
(1,17)	1:68:A:ASP:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	3	11.11
(1,33)	1:72:A:HIS:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	7	10.82

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,108)	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	1:95:B:GLN:N	19	10.78
(1,18)	1:68:B:ASP:C	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	18	10.73
(1,11)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:ASP:N	20	10.69
(1,34)	1:72:B:HIS:C	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	17	10.65
(1,107)	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	1:95:A:GLN:N	13	10.49
(1,18)	1:68:B:ASP:C	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	1	10.45
(1,33)	1:72:A:HIS:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	14	10.44
(1,18)	1:68:B:ASP:C	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	20	10.16
(1,108)	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	1:95:B:GLN:N	17	10.11
(1,107)	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	1:95:A:GLN:N	18	10.1
(1,40)	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	1:75:B:LEU:N	18	10.07
(1,108)	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	1:95:B:GLN:N	11	9.82
(1,34)	1:72:B:HIS:C	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	8	9.73
(1,26)	1:70:B:SER:C	1:71:B:ARG:N	1:71:B:ARG:CA	1:71:B:ARG:C	15	9.66
(1,110)	1:94:B:ALA:C	1:95:B:GLN:N	1:95:B:GLN:CA	1:95:B:GLN:C	16	9.56
(1,36)	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	1:74:B:LYS:N	6	9.49
(1,25)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	17	9.45
(1,18)	1:68:B:ASP:C	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	14	9.22
(1,17)	1:68:A:ASP:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	9	9.14
(1,37)	1:73:A:SER:C	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	19	9.1
(1,106)	1:93:B:ARG:C	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	12	9.07
(1,30)	1:71:B:ARG:C	1:72:B:HIS:N	1:72:B:HIS:CA	1:72:B:HIS:C	8	8.97
(1,107)	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	1:95:A:GLN:N	11	8.95
(1,34)	1:72:B:HIS:C	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	18	8.87
(1,19)	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1:70:A:SER:N	1	8.86
(1,19)	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1:70:A:SER:N	9	8.8
(1,106)	1:93:B:ARG:C	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	8	8.78
(1,20)	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	1:70:B:SER:N	17	8.77
(1,17)	1:68:A:ASP:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	12	8.77
(1,20)	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	1:70:B:SER:N	7	8.74
(1,110)	1:94:B:ALA:C	1:95:B:GLN:N	1:95:B:GLN:CA	1:95:B:GLN:C	4	8.7
(1,105)	1:93:A:ARG:C	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	2	8.7
(1,107)	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	1:95:A:GLN:N	16	8.62
(1,106)	1:93:B:ARG:C	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	15	8.58
(1,110)	1:94:B:ALA:C	1:95:B:GLN:N	1:95:B:GLN:CA	1:95:B:GLN:C	7	8.57
(1,20)	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	1:70:B:SER:N	12	8.56
(1,17)	1:68:A:ASP:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	19	8.56
(1,20)	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	1:70:B:SER:N	5	8.53
(1,19)	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1:70:A:SER:N	17	8.47
(1,109)	1:94:A:ALA:C	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	11	8.43
(1,18)	1:68:B:ASP:C	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	16	8.17
(1,20)	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	1:70:B:SER:N	4	8.15
(1,34)	1:72:B:HIS:C	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	15	7.99
(1,20)	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	1:70:B:SER:N	2	7.96
(1,110)	1:94:B:ALA:C	1:95:B:GLN:N	1:95:B:GLN:CA	1:95:B:GLN:C	15	7.92
(1,17)	1:68:A:ASP:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	20	7.83
(1,19)	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1:70:A:SER:N	7	7.73
(1,12)	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	1:68:B:ASP:N	17	7.72
(1,30)	1:71:B:ARG:C	1:72:B:HIS:N	1:72:B:HIS:CA	1:72:B:HIS:C	11	7.65
(1,18)	1:68:B:ASP:C	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	15	7.54
(1,38)	1:73:B:SER:C	1:74:B:LYS:N	1:74:B:LYS:CA	1:74:B:LYS:C	2	7.47

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,107)	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	1:95:A:GLN:N	1	7.35
(1,17)	1:68:A:ASP:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	2	7.29
(1,26)	1:70:B:SER:C	1:71:B:ARG:N	1:71:B:ARG:CA	1:71:B:ARG:C	9	7.26
(1,11)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:ASP:N	10	7.2
(1,19)	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1:70:A:SER:N	4	7.14
(1,12)	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	1:68:B:ASP:N	18	7.01
(1,17)	1:68:A:ASP:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	18	6.9
(1,110)	1:94:B:ALA:C	1:95:B:GLN:N	1:95:B:GLN:CA	1:95:B:GLN:C	1	6.89
(1,105)	1:93:A:ARG:C	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	1	6.83
(1,29)	1:71:A:ARG:C	1:72:A:HIS:N	1:72:A:HIS:CA	1:72:A:HIS:C	14	6.66
(1,25)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	2	6.59
(1,34)	1:72:B:HIS:C	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	14	6.5
(1,106)	1:93:B:ARG:C	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	1	6.42
(1,110)	1:94:B:ALA:C	1:95:B:GLN:N	1:95:B:GLN:CA	1:95:B:GLN:C	14	6.22
(1,30)	1:71:B:ARG:C	1:72:B:HIS:N	1:72:B:HIS:CA	1:72:B:HIS:C	14	6.13
(1,107)	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	1:95:A:GLN:N	3	6.11
(1,106)	1:93:B:ARG:C	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	7	5.94
(1,110)	1:94:B:ALA:C	1:95:B:GLN:N	1:95:B:GLN:CA	1:95:B:GLN:C	9	5.93
(1,33)	1:72:A:HIS:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	19	5.85
(1,19)	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1:70:A:SER:N	14	5.81
(1,110)	1:94:B:ALA:C	1:95:B:GLN:N	1:95:B:GLN:CA	1:95:B:GLN:C	13	5.8
(1,107)	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	1:95:A:GLN:N	5	5.71
(1,18)	1:68:B:ASP:C	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	19	5.69
(1,20)	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	1:70:B:SER:N	6	5.63
(1,12)	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	1:68:B:ASP:N	5	5.59
(1,33)	1:72:A:HIS:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	13	5.3
(1,34)	1:72:B:HIS:C	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	3	5.18
(1,34)	1:72:B:HIS:C	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	13	5.15
(1,34)	1:72:B:HIS:C	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	20	5.09
(1,107)	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	1:95:A:GLN:N	4	5.05
(1,108)	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	1:95:B:GLN:N	5	4.94
(1,18)	1:68:B:ASP:C	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	3	4.92
(1,11)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:ASP:N	3	4.91
(1,30)	1:71:B:ARG:C	1:72:B:HIS:N	1:72:B:HIS:CA	1:72:B:HIS:C	16	4.85
(1,17)	1:68:A:ASP:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	17	4.79
(1,107)	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	1:95:A:GLN:N	15	4.76
(1,106)	1:93:B:ARG:C	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	5	4.73
(1,25)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	8	4.73
(1,20)	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	1:70:B:SER:N	16	4.56
(1,25)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	16	4.55
(1,109)	1:94:A:ALA:C	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	13	4.52
(1,19)	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1:70:A:SER:N	15	4.44
(1,19)	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1:70:A:SER:N	19	4.44
(1,108)	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	1:95:B:GLN:N	16	4.25
(1,17)	1:68:A:ASP:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	10	4.21
(1,33)	1:72:A:HIS:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	12	4.17
(1,32)	1:72:B:HIS:N	1:72:B:HIS:CA	1:72:B:HIS:C	1:73:B:SER:N	6	4.15
(1,107)	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	1:95:A:GLN:N	10	4.1
(1,19)	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1:70:A:SER:N	20	4.04
(1,19)	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1:70:A:SER:N	11	4.03
(1,26)	1:70:B:SER:C	1:71:B:ARG:N	1:71:B:ARG:CA	1:71:B:ARG:C	5	3.99

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,20)	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	1:70:B:SER:N	14	3.9
(1,30)	1:71:B:ARG:C	1:72:B:HIS:N	1:72:B:HIS:CA	1:72:B:HIS:C	1	3.87
(1,34)	1:72:B:HIS:C	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	5	3.8
(1,34)	1:72:B:HIS:C	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	10	3.67
(1,19)	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1:70:A:SER:N	8	3.64
(1,26)	1:70:B:SER:C	1:71:B:ARG:N	1:71:B:ARG:CA	1:71:B:ARG:C	1	3.51
(1,17)	1:68:A:ASP:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	14	3.5
(1,17)	1:68:A:ASP:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	5	3.25
(1,20)	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	1:70:B:SER:N	9	3.16
(1,108)	1:94:B:ALA:N	1:94:B:ALA:CA	1:94:B:ALA:C	1:95:B:GLN:N	20	3.13
(1,25)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	14	3.13
(1,20)	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	1:70:B:SER:N	3	3.03
(1,33)	1:72:A:HIS:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	16	3.01
(1,9)	1:66:A:LYS:C	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	17	3.0
(1,10)	1:66:B:LYS:C	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	13	2.97
(1,17)	1:68:A:ASP:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	6	2.92
(1,34)	1:72:B:HIS:C	1:73:B:SER:N	1:73:B:SER:CA	1:73:B:SER:C	4	2.9
(1,31)	1:72:A:HIS:N	1:72:A:HIS:CA	1:72:A:HIS:C	1:73:A:SER:N	1	2.86
(1,9)	1:66:A:LYS:C	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	20	2.84
(1,26)	1:70:B:SER:C	1:71:B:ARG:N	1:71:B:ARG:CA	1:71:B:ARG:C	10	2.65
(1,20)	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	1:70:B:SER:N	1	2.57
(1,33)	1:72:A:HIS:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	4	2.55
(1,20)	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	1:70:B:SER:N	18	2.37
(1,19)	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	1:70:A:SER:N	6	2.34
(1,25)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	12	2.28
(1,33)	1:72:A:HIS:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	9	2.17
(1,12)	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	1:68:B:ASP:N	15	2.01
(1,26)	1:70:B:SER:C	1:71:B:ARG:N	1:71:B:ARG:CA	1:71:B:ARG:C	20	1.84
(1,17)	1:68:A:ASP:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	16	1.81
(1,10)	1:66:B:LYS:C	1:67:B:LYS:N	1:67:B:LYS:CA	1:67:B:LYS:C	9	1.79
(1,25)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	20	1.74
(1,31)	1:72:A:HIS:N	1:72:A:HIS:CA	1:72:A:HIS:C	1:73:A:SER:N	15	1.46
(1,107)	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	1:95:A:GLN:N	7	1.43
(1,31)	1:72:A:HIS:N	1:72:A:HIS:CA	1:72:A:HIS:C	1:73:A:SER:N	20	1.3
(1,20)	1:69:B:SER:N	1:69:B:SER:CA	1:69:B:SER:C	1:70:B:SER:N	11	1.3
(1,35)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LYS:N	14	1.21
(1,26)	1:70:B:SER:C	1:71:B:ARG:N	1:71:B:ARG:CA	1:71:B:ARG:C	11	1.11