



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2MB9 / pdb_00002mb9
BMRB ID : 19392
Title : Human Bcl10 CARD
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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

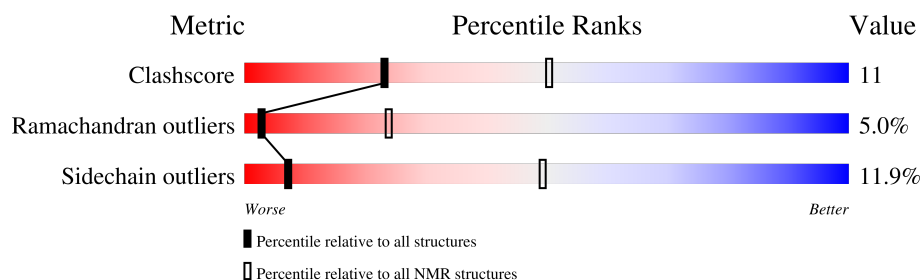
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

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	118	

2 Ensemble composition and analysis

This entry contains 10 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:12-A:115 (104)	2.23	2

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 3 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 5, 7
2	3, 9
3	4, 6
Single-model clusters	8; 10

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1822 atoms, of which 936 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called B-cell lymphoma/leukemia 10.

Mol	Chain	Residues	Atoms						Trace
1	A	106	Total	C	H	N	O	S	0
			1822	552	936	165	167	2	

There are 4 discrepancies between the modelled and reference sequences:

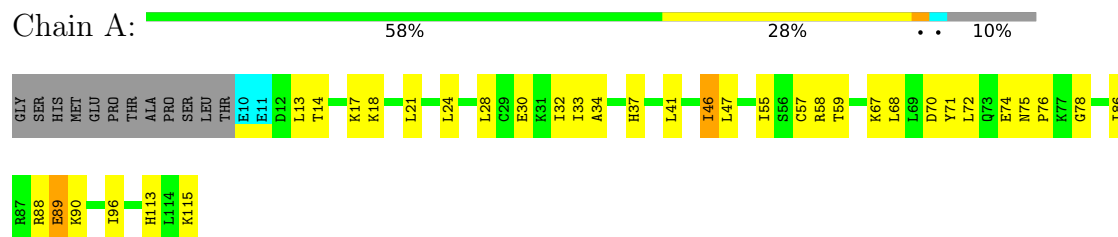
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP O95999
A	-1	SER	-	expression tag	UNP O95999
A	0	HIS	-	expression tag	UNP O95999
A	53	ARG	GLU	engineered mutation	UNP O95999

4 Residue-property plots [i](#)

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: B-cell lymphoma/leukemia 10

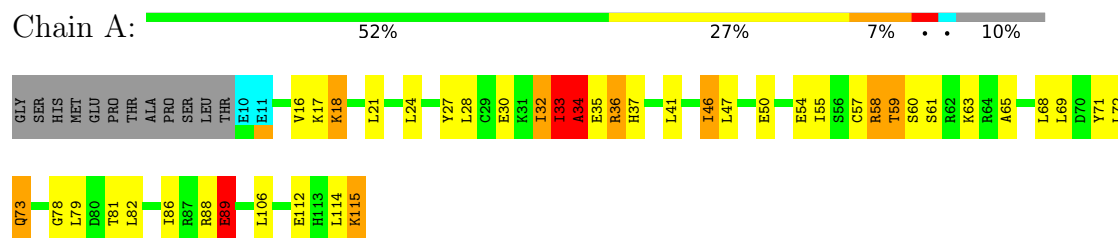


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

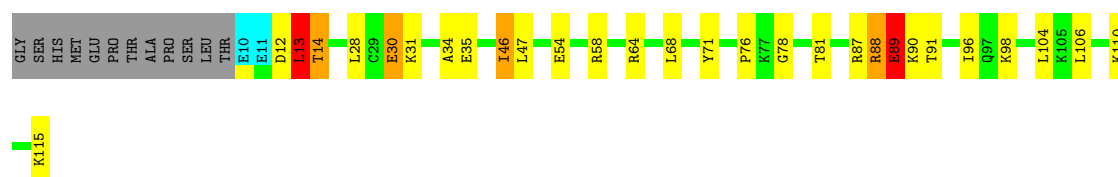
- Molecule 1: B-cell lymphoma/leukemia 10



4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: B-cell lymphoma/leukemia 10

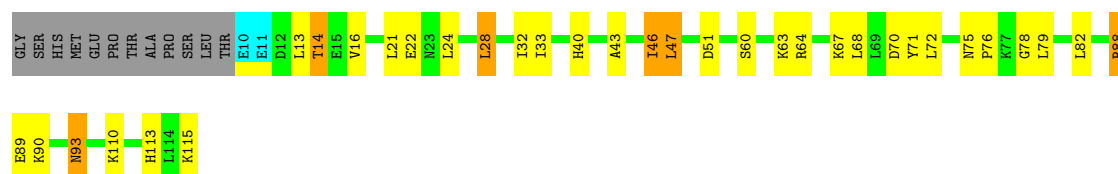




4.2.3 Score per residue for model 3

- Molecule 1: B-cell lymphoma/leukemia 10

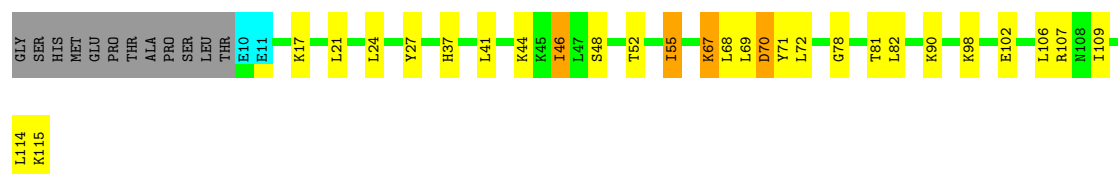
Chain A: 59% 24% 5% 10%



4.2.4 Score per residue for model 4

- Molecule 1: B-cell lymphoma/leukemia 10

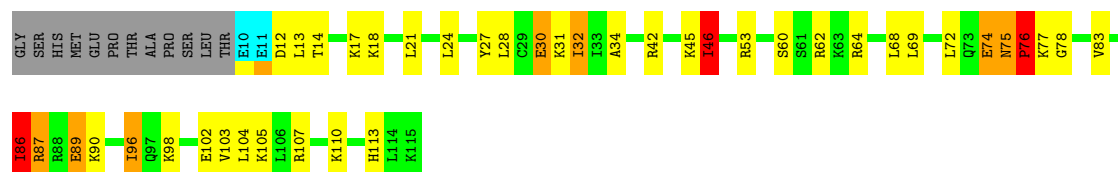
Chain A: 64% 20% 10%



4.2.5 Score per residue for model 5

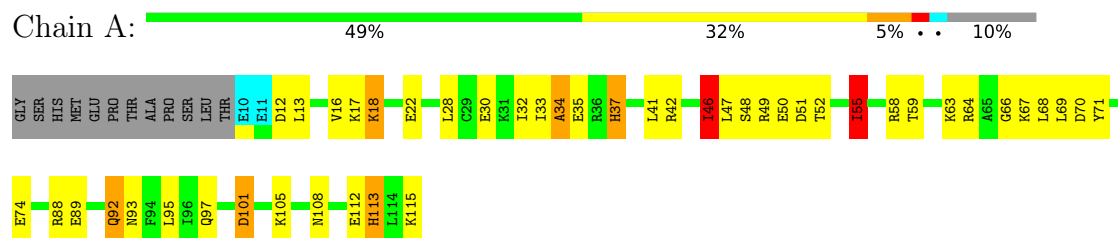
- Molecule 1: B-cell lymphoma/leukemia 10

Chain A: 53% 27% 6% 10%



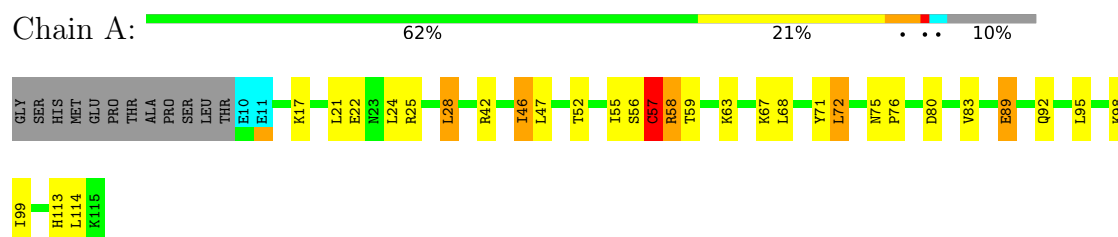
4.2.6 Score per residue for model 6

- Molecule 1: B-cell lymphoma/leukemia 10



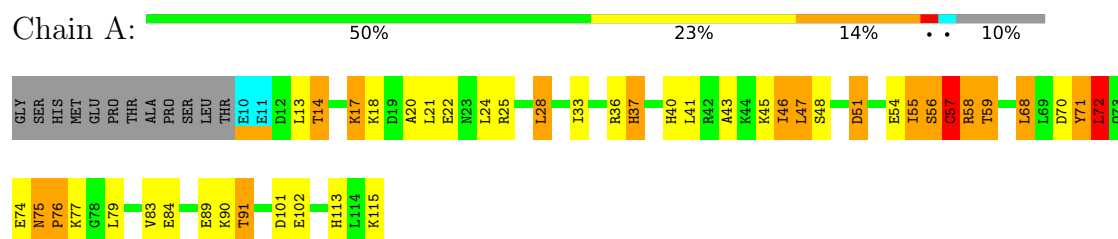
4.2.7 Score per residue for model 7

- Molecule 1: B-cell lymphoma/leukemia 10



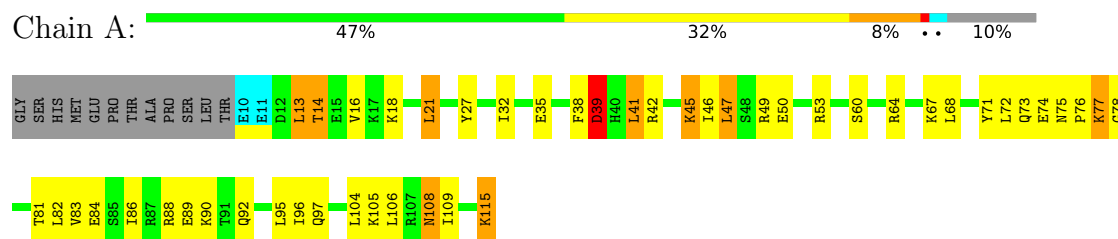
4.2.8 Score per residue for model 8

- Molecule 1: B-cell lymphoma/leukemia 10



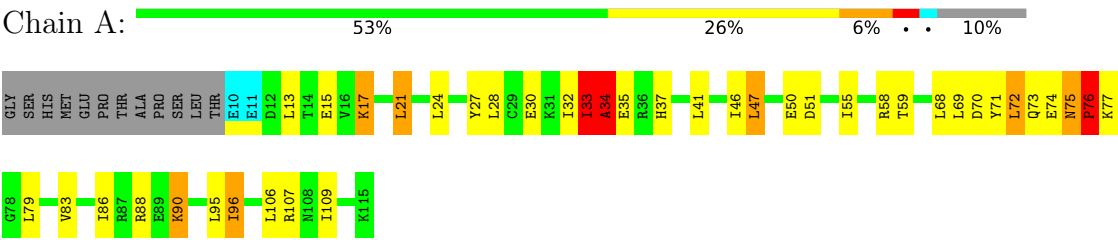
4.2.9 Score per residue for model 9

- Molecule 1: B-cell lymphoma/leukemia 10



4.2.10 Score per residue for model 10

- Molecule 1: B-cell lymphoma/leukemia 10



5 Refinement protocol and experimental data overview

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

Of the 1000 calculated structures, 10 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	structure solution	
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	1359
Number of shifts mapped to atoms	1251
Number of unparsed shifts	0
Number of shifts with mapping errors	108
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

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	1.26±0.07	3±2/875 (0.3± 0.2%)	1.37±0.05	7±4/1166 (0.6± 0.3%)
All	All	1.26	28/8750 (0.3%)	1.37	69/11660 (0.6%)

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	0.9±0.7
All	All	0	9

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	74	GLU	C-N	-8.70	1.26	1.33	5	1
1	A	39	ASP	N-CA	7.52	1.55	1.46	9	1
1	A	58	ARG	N-CA	7.15	1.55	1.46	8	3
1	A	14	THR	C-N	7.03	1.43	1.33	2	1
1	A	34	ALA	C-N	-6.62	1.23	1.33	1	3
1	A	55	ILE	N-CA	6.35	1.54	1.46	6	2
1	A	32	ILE	CA-CB	6.19	1.59	1.53	5	1
1	A	33	ILE	CA-C	6.10	1.60	1.52	10	1
1	A	91	THR	CA-C	5.91	1.60	1.52	2	1
1	A	90	LYS	N-CA	5.85	1.53	1.46	10	1
1	A	35	GLU	N-CA	-5.64	1.38	1.46	1	1
1	A	75	ASN	N-CA	-5.61	1.41	1.46	5	1
1	A	76	PRO	N-CA	5.52	1.54	1.47	10	1
1	A	39	ASP	C-N	-5.49	1.26	1.33	9	1
1	A	56	SER	CA-C	5.43	1.60	1.52	8	1
1	A	76	PRO	C-N	-5.33	1.26	1.33	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	20	ALA	N-CA	5.21	1.52	1.46	8	1
1	A	33	ILE	N-CA	-5.19	1.39	1.46	6	3
1	A	59	THR	CA-C	5.11	1.59	1.52	1	2
1	A	86	ILE	CA-CB	5.01	1.60	1.54	5	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	14	THR	CA-C-O	-12.48	104.46	119.18	2	1
1	A	14	THR	CA-CB-CG2	-11.99	90.12	110.50	2	1
1	A	13	LEU	CA-C-N	-10.05	106.61	122.29	2	1
1	A	13	LEU	C-N-CA	-10.05	106.61	122.29	2	1
1	A	14	THR	CA-CB-OG1	8.60	122.50	109.60	2	1
1	A	14	THR	N-CA-C	8.46	123.99	112.90	8	3
1	A	34	ALA	N-CA-CB	-8.30	96.46	110.49	1	1
1	A	75	ASN	CA-C-N	7.87	129.68	119.84	5	5
1	A	75	ASN	C-N-CA	7.87	129.68	119.84	5	5
1	A	33	ILE	CA-C-N	7.45	135.78	121.54	1	2
1	A	33	ILE	C-N-CA	7.45	135.78	121.54	1	2
1	A	113	HIS	N-CA-C	7.45	122.12	112.89	8	1
1	A	35	GLU	N-CA-C	-7.22	104.47	113.28	1	2
1	A	88	ARG	CA-C-N	6.95	134.81	121.54	2	1
1	A	88	ARG	C-N-CA	6.95	134.81	121.54	2	1
1	A	83	VAL	N-CA-C	6.71	118.28	110.62	8	1
1	A	70	ASP	CA-CB-CG	6.52	119.12	112.60	4	1
1	A	74	GLU	N-CA-C	6.44	119.26	111.40	9	2
1	A	57	CYS	CA-C-N	6.35	133.66	121.54	1	3
1	A	57	CYS	C-N-CA	6.35	133.66	121.54	1	3
1	A	34	ALA	CB-CA-C	-6.28	97.93	110.42	1	1
1	A	34	ALA	N-CA-C	6.23	124.08	110.80	1	2
1	A	108	ASN	CA-CB-CG	6.19	118.79	112.60	9	1
1	A	41	LEU	N-CA-C	6.14	119.88	112.38	10	1
1	A	32	ILE	CA-C-N	-6.11	115.08	122.90	6	2
1	A	32	ILE	C-N-CA	-6.11	115.08	122.90	6	2
1	A	75	ASN	CA-C-O	-6.08	115.16	121.06	10	1
1	A	46	ILE	CB-CA-C	-6.04	103.88	112.22	5	1
1	A	91	THR	N-CA-C	-6.04	105.17	112.54	8	1
1	A	113	HIS	CA-CB-CG	5.72	119.52	113.80	7	3
1	A	56	SER	CA-C-N	5.59	132.22	121.54	8	2
1	A	56	SER	C-N-CA	5.59	132.22	121.54	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	75	ASN	CA-CB-CG	5.55	118.16	112.60	8	1
1	A	60	SER	N-CA-C	-5.36	101.17	108.24	5	1
1	A	73	GLN	N-CA-C	5.28	119.40	111.96	10	1
1	A	74	GLU	N-CA-CB	-5.21	101.69	110.49	10	1
1	A	58	ARG	N-CA-C	5.14	121.76	110.80	7	2
1	A	76	PRO	N-CA-C	5.13	123.03	112.47	5	1
1	A	72	LEU	CA-C-N	-5.08	111.83	121.54	8	1
1	A	72	LEU	C-N-CA	-5.08	111.83	121.54	8	1
1	A	89	GLU	N-CA-C	5.04	121.55	110.80	2	1
1	A	73	GLN	CA-C-N	-5.04	112.29	120.71	9	1
1	A	73	GLN	C-N-CA	-5.04	112.29	120.71	9	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	36	ARG	Peptide,Sidechain	2
1	A	37	HIS	Peptide	1
1	A	107	ARG	Sidechain	1
1	A	64	ARG	Sidechain	1
1	A	49	ARG	Sidechain	1
1	A	42	ARG	Sidechain	1
1	A	25	ARG	Sidechain	1
1	A	33	ILE	Peptide	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	868	924	921	20±6
All	All	8680	9240	9210	199

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:ILE:HB	1:A:47:LEU:HD22	0.74	1.57	3	2
1:A:13:LEU:HD23	1:A:104:LEU:HA	0.72	1.60	2	2
1:A:47:LEU:HD21	1:A:72:LEU:HD11	0.69	1.64	3	1
1:A:13:LEU:HD11	1:A:107:ARG:CZ	0.66	2.21	5	1
1:A:17:LYS:O	1:A:21:LEU:HG	0.65	1.91	5	5
1:A:32:ILE:HG12	1:A:33:ILE:HG22	0.63	1.71	10	1
1:A:83:VAL:HA	1:A:86:ILE:HG12	0.61	1.71	9	1
1:A:27:TYR:CE1	1:A:28:LEU:HG	0.61	2.30	10	1
1:A:68:LEU:O	1:A:72:LEU:HG	0.61	1.96	10	5
1:A:47:LEU:HG	1:A:71:TYR:CE2	0.60	2.30	3	1
1:A:13:LEU:O	1:A:16:VAL:HG22	0.60	1.97	3	3
1:A:70:ASP:O	1:A:76:PRO:HA	0.59	1.97	10	2
1:A:115:LYS:HA	1:A:115:LYS:NZ	0.59	2.13	9	2
1:A:24:LEU:O	1:A:28:LEU:HB2	0.58	1.98	8	4
1:A:69:LEU:HA	1:A:72:LEU:HD12	0.57	1.75	1	2
1:A:38:PHE:CD2	1:A:41:LEU:HG	0.56	2.34	9	1
1:A:12:ASP:O	1:A:110:LYS:HD2	0.56	2.01	2	1
1:A:59:THR:HG23	1:A:64:ARG:HB3	0.55	1.78	6	1
1:A:68:LEU:HA	1:A:71:TYR:CZ	0.55	2.36	6	3
1:A:18:LYS:HE2	1:A:73:GLN:O	0.55	2.02	1	1
1:A:46:ILE:HG21	1:A:78:GLY:HA2	0.55	1.79	3	1
1:A:87:ARG:HA	1:A:96:ILE:HD11	0.54	1.80	5	1
1:A:83:VAL:HA	1:A:86:ILE:CG1	0.53	2.33	9	1
1:A:46:ILE:HD12	1:A:46:ILE:H	0.53	1.62	2	3
1:A:79:LEU:HD12	1:A:79:LEU:H	0.52	1.65	10	2
1:A:87:ARG:HA	1:A:96:ILE:CD1	0.52	2.34	5	1
1:A:63:LYS:O	1:A:67:LYS:HG2	0.52	2.04	6	1
1:A:88:ARG:NE	1:A:88:ARG:HA	0.52	2.20	10	1
1:A:35:GLU:O	1:A:39:ASP:HB3	0.52	2.04	9	1
1:A:34:ALA:HB1	1:A:68:LEU:HD23	0.51	1.82	5	1
1:A:47:LEU:HD21	1:A:71:TYR:CE1	0.51	2.41	8	1
1:A:22:GLU:OE1	1:A:22:GLU:HA	0.51	2.06	3	1
1:A:65:ALA:O	1:A:69:LEU:HG	0.51	2.06	1	1
1:A:47:LEU:HB3	1:A:51:ASP:OD2	0.51	2.06	8	2
1:A:24:LEU:HA	1:A:27:TYR:CZ	0.50	2.41	1	2
1:A:51:ASP:OD2	1:A:55:ILE:HG22	0.50	2.07	6	1
1:A:77:LYS:NZ	1:A:77:LYS:HA	0.50	2.22	9	1
1:A:68:LEU:HA	1:A:71:TYR:CE1	0.50	2.42	2	4
1:A:80:ASP:O	1:A:83:VAL:HG12	0.50	2.05	7	1
1:A:46:ILE:HG23	1:A:47:LEU:HD22	0.50	1.83	10	1
1:A:87:ARG:C	1:A:89:GLU:H	0.50	2.14	2	1
1:A:37:HIS:HB2	1:A:41:LEU:HD12	0.50	1.84	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:HIS:O	1:A:43:ALA:HB3	0.50	2.06	8	2
1:A:68:LEU:HD12	1:A:71:TYR:CE1	0.50	2.42	4	3
1:A:30:GLU:HA	1:A:62:ARG:NH1	0.49	2.22	5	1
1:A:46:ILE:H	1:A:46:ILE:HD12	0.49	1.67	1	4
1:A:68:LEU:O	1:A:72:LEU:HD13	0.49	2.08	3	1
1:A:78:GLY:O	1:A:81:THR:HB	0.49	2.07	1	3
1:A:48:SER:HA	1:A:52:THR:CB	0.49	2.38	6	2
1:A:16:VAL:HG21	1:A:106:LEU:HB3	0.49	1.85	1	1
1:A:115:LYS:HA	1:A:115:LYS:CE	0.49	2.38	1	1
1:A:72:LEU:HD11	1:A:82:LEU:HD11	0.49	1.83	1	2
1:A:46:ILE:CG2	1:A:78:GLY:HA2	0.49	2.38	3	1
1:A:48:SER:HB2	1:A:51:ASP:OD1	0.48	2.08	8	1
1:A:67:LYS:O	1:A:67:LYS:HD3	0.48	2.08	9	1
1:A:106:LEU:O	1:A:109:ILE:HB	0.48	2.08	9	2
1:A:18:LYS:O	1:A:22:GLU:HG2	0.48	2.09	6	1
1:A:55:ILE:O	1:A:59:THR:HB	0.48	2.08	10	1
1:A:34:ALA:CB	1:A:68:LEU:HD22	0.48	2.38	1	2
1:A:57:CYS:SG	1:A:67:LYS:HG3	0.48	2.49	7	1
1:A:68:LEU:HD12	1:A:71:TYR:CE2	0.48	2.44	1	2
1:A:86:ILE:O	1:A:96:ILE:HD12	0.47	2.09	10	1
1:A:51:ASP:O	1:A:55:ILE:HG23	0.47	2.09	10	1
1:A:115:LYS:HA	1:A:115:LYS:HZ3	0.47	1.68	9	1
1:A:46:ILE:HD13	1:A:46:ILE:H	0.47	1.69	7	1
1:A:47:LEU:HD12	1:A:71:TYR:CD1	0.47	2.44	1	1
1:A:30:GLU:OE2	1:A:31:LYS:HG2	0.47	2.09	2	1
1:A:35:GLU:OE1	1:A:64:ARG:HD2	0.47	2.10	2	1
1:A:34:ALA:O	1:A:37:HIS:HB3	0.47	2.10	6	1
1:A:28:LEU:O	1:A:32:ILE:HG22	0.47	2.09	5	2
1:A:53:ARG:O	1:A:53:ARG:HD3	0.47	2.10	5	1
1:A:75:ASN:O	1:A:77:LYS:N	0.47	2.48	10	3
1:A:88:ARG:O	1:A:88:ARG:HD3	0.47	2.10	1	1
1:A:46:ILE:HG21	1:A:72:LEU:HD22	0.47	1.87	4	1
1:A:41:LEU:CD1	1:A:68:LEU:HD13	0.47	2.39	8	1
1:A:79:LEU:HD12	1:A:79:LEU:N	0.46	2.25	10	2
1:A:89:GLU:CB	1:A:96:ILE:HG13	0.46	2.41	2	1
1:A:102:GLU:O	1:A:106:LEU:HB2	0.46	2.11	4	1
1:A:14:THR:O	1:A:17:LYS:HG3	0.46	2.10	8	1
1:A:60:SER:CB	1:A:64:ARG:HG3	0.46	2.39	3	1
1:A:68:LEU:HA	1:A:71:TYR:CE2	0.46	2.46	7	2
1:A:41:LEU:CD2	1:A:46:ILE:HD11	0.45	2.41	1	1
1:A:42:ARG:O	1:A:45:LYS:HG3	0.45	2.11	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:GLU:H	1:A:89:GLU:CD	0.45	2.19	5	1
1:A:95:LEU:O	1:A:99:ILE:HG13	0.45	2.12	7	1
1:A:34:ALA:HB2	1:A:41:LEU:HB2	0.45	1.87	1	1
1:A:47:LEU:HG	1:A:71:TYR:CZ	0.45	2.46	3	1
1:A:49:ARG:HD2	1:A:50:GLU:OE2	0.45	2.12	9	1
1:A:88:ARG:HD3	1:A:88:ARG:O	0.45	2.11	6	1
1:A:35:GLU:OE1	1:A:64:ARG:HD3	0.45	2.12	9	1
1:A:60:SER:O	1:A:64:ARG:HG3	0.45	2.12	9	1
1:A:106:LEU:O	1:A:109:ILE:HG22	0.45	2.12	10	1
1:A:72:LEU:HB3	1:A:78:GLY:HA3	0.45	1.88	5	1
1:A:110:LYS:O	1:A:113:HIS:HB3	0.45	2.12	3	2
1:A:54:GLU:O	1:A:58:ARG:HG2	0.44	2.12	2	1
1:A:83:VAL:O	1:A:87:ARG:HG3	0.44	2.13	5	1
1:A:37:HIS:HB2	1:A:41:LEU:CD1	0.44	2.42	6	1
1:A:35:GLU:OE2	1:A:64:ARG:HD2	0.44	2.11	6	1
1:A:81:THR:O	1:A:84:GLU:HB3	0.44	2.12	9	1
1:A:69:LEU:HD13	1:A:79:LEU:HD21	0.44	1.89	10	1
1:A:47:LEU:HD21	1:A:72:LEU:HB3	0.44	1.89	9	1
1:A:87:ARG:O	1:A:96:ILE:HD11	0.43	2.13	5	1
1:A:67:LYS:O	1:A:70:ASP:HB3	0.43	2.13	4	2
1:A:13:LEU:O	1:A:103:VAL:HG13	0.43	2.13	5	1
1:A:86:ILE:HA	1:A:89:GLU:HB2	0.43	1.90	1	1
1:A:93:ASN:O	1:A:97:GLN:HG2	0.43	2.13	6	1
1:A:17:LYS:HB3	1:A:17:LYS:NZ	0.43	2.28	10	1
1:A:89:GLU:HB3	1:A:96:ILE:HG13	0.43	1.89	2	1
1:A:78:GLY:O	1:A:82:LEU:HG	0.43	2.12	9	1
1:A:34:ALA:HB2	1:A:68:LEU:HD22	0.43	1.90	10	1
1:A:66:GLY:O	1:A:70:ASP:HB2	0.43	2.14	6	1
1:A:22:GLU:CD	1:A:77:LYS:HD3	0.43	2.38	8	1
1:A:21:LEU:HD23	1:A:79:LEU:CD1	0.43	2.44	10	1
1:A:79:LEU:H	1:A:79:LEU:CD1	0.43	2.26	8	2
1:A:49:ARG:O	1:A:53:ARG:HG3	0.43	2.13	9	1
1:A:32:ILE:HG12	1:A:33:ILE:H	0.43	1.74	10	1
1:A:13:LEU:CD2	1:A:104:LEU:HA	0.42	2.44	9	1
1:A:33:ILE:HG13	1:A:34:ALA:H	0.42	1.74	1	2
1:A:55:ILE:C	1:A:57:CYS:H	0.42	2.23	8	1
1:A:88:ARG:NH2	1:A:89:GLU:HA	0.42	2.29	3	1
1:A:69:LEU:HA	1:A:72:LEU:CD1	0.42	2.45	5	2
1:A:79:LEU:HD23	1:A:82:LEU:HD12	0.42	1.92	3	1
1:A:98:LYS:O	1:A:102:GLU:HG2	0.42	2.13	5	1
1:A:101:ASP:O	1:A:105:LYS:HG3	0.42	2.14	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ILE:CG1	1:A:33:ILE:N	0.42	2.83	1	1
1:A:44:LYS:HD2	1:A:81:THR:HG23	0.42	1.90	4	1
1:A:70:ASP:HA	1:A:76:PRO:O	0.42	2.15	8	1
1:A:22:GLU:O	1:A:25:ARG:HB3	0.41	2.15	7	1
1:A:18:LYS:HA	1:A:21:LEU:HB2	0.41	1.92	9	1
1:A:37:HIS:O	1:A:41:LEU:HG	0.41	2.15	4	1
1:A:83:VAL:HA	1:A:86:ILE:CG2	0.41	2.46	5	1
1:A:28:LEU:O	1:A:32:ILE:HB	0.41	2.16	1	1
1:A:42:ARG:HD2	1:A:42:ARG:H	0.41	1.74	9	1
1:A:30:GLU:OE1	1:A:31:LYS:NZ	0.41	2.52	5	1
1:A:51:ASP:OD1	1:A:58:ARG:HD2	0.41	2.15	6	1
1:A:86:ILE:O	1:A:89:GLU:HB2	0.41	2.15	1	1
1:A:28:LEU:CD2	1:A:95:LEU:HD12	0.41	2.46	10	1
1:A:33:ILE:HG13	1:A:34:ALA:N	0.41	2.30	10	1
1:A:33:ILE:CG1	1:A:34:ALA:H	0.41	2.29	1	1
1:A:82:LEU:O	1:A:86:ILE:HG13	0.41	2.16	1	1
1:A:12:ASP:OD2	1:A:107:ARG:HB2	0.41	2.16	5	1
1:A:83:VAL:HA	1:A:86:ILE:HG23	0.41	1.93	5	1
1:A:92:GLN:HG3	1:A:93:ASN:H	0.41	1.75	6	1
1:A:63:LYS:O	1:A:67:LYS:HB2	0.41	2.16	7	1
1:A:21:LEU:HD13	1:A:24:LEU:HD13	0.40	1.91	3	1
1:A:45:LYS:HB2	1:A:45:LYS:NZ	0.40	2.31	9	1
1:A:16:VAL:HG11	1:A:106:LEU:O	0.40	2.16	1	1
1:A:89:GLU:O	1:A:91:THR:N	0.40	2.54	8	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	103/118 (87%)	85±6 (83±5%)	12±4 (12±4%)	5±2 (5±2%)	3	24
All	All	1030/1180 (87%)	853 (83%)	125 (12%)	52 (5%)	3	24

All 24 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	76	PRO	7
1	A	89	GLU	5
1	A	90	LYS	4
1	A	58	ARG	3
1	A	59	THR	3
1	A	37	HIS	3
1	A	92	GLN	3
1	A	33	ILE	2
1	A	34	ALA	2
1	A	14	THR	2
1	A	55	ILE	2
1	A	17	LYS	2
1	A	57	CYS	2
1	A	72	LEU	2
1	A	60	SER	1
1	A	61	SER	1
1	A	93	ASN	1
1	A	87	ARG	1
1	A	46	ILE	1
1	A	56	SER	1
1	A	39	ASP	1
1	A	41	LEU	1
1	A	88	ARG	1
1	A	107	ARG	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	98/110 (89%)	86±3 (88±3%)	12±3 (12±3%)	7	49
All	All	980/1100 (89%)	863 (88%)	117 (12%)	7	49

All 54 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	46	ILE	8
1	A	115	LYS	7

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Mol	Chain	Res	Type	Models (Total)
1	A	47	LEU	7
1	A	30	GLU	5
1	A	28	LEU	5
1	A	18	LYS	4
1	A	89	GLU	4
1	A	13	LEU	4
1	A	50	GLU	3
1	A	55	ILE	3
1	A	114	LEU	3
1	A	90	LYS	3
1	A	98	LYS	3
1	A	96	ILE	3
1	A	54	GLU	2
1	A	63	LYS	2
1	A	112	GLU	2
1	A	14	THR	2
1	A	88	ARG	2
1	A	69	LEU	2
1	A	27	TYR	2
1	A	74	GLU	2
1	A	76	PRO	2
1	A	105	LYS	2
1	A	95	LEU	2
1	A	101	ASP	2
1	A	108	ASN	2
1	A	45	LYS	2
1	A	21	LEU	2
1	A	36	ARG	1
1	A	73	GLN	1
1	A	79	LEU	1
1	A	106	LEU	1
1	A	93	ASN	1
1	A	67	LYS	1
1	A	86	ILE	1
1	A	12	ASP	1
1	A	42	ARG	1
1	A	113	HIS	1
1	A	52	THR	1
1	A	72	LEU	1
1	A	75	ASN	1
1	A	51	ASP	1
1	A	68	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	71	TYR	1
1	A	84	GLU	1
1	A	102	GLU	1
1	A	32	ILE	1
1	A	77	LYS	1
1	A	97	GLN	1
1	A	15	GLU	1
1	A	17	LYS	1
1	A	58	ARG	1
1	A	83	VAL	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 79% for the well-defined parts and 79% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_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	1359
Number of shifts mapped to atoms	1251
Number of unparsed shifts	0
Number of shifts with mapping errors	108
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. All 108 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	0	HIS	HA	4.652	.	1
1	A	0	HIS	HB2	3.185	.	.
1	A	0	HIS	HB3	3.113	.	.
1	A	0	HIS	C	174.666	.	1
1	A	0	HIS	CA	56.088	.	1
1	A	0	HIS	CB	29.966	.	1
1	A	1	MET	H	8.307	.	1
1	A	1	MET	HA	4.437	.	1
1	A	1	MET	HB2	1.905	.	.
1	A	1	MET	HB3	2.014	.	.
1	A	1	MET	HG2	2.43	.	.
1	A	1	MET	HG3	2.478	.	.
1	A	1	MET	C	175.646	.	1
1	A	1	MET	CA	55.201	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	CB	33.069	.	1
1	A	1	MET	CG	31.995	.	1
1	A	1	MET	N	122.021	.	1
1	A	2	GLU	H	8.395	.	1
1	A	2	GLU	HA	4.57	.	1
1	A	2	GLU	HB2	1.883	.	.
1	A	2	GLU	HB3	2.034	.	.
1	A	2	GLU	HG2	2.436	.	.
1	A	2	GLU	HG3	2.287	.	.
1	A	2	GLU	C	174.62	.	1
1	A	2	GLU	CA	54.377	.	1
1	A	2	GLU	CB	29.731	.	1
1	A	2	GLU	CG	36.178	.	1
1	A	2	GLU	N	123.797	.	1
1	A	3	PRO	HA	4.466	.	1
1	A	3	PRO	HB2	2.289	.	.
1	A	3	PRO	HB3	1.923	.	.
1	A	3	PRO	HD2	3.792	.	.
1	A	3	PRO	HD3	3.726	.	.
1	A	3	PRO	HG2	2.129	.	.
1	A	3	PRO	HG3	2.017	.	.
1	A	3	PRO	C	177.015	.	1
1	A	3	PRO	CA	63.241	.	1
1	A	3	PRO	CB	32.172	.	1
1	A	3	PRO	CD	50.718	.	1
1	A	3	PRO	CG	27.418	.	1
1	A	4	THR	H	8.162	.	1
1	A	4	THR	HA	4.263	.	1
1	A	4	THR	HB	4.154	.	1
1	A	4	THR	HG21	1.199	.	1
1	A	4	THR	HG22	1.199	.	1
1	A	4	THR	HG23	1.199	.	1
1	A	4	THR	C	173.995	.	1
1	A	4	THR	CA	61.765	.	1
1	A	4	THR	CB	69.933	.	1
1	A	4	THR	CG2	21.692	.	1
1	A	4	THR	N	114.442	.	1
1	A	5	ALA	H	8.26	.	1
1	A	5	ALA	HA	4.605	.	1
1	A	5	ALA	HB1	1.357	.	1
1	A	5	ALA	HB2	1.357	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	ALA	HB3	1.357	.	1
1	A	5	ALA	C	175.299	.	1
1	A	5	ALA	CA	50.553	.	1
1	A	5	ALA	CB	18.453	.	1
1	A	5	ALA	N	127.909	.	1
1	A	6	PRO	HA	4.457	.	1
1	A	6	PRO	HB2	1.876	.	.
1	A	6	PRO	HB3	2.281	.	.
1	A	6	PRO	HD2	3.795	.	.
1	A	6	PRO	HD3	3.631	.	.
1	A	6	PRO	HG3	1.996	.	.
1	A	6	PRO	C	176.161	.	1
1	A	6	PRO	CA	63.09	.	1
1	A	6	PRO	CB	32.322	.	1
1	A	6	PRO	CD	50.452	.	1
1	A	6	PRO	CG	27.419	.	1
1	A	7	SER	H	8.249	.	1
1	A	7	SER	HA	4.497	.	1
1	A	7	SER	HB2	3.603	.	.
1	A	7	SER	HB3	3.808	.	.
1	A	7	SER	C	173.813	.	1
1	A	7	SER	CA	57.676	.	1
1	A	7	SER	CB	64.673	.	1
1	A	7	SER	N	115.227	.	1
1	A	8	LEU	H	8.22	.	1
1	A	8	LEU	HA	4.656	.	1
1	A	8	LEU	HB2	1.771	.	.
1	A	8	LEU	HB3	1.659	.	.
1	A	8	LEU	HD11	0.828	.	.
1	A	8	LEU	HD12	0.828	.	.
1	A	8	LEU	HD13	0.828	.	.
1	A	8	LEU	HD21	0.887	.	.
1	A	8	LEU	HD22	0.887	.	.
1	A	8	LEU	HD23	0.887	.	.
1	A	8	LEU	HG	1.144	.	1
1	A	8	LEU	C	177.893	.	1
1	A	8	LEU	CA	54.606	.	1
1	A	8	LEU	CB	42.854	.	1
1	A	8	LEU	CD1	24.08	.	.
1	A	8	LEU	CD2	26.304	.	.
1	A	8	LEU	CG	29.169	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	8	LEU	N	122.306	.	1
1	A	9	THR	H	9.056	.	1
1	A	9	THR	HA	4.449	.	1
1	A	9	THR	HB	4.648	.	1
1	A	9	THR	HG21	1.343	.	1
1	A	9	THR	HG22	1.343	.	1
1	A	9	THR	HG23	1.343	.	1
1	A	9	THR	C	175.386	.	1
1	A	9	THR	CA	61.076	.	1
1	A	9	THR	CB	71.33	.	1
1	A	9	THR	CG2	22.29	.	1
1	A	9	THR	N	114.593	.	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	115	-0.58 ± 0.17	Should be checked
$^{13}\text{C}_\beta$	113	0.17 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	115	-0.49 ± 0.14	None needed (< 0.5 ppm)
^{15}N	109	0.63 ± 0.31	Should be applied

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 79%, i.e. 1234 atoms were assigned a chemical shift out of a possible 1567. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	512/520 (98%)	206/209 (99%)	206/208 (99%)	100/103 (97%)
Sidechain	708/985 (72%)	489/631 (77%)	212/301 (70%)	7/53 (13%)
Aromatic	14/62 (23%)	14/30 (47%)	0/26 (0%)	0/6 (0%)
Overall	1234/1567 (79%)	709/870 (81%)	418/535 (78%)	107/162 (66%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1251 atoms were assigned a chemical shift out of a possible 1591. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	522/530 (98%)	210/213 (99%)	210/212 (99%)	102/105 (97%)
Sidechain	715/999 (72%)	493/639 (77%)	215/307 (70%)	7/53 (13%)
Aromatic	14/62 (23%)	14/30 (47%)	0/26 (0%)	0/6 (0%)
Overall	1251/1591 (79%)	717/882 (81%)	425/545 (78%)	109/164 (66%)

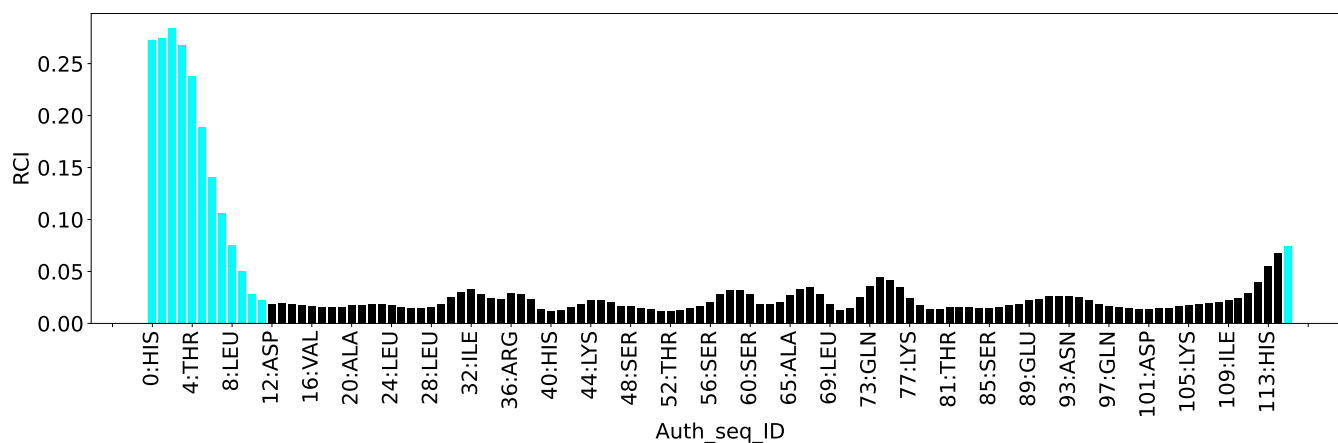
7.1.4 Statistically unusual chemical shifts [i](#)

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	1291
Intra-residue ($ i-j =0$)	681
Sequential ($ i-j =1$)	296
Medium range ($ i-j >1$ and $ i-j <5$)	150
Long range ($ i-j \geq 5$)	164
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	203
Number of unmapped restraints	0
Number of restraints per residue	12.7
Number of long range restraints per residue ¹	1.4

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)	39.7	0.2
0.2-0.5 (Medium)	39.8	0.5
>0.5 (Large)	103.8	5.93

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)	33.2	9.91
10.0-20.0 (Medium)	2.7	18.83
>20.0 (Large)	0.2	28.36

9 Distance violation analysis ⓘ

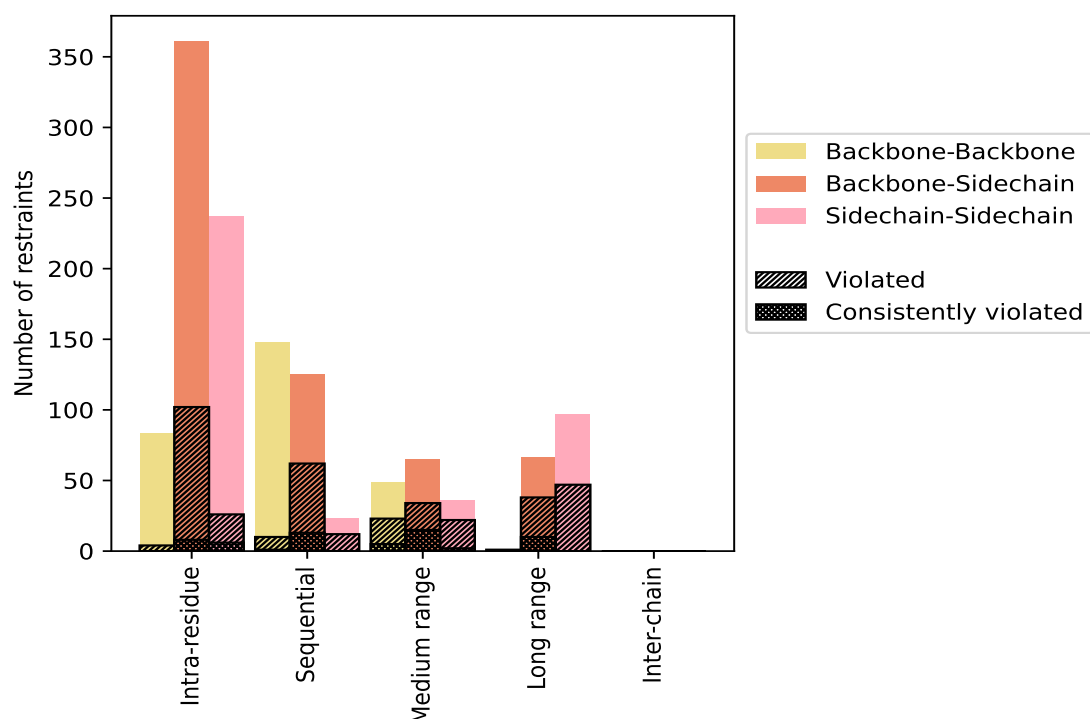
9.1 Summary of distance violations ⓘ

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)	681	52.7	132	19.4	10.2	14	2.1	1.1
Backbone-Backbone	83	6.4	4	4.8	0.3	0	0.0	0.0
Backbone-Sidechain	361	28.0	102	28.3	7.9	8	2.2	0.6
Sidechain-Sidechain	237	18.4	26	11.0	2.0	6	2.5	0.5
Sequential (i-j =1)	296	22.9	84	28.4	6.5	14	4.7	1.1
Backbone-Backbone	148	11.5	10	6.8	0.8	1	0.7	0.1
Backbone-Sidechain	125	9.7	62	49.6	4.8	13	10.4	1.0
Sidechain-Sidechain	23	1.8	12	52.2	0.9	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	150	11.6	79	52.7	6.1	22	14.7	1.7
Backbone-Backbone	49	3.8	23	46.9	1.8	5	10.2	0.4
Backbone-Sidechain	65	5.0	34	52.3	2.6	15	23.1	1.2
Sidechain-Sidechain	36	2.8	22	61.1	1.7	2	5.6	0.2
Long range (i-j ≥5)	164	12.7	86	52.4	6.7	10	6.1	0.8
Backbone-Backbone	1	0.1	1	100.0	0.1	0	0.0	0.0
Backbone-Sidechain	66	5.1	38	57.6	2.9	10	15.2	0.8
Sidechain-Sidechain	97	7.5	47	48.5	3.6	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1291	100.0	381	29.5	29.5	60	4.6	4.6
Backbone-Backbone	281	21.8	38	13.5	2.9	6	2.1	0.5
Backbone-Sidechain	617	47.8	236	38.2	18.3	46	7.5	3.6
Sidechain-Sidechain	393	30.4	107	27.2	8.3	8	2.0	0.6

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

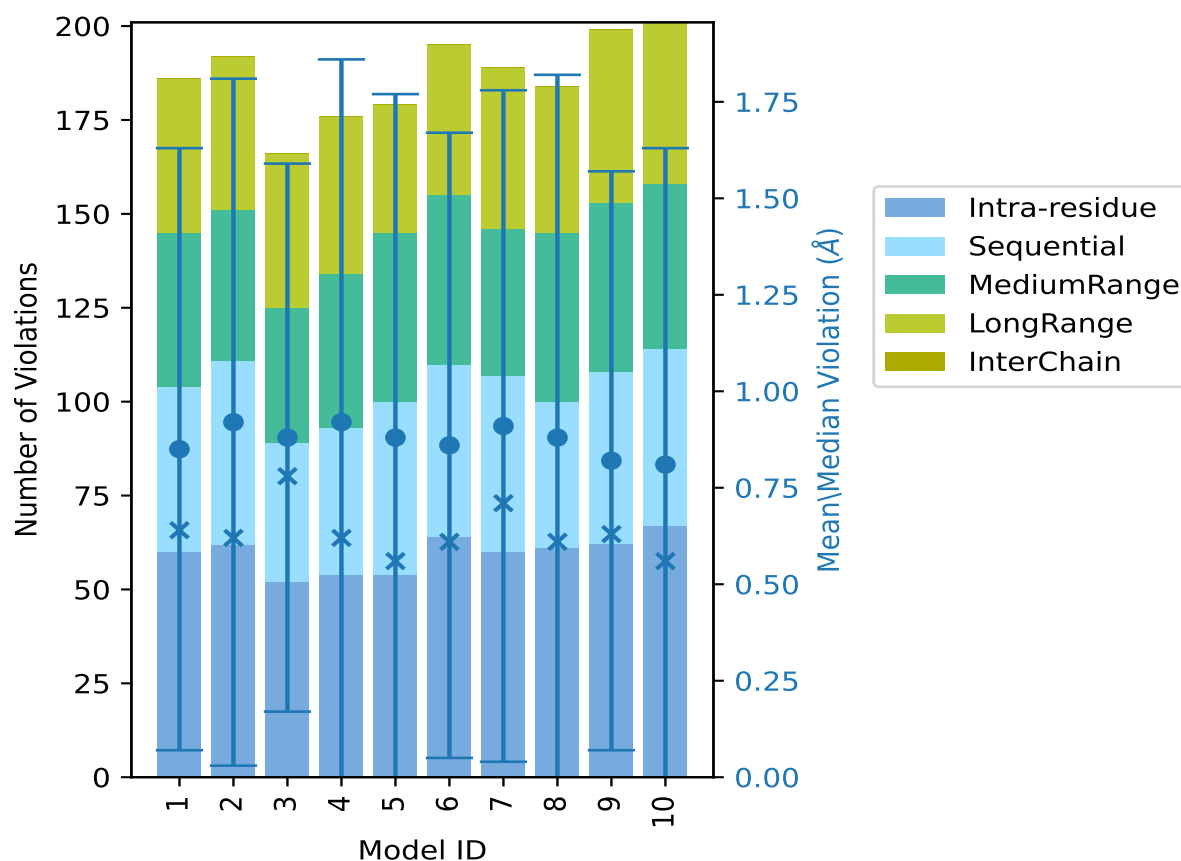
9.2 Distance violation statistics for each model [i](#)

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	60	44	41	41	0	186	0.85	4.14	0.78	0.64
2	62	49	40	41	0	192	0.92	4.59	0.89	0.62
3	52	37	36	41	0	166	0.88	3.73	0.71	0.78
4	54	39	41	42	0	176	0.92	5.93	0.94	0.62
5	54	46	45	34	0	179	0.88	5.08	0.89	0.56
6	64	46	45	40	0	195	0.86	3.52	0.81	0.61
7	60	47	39	43	0	189	0.91	4.74	0.87	0.71
8	61	39	45	39	0	184	0.88	4.94	0.94	0.61
9	62	46	45	46	0	199	0.82	3.32	0.75	0.63
10	67	47	44	43	0	201	0.81	4.98	0.82	0.56

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 [i](#)



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

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 910(IR:549, SQ:212, MR:71, LR:78, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
36	19	13	21	0	89	1	10.0
13	8	18	11	0	50	2	20.0
15	5	4	9	0	33	3	30.0

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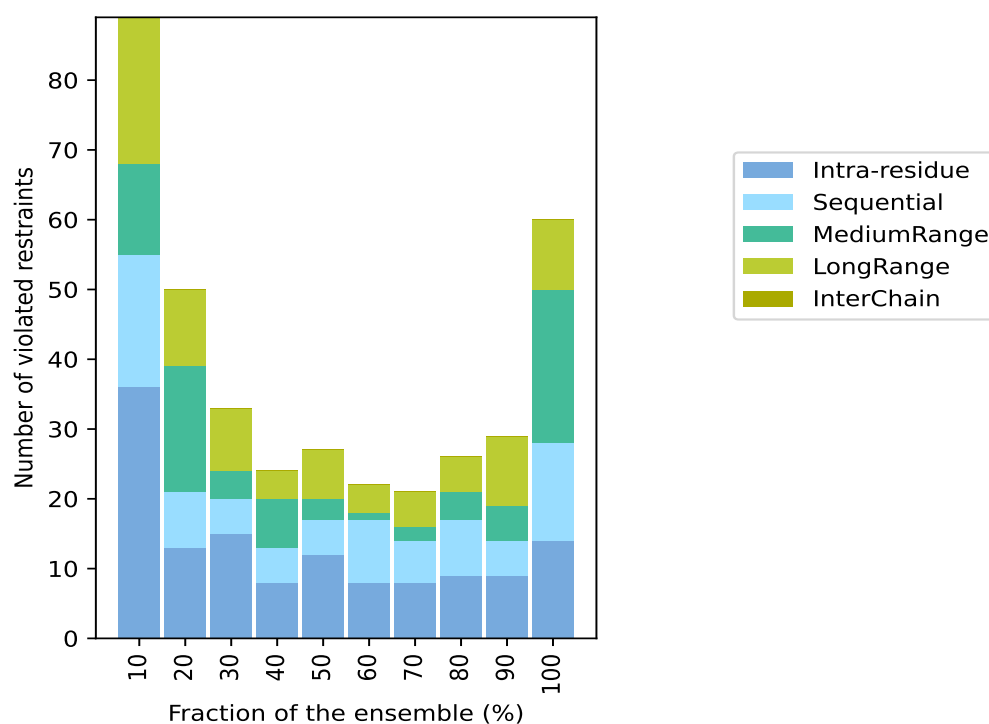
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
8	5	7	4	0	24	4	40.0
12	5	3	7	0	27	5	50.0
8	9	1	4	0	22	6	60.0
8	6	2	5	0	21	7	70.0
9	8	4	5	0	26	8	80.0
9	5	5	10	0	29	9	90.0
14	14	22	10	0	60	10	100.0

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 ⓘ

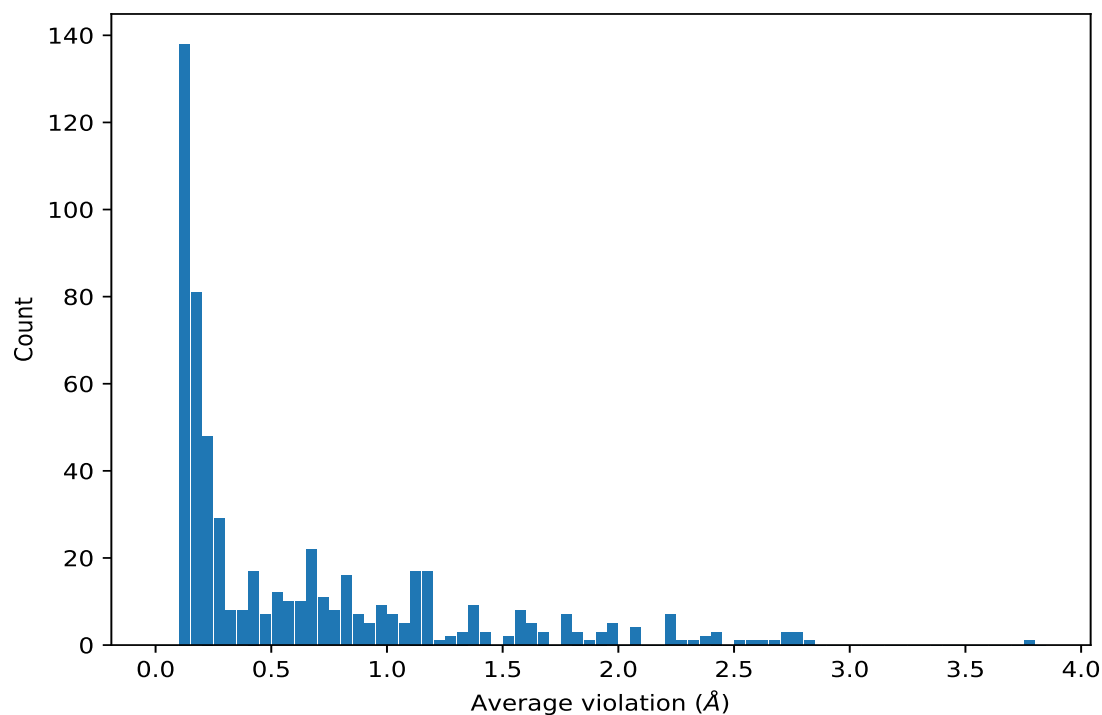


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



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

The following table provides the mean and the standard deviation of 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)
(1,347)	1:64:A:ARG:H	1:35:A:GLU:HG3	10	3.79	1.27	3.54
(1,210)	1:74:A:GLU:H	1:70:A:ASP:HA	10	2.81	0.94	2.7
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD11	10	2.74	0.62	3.05
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD12	10	2.74	0.62	3.05
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD13	10	2.74	0.62	3.05
(1,160)	1:70:A:ASP:H	1:71:A:TYR:HB2	10	2.69	0.44	2.78
(1,861)	1:54:A:GLU:H	1:51:A:ASP:HB3	10	2.64	0.4	2.76
(1,1167)	1:53:A:ARG:H	1:55:A:ILE:HG12	10	2.52	1.04	2.24
(1,997)	1:106:A:LEU:H	1:104:A:LEU:HB2	10	2.44	0.22	2.46
(1,312)	1:107:A:ARG:H	1:110:A:LYS:HB2	10	2.43	0.19	2.41
(1,574)	1:67:A:LYS:H	1:68:A:LEU:HB2	10	2.42	0.36	2.24
(1,755)	1:56:A:SER:H	1:64:A:ARG:HG3	10	2.38	1.23	2.5
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD21	10	2.07	0.97	1.94
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD22	10	2.07	0.97	1.94
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD23	10	2.07	0.97	1.94

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,938)	1:102:A:GLU:HB3	1:106:A:LEU:HG	10	1.98	1.1	1.36
(1,510)	1:97:A:GLN:HE22	1:97:A:GLN:HB3	10	1.9	0.44	1.91
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD21	10	1.83	0.9	2.38
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD22	10	1.83	0.9	2.38
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD23	10	1.83	0.9	2.38
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD21	10	1.77	0.5	1.9
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD22	10	1.77	0.5	1.9
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD23	10	1.77	0.5	1.9
(1,933)	1:63:A:LYS:H	1:64:A:ARG:HB2	10	1.7	0.77	1.36
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD11	10	1.63	1.02	1.35
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD12	10	1.63	1.02	1.35
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD13	10	1.63	1.02	1.35
(1,872)	1:45:A:LYS:H	1:41:A:LEU:HA	10	1.56	0.61	1.58
(1,1059)	1:98:A:LYS:H	1:96:A:ILE:HB	10	1.43	0.2	1.46
(1,952)	1:82:A:LEU:H	1:84:A:GLU:HB2	10	1.41	1.04	1.08
(1,987)	1:32:A:ILE:H	1:28:A:LEU:HB2	10	1.39	0.48	1.27
(1,922)	1:106:A:LEU:H	1:106:A:LEU:HG	10	1.38	0.14	1.35
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD21	10	1.36	0.4	1.43
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD22	10	1.36	0.4	1.43
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD23	10	1.36	0.4	1.43
(1,21)	1:97:A:GLN:H	1:98:A:LYS:HB2	10	1.35	0.21	1.29
(1,502)	1:31:A:LYS:H	1:28:A:LEU:HB2	10	1.31	0.27	1.23
(1,913)	1:63:A:LYS:H	1:63:A:LYS:HD2	10	1.3	0.2	1.22
(1,450)	1:108:A:ASN:HD22	1:108:A:ASN:HB3	10	1.22	0.08	1.24
(1,8)	1:42:A:ARG:H	1:45:A:LYS:HG2	10	1.17	0.06	1.17
(1,948)	1:20:A:ALA:H	1:18:A:LYS:HB2	10	1.15	0.18	1.16
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD11	10	1.15	0.44	1.19
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD12	10	1.15	0.44	1.19
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD13	10	1.15	0.44	1.19
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD11	10	1.15	0.44	1.19
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD12	10	1.15	0.44	1.19
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD13	10	1.15	0.44	1.19
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG21	10	1.09	0.5	1.2
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG22	10	1.09	0.5	1.2
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG23	10	1.09	0.5	1.2
(1,534)	1:92:A:GLN:HE22	1:92:A:GLN:HG3	10	1.03	0.25	1.2
(1,927)	1:14:A:THR:H	1:12:A:ASP:HB2	10	1.02	0.18	1.04
(1,1168)	1:54:A:GLU:H	1:56:A:SER:H	10	1.01	0.46	0.9
(1,1277)	1:107:A:ARG:H	1:106:A:LEU:HB3	10	1.0	0.23	1.09
(1,1122)	1:97:A:GLN:H	1:99:A:ILE:HB	10	1.0	0.48	0.9
(1,1052)	1:23:A:ASN:HD22	1:23:A:ASN:HB3	10	0.94	0.19	0.96
(1,6)	1:27:A:TYR:H	1:23:A:ASN:HB2	10	0.91	0.24	0.9

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,607)	1:19:A:ASP:H	1:18:A:LYS:HB2	10	0.89	0.43	0.88
(1,599)	1:88:A:ARG:H	1:88:A:ARG:HG3	10	0.88	0.28	0.94
(1,444)	1:46:A:ILE:H	1:45:A:LYS:HB2	10	0.87	0.12	0.91
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG21	10	0.86	0.27	0.79
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG22	10	0.86	0.27	0.79
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG23	10	0.86	0.27	0.79
(1,158)	1:66:A:GLY:H	1:67:A:LYS:HB3	10	0.84	0.57	0.76
(1,241)	1:12:A:ASP:H	1:13:A:LEU:HA	10	0.84	0.13	0.83
(1,1013)	1:64:A:ARG:H	1:62:A:ARG:HB3	10	0.8	0.27	0.72
(1,386)	1:16:A:VAL:H	1:16:A:VAL:HB	10	0.79	0.03	0.78
(1,1211)	1:71:A:TYR:HD1	1:68:A:LEU:HB3	10	0.72	0.26	0.62
(1,1211)	1:71:A:TYR:HD2	1:68:A:LEU:HB3	10	0.72	0.26	0.62
(1,1206)	1:69:A:LEU:H	1:69:A:LEU:HB3	10	0.7	0.08	0.72
(1,730)	1:84:A:GLU:H	1:83:A:VAL:HB	10	0.66	0.06	0.67
(1,1088)	1:101:A:ASP:H	1:99:A:ILE:HB	10	0.64	0.28	0.58
(1,513)	1:112:A:GLU:H	1:114:A:LEU:H	10	0.52	0.23	0.62
(1,544)	1:70:A:ASP:H	1:68:A:LEU:HA	10	0.5	0.15	0.47
(1,239)	1:93:A:ASN:HD22	1:93:A:ASN:HB3	10	0.4	0.14	0.4
(1,597)	1:46:A:ILE:H	1:45:A:LYS:HG3	10	0.39	0.09	0.38
(1,1046)	1:17:A:LYS:H	1:16:A:VAL:HB	10	0.38	0.09	0.38
(1,813)	1:73:A:GLN:HE22	1:73:A:GLN:HG2	10	0.31	0.06	0.29
(1,27)	1:27:A:TYR:H	1:27:A:TYR:HB2	10	0.23	0.03	0.24
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG21	10	0.2	0.03	0.2
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG22	10	0.2	0.03	0.2
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG23	10	0.2	0.03	0.2
(1,291)	1:16:A:VAL:HG21	1:16:A:VAL:HA	10	0.2	0.03	0.2
(1,291)	1:16:A:VAL:HG22	1:16:A:VAL:HA	10	0.2	0.03	0.2
(1,291)	1:16:A:VAL:HG23	1:16:A:VAL:HA	10	0.2	0.03	0.2
(1,1156)	1:75:A:ASN:H	1:18:A:LYS:HE3	9	2.56	1.46	2.56
(1,666)	1:65:A:ALA:H	1:35:A:GLU:HG3	9	2.24	0.83	2.39
(1,131)	1:81:A:THR:HG21	1:72:A:LEU:HB3	9	2.23	0.46	2.31
(1,131)	1:81:A:THR:HG22	1:72:A:LEU:HB3	9	2.23	0.46	2.31
(1,131)	1:81:A:THR:HG23	1:72:A:LEU:HB3	9	2.23	0.46	2.31
(1,655)	1:47:A:LEU:HD11	1:68:A:LEU:HB3	9	2.22	0.69	2.13
(1,655)	1:47:A:LEU:HD12	1:68:A:LEU:HB3	9	2.22	0.69	2.13
(1,655)	1:47:A:LEU:HD13	1:68:A:LEU:HB3	9	2.22	0.69	2.13
(1,1212)	1:55:A:ILE:H	1:51:A:ASP:HB3	9	1.97	0.82	2.0
(1,430)	1:16:A:VAL:H	1:15:A:GLU:HG2	9	1.41	0.31	1.47
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD11	9	1.35	0.29	1.23
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD12	9	1.35	0.29	1.23
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD13	9	1.35	0.29	1.23
(1,278)	1:29:A:CYS:H	1:30:A:GLU:HB2	9	1.27	0.74	1.04

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,169)	1:97:A:GLN:HE21	1:97:A:GLN:HB3	9	1.25	0.29	1.25
(1,83)	1:88:A:ARG:H	1:87:A:ARG:HB2	9	1.18	0.32	1.28
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB1	9	1.15	0.31	1.19
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB2	9	1.15	0.31	1.19
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB3	9	1.15	0.31	1.19
(1,1049)	1:74:A:GLU:H	1:74:A:GLU:HG2	9	1.1	0.74	1.51
(1,1253)	1:54:A:GLU:H	1:57:A:CYS:H	9	1.03	0.64	0.75
(1,920)	1:88:A:ARG:H	1:88:A:ARG:HG2	9	1.03	0.17	1.1
(1,880)	1:32:A:ILE:HD11	1:86:A:ILE:HG13	9	0.98	0.58	0.72
(1,880)	1:32:A:ILE:HD12	1:86:A:ILE:HG13	9	0.98	0.58	0.72
(1,880)	1:32:A:ILE:HD13	1:86:A:ILE:HG13	9	0.98	0.58	0.72
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD21	9	0.97	0.4	1.06
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD22	9	0.97	0.4	1.06
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD23	9	0.97	0.4	1.06
(1,178)	1:105:A:LYS:H	1:105:A:LYS:HD2	9	0.96	0.46	1.25
(1,371)	1:71:A:TYR:H	1:71:A:TYR:HB2	9	0.93	0.05	0.92
(1,185)	1:46:A:ILE:H	1:44:A:LYS:HB3	9	0.87	0.29	0.79
(1,269)	1:55:A:ILE:H	1:55:A:ILE:HB	9	0.78	0.25	0.89
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD11	9	0.7	1.51	0.15
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD12	9	0.7	1.51	0.15
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD13	9	0.7	1.51	0.15
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD11	9	0.7	1.51	0.15
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD12	9	0.7	1.51	0.15
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD13	9	0.7	1.51	0.15
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD11	9	0.7	1.51	0.15
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD12	9	0.7	1.51	0.15
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD13	9	0.7	1.51	0.15
(1,635)	1:32:A:ILE:H	1:31:A:LYS:HB2	9	0.62	0.41	0.52
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG21	9	0.57	0.25	0.45
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG22	9	0.57	0.25	0.45
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG23	9	0.57	0.25	0.45
(1,732)	1:36:A:ARG:H	1:35:A:GLU:HB2	9	0.34	0.16	0.33
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG21	9	0.28	0.02	0.27
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG22	9	0.28	0.02	0.27
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG23	9	0.28	0.02	0.27
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD11	9	0.25	0.07	0.25
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD12	9	0.25	0.07	0.25
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD13	9	0.25	0.07	0.25
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD11	9	0.25	0.07	0.25
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD12	9	0.25	0.07	0.25
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD13	9	0.25	0.07	0.25
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD11	9	0.25	0.07	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD12	9	0.25	0.07	0.25
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD13	9	0.25	0.07	0.25
(1,28)	1:102:A:GLU:HA	1:102:A:GLU:HG3	9	0.24	0.06	0.26
(1,770)	1:47:A:LEU:H	1:47:A:LEU:HB3	9	0.22	0.06	0.2
(1,1108)	1:65:A:ALA:HA	1:35:A:GLU:HB2	9	0.19	0.05	0.19
(1,679)	1:64:A:ARG:HB3	1:35:A:GLU:HG3	8	2.26	1.12	2.38
(1,1208)	1:59:A:THR:HG21	1:67:A:LYS:HB3	8	1.93	0.81	2.3
(1,1208)	1:59:A:THR:HG22	1:67:A:LYS:HB3	8	1.93	0.81	2.3
(1,1208)	1:59:A:THR:HG23	1:67:A:LYS:HB3	8	1.93	0.81	2.3
(1,1269)	1:78:A:GLY:H	1:72:A:LEU:H	8	1.66	0.55	1.66
(1,658)	1:51:A:ASP:HA	1:54:A:GLU:HG3	8	1.63	0.96	1.47
(1,332)	1:74:A:GLU:H	1:73:A:GLN:HG2	8	1.6	0.25	1.57
(1,5)	1:73:A:GLN:H	1:73:A:GLN:HG2	8	1.55	0.28	1.51
(1,756)	1:73:A:GLN:H	1:73:A:GLN:HE22	8	1.14	0.19	1.21
(1,1227)	1:10:A:GLU:H	1:11:A:GLU:HG2	8	1.1	0.99	0.74
(1,251)	1:74:A:GLU:H	1:74:A:GLU:HG3	8	0.91	0.41	1.04
(1,1068)	1:39:A:ASP:H	1:39:A:ASP:HB2	8	0.83	0.06	0.82
(1,628)	1:106:A:LEU:HB3	1:13:A:LEU:HB3	8	0.74	0.53	0.58
(1,719)	1:18:A:LYS:H	1:18:A:LYS:HD3	8	0.73	0.43	0.72
(1,250)	1:24:A:LEU:HD11	1:102:A:GLU:HB3	8	0.67	0.42	0.52
(1,250)	1:24:A:LEU:HD12	1:102:A:GLU:HB3	8	0.67	0.42	0.52
(1,250)	1:24:A:LEU:HD13	1:102:A:GLU:HB3	8	0.67	0.42	0.52
(1,726)	1:93:A:ASN:H	1:94:A:PHE:HB2	8	0.65	0.56	0.45
(1,995)	1:30:A:GLU:H	1:30:A:GLU:HB3	8	0.59	0.26	0.57
(1,600)	1:39:A:ASP:H	1:38:A:PHE:HB2	8	0.51	0.18	0.52
(1,1024)	1:39:A:ASP:H	1:38:A:PHE:HB2	8	0.51	0.18	0.52
(1,103)	1:47:A:LEU:H	1:48:A:SER:HA	8	0.49	0.15	0.5
(1,1191)	1:11:A:GLU:H	1:14:A:THR:H	8	0.44	0.12	0.47
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG21	8	0.34	0.08	0.32
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG22	8	0.34	0.08	0.32
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG23	8	0.34	0.08	0.32
(1,1176)	1:32:A:ILE:H	1:32:A:ILE:HG13	8	0.2	0.06	0.19
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD11	8	0.19	0.05	0.2
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD12	8	0.19	0.05	0.2
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD13	8	0.19	0.05	0.2
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD11	8	0.19	0.05	0.2
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD12	8	0.19	0.05	0.2
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD13	8	0.19	0.05	0.2
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD11	8	0.19	0.05	0.2
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD12	8	0.19	0.05	0.2
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD13	8	0.19	0.05	0.2
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG21	8	0.15	0.03	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG22	8	0.15	0.03	0.14
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG23	8	0.15	0.03	0.14
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG21	8	0.15	0.03	0.14
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG22	8	0.15	0.03	0.14
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG23	8	0.15	0.03	0.14
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG21	8	0.15	0.03	0.14
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG22	8	0.15	0.03	0.14
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG23	8	0.15	0.03	0.14
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG21	8	0.15	0.03	0.14
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG22	8	0.15	0.03	0.14
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG23	8	0.15	0.03	0.14
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG21	8	0.15	0.03	0.14
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG22	8	0.15	0.03	0.14
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG23	8	0.15	0.03	0.14
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG21	8	0.15	0.03	0.14
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG22	8	0.15	0.03	0.14
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG23	8	0.15	0.03	0.14
(1,964)	1:102:A:GLU:H	1:102:A:GLU:HB3	8	0.14	0.01	0.14
(1,669)	1:10:A:GLU:HG2	1:10:A:GLU:HA	8	0.12	0.01	0.12
(1,468)	1:77:A:LYS:HE3	1:77:A:LYS:HB2	7	1.3	0.55	1.34
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD11	7	0.85	0.37	0.89
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD12	7	0.85	0.37	0.89
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD13	7	0.85	0.37	0.89
(1,801)	1:89:A:GLU:H	1:88:A:ARG:HB2	7	0.82	0.22	0.9
(1,877)	1:55:A:ILE:HG21	1:68:A:LEU:HB3	7	0.8	0.53	0.68
(1,877)	1:55:A:ILE:HG22	1:68:A:LEU:HB3	7	0.8	0.53	0.68
(1,877)	1:55:A:ILE:HG23	1:68:A:LEU:HB3	7	0.8	0.53	0.68
(1,68)	1:54:A:GLU:HA	1:54:A:GLU:HG3	7	0.8	0.32	0.83
(1,265)	1:73:A:GLN:H	1:71:A:TYR:HA	7	0.74	0.77	0.27
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD21	7	0.74	0.25	0.84
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD22	7	0.74	0.25	0.84
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD23	7	0.74	0.25	0.84
(1,382)	1:54:A:GLU:H	1:54:A:GLU:HG3	7	0.73	0.32	0.92
(1,975)	1:54:A:GLU:H	1:54:A:GLU:HG3	7	0.73	0.32	0.92
(1,152)	1:16:A:VAL:H	1:106:A:LEU:HB2	7	0.55	0.39	0.42
(1,274)	1:115:A:LYS:H	1:114:A:LEU:HB3	7	0.52	0.37	0.57
(1,447)	1:31:A:LYS:H	1:32:A:ILE:HB	7	0.44	0.2	0.48
(1,180)	1:98:A:LYS:H	1:99:A:ILE:HG12	7	0.43	0.55	0.23
(1,942)	1:114:A:LEU:HD11	1:114:A:LEU:HB3	7	0.43	0.01	0.43
(1,942)	1:114:A:LEU:HD12	1:114:A:LEU:HB3	7	0.43	0.01	0.43
(1,942)	1:114:A:LEU:HD13	1:114:A:LEU:HB3	7	0.43	0.01	0.43
(1,620)	1:40:A:HIS:H	1:39:A:ASP:HB3	7	0.28	0.08	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG21	7	0.27	0.08	0.31
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG22	7	0.27	0.08	0.31
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG23	7	0.27	0.08	0.31
(1,935)	1:97:A:GLN:H	1:96:A:ILE:HG13	7	0.23	0.06	0.22
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG21	7	0.19	0.05	0.19
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG22	7	0.19	0.05	0.19
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG23	7	0.19	0.05	0.19
(1,1155)	1:71:A:TYR:HD1	1:68:A:LEU:HG	7	0.18	0.03	0.19
(1,1155)	1:71:A:TYR:HD2	1:68:A:LEU:HG	7	0.18	0.03	0.19
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD11	7	0.17	0.05	0.13
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD12	7	0.17	0.05	0.13
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD13	7	0.17	0.05	0.13
(1,308)	1:104:A:LEU:HA	1:13:A:LEU:HB2	7	0.16	0.05	0.15
(1,73)	1:115:A:LYS:H	1:114:A:LEU:H	6	1.5	0.13	1.54
(1,375)	1:114:A:LEU:H	1:115:A:LYS:H	6	1.5	0.13	1.54
(1,92)	1:42:A:ARG:HD2	1:41:A:LEU:HB3	6	1.13	0.43	1.16
(1,560)	1:22:A:GLU:H	1:22:A:GLU:HG2	6	1.08	0.06	1.08
(1,654)	1:29:A:CYS:H	1:30:A:GLU:HB3	6	0.93	0.1	0.94
(1,19)	1:82:A:LEU:HD21	1:46:A:ILE:HG13	6	0.79	0.6	0.6
(1,19)	1:82:A:LEU:HD22	1:46:A:ILE:HG13	6	0.79	0.6	0.6
(1,19)	1:82:A:LEU:HD23	1:46:A:ILE:HG13	6	0.79	0.6	0.6
(1,129)	1:74:A:GLU:H	1:73:A:GLN:HB3	6	0.67	0.33	0.72
(1,854)	1:54:A:GLU:H	1:53:A:ARG:HB3	6	0.63	0.24	0.69
(1,960)	1:28:A:LEU:H	1:28:A:LEU:HG	6	0.6	0.31	0.5
(1,863)	1:114:A:LEU:H	1:114:A:LEU:HB3	6	0.56	0.05	0.57
(1,74)	1:68:A:LEU:H	1:55:A:ILE:HB	6	0.51	0.37	0.43
(1,227)	1:98:A:LYS:H	1:97:A:GLN:HB2	6	0.43	0.14	0.39
(1,460)	1:50:A:GLU:HA	1:50:A:GLU:HG3	6	0.4	0.19	0.33
(1,452)	1:102:A:GLU:H	1:24:A:LEU:HD11	6	0.38	0.21	0.38
(1,452)	1:102:A:GLU:H	1:24:A:LEU:HD12	6	0.38	0.21	0.38
(1,452)	1:102:A:GLU:H	1:24:A:LEU:HD13	6	0.38	0.21	0.38
(1,339)	1:105:A:LYS:H	1:104:A:LEU:HB3	6	0.34	0.08	0.36
(1,1094)	1:89:A:GLU:H	1:88:A:ARG:HB3	6	0.32	0.14	0.26
(1,24)	1:52:A:THR:H	1:52:A:THR:HG21	6	0.26	0.08	0.26
(1,24)	1:52:A:THR:H	1:52:A:THR:HG22	6	0.26	0.08	0.26
(1,24)	1:52:A:THR:H	1:52:A:THR:HG23	6	0.26	0.08	0.26
(1,736)	1:49:A:ARG:HD2	1:49:A:ARG:HG3	6	0.18	0.02	0.18
(1,145)	1:16:A:VAL:H	1:16:A:VAL:HG21	6	0.16	0.06	0.16
(1,145)	1:16:A:VAL:H	1:16:A:VAL:HG22	6	0.16	0.06	0.16
(1,145)	1:16:A:VAL:H	1:16:A:VAL:HG23	6	0.16	0.06	0.16
(1,994)	1:40:A:HIS:H	1:40:A:HIS:HB3	6	0.16	0.03	0.16
(1,348)	1:109:A:ILE:HA	1:16:A:VAL:HG11	6	0.13	0.03	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,348)	1:109:A:ILE:HA	1:16:A:VAL:HG12	6	0.13	0.03	0.13
(1,348)	1:109:A:ILE:HA	1:16:A:VAL:HG13	6	0.13	0.03	0.13
(1,1160)	1:20:A:ALA:HB1	1:24:A:LEU:HD11	6	0.13	0.03	0.12
(1,1160)	1:20:A:ALA:HB1	1:24:A:LEU:HD12	6	0.13	0.03	0.12
(1,1160)	1:20:A:ALA:HB1	1:24:A:LEU:HD13	6	0.13	0.03	0.12
(1,1160)	1:20:A:ALA:HB2	1:24:A:LEU:HD11	6	0.13	0.03	0.12
(1,1160)	1:20:A:ALA:HB2	1:24:A:LEU:HD12	6	0.13	0.03	0.12
(1,1160)	1:20:A:ALA:HB2	1:24:A:LEU:HD13	6	0.13	0.03	0.12
(1,1160)	1:20:A:ALA:HB3	1:24:A:LEU:HD11	6	0.13	0.03	0.12
(1,1160)	1:20:A:ALA:HB3	1:24:A:LEU:HD12	6	0.13	0.03	0.12
(1,1160)	1:20:A:ALA:HB3	1:24:A:LEU:HD13	6	0.13	0.03	0.12
(1,632)	1:89:A:GLU:HB3	1:92:A:GLN:HB3	5	2.33	1.19	2.54
(1,438)	1:52:A:THR:H	1:47:A:LEU:HB3	5	1.79	1.31	1.34
(1,149)	1:78:A:GLY:H	1:21:A:LEU:HD11	5	1.59	0.67	2.0
(1,149)	1:78:A:GLY:H	1:21:A:LEU:HD12	5	1.59	0.67	2.0
(1,149)	1:78:A:GLY:H	1:21:A:LEU:HD13	5	1.59	0.67	2.0
(1,849)	1:78:A:GLY:H	1:75:A:ASN:HB3	5	1.07	0.32	0.9
(1,659)	1:63:A:LYS:H	1:62:A:ARG:HG3	5	0.81	0.22	0.77
(1,916)	1:36:A:ARG:H	1:36:A:ARG:HG3	5	0.81	0.3	0.82
(1,286)	1:85:A:SER:H	1:85:A:SER:HB3	5	0.79	0.02	0.78
(1,884)	1:89:A:GLU:H	1:89:A:GLU:HG2	5	0.79	0.25	0.75
(1,150)	1:31:A:LYS:H	1:31:A:LYS:HG2	5	0.7	0.28	0.79
(1,267)	1:95:A:LEU:H	1:95:A:LEU:HG	5	0.67	0.16	0.67
(1,727)	1:15:A:GLU:H	1:12:A:ASP:HA	5	0.65	0.28	0.55
(1,88)	1:108:A:ASN:H	1:107:A:ARG:HB3	5	0.61	0.14	0.58
(1,424)	1:11:A:GLU:H	1:11:A:GLU:HB2	5	0.61	0.17	0.68
(1,390)	1:96:A:ILE:H	1:95:A:LEU:HG	5	0.56	0.23	0.58
(1,817)	1:42:A:ARG:H	1:41:A:LEU:HB2	5	0.36	0.14	0.32
(1,470)	1:16:A:VAL:HG21	1:106:A:LEU:HB3	5	0.3	0.17	0.21
(1,470)	1:16:A:VAL:HG22	1:106:A:LEU:HB3	5	0.3	0.17	0.21
(1,470)	1:16:A:VAL:HG23	1:106:A:LEU:HB3	5	0.3	0.17	0.21
(1,791)	1:62:A:ARG:HB3	1:62:A:ARG:HG3	5	0.2	0.01	0.21
(1,565)	1:44:A:LYS:H	1:44:A:LYS:HD2	5	0.2	0.11	0.18
(1,619)	1:87:A:ARG:HA	1:96:A:ILE:HG21	5	0.18	0.06	0.18
(1,619)	1:87:A:ARG:HA	1:96:A:ILE:HG22	5	0.18	0.06	0.18
(1,619)	1:87:A:ARG:HA	1:96:A:ILE:HG23	5	0.18	0.06	0.18
(1,772)	1:71:A:TYR:HE1	1:55:A:ILE:HB	5	0.18	0.06	0.17
(1,772)	1:71:A:TYR:HE2	1:55:A:ILE:HB	5	0.18	0.06	0.17
(1,694)	1:36:A:ARG:H	1:36:A:ARG:HB3	5	0.18	0.05	0.15
(1,1034)	1:79:A:LEU:H	1:79:A:LEU:HB3	5	0.18	0.06	0.16
(1,350)	1:27:A:TYR:HE1	1:28:A:LEU:HB2	5	0.18	0.04	0.17
(1,350)	1:27:A:TYR:HE2	1:28:A:LEU:HB2	5	0.18	0.04	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,642)	1:73:A:GLN:HA	1:73:A:GLN:HG2	5	0.18	0.02	0.17
(1,956)	1:34:A:ALA:HB1	1:41:A:LEU:HD11	5	0.14	0.02	0.13
(1,956)	1:34:A:ALA:HB1	1:41:A:LEU:HD12	5	0.14	0.02	0.13
(1,956)	1:34:A:ALA:HB1	1:41:A:LEU:HD13	5	0.14	0.02	0.13
(1,956)	1:34:A:ALA:HB2	1:41:A:LEU:HD11	5	0.14	0.02	0.13
(1,956)	1:34:A:ALA:HB2	1:41:A:LEU:HD12	5	0.14	0.02	0.13
(1,956)	1:34:A:ALA:HB2	1:41:A:LEU:HD13	5	0.14	0.02	0.13
(1,956)	1:34:A:ALA:HB3	1:41:A:LEU:HD11	5	0.14	0.02	0.13
(1,956)	1:34:A:ALA:HB3	1:41:A:LEU:HD12	5	0.14	0.02	0.13
(1,956)	1:34:A:ALA:HB3	1:41:A:LEU:HD13	5	0.14	0.02	0.13
(1,1118)	1:72:A:LEU:HA	1:46:A:ILE:HG21	5	0.13	0.03	0.12
(1,1118)	1:72:A:LEU:HA	1:46:A:ILE:HG22	5	0.13	0.03	0.12
(1,1118)	1:72:A:LEU:HA	1:46:A:ILE:HG23	5	0.13	0.03	0.12
(1,705)	1:111:A:LEU:H	1:111:A:LEU:HB3	5	0.12	0.01	0.12
(1,745)	1:18:A:LYS:HE3	1:21:A:LEU:HD11	4	2.77	1.04	2.92
(1,745)	1:18:A:LYS:HE3	1:21:A:LEU:HD12	4	2.77	1.04	2.92
(1,745)	1:18:A:LYS:HE3	1:21:A:LEU:HD13	4	2.77	1.04	2.92
(1,1021)	1:92:A:GLN:HB2	1:89:A:GLU:HB3	4	2.39	0.7	2.45
(1,915)	1:21:A:LEU:HD11	1:79:A:LEU:HB3	4	1.19	1.43	0.44
(1,915)	1:21:A:LEU:HD12	1:79:A:LEU:HB3	4	1.19	1.43	0.44
(1,915)	1:21:A:LEU:HD13	1:79:A:LEU:HB3	4	1.19	1.43	0.44
(1,685)	1:53:A:ARG:H	1:56:A:SER:H	4	0.99	0.51	0.94
(1,1069)	1:38:A:PHE:H	1:36:A:ARG:H	4	0.98	0.25	0.84
(1,1035)	1:74:A:GLU:H	1:73:A:GLN:HG3	4	0.84	0.31	0.68
(1,687)	1:97:A:GLN:H	1:97:A:GLN:HB3	4	0.66	0.27	0.81
(1,1018)	1:50:A:GLU:H	1:51:A:ASP:HB2	4	0.53	0.34	0.38
(1,130)	1:16:A:VAL:H	1:13:A:LEU:HA	4	0.46	0.18	0.46
(1,520)	1:14:A:THR:H	1:11:A:GLU:HA	4	0.44	0.26	0.38
(1,402)	1:51:A:ASP:H	1:50:A:GLU:HB2	4	0.41	0.13	0.38
(1,955)	1:73:A:GLN:H	1:73:A:GLN:HB3	4	0.36	0.1	0.38
(1,364)	1:14:A:THR:H	1:14:A:THR:HB	4	0.26	0.09	0.29
(1,448)	1:47:A:LEU:H	1:46:A:ILE:H	4	0.24	0.03	0.24
(1,1198)	1:108:A:ASN:HD22	1:108:A:ASN:HB2	4	0.16	0.06	0.15
(1,1126)	1:53:A:ARG:H	1:53:A:ARG:HB3	4	0.15	0.03	0.15
(1,1283)	1:47:A:LEU:HD11	1:71:A:TYR:HB2	4	0.15	0.04	0.14
(1,1283)	1:47:A:LEU:HD12	1:71:A:TYR:HB2	4	0.15	0.04	0.14
(1,1283)	1:47:A:LEU:HD13	1:71:A:TYR:HB2	4	0.15	0.04	0.14
(1,523)	1:73:A:GLN:HE21	1:18:A:LYS:HE2	4	0.15	0.02	0.15
(1,469)	1:57:A:CYS:H	1:57:A:CYS:HB3	4	0.14	0.02	0.14
(1,533)	1:79:A:LEU:HD11	1:80:A:ASP:HA	4	0.14	0.04	0.12
(1,533)	1:79:A:LEU:HD12	1:80:A:ASP:HA	4	0.14	0.04	0.12
(1,533)	1:79:A:LEU:HD13	1:80:A:ASP:HA	4	0.14	0.04	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,65)	1:63:A:LYS:HE2	1:63:A:LYS:HD2	4	0.14	0.01	0.14
(1,361)	1:27:A:TYR:HD1	1:95:A:LEU:HD11	4	0.14	0.03	0.14
(1,361)	1:27:A:TYR:HD1	1:95:A:LEU:HD12	4	0.14	0.03	0.14
(1,361)	1:27:A:TYR:HD1	1:95:A:LEU:HD13	4	0.14	0.03	0.14
(1,361)	1:27:A:TYR:HD2	1:95:A:LEU:HD11	4	0.14	0.03	0.14
(1,361)	1:27:A:TYR:HD2	1:95:A:LEU:HD12	4	0.14	0.03	0.14
(1,361)	1:27:A:TYR:HD2	1:95:A:LEU:HD13	4	0.14	0.03	0.14
(1,930)	1:16:A:VAL:HG21	1:13:A:LEU:HA	4	0.13	0.01	0.13
(1,930)	1:16:A:VAL:HG22	1:13:A:LEU:HA	4	0.13	0.01	0.13
(1,930)	1:16:A:VAL:HG23	1:13:A:LEU:HA	4	0.13	0.01	0.13
(1,17)	1:31:A:LYS:HB2	1:31:A:LYS:HD2	4	0.1	0.0	0.1
(1,886)	1:96:A:ILE:HD11	1:89:A:GLU:HB2	3	1.75	2.14	0.24
(1,886)	1:96:A:ILE:HD12	1:89:A:GLU:HB2	3	1.75	2.14	0.24
(1,886)	1:96:A:ILE:HD13	1:89:A:GLU:HB2	3	1.75	2.14	0.24
(1,474)	1:71:A:TYR:HE1	1:55:A:ILE:H	3	0.66	0.35	0.88
(1,474)	1:71:A:TYR:HE2	1:55:A:ILE:H	3	0.66	0.35	0.88
(1,327)	1:63:A:LYS:HE3	1:63:A:LYS:HG2	3	0.59	0.2	0.71
(1,357)	1:107:A:ARG:H	1:106:A:LEU:HD21	3	0.5	0.23	0.61
(1,357)	1:107:A:ARG:H	1:106:A:LEU:HD22	3	0.5	0.23	0.61
(1,357)	1:107:A:ARG:H	1:106:A:LEU:HD23	3	0.5	0.23	0.61
(1,1246)	1:46:A:ILE:H	1:81:A:THR:HG21	3	0.49	0.19	0.61
(1,1246)	1:46:A:ILE:H	1:81:A:THR:HG22	3	0.49	0.19	0.61
(1,1246)	1:46:A:ILE:H	1:81:A:THR:HG23	3	0.49	0.19	0.61
(1,716)	1:99:A:ILE:H	1:98:A:LYS:HB3	3	0.3	0.19	0.2
(1,488)	1:49:A:ARG:HD2	1:49:A:ARG:HB2	3	0.28	0.09	0.34
(1,764)	1:32:A:ILE:HG13	1:69:A:LEU:HD21	3	0.28	0.11	0.35
(1,764)	1:32:A:ILE:HG13	1:69:A:LEU:HD22	3	0.28	0.11	0.35
(1,764)	1:32:A:ILE:HG13	1:69:A:LEU:HD23	3	0.28	0.11	0.35
(1,1258)	1:88:A:ARG:HA	1:88:A:ARG:HG3	3	0.24	0.04	0.24
(1,1029)	1:97:A:GLN:HG3	1:97:A:GLN:HB3	3	0.21	0.0	0.21
(1,319)	1:72:A:LEU:HD21	1:72:A:LEU:HA	3	0.2	0.07	0.21
(1,319)	1:72:A:LEU:HD22	1:72:A:LEU:HA	3	0.2	0.07	0.21
(1,319)	1:72:A:LEU:HD23	1:72:A:LEU:HA	3	0.2	0.07	0.21
(1,1220)	1:74:A:GLU:HG3	1:74:A:GLU:HB3	3	0.18	0.02	0.19
(1,1096)	1:69:A:LEU:HA	1:72:A:LEU:HD21	3	0.18	0.03	0.18
(1,1096)	1:69:A:LEU:HA	1:72:A:LEU:HD22	3	0.18	0.03	0.18
(1,1096)	1:69:A:LEU:HA	1:72:A:LEU:HD23	3	0.18	0.03	0.18
(1,1158)	1:78:A:GLY:HA3	1:72:A:LEU:HD21	3	0.18	0.09	0.14
(1,1158)	1:78:A:GLY:HA3	1:72:A:LEU:HD22	3	0.18	0.09	0.14
(1,1158)	1:78:A:GLY:HA3	1:72:A:LEU:HD23	3	0.18	0.09	0.14
(1,240)	1:34:A:ALA:HB1	1:35:A:GLU:HA	3	0.17	0.01	0.18
(1,240)	1:34:A:ALA:HB2	1:35:A:GLU:HA	3	0.17	0.01	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,240)	1:34:A:ALA:HB3	1:35:A:GLU:HA	3	0.17	0.01	0.18
(1,644)	1:79:A:LEU:HD11	1:82:A:LEU:HD21	3	0.17	0.04	0.14
(1,644)	1:79:A:LEU:HD11	1:82:A:LEU:HD22	3	0.17	0.04	0.14
(1,644)	1:79:A:LEU:HD11	1:82:A:LEU:HD23	3	0.17	0.04	0.14
(1,644)	1:79:A:LEU:HD12	1:82:A:LEU:HD21	3	0.17	0.04	0.14
(1,644)	1:79:A:LEU:HD12	1:82:A:LEU:HD22	3	0.17	0.04	0.14
(1,644)	1:79:A:LEU:HD12	1:82:A:LEU:HD23	3	0.17	0.04	0.14
(1,644)	1:79:A:LEU:HD13	1:82:A:LEU:HD21	3	0.17	0.04	0.14
(1,644)	1:79:A:LEU:HD13	1:82:A:LEU:HD22	3	0.17	0.04	0.14
(1,644)	1:79:A:LEU:HD13	1:82:A:LEU:HD23	3	0.17	0.04	0.14
(1,993)	1:10:A:GLU:HA	1:10:A:GLU:HB2	3	0.17	0.0	0.17
(1,1005)	1:82:A:LEU:HD11	1:72:A:LEU:HD21	3	0.17	0.05	0.16
(1,1005)	1:82:A:LEU:HD11	1:72:A:LEU:HD22	3	0.17	0.05	0.16
(1,1005)	1:82:A:LEU:HD11	1:72:A:LEU:HD23	3	0.17	0.05	0.16
(1,1005)	1:82:A:LEU:HD12	1:72:A:LEU:HD21	3	0.17	0.05	0.16
(1,1005)	1:82:A:LEU:HD12	1:72:A:LEU:HD22	3	0.17	0.05	0.16
(1,1005)	1:82:A:LEU:HD12	1:72:A:LEU:HD23	3	0.17	0.05	0.16
(1,1005)	1:82:A:LEU:HD13	1:72:A:LEU:HD21	3	0.17	0.05	0.16
(1,1005)	1:82:A:LEU:HD13	1:72:A:LEU:HD22	3	0.17	0.05	0.16
(1,1005)	1:82:A:LEU:HD13	1:72:A:LEU:HD23	3	0.17	0.05	0.16
(1,1224)	1:19:A:ASP:H	1:19:A:ASP:HB3	3	0.16	0.0	0.16
(1,779)	1:79:A:LEU:HD11	1:25:A:ARG:HB2	3	0.16	0.01	0.15
(1,779)	1:79:A:LEU:HD12	1:25:A:ARG:HB2	3	0.16	0.01	0.15
(1,779)	1:79:A:LEU:HD13	1:25:A:ARG:HB2	3	0.16	0.01	0.15
(1,1027)	1:49:A:ARG:HA	1:49:A:ARG:HB2	3	0.15	0.01	0.15
(1,1280)	1:24:A:LEU:HD21	1:24:A:LEU:HA	3	0.15	0.01	0.15
(1,1280)	1:24:A:LEU:HD22	1:24:A:LEU:HA	3	0.15	0.01	0.15
(1,1280)	1:24:A:LEU:HD23	1:24:A:LEU:HA	3	0.15	0.01	0.15
(1,205)	1:105:A:LYS:HA	1:105:A:LYS:HB2	3	0.15	0.0	0.15
(1,1017)	1:36:A:ARG:HA	1:36:A:ARG:HG3	3	0.15	0.04	0.15
(1,1194)	1:64:A:ARG:HA	1:63:A:LYS:HD2	3	0.14	0.02	0.16
(1,109)	1:71:A:TYR:HD1	1:68:A:LEU:HB2	3	0.14	0.01	0.14
(1,109)	1:71:A:TYR:HD2	1:68:A:LEU:HB2	3	0.14	0.01	0.14
(1,1083)	1:109:A:ILE:HG21	1:106:A:LEU:HA	3	0.14	0.03	0.13
(1,1083)	1:109:A:ILE:HG22	1:106:A:LEU:HA	3	0.14	0.03	0.13
(1,1083)	1:109:A:ILE:HG23	1:106:A:LEU:HA	3	0.14	0.03	0.13
(1,408)	1:84:A:GLU:HA	1:83:A:VAL:HG21	3	0.13	0.0	0.13
(1,408)	1:84:A:GLU:HA	1:83:A:VAL:HG22	3	0.13	0.0	0.13
(1,408)	1:84:A:GLU:HA	1:83:A:VAL:HG23	3	0.13	0.0	0.13
(1,680)	1:21:A:LEU:H	1:21:A:LEU:HB3	3	0.13	0.02	0.12
(1,71)	1:95:A:LEU:HD21	1:86:A:ILE:HD11	3	0.12	0.01	0.12
(1,71)	1:95:A:LEU:HD21	1:86:A:ILE:HD12	3	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,71)	1:95:A:LEU:HD21	1:86:A:ILE:HD13	3	0.12	0.01	0.12
(1,71)	1:95:A:LEU:HD22	1:86:A:ILE:HD11	3	0.12	0.01	0.12
(1,71)	1:95:A:LEU:HD22	1:86:A:ILE:HD12	3	0.12	0.01	0.12
(1,71)	1:95:A:LEU:HD22	1:86:A:ILE:HD13	3	0.12	0.01	0.12
(1,71)	1:95:A:LEU:HD23	1:86:A:ILE:HD11	3	0.12	0.01	0.12
(1,71)	1:95:A:LEU:HD23	1:86:A:ILE:HD12	3	0.12	0.01	0.12
(1,71)	1:95:A:LEU:HD23	1:86:A:ILE:HD13	3	0.12	0.01	0.12
(1,2)	1:32:A:ILE:H	1:32:A:ILE:HG12	3	0.12	0.02	0.11
(1,584)	1:79:A:LEU:HD21	1:69:A:LEU:HB2	3	0.11	0.01	0.11
(1,584)	1:79:A:LEU:HD22	1:69:A:LEU:HB2	3	0.11	0.01	0.11
(1,584)	1:79:A:LEU:HD23	1:69:A:LEU:HB2	3	0.11	0.01	0.11
(1,546)	1:89:A:GLU:H	1:89:A:GLU:HB3	3	0.11	0.0	0.11
(1,686)	1:56:A:SER:H	1:53:A:ARG:HA	2	2.09	0.14	2.09
(1,530)	1:59:A:THR:HG21	1:64:A:ARG:HG2	2	1.97	1.76	1.97
(1,530)	1:59:A:THR:HG22	1:64:A:ARG:HG2	2	1.97	1.76	1.97
(1,530)	1:59:A:THR:HG23	1:64:A:ARG:HG2	2	1.97	1.76	1.97
(1,540)	1:95:A:LEU:HA	1:99:A:ILE:HG13	2	1.66	0.95	1.66
(1,293)	1:47:A:LEU:HD11	1:51:A:ASP:HB3	2	1.56	0.56	1.56
(1,293)	1:47:A:LEU:HD12	1:51:A:ASP:HB3	2	1.56	0.56	1.56
(1,293)	1:47:A:LEU:HD13	1:51:A:ASP:HB3	2	1.56	0.56	1.56
(1,418)	1:33:A:ILE:HG21	1:65:A:ALA:HB1	2	1.19	1.05	1.19
(1,418)	1:33:A:ILE:HG21	1:65:A:ALA:HB2	2	1.19	1.05	1.19
(1,418)	1:33:A:ILE:HG21	1:65:A:ALA:HB3	2	1.19	1.05	1.19
(1,418)	1:33:A:ILE:HG22	1:65:A:ALA:HB1	2	1.19	1.05	1.19
(1,418)	1:33:A:ILE:HG22	1:65:A:ALA:HB2	2	1.19	1.05	1.19
(1,418)	1:33:A:ILE:HG22	1:65:A:ALA:HB3	2	1.19	1.05	1.19
(1,418)	1:33:A:ILE:HG23	1:65:A:ALA:HB1	2	1.19	1.05	1.19
(1,418)	1:33:A:ILE:HG23	1:65:A:ALA:HB2	2	1.19	1.05	1.19
(1,418)	1:33:A:ILE:HG23	1:65:A:ALA:HB3	2	1.19	1.05	1.19
(1,11)	1:81:A:THR:HG21	1:46:A:ILE:HG13	2	1.16	0.67	1.16
(1,11)	1:81:A:THR:HG22	1:46:A:ILE:HG13	2	1.16	0.67	1.16
(1,11)	1:81:A:THR:HG23	1:46:A:ILE:HG13	2	1.16	0.67	1.16
(1,442)	1:34:A:ALA:HB1	1:32:A:ILE:HG12	2	1.12	0.82	1.12
(1,442)	1:34:A:ALA:HB2	1:32:A:ILE:HG12	2	1.12	0.82	1.12
(1,442)	1:34:A:ALA:HB3	1:32:A:ILE:HG12	2	1.12	0.82	1.12
(1,284)	1:84:A:GLU:H	1:84:A:GLU:HB3	2	0.8	0.03	0.8
(1,1066)	1:72:A:LEU:H	1:72:A:LEU:HB2	2	0.76	0.01	0.76
(1,990)	1:101:A:ASP:H	1:97:A:GLN:HA	2	0.74	0.58	0.74
(1,224)	1:74:A:GLU:H	1:72:A:LEU:HA	2	0.64	0.16	0.64
(1,982)	1:71:A:TYR:H	1:73:A:GLN:H	2	0.64	0.15	0.64
(1,781)	1:21:A:LEU:HB3	1:24:A:LEU:HD21	2	0.62	0.47	0.62
(1,781)	1:21:A:LEU:HB3	1:24:A:LEU:HD22	2	0.62	0.47	0.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,781)	1:21:A:LEU:HB3	1:24:A:LEU:HD23	2	0.62	0.47	0.62
(1,564)	1:80:A:ASP:H	1:79:A:LEU:HB2	2	0.56	0.05	0.56
(1,298)	1:97:A:GLN:HA	1:97:A:GLN:HG3	2	0.52	0.26	0.52
(1,811)	1:47:A:LEU:H	1:46:A:ILE:HB	2	0.52	0.4	0.52
(1,802)	1:27:A:TYR:HE1	1:23:A:ASN:HB3	2	0.45	0.11	0.45
(1,802)	1:27:A:TYR:HE2	1:23:A:ASN:HB3	2	0.45	0.11	0.45
(1,148)	1:42:A:ARG:HD3	1:52:A:THR:HG21	2	0.44	0.29	0.44
(1,148)	1:42:A:ARG:HD3	1:52:A:THR:HG22	2	0.44	0.29	0.44
(1,148)	1:42:A:ARG:HD3	1:52:A:THR:HG23	2	0.44	0.29	0.44
(1,508)	1:106:A:LEU:HD11	1:106:A:LEU:HB3	2	0.42	0.01	0.42
(1,508)	1:106:A:LEU:HD12	1:106:A:LEU:HB3	2	0.42	0.01	0.42
(1,508)	1:106:A:LEU:HD13	1:106:A:LEU:HB3	2	0.42	0.01	0.42
(1,1278)	1:34:A:ALA:H	1:33:A:ILE:HA	2	0.39	0.08	0.39
(1,647)	1:73:A:GLN:HE21	1:73:A:GLN:HG3	2	0.33	0.22	0.33
(1,3)	1:56:A:SER:H	1:55:A:ILE:HG13	2	0.29	0.13	0.29
(1,1109)	1:83:A:VAL:HG11	1:86:A:ILE:HD11	2	0.24	0.08	0.24
(1,1109)	1:83:A:VAL:HG11	1:86:A:ILE:HD12	2	0.24	0.08	0.24
(1,1109)	1:83:A:VAL:HG11	1:86:A:ILE:HD13	2	0.24	0.08	0.24
(1,1109)	1:83:A:VAL:HG12	1:86:A:ILE:HD11	2	0.24	0.08	0.24
(1,1109)	1:83:A:VAL:HG12	1:86:A:ILE:HD12	2	0.24	0.08	0.24
(1,1109)	1:83:A:VAL:HG12	1:86:A:ILE:HD13	2	0.24	0.08	0.24
(1,1109)	1:83:A:VAL:HG13	1:86:A:ILE:HD11	2	0.24	0.08	0.24
(1,1109)	1:83:A:VAL:HG13	1:86:A:ILE:HD12	2	0.24	0.08	0.24
(1,1109)	1:83:A:VAL:HG13	1:86:A:ILE:HD13	2	0.24	0.08	0.24
(1,1032)	1:63:A:LYS:HE3	1:63:A:LYS:HD2	2	0.24	0.01	0.24
(1,259)	1:53:A:ARG:HA	1:53:A:ARG:HG3	2	0.23	0.01	0.23
(1,743)	1:47:A:LEU:HD11	1:47:A:LEU:HA	2	0.22	0.01	0.22
(1,743)	1:47:A:LEU:HD12	1:47:A:LEU:HA	2	0.22	0.01	0.22
(1,743)	1:47:A:LEU:HD13	1:47:A:LEU:HA	2	0.22	0.01	0.22
(1,937)	1:111:A:LEU:H	1:110:A:LYS:HG3	2	0.22	0.04	0.22
(1,1241)	1:96:A:ILE:HD11	1:93:A:ASN:HA	2	0.22	0.07	0.22
(1,1241)	1:96:A:ILE:HD12	1:93:A:ASN:HA	2	0.22	0.07	0.22
(1,1241)	1:96:A:ILE:HD13	1:93:A:ASN:HA	2	0.22	0.07	0.22
(1,246)	1:45:A:LYS:H	1:45:A:LYS:HG2	2	0.22	0.08	0.22
(1,943)	1:47:A:LEU:HD21	1:72:A:LEU:HD21	2	0.2	0.0	0.2
(1,943)	1:47:A:LEU:HD21	1:72:A:LEU:HD22	2	0.2	0.0	0.2
(1,943)	1:47:A:LEU:HD21	1:72:A:LEU:HD23	2	0.2	0.0	0.2
(1,943)	1:47:A:LEU:HD22	1:72:A:LEU:HD21	2	0.2	0.0	0.2
(1,943)	1:47:A:LEU:HD22	1:72:A:LEU:HD22	2	0.2	0.0	0.2
(1,943)	1:47:A:LEU:HD22	1:72:A:LEU:HD23	2	0.2	0.0	0.2
(1,943)	1:47:A:LEU:HD23	1:72:A:LEU:HD21	2	0.2	0.0	0.2
(1,943)	1:47:A:LEU:HD23	1:72:A:LEU:HD22	2	0.2	0.0	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,943)	1:47:A:LEU:HD23	1:72:A:LEU:HD23	2	0.2	0.0	0.2
(1,378)	1:83:A:VAL:HB	1:82:A:LEU:HB2	2	0.2	0.09	0.2
(1,1181)	1:19:A:ASP:H	1:16:A:VAL:HA	2	0.18	0.02	0.18
(1,153)	1:114:A:LEU:HD11	1:115:A:LYS:HA	2	0.18	0.06	0.18
(1,153)	1:114:A:LEU:HD12	1:115:A:LYS:HA	2	0.18	0.06	0.18
(1,153)	1:114:A:LEU:HD13	1:115:A:LYS:HA	2	0.18	0.06	0.18
(1,1111)	1:38:A:PHE:HD1	1:52:A:THR:HG21	2	0.18	0.06	0.18
(1,1111)	1:38:A:PHE:HD1	1:52:A:THR:HG22	2	0.18	0.06	0.18
(1,1111)	1:38:A:PHE:HD1	1:52:A:THR:HG23	2	0.18	0.06	0.18
(1,1111)	1:38:A:PHE:HD2	1:52:A:THR:HG21	2	0.18	0.06	0.18
(1,1111)	1:38:A:PHE:HD2	1:52:A:THR:HG22	2	0.18	0.06	0.18
(1,1111)	1:38:A:PHE:HD2	1:52:A:THR:HG23	2	0.18	0.06	0.18
(1,115)	1:16:A:VAL:HG21	1:15:A:GLU:HB2	2	0.16	0.06	0.16
(1,115)	1:16:A:VAL:HG22	1:15:A:GLU:HB2	2	0.16	0.06	0.16
(1,115)	1:16:A:VAL:HG23	1:15:A:GLU:HB2	2	0.16	0.06	0.16
(1,413)	1:79:A:LEU:H	1:79:A:LEU:HD11	2	0.15	0.02	0.15
(1,413)	1:79:A:LEU:H	1:79:A:LEU:HD12	2	0.15	0.02	0.15
(1,413)	1:79:A:LEU:H	1:79:A:LEU:HD13	2	0.15	0.02	0.15
(1,918)	1:49:A:ARG:HA	1:52:A:THR:HG21	2	0.15	0.03	0.15
(1,918)	1:49:A:ARG:HA	1:52:A:THR:HG22	2	0.15	0.03	0.15
(1,918)	1:49:A:ARG:HA	1:52:A:THR:HG23	2	0.15	0.03	0.15
(1,924)	1:87:A:ARG:HB2	1:84:A:GLU:HA	2	0.15	0.02	0.15
(1,113)	1:69:A:LEU:HD21	1:34:A:ALA:HB1	2	0.14	0.04	0.14
(1,113)	1:69:A:LEU:HD21	1:34:A:ALA:HB2	2	0.14	0.04	0.14
(1,113)	1:69:A:LEU:HD21	1:34:A:ALA:HB3	2	0.14	0.04	0.14
(1,113)	1:69:A:LEU:HD22	1:34:A:ALA:HB1	2	0.14	0.04	0.14
(1,113)	1:69:A:LEU:HD22	1:34:A:ALA:HB2	2	0.14	0.04	0.14
(1,113)	1:69:A:LEU:HD22	1:34:A:ALA:HB3	2	0.14	0.04	0.14
(1,113)	1:69:A:LEU:HD23	1:34:A:ALA:HB1	2	0.14	0.04	0.14
(1,113)	1:69:A:LEU:HD23	1:34:A:ALA:HB2	2	0.14	0.04	0.14
(1,113)	1:69:A:LEU:HD23	1:34:A:ALA:HB3	2	0.14	0.04	0.14
(1,1031)	1:65:A:ALA:HA	1:69:A:LEU:HG	2	0.14	0.01	0.14
(1,1104)	1:45:A:LYS:HG2	1:42:A:ARG:HA	2	0.14	0.02	0.14
(1,491)	1:70:A:ASP:H	1:70:A:ASP:HB3	2	0.13	0.01	0.13
(1,850)	1:73:A:GLN:HG2	1:79:A:LEU:HD11	2	0.13	0.03	0.13
(1,850)	1:73:A:GLN:HG2	1:79:A:LEU:HD12	2	0.13	0.03	0.13
(1,850)	1:73:A:GLN:HG2	1:79:A:LEU:HD13	2	0.13	0.03	0.13
(1,1207)	1:24:A:LEU:HD11	1:28:A:LEU:HG	2	0.13	0.02	0.13
(1,1207)	1:24:A:LEU:HD12	1:28:A:LEU:HG	2	0.13	0.02	0.13
(1,1207)	1:24:A:LEU:HD13	1:28:A:LEU:HG	2	0.13	0.02	0.13
(1,351)	1:81:A:THR:HG21	1:46:A:ILE:HG21	2	0.12	0.01	0.12
(1,351)	1:81:A:THR:HG21	1:46:A:ILE:HG22	2	0.12	0.01	0.12

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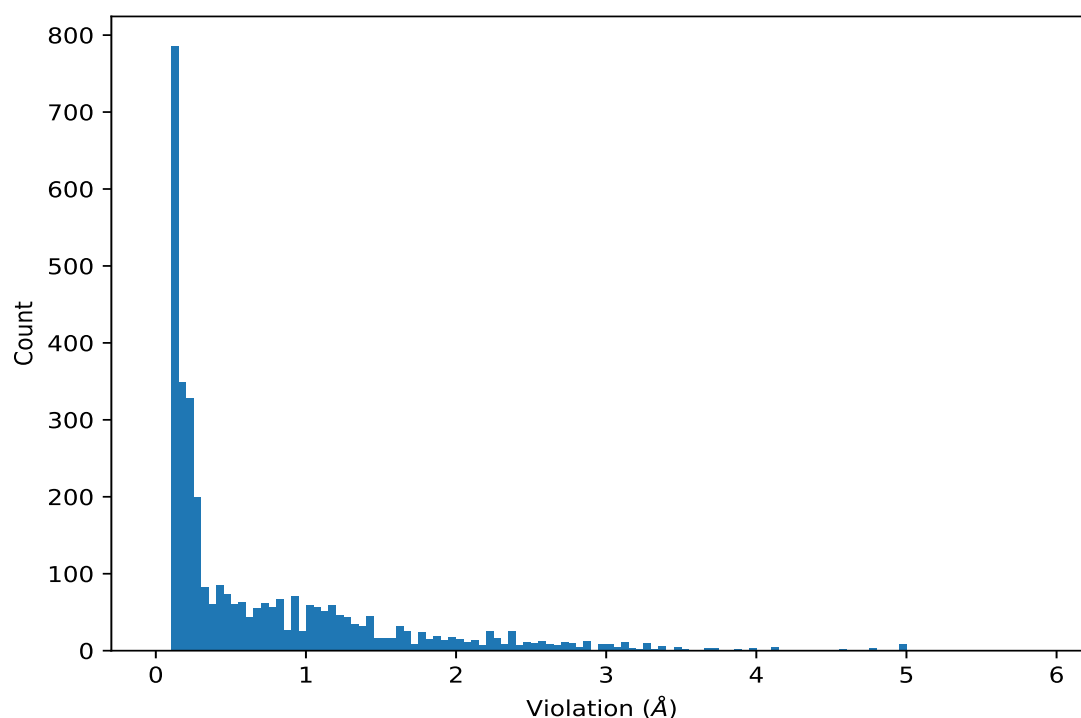
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,351)	1:81:A:THR:HG21	1:46:A:ILE:HG23	2	0.12	0.01	0.12
(1,351)	1:81:A:THR:HG22	1:46:A:ILE:HG21	2	0.12	0.01	0.12
(1,351)	1:81:A:THR:HG22	1:46:A:ILE:HG22	2	0.12	0.01	0.12
(1,351)	1:81:A:THR:HG22	1:46:A:ILE:HG23	2	0.12	0.01	0.12
(1,351)	1:81:A:THR:HG23	1:46:A:ILE:HG21	2	0.12	0.01	0.12
(1,351)	1:81:A:THR:HG23	1:46:A:ILE:HG22	2	0.12	0.01	0.12
(1,351)	1:81:A:THR:HG23	1:46:A:ILE:HG23	2	0.12	0.01	0.12
(1,132)	1:95:A:LEU:HD21	1:31:A:LYS:HB2	2	0.12	0.0	0.12
(1,132)	1:95:A:LEU:HD22	1:31:A:LYS:HB2	2	0.12	0.0	0.12
(1,132)	1:95:A:LEU:HD23	1:31:A:LYS:HB2	2	0.12	0.0	0.12
(1,314)	1:25:A:ARG:HA	1:69:A:LEU:HG	2	0.12	0.0	0.12
(1,197)	1:30:A:GLU:H	1:30:A:GLU:HA	2	0.11	0.0	0.11
(1,785)	1:112:A:GLU:H	1:112:A:GLU:HA	2	0.11	0.0	0.11
(1,1166)	1:14:A:THR:HG21	1:10:A:GLU:HB2	2	0.11	0.0	0.11
(1,1166)	1:14:A:THR:HG22	1:10:A:GLU:HB2	2	0.11	0.0	0.11
(1,1166)	1:14:A:THR:HG23	1:10:A:GLU:HB2	2	0.11	0.0	0.11

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)
(1,347)	1:64:A:ARG:H	1:35:A:GLU:HG3	4	5.93
(1,347)	1:64:A:ARG:H	1:35:A:GLU:HG3	5	5.08
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD11	10	4.98
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD12	10	4.98
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD13	10	4.98
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD11	10	4.98
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD12	10	4.98
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD13	10	4.98
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD11	10	4.98
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD12	10	4.98
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD13	10	4.98
(1,347)	1:64:A:ARG:H	1:35:A:GLU:HG3	8	4.94
(1,886)	1:96:A:ILE:HD11	1:89:A:GLU:HB2	5	4.78
(1,886)	1:96:A:ILE:HD12	1:89:A:GLU:HB2	5	4.78
(1,886)	1:96:A:ILE:HD13	1:89:A:GLU:HB2	5	4.78
(1,1167)	1:53:A:ARG:H	1:55:A:ILE:HG12	7	4.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:64:A:ARG:H	1:35:A:GLU:HG3	2	4.59
(1,1156)	1:75:A:ASN:H	1:18:A:LYS:HE3	7	4.55
(1,938)	1:102:A:GLU:HB3	1:106:A:LEU:HG	8	4.52
(1,952)	1:82:A:LEU:H	1:84:A:GLU:HB2	8	4.31
(1,1156)	1:75:A:ASN:H	1:18:A:LYS:HE3	8	4.29
(1,210)	1:74:A:GLU:H	1:70:A:ASP:HA	8	4.19
(1,755)	1:56:A:SER:H	1:64:A:ARG:HG3	1	4.14
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD21	4	4.12
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD22	4	4.12
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD23	4	4.12
(1,210)	1:74:A:GLU:H	1:70:A:ASP:HA	4	4.12
(1,1167)	1:53:A:ARG:H	1:55:A:ILE:HG12	8	4.01
(1,745)	1:18:A:LYS:HE3	1:21:A:LEU:HD11	10	3.96
(1,745)	1:18:A:LYS:HE3	1:21:A:LEU:HD12	10	3.96
(1,745)	1:18:A:LYS:HE3	1:21:A:LEU:HD13	10	3.96
(1,1156)	1:75:A:ASN:H	1:18:A:LYS:HE3	2	3.91
(1,755)	1:56:A:SER:H	1:64:A:ARG:HG3	7	3.89
(1,632)	1:89:A:GLU:HB3	1:92:A:GLN:HB3	5	3.88
(1,347)	1:64:A:ARG:H	1:35:A:GLU:HG3	7	3.77
(1,530)	1:59:A:THR:HG21	1:64:A:ARG:HG2	3	3.73
(1,530)	1:59:A:THR:HG22	1:64:A:ARG:HG2	3	3.73
(1,530)	1:59:A:THR:HG23	1:64:A:ARG:HG2	3	3.73
(1,915)	1:21:A:LEU:HD11	1:79:A:LEU:HB3	10	3.67
(1,915)	1:21:A:LEU:HD12	1:79:A:LEU:HB3	10	3.67
(1,915)	1:21:A:LEU:HD13	1:79:A:LEU:HB3	10	3.67
(1,679)	1:64:A:ARG:HB3	1:35:A:GLU:HG3	2	3.64
(1,210)	1:74:A:GLU:H	1:70:A:ASP:HA	10	3.59
(1,755)	1:56:A:SER:H	1:64:A:ARG:HG3	6	3.52
(1,679)	1:64:A:ARG:HB3	1:35:A:GLU:HG3	4	3.52
(1,745)	1:18:A:LYS:HE3	1:21:A:LEU:HD11	2	3.46
(1,745)	1:18:A:LYS:HE3	1:21:A:LEU:HD12	2	3.46
(1,745)	1:18:A:LYS:HE3	1:21:A:LEU:HD13	2	3.46
(1,666)	1:65:A:ALA:H	1:35:A:GLU:HG3	4	3.46
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD11	7	3.4
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD12	7	3.4
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD13	7	3.4
(1,1212)	1:55:A:ILE:H	1:51:A:ASP:HB3	7	3.39
(1,438)	1:52:A:THR:H	1:47:A:LEU:HB3	6	3.38
(1,658)	1:51:A:ASP:HA	1:54:A:GLU:HG3	2	3.36
(1,1227)	1:10:A:GLU:H	1:11:A:GLU:HG2	2	3.34
(1,347)	1:64:A:ARG:H	1:35:A:GLU:HG3	9	3.32
(1,438)	1:52:A:THR:H	1:47:A:LEU:HB3	4	3.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,210)	1:74:A:GLU:H	1:70:A:ASP:HA	9	3.3
(1,1021)	1:92:A:GLN:HB2	1:89:A:GLU:HB3	1	3.28
(1,755)	1:56:A:SER:H	1:64:A:ARG:HG3	8	3.28
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD11	10	3.27
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD12	10	3.27
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD13	10	3.27
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD21	5	3.25
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD22	5	3.25
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD23	5	3.25
(1,160)	1:70:A:ASP:H	1:71:A:TYR:HB2	3	3.24
(1,347)	1:64:A:ARG:H	1:35:A:GLU:HG3	6	3.21
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD11	6	3.16
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD12	6	3.16
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD13	6	3.16
(1,1208)	1:59:A:THR:HG21	1:67:A:LYS:HB3	2	3.15
(1,1208)	1:59:A:THR:HG22	1:67:A:LYS:HB3	2	3.15
(1,1208)	1:59:A:THR:HG23	1:67:A:LYS:HB3	2	3.15
(1,347)	1:64:A:ARG:H	1:35:A:GLU:HG3	10	3.15
(1,632)	1:89:A:GLU:HB3	1:92:A:GLN:HB3	1	3.14
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD11	3	3.12
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD12	3	3.12
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD13	3	3.12
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD11	7	3.11
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD12	7	3.11
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD13	7	3.11
(1,574)	1:67:A:LYS:H	1:68:A:LEU:HB2	4	3.09
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD11	5	3.09
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD12	5	3.09
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD13	5	3.09
(1,938)	1:102:A:GLU:HB3	1:106:A:LEU:HG	10	3.08
(1,861)	1:54:A:GLU:H	1:51:A:ASP:HB3	1	3.03
(1,666)	1:65:A:ALA:H	1:35:A:GLU:HG3	5	3.02
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD11	9	3.01
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD12	9	3.01
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD13	9	3.01
(1,655)	1:47:A:LEU:HD11	1:68:A:LEU:HB3	9	3.0
(1,655)	1:47:A:LEU:HD12	1:68:A:LEU:HB3	9	3.0
(1,655)	1:47:A:LEU:HD13	1:68:A:LEU:HB3	9	3.0
(1,861)	1:54:A:GLU:H	1:51:A:ASP:HB3	6	2.98
(1,679)	1:64:A:ARG:HB3	1:35:A:GLU:HG3	8	2.97
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD11	4	2.97
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD12	4	2.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD13	4	2.97
(1,655)	1:47:A:LEU:HD11	1:68:A:LEU:HB3	2	2.95
(1,655)	1:47:A:LEU:HD12	1:68:A:LEU:HB3	2	2.95
(1,655)	1:47:A:LEU:HD13	1:68:A:LEU:HB3	2	2.95
(1,574)	1:67:A:LYS:H	1:68:A:LEU:HB2	8	2.95
(1,160)	1:70:A:ASP:H	1:71:A:TYR:HB2	2	2.91
(1,861)	1:54:A:GLU:H	1:51:A:ASP:HB3	9	2.9
(1,666)	1:65:A:ALA:H	1:35:A:GLU:HG3	8	2.88
(1,666)	1:65:A:ALA:H	1:35:A:GLU:HG3	2	2.87
(1,655)	1:47:A:LEU:HD11	1:68:A:LEU:HB3	7	2.87
(1,655)	1:47:A:LEU:HD12	1:68:A:LEU:HB3	7	2.87
(1,655)	1:47:A:LEU:HD13	1:68:A:LEU:HB3	7	2.87
(1,160)	1:70:A:ASP:H	1:71:A:TYR:HB2	1	2.87
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD11	2	2.87
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD12	2	2.87
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD13	2	2.87
(1,933)	1:63:A:LYS:H	1:64:A:ARG:HB2	2	2.86
(1,160)	1:70:A:ASP:H	1:71:A:TYR:HB2	9	2.85
(1,861)	1:54:A:GLU:H	1:51:A:ASP:HB3	3	2.84
(1,997)	1:106:A:LEU:H	1:104:A:LEU:HB2	6	2.83
(1,574)	1:67:A:LYS:H	1:68:A:LEU:HB2	6	2.82
(1,160)	1:70:A:ASP:H	1:71:A:TYR:HB2	8	2.82
(1,1212)	1:55:A:ILE:H	1:51:A:ASP:HB3	2	2.8
(1,1167)	1:53:A:ARG:H	1:55:A:ILE:HG12	6	2.79
(1,933)	1:63:A:LYS:H	1:64:A:ARG:HB2	5	2.79
(1,861)	1:54:A:GLU:H	1:51:A:ASP:HB3	7	2.77
(1,655)	1:47:A:LEU:HD11	1:68:A:LEU:HB3	1	2.77
(1,655)	1:47:A:LEU:HD12	1:68:A:LEU:HB3	1	2.77
(1,655)	1:47:A:LEU:HD13	1:68:A:LEU:HB3	1	2.77
(1,933)	1:63:A:LYS:H	1:64:A:ARG:HB2	6	2.76
(1,861)	1:54:A:GLU:H	1:51:A:ASP:HB3	5	2.75
(1,160)	1:70:A:ASP:H	1:71:A:TYR:HB2	10	2.75
(1,210)	1:74:A:GLU:H	1:70:A:ASP:HA	6	2.74
(1,160)	1:70:A:ASP:H	1:71:A:TYR:HB2	7	2.74
(1,1021)	1:92:A:GLN:HB2	1:89:A:GLU:HB3	9	2.73
(1,1156)	1:75:A:ASN:H	1:18:A:LYS:HE3	6	2.71
(1,938)	1:102:A:GLU:HB3	1:106:A:LEU:HG	4	2.71
(1,131)	1:81:A:THR:HG21	1:72:A:LEU:HB3	4	2.71
(1,131)	1:81:A:THR:HG22	1:72:A:LEU:HB3	4	2.71
(1,131)	1:81:A:THR:HG23	1:72:A:LEU:HB3	4	2.71
(1,131)	1:81:A:THR:HG21	1:72:A:LEU:HB3	7	2.71
(1,131)	1:81:A:THR:HG22	1:72:A:LEU:HB3	7	2.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,131)	1:81:A:THR:HG23	1:72:A:LEU:HB3	7	2.71
(1,861)	1:54:A:GLU:H	1:51:A:ASP:HB3	8	2.69
(1,997)	1:106:A:LEU:H	1:104:A:LEU:HB2	8	2.68
(1,679)	1:64:A:ARG:HB3	1:35:A:GLU:HG3	5	2.67
(1,160)	1:70:A:ASP:H	1:71:A:TYR:HB2	4	2.67
(1,312)	1:107:A:ARG:H	1:110:A:LYS:HB2	2	2.66
(1,312)	1:107:A:ARG:H	1:110:A:LYS:HB2	9	2.66
(1,210)	1:74:A:GLU:H	1:70:A:ASP:HA	7	2.66
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD21	9	2.65
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD22	9	2.65
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD23	9	2.65
(1,312)	1:107:A:ARG:H	1:110:A:LYS:HB2	5	2.65
(1,997)	1:106:A:LEU:H	1:104:A:LEU:HB2	10	2.63
(1,540)	1:95:A:LEU:HA	1:99:A:ILE:HG13	4	2.61
(1,160)	1:70:A:ASP:H	1:71:A:TYR:HB2	6	2.61
(1,755)	1:56:A:SER:H	1:64:A:ARG:HG3	5	2.6
(1,658)	1:51:A:ASP:HA	1:54:A:GLU:HG3	1	2.59
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD11	8	2.59
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD12	8	2.59
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD13	8	2.59
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD21	6	2.58
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD22	6	2.58
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD23	6	2.58
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD21	6	2.57
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD22	6	2.57
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD23	6	2.57
(1,210)	1:74:A:GLU:H	1:70:A:ASP:HA	1	2.57
(1,1156)	1:75:A:ASN:H	1:18:A:LYS:HE3	10	2.56
(1,997)	1:106:A:LEU:H	1:104:A:LEU:HB2	3	2.54
(1,632)	1:89:A:GLU:HB3	1:92:A:GLN:HB3	9	2.54
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD21	5	2.54
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD22	5	2.54
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD23	5	2.54
(1,312)	1:107:A:ARG:H	1:110:A:LYS:HB2	4	2.54
(1,1269)	1:78:A:GLY:H	1:72:A:LEU:H	6	2.53
(1,872)	1:45:A:LYS:H	1:41:A:LEU:HA	7	2.52
(1,510)	1:97:A:GLN:HE22	1:97:A:GLN:HB3	10	2.52
(1,997)	1:106:A:LEU:H	1:104:A:LEU:HB2	5	2.5
(1,1167)	1:53:A:ARG:H	1:55:A:ILE:HG12	1	2.48
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD21	10	2.48
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD22	10	2.48
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD23	10	2.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD11	9	2.48
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD12	9	2.48
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD13	9	2.48
(1,131)	1:81:A:THR:HG21	1:72:A:LEU:HB3	3	2.47
(1,131)	1:81:A:THR:HG22	1:72:A:LEU:HB3	3	2.47
(1,131)	1:81:A:THR:HG23	1:72:A:LEU:HB3	3	2.47
(1,312)	1:107:A:ARG:H	1:110:A:LYS:HB2	6	2.46
(1,1208)	1:59:A:THR:HG21	1:67:A:LYS:HB3	6	2.44
(1,1208)	1:59:A:THR:HG22	1:67:A:LYS:HB3	6	2.44
(1,1208)	1:59:A:THR:HG23	1:67:A:LYS:HB3	6	2.44
(1,997)	1:106:A:LEU:H	1:104:A:LEU:HB2	7	2.43
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD21	1	2.41
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD22	1	2.41
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD23	1	2.41
(1,861)	1:54:A:GLU:H	1:51:A:ASP:HB3	10	2.4
(1,755)	1:56:A:SER:H	1:64:A:ARG:HG3	2	2.4
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD21	9	2.4
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD22	9	2.4
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD23	9	2.4
(1,987)	1:32:A:ILE:H	1:28:A:LEU:HB2	4	2.39
(1,861)	1:54:A:GLU:H	1:51:A:ASP:HB3	2	2.39
(1,666)	1:65:A:ALA:H	1:35:A:GLU:HG3	9	2.39
(1,1208)	1:59:A:THR:HG21	1:67:A:LYS:HB3	5	2.38
(1,1208)	1:59:A:THR:HG22	1:67:A:LYS:HB3	5	2.38
(1,1208)	1:59:A:THR:HG23	1:67:A:LYS:HB3	5	2.38
(1,745)	1:18:A:LYS:HE3	1:21:A:LEU:HD11	6	2.38
(1,745)	1:18:A:LYS:HE3	1:21:A:LEU:HD12	6	2.38
(1,745)	1:18:A:LYS:HE3	1:21:A:LEU:HD13	6	2.38
(1,347)	1:64:A:ARG:H	1:35:A:GLU:HG3	3	2.38
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD21	2	2.37
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD22	2	2.37
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD23	2	2.37
(1,1208)	1:59:A:THR:HG21	1:67:A:LYS:HB3	1	2.36
(1,1208)	1:59:A:THR:HG22	1:67:A:LYS:HB3	1	2.36
(1,1208)	1:59:A:THR:HG23	1:67:A:LYS:HB3	1	2.36
(1,312)	1:107:A:ARG:H	1:110:A:LYS:HB2	3	2.36
(1,131)	1:81:A:THR:HG21	1:72:A:LEU:HB3	5	2.35
(1,131)	1:81:A:THR:HG22	1:72:A:LEU:HB3	5	2.35
(1,131)	1:81:A:THR:HG23	1:72:A:LEU:HB3	5	2.35
(1,312)	1:107:A:ARG:H	1:110:A:LYS:HB2	7	2.34
(1,1167)	1:53:A:ARG:H	1:55:A:ILE:HG12	4	2.33
(1,938)	1:102:A:GLU:HB3	1:106:A:LEU:HG	6	2.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,574)	1:67:A:LYS:H	1:68:A:LEU:HB2	5	2.32
(1,510)	1:97:A:GLN:HE22	1:97:A:GLN:HB3	2	2.31
(1,312)	1:107:A:ARG:H	1:110:A:LYS:HB2	1	2.31
(1,131)	1:81:A:THR:HG21	1:72:A:LEU:HB3	6	2.31
(1,131)	1:81:A:THR:HG22	1:72:A:LEU:HB3	6	2.31
(1,131)	1:81:A:THR:HG23	1:72:A:LEU:HB3	6	2.31
(1,1212)	1:55:A:ILE:H	1:51:A:ASP:HB3	1	2.3
(1,574)	1:67:A:LYS:H	1:68:A:LEU:HB2	1	2.3
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD21	7	2.3
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD22	7	2.3
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD23	7	2.3
(1,510)	1:97:A:GLN:HE22	1:97:A:GLN:HB3	9	2.29
(1,278)	1:29:A:CYS:H	1:30:A:GLU:HB2	1	2.29
(1,872)	1:45:A:LYS:H	1:41:A:LEU:HA	2	2.28
(1,312)	1:107:A:ARG:H	1:110:A:LYS:HB2	8	2.28
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD11	5	2.28
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD12	5	2.28
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD13	5	2.28
(1,1269)	1:78:A:GLY:H	1:72:A:LEU:H	1	2.27
(1,278)	1:29:A:CYS:H	1:30:A:GLU:HB2	10	2.27
(1,997)	1:106:A:LEU:H	1:104:A:LEU:HB2	4	2.26
(1,510)	1:97:A:GLN:HE22	1:97:A:GLN:HB3	5	2.25
(1,1208)	1:59:A:THR:HG21	1:67:A:LYS:HB3	3	2.24
(1,1208)	1:59:A:THR:HG22	1:67:A:LYS:HB3	3	2.24
(1,1208)	1:59:A:THR:HG23	1:67:A:LYS:HB3	3	2.24
(1,418)	1:33:A:ILE:HG21	1:65:A:ALA:HB1	1	2.24
(1,418)	1:33:A:ILE:HG21	1:65:A:ALA:HB2	1	2.24
(1,418)	1:33:A:ILE:HG21	1:65:A:ALA:HB3	1	2.24
(1,418)	1:33:A:ILE:HG22	1:65:A:ALA:HB1	1	2.24
(1,418)	1:33:A:ILE:HG22	1:65:A:ALA:HB2	1	2.24
(1,418)	1:33:A:ILE:HG22	1:65:A:ALA:HB3	1	2.24
(1,418)	1:33:A:ILE:HG23	1:65:A:ALA:HB1	1	2.24
(1,418)	1:33:A:ILE:HG23	1:65:A:ALA:HB2	1	2.24
(1,418)	1:33:A:ILE:HG23	1:65:A:ALA:HB3	1	2.24
(1,131)	1:81:A:THR:HG21	1:72:A:LEU:HB3	9	2.24
(1,131)	1:81:A:THR:HG22	1:72:A:LEU:HB3	9	2.24
(1,131)	1:81:A:THR:HG23	1:72:A:LEU:HB3	9	2.24
(1,1156)	1:75:A:ASN:H	1:18:A:LYS:HE3	9	2.23
(1,1122)	1:97:A:GLN:H	1:99:A:ILE:HB	4	2.23
(1,686)	1:56:A:SER:H	1:53:A:ARG:HA	4	2.23
(1,1156)	1:75:A:ASN:H	1:18:A:LYS:HE3	3	2.21
(1,997)	1:106:A:LEU:H	1:104:A:LEU:HB2	1	2.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,872)	1:45:A:LYS:H	1:41:A:LEU:HA	5	2.21
(1,149)	1:78:A:GLY:H	1:21:A:LEU:HD11	9	2.21
(1,149)	1:78:A:GLY:H	1:21:A:LEU:HD12	9	2.21
(1,149)	1:78:A:GLY:H	1:21:A:LEU:HD13	9	2.21
(1,997)	1:106:A:LEU:H	1:104:A:LEU:HB2	9	2.2
(1,574)	1:67:A:LYS:H	1:68:A:LEU:HB2	10	2.19
(1,1021)	1:92:A:GLN:HB2	1:89:A:GLU:HB3	5	2.17
(1,997)	1:106:A:LEU:H	1:104:A:LEU:HB2	2	2.17
(1,574)	1:67:A:LYS:H	1:68:A:LEU:HB2	7	2.17
(1,1167)	1:53:A:ARG:H	1:55:A:ILE:HG12	9	2.16
(1,658)	1:51:A:ASP:HA	1:54:A:GLU:HG3	7	2.16
(1,574)	1:67:A:LYS:H	1:68:A:LEU:HB2	9	2.16
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD21	8	2.14
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD22	8	2.14
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD23	8	2.14
(1,1212)	1:55:A:ILE:H	1:51:A:ASP:HB3	8	2.13
(1,655)	1:47:A:LEU:HD11	1:68:A:LEU:HB3	8	2.13
(1,655)	1:47:A:LEU:HD12	1:68:A:LEU:HB3	8	2.13
(1,655)	1:47:A:LEU:HD13	1:68:A:LEU:HB3	8	2.13
(1,574)	1:67:A:LYS:H	1:68:A:LEU:HB2	2	2.13
(1,293)	1:47:A:LEU:HD11	1:51:A:ASP:HB3	4	2.12
(1,293)	1:47:A:LEU:HD12	1:51:A:ASP:HB3	4	2.12
(1,293)	1:47:A:LEU:HD13	1:51:A:ASP:HB3	4	2.12
(1,131)	1:81:A:THR:HG21	1:72:A:LEU:HB3	2	2.11
(1,131)	1:81:A:THR:HG22	1:72:A:LEU:HB3	2	2.11
(1,131)	1:81:A:THR:HG23	1:72:A:LEU:HB3	2	2.11
(1,1253)	1:54:A:GLU:H	1:57:A:CYS:H	8	2.09
(1,574)	1:67:A:LYS:H	1:68:A:LEU:HB2	3	2.09
(1,131)	1:81:A:THR:HG21	1:72:A:LEU:HB3	1	2.09
(1,131)	1:81:A:THR:HG22	1:72:A:LEU:HB3	1	2.09
(1,131)	1:81:A:THR:HG23	1:72:A:LEU:HB3	1	2.09
(1,1167)	1:53:A:ARG:H	1:55:A:ILE:HG12	2	2.08
(1,679)	1:64:A:ARG:HB3	1:35:A:GLU:HG3	10	2.08
(1,19)	1:82:A:LEU:HD21	1:46:A:ILE:HG13	10	2.07
(1,19)	1:82:A:LEU:HD22	1:46:A:ILE:HG13	10	2.07
(1,19)	1:82:A:LEU:HD23	1:46:A:ILE:HG13	10	2.07
(1,210)	1:74:A:GLU:H	1:70:A:ASP:HA	5	2.06
(1,726)	1:93:A:ASN:H	1:94:A:PHE:HB2	2	2.05
(1,312)	1:107:A:ARG:H	1:110:A:LYS:HB2	10	2.05
(1,510)	1:97:A:GLN:HE22	1:97:A:GLN:HB3	1	2.04
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD21	1	2.02
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD22	1	2.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD23	1	2.02
(1,1167)	1:53:A:ARG:H	1:55:A:ILE:HG12	3	2.01
(1,149)	1:78:A:GLY:H	1:21:A:LEU:HD11	2	2.01
(1,149)	1:78:A:GLY:H	1:21:A:LEU:HD12	2	2.01
(1,149)	1:78:A:GLY:H	1:21:A:LEU:HD13	2	2.01
(1,1212)	1:55:A:ILE:H	1:51:A:ASP:HB3	5	2.0
(1,1049)	1:74:A:GLU:H	1:74:A:GLU:HG2	8	2.0
(1,149)	1:78:A:GLY:H	1:21:A:LEU:HD11	3	2.0
(1,149)	1:78:A:GLY:H	1:21:A:LEU:HD12	3	2.0
(1,149)	1:78:A:GLY:H	1:21:A:LEU:HD13	3	2.0
(1,679)	1:64:A:ARG:HB3	1:35:A:GLU:HG3	9	1.99
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD21	4	1.99
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD22	4	1.99
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD23	4	1.99
(1,468)	1:77:A:LYS:HE3	1:77:A:LYS:HB2	2	1.99
(1,332)	1:74:A:GLU:H	1:73:A:GLN:HG2	7	1.99
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD21	2	1.98
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD22	2	1.98
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD23	2	1.98
(1,278)	1:29:A:CYS:H	1:30:A:GLU:HB2	2	1.98
(1,265)	1:73:A:GLN:H	1:71:A:TYR:HA	10	1.98
(1,468)	1:77:A:LYS:HE3	1:77:A:LYS:HB2	9	1.97
(1,1212)	1:55:A:ILE:H	1:51:A:ASP:HB3	9	1.96
(1,686)	1:56:A:SER:H	1:53:A:ARG:HA	6	1.96
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD21	3	1.96
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD22	3	1.96
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD23	3	1.96
(1,1269)	1:78:A:GLY:H	1:72:A:LEU:H	4	1.95
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD21	2	1.95
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD22	2	1.95
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD23	2	1.95
(1,1168)	1:54:A:GLU:H	1:56:A:SER:H	4	1.94
(1,1049)	1:74:A:GLU:H	1:74:A:GLU:HG2	1	1.94
(1,442)	1:34:A:ALA:HB1	1:32:A:ILE:HG12	10	1.93
(1,442)	1:34:A:ALA:HB2	1:32:A:ILE:HG12	10	1.93
(1,442)	1:34:A:ALA:HB3	1:32:A:ILE:HG12	10	1.93
(1,655)	1:47:A:LEU:HD11	1:68:A:LEU:HB3	4	1.91
(1,655)	1:47:A:LEU:HD12	1:68:A:LEU:HB3	4	1.91
(1,655)	1:47:A:LEU:HD13	1:68:A:LEU:HB3	4	1.91
(1,265)	1:73:A:GLN:H	1:71:A:TYR:HA	8	1.91
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD21	3	1.9
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD22	3	1.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD23	3	1.9
(1,1227)	1:10:A:GLU:H	1:11:A:GLU:HG2	6	1.89
(1,332)	1:74:A:GLU:H	1:73:A:GLN:HG2	2	1.88
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD11	3	1.87
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD12	3	1.87
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD13	3	1.87
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD11	3	1.87
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD12	3	1.87
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD13	3	1.87
(1,158)	1:66:A:GLY:H	1:67:A:LYS:HB3	6	1.87
(1,5)	1:73:A:GLN:H	1:73:A:GLN:HG2	7	1.87
(1,1253)	1:54:A:GLU:H	1:57:A:CYS:H	7	1.86
(1,913)	1:63:A:LYS:H	1:63:A:LYS:HD2	7	1.86
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD21	5	1.86
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD22	5	1.86
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD23	5	1.86
(1,5)	1:73:A:GLN:H	1:73:A:GLN:HG2	2	1.86
(1,880)	1:32:A:ILE:HD11	1:86:A:ILE:HG13	9	1.84
(1,880)	1:32:A:ILE:HD12	1:86:A:ILE:HG13	9	1.84
(1,880)	1:32:A:ILE:HD13	1:86:A:ILE:HG13	9	1.84
(1,5)	1:73:A:GLN:H	1:73:A:GLN:HG2	9	1.84
(1,987)	1:32:A:ILE:H	1:28:A:LEU:HB2	10	1.83
(1,11)	1:81:A:THR:HG21	1:46:A:ILE:HG13	7	1.83
(1,11)	1:81:A:THR:HG22	1:46:A:ILE:HG13	7	1.83
(1,11)	1:81:A:THR:HG23	1:46:A:ILE:HG13	7	1.83
(1,933)	1:63:A:LYS:H	1:64:A:ARG:HB2	3	1.82
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD21	2	1.81
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD22	2	1.81
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD23	2	1.81
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD11	10	1.8
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD12	10	1.8
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD13	10	1.8
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD21	9	1.79
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD22	9	1.79
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD23	9	1.79
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD21	6	1.79
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD22	6	1.79
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD23	6	1.79
(1,987)	1:32:A:ILE:H	1:28:A:LEU:HB2	3	1.79
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG21	8	1.79
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG22	8	1.79
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG23	8	1.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD11	1	1.79
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD12	1	1.79
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD13	1	1.79
(1,1168)	1:54:A:GLU:H	1:56:A:SER:H	6	1.78
(1,655)	1:47:A:LEU:HD11	1:68:A:LEU:HB3	6	1.78
(1,655)	1:47:A:LEU:HD12	1:68:A:LEU:HB3	6	1.78
(1,655)	1:47:A:LEU:HD13	1:68:A:LEU:HB3	6	1.78
(1,510)	1:97:A:GLN:HE22	1:97:A:GLN:HB3	8	1.78
(1,180)	1:98:A:LYS:H	1:99:A:ILE:HG12	4	1.78
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD21	7	1.76
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD22	7	1.76
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD23	7	1.76
(1,872)	1:45:A:LYS:H	1:41:A:LEU:HA	1	1.76
(1,332)	1:74:A:GLU:H	1:73:A:GLN:HG2	5	1.76
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD11	4	1.74
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD12	4	1.74
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD13	4	1.74
(1,922)	1:106:A:LEU:H	1:106:A:LEU:HG	4	1.74
(1,158)	1:66:A:GLY:H	1:67:A:LYS:HB3	1	1.74
(1,1269)	1:78:A:GLY:H	1:72:A:LEU:H	9	1.73
(1,92)	1:42:A:ARG:HD2	1:41:A:LEU:HB3	1	1.72
(1,169)	1:97:A:GLN:HE21	1:97:A:GLN:HB3	10	1.71
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD21	4	1.7
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD22	4	1.7
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD23	4	1.7
(1,502)	1:31:A:LYS:H	1:28:A:LEU:HB2	3	1.7
(1,430)	1:16:A:VAL:H	1:15:A:GLU:HG2	4	1.7
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD11	5	1.69
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD12	5	1.69
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD13	5	1.69
(1,250)	1:24:A:LEU:HD11	1:102:A:GLU:HB3	4	1.69
(1,250)	1:24:A:LEU:HD12	1:102:A:GLU:HB3	4	1.69
(1,250)	1:24:A:LEU:HD13	1:102:A:GLU:HB3	4	1.69
(1,1212)	1:55:A:ILE:H	1:51:A:ASP:HB3	3	1.68
(1,685)	1:53:A:ARG:H	1:56:A:SER:H	4	1.68
(1,666)	1:65:A:ALA:H	1:35:A:GLU:HG3	7	1.68
(1,658)	1:51:A:ASP:HA	1:54:A:GLU:HG3	3	1.68
(1,510)	1:97:A:GLN:HE22	1:97:A:GLN:HB3	4	1.68
(1,655)	1:47:A:LEU:HD11	1:68:A:LEU:HB3	3	1.67
(1,655)	1:47:A:LEU:HD12	1:68:A:LEU:HB3	3	1.67
(1,655)	1:47:A:LEU:HD13	1:68:A:LEU:HB3	3	1.67
(1,502)	1:31:A:LYS:H	1:28:A:LEU:HB2	8	1.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,880)	1:32:A:ILE:HD11	1:86:A:ILE:HG13	1	1.66
(1,880)	1:32:A:ILE:HD12	1:86:A:ILE:HG13	1	1.66
(1,880)	1:32:A:ILE:HD13	1:86:A:ILE:HG13	1	1.66
(1,628)	1:106:A:LEU:HB3	1:13:A:LEU:HB3	10	1.66
(1,21)	1:97:A:GLN:H	1:98:A:LYS:HB2	9	1.66
(1,952)	1:82:A:LEU:H	1:84:A:GLU:HB2	10	1.65
(1,872)	1:45:A:LYS:H	1:41:A:LEU:HA	10	1.65
(1,375)	1:114:A:LEU:H	1:115:A:LYS:H	7	1.65
(1,73)	1:115:A:LYS:H	1:114:A:LEU:H	7	1.65
(1,502)	1:31:A:LYS:H	1:28:A:LEU:HB2	1	1.64
(1,1059)	1:98:A:LYS:H	1:96:A:ILE:HB	6	1.63
(1,1049)	1:74:A:GLU:H	1:74:A:GLU:HG2	7	1.63
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD11	4	1.63
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD12	4	1.63
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD13	4	1.63
(1,952)	1:82:A:LEU:H	1:84:A:GLU:HB2	5	1.63
(1,849)	1:78:A:GLY:H	1:75:A:ASN:HB3	9	1.63
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD11	4	1.63
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD12	4	1.63
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD13	4	1.63
(1,430)	1:16:A:VAL:H	1:15:A:GLU:HG2	10	1.63
(1,1059)	1:98:A:LYS:H	1:96:A:ILE:HB	2	1.62
(1,169)	1:97:A:GLN:HE21	1:97:A:GLN:HB3	8	1.62
(1,861)	1:54:A:GLU:H	1:51:A:ASP:HB3	4	1.61
(1,632)	1:89:A:GLU:HB3	1:92:A:GLN:HB3	6	1.61
(1,510)	1:97:A:GLN:HE22	1:97:A:GLN:HB3	6	1.61
(1,375)	1:114:A:LEU:H	1:115:A:LYS:H	5	1.61
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB1	3	1.61
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB2	3	1.61
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB3	3	1.61
(1,73)	1:115:A:LYS:H	1:114:A:LEU:H	5	1.61
(1,21)	1:97:A:GLN:H	1:98:A:LYS:HB2	1	1.61
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD21	6	1.6
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD22	6	1.6
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD23	6	1.6
(1,278)	1:29:A:CYS:H	1:30:A:GLU:HB2	3	1.6
(1,21)	1:97:A:GLN:H	1:98:A:LYS:HB2	2	1.6
(1,666)	1:65:A:ALA:H	1:35:A:GLU:HG3	6	1.59
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG21	4	1.59
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG22	4	1.59
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG23	4	1.59
(1,1269)	1:78:A:GLY:H	1:72:A:LEU:H	2	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1049)	1:74:A:GLU:H	1:74:A:GLU:HG2	2	1.58
(1,375)	1:114:A:LEU:H	1:115:A:LYS:H	6	1.58
(1,347)	1:64:A:ARG:H	1:35:A:GLU:HG3	1	1.58
(1,332)	1:74:A:GLU:H	1:73:A:GLN:HG2	4	1.58
(1,73)	1:115:A:LYS:H	1:114:A:LEU:H	6	1.58
(1,877)	1:55:A:ILE:HG21	1:68:A:LEU:HB3	9	1.57
(1,877)	1:55:A:ILE:HG22	1:68:A:LEU:HB3	9	1.57
(1,877)	1:55:A:ILE:HG23	1:68:A:LEU:HB3	9	1.57
(1,430)	1:16:A:VAL:H	1:15:A:GLU:HG2	1	1.57
(1,332)	1:74:A:GLU:H	1:73:A:GLN:HG2	6	1.56
(1,1059)	1:98:A:LYS:H	1:96:A:ILE:HB	9	1.55
(1,987)	1:32:A:ILE:H	1:28:A:LEU:HB2	1	1.54
(1,5)	1:73:A:GLN:H	1:73:A:GLN:HG2	6	1.54
(1,510)	1:97:A:GLN:HE22	1:97:A:GLN:HB3	7	1.53
(1,1049)	1:74:A:GLU:H	1:74:A:GLU:HG2	10	1.51
(1,880)	1:32:A:ILE:HD11	1:86:A:ILE:HG13	10	1.51
(1,880)	1:32:A:ILE:HD12	1:86:A:ILE:HG13	10	1.51
(1,880)	1:32:A:ILE:HD13	1:86:A:ILE:HG13	10	1.51
(1,872)	1:45:A:LYS:H	1:41:A:LEU:HA	4	1.51
(1,375)	1:114:A:LEU:H	1:115:A:LYS:H	2	1.51
(1,83)	1:88:A:ARG:H	1:87:A:ARG:HB2	8	1.51
(1,73)	1:115:A:LYS:H	1:114:A:LEU:H	2	1.51
(1,1059)	1:98:A:LYS:H	1:96:A:ILE:HB	1	1.5
(1,468)	1:77:A:LYS:HE3	1:77:A:LYS:HB2	1	1.5
(1,430)	1:16:A:VAL:H	1:15:A:GLU:HG2	8	1.5
(1,332)	1:74:A:GLU:H	1:73:A:GLN:HG2	1	1.5
(1,178)	1:105:A:LYS:H	1:105:A:LYS:HD2	10	1.5
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG21	2	1.49
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG22	2	1.49
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG23	2	1.49
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD21	4	1.49
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD22	4	1.49
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD23	4	1.49
(1,251)	1:74:A:GLU:H	1:74:A:GLU:HG3	8	1.49
(1,1167)	1:53:A:ARG:H	1:55:A:ILE:HG12	5	1.48
(1,5)	1:73:A:GLN:H	1:73:A:GLN:HG2	3	1.48
(1,1253)	1:54:A:GLU:H	1:57:A:CYS:H	6	1.47
(1,719)	1:18:A:LYS:H	1:18:A:LYS:HD3	10	1.47
(1,430)	1:16:A:VAL:H	1:15:A:GLU:HG2	6	1.47
(1,83)	1:88:A:ARG:H	1:87:A:ARG:HB2	4	1.47
(1,1059)	1:98:A:LYS:H	1:96:A:ILE:HB	5	1.46
(1,1059)	1:98:A:LYS:H	1:96:A:ILE:HB	10	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,607)	1:19:A:ASP:H	1:18:A:LYS:HB2	3	1.46
(1,1269)	1:78:A:GLY:H	1:72:A:LEU:H	7	1.45
(1,1059)	1:98:A:LYS:H	1:96:A:ILE:HB	3	1.45
(1,160)	1:70:A:ASP:H	1:71:A:TYR:HB2	5	1.45
(1,83)	1:88:A:ARG:H	1:87:A:ARG:HB2	10	1.45
(1,21)	1:97:A:GLN:H	1:98:A:LYS:HB2	6	1.45
(1,5)	1:73:A:GLN:H	1:73:A:GLN:HG2	5	1.45
(1,952)	1:82:A:LEU:H	1:84:A:GLU:HB2	3	1.44
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD21	8	1.44
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD22	8	1.44
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD23	8	1.44
(1,210)	1:74:A:GLU:H	1:70:A:ASP:HA	2	1.44
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB1	2	1.44
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB2	2	1.44
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB3	2	1.44
(1,1088)	1:101:A:ASP:H	1:99:A:ILE:HB	4	1.43
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD21	3	1.43
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD22	3	1.43
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD23	3	1.43
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD21	8	1.43
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD22	8	1.43
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD23	8	1.43
(1,922)	1:106:A:LEU:H	1:106:A:LEU:HG	7	1.43
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG21	1	1.43
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG22	1	1.43
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG23	1	1.43
(1,628)	1:106:A:LEU:HB3	1:13:A:LEU:HB3	7	1.43
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD11	4	1.43
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD12	4	1.43
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD13	4	1.43
(1,92)	1:42:A:ARG:HD2	1:41:A:LEU:HB3	8	1.43
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD11	8	1.42
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD12	8	1.42
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD13	8	1.42
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD11	7	1.42
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD12	7	1.42
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD13	7	1.42
(1,913)	1:63:A:LYS:H	1:63:A:LYS:HD2	9	1.42
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD11	7	1.42
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD12	7	1.42
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD13	7	1.42
(1,430)	1:16:A:VAL:H	1:15:A:GLU:HG2	9	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,210)	1:74:A:GLU:H	1:70:A:ASP:HA	3	1.42
(1,1069)	1:38:A:PHE:H	1:36:A:ARG:H	1	1.41
(1,1059)	1:98:A:LYS:H	1:96:A:ILE:HB	7	1.41
(1,933)	1:63:A:LYS:H	1:64:A:ARG:HB2	7	1.41
(1,880)	1:32:A:ILE:HD11	1:86:A:ILE:HG13	8	1.4
(1,880)	1:32:A:ILE:HD12	1:86:A:ILE:HG13	8	1.4
(1,880)	1:32:A:ILE:HD13	1:86:A:ILE:HG13	8	1.4
(1,430)	1:16:A:VAL:H	1:15:A:GLU:HG2	3	1.4
(1,6)	1:27:A:TYR:H	1:23:A:ASN:HB2	8	1.4
(1,938)	1:102:A:GLU:HB3	1:106:A:LEU:HG	3	1.39
(1,68)	1:54:A:GLU:HA	1:54:A:GLU:HG3	6	1.39
(1,1021)	1:92:A:GLN:HB2	1:89:A:GLU:HB3	6	1.38
(1,922)	1:106:A:LEU:H	1:106:A:LEU:HG	2	1.38
(1,922)	1:106:A:LEU:H	1:106:A:LEU:HG	10	1.38
(1,607)	1:19:A:ASP:H	1:18:A:LYS:HB2	7	1.38
(1,430)	1:16:A:VAL:H	1:15:A:GLU:HG2	5	1.38
(1,178)	1:105:A:LYS:H	1:105:A:LYS:HD2	1	1.38
(1,1253)	1:54:A:GLU:H	1:57:A:CYS:H	4	1.37
(1,1035)	1:74:A:GLU:H	1:73:A:GLN:HG3	5	1.37
(1,948)	1:20:A:ALA:H	1:18:A:LYS:HB2	2	1.37
(1,948)	1:20:A:ALA:H	1:18:A:LYS:HB2	3	1.37
(1,922)	1:106:A:LEU:H	1:106:A:LEU:HG	1	1.37
(1,149)	1:78:A:GLY:H	1:21:A:LEU:HD11	6	1.37
(1,149)	1:78:A:GLY:H	1:21:A:LEU:HD12	6	1.37
(1,149)	1:78:A:GLY:H	1:21:A:LEU:HD13	6	1.37
(1,5)	1:73:A:GLN:H	1:73:A:GLN:HG2	1	1.37
(1,607)	1:19:A:ASP:H	1:18:A:LYS:HB2	2	1.36
(1,332)	1:74:A:GLU:H	1:73:A:GLN:HG2	3	1.36
(1,877)	1:55:A:ILE:HG21	1:68:A:LEU:HB3	3	1.35
(1,877)	1:55:A:ILE:HG22	1:68:A:LEU:HB3	3	1.35
(1,877)	1:55:A:ILE:HG23	1:68:A:LEU:HB3	3	1.35
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG21	5	1.35
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG22	5	1.35
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG23	5	1.35
(1,375)	1:114:A:LEU:H	1:115:A:LYS:H	3	1.35
(1,73)	1:115:A:LYS:H	1:114:A:LEU:H	3	1.35
(1,468)	1:77:A:LYS:HE3	1:77:A:LYS:HB2	6	1.34
(1,438)	1:52:A:THR:H	1:47:A:LEU:HB3	7	1.34
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD11	2	1.34
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD12	2	1.34
(1,321)	1:17:A:LYS:H	1:106:A:LEU:HD13	2	1.34
(1,922)	1:106:A:LEU:H	1:106:A:LEU:HG	3	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,922)	1:106:A:LEU:H	1:106:A:LEU:HG	9	1.33
(1,756)	1:73:A:GLN:H	1:73:A:GLN:HE22	9	1.33
(1,178)	1:105:A:LYS:H	1:105:A:LYS:HD2	7	1.33
(1,169)	1:97:A:GLN:HE21	1:97:A:GLN:HB3	9	1.33
(1,21)	1:97:A:GLN:H	1:98:A:LYS:HB2	3	1.33
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD21	7	1.32
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD22	7	1.32
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD23	7	1.32
(1,990)	1:101:A:ASP:H	1:97:A:GLN:HA	10	1.32
(1,987)	1:32:A:ILE:H	1:28:A:LEU:HB2	8	1.32
(1,938)	1:102:A:GLU:HB3	1:106:A:LEU:HG	2	1.32
(1,933)	1:63:A:LYS:H	1:64:A:ARG:HB2	1	1.32
(1,922)	1:106:A:LEU:H	1:106:A:LEU:HG	8	1.32
(1,913)	1:63:A:LYS:H	1:63:A:LYS:HD2	3	1.32
(1,178)	1:105:A:LYS:H	1:105:A:LYS:HD2	3	1.32
(1,1122)	1:97:A:GLN:H	1:99:A:ILE:HB	8	1.31
(1,375)	1:114:A:LEU:H	1:115:A:LYS:H	9	1.31
(1,185)	1:46:A:ILE:H	1:44:A:LYS:HB3	4	1.31
(1,83)	1:88:A:ARG:H	1:87:A:ARG:HB2	6	1.31
(1,73)	1:115:A:LYS:H	1:114:A:LEU:H	9	1.31
(1,1059)	1:98:A:LYS:H	1:96:A:ILE:HB	4	1.3
(1,1013)	1:64:A:ARG:H	1:62:A:ARG:HB3	2	1.3
(1,948)	1:20:A:ALA:H	1:18:A:LYS:HB2	7	1.3
(1,927)	1:14:A:THR:H	1:12:A:ASP:HB2	9	1.3
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG21	3	1.3
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG22	3	1.3
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG23	3	1.3
(1,502)	1:31:A:LYS:H	1:28:A:LEU:HB2	6	1.3
(1,74)	1:68:A:LEU:H	1:55:A:ILE:HB	9	1.3
(1,756)	1:73:A:GLN:H	1:73:A:GLN:HE22	2	1.29
(1,685)	1:53:A:ARG:H	1:56:A:SER:H	6	1.29
(1,635)	1:32:A:ILE:H	1:31:A:LYS:HB2	3	1.29
(1,599)	1:88:A:ARG:H	1:88:A:ARG:HG3	1	1.29
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB1	8	1.29
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB2	8	1.29
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB3	8	1.29
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB1	9	1.29
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB2	9	1.29
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB3	9	1.29
(1,948)	1:20:A:ALA:H	1:18:A:LYS:HB2	6	1.28
(1,913)	1:63:A:LYS:H	1:63:A:LYS:HD2	2	1.28
(1,666)	1:65:A:ALA:H	1:35:A:GLU:HG3	3	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,599)	1:88:A:ARG:H	1:88:A:ARG:HG3	5	1.28
(1,450)	1:108:A:ASN:HD22	1:108:A:ASN:HB3	7	1.28
(1,83)	1:88:A:ARG:H	1:87:A:ARG:HB2	2	1.28
(1,745)	1:18:A:LYS:HE3	1:21:A:LEU:HD11	7	1.27
(1,745)	1:18:A:LYS:HE3	1:21:A:LEU:HD12	7	1.27
(1,745)	1:18:A:LYS:HE3	1:21:A:LEU:HD13	7	1.27
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD11	3	1.27
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD12	3	1.27
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD13	3	1.27
(1,1277)	1:107:A:ARG:H	1:106:A:LEU:HB3	6	1.26
(1,658)	1:51:A:ASP:HA	1:54:A:GLU:HG3	10	1.26
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD21	6	1.26
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD22	6	1.26
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD23	6	1.26
(1,251)	1:74:A:GLU:H	1:74:A:GLU:HG3	10	1.26
(1,152)	1:16:A:VAL:H	1:106:A:LEU:HB2	4	1.26
(1,83)	1:88:A:ARG:H	1:87:A:ARG:HB2	3	1.26
(1,1208)	1:59:A:THR:HG21	1:67:A:LYS:HB3	7	1.25
(1,1208)	1:59:A:THR:HG22	1:67:A:LYS:HB3	7	1.25
(1,1208)	1:59:A:THR:HG23	1:67:A:LYS:HB3	7	1.25
(1,938)	1:102:A:GLU:HB3	1:106:A:LEU:HG	1	1.25
(1,927)	1:14:A:THR:H	1:12:A:ASP:HB2	3	1.25
(1,922)	1:106:A:LEU:H	1:106:A:LEU:HG	6	1.25
(1,756)	1:73:A:GLN:H	1:73:A:GLN:HE22	5	1.25
(1,534)	1:92:A:GLN:HE22	1:92:A:GLN:HG3	10	1.25
(1,450)	1:108:A:ASN:HD22	1:108:A:ASN:HB3	3	1.25
(1,450)	1:108:A:ASN:HD22	1:108:A:ASN:HB3	6	1.25
(1,178)	1:105:A:LYS:H	1:105:A:LYS:HD2	4	1.25
(1,169)	1:97:A:GLN:HE21	1:97:A:GLN:HB3	2	1.25
(1,169)	1:97:A:GLN:HE21	1:97:A:GLN:HB3	4	1.25
(1,21)	1:97:A:GLN:H	1:98:A:LYS:HB2	5	1.25
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD11	1	1.24
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD12	1	1.24
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD13	1	1.24
(1,756)	1:73:A:GLN:H	1:73:A:GLN:HE22	3	1.24
(1,534)	1:92:A:GLN:HE22	1:92:A:GLN:HG3	8	1.24
(1,534)	1:92:A:GLN:HE22	1:92:A:GLN:HG3	9	1.24
(1,502)	1:31:A:LYS:H	1:28:A:LEU:HB2	7	1.24
(1,450)	1:108:A:ASN:HD22	1:108:A:ASN:HB3	1	1.24
(1,450)	1:108:A:ASN:HD22	1:108:A:ASN:HB3	2	1.24
(1,450)	1:108:A:ASN:HD22	1:108:A:ASN:HB3	4	1.24
(1,450)	1:108:A:ASN:HD22	1:108:A:ASN:HB3	8	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,450)	1:108:A:ASN:HD22	1:108:A:ASN:HB3	10	1.24
(1,8)	1:42:A:ARG:H	1:45:A:LYS:HG2	7	1.24
(1,8)	1:42:A:ARG:H	1:45:A:LYS:HG2	9	1.24
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD11	8	1.23
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD12	8	1.23
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD13	8	1.23
(1,1052)	1:23:A:ASN:HD22	1:23:A:ASN:HB3	7	1.23
(1,952)	1:82:A:LEU:H	1:84:A:GLU:HB2	7	1.23
(1,450)	1:108:A:ASN:HD22	1:108:A:ASN:HB3	5	1.23
(1,1277)	1:107:A:ARG:H	1:106:A:LEU:HB3	5	1.22
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD11	5	1.22
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD12	5	1.22
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD13	5	1.22
(1,987)	1:32:A:ILE:H	1:28:A:LEU:HB2	6	1.22
(1,933)	1:63:A:LYS:H	1:64:A:ARG:HB2	10	1.22
(1,922)	1:106:A:LEU:H	1:106:A:LEU:HG	5	1.22
(1,913)	1:63:A:LYS:H	1:63:A:LYS:HD2	1	1.22
(1,913)	1:63:A:LYS:H	1:63:A:LYS:HD2	6	1.22
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD11	5	1.22
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD12	5	1.22
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD13	5	1.22
(1,719)	1:18:A:LYS:H	1:18:A:LYS:HD3	5	1.22
(1,534)	1:92:A:GLN:HE22	1:92:A:GLN:HG3	1	1.22
(1,502)	1:31:A:LYS:H	1:28:A:LEU:HB2	10	1.22
(1,21)	1:97:A:GLN:H	1:98:A:LYS:HB2	7	1.22
(1,21)	1:97:A:GLN:H	1:98:A:LYS:HB2	8	1.22
(1,8)	1:42:A:ARG:H	1:45:A:LYS:HG2	1	1.22
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD11	1	1.21
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD12	1	1.21
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD13	1	1.21
(1,933)	1:63:A:LYS:H	1:64:A:ARG:HB2	9	1.21
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD11	1	1.21
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD12	1	1.21
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD13	1	1.21
(1,534)	1:92:A:GLN:HE22	1:92:A:GLN:HG3	5	1.21
(1,1052)	1:23:A:ASN:HD22	1:23:A:ASN:HB3	1	1.2
(1,755)	1:56:A:SER:H	1:64:A:ARG:HG3	9	1.2
(1,534)	1:92:A:GLN:HE22	1:92:A:GLN:HG3	6	1.2
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD21	10	1.2
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD22	10	1.2
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD23	10	1.2
(1,332)	1:74:A:GLU:H	1:73:A:GLN:HG2	9	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:42:A:ARG:H	1:45:A:LYS:HG2	2	1.2
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD11	3	1.19
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD12	3	1.19
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD13	3	1.19
(1,920)	1:88:A:ARG:H	1:88:A:ARG:HG2	2	1.19
(1,913)	1:63:A:LYS:H	1:63:A:LYS:HD2	5	1.19
(1,913)	1:63:A:LYS:H	1:63:A:LYS:HD2	8	1.19
(1,849)	1:78:A:GLY:H	1:75:A:ASN:HB3	8	1.19
(1,756)	1:73:A:GLN:H	1:73:A:GLN:HE22	6	1.19
(1,502)	1:31:A:LYS:H	1:28:A:LEU:HB2	5	1.19
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB1	7	1.19
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB2	7	1.19
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB3	7	1.19
(1,158)	1:66:A:GLY:H	1:67:A:LYS:HB3	7	1.19
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD11	8	1.19
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD12	8	1.19
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD13	8	1.19
(1,8)	1:42:A:ARG:H	1:45:A:LYS:HG2	10	1.19
(1,1013)	1:64:A:ARG:H	1:62:A:ARG:HB3	9	1.18
(1,987)	1:32:A:ILE:H	1:28:A:LEU:HB2	7	1.18
(1,920)	1:88:A:ARG:H	1:88:A:ARG:HG2	7	1.18
(1,920)	1:88:A:ARG:H	1:88:A:ARG:HG2	8	1.18
(1,877)	1:55:A:ILE:HG21	1:68:A:LEU:HB3	7	1.18
(1,877)	1:55:A:ILE:HG22	1:68:A:LEU:HB3	7	1.18
(1,877)	1:55:A:ILE:HG23	1:68:A:LEU:HB3	7	1.18
(1,92)	1:42:A:ARG:HD2	1:41:A:LEU:HB3	3	1.18
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD11	9	1.17
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD12	9	1.17
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD13	9	1.17
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD11	2	1.17
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD12	2	1.17
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD13	2	1.17
(1,948)	1:20:A:ALA:H	1:18:A:LYS:HB2	4	1.17
(1,913)	1:63:A:LYS:H	1:63:A:LYS:HD2	10	1.17
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD11	2	1.17
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD12	2	1.17
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD13	2	1.17
(1,169)	1:97:A:GLN:HE21	1:97:A:GLN:HB3	5	1.17
(1,95)	1:27:A:TYR:HE1	1:102:A:GLU:HG3	8	1.17
(1,95)	1:27:A:TYR:HE2	1:102:A:GLU:HG3	8	1.17
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD21	10	1.16
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD22	10	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD23	10	1.16
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD21	1	1.16
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD22	1	1.16
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD23	1	1.16
(1,948)	1:20:A:ALA:H	1:18:A:LYS:HB2	10	1.16
(1,756)	1:73:A:GLN:H	1:73:A:GLN:HE22	7	1.16
(1,607)	1:19:A:ASP:H	1:18:A:LYS:HB2	10	1.16
(1,502)	1:31:A:LYS:H	1:28:A:LEU:HB2	4	1.16
(1,468)	1:77:A:LYS:HE3	1:77:A:LYS:HB2	4	1.16
(1,8)	1:42:A:ARG:H	1:45:A:LYS:HG2	6	1.16
(1,1277)	1:107:A:ARG:H	1:106:A:LEU:HB3	9	1.15
(1,1167)	1:53:A:ARG:H	1:55:A:ILE:HG12	10	1.15
(1,1122)	1:97:A:GLN:H	1:99:A:ILE:HB	5	1.15
(1,872)	1:45:A:LYS:H	1:41:A:LEU:HA	9	1.15
(1,560)	1:22:A:GLU:H	1:22:A:GLU:HG2	1	1.15
(1,560)	1:22:A:GLU:H	1:22:A:GLU:HG2	9	1.15
(1,502)	1:31:A:LYS:H	1:28:A:LEU:HB2	2	1.15
(1,251)	1:74:A:GLU:H	1:74:A:GLU:HG3	1	1.15
(1,185)	1:46:A:ILE:H	1:44:A:LYS:HB3	3	1.15
(1,92)	1:42:A:ARG:HD2	1:41:A:LEU:HB3	5	1.15
(1,8)	1:42:A:ARG:H	1:45:A:LYS:HG2	3	1.15
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD11	9	1.14
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD12	9	1.14
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD13	9	1.14
(1,916)	1:36:A:ARG:H	1:36:A:ARG:HG3	2	1.14
(1,169)	1:97:A:GLN:HE21	1:97:A:GLN:HB3	7	1.14
(1,8)	1:42:A:ARG:H	1:45:A:LYS:HG2	8	1.14
(1,1277)	1:107:A:ARG:H	1:106:A:LEU:HB3	10	1.13
(1,1227)	1:10:A:GLU:H	1:11:A:GLU:HG2	1	1.13
(1,938)	1:102:A:GLU:HB3	1:106:A:LEU:HG	7	1.13
(1,927)	1:14:A:THR:H	1:12:A:ASP:HB2	4	1.13
(1,884)	1:89:A:GLU:H	1:89:A:GLU:HG2	9	1.13
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB1	4	1.13
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB2	4	1.13
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB3	4	1.13
(1,8)	1:42:A:ARG:H	1:45:A:LYS:HG2	5	1.13
(1,920)	1:88:A:ARG:H	1:88:A:ARG:HG2	1	1.12
(1,913)	1:63:A:LYS:H	1:63:A:LYS:HD2	4	1.12
(1,431)	1:87:A:ARG:H	1:86:A:ILE:HB	5	1.12
(1,169)	1:97:A:GLN:HE21	1:97:A:GLN:HB3	6	1.12
(1,1018)	1:50:A:GLU:H	1:51:A:ASP:HB2	5	1.11
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG21	2	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG22	2	1.11
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG23	2	1.11
(1,1277)	1:107:A:ARG:H	1:106:A:LEU:HB3	3	1.1
(1,960)	1:28:A:LEU:H	1:28:A:LEU:HG	4	1.1
(1,927)	1:14:A:THR:H	1:12:A:ASP:HB2	8	1.1
(1,920)	1:88:A:ARG:H	1:88:A:ARG:HG2	6	1.1
(1,560)	1:22:A:GLU:H	1:22:A:GLU:HG2	2	1.1
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD21	1	1.1
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD22	1	1.1
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD23	1	1.1
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD21	7	1.1
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD22	7	1.1
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD23	7	1.1
(1,274)	1:115:A:LYS:H	1:114:A:LEU:HB3	10	1.1
(1,241)	1:12:A:ASP:H	1:13:A:LEU:HA	6	1.1
(1,150)	1:31:A:LYS:H	1:31:A:LYS:HG2	3	1.1
(1,83)	1:88:A:ARG:H	1:87:A:ARG:HB2	7	1.1
(1,21)	1:97:A:GLN:H	1:98:A:LYS:HB2	4	1.1
(1,6)	1:27:A:TYR:H	1:23:A:ASN:HB2	7	1.1
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD11	9	1.09
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD12	9	1.09
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD13	9	1.09
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD11	9	1.09
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD12	9	1.09
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD13	9	1.09
(1,781)	1:21:A:LEU:HB3	1:24:A:LEU:HD21	10	1.09
(1,781)	1:21:A:LEU:HB3	1:24:A:LEU:HD22	10	1.09
(1,781)	1:21:A:LEU:HB3	1:24:A:LEU:HD23	10	1.09
(1,654)	1:29:A:CYS:H	1:30:A:GLU:HB3	7	1.09
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG21	1	1.09
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG22	1	1.09
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG23	1	1.09
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB1	5	1.09
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB2	5	1.09
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB3	5	1.09
(1,6)	1:27:A:TYR:H	1:23:A:ASN:HB2	6	1.09
(1,1277)	1:107:A:ARG:H	1:106:A:LEU:HB3	8	1.08
(1,659)	1:63:A:LYS:H	1:62:A:ARG:HG3	2	1.08
(1,185)	1:46:A:ILE:H	1:44:A:LYS:HB3	7	1.08
(1,131)	1:81:A:THR:HG21	1:72:A:LEU:HB3	8	1.08
(1,131)	1:81:A:THR:HG22	1:72:A:LEU:HB3	8	1.08
(1,131)	1:81:A:THR:HG23	1:72:A:LEU:HB3	8	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,948)	1:20:A:ALA:H	1:18:A:LYS:HB2	9	1.07
(1,938)	1:102:A:GLU:HB3	1:106:A:LEU:HG	5	1.07
(1,916)	1:36:A:ARG:H	1:36:A:ARG:HG3	3	1.07
(1,801)	1:89:A:GLU:H	1:88:A:ARG:HB2	6	1.07
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG21	2	1.07
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG22	2	1.07
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG23	2	1.07
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD21	8	1.07
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD22	8	1.07
(1,500)	1:36:A:ARG:H	1:68:A:LEU:HD23	8	1.07
(1,21)	1:97:A:GLN:H	1:98:A:LYS:HB2	10	1.07
(1,1052)	1:23:A:ASN:HD22	1:23:A:ASN:HB3	6	1.06
(1,948)	1:20:A:ALA:H	1:18:A:LYS:HB2	5	1.06
(1,755)	1:56:A:SER:H	1:64:A:ARG:HG3	10	1.06
(1,635)	1:32:A:ILE:H	1:31:A:LYS:HB2	4	1.06
(1,635)	1:32:A:ILE:H	1:31:A:LYS:HB2	10	1.06
(1,560)	1:22:A:GLU:H	1:22:A:GLU:HG2	8	1.06
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD21	3	1.06
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD22	3	1.06
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD23	3	1.06
(1,1211)	1:71:A:TYR:HD1	1:68:A:LEU:HB3	4	1.05
(1,1211)	1:71:A:TYR:HD2	1:68:A:LEU:HB3	4	1.05
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD11	2	1.05
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD12	2	1.05
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD13	2	1.05
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD11	7	1.05
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD12	7	1.05
(1,1152)	1:72:A:LEU:H	1:79:A:LEU:HD13	7	1.05
(1,872)	1:45:A:LYS:H	1:41:A:LEU:HA	6	1.05
(1,659)	1:63:A:LYS:H	1:62:A:ARG:HG3	4	1.05
(1,560)	1:22:A:GLU:H	1:22:A:GLU:HG2	7	1.05
(1,524)	1:86:A:ILE:H	1:86:A:ILE:HG12	5	1.05
(1,251)	1:74:A:GLU:H	1:74:A:GLU:HG3	7	1.05
(1,6)	1:27:A:TYR:H	1:23:A:ASN:HB2	5	1.05
(1,1211)	1:71:A:TYR:HD1	1:68:A:LEU:HB3	6	1.04
(1,1211)	1:71:A:TYR:HD2	1:68:A:LEU:HB3	6	1.04
(1,1168)	1:54:A:GLU:H	1:56:A:SER:H	8	1.04
(1,1165)	1:26:A:VAL:H	1:26:A:VAL:HG21	1	1.04
(1,1165)	1:26:A:VAL:H	1:26:A:VAL:HG22	1	1.04
(1,1165)	1:26:A:VAL:H	1:26:A:VAL:HG23	1	1.04
(1,927)	1:14:A:THR:H	1:12:A:ASP:HB2	1	1.04
(1,801)	1:89:A:GLU:H	1:88:A:ARG:HB2	7	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,727)	1:15:A:GLU:H	1:12:A:ASP:HA	9	1.04
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG21	6	1.04
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG22	6	1.04
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG23	6	1.04
(1,599)	1:88:A:ARG:H	1:88:A:ARG:HG3	3	1.04
(1,278)	1:29:A:CYS:H	1:30:A:GLU:HB2	7	1.04
(1,129)	1:74:A:GLU:H	1:73:A:GLN:HB3	10	1.04
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD11	6	1.03
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD12	6	1.03
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD13	6	1.03
(1,938)	1:102:A:GLU:HB3	1:106:A:LEU:HG	9	1.03
(1,927)	1:14:A:THR:H	1:12:A:ASP:HB2	10	1.03
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD11	6	1.03
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD12	6	1.03
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD13	6	1.03
(1,371)	1:71:A:TYR:H	1:71:A:TYR:HB2	8	1.03
(1,1277)	1:107:A:ARG:H	1:106:A:LEU:HB3	7	1.02
(1,1269)	1:78:A:GLY:H	1:72:A:LEU:H	3	1.02
(1,1211)	1:71:A:TYR:HD1	1:68:A:LEU:HB3	10	1.02
(1,1211)	1:71:A:TYR:HD2	1:68:A:LEU:HB3	10	1.02
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD21	5	1.02
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD22	5	1.02
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD23	5	1.02
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG21	3	1.02
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG22	3	1.02
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG23	3	1.02
(1,552)	1:99:A:ILE:H	1:99:A:ILE:HG13	4	1.02
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD21	5	1.02
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD22	5	1.02
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD23	5	1.02
(1,251)	1:74:A:GLU:H	1:74:A:GLU:HG3	2	1.02
(1,185)	1:46:A:ILE:H	1:44:A:LYS:HB3	2	1.02
(1,101)	1:99:A:ILE:H	1:99:A:ILE:HG13	4	1.02
(1,679)	1:64:A:ARG:HB3	1:35:A:GLU:HG3	6	1.01
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG21	6	1.01
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG22	6	1.01
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG23	6	1.01
(1,510)	1:97:A:GLN:HE22	1:97:A:GLN:HB3	3	1.01
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD21	1	1.01
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD22	1	1.01
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD23	1	1.01
(1,110)	1:11:A:GLU:H	1:10:A:GLU:HG2	7	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:42:A:ARG:H	1:45:A:LYS:HG2	4	1.01
(1,6)	1:27:A:TYR:H	1:23:A:ASN:HB2	2	1.01
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD11	4	1.0
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD12	4	1.0
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD13	4	1.0
(1,1122)	1:97:A:GLN:H	1:99:A:ILE:HB	10	1.0
(1,293)	1:47:A:LEU:HD11	1:51:A:ASP:HB3	6	1.0
(1,293)	1:47:A:LEU:HD12	1:51:A:ASP:HB3	6	1.0
(1,293)	1:47:A:LEU:HD13	1:51:A:ASP:HB3	6	1.0
(1,1052)	1:23:A:ASN:HD22	1:23:A:ASN:HB3	8	0.99
(1,801)	1:89:A:GLU:H	1:88:A:ARG:HB2	1	0.99
(1,756)	1:73:A:GLN:H	1:73:A:GLN:HE22	4	0.99
(1,654)	1:29:A:CYS:H	1:30:A:GLU:HB3	10	0.99
(1,599)	1:88:A:ARG:H	1:88:A:ARG:HG3	8	0.99
(1,450)	1:108:A:ASN:HD22	1:108:A:ASN:HB3	9	0.99
(1,5)	1:73:A:GLN:H	1:73:A:GLN:HG2	4	0.99
(1,560)	1:22:A:GLU:H	1:22:A:GLU:HG2	10	0.98
(1,152)	1:16:A:VAL:H	1:106:A:LEU:HB2	2	0.98
(1,92)	1:42:A:ARG:HD2	1:41:A:LEU:HB3	2	0.98
(1,975)	1:54:A:GLU:H	1:54:A:GLU:HG3	10	0.97
(1,920)	1:88:A:ARG:H	1:88:A:ARG:HG2	5	0.97
(1,654)	1:29:A:CYS:H	1:30:A:GLU:HB3	8	0.97
(1,628)	1:106:A:LEU:HB3	1:13:A:LEU:HB3	6	0.97
(1,607)	1:19:A:ASP:H	1:18:A:LYS:HB2	4	0.97
(1,444)	1:46:A:ILE:H	1:45:A:LYS:HB2	4	0.97
(1,382)	1:54:A:GLU:H	1:54:A:GLU:HG3	10	0.97
(1,241)	1:12:A:ASP:H	1:13:A:LEU:HA	8	0.97
(1,129)	1:74:A:GLU:H	1:73:A:GLN:HB3	8	0.97
(1,1122)	1:97:A:GLN:H	1:99:A:ILE:HB	7	0.96
(1,1052)	1:23:A:ASN:HD22	1:23:A:ASN:HB3	2	0.96
(1,927)	1:14:A:THR:H	1:12:A:ASP:HB2	2	0.96
(1,920)	1:88:A:ARG:H	1:88:A:ARG:HG2	3	0.96
(1,371)	1:71:A:TYR:H	1:71:A:TYR:HB2	2	0.96
(1,371)	1:71:A:TYR:H	1:71:A:TYR:HB2	3	0.96
(1,1052)	1:23:A:ASN:HD22	1:23:A:ASN:HB3	3	0.95
(1,1013)	1:64:A:ARG:H	1:62:A:ARG:HB3	3	0.95
(1,987)	1:32:A:ILE:H	1:28:A:LEU:HB2	5	0.95
(1,884)	1:89:A:GLU:H	1:89:A:GLU:HG2	8	0.95
(1,666)	1:65:A:ALA:H	1:35:A:GLU:HG3	10	0.95
(1,599)	1:88:A:ARG:H	1:88:A:ARG:HG3	9	0.95
(1,118)	1:97:A:GLN:H	1:97:A:GLN:HB2	8	0.95
(1,68)	1:54:A:GLU:HA	1:54:A:GLU:HG3	5	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1208)	1:59:A:THR:HG21	1:67:A:LYS:HB3	8	0.94
(1,1208)	1:59:A:THR:HG22	1:67:A:LYS:HB3	8	0.94
(1,1208)	1:59:A:THR:HG23	1:67:A:LYS:HB3	8	0.94
(1,1168)	1:54:A:GLU:H	1:56:A:SER:H	7	0.94
(1,1168)	1:54:A:GLU:H	1:56:A:SER:H	9	0.94
(1,1068)	1:39:A:ASP:H	1:39:A:ASP:HB2	10	0.94
(1,975)	1:54:A:GLU:H	1:54:A:GLU:HG3	1	0.94
(1,975)	1:54:A:GLU:H	1:54:A:GLU:HG3	5	0.94
(1,948)	1:20:A:ALA:H	1:18:A:LYS:HB2	8	0.94
(1,920)	1:88:A:ARG:H	1:88:A:ARG:HG2	9	0.94
(1,854)	1:54:A:GLU:H	1:53:A:ARG:HB3	1	0.94
(1,599)	1:88:A:ARG:H	1:88:A:ARG:HG3	7	0.94
(1,444)	1:46:A:ILE:H	1:45:A:LYS:HB2	9	0.94
(1,382)	1:54:A:GLU:H	1:54:A:GLU:HG3	1	0.94
(1,382)	1:54:A:GLU:H	1:54:A:GLU:HG3	5	0.94
(1,371)	1:71:A:TYR:H	1:71:A:TYR:HB2	7	0.94
(1,1211)	1:71:A:TYR:HD1	1:68:A:LEU:HB3	8	0.93
(1,1211)	1:71:A:TYR:HD2	1:68:A:LEU:HB3	8	0.93
(1,1052)	1:23:A:ASN:HD22	1:23:A:ASN:HB3	9	0.93
(1,987)	1:32:A:ILE:H	1:28:A:LEU:HB2	2	0.93
(1,952)	1:82:A:LEU:H	1:84:A:GLU:HB2	6	0.93
(1,952)	1:82:A:LEU:H	1:84:A:GLU:HB2	9	0.93
(1,534)	1:92:A:GLN:HE22	1:92:A:GLN:HG3	3	0.93
(1,474)	1:71:A:TYR:HE1	1:55:A:ILE:H	3	0.93
(1,474)	1:71:A:TYR:HE2	1:55:A:ILE:H	3	0.93
(1,269)	1:55:A:ILE:H	1:55:A:ILE:HB	4	0.93
(1,158)	1:66:A:GLY:H	1:67:A:LYS:HB3	3	0.93
(1,1013)	1:64:A:ARG:H	1:62:A:ARG:HB3	6	0.92
(1,995)	1:30:A:GLU:H	1:30:A:GLU:HB3	7	0.92
(1,975)	1:54:A:GLU:H	1:54:A:GLU:HG3	2	0.92
(1,382)	1:54:A:GLU:H	1:54:A:GLU:HG3	2	0.92
(1,371)	1:71:A:TYR:H	1:71:A:TYR:HB2	6	0.92
(1,371)	1:71:A:TYR:H	1:71:A:TYR:HB2	9	0.92
(1,269)	1:55:A:ILE:H	1:55:A:ILE:HB	3	0.92
(1,269)	1:55:A:ILE:H	1:55:A:ILE:HB	9	0.92
(1,129)	1:74:A:GLU:H	1:73:A:GLN:HB3	5	0.92
(1,1086)	1:15:A:GLU:H	1:15:A:GLU:HB2	2	0.91
(1,1068)	1:39:A:ASP:H	1:39:A:ASP:HB2	8	0.91
(1,1059)	1:98:A:LYS:H	1:96:A:ILE:HB	8	0.91
(1,933)	1:63:A:LYS:H	1:64:A:ARG:HB2	8	0.91
(1,927)	1:14:A:THR:H	1:12:A:ASP:HB2	7	0.91
(1,811)	1:47:A:LEU:H	1:46:A:ILE:HB	10	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:29:A:CYS:H	1:30:A:GLU:HB3	9	0.91
(1,535)	1:18:A:LYS:H	1:18:A:LYS:HB2	7	0.91
(1,444)	1:46:A:ILE:H	1:45:A:LYS:HB2	2	0.91
(1,444)	1:46:A:ILE:H	1:45:A:LYS:HB2	3	0.91
(1,444)	1:46:A:ILE:H	1:45:A:LYS:HB2	5	0.91
(1,444)	1:46:A:ILE:H	1:45:A:LYS:HB2	8	0.91
(1,371)	1:71:A:TYR:H	1:71:A:TYR:HB2	4	0.91
(1,267)	1:95:A:LEU:H	1:95:A:LEU:HG	6	0.91
(1,975)	1:54:A:GLU:H	1:54:A:GLU:HG3	7	0.9
(1,960)	1:28:A:LEU:H	1:28:A:LEU:HG	3	0.9
(1,872)	1:45:A:LYS:H	1:41:A:LEU:HA	3	0.9
(1,849)	1:78:A:GLY:H	1:75:A:ASN:HB3	10	0.9
(1,801)	1:89:A:GLU:H	1:88:A:ARG:HB2	8	0.9
(1,755)	1:56:A:SER:H	1:64:A:ARG:HG3	3	0.9
(1,727)	1:15:A:GLU:H	1:12:A:ASP:HA	3	0.9
(1,444)	1:46:A:ILE:H	1:45:A:LYS:HB2	1	0.9
(1,382)	1:54:A:GLU:H	1:54:A:GLU:HG3	7	0.9
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD21	7	0.9
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD22	7	0.9
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD23	7	0.9
(1,269)	1:55:A:ILE:H	1:55:A:ILE:HB	10	0.9
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD11	10	0.89
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD12	10	0.89
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD13	10	0.89
(1,849)	1:78:A:GLY:H	1:75:A:ASN:HB3	5	0.89
(1,658)	1:51:A:ASP:HA	1:54:A:GLU:HG3	4	0.89
(1,655)	1:47:A:LEU:HD11	1:68:A:LEU:HB3	10	0.89
(1,655)	1:47:A:LEU:HD12	1:68:A:LEU:HB3	10	0.89
(1,655)	1:47:A:LEU:HD13	1:68:A:LEU:HB3	10	0.89
(1,269)	1:55:A:ILE:H	1:55:A:ILE:HB	6	0.89
(1,1216)	1:35:A:GLU:H	1:33:A:ILE:HG21	1	0.88
(1,1216)	1:35:A:GLU:H	1:33:A:ILE:HG22	1	0.88
(1,1216)	1:35:A:GLU:H	1:33:A:ILE:HG23	1	0.88
(1,474)	1:71:A:TYR:HE1	1:55:A:ILE:H	9	0.88
(1,474)	1:71:A:TYR:HE2	1:55:A:ILE:H	9	0.88
(1,444)	1:46:A:ILE:H	1:45:A:LYS:HB2	7	0.88
(1,371)	1:71:A:TYR:H	1:71:A:TYR:HB2	10	0.88
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD21	9	0.88
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD22	9	0.88
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD23	9	0.88
(1,241)	1:12:A:ASP:H	1:13:A:LEU:HA	1	0.88
(1,952)	1:82:A:LEU:H	1:84:A:GLU:HB2	4	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,726)	1:93:A:ASN:H	1:94:A:PHE:HB2	3	0.87
(1,658)	1:51:A:ASP:HA	1:54:A:GLU:HG3	9	0.87
(1,444)	1:46:A:ILE:H	1:45:A:LYS:HB2	6	0.87
(1,1069)	1:38:A:PHE:H	1:36:A:ARG:H	10	0.86
(1,995)	1:30:A:GLU:H	1:30:A:GLU:HB3	9	0.86
(1,371)	1:71:A:TYR:H	1:71:A:TYR:HB2	1	0.86
(1,1168)	1:54:A:GLU:H	1:56:A:SER:H	5	0.85
(1,278)	1:29:A:CYS:H	1:30:A:GLU:HB2	8	0.85
(1,269)	1:55:A:ILE:H	1:55:A:ILE:HB	2	0.85
(1,269)	1:55:A:ILE:H	1:55:A:ILE:HB	5	0.85
(1,241)	1:12:A:ASP:H	1:13:A:LEU:HA	4	0.85
(1,1122)	1:97:A:GLN:H	1:99:A:ILE:HB	3	0.84
(1,755)	1:56:A:SER:H	1:64:A:ARG:HG3	4	0.84
(1,390)	1:96:A:ILE:H	1:95:A:LEU:HG	2	0.84
(1,386)	1:16:A:VAL:H	1:16:A:VAL:HB	5	0.84
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD21	10	0.84
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD22	10	0.84
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD23	10	0.84
(1,1069)	1:38:A:PHE:H	1:36:A:ARG:H	8	0.83
(1,1068)	1:39:A:ASP:H	1:39:A:ASP:HB2	5	0.83
(1,1068)	1:39:A:ASP:H	1:39:A:ASP:HB2	9	0.83
(1,995)	1:30:A:GLU:H	1:30:A:GLU:HB3	8	0.83
(1,719)	1:18:A:LYS:H	1:18:A:LYS:HD3	2	0.83
(1,719)	1:18:A:LYS:H	1:18:A:LYS:HD3	9	0.83
(1,687)	1:97:A:GLN:H	1:97:A:GLN:HB3	7	0.83
(1,520)	1:14:A:THR:H	1:11:A:GLU:HA	3	0.83
(1,493)	1:111:A:LEU:H	1:111:A:LEU:HB2	7	0.83
(1,386)	1:16:A:VAL:H	1:16:A:VAL:HB	3	0.83
(1,286)	1:85:A:SER:H	1:85:A:SER:HB3	7	0.83
(1,284)	1:84:A:GLU:H	1:84:A:GLU:HB3	3	0.83
(1,241)	1:12:A:ASP:H	1:13:A:LEU:HA	2	0.83
(1,241)	1:12:A:ASP:H	1:13:A:LEU:HA	9	0.83
(1,68)	1:54:A:GLU:HA	1:54:A:GLU:HG3	1	0.83
(1,68)	1:54:A:GLU:HA	1:54:A:GLU:HG3	8	0.83
(1,68)	1:54:A:GLU:HA	1:54:A:GLU:HG3	9	0.83
(1,1069)	1:38:A:PHE:H	1:36:A:ARG:H	6	0.82
(1,916)	1:36:A:ARG:H	1:36:A:ARG:HG3	4	0.82
(1,687)	1:97:A:GLN:H	1:97:A:GLN:HB3	6	0.82
(1,654)	1:29:A:CYS:H	1:30:A:GLU:HB3	6	0.82
(1,502)	1:31:A:LYS:H	1:28:A:LEU:HB2	9	0.82
(1,460)	1:50:A:GLU:HA	1:50:A:GLU:HG3	6	0.82
(1,274)	1:115:A:LYS:H	1:114:A:LEU:HB3	8	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,241)	1:12:A:ASP:H	1:13:A:LEU:HA	7	0.82
(1,158)	1:66:A:GLY:H	1:67:A:LYS:HB3	2	0.82
(1,150)	1:31:A:LYS:H	1:31:A:LYS:HG2	7	0.82
(1,1277)	1:107:A:ARG:H	1:106:A:LEU:HB3	1	0.81
(1,1227)	1:10:A:GLU:H	1:11:A:GLU:HG2	7	0.81
(1,1068)	1:39:A:ASP:H	1:39:A:ASP:HB2	6	0.81
(1,628)	1:106:A:LEU:HB3	1:13:A:LEU:HB3	5	0.81
(1,386)	1:16:A:VAL:H	1:16:A:VAL:HB	8	0.81
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD21	1	0.81
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD22	1	0.81
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD23	1	0.81
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB1	6	0.81
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB2	6	0.81
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB3	6	0.81
(1,88)	1:108:A:ASN:H	1:107:A:ARG:HB3	2	0.81
(1,1068)	1:39:A:ASP:H	1:39:A:ASP:HB2	1	0.8
(1,1068)	1:39:A:ASP:H	1:39:A:ASP:HB2	3	0.8
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD21	9	0.8
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD22	9	0.8
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD23	9	0.8
(1,854)	1:54:A:GLU:H	1:53:A:ARG:HB3	8	0.8
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG21	7	0.8
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG22	7	0.8
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG23	7	0.8
(1,687)	1:97:A:GLN:H	1:97:A:GLN:HB3	4	0.8
(1,607)	1:19:A:ASP:H	1:18:A:LYS:HB2	9	0.8
(1,286)	1:85:A:SER:H	1:85:A:SER:HB3	6	0.8
(1,250)	1:24:A:LEU:HD11	1:102:A:GLU:HB3	3	0.8
(1,250)	1:24:A:LEU:HD12	1:102:A:GLU:HB3	3	0.8
(1,250)	1:24:A:LEU:HD13	1:102:A:GLU:HB3	3	0.8
(1,224)	1:74:A:GLU:H	1:72:A:LEU:HA	8	0.8
(1,1206)	1:69:A:LEU:H	1:69:A:LEU:HB3	1	0.79
(1,854)	1:54:A:GLU:H	1:53:A:ARG:HB3	4	0.79
(1,654)	1:29:A:CYS:H	1:30:A:GLU:HB3	1	0.79
(1,386)	1:16:A:VAL:H	1:16:A:VAL:HB	4	0.79
(1,386)	1:16:A:VAL:H	1:16:A:VAL:HB	10	0.79
(1,241)	1:12:A:ASP:H	1:13:A:LEU:HA	10	0.79
(1,185)	1:46:A:ILE:H	1:44:A:LYS:HB3	1	0.79
(1,150)	1:31:A:LYS:H	1:31:A:LYS:HG2	9	0.79
(1,6)	1:27:A:TYR:H	1:23:A:ASN:HB2	3	0.79
(1,1269)	1:78:A:GLY:H	1:72:A:LEU:H	5	0.78
(1,1168)	1:54:A:GLU:H	1:56:A:SER:H	3	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1024)	1:39:A:ASP:H	1:38:A:PHE:HB2	9	0.78
(1,982)	1:71:A:TYR:H	1:73:A:GLN:H	10	0.78
(1,948)	1:20:A:ALA:H	1:18:A:LYS:HB2	1	0.78
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG21	8	0.78
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG22	8	0.78
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG23	8	0.78
(1,600)	1:39:A:ASP:H	1:38:A:PHE:HB2	9	0.78
(1,544)	1:70:A:ASP:H	1:68:A:LEU:HA	8	0.78
(1,386)	1:16:A:VAL:H	1:16:A:VAL:HB	6	0.78
(1,386)	1:16:A:VAL:H	1:16:A:VAL:HB	7	0.78
(1,298)	1:97:A:GLN:HA	1:97:A:GLN:HG3	8	0.78
(1,286)	1:85:A:SER:H	1:85:A:SER:HB3	1	0.78
(1,267)	1:95:A:LEU:H	1:95:A:LEU:HG	2	0.78
(1,19)	1:82:A:LEU:HD21	1:46:A:ILE:HG13	7	0.78
(1,19)	1:82:A:LEU:HD22	1:46:A:ILE:HG13	7	0.78
(1,19)	1:82:A:LEU:HD23	1:46:A:ILE:HG13	7	0.78
(1,1206)	1:69:A:LEU:H	1:69:A:LEU:HB3	9	0.77
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG21	10	0.77
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG22	10	0.77
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG23	10	0.77
(1,659)	1:63:A:LYS:H	1:62:A:ARG:HG3	5	0.77
(1,607)	1:19:A:ASP:H	1:18:A:LYS:HB2	5	0.77
(1,386)	1:16:A:VAL:H	1:16:A:VAL:HB	1	0.77
(1,386)	1:16:A:VAL:H	1:16:A:VAL:HB	2	0.77
(1,286)	1:85:A:SER:H	1:85:A:SER:HB3	5	0.77
(1,286)	1:85:A:SER:H	1:85:A:SER:HB3	10	0.77
(1,284)	1:84:A:GLU:H	1:84:A:GLU:HB3	7	0.77
(1,274)	1:115:A:LYS:H	1:114:A:LEU:HB3	7	0.77
(1,251)	1:74:A:GLU:H	1:74:A:GLU:HG3	9	0.77
(1,241)	1:12:A:ASP:H	1:13:A:LEU:HA	5	0.77
(1,103)	1:47:A:LEU:H	1:48:A:SER:HA	3	0.77
(1,1206)	1:69:A:LEU:H	1:69:A:LEU:HB3	5	0.76
(1,1066)	1:72:A:LEU:H	1:72:A:LEU:HB2	9	0.76
(1,390)	1:96:A:ILE:H	1:95:A:LEU:HG	7	0.76
(1,386)	1:16:A:VAL:H	1:16:A:VAL:HB	9	0.76
(1,185)	1:46:A:ILE:H	1:44:A:LYS:HB3	8	0.76
(1,1253)	1:54:A:GLU:H	1:57:A:CYS:H	1	0.75
(1,1068)	1:39:A:ASP:H	1:39:A:ASP:HB2	4	0.75
(1,1066)	1:72:A:LEU:H	1:72:A:LEU:HB2	7	0.75
(1,927)	1:14:A:THR:H	1:12:A:ASP:HB2	5	0.75
(1,884)	1:89:A:GLU:H	1:89:A:GLU:HG2	1	0.75
(1,513)	1:112:A:GLU:H	1:114:A:LEU:H	8	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	1:63:A:LYS:HE3	1:63:A:LYS:HG2	1	0.75
(1,250)	1:24:A:LEU:HD11	1:102:A:GLU:HB3	6	0.75
(1,250)	1:24:A:LEU:HD12	1:102:A:GLU:HB3	6	0.75
(1,250)	1:24:A:LEU:HD13	1:102:A:GLU:HB3	6	0.75
(1,1277)	1:107:A:ARG:H	1:106:A:LEU:HB3	2	0.74
(1,1206)	1:69:A:LEU:H	1:69:A:LEU:HB3	8	0.74
(1,1013)	1:64:A:ARG:H	1:62:A:ARG:HB3	5	0.74
(1,987)	1:32:A:ILE:H	1:28:A:LEU:HB2	9	0.74
(1,884)	1:89:A:GLU:H	1:89:A:GLU:HG2	6	0.74
(1,801)	1:89:A:GLU:H	1:88:A:ARG:HB2	9	0.74
(1,599)	1:88:A:ARG:H	1:88:A:ARG:HG3	2	0.74
(1,513)	1:112:A:GLU:H	1:114:A:LEU:H	6	0.74
(1,513)	1:112:A:GLU:H	1:114:A:LEU:H	10	0.74
(1,185)	1:46:A:ILE:H	1:44:A:LYS:HB3	5	0.74
(1,1212)	1:55:A:ILE:H	1:51:A:ASP:HB3	6	0.73
(1,1206)	1:69:A:LEU:H	1:69:A:LEU:HB3	10	0.73
(1,1052)	1:23:A:ASN:HD22	1:23:A:ASN:HB3	10	0.73
(1,1035)	1:74:A:GLU:H	1:73:A:GLN:HG3	6	0.73
(1,849)	1:78:A:GLY:H	1:75:A:ASN:HB3	2	0.73
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG21	1	0.73
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG22	1	0.73
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG23	1	0.73
(1,730)	1:84:A:GLU:H	1:83:A:VAL:HB	10	0.73
(1,513)	1:112:A:GLU:H	1:114:A:LEU:H	5	0.73
(1,148)	1:42:A:ARG:HD3	1:52:A:THR:HG21	7	0.73
(1,148)	1:42:A:ARG:HD3	1:52:A:THR:HG22	7	0.73
(1,148)	1:42:A:ARG:HD3	1:52:A:THR:HG23	7	0.73
(1,6)	1:27:A:TYR:H	1:23:A:ASN:HB2	9	0.73
(1,1206)	1:69:A:LEU:H	1:69:A:LEU:HB3	2	0.72
(1,1168)	1:54:A:GLU:H	1:56:A:SER:H	2	0.72
(1,1088)	1:101:A:ASP:H	1:99:A:ILE:HB	10	0.72
(1,1049)	1:74:A:GLU:H	1:74:A:GLU:HG2	5	0.72
(1,933)	1:63:A:LYS:H	1:64:A:ARG:HB2	4	0.72
(1,927)	1:14:A:THR:H	1:12:A:ASP:HB2	6	0.72
(1,880)	1:32:A:ILE:HD11	1:86:A:ILE:HG13	3	0.72
(1,880)	1:32:A:ILE:HD12	1:86:A:ILE:HG13	3	0.72
(1,880)	1:32:A:ILE:HD13	1:86:A:ILE:HG13	3	0.72
(1,278)	1:29:A:CYS:H	1:30:A:GLU:HB2	9	0.72
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD11	5	0.71
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD12	5	0.71
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD13	5	0.71
(1,1212)	1:55:A:ILE:H	1:51:A:ASP:HB3	10	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD21	10	0.71
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD22	10	0.71
(1,1015)	1:27:A:TYR:H	1:28:A:LEU:HD23	10	0.71
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG21	8	0.71
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG22	8	0.71
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG23	8	0.71
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG21	9	0.71
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG22	9	0.71
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG23	9	0.71
(1,756)	1:73:A:GLN:H	1:73:A:GLN:HE22	1	0.71
(1,732)	1:36:A:ARG:H	1:35:A:GLU:HB2	1	0.71
(1,730)	1:84:A:GLU:H	1:83:A:VAL:HB	2	0.71
(1,540)	1:95:A:LEU:HA	1:99:A:ILE:HG13	5	0.71
(1,424)	1:11:A:GLU:H	1:11:A:GLU:HB2	7	0.71
(1,357)	1:107:A:ARG:H	1:106:A:LEU:HD21	8	0.71
(1,357)	1:107:A:ARG:H	1:106:A:LEU:HD22	8	0.71
(1,357)	1:107:A:ARG:H	1:106:A:LEU:HD23	8	0.71
(1,327)	1:63:A:LYS:HE3	1:63:A:LYS:HG2	3	0.71
(1,185)	1:46:A:ILE:H	1:44:A:LYS:HB3	9	0.71
(1,178)	1:105:A:LYS:H	1:105:A:LYS:HD2	6	0.71
(1,88)	1:108:A:ASN:H	1:107:A:ARG:HB3	10	0.71
(1,19)	1:82:A:LEU:HD21	1:46:A:ILE:HG13	2	0.71
(1,19)	1:82:A:LEU:HD22	1:46:A:ILE:HG13	2	0.71
(1,19)	1:82:A:LEU:HD23	1:46:A:ILE:HG13	2	0.71
(1,1052)	1:23:A:ASN:HD22	1:23:A:ASN:HB3	5	0.7
(1,1024)	1:39:A:ASP:H	1:38:A:PHE:HB2	10	0.7
(1,916)	1:36:A:ARG:H	1:36:A:ARG:HG3	9	0.7
(1,635)	1:32:A:ILE:H	1:31:A:LYS:HB2	1	0.7
(1,600)	1:39:A:ASP:H	1:38:A:PHE:HB2	10	0.7
(1,447)	1:31:A:LYS:H	1:32:A:ILE:HB	9	0.7
(1,158)	1:66:A:GLY:H	1:67:A:LYS:HB3	9	0.7
(1,130)	1:16:A:VAL:H	1:13:A:LEU:HA	2	0.7
(1,111)	1:89:A:GLU:H	1:87:A:ARG:HA	5	0.7
(1,83)	1:88:A:ARG:H	1:87:A:ARG:HB2	9	0.7
(1,1206)	1:69:A:LEU:H	1:69:A:LEU:HB3	3	0.69
(1,1206)	1:69:A:LEU:H	1:69:A:LEU:HB3	7	0.69
(1,1013)	1:64:A:ARG:H	1:62:A:ARG:HB3	4	0.69
(1,730)	1:84:A:GLU:H	1:83:A:VAL:HB	3	0.69
(1,730)	1:84:A:GLU:H	1:83:A:VAL:HB	8	0.69
(1,661)	1:83:A:VAL:H	1:83:A:VAL:HB	10	0.69
(1,544)	1:70:A:ASP:H	1:68:A:LEU:HA	3	0.69
(1,534)	1:92:A:GLN:HE22	1:92:A:GLN:HG3	2	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,513)	1:112:A:GLU:H	1:114:A:LEU:H	3	0.69
(1,424)	1:11:A:GLU:H	1:11:A:GLU:HB2	10	0.69
(1,227)	1:98:A:LYS:H	1:97:A:GLN:HB2	8	0.69
(1,6)	1:27:A:TYR:H	1:23:A:ASN:HB2	1	0.69
(1,877)	1:55:A:ILE:HG21	1:68:A:LEU:HB3	10	0.68
(1,877)	1:55:A:ILE:HG22	1:68:A:LEU:HB3	10	0.68
(1,877)	1:55:A:ILE:HG23	1:68:A:LEU:HB3	10	0.68
(1,534)	1:92:A:GLN:HE22	1:92:A:GLN:HG3	7	0.68
(1,438)	1:52:A:THR:H	1:47:A:LEU:HB3	2	0.68
(1,424)	1:11:A:GLU:H	1:11:A:GLU:HB2	1	0.68
(1,424)	1:11:A:GLU:H	1:11:A:GLU:HB2	3	0.68
(1,1208)	1:59:A:THR:HG21	1:67:A:LYS:HB3	4	0.67
(1,1208)	1:59:A:THR:HG22	1:67:A:LYS:HB3	4	0.67
(1,1208)	1:59:A:THR:HG23	1:67:A:LYS:HB3	4	0.67
(1,1052)	1:23:A:ASN:HD22	1:23:A:ASN:HB3	4	0.67
(1,730)	1:84:A:GLU:H	1:83:A:VAL:HB	1	0.67
(1,730)	1:84:A:GLU:H	1:83:A:VAL:HB	9	0.67
(1,544)	1:70:A:ASP:H	1:68:A:LEU:HA	1	0.67
(1,468)	1:77:A:LYS:HE3	1:77:A:LYS:HB2	7	0.67
(1,267)	1:95:A:LEU:H	1:95:A:LEU:HG	9	0.67
(1,1227)	1:10:A:GLU:H	1:11:A:GLU:HG2	8	0.66
(1,1122)	1:97:A:GLN:H	1:99:A:ILE:HB	9	0.66
(1,1013)	1:64:A:ARG:H	1:62:A:ARG:HB3	10	0.66
(1,599)	1:88:A:ARG:H	1:88:A:ARG:HG3	6	0.66
(1,452)	1:102:A:GLU:H	1:24:A:LEU:HD11	4	0.66
(1,452)	1:102:A:GLU:H	1:24:A:LEU:HD12	4	0.66
(1,452)	1:102:A:GLU:H	1:24:A:LEU:HD13	4	0.66
(1,447)	1:31:A:LYS:H	1:32:A:ILE:HB	6	0.66
(1,269)	1:55:A:ILE:H	1:55:A:ILE:HB	1	0.66
(1,6)	1:27:A:TYR:H	1:23:A:ASN:HB2	10	0.66
(1,952)	1:82:A:LEU:H	1:84:A:GLU:HB2	1	0.65
(1,808)	1:72:A:LEU:HD21	1:46:A:ILE:HG13	2	0.65
(1,808)	1:72:A:LEU:HD22	1:46:A:ILE:HG13	2	0.65
(1,808)	1:72:A:LEU:HD23	1:46:A:ILE:HG13	2	0.65
(1,730)	1:84:A:GLU:H	1:83:A:VAL:HB	4	0.65
(1,534)	1:92:A:GLN:HE22	1:92:A:GLN:HG3	4	0.65
(1,215)	1:27:A:TYR:H	1:26:A:VAL:HB	1	0.65
(1,1246)	1:46:A:ILE:H	1:81:A:THR:HG21	8	0.64
(1,1246)	1:46:A:ILE:H	1:81:A:THR:HG22	8	0.64
(1,1246)	1:46:A:ILE:H	1:81:A:THR:HG23	8	0.64
(1,1122)	1:97:A:GLN:H	1:99:A:ILE:HB	6	0.64
(1,1088)	1:101:A:ASP:H	1:99:A:ILE:HB	1	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1088)	1:101:A:ASP:H	1:99:A:ILE:HB	8	0.64
(1,1035)	1:74:A:GLU:H	1:73:A:GLN:HG3	4	0.64
(1,169)	1:97:A:GLN:HE21	1:97:A:GLN:HB3	1	0.64
(1,1122)	1:97:A:GLN:H	1:99:A:ILE:HB	2	0.63
(1,1094)	1:89:A:GLU:H	1:88:A:ARG:HB3	10	0.63
(1,920)	1:88:A:ARG:H	1:88:A:ARG:HG2	4	0.63
(1,730)	1:84:A:GLU:H	1:83:A:VAL:HB	6	0.63
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG21	9	0.63
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG22	9	0.63
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG23	9	0.63
(1,1211)	1:71:A:TYR:HD1	1:68:A:LEU:HB3	9	0.62
(1,1211)	1:71:A:TYR:HD2	1:68:A:LEU:HB3	9	0.62
(1,1088)	1:101:A:ASP:H	1:99:A:ILE:HB	7	0.62
(1,730)	1:84:A:GLU:H	1:83:A:VAL:HB	5	0.62
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG21	4	0.62
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG22	4	0.62
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG23	4	0.62
(1,1246)	1:46:A:ILE:H	1:81:A:THR:HG21	10	0.61
(1,1246)	1:46:A:ILE:H	1:81:A:THR:HG22	10	0.61
(1,1246)	1:46:A:ILE:H	1:81:A:THR:HG23	10	0.61
(1,1211)	1:71:A:TYR:HD1	1:68:A:LEU:HB3	2	0.61
(1,1211)	1:71:A:TYR:HD2	1:68:A:LEU:HB3	2	0.61
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD21	8	0.61
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD22	8	0.61
(1,1146)	1:28:A:LEU:H	1:79:A:LEU:HD23	8	0.61
(1,1035)	1:74:A:GLU:H	1:73:A:GLN:HG3	1	0.61
(1,1013)	1:64:A:ARG:H	1:62:A:ARG:HB3	8	0.61
(1,872)	1:45:A:LYS:H	1:41:A:LEU:HA	8	0.61
(1,863)	1:114:A:LEU:H	1:114:A:LEU:HB3	3	0.61
(1,863)	1:114:A:LEU:H	1:114:A:LEU:HB3	6	0.61
(1,659)	1:63:A:LYS:H	1:62:A:ARG:HG3	3	0.61
(1,564)	1:80:A:ASP:H	1:79:A:LEU:HB2	6	0.61
(1,357)	1:107:A:ARG:H	1:106:A:LEU:HD21	4	0.61
(1,357)	1:107:A:ARG:H	1:106:A:LEU:HD22	4	0.61
(1,357)	1:107:A:ARG:H	1:106:A:LEU:HD23	4	0.61
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD11	6	0.61
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD12	6	0.61
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD13	6	0.61
(1,6)	1:27:A:TYR:H	1:23:A:ASN:HB2	4	0.61
(1,1211)	1:71:A:TYR:HD1	1:68:A:LEU:HB3	3	0.6
(1,1211)	1:71:A:TYR:HD2	1:68:A:LEU:HB3	3	0.6
(1,719)	1:18:A:LYS:H	1:18:A:LYS:HD3	7	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD21	9	0.6
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD22	9	0.6
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD23	9	0.6
(1,402)	1:51:A:ASP:H	1:50:A:GLU:HB2	6	0.6
(1,1024)	1:39:A:ASP:H	1:38:A:PHE:HB2	7	0.59
(1,877)	1:55:A:ILE:HG21	1:68:A:LEU:HB3	8	0.59
(1,877)	1:55:A:ILE:HG22	1:68:A:LEU:HB3	8	0.59
(1,877)	1:55:A:ILE:HG23	1:68:A:LEU:HB3	8	0.59
(1,863)	1:114:A:LEU:H	1:114:A:LEU:HB3	9	0.59
(1,854)	1:54:A:GLU:H	1:53:A:ARG:HB3	6	0.59
(1,600)	1:39:A:ASP:H	1:38:A:PHE:HB2	7	0.59
(1,430)	1:16:A:VAL:H	1:15:A:GLU:HG2	7	0.59
(1,103)	1:47:A:LEU:H	1:48:A:SER:HA	9	0.59
(1,1211)	1:71:A:TYR:HD1	1:68:A:LEU:HB3	1	0.58
(1,1211)	1:71:A:TYR:HD2	1:68:A:LEU:HB3	1	0.58
(1,1206)	1:69:A:LEU:H	1:69:A:LEU:HB3	6	0.58
(1,726)	1:93:A:ASN:H	1:94:A:PHE:HB2	10	0.58
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG21	9	0.58
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG22	9	0.58
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG23	9	0.58
(1,685)	1:53:A:ARG:H	1:56:A:SER:H	8	0.58
(1,390)	1:96:A:ILE:H	1:95:A:LEU:HG	6	0.58
(1,88)	1:108:A:ASN:H	1:107:A:ARG:HB3	6	0.58
(1,83)	1:88:A:ARG:H	1:87:A:ARG:HB2	1	0.58
(1,1191)	1:11:A:GLU:H	1:14:A:THR:H	2	0.57
(1,1168)	1:54:A:GLU:H	1:56:A:SER:H	10	0.57
(1,995)	1:30:A:GLU:H	1:30:A:GLU:HB3	1	0.57
(1,995)	1:30:A:GLU:H	1:30:A:GLU:HB3	6	0.57
(1,960)	1:28:A:LEU:H	1:28:A:LEU:HG	7	0.57
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD21	2	0.57
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD22	2	0.57
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD23	2	0.57
(1,452)	1:102:A:GLU:H	1:24:A:LEU:HD11	3	0.57
(1,452)	1:102:A:GLU:H	1:24:A:LEU:HD12	3	0.57
(1,452)	1:102:A:GLU:H	1:24:A:LEU:HD13	3	0.57
(1,274)	1:115:A:LYS:H	1:114:A:LEU:HB3	2	0.57
(1,995)	1:30:A:GLU:H	1:30:A:GLU:HB3	10	0.56
(1,863)	1:114:A:LEU:H	1:114:A:LEU:HB3	10	0.56
(1,817)	1:42:A:ARG:H	1:41:A:LEU:HB2	5	0.56
(1,802)	1:27:A:TYR:HE1	1:23:A:ASN:HB3	1	0.56
(1,802)	1:27:A:TYR:HE2	1:23:A:ASN:HB3	1	0.56
(1,716)	1:99:A:ILE:H	1:98:A:LYS:HB3	10	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,659)	1:63:A:LYS:H	1:62:A:ARG:HG3	10	0.56
(1,250)	1:24:A:LEU:HD11	1:102:A:GLU:HB3	2	0.56
(1,250)	1:24:A:LEU:HD12	1:102:A:GLU:HB3	2	0.56
(1,250)	1:24:A:LEU:HD13	1:102:A:GLU:HB3	2	0.56
(1,150)	1:31:A:LYS:H	1:31:A:LYS:HG2	10	0.56
(1,88)	1:108:A:ASN:H	1:107:A:ARG:HB3	3	0.56
(1,1206)	1:69:A:LEU:H	1:69:A:LEU:HB3	4	0.55
(1,1191)	1:11:A:GLU:H	1:14:A:THR:H	4	0.55
(1,727)	1:15:A:GLU:H	1:12:A:ASP:HA	8	0.55
(1,647)	1:73:A:GLN:HE21	1:73:A:GLN:HG3	1	0.55
(1,267)	1:95:A:LEU:H	1:95:A:LEU:HG	7	0.55
(1,241)	1:12:A:ASP:H	1:13:A:LEU:HA	3	0.55
(1,239)	1:93:A:ASN:HD22	1:93:A:ASN:HB3	8	0.55
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD11	10	0.55
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD12	10	0.55
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD13	10	0.55
(1,130)	1:16:A:VAL:H	1:13:A:LEU:HA	8	0.55
(1,103)	1:47:A:LEU:H	1:48:A:SER:HA	8	0.55
(1,1253)	1:54:A:GLU:H	1:57:A:CYS:H	2	0.54
(1,1191)	1:11:A:GLU:H	1:14:A:THR:H	8	0.54
(1,1088)	1:101:A:ASP:H	1:99:A:ILE:HB	9	0.54
(1,1013)	1:64:A:ARG:H	1:62:A:ARG:HB3	1	0.54
(1,544)	1:70:A:ASP:H	1:68:A:LEU:HA	10	0.54
(1,513)	1:112:A:GLU:H	1:114:A:LEU:H	9	0.54
(1,470)	1:16:A:VAL:HG21	1:106:A:LEU:HB3	6	0.54
(1,470)	1:16:A:VAL:HG22	1:106:A:LEU:HB3	6	0.54
(1,470)	1:16:A:VAL:HG23	1:106:A:LEU:HB3	6	0.54
(1,239)	1:93:A:ASN:HD22	1:93:A:ASN:HB3	2	0.54
(1,239)	1:93:A:ASN:HD22	1:93:A:ASN:HB3	3	0.54
(1,239)	1:93:A:ASN:HD22	1:93:A:ASN:HB3	7	0.54
(1,1122)	1:97:A:GLN:H	1:99:A:ILE:HB	1	0.53
(1,520)	1:14:A:THR:H	1:11:A:GLU:HA	9	0.53
(1,447)	1:31:A:LYS:H	1:32:A:ILE:HB	8	0.53
(1,444)	1:46:A:ILE:H	1:45:A:LYS:HB2	10	0.53
(1,265)	1:73:A:GLN:H	1:71:A:TYR:HA	7	0.53
(1,239)	1:93:A:ASN:HD22	1:93:A:ASN:HB3	4	0.53
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB1	10	0.53
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB2	10	0.53
(1,183)	1:69:A:LEU:H	1:65:A:ALA:HB3	10	0.53
(1,1088)	1:101:A:ASP:H	1:99:A:ILE:HB	3	0.52
(1,1024)	1:39:A:ASP:H	1:38:A:PHE:HB2	5	0.52
(1,863)	1:114:A:LEU:H	1:114:A:LEU:HB3	2	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,801)	1:89:A:GLU:H	1:88:A:ARG:HB2	2	0.52
(1,635)	1:32:A:ILE:H	1:31:A:LYS:HB2	5	0.52
(1,600)	1:39:A:ASP:H	1:38:A:PHE:HB2	5	0.52
(1,597)	1:46:A:ILE:H	1:45:A:LYS:HG3	6	0.52
(1,544)	1:70:A:ASP:H	1:68:A:LEU:HA	7	0.52
(1,452)	1:102:A:GLU:H	1:24:A:LEU:HD11	1	0.52
(1,452)	1:102:A:GLU:H	1:24:A:LEU:HD12	1	0.52
(1,452)	1:102:A:GLU:H	1:24:A:LEU:HD13	1	0.52
(1,129)	1:74:A:GLU:H	1:73:A:GLN:HB3	7	0.52
(1,74)	1:68:A:LEU:H	1:55:A:ILE:HB	4	0.52
(1,1211)	1:71:A:TYR:HD1	1:68:A:LEU:HB3	7	0.51
(1,1211)	1:71:A:TYR:HD2	1:68:A:LEU:HB3	7	0.51
(1,1046)	1:17:A:LYS:H	1:16:A:VAL:HB	3	0.51
(1,1024)	1:39:A:ASP:H	1:38:A:PHE:HB2	3	0.51
(1,915)	1:21:A:LEU:HD11	1:79:A:LEU:HB3	9	0.51
(1,915)	1:21:A:LEU:HD12	1:79:A:LEU:HB3	9	0.51
(1,915)	1:21:A:LEU:HD13	1:79:A:LEU:HB3	9	0.51
(1,801)	1:89:A:GLU:H	1:88:A:ARG:HB2	3	0.51
(1,719)	1:18:A:LYS:H	1:18:A:LYS:HD3	6	0.51
(1,600)	1:39:A:ASP:H	1:38:A:PHE:HB2	3	0.51
(1,564)	1:80:A:ASP:H	1:79:A:LEU:HB2	2	0.51
(1,227)	1:98:A:LYS:H	1:97:A:GLN:HB2	5	0.51
(1,178)	1:105:A:LYS:H	1:105:A:LYS:HD2	2	0.51
(1,103)	1:47:A:LEU:H	1:48:A:SER:HA	1	0.51
(1,58)	1:27:A:TYR:HD1	1:28:A:LEU:HB3	10	0.51
(1,58)	1:27:A:TYR:HD2	1:28:A:LEU:HB3	10	0.51
(1,1277)	1:107:A:ARG:H	1:106:A:LEU:HB3	4	0.5
(1,1191)	1:11:A:GLU:H	1:14:A:THR:H	3	0.5
(1,1168)	1:54:A:GLU:H	1:56:A:SER:H	1	0.5
(1,1046)	1:17:A:LYS:H	1:16:A:VAL:HB	5	0.5
(1,880)	1:32:A:ILE:HD11	1:86:A:ILE:HG13	7	0.5
(1,880)	1:32:A:ILE:HD12	1:86:A:ILE:HG13	7	0.5
(1,880)	1:32:A:ILE:HD13	1:86:A:ILE:HG13	7	0.5
(1,730)	1:84:A:GLU:H	1:83:A:VAL:HB	7	0.5
(1,607)	1:19:A:ASP:H	1:18:A:LYS:HB2	6	0.5
(1,597)	1:46:A:ILE:H	1:45:A:LYS:HG3	7	0.5
(1,158)	1:66:A:GLY:H	1:67:A:LYS:HB3	8	0.5
(1,982)	1:71:A:TYR:H	1:73:A:GLN:H	8	0.49
(1,817)	1:42:A:ARG:H	1:41:A:LEU:HB2	7	0.49
(1,726)	1:93:A:ASN:H	1:94:A:PHE:HB2	5	0.49
(1,278)	1:29:A:CYS:H	1:30:A:GLU:HB2	6	0.49
(1,152)	1:16:A:VAL:H	1:106:A:LEU:HB2	1	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:82:A:LEU:HD21	1:46:A:ILE:HG13	9	0.49
(1,19)	1:82:A:LEU:HD22	1:46:A:ILE:HG13	9	0.49
(1,19)	1:82:A:LEU:HD23	1:46:A:ILE:HG13	9	0.49
(1,11)	1:81:A:THR:HG21	1:46:A:ILE:HG13	10	0.49
(1,11)	1:81:A:THR:HG22	1:46:A:ILE:HG13	10	0.49
(1,11)	1:81:A:THR:HG23	1:46:A:ILE:HG13	10	0.49
(1,1088)	1:101:A:ASP:H	1:99:A:ILE:HB	5	0.48
(1,635)	1:32:A:ILE:H	1:31:A:LYS:HB2	6	0.48
(1,599)	1:88:A:ARG:H	1:88:A:ARG:HG3	4	0.48
(1,498)	1:66:A:GLY:H	1:63:A:LYS:HA	5	0.48
(1,447)	1:31:A:LYS:H	1:32:A:ILE:HB	2	0.48
(1,224)	1:74:A:GLU:H	1:72:A:LEU:HA	10	0.48
(1,103)	1:47:A:LEU:H	1:48:A:SER:HA	7	0.48
(1,1278)	1:34:A:ALA:H	1:33:A:ILE:HA	10	0.47
(1,1253)	1:54:A:GLU:H	1:57:A:CYS:H	9	0.47
(1,1227)	1:10:A:GLU:H	1:11:A:GLU:HG2	10	0.47
(1,1046)	1:17:A:LYS:H	1:16:A:VAL:HB	9	0.47
(1,1024)	1:39:A:ASP:H	1:38:A:PHE:HB2	6	0.47
(1,952)	1:82:A:LEU:H	1:84:A:GLU:HB2	2	0.47
(1,880)	1:32:A:ILE:HD11	1:86:A:ILE:HG13	4	0.47
(1,880)	1:32:A:ILE:HD12	1:86:A:ILE:HG13	4	0.47
(1,880)	1:32:A:ILE:HD13	1:86:A:ILE:HG13	4	0.47
(1,863)	1:114:A:LEU:H	1:114:A:LEU:HB3	5	0.47
(1,600)	1:39:A:ASP:H	1:38:A:PHE:HB2	6	0.47
(1,599)	1:88:A:ARG:H	1:88:A:ARG:HG3	10	0.47
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD21	7	0.47
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD22	7	0.47
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD23	7	0.47
(1,470)	1:16:A:VAL:HG21	1:106:A:LEU:HB3	10	0.47
(1,470)	1:16:A:VAL:HG22	1:106:A:LEU:HB3	10	0.47
(1,470)	1:16:A:VAL:HG23	1:106:A:LEU:HB3	10	0.47
(1,402)	1:51:A:ASP:H	1:50:A:GLU:HB2	7	0.47
(1,250)	1:24:A:LEU:HD11	1:102:A:GLU:HB3	1	0.47
(1,250)	1:24:A:LEU:HD12	1:102:A:GLU:HB3	1	0.47
(1,250)	1:24:A:LEU:HD13	1:102:A:GLU:HB3	1	0.47
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD11	3	0.46
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD12	3	0.46
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD13	3	0.46
(1,955)	1:73:A:GLN:H	1:73:A:GLN:HB3	8	0.46
(1,942)	1:114:A:LEU:HD11	1:114:A:LEU:HB3	10	0.46
(1,942)	1:114:A:LEU:HD12	1:114:A:LEU:HB3	10	0.46
(1,942)	1:114:A:LEU:HD13	1:114:A:LEU:HB3	10	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,854)	1:54:A:GLU:H	1:53:A:ARG:HB3	9	0.46
(1,632)	1:89:A:GLU:HB3	1:92:A:GLN:HB3	8	0.46
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD21	4	0.46
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD22	4	0.46
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD23	4	0.46
(1,1018)	1:50:A:GLU:H	1:51:A:ASP:HB2	10	0.45
(1,813)	1:73:A:GLN:HE22	1:73:A:GLN:HG2	10	0.45
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG21	7	0.45
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG22	7	0.45
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG23	7	0.45
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG21	5	0.45
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG22	5	0.45
(1,693)	1:17:A:LYS:H	1:103:A:VAL:HG23	5	0.45
(1,620)	1:40:A:HIS:H	1:39:A:ASP:HB3	4	0.45
(1,597)	1:46:A:ILE:H	1:45:A:LYS:HG3	5	0.45
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD21	3	0.45
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD22	3	0.45
(1,570)	1:103:A:VAL:H	1:104:A:LEU:HD23	3	0.45
(1,468)	1:77:A:LYS:HE3	1:77:A:LYS:HB2	10	0.45
(1,339)	1:105:A:LYS:H	1:104:A:LEU:HB3	6	0.45
(1,267)	1:95:A:LEU:H	1:95:A:LEU:HG	10	0.45
(1,178)	1:105:A:LYS:H	1:105:A:LYS:HD2	5	0.45
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG21	7	0.45
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG22	7	0.45
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG23	7	0.45
(1,68)	1:54:A:GLU:HA	1:54:A:GLU:HG3	2	0.45
(1,1191)	1:11:A:GLU:H	1:14:A:THR:H	9	0.44
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD11	10	0.44
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD12	10	0.44
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD13	10	0.44
(1,955)	1:73:A:GLN:H	1:73:A:GLN:HB3	4	0.44
(1,942)	1:114:A:LEU:HD11	1:114:A:LEU:HB3	2	0.44
(1,942)	1:114:A:LEU:HD12	1:114:A:LEU:HB3	2	0.44
(1,942)	1:114:A:LEU:HD13	1:114:A:LEU:HB3	2	0.44
(1,942)	1:114:A:LEU:HD11	1:114:A:LEU:HB3	8	0.44
(1,942)	1:114:A:LEU:HD12	1:114:A:LEU:HB3	8	0.44
(1,942)	1:114:A:LEU:HD13	1:114:A:LEU:HB3	8	0.44
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD11	10	0.44
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD12	10	0.44
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD13	10	0.44
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG21	7	0.44
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG22	7	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG23	7	0.44
(1,74)	1:68:A:LEU:H	1:55:A:ILE:HB	10	0.44
(1,942)	1:114:A:LEU:HD11	1:114:A:LEU:HB3	5	0.43
(1,942)	1:114:A:LEU:HD12	1:114:A:LEU:HB3	5	0.43
(1,942)	1:114:A:LEU:HD13	1:114:A:LEU:HB3	5	0.43
(1,942)	1:114:A:LEU:HD11	1:114:A:LEU:HB3	6	0.43
(1,942)	1:114:A:LEU:HD12	1:114:A:LEU:HB3	6	0.43
(1,942)	1:114:A:LEU:HD13	1:114:A:LEU:HB3	6	0.43
(1,732)	1:36:A:ARG:H	1:35:A:GLU:HB2	2	0.43
(1,597)	1:46:A:ILE:H	1:45:A:LYS:HG3	4	0.43
(1,390)	1:96:A:ILE:H	1:95:A:LEU:HG	10	0.43
(1,103)	1:47:A:LEU:H	1:48:A:SER:HA	5	0.43
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG21	3	0.43
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG22	3	0.43
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG23	3	0.43
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG21	9	0.43
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG22	9	0.43
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG23	9	0.43
(1,1088)	1:101:A:ASP:H	1:99:A:ILE:HB	6	0.42
(1,960)	1:28:A:LEU:H	1:28:A:LEU:HG	6	0.42
(1,942)	1:114:A:LEU:HD11	1:114:A:LEU:HB3	9	0.42
(1,942)	1:114:A:LEU:HD12	1:114:A:LEU:HB3	9	0.42
(1,942)	1:114:A:LEU:HD13	1:114:A:LEU:HB3	9	0.42
(1,880)	1:32:A:ILE:HD11	1:86:A:ILE:HG13	6	0.42
(1,880)	1:32:A:ILE:HD12	1:86:A:ILE:HG13	6	0.42
(1,880)	1:32:A:ILE:HD13	1:86:A:ILE:HG13	6	0.42
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG21	3	0.42
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG22	3	0.42
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG23	3	0.42
(1,685)	1:53:A:ARG:H	1:56:A:SER:H	7	0.42
(1,544)	1:70:A:ASP:H	1:68:A:LEU:HA	9	0.42
(1,508)	1:106:A:LEU:HD11	1:106:A:LEU:HB3	8	0.42
(1,508)	1:106:A:LEU:HD12	1:106:A:LEU:HB3	8	0.42
(1,508)	1:106:A:LEU:HD13	1:106:A:LEU:HB3	8	0.42
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD21	3	0.42
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD22	3	0.42
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD23	3	0.42
(1,227)	1:98:A:LYS:H	1:97:A:GLN:HB2	2	0.42
(1,152)	1:16:A:VAL:H	1:106:A:LEU:HB2	7	0.42
(1,74)	1:68:A:LEU:H	1:55:A:ILE:HB	3	0.42
(1,3)	1:56:A:SER:H	1:55:A:ILE:HG13	7	0.42
(1,1013)	1:64:A:ARG:H	1:62:A:ARG:HB3	7	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,942)	1:114:A:LEU:HD11	1:114:A:LEU:HB3	3	0.41
(1,942)	1:114:A:LEU:HD12	1:114:A:LEU:HB3	3	0.41
(1,942)	1:114:A:LEU:HD13	1:114:A:LEU:HB3	3	0.41
(1,727)	1:15:A:GLU:H	1:12:A:ASP:HA	2	0.41
(1,726)	1:93:A:ASN:H	1:94:A:PHE:HB2	4	0.41
(1,565)	1:44:A:LYS:H	1:44:A:LYS:HD2	10	0.41
(1,508)	1:106:A:LEU:HD11	1:106:A:LEU:HB3	4	0.41
(1,508)	1:106:A:LEU:HD12	1:106:A:LEU:HB3	4	0.41
(1,508)	1:106:A:LEU:HD13	1:106:A:LEU:HB3	4	0.41
(1,250)	1:24:A:LEU:HD11	1:102:A:GLU:HB3	7	0.41
(1,250)	1:24:A:LEU:HD12	1:102:A:GLU:HB3	7	0.41
(1,250)	1:24:A:LEU:HD13	1:102:A:GLU:HB3	7	0.41
(1,24)	1:52:A:THR:H	1:52:A:THR:HG21	8	0.41
(1,24)	1:52:A:THR:H	1:52:A:THR:HG22	8	0.41
(1,24)	1:52:A:THR:H	1:52:A:THR:HG23	8	0.41
(1,19)	1:82:A:LEU:HD21	1:46:A:ILE:HG13	8	0.41
(1,19)	1:82:A:LEU:HD22	1:46:A:ILE:HG13	8	0.41
(1,19)	1:82:A:LEU:HD23	1:46:A:ILE:HG13	8	0.41
(1,1046)	1:17:A:LYS:H	1:16:A:VAL:HB	1	0.4
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD11	8	0.4
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD12	8	0.4
(1,1042)	1:103:A:VAL:H	1:24:A:LEU:HD13	8	0.4
(1,836)	1:89:A:GLU:H	1:87:A:ARG:H	5	0.4
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD11	8	0.4
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD12	8	0.4
(1,806)	1:103:A:VAL:H	1:24:A:LEU:HD13	8	0.4
(1,732)	1:36:A:ARG:H	1:35:A:GLU:HB2	8	0.4
(1,1191)	1:11:A:GLU:H	1:14:A:THR:H	10	0.39
(1,1046)	1:17:A:LYS:H	1:16:A:VAL:HB	7	0.39
(1,813)	1:73:A:GLN:HE22	1:73:A:GLN:HG2	8	0.39
(1,732)	1:36:A:ARG:H	1:35:A:GLU:HB2	6	0.39
(1,726)	1:93:A:ASN:H	1:94:A:PHE:HB2	1	0.39
(1,544)	1:70:A:ASP:H	1:68:A:LEU:HA	2	0.39
(1,513)	1:112:A:GLU:H	1:114:A:LEU:H	4	0.39
(1,460)	1:50:A:GLU:HA	1:50:A:GLU:HG3	10	0.39
(1,339)	1:105:A:LYS:H	1:104:A:LEU:HB3	4	0.39
(1,129)	1:74:A:GLU:H	1:73:A:GLN:HB3	2	0.39
(1,88)	1:108:A:ASN:H	1:107:A:ARG:HB3	5	0.39
(1,1253)	1:54:A:GLU:H	1:57:A:CYS:H	10	0.38
(1,1088)	1:101:A:ASP:H	1:99:A:ILE:HB	2	0.38
(1,1046)	1:17:A:LYS:H	1:16:A:VAL:HB	8	0.38
(1,915)	1:21:A:LEU:HD11	1:79:A:LEU:HB3	2	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,915)	1:21:A:LEU:HD12	1:79:A:LEU:HB3	2	0.38
(1,915)	1:21:A:LEU:HD13	1:79:A:LEU:HB3	2	0.38
(1,640)	1:34:A:ALA:HB1	1:68:A:LEU:HB3	1	0.38
(1,640)	1:34:A:ALA:HB2	1:68:A:LEU:HB3	1	0.38
(1,640)	1:34:A:ALA:HB3	1:68:A:LEU:HB3	1	0.38
(1,597)	1:46:A:ILE:H	1:45:A:LYS:HG3	1	0.38
(1,597)	1:46:A:ILE:H	1:45:A:LYS:HG3	8	0.38
(1,149)	1:78:A:GLY:H	1:21:A:LEU:HD11	10	0.38
(1,149)	1:78:A:GLY:H	1:21:A:LEU:HD12	10	0.38
(1,149)	1:78:A:GLY:H	1:21:A:LEU:HD13	10	0.38
(1,1156)	1:75:A:ASN:H	1:18:A:LYS:HE3	4	0.37
(1,1046)	1:17:A:LYS:H	1:16:A:VAL:HB	6	0.37
(1,884)	1:89:A:GLU:H	1:89:A:GLU:HG2	7	0.37
(1,770)	1:47:A:LEU:H	1:47:A:LEU:HB3	10	0.37
(1,764)	1:32:A:ILE:HG13	1:69:A:LEU:HD21	9	0.37
(1,764)	1:32:A:ILE:HG13	1:69:A:LEU:HD22	9	0.37
(1,764)	1:32:A:ILE:HG13	1:69:A:LEU:HD23	9	0.37
(1,597)	1:46:A:ILE:H	1:45:A:LYS:HG3	2	0.37
(1,597)	1:46:A:ILE:H	1:45:A:LYS:HG3	3	0.37
(1,339)	1:105:A:LYS:H	1:104:A:LEU:HB3	7	0.37
(1,130)	1:16:A:VAL:H	1:13:A:LEU:HA	4	0.37
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG21	5	0.37
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG22	5	0.37
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG23	5	0.37
(1,1024)	1:39:A:ASP:H	1:38:A:PHE:HB2	2	0.36
(1,874)	1:74:A:GLU:H	1:75:A:ASN:H	8	0.36
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG21	5	0.36
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG22	5	0.36
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG23	5	0.36
(1,600)	1:39:A:ASP:H	1:38:A:PHE:HB2	2	0.36
(1,597)	1:46:A:ILE:H	1:45:A:LYS:HG3	9	0.36
(1,544)	1:70:A:ASP:H	1:68:A:LEU:HA	4	0.36
(1,488)	1:49:A:ARG:HD2	1:49:A:ARG:HB2	2	0.36
(1,460)	1:50:A:GLU:HA	1:50:A:GLU:HG3	3	0.36
(1,227)	1:98:A:LYS:H	1:97:A:GLN:HB2	9	0.36
(1,152)	1:16:A:VAL:H	1:106:A:LEU:HB2	9	0.36
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD11	3	0.36
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD12	3	0.36
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD13	3	0.36
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD11	3	0.36
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD12	3	0.36
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD13	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD11	3	0.36
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD12	3	0.36
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD13	3	0.36
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG21	7	0.35
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG22	7	0.35
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG23	7	0.35
(1,960)	1:28:A:LEU:H	1:28:A:LEU:HG	2	0.35
(1,935)	1:97:A:GLN:H	1:96:A:ILE:HG13	6	0.35
(1,887)	1:84:A:GLU:H	1:81:A:THR:HA	8	0.35
(1,764)	1:32:A:ILE:HG13	1:69:A:LEU:HD21	5	0.35
(1,764)	1:32:A:ILE:HG13	1:69:A:LEU:HD22	5	0.35
(1,764)	1:32:A:ILE:HG13	1:69:A:LEU:HD23	5	0.35
(1,628)	1:106:A:LEU:HB3	1:13:A:LEU:HB3	8	0.35
(1,544)	1:70:A:ASP:H	1:68:A:LEU:HA	5	0.35
(1,364)	1:14:A:THR:H	1:14:A:THR:HB	2	0.35
(1,1253)	1:54:A:GLU:H	1:57:A:CYS:H	5	0.34
(1,1191)	1:11:A:GLU:H	1:14:A:THR:H	7	0.34
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG21	1	0.34
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG22	1	0.34
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG23	1	0.34
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG21	2	0.34
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG22	2	0.34
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG23	2	0.34
(1,1046)	1:17:A:LYS:H	1:16:A:VAL:HB	4	0.34
(1,802)	1:27:A:TYR:HE1	1:23:A:ASN:HB3	4	0.34
(1,802)	1:27:A:TYR:HE2	1:23:A:ASN:HB3	4	0.34
(1,727)	1:15:A:GLU:H	1:12:A:ASP:HA	6	0.34
(1,488)	1:49:A:ARG:HD2	1:49:A:ARG:HB2	1	0.34
(1,339)	1:105:A:LYS:H	1:104:A:LEU:HB3	10	0.34
(1,250)	1:24:A:LEU:HD11	1:102:A:GLU:HB3	9	0.34
(1,250)	1:24:A:LEU:HD12	1:102:A:GLU:HB3	9	0.34
(1,250)	1:24:A:LEU:HD13	1:102:A:GLU:HB3	9	0.34
(1,227)	1:98:A:LYS:H	1:97:A:GLN:HB2	1	0.34
(1,92)	1:42:A:ARG:HD2	1:41:A:LEU:HB3	7	0.34
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD11	8	0.34
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD12	8	0.34
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD13	8	0.34
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD11	8	0.34
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD12	8	0.34
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD13	8	0.34
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD11	8	0.34
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD12	8	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD13	8	0.34
(1,732)	1:36:A:ARG:H	1:35:A:GLU:HB2	10	0.33
(1,364)	1:14:A:THR:H	1:14:A:THR:HB	5	0.33
(1,250)	1:24:A:LEU:HD11	1:102:A:GLU:HB3	5	0.33
(1,250)	1:24:A:LEU:HD12	1:102:A:GLU:HB3	5	0.33
(1,250)	1:24:A:LEU:HD13	1:102:A:GLU:HB3	5	0.33
(1,180)	1:98:A:LYS:H	1:99:A:ILE:HG12	7	0.33
(1,1109)	1:83:A:VAL:HG11	1:86:A:ILE:HD11	9	0.32
(1,1109)	1:83:A:VAL:HG11	1:86:A:ILE:HD12	9	0.32
(1,1109)	1:83:A:VAL:HG11	1:86:A:ILE:HD13	9	0.32
(1,1109)	1:83:A:VAL:HG12	1:86:A:ILE:HD11	9	0.32
(1,1109)	1:83:A:VAL:HG12	1:86:A:ILE:HD12	9	0.32
(1,1109)	1:83:A:VAL:HG12	1:86:A:ILE:HD13	9	0.32
(1,1109)	1:83:A:VAL:HG13	1:86:A:ILE:HD11	9	0.32
(1,1109)	1:83:A:VAL:HG13	1:86:A:ILE:HD12	9	0.32
(1,1109)	1:83:A:VAL:HG13	1:86:A:ILE:HD13	9	0.32
(1,1018)	1:50:A:GLU:H	1:51:A:ASP:HB2	8	0.32
(1,955)	1:73:A:GLN:H	1:73:A:GLN:HB3	10	0.32
(1,817)	1:42:A:ARG:H	1:41:A:LEU:HB2	2	0.32
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG21	4	0.32
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG22	4	0.32
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG23	4	0.32
(1,544)	1:70:A:ASP:H	1:68:A:LEU:HA	6	0.32
(1,322)	1:42:A:ARG:HD2	1:42:A:ARG:HB2	3	0.32
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD11	4	0.32
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD12	4	0.32
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD13	4	0.32
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD11	4	0.32
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD12	4	0.32
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD13	4	0.32
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD11	4	0.32
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD12	4	0.32
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD13	4	0.32
(1,1278)	1:34:A:ALA:H	1:33:A:ILE:HA	1	0.31
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG21	9	0.31
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG22	9	0.31
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG23	9	0.31
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG21	10	0.31
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG22	10	0.31
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG23	10	0.31
(1,628)	1:106:A:LEU:HB3	1:13:A:LEU:HB3	9	0.31
(1,513)	1:112:A:GLU:H	1:114:A:LEU:H	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,68)	1:54:A:GLU:HA	1:54:A:GLU:HG3	10	0.31
(1,28)	1:102:A:GLU:HA	1:102:A:GLU:HG3	9	0.31
(1,1227)	1:10:A:GLU:H	1:11:A:GLU:HG2	4	0.3
(1,1176)	1:32:A:ILE:H	1:32:A:ILE:HG13	9	0.3
(1,1158)	1:78:A:GLY:HA3	1:72:A:LEU:HD21	6	0.3
(1,1158)	1:78:A:GLY:HA3	1:72:A:LEU:HD22	6	0.3
(1,1158)	1:78:A:GLY:HA3	1:72:A:LEU:HD23	6	0.3
(1,1094)	1:89:A:GLU:H	1:88:A:ARG:HB3	1	0.3
(1,1067)	1:34:A:ALA:HA	1:68:A:LEU:HD21	1	0.3
(1,1067)	1:34:A:ALA:HA	1:68:A:LEU:HD22	1	0.3
(1,1067)	1:34:A:ALA:HA	1:68:A:LEU:HD23	1	0.3
(1,916)	1:36:A:ARG:H	1:36:A:ARG:HG3	1	0.3
(1,813)	1:73:A:GLN:HE22	1:73:A:GLN:HG2	4	0.3
(1,813)	1:73:A:GLN:HE22	1:73:A:GLN:HG2	9	0.3
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG21	6	0.3
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG22	6	0.3
(1,758)	1:106:A:LEU:H	1:16:A:VAL:HG23	6	0.3
(1,620)	1:40:A:HIS:H	1:39:A:ASP:HB3	1	0.3
(1,620)	1:40:A:HIS:H	1:39:A:ASP:HB3	5	0.3
(1,607)	1:19:A:ASP:H	1:18:A:LYS:HB2	1	0.3
(1,460)	1:50:A:GLU:HA	1:50:A:GLU:HG3	2	0.3
(1,448)	1:47:A:LEU:H	1:46:A:ILE:H	1	0.3
(1,442)	1:34:A:ALA:HB1	1:32:A:ILE:HG12	1	0.3
(1,442)	1:34:A:ALA:HB2	1:32:A:ILE:HG12	1	0.3
(1,442)	1:34:A:ALA:HB3	1:32:A:ILE:HG12	1	0.3
(1,327)	1:63:A:LYS:HE3	1:63:A:LYS:HG2	2	0.3
(1,246)	1:45:A:LYS:H	1:45:A:LYS:HG2	4	0.3
(1,103)	1:47:A:LEU:H	1:48:A:SER:HA	10	0.3
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD11	2	0.29
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD12	2	0.29
(1,1234)	1:86:A:ILE:H	1:96:A:ILE:HD13	2	0.29
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD11	6	0.29
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD12	6	0.29
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD13	6	0.29
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD11	6	0.29
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD12	6	0.29
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD13	6	0.29
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD11	6	0.29
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD12	6	0.29
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD13	6	0.29
(1,813)	1:73:A:GLN:HE22	1:73:A:GLN:HG2	3	0.29
(1,813)	1:73:A:GLN:HE22	1:73:A:GLN:HG2	5	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,772)	1:71:A:TYR:HE1	1:55:A:ILE:HB	2	0.29
(1,772)	1:71:A:TYR:HE2	1:55:A:ILE:HB	2	0.29
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG21	3	0.29
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG22	3	0.29
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG23	3	0.29
(1,620)	1:40:A:HIS:H	1:39:A:ASP:HB3	9	0.29
(1,619)	1:87:A:ARG:HA	1:96:A:ILE:HG21	5	0.29
(1,619)	1:87:A:ARG:HA	1:96:A:ILE:HG22	5	0.29
(1,619)	1:87:A:ARG:HA	1:96:A:ILE:HG23	5	0.29
(1,447)	1:31:A:LYS:H	1:32:A:ILE:HB	7	0.29
(1,402)	1:51:A:ASP:H	1:50:A:GLU:HB2	1	0.29
(1,402)	1:51:A:ASP:H	1:50:A:GLU:HB2	2	0.29
(1,185)	1:46:A:ILE:H	1:44:A:LYS:HB3	6	0.29
(1,28)	1:102:A:GLU:HA	1:102:A:GLU:HG3	5	0.29
(1,1258)	1:88:A:ARG:HA	1:88:A:ARG:HG3	10	0.28
(1,1241)	1:96:A:ILE:HD11	1:93:A:ASN:HA	5	0.28
(1,1241)	1:96:A:ILE:HD12	1:93:A:ASN:HA	5	0.28
(1,1241)	1:96:A:ILE:HD13	1:93:A:ASN:HA	5	0.28
(1,1049)	1:74:A:GLU:H	1:74:A:GLU:HG2	9	0.28
(1,1034)	1:79:A:LEU:H	1:79:A:LEU:HB3	9	0.28
(1,813)	1:73:A:GLN:HE22	1:73:A:GLN:HG2	1	0.28
(1,813)	1:73:A:GLN:HE22	1:73:A:GLN:HG2	2	0.28
(1,813)	1:73:A:GLN:HE22	1:73:A:GLN:HG2	6	0.28
(1,813)	1:73:A:GLN:HE22	1:73:A:GLN:HG2	7	0.28
(1,726)	1:93:A:ASN:H	1:94:A:PHE:HB2	6	0.28
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG21	5	0.28
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG22	5	0.28
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG23	5	0.28
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG21	8	0.28
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG22	8	0.28
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG23	8	0.28
(1,378)	1:83:A:VAL:HB	1:82:A:LEU:HB2	10	0.28
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD21	2	0.28
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD22	2	0.28
(1,353)	1:20:A:ALA:H	1:106:A:LEU:HD23	2	0.28
(1,319)	1:72:A:LEU:HD21	1:72:A:LEU:HA	9	0.28
(1,319)	1:72:A:LEU:HD22	1:72:A:LEU:HA	9	0.28
(1,319)	1:72:A:LEU:HD23	1:72:A:LEU:HA	9	0.28
(1,251)	1:74:A:GLU:H	1:74:A:GLU:HG3	6	0.28
(1,239)	1:93:A:ASN:HD22	1:93:A:ASN:HB3	6	0.28
(1,180)	1:98:A:LYS:H	1:99:A:ILE:HG12	3	0.28
(1,158)	1:66:A:GLY:H	1:67:A:LYS:HB3	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,103)	1:47:A:LEU:H	1:48:A:SER:HA	2	0.28
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG21	2	0.28
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG22	2	0.28
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG23	2	0.28
(1,1176)	1:32:A:ILE:H	1:32:A:ILE:HG13	4	0.27
(1,1046)	1:17:A:LYS:H	1:16:A:VAL:HB	10	0.27
(1,715)	1:35:A:GLU:H	1:35:A:GLU:HG2	10	0.27
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG21	1	0.27
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG22	1	0.27
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG23	1	0.27
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG21	2	0.27
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG22	2	0.27
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG23	2	0.27
(1,438)	1:52:A:THR:H	1:47:A:LEU:HB3	1	0.27
(1,424)	1:11:A:GLU:H	1:11:A:GLU:HB2	8	0.27
(1,298)	1:97:A:GLN:HA	1:97:A:GLN:HG3	6	0.27
(1,265)	1:73:A:GLN:H	1:71:A:TYR:HA	9	0.27
(1,251)	1:74:A:GLU:H	1:74:A:GLU:HG3	4	0.27
(1,239)	1:93:A:ASN:HD22	1:93:A:ASN:HB3	9	0.27
(1,227)	1:98:A:LYS:H	1:97:A:GLN:HB2	3	0.27
(1,145)	1:16:A:VAL:H	1:16:A:VAL:HG21	2	0.27
(1,145)	1:16:A:VAL:H	1:16:A:VAL:HG22	2	0.27
(1,145)	1:16:A:VAL:H	1:16:A:VAL:HG23	2	0.27
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD11	6	0.27
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD12	6	0.27
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD13	6	0.27
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD11	6	0.27
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD12	6	0.27
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD13	6	0.27
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD11	6	0.27
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD12	6	0.27
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD13	6	0.27
(1,28)	1:102:A:GLU:HA	1:102:A:GLU:HG3	6	0.27
(1,28)	1:102:A:GLU:HA	1:102:A:GLU:HG3	10	0.27
(1,24)	1:52:A:THR:H	1:52:A:THR:HG21	9	0.27
(1,24)	1:52:A:THR:H	1:52:A:THR:HG22	9	0.27
(1,24)	1:52:A:THR:H	1:52:A:THR:HG23	9	0.27
(1,1198)	1:108:A:ASN:HD22	1:108:A:ASN:HB2	9	0.26
(1,1108)	1:65:A:ALA:HA	1:35:A:GLU:HB2	4	0.26
(1,1094)	1:89:A:GLU:H	1:88:A:ARG:HB3	4	0.26
(1,1094)	1:89:A:GLU:H	1:88:A:ARG:HB3	7	0.26
(1,937)	1:111:A:LEU:H	1:110:A:LYS:HG3	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,935)	1:97:A:GLN:H	1:96:A:ILE:HG13	2	0.26
(1,880)	1:32:A:ILE:HD11	1:86:A:ILE:HG13	2	0.26
(1,880)	1:32:A:ILE:HD12	1:86:A:ILE:HG13	2	0.26
(1,880)	1:32:A:ILE:HD13	1:86:A:ILE:HG13	2	0.26
(1,770)	1:47:A:LEU:H	1:47:A:LEU:HB3	1	0.26
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG21	6	0.26
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG22	6	0.26
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG23	6	0.26
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG21	7	0.26
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG22	7	0.26
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG23	7	0.26
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG21	9	0.26
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG22	9	0.26
(1,630)	1:99:A:ILE:H	1:99:A:ILE:HG23	9	0.26
(1,620)	1:40:A:HIS:H	1:39:A:ASP:HB3	3	0.26
(1,528)	1:31:A:LYS:H	1:28:A:LEU:HB3	3	0.26
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG21	1	0.26
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG22	1	0.26
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG23	1	0.26
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG21	8	0.26
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG22	8	0.26
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG23	8	0.26
(1,460)	1:50:A:GLU:HA	1:50:A:GLU:HG3	7	0.26
(1,460)	1:50:A:GLU:HA	1:50:A:GLU:HG3	9	0.26
(1,447)	1:31:A:LYS:H	1:32:A:ILE:HB	5	0.26
(1,339)	1:105:A:LYS:H	1:104:A:LEU:HB3	3	0.26
(1,239)	1:93:A:ASN:HD22	1:93:A:ASN:HB3	1	0.26
(1,239)	1:93:A:ASN:HD22	1:93:A:ASN:HB3	5	0.26
(1,239)	1:93:A:ASN:HD22	1:93:A:ASN:HB3	10	0.26
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG21	4	0.26
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG22	4	0.26
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG23	4	0.26
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG21	6	0.26
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG22	6	0.26
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG23	6	0.26
(1,28)	1:102:A:GLU:HA	1:102:A:GLU:HG3	2	0.26
(1,27)	1:27:A:TYR:H	1:27:A:TYR:HB2	1	0.26
(1,27)	1:27:A:TYR:H	1:27:A:TYR:HB2	2	0.26
(1,27)	1:27:A:TYR:H	1:27:A:TYR:HB2	6	0.26
(1,24)	1:52:A:THR:H	1:52:A:THR:HG21	3	0.26
(1,24)	1:52:A:THR:H	1:52:A:THR:HG22	3	0.26
(1,24)	1:52:A:THR:H	1:52:A:THR:HG23	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:52:A:THR:H	1:52:A:THR:HG21	10	0.26
(1,24)	1:52:A:THR:H	1:52:A:THR:HG22	10	0.26
(1,24)	1:52:A:THR:H	1:52:A:THR:HG23	10	0.26
(1,19)	1:82:A:LEU:HD21	1:46:A:ILE:HG13	3	0.26
(1,19)	1:82:A:LEU:HD22	1:46:A:ILE:HG13	3	0.26
(1,19)	1:82:A:LEU:HD23	1:46:A:ILE:HG13	3	0.26
(1,1032)	1:63:A:LYS:HE3	1:63:A:LYS:HD2	9	0.25
(1,995)	1:30:A:GLU:H	1:30:A:GLU:HB3	2	0.25
(1,960)	1:28:A:LEU:H	1:28:A:LEU:HG	8	0.25
(1,817)	1:42:A:ARG:H	1:41:A:LEU:HB2	10	0.25
(1,732)	1:36:A:ARG:H	1:35:A:GLU:HB2	9	0.25
(1,452)	1:102:A:GLU:H	1:24:A:LEU:HD11	9	0.25
(1,452)	1:102:A:GLU:H	1:24:A:LEU:HD12	9	0.25
(1,452)	1:102:A:GLU:H	1:24:A:LEU:HD13	9	0.25
(1,448)	1:47:A:LEU:H	1:46:A:ILE:H	7	0.25
(1,364)	1:14:A:THR:H	1:14:A:THR:HB	8	0.25
(1,350)	1:27:A:TYR:HE1	1:28:A:LEU:HB2	9	0.25
(1,350)	1:27:A:TYR:HE2	1:28:A:LEU:HB2	9	0.25
(1,265)	1:73:A:GLN:H	1:71:A:TYR:HA	5	0.25
(1,150)	1:31:A:LYS:H	1:31:A:LYS:HG2	1	0.25
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD11	10	0.25
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD12	10	0.25
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD13	10	0.25
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD11	10	0.25
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD12	10	0.25
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD13	10	0.25
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD11	10	0.25
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD12	10	0.25
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD13	10	0.25
(1,28)	1:102:A:GLU:HA	1:102:A:GLU:HG3	3	0.25
(1,24)	1:52:A:THR:H	1:52:A:THR:HG21	6	0.25
(1,24)	1:52:A:THR:H	1:52:A:THR:HG22	6	0.25
(1,24)	1:52:A:THR:H	1:52:A:THR:HG23	6	0.25
(1,1258)	1:88:A:ARG:HA	1:88:A:ARG:HG3	1	0.24
(1,1156)	1:75:A:ASN:H	1:18:A:LYS:HE3	5	0.24
(1,1111)	1:38:A:PHE:HD1	1:52:A:THR:HG21	9	0.24
(1,1111)	1:38:A:PHE:HD1	1:52:A:THR:HG22	9	0.24
(1,1111)	1:38:A:PHE:HD1	1:52:A:THR:HG23	9	0.24
(1,1111)	1:38:A:PHE:HD2	1:52:A:THR:HG21	9	0.24
(1,1111)	1:38:A:PHE:HD2	1:52:A:THR:HG22	9	0.24
(1,1111)	1:38:A:PHE:HD2	1:52:A:THR:HG23	9	0.24
(1,1018)	1:50:A:GLU:H	1:51:A:ASP:HB2	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,975)	1:54:A:GLU:H	1:54:A:GLU:HG3	9	0.24
(1,974)	1:89:A:GLU:H	1:88:A:ARG:H	9	0.24
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD11	5	0.24
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD12	5	0.24
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD13	5	0.24
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD11	6	0.24
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD12	6	0.24
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD13	6	0.24
(1,935)	1:97:A:GLN:H	1:96:A:ILE:HG13	7	0.24
(1,886)	1:96:A:ILE:HD11	1:89:A:GLU:HB2	1	0.24
(1,886)	1:96:A:ILE:HD12	1:89:A:GLU:HB2	1	0.24
(1,886)	1:96:A:ILE:HD13	1:89:A:GLU:HB2	1	0.24
(1,886)	1:96:A:ILE:HD11	1:89:A:GLU:HB2	7	0.24
(1,886)	1:96:A:ILE:HD12	1:89:A:GLU:HB2	7	0.24
(1,886)	1:96:A:ILE:HD13	1:89:A:GLU:HB2	7	0.24
(1,694)	1:36:A:ARG:H	1:36:A:ARG:HB3	4	0.24
(1,628)	1:106:A:LEU:HB3	1:13:A:LEU:HB3	4	0.24
(1,620)	1:40:A:HIS:H	1:39:A:ASP:HB3	6	0.24
(1,549)	1:65:A:ALA:HB1	1:33:A:ILE:HG21	1	0.24
(1,549)	1:65:A:ALA:HB1	1:33:A:ILE:HG22	1	0.24
(1,549)	1:65:A:ALA:HB1	1:33:A:ILE:HG23	1	0.24
(1,549)	1:65:A:ALA:HB2	1:33:A:ILE:HG21	1	0.24
(1,549)	1:65:A:ALA:HB2	1:33:A:ILE:HG22	1	0.24
(1,549)	1:65:A:ALA:HB2	1:33:A:ILE:HG23	1	0.24
(1,549)	1:65:A:ALA:HB3	1:33:A:ILE:HG21	1	0.24
(1,549)	1:65:A:ALA:HB3	1:33:A:ILE:HG22	1	0.24
(1,549)	1:65:A:ALA:HB3	1:33:A:ILE:HG23	1	0.24
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD11	3	0.24
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD12	3	0.24
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD13	3	0.24
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD11	3	0.24
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD12	3	0.24
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD13	3	0.24
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD11	3	0.24
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD12	3	0.24
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD13	3	0.24
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD11	9	0.24
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD12	9	0.24
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD13	9	0.24
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD11	9	0.24
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD12	9	0.24
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD13	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD11	9	0.24
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD12	9	0.24
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD13	9	0.24
(1,382)	1:54:A:GLU:H	1:54:A:GLU:HG3	9	0.24
(1,291)	1:16:A:VAL:HG21	1:16:A:VAL:HA	3	0.24
(1,291)	1:16:A:VAL:HG22	1:16:A:VAL:HA	3	0.24
(1,291)	1:16:A:VAL:HG23	1:16:A:VAL:HA	3	0.24
(1,259)	1:53:A:ARG:HA	1:53:A:ARG:HG3	5	0.24
(1,153)	1:114:A:LEU:HD11	1:115:A:LYS:HA	3	0.24
(1,153)	1:114:A:LEU:HD12	1:115:A:LYS:HA	3	0.24
(1,153)	1:114:A:LEU:HD13	1:115:A:LYS:HA	3	0.24
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG21	3	0.24
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG22	3	0.24
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG23	3	0.24
(1,27)	1:27:A:TYR:H	1:27:A:TYR:HB2	5	0.24
(1,27)	1:27:A:TYR:H	1:27:A:TYR:HB2	9	0.24
(1,1176)	1:32:A:ILE:H	1:32:A:ILE:HG13	2	0.23
(1,1169)	1:73:A:GLN:H	1:72:A:LEU:H	8	0.23
(1,1155)	1:71:A:TYR:HD1	1:68:A:LEU:HG	4	0.23
(1,1155)	1:71:A:TYR:HD2	1:68:A:LEU:HG	4	0.23
(1,1094)	1:89:A:GLU:H	1:88:A:ARG:HB3	2	0.23
(1,1032)	1:63:A:LYS:HE3	1:63:A:LYS:HD2	4	0.23
(1,1005)	1:82:A:LEU:HD11	1:72:A:LEU:HD21	1	0.23
(1,1005)	1:82:A:LEU:HD11	1:72:A:LEU:HD22	1	0.23
(1,1005)	1:82:A:LEU:HD11	1:72:A:LEU:HD23	1	0.23
(1,1005)	1:82:A:LEU:HD12	1:72:A:LEU:HD21	1	0.23
(1,1005)	1:82:A:LEU:HD12	1:72:A:LEU:HD22	1	0.23
(1,1005)	1:82:A:LEU:HD12	1:72:A:LEU:HD23	1	0.23
(1,1005)	1:82:A:LEU:HD13	1:72:A:LEU:HD21	1	0.23
(1,1005)	1:82:A:LEU:HD13	1:72:A:LEU:HD22	1	0.23
(1,1005)	1:82:A:LEU:HD13	1:72:A:LEU:HD23	1	0.23
(1,854)	1:54:A:GLU:H	1:53:A:ARG:HB3	2	0.23
(1,743)	1:47:A:LEU:HD11	1:47:A:LEU:HA	5	0.23
(1,743)	1:47:A:LEU:HD12	1:47:A:LEU:HA	5	0.23
(1,743)	1:47:A:LEU:HD13	1:47:A:LEU:HA	5	0.23
(1,694)	1:36:A:ARG:H	1:36:A:ARG:HB3	9	0.23
(1,679)	1:64:A:ARG:HB3	1:35:A:GLU:HG3	7	0.23
(1,658)	1:51:A:ASP:HA	1:54:A:GLU:HG3	6	0.23
(1,513)	1:112:A:GLU:H	1:114:A:LEU:H	7	0.23
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD21	10	0.23
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD22	10	0.23
(1,497)	1:47:A:LEU:H	1:41:A:LEU:HD23	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,308)	1:104:A:LEU:HA	1:13:A:LEU:HB2	2	0.23
(1,308)	1:104:A:LEU:HA	1:13:A:LEU:HB2	5	0.23
(1,278)	1:29:A:CYS:H	1:30:A:GLU:HB2	4	0.23
(1,180)	1:98:A:LYS:H	1:99:A:ILE:HG12	8	0.23
(1,178)	1:105:A:LYS:H	1:105:A:LYS:HD2	9	0.23
(1,158)	1:66:A:GLY:H	1:67:A:LYS:HB3	10	0.23
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG21	1	0.23
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG22	1	0.23
(1,85)	1:82:A:LEU:H	1:83:A:VAL:HG23	1	0.23
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD11	2	0.23
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD12	2	0.23
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD13	2	0.23
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD11	2	0.23
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD12	2	0.23
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD13	2	0.23
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD11	2	0.23
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD12	2	0.23
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD13	2	0.23
(1,27)	1:27:A:TYR:H	1:27:A:TYR:HB2	3	0.23
(1,27)	1:27:A:TYR:H	1:27:A:TYR:HB2	7	0.23
(1,1283)	1:47:A:LEU:HD11	1:71:A:TYR:HB2	3	0.22
(1,1283)	1:47:A:LEU:HD12	1:71:A:TYR:HB2	3	0.22
(1,1283)	1:47:A:LEU:HD13	1:71:A:TYR:HB2	3	0.22
(1,1246)	1:46:A:ILE:H	1:81:A:THR:HG21	9	0.22
(1,1246)	1:46:A:ILE:H	1:81:A:THR:HG22	9	0.22
(1,1246)	1:46:A:ILE:H	1:81:A:THR:HG23	9	0.22
(1,1211)	1:71:A:TYR:HD1	1:68:A:LEU:HB3	5	0.22
(1,1211)	1:71:A:TYR:HD2	1:68:A:LEU:HB3	5	0.22
(1,1108)	1:65:A:ALA:HA	1:35:A:GLU:HB2	2	0.22
(1,1108)	1:65:A:ALA:HA	1:35:A:GLU:HB2	5	0.22
(1,1108)	1:65:A:ALA:HA	1:35:A:GLU:HB2	8	0.22
(1,1096)	1:69:A:LEU:HA	1:72:A:LEU:HD21	1	0.22
(1,1096)	1:69:A:LEU:HA	1:72:A:LEU:HD22	1	0.22
(1,1096)	1:69:A:LEU:HA	1:72:A:LEU:HD23	1	0.22
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD11	8	0.22
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD12	8	0.22
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD13	8	0.22
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD11	8	0.22
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD12	8	0.22
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD13	8	0.22
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD11	8	0.22
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD12	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD13	8	0.22
(1,975)	1:54:A:GLU:H	1:54:A:GLU:HG3	6	0.22
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD11	3	0.22
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD12	3	0.22
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD13	3	0.22
(1,935)	1:97:A:GLN:H	1:96:A:ILE:HG13	1	0.22
(1,791)	1:62:A:ARG:HB3	1:62:A:ARG:HG3	3	0.22
(1,770)	1:47:A:LEU:H	1:47:A:LEU:HB3	6	0.22
(1,743)	1:47:A:LEU:HD11	1:47:A:LEU:HA	1	0.22
(1,743)	1:47:A:LEU:HD12	1:47:A:LEU:HA	1	0.22
(1,743)	1:47:A:LEU:HD13	1:47:A:LEU:HA	1	0.22
(1,732)	1:36:A:ARG:H	1:35:A:GLU:HB2	4	0.22
(1,644)	1:79:A:LEU:HD11	1:82:A:LEU:HD21	3	0.22
(1,644)	1:79:A:LEU:HD11	1:82:A:LEU:HD22	3	0.22
(1,644)	1:79:A:LEU:HD11	1:82:A:LEU:HD23	3	0.22
(1,644)	1:79:A:LEU:HD12	1:82:A:LEU:HD21	3	0.22
(1,644)	1:79:A:LEU:HD12	1:82:A:LEU:HD22	3	0.22
(1,644)	1:79:A:LEU:HD12	1:82:A:LEU:HD23	3	0.22
(1,644)	1:79:A:LEU:HD13	1:82:A:LEU:HD21	3	0.22
(1,644)	1:79:A:LEU:HD13	1:82:A:LEU:HD22	3	0.22
(1,644)	1:79:A:LEU:HD13	1:82:A:LEU:HD23	3	0.22
(1,607)	1:19:A:ASP:H	1:18:A:LYS:HB2	8	0.22
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG21	2	0.22
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG22	2	0.22
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG23	2	0.22
(1,520)	1:14:A:THR:H	1:11:A:GLU:HA	4	0.22
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD11	10	0.22
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD12	10	0.22
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD13	10	0.22
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD11	10	0.22
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD12	10	0.22
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD13	10	0.22
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD11	10	0.22
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD12	10	0.22
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD13	10	0.22
(1,448)	1:47:A:LEU:H	1:46:A:ILE:H	4	0.22
(1,382)	1:54:A:GLU:H	1:54:A:GLU:HG3	6	0.22
(1,291)	1:16:A:VAL:HG21	1:16:A:VAL:HA	5	0.22
(1,291)	1:16:A:VAL:HG22	1:16:A:VAL:HA	5	0.22
(1,291)	1:16:A:VAL:HG23	1:16:A:VAL:HA	5	0.22
(1,291)	1:16:A:VAL:HG21	1:16:A:VAL:HA	6	0.22
(1,291)	1:16:A:VAL:HG22	1:16:A:VAL:HA	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,291)	1:16:A:VAL:HG23	1:16:A:VAL:HA	6	0.22
(1,291)	1:16:A:VAL:HG21	1:16:A:VAL:HA	9	0.22
(1,291)	1:16:A:VAL:HG22	1:16:A:VAL:HA	9	0.22
(1,291)	1:16:A:VAL:HG23	1:16:A:VAL:HA	9	0.22
(1,259)	1:53:A:ARG:HA	1:53:A:ARG:HG3	1	0.22
(1,190)	1:107:A:ARG:HB2	1:107:A:ARG:HG3	9	0.22
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG21	5	0.22
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG22	5	0.22
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG23	5	0.22
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG21	6	0.22
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG22	6	0.22
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG23	6	0.22
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG21	9	0.22
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG22	9	0.22
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG23	9	0.22
(1,115)	1:16:A:VAL:HG21	1:15:A:GLU:HB2	2	0.22
(1,115)	1:16:A:VAL:HG22	1:15:A:GLU:HB2	2	0.22
(1,115)	1:16:A:VAL:HG23	1:15:A:GLU:HB2	2	0.22
(1,1284)	1:98:A:LYS:H	1:95:A:LEU:HA	9	0.21
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG21	5	0.21
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG22	5	0.21
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG23	5	0.21
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG21	5	0.21
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG22	5	0.21
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG23	5	0.21
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG21	5	0.21
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG22	5	0.21
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG23	5	0.21
(1,1181)	1:19:A:ASP:H	1:16:A:VAL:HA	8	0.21
(1,1094)	1:89:A:GLU:H	1:88:A:ARG:HB3	6	0.21
(1,1046)	1:17:A:LYS:H	1:16:A:VAL:HB	2	0.21
(1,1029)	1:97:A:GLN:HG3	1:97:A:GLN:HB3	3	0.21
(1,1029)	1:97:A:GLN:HG3	1:97:A:GLN:HB3	7	0.21
(1,994)	1:40:A:HIS:H	1:40:A:HIS:HB3	5	0.21
(1,955)	1:73:A:GLN:H	1:73:A:GLN:HB3	1	0.21
(1,943)	1:47:A:LEU:HD21	1:72:A:LEU:HD21	7	0.21
(1,943)	1:47:A:LEU:HD21	1:72:A:LEU:HD22	7	0.21
(1,943)	1:47:A:LEU:HD21	1:72:A:LEU:HD23	7	0.21
(1,943)	1:47:A:LEU:HD22	1:72:A:LEU:HD21	7	0.21
(1,943)	1:47:A:LEU:HD22	1:72:A:LEU:HD22	7	0.21
(1,943)	1:47:A:LEU:HD22	1:72:A:LEU:HD23	7	0.21
(1,943)	1:47:A:LEU:HD23	1:72:A:LEU:HD21	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,943)	1:47:A:LEU:HD23	1:72:A:LEU:HD22	7	0.21
(1,943)	1:47:A:LEU:HD23	1:72:A:LEU:HD23	7	0.21
(1,931)	1:12:A:ASP:H	1:11:A:GLU:HB2	2	0.21
(1,915)	1:21:A:LEU:HD11	1:79:A:LEU:HB3	4	0.21
(1,915)	1:21:A:LEU:HD12	1:79:A:LEU:HB3	4	0.21
(1,915)	1:21:A:LEU:HD13	1:79:A:LEU:HB3	4	0.21
(1,791)	1:62:A:ARG:HB3	1:62:A:ARG:HG3	8	0.21
(1,791)	1:62:A:ARG:HB3	1:62:A:ARG:HG3	10	0.21
(1,770)	1:47:A:LEU:H	1:47:A:LEU:HB3	8	0.21
(1,642)	1:73:A:GLN:HA	1:73:A:GLN:HG2	9	0.21
(1,614)	1:115:A:LYS:HE3	1:115:A:LYS:HD3	10	0.21
(1,533)	1:79:A:LEU:HD11	1:80:A:ASP:HA	9	0.21
(1,533)	1:79:A:LEU:HD12	1:80:A:ASP:HA	9	0.21
(1,533)	1:79:A:LEU:HD13	1:80:A:ASP:HA	9	0.21
(1,530)	1:59:A:THR:HG21	1:64:A:ARG:HG2	1	0.21
(1,530)	1:59:A:THR:HG22	1:64:A:ARG:HG2	1	0.21
(1,530)	1:59:A:THR:HG23	1:64:A:ARG:HG2	1	0.21
(1,470)	1:16:A:VAL:HG21	1:106:A:LEU:HB3	7	0.21
(1,470)	1:16:A:VAL:HG22	1:106:A:LEU:HB3	7	0.21
(1,470)	1:16:A:VAL:HG23	1:106:A:LEU:HB3	7	0.21
(1,448)	1:47:A:LEU:H	1:46:A:ILE:H	6	0.21
(1,319)	1:72:A:LEU:HD21	1:72:A:LEU:HA	7	0.21
(1,319)	1:72:A:LEU:HD22	1:72:A:LEU:HA	7	0.21
(1,319)	1:72:A:LEU:HD23	1:72:A:LEU:HA	7	0.21
(1,145)	1:16:A:VAL:H	1:16:A:VAL:HG21	8	0.21
(1,145)	1:16:A:VAL:H	1:16:A:VAL:HG22	8	0.21
(1,145)	1:16:A:VAL:H	1:16:A:VAL:HG23	8	0.21
(1,130)	1:16:A:VAL:H	1:13:A:LEU:HA	1	0.21
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG21	5	0.21
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG22	5	0.21
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG23	5	0.21
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG21	5	0.21
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG22	5	0.21
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG23	5	0.21
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG21	5	0.21
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG22	5	0.21
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG23	5	0.21
(1,28)	1:102:A:GLU:HA	1:102:A:GLU:HG3	7	0.21
(1,27)	1:27:A:TYR:H	1:27:A:TYR:HB2	4	0.21
(1,27)	1:27:A:TYR:H	1:27:A:TYR:HB2	10	0.21
(1,1220)	1:74:A:GLU:HG3	1:74:A:GLU:HB3	3	0.2
(1,1176)	1:32:A:ILE:H	1:32:A:ILE:HG13	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1155)	1:71:A:TYR:HD1	1:68:A:LEU:HG	1	0.2
(1,1155)	1:71:A:TYR:HD2	1:68:A:LEU:HG	1	0.2
(1,1155)	1:71:A:TYR:HD1	1:68:A:LEU:HG	6	0.2
(1,1155)	1:71:A:TYR:HD2	1:68:A:LEU:HG	6	0.2
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG21	4	0.2
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG22	4	0.2
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG23	4	0.2
(1,1034)	1:79:A:LEU:H	1:79:A:LEU:HB3	7	0.2
(1,1029)	1:97:A:GLN:HG3	1:97:A:GLN:HB3	4	0.2
(1,1017)	1:36:A:ARG:HA	1:36:A:ARG:HG3	1	0.2
(1,943)	1:47:A:LEU:HD21	1:72:A:LEU:HD21	1	0.2
(1,943)	1:47:A:LEU:HD21	1:72:A:LEU:HD22	1	0.2
(1,943)	1:47:A:LEU:HD21	1:72:A:LEU:HD23	1	0.2
(1,943)	1:47:A:LEU:HD22	1:72:A:LEU:HD21	1	0.2
(1,943)	1:47:A:LEU:HD22	1:72:A:LEU:HD22	1	0.2
(1,943)	1:47:A:LEU:HD22	1:72:A:LEU:HD23	1	0.2
(1,943)	1:47:A:LEU:HD23	1:72:A:LEU:HD21	1	0.2
(1,943)	1:47:A:LEU:HD23	1:72:A:LEU:HD22	1	0.2
(1,943)	1:47:A:LEU:HD23	1:72:A:LEU:HD23	1	0.2
(1,935)	1:97:A:GLN:H	1:96:A:ILE:HG13	10	0.2
(1,827)	1:76:A:PRO:HD3	1:75:A:ASN:HA	9	0.2
(1,817)	1:42:A:ARG:H	1:41:A:LEU:HB2	1	0.2
(1,791)	1:62:A:ARG:HB3	1:62:A:ARG:HG3	9	0.2
(1,770)	1:47:A:LEU:H	1:47:A:LEU:HB3	4	0.2
(1,770)	1:47:A:LEU:H	1:47:A:LEU:HB3	9	0.2
(1,741)	1:82:A:LEU:HD21	1:46:A:ILE:HD11	10	0.2
(1,741)	1:82:A:LEU:HD21	1:46:A:ILE:HD12	10	0.2
(1,741)	1:82:A:LEU:HD21	1:46:A:ILE:HD13	10	0.2
(1,741)	1:82:A:LEU:HD22	1:46:A:ILE:HD11	10	0.2
(1,741)	1:82:A:LEU:HD22	1:46:A:ILE:HD12	10	0.2
(1,741)	1:82:A:LEU:HD22	1:46:A:ILE:HD13	10	0.2
(1,741)	1:82:A:LEU:HD23	1:46:A:ILE:HD11	10	0.2
(1,741)	1:82:A:LEU:HD23	1:46:A:ILE:HD12	10	0.2
(1,741)	1:82:A:LEU:HD23	1:46:A:ILE:HD13	10	0.2
(1,736)	1:49:A:ARG:HD2	1:49:A:ARG:HG3	8	0.2
(1,736)	1:49:A:ARG:HD2	1:49:A:ARG:HG3	10	0.2
(1,716)	1:99:A:ILE:H	1:98:A:LYS:HB3	9	0.2
(1,619)	1:87:A:ARG:HA	1:96:A:ILE:HG21	6	0.2
(1,619)	1:87:A:ARG:HA	1:96:A:ILE:HG22	6	0.2
(1,619)	1:87:A:ARG:HA	1:96:A:ILE:HG23	6	0.2
(1,576)	1:75:A:ASN:HA	1:76:A:PRO:HD3	9	0.2
(1,565)	1:44:A:LYS:H	1:44:A:LYS:HD2	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,520)	1:14:A:THR:H	1:11:A:GLU:HA	8	0.2
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD11	2	0.2
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD12	2	0.2
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD13	2	0.2
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD11	2	0.2
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD12	2	0.2
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD13	2	0.2
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD11	2	0.2
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD12	2	0.2
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD13	2	0.2
(1,339)	1:105:A:LYS:H	1:104:A:LEU:HB3	5	0.2
(1,291)	1:16:A:VAL:HG21	1:16:A:VAL:HA	4	0.2
(1,291)	1:16:A:VAL:HG22	1:16:A:VAL:HA	4	0.2
(1,291)	1:16:A:VAL:HG23	1:16:A:VAL:HA	4	0.2
(1,291)	1:16:A:VAL:HG21	1:16:A:VAL:HA	7	0.2
(1,291)	1:16:A:VAL:HG22	1:16:A:VAL:HA	7	0.2
(1,291)	1:16:A:VAL:HG23	1:16:A:VAL:HA	7	0.2
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG21	4	0.2
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG22	4	0.2
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG23	4	0.2
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG21	7	0.2
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG22	7	0.2
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG23	7	0.2
(1,74)	1:68:A:LEU:H	1:55:A:ILE:HB	6	0.2
(1,74)	1:68:A:LEU:H	1:55:A:ILE:HB	8	0.2
(1,1258)	1:88:A:ARG:HA	1:88:A:ARG:HG3	6	0.19
(1,1220)	1:74:A:GLU:HG3	1:74:A:GLU:HB3	10	0.19
(1,1201)	1:77:A:LYS:H	1:77:A:LYS:HB2	4	0.19
(1,1160)	1:20:A:ALA:HB1	1:24:A:LEU:HD11	2	0.19
(1,1160)	1:20:A:ALA:HB1	1:24:A:LEU:HD12	2	0.19
(1,1160)	1:20:A:ALA:HB1	1:24:A:LEU:HD13	2	0.19
(1,1160)	1:20:A:ALA:HB2	1:24:A:LEU:HD11	2	0.19
(1,1160)	1:20:A:ALA:HB2	1:24:A:LEU:HD12	2	0.19
(1,1160)	1:20:A:ALA:HB2	1:24:A:LEU:HD13	2	0.19
(1,1160)	1:20:A:ALA:HB3	1:24:A:LEU:HD11	2	0.19
(1,1160)	1:20:A:ALA:HB3	1:24:A:LEU:HD12	2	0.19
(1,1160)	1:20:A:ALA:HB3	1:24:A:LEU:HD13	2	0.19
(1,1155)	1:71:A:TYR:HD1	1:68:A:LEU:HG	7	0.19
(1,1155)	1:71:A:TYR:HD2	1:68:A:LEU:HG	7	0.19
(1,1126)	1:53:A:ARG:H	1:53:A:ARG:HB3	9	0.19
(1,1118)	1:72:A:LEU:HA	1:46:A:ILE:HG21	2	0.19
(1,1118)	1:72:A:LEU:HA	1:46:A:ILE:HG22	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1118)	1:72:A:LEU:HA	1:46:A:ILE:HG23	2	0.19
(1,1108)	1:65:A:ALA:HA	1:35:A:GLU:HB2	9	0.19
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG21	8	0.19
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG22	8	0.19
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG23	8	0.19
(1,994)	1:40:A:HIS:H	1:40:A:HIS:HB3	2	0.19
(1,937)	1:111:A:LEU:H	1:110:A:LYS:HG3	6	0.19
(1,935)	1:97:A:GLN:H	1:96:A:ILE:HG13	5	0.19
(1,750)	1:92:A:GLN:HE21	1:91:A:THR:HB	9	0.19
(1,732)	1:36:A:ARG:H	1:35:A:GLU:HB2	5	0.19
(1,719)	1:18:A:LYS:H	1:18:A:LYS:HD3	1	0.19
(1,687)	1:97:A:GLN:H	1:97:A:GLN:HB3	9	0.19
(1,681)	1:13:A:LEU:H	1:13:A:LEU:HB2	2	0.19
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG21	10	0.19
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG22	10	0.19
(1,643)	1:87:A:ARG:H	1:96:A:ILE:HG23	10	0.19
(1,642)	1:73:A:GLN:HA	1:73:A:GLN:HG2	8	0.19
(1,628)	1:106:A:LEU:HB3	1:13:A:LEU:HB3	1	0.19
(1,591)	1:93:A:ASN:H	1:93:A:ASN:HB3	8	0.19
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG21	5	0.19
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG22	5	0.19
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG23	5	0.19
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD11	5	0.19
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD12	5	0.19
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD13	5	0.19
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD11	5	0.19
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD12	5	0.19
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD13	5	0.19
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD11	5	0.19
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD12	5	0.19
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD13	5	0.19
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD11	7	0.19
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD12	7	0.19
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD13	7	0.19
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD11	7	0.19
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD12	7	0.19
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD13	7	0.19
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD11	7	0.19
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD12	7	0.19
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD13	7	0.19
(1,390)	1:96:A:ILE:H	1:95:A:LEU:HG	1	0.19
(1,357)	1:107:A:ARG:H	1:106:A:LEU:HD21	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,357)	1:107:A:ARG:H	1:106:A:LEU:HD22	2	0.19
(1,357)	1:107:A:ARG:H	1:106:A:LEU:HD23	2	0.19
(1,348)	1:109:A:ILE:HA	1:16:A:VAL:HG11	5	0.19
(1,348)	1:109:A:ILE:HA	1:16:A:VAL:HG12	5	0.19
(1,348)	1:109:A:ILE:HA	1:16:A:VAL:HG13	5	0.19
(1,337)	1:20:A:ALA:H	1:106:A:LEU:HD11	4	0.19
(1,337)	1:20:A:ALA:H	1:106:A:LEU:HD12	4	0.19
(1,337)	1:20:A:ALA:H	1:106:A:LEU:HD13	4	0.19
(1,274)	1:115:A:LYS:H	1:114:A:LEU:HB3	5	0.19
(1,229)	1:93:A:ASN:H	1:93:A:ASN:HB3	8	0.19
(1,99)	1:20:A:ALA:H	1:106:A:LEU:HD11	4	0.19
(1,99)	1:20:A:ALA:H	1:106:A:LEU:HD12	4	0.19
(1,99)	1:20:A:ALA:H	1:106:A:LEU:HD13	4	0.19
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD11	9	0.19
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD12	9	0.19
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD13	9	0.19
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD11	9	0.19
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD12	9	0.19
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD13	9	0.19
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD11	9	0.19
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD12	9	0.19
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD13	9	0.19
(1,1227)	1:10:A:GLU:H	1:11:A:GLU:HG2	5	0.18
(1,1191)	1:11:A:GLU:H	1:14:A:THR:H	5	0.18
(1,1176)	1:32:A:ILE:H	1:32:A:ILE:HG13	7	0.18
(1,1176)	1:32:A:ILE:H	1:32:A:ILE:HG13	8	0.18
(1,1096)	1:69:A:LEU:HA	1:72:A:LEU:HD21	8	0.18
(1,1096)	1:69:A:LEU:HA	1:72:A:LEU:HD22	8	0.18
(1,1096)	1:69:A:LEU:HA	1:72:A:LEU:HD23	8	0.18
(1,1083)	1:109:A:ILE:HG21	1:106:A:LEU:HA	6	0.18
(1,1083)	1:109:A:ILE:HG22	1:106:A:LEU:HA	6	0.18
(1,1083)	1:109:A:ILE:HG23	1:106:A:LEU:HA	6	0.18
(1,956)	1:34:A:ALA:HB1	1:41:A:LEU:HD11	2	0.18
(1,956)	1:34:A:ALA:HB1	1:41:A:LEU:HD12	2	0.18
(1,956)	1:34:A:ALA:HB1	1:41:A:LEU:HD13	2	0.18
(1,956)	1:34:A:ALA:HB2	1:41:A:LEU:HD11	2	0.18
(1,956)	1:34:A:ALA:HB2	1:41:A:LEU:HD12	2	0.18
(1,956)	1:34:A:ALA:HB2	1:41:A:LEU:HD13	2	0.18
(1,956)	1:34:A:ALA:HB3	1:41:A:LEU:HD11	2	0.18
(1,956)	1:34:A:ALA:HB3	1:41:A:LEU:HD12	2	0.18
(1,956)	1:34:A:ALA:HB3	1:41:A:LEU:HD13	2	0.18
(1,918)	1:49:A:ARG:HA	1:52:A:THR:HG21	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,918)	1:49:A:ARG:HA	1:52:A:THR:HG22	6	0.18
(1,918)	1:49:A:ARG:HA	1:52:A:THR:HG23	6	0.18
(1,791)	1:62:A:ARG:HB3	1:62:A:ARG:HG3	6	0.18
(1,770)	1:47:A:LEU:H	1:47:A:LEU:HB3	2	0.18
(1,770)	1:47:A:LEU:H	1:47:A:LEU:HB3	5	0.18
(1,736)	1:49:A:ARG:HD2	1:49:A:ARG:HG3	3	0.18
(1,728)	1:14:A:THR:HA	1:14:A:THR:HG21	2	0.18
(1,728)	1:14:A:THR:HA	1:14:A:THR:HG22	2	0.18
(1,728)	1:14:A:THR:HA	1:14:A:THR:HG23	2	0.18
(1,719)	1:18:A:LYS:H	1:18:A:LYS:HD3	3	0.18
(1,619)	1:87:A:ARG:HA	1:96:A:ILE:HG21	2	0.18
(1,619)	1:87:A:ARG:HA	1:96:A:ILE:HG22	2	0.18
(1,619)	1:87:A:ARG:HA	1:96:A:ILE:HG23	2	0.18
(1,565)	1:44:A:LYS:H	1:44:A:LYS:HD2	5	0.18
(1,485)	1:14:A:THR:HG21	1:14:A:THR:HA	2	0.18
(1,485)	1:14:A:THR:HG22	1:14:A:THR:HA	2	0.18
(1,485)	1:14:A:THR:HG23	1:14:A:THR:HA	2	0.18
(1,452)	1:102:A:GLU:H	1:24:A:LEU:HD11	7	0.18
(1,452)	1:102:A:GLU:H	1:24:A:LEU:HD12	7	0.18
(1,452)	1:102:A:GLU:H	1:24:A:LEU:HD13	7	0.18
(1,291)	1:16:A:VAL:HG21	1:16:A:VAL:HA	1	0.18
(1,291)	1:16:A:VAL:HG22	1:16:A:VAL:HA	1	0.18
(1,291)	1:16:A:VAL:HG23	1:16:A:VAL:HA	1	0.18
(1,240)	1:34:A:ALA:HB1	1:35:A:GLU:HA	6	0.18
(1,240)	1:34:A:ALA:HB2	1:35:A:GLU:HA	6	0.18
(1,240)	1:34:A:ALA:HB3	1:35:A:GLU:HA	6	0.18
(1,240)	1:34:A:ALA:HB1	1:35:A:GLU:HA	10	0.18
(1,240)	1:34:A:ALA:HB2	1:35:A:GLU:HA	10	0.18
(1,240)	1:34:A:ALA:HB3	1:35:A:GLU:HA	10	0.18
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD11	1	0.18
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD12	1	0.18
(1,151)	1:47:A:LEU:H	1:41:A:LEU:HD13	1	0.18
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG21	1	0.18
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG22	1	0.18
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG23	1	0.18
(1,113)	1:69:A:LEU:HD21	1:34:A:ALA:HB1	1	0.18
(1,113)	1:69:A:LEU:HD21	1:34:A:ALA:HB2	1	0.18
(1,113)	1:69:A:LEU:HD21	1:34:A:ALA:HB3	1	0.18
(1,113)	1:69:A:LEU:HD22	1:34:A:ALA:HB1	1	0.18
(1,113)	1:69:A:LEU:HD22	1:34:A:ALA:HB2	1	0.18
(1,113)	1:69:A:LEU:HD22	1:34:A:ALA:HB3	1	0.18
(1,113)	1:69:A:LEU:HD23	1:34:A:ALA:HB1	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,113)	1:69:A:LEU:HD23	1:34:A:ALA:HB2	1	0.18
(1,113)	1:69:A:LEU:HD23	1:34:A:ALA:HB3	1	0.18
(1,81)	1:50:A:GLU:H	1:50:A:GLU:HB2	6	0.18
(1,60)	1:108:A:ASN:H	1:108:A:ASN:HB2	6	0.18
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD11	7	0.18
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD12	7	0.18
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD13	7	0.18
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD11	7	0.18
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD12	7	0.18
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD13	7	0.18
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD11	7	0.18
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD12	7	0.18
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD13	7	0.18
(1,1280)	1:24:A:LEU:HD21	1:24:A:LEU:HA	8	0.17
(1,1280)	1:24:A:LEU:HD22	1:24:A:LEU:HA	8	0.17
(1,1280)	1:24:A:LEU:HD23	1:24:A:LEU:HA	8	0.17
(1,1224)	1:19:A:ASP:H	1:19:A:ASP:HB3	7	0.17
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG21	4	0.17
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG22	4	0.17
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG23	4	0.17
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG21	4	0.17
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG22	4	0.17
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG23	4	0.17
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG21	4	0.17
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG22	4	0.17
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG23	4	0.17
(1,1155)	1:71:A:TYR:HD1	1:68:A:LEU:HG	2	0.17
(1,1155)	1:71:A:TYR:HD2	1:68:A:LEU:HG	2	0.17
(1,1155)	1:71:A:TYR:HD1	1:68:A:LEU:HG	9	0.17
(1,1155)	1:71:A:TYR:HD2	1:68:A:LEU:HG	9	0.17
(1,1126)	1:53:A:ARG:H	1:53:A:ARG:HB3	8	0.17
(1,1109)	1:83:A:VAL:HG11	1:86:A:ILE:HD11	5	0.17
(1,1109)	1:83:A:VAL:HG11	1:86:A:ILE:HD12	5	0.17
(1,1109)	1:83:A:VAL:HG11	1:86:A:ILE:HD13	5	0.17
(1,1109)	1:83:A:VAL:HG12	1:86:A:ILE:HD11	5	0.17
(1,1109)	1:83:A:VAL:HG12	1:86:A:ILE:HD12	5	0.17
(1,1109)	1:83:A:VAL:HG12	1:86:A:ILE:HD13	5	0.17
(1,1109)	1:83:A:VAL:HG13	1:86:A:ILE:HD11	5	0.17
(1,1109)	1:83:A:VAL:HG13	1:86:A:ILE:HD12	5	0.17
(1,1109)	1:83:A:VAL:HG13	1:86:A:ILE:HD13	5	0.17
(1,1027)	1:49:A:ARG:HA	1:49:A:ARG:HB2	6	0.17
(1,1024)	1:39:A:ASP:H	1:38:A:PHE:HB2	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,995)	1:30:A:GLU:H	1:30:A:GLU:HB3	5	0.17
(1,994)	1:40:A:HIS:H	1:40:A:HIS:HB3	1	0.17
(1,993)	1:10:A:GLU:HA	1:10:A:GLU:HB2	4	0.17
(1,993)	1:10:A:GLU:HA	1:10:A:GLU:HB2	7	0.17
(1,870)	1:33:A:ILE:HB	1:36:A:ARG:HB2	1	0.17
(1,852)	1:96:A:ILE:H	1:96:A:ILE:HG12	5	0.17
(1,779)	1:79:A:LEU:HD11	1:25:A:ARG:HB2	9	0.17
(1,779)	1:79:A:LEU:HD12	1:25:A:ARG:HB2	9	0.17
(1,779)	1:79:A:LEU:HD13	1:25:A:ARG:HB2	9	0.17
(1,772)	1:71:A:TYR:HE1	1:55:A:ILE:HB	5	0.17
(1,772)	1:71:A:TYR:HE2	1:55:A:ILE:HB	5	0.17
(1,772)	1:71:A:TYR:HE1	1:55:A:ILE:HB	10	0.17
(1,772)	1:71:A:TYR:HE2	1:55:A:ILE:HB	10	0.17
(1,736)	1:49:A:ARG:HD2	1:49:A:ARG:HG3	6	0.17
(1,677)	1:27:A:TYR:HE1	1:24:A:LEU:HD11	9	0.17
(1,677)	1:27:A:TYR:HE1	1:24:A:LEU:HD12	9	0.17
(1,677)	1:27:A:TYR:HE1	1:24:A:LEU:HD13	9	0.17
(1,677)	1:27:A:TYR:HE2	1:24:A:LEU:HD11	9	0.17
(1,677)	1:27:A:TYR:HE2	1:24:A:LEU:HD12	9	0.17
(1,677)	1:27:A:TYR:HE2	1:24:A:LEU:HD13	9	0.17
(1,642)	1:73:A:GLN:HA	1:73:A:GLN:HG2	10	0.17
(1,600)	1:39:A:ASP:H	1:38:A:PHE:HB2	4	0.17
(1,597)	1:46:A:ILE:H	1:45:A:LYS:HG3	10	0.17
(1,523)	1:73:A:GLN:HE21	1:18:A:LYS:HE2	1	0.17
(1,501)	1:96:A:ILE:H	1:96:A:ILE:HG12	5	0.17
(1,474)	1:71:A:TYR:HE1	1:55:A:ILE:H	10	0.17
(1,474)	1:71:A:TYR:HE2	1:55:A:ILE:H	10	0.17
(1,470)	1:16:A:VAL:HG21	1:106:A:LEU:HB3	9	0.17
(1,470)	1:16:A:VAL:HG22	1:106:A:LEU:HB3	9	0.17
(1,470)	1:16:A:VAL:HG23	1:106:A:LEU:HB3	9	0.17
(1,469)	1:57:A:CYS:H	1:57:A:CYS:HB3	9	0.17
(1,413)	1:79:A:LEU:H	1:79:A:LEU:HD11	8	0.17
(1,413)	1:79:A:LEU:H	1:79:A:LEU:HD12	8	0.17
(1,413)	1:79:A:LEU:H	1:79:A:LEU:HD13	8	0.17
(1,350)	1:27:A:TYR:HE1	1:28:A:LEU:HB2	1	0.17
(1,350)	1:27:A:TYR:HE2	1:28:A:LEU:HB2	1	0.17
(1,350)	1:27:A:TYR:HE1	1:28:A:LEU:HB2	5	0.17
(1,350)	1:27:A:TYR:HE2	1:28:A:LEU:HB2	5	0.17
(1,308)	1:104:A:LEU:HA	1:13:A:LEU:HB2	6	0.17
(1,291)	1:16:A:VAL:HG21	1:16:A:VAL:HA	8	0.17
(1,291)	1:16:A:VAL:HG22	1:16:A:VAL:HA	8	0.17
(1,291)	1:16:A:VAL:HG23	1:16:A:VAL:HA	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,291)	1:16:A:VAL:HG21	1:16:A:VAL:HA	10	0.17
(1,291)	1:16:A:VAL:HG22	1:16:A:VAL:HA	10	0.17
(1,291)	1:16:A:VAL:HG23	1:16:A:VAL:HA	10	0.17
(1,180)	1:98:A:LYS:H	1:99:A:ILE:HG12	1	0.17
(1,152)	1:16:A:VAL:H	1:106:A:LEU:HB2	3	0.17
(1,145)	1:16:A:VAL:H	1:16:A:VAL:HG21	1	0.17
(1,145)	1:16:A:VAL:H	1:16:A:VAL:HG22	1	0.17
(1,145)	1:16:A:VAL:H	1:16:A:VAL:HG23	1	0.17
(1,129)	1:74:A:GLU:H	1:73:A:GLN:HB3	9	0.17
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG21	8	0.17
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG22	8	0.17
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG23	8	0.17
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG21	10	0.17
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG22	10	0.17
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG23	10	0.17
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG21	4	0.17
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG22	4	0.17
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG23	4	0.17
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG21	4	0.17
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG22	4	0.17
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG23	4	0.17
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG21	4	0.17
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG22	4	0.17
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG23	4	0.17
(1,1224)	1:19:A:ASP:H	1:19:A:ASP:HB3	2	0.16
(1,1224)	1:19:A:ASP:H	1:19:A:ASP:HB3	10	0.16
(1,1220)	1:74:A:GLU:HG3	1:74:A:GLU:HB3	2	0.16
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG21	9	0.16
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG22	9	0.16
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG23	9	0.16
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG21	9	0.16
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG22	9	0.16
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG23	9	0.16
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG21	9	0.16
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG22	9	0.16
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG23	9	0.16
(1,1194)	1:64:A:ARG:HA	1:63:A:LYS:HD2	4	0.16
(1,1194)	1:64:A:ARG:HA	1:63:A:LYS:HD2	6	0.16
(1,1181)	1:19:A:ASP:H	1:16:A:VAL:HA	6	0.16
(1,1108)	1:65:A:ALA:HA	1:35:A:GLU:HB2	3	0.16
(1,1108)	1:65:A:ALA:HA	1:35:A:GLU:HB2	6	0.16
(1,1104)	1:45:A:LYS:HG2	1:42:A:ARG:HA	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD11	5	0.16
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD12	5	0.16
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD13	5	0.16
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD11	5	0.16
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD12	5	0.16
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD13	5	0.16
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD11	5	0.16
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD12	5	0.16
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD13	5	0.16
(1,1034)	1:79:A:LEU:H	1:79:A:LEU:HB3	8	0.16
(1,1005)	1:82:A:LEU:HD11	1:72:A:LEU:HD21	6	0.16
(1,1005)	1:82:A:LEU:HD11	1:72:A:LEU:HD22	6	0.16
(1,1005)	1:82:A:LEU:HD11	1:72:A:LEU:HD23	6	0.16
(1,1005)	1:82:A:LEU:HD12	1:72:A:LEU:HD21	6	0.16
(1,1005)	1:82:A:LEU:HD12	1:72:A:LEU:HD22	6	0.16
(1,1005)	1:82:A:LEU:HD12	1:72:A:LEU:HD23	6	0.16
(1,1005)	1:82:A:LEU:HD13	1:72:A:LEU:HD21	6	0.16
(1,1005)	1:82:A:LEU:HD13	1:72:A:LEU:HD22	6	0.16
(1,1005)	1:82:A:LEU:HD13	1:72:A:LEU:HD23	6	0.16
(1,993)	1:10:A:GLU:HA	1:10:A:GLU:HB2	5	0.16
(1,968)	1:53:A:ARG:HA	1:53:A:ARG:HG2	7	0.16
(1,964)	1:102:A:GLU:H	1:102:A:GLU:HB3	4	0.16
(1,956)	1:34:A:ALA:HB1	1:41:A:LEU:HD11	1	0.16
(1,956)	1:34:A:ALA:HB1	1:41:A:LEU:HD12	1	0.16
(1,956)	1:34:A:ALA:HB1	1:41:A:LEU:HD13	1	0.16
(1,956)	1:34:A:ALA:HB2	1:41:A:LEU:HD11	1	0.16
(1,956)	1:34:A:ALA:HB2	1:41:A:LEU:HD12	1	0.16
(1,956)	1:34:A:ALA:HB2	1:41:A:LEU:HD13	1	0.16
(1,956)	1:34:A:ALA:HB3	1:41:A:LEU:HD11	1	0.16
(1,956)	1:34:A:ALA:HB3	1:41:A:LEU:HD12	1	0.16
(1,956)	1:34:A:ALA:HB3	1:41:A:LEU:HD13	1	0.16
(1,924)	1:87:A:ARG:HB2	1:84:A:GLU:HA	5	0.16
(1,850)	1:73:A:GLN:HG2	1:79:A:LEU:HD11	8	0.16
(1,850)	1:73:A:GLN:HG2	1:79:A:LEU:HD12	8	0.16
(1,850)	1:73:A:GLN:HG2	1:79:A:LEU:HD13	8	0.16
(1,736)	1:49:A:ARG:HD2	1:49:A:ARG:HG3	5	0.16
(1,642)	1:73:A:GLN:HA	1:73:A:GLN:HG2	2	0.16
(1,635)	1:32:A:ILE:H	1:31:A:LYS:HB2	2	0.16
(1,635)	1:32:A:ILE:H	1:31:A:LYS:HB2	7	0.16
(1,523)	1:73:A:GLN:HE21	1:18:A:LYS:HE2	8	0.16
(1,361)	1:27:A:TYR:HD1	1:95:A:LEU:HD11	1	0.16
(1,361)	1:27:A:TYR:HD1	1:95:A:LEU:HD12	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,361)	1:27:A:TYR:HD1	1:95:A:LEU:HD13	1	0.16
(1,361)	1:27:A:TYR:HD2	1:95:A:LEU:HD11	1	0.16
(1,361)	1:27:A:TYR:HD2	1:95:A:LEU:HD12	1	0.16
(1,361)	1:27:A:TYR:HD2	1:95:A:LEU:HD13	1	0.16
(1,361)	1:27:A:TYR:HD1	1:95:A:LEU:HD11	3	0.16
(1,361)	1:27:A:TYR:HD1	1:95:A:LEU:HD12	3	0.16
(1,361)	1:27:A:TYR:HD1	1:95:A:LEU:HD13	3	0.16
(1,361)	1:27:A:TYR:HD2	1:95:A:LEU:HD11	3	0.16
(1,361)	1:27:A:TYR:HD2	1:95:A:LEU:HD12	3	0.16
(1,361)	1:27:A:TYR:HD2	1:95:A:LEU:HD13	3	0.16
(1,291)	1:16:A:VAL:HG21	1:16:A:VAL:HA	2	0.16
(1,291)	1:16:A:VAL:HG22	1:16:A:VAL:HA	2	0.16
(1,291)	1:16:A:VAL:HG23	1:16:A:VAL:HA	2	0.16
(1,265)	1:73:A:GLN:H	1:71:A:TYR:HA	1	0.16
(1,205)	1:105:A:LYS:HA	1:105:A:LYS:HB2	8	0.16
(1,148)	1:42:A:ARG:HD3	1:52:A:THR:HG21	4	0.16
(1,148)	1:42:A:ARG:HD3	1:52:A:THR:HG22	4	0.16
(1,148)	1:42:A:ARG:HD3	1:52:A:THR:HG23	4	0.16
(1,146)	1:68:A:LEU:HD11	1:72:A:LEU:HG	3	0.16
(1,146)	1:68:A:LEU:HD12	1:72:A:LEU:HG	3	0.16
(1,146)	1:68:A:LEU:HD13	1:72:A:LEU:HG	3	0.16
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG21	2	0.16
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG22	2	0.16
(1,126)	1:16:A:VAL:HA	1:16:A:VAL:HG23	2	0.16
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG21	9	0.16
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG22	9	0.16
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG23	9	0.16
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG21	9	0.16
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG22	9	0.16
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG23	9	0.16
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG21	9	0.16
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG22	9	0.16
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG23	9	0.16
(1,84)	1:73:A:GLN:HE22	1:18:A:LYS:HA	10	0.16
(1,65)	1:63:A:LYS:HE2	1:63:A:LYS:HD2	6	0.16
(1,28)	1:102:A:GLU:HA	1:102:A:GLU:HG3	1	0.16
(1,27)	1:27:A:TYR:H	1:27:A:TYR:HB2	8	0.16
(1,3)	1:56:A:SER:H	1:55:A:ILE:HG13	8	0.16
(1,1283)	1:47:A:LEU:HD11	1:71:A:TYR:HB2	9	0.15
(1,1283)	1:47:A:LEU:HD12	1:71:A:TYR:HB2	9	0.15
(1,1283)	1:47:A:LEU:HD13	1:71:A:TYR:HB2	9	0.15
(1,1280)	1:24:A:LEU:HD21	1:24:A:LEU:HA	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1280)	1:24:A:LEU:HD22	1:24:A:LEU:HA	10	0.15
(1,1280)	1:24:A:LEU:HD23	1:24:A:LEU:HA	10	0.15
(1,1241)	1:96:A:ILE:HD11	1:93:A:ASN:HA	6	0.15
(1,1241)	1:96:A:ILE:HD12	1:93:A:ASN:HA	6	0.15
(1,1241)	1:96:A:ILE:HD13	1:93:A:ASN:HA	6	0.15
(1,1207)	1:24:A:LEU:HD11	1:28:A:LEU:HG	10	0.15
(1,1207)	1:24:A:LEU:HD12	1:28:A:LEU:HG	10	0.15
(1,1207)	1:24:A:LEU:HD13	1:28:A:LEU:HG	10	0.15
(1,1198)	1:108:A:ASN:HD22	1:108:A:ASN:HB2	6	0.15
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG21	3	0.15
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG22	3	0.15
(1,1097)	1:91:A:THR:H	1:91:A:THR:HG23	3	0.15
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD11	7	0.15
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD12	7	0.15
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD13	7	0.15
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD11	7	0.15
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD12	7	0.15
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD13	7	0.15
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD11	7	0.15
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD12	7	0.15
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD13	7	0.15
(1,1031)	1:65:A:ALA:HA	1:69:A:LEU:HG	4	0.15
(1,1027)	1:49:A:ARG:HA	1:49:A:ARG:HB2	8	0.15
(1,1017)	1:36:A:ARG:HA	1:36:A:ARG:HG3	9	0.15
(1,990)	1:101:A:ASP:H	1:97:A:GLN:HA	5	0.15
(1,781)	1:21:A:LEU:HB3	1:24:A:LEU:HD21	9	0.15
(1,781)	1:21:A:LEU:HB3	1:24:A:LEU:HD22	9	0.15
(1,781)	1:21:A:LEU:HB3	1:24:A:LEU:HD23	9	0.15
(1,779)	1:79:A:LEU:HD11	1:25:A:ARG:HB2	5	0.15
(1,779)	1:79:A:LEU:HD12	1:25:A:ARG:HB2	5	0.15
(1,779)	1:79:A:LEU:HD13	1:25:A:ARG:HB2	5	0.15
(1,779)	1:79:A:LEU:HD11	1:25:A:ARG:HB2	6	0.15
(1,779)	1:79:A:LEU:HD12	1:25:A:ARG:HB2	6	0.15
(1,779)	1:79:A:LEU:HD13	1:25:A:ARG:HB2	6	0.15
(1,770)	1:47:A:LEU:H	1:47:A:LEU:HB3	3	0.15
(1,732)	1:36:A:ARG:H	1:35:A:GLU:HB2	7	0.15
(1,726)	1:93:A:ASN:H	1:94:A:PHE:HB2	8	0.15
(1,694)	1:36:A:ARG:H	1:36:A:ARG:HB3	5	0.15
(1,694)	1:36:A:ARG:H	1:36:A:ARG:HB3	7	0.15
(1,680)	1:21:A:LEU:H	1:21:A:LEU:HB3	5	0.15
(1,669)	1:10:A:GLU:HG2	1:10:A:GLU:HA	1	0.15
(1,642)	1:73:A:GLN:HA	1:73:A:GLN:HG2	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,620)	1:40:A:HIS:H	1:39:A:ASP:HB3	10	0.15
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG21	4	0.15
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG22	4	0.15
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG23	4	0.15
(1,488)	1:49:A:ARG:HD2	1:49:A:ARG:HB2	9	0.15
(1,350)	1:27:A:TYR:HE1	1:28:A:LEU:HB2	10	0.15
(1,350)	1:27:A:TYR:HE2	1:28:A:LEU:HB2	10	0.15
(1,308)	1:104:A:LEU:HA	1:13:A:LEU:HB2	8	0.15
(1,240)	1:34:A:ALA:HB1	1:35:A:GLU:HA	8	0.15
(1,240)	1:34:A:ALA:HB2	1:35:A:GLU:HA	8	0.15
(1,240)	1:34:A:ALA:HB3	1:35:A:GLU:HA	8	0.15
(1,205)	1:105:A:LYS:HA	1:105:A:LYS:HB2	2	0.15
(1,205)	1:105:A:LYS:HA	1:105:A:LYS:HB2	6	0.15
(1,158)	1:66:A:GLY:H	1:67:A:LYS:HB3	5	0.15
(1,152)	1:16:A:VAL:H	1:106:A:LEU:HB2	8	0.15
(1,109)	1:71:A:TYR:HD1	1:68:A:LEU:HB2	4	0.15
(1,109)	1:71:A:TYR:HD2	1:68:A:LEU:HB2	4	0.15
(1,2)	1:32:A:ILE:H	1:32:A:ILE:HG12	10	0.15
(1,1280)	1:24:A:LEU:HD21	1:24:A:LEU:HA	5	0.14
(1,1280)	1:24:A:LEU:HD22	1:24:A:LEU:HA	5	0.14
(1,1280)	1:24:A:LEU:HD23	1:24:A:LEU:HA	5	0.14
(1,1198)	1:108:A:ASN:HD22	1:108:A:ASN:HB2	7	0.14
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG21	1	0.14
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG22	1	0.14
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG23	1	0.14
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG21	1	0.14
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG22	1	0.14
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG23	1	0.14
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG21	1	0.14
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG22	1	0.14
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG23	1	0.14
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG21	2	0.14
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG22	2	0.14
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG23	2	0.14
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG21	2	0.14
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG22	2	0.14
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG23	2	0.14
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG21	2	0.14
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG22	2	0.14
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG23	2	0.14
(1,1160)	1:20:A:ALA:HB1	1:24:A:LEU:HD11	3	0.14
(1,1160)	1:20:A:ALA:HB1	1:24:A:LEU:HD12	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1160)	1:20:A:ALA:HB1	1:24:A:LEU:HD13	3	0.14
(1,1160)	1:20:A:ALA:HB2	1:24:A:LEU:HD11	3	0.14
(1,1160)	1:20:A:ALA:HB2	1:24:A:LEU:HD12	3	0.14
(1,1160)	1:20:A:ALA:HB2	1:24:A:LEU:HD13	3	0.14
(1,1160)	1:20:A:ALA:HB3	1:24:A:LEU:HD11	3	0.14
(1,1160)	1:20:A:ALA:HB3	1:24:A:LEU:HD12	3	0.14
(1,1160)	1:20:A:ALA:HB3	1:24:A:LEU:HD13	3	0.14
(1,1160)	1:20:A:ALA:HB1	1:24:A:LEU:HD11	6	0.14
(1,1160)	1:20:A:ALA:HB1	1:24:A:LEU:HD12	6	0.14
(1,1160)	1:20:A:ALA:HB1	1:24:A:LEU:HD13	6	0.14
(1,1160)	1:20:A:ALA:HB2	1:24:A:LEU:HD11	6	0.14
(1,1160)	1:20:A:ALA:HB2	1:24:A:LEU:HD12	6	0.14
(1,1160)	1:20:A:ALA:HB2	1:24:A:LEU:HD13	6	0.14
(1,1160)	1:20:A:ALA:HB3	1:24:A:LEU:HD11	6	0.14
(1,1160)	1:20:A:ALA:HB3	1:24:A:LEU:HD12	6	0.14
(1,1160)	1:20:A:ALA:HB3	1:24:A:LEU:HD13	6	0.14
(1,1158)	1:78:A:GLY:HA3	1:72:A:LEU:HD21	2	0.14
(1,1158)	1:78:A:GLY:HA3	1:72:A:LEU:HD22	2	0.14
(1,1158)	1:78:A:GLY:HA3	1:72:A:LEU:HD23	2	0.14
(1,1125)	1:13:A:LEU:HG	1:107:A:ARG:HA	2	0.14
(1,1096)	1:69:A:LEU:HA	1:72:A:LEU:HD21	6	0.14
(1,1096)	1:69:A:LEU:HA	1:72:A:LEU:HD22	6	0.14
(1,1096)	1:69:A:LEU:HA	1:72:A:LEU:HD23	6	0.14
(1,1027)	1:49:A:ARG:HA	1:49:A:ARG:HB2	10	0.14
(1,994)	1:40:A:HIS:H	1:40:A:HIS:HB3	3	0.14
(1,980)	1:95:A:LEU:HD21	1:27:A:TYR:HE1	9	0.14
(1,980)	1:95:A:LEU:HD21	1:27:A:TYR:HE2	9	0.14
(1,980)	1:95:A:LEU:HD22	1:27:A:TYR:HE1	9	0.14
(1,980)	1:95:A:LEU:HD22	1:27:A:TYR:HE2	9	0.14
(1,980)	1:95:A:LEU:HD23	1:27:A:TYR:HE1	9	0.14
(1,980)	1:95:A:LEU:HD23	1:27:A:TYR:HE2	9	0.14
(1,964)	1:102:A:GLU:H	1:102:A:GLU:HB3	1	0.14
(1,964)	1:102:A:GLU:H	1:102:A:GLU:HB3	2	0.14
(1,964)	1:102:A:GLU:H	1:102:A:GLU:HB3	5	0.14
(1,964)	1:102:A:GLU:H	1:102:A:GLU:HB3	6	0.14
(1,964)	1:102:A:GLU:H	1:102:A:GLU:HB3	9	0.14
(1,930)	1:16:A:VAL:HG21	1:13:A:LEU:HA	9	0.14
(1,930)	1:16:A:VAL:HG22	1:13:A:LEU:HA	9	0.14
(1,930)	1:16:A:VAL:HG23	1:13:A:LEU:HA	9	0.14
(1,841)	1:107:A:ARG:HA	1:110:A:LYS:HB2	2	0.14
(1,772)	1:71:A:TYR:HE1	1:55:A:ILE:HB	4	0.14
(1,772)	1:71:A:TYR:HE2	1:55:A:ILE:HB	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,736)	1:49:A:ARG:HD2	1:49:A:ARG:HG3	9	0.14
(1,716)	1:99:A:ILE:H	1:98:A:LYS:HB3	5	0.14
(1,669)	1:10:A:GLU:HG2	1:10:A:GLU:HA	7	0.14
(1,644)	1:79:A:LEU:HD11	1:82:A:LEU:HD21	1	0.14
(1,644)	1:79:A:LEU:HD11	1:82:A:LEU:HD22	1	0.14
(1,644)	1:79:A:LEU:HD11	1:82:A:LEU:HD23	1	0.14
(1,644)	1:79:A:LEU:HD12	1:82:A:LEU:HD21	1	0.14
(1,644)	1:79:A:LEU:HD12	1:82:A:LEU:HD22	1	0.14
(1,644)	1:79:A:LEU:HD12	1:82:A:LEU:HD23	1	0.14
(1,644)	1:79:A:LEU:HD13	1:82:A:LEU:HD21	1	0.14
(1,644)	1:79:A:LEU:HD13	1:82:A:LEU:HD22	1	0.14
(1,644)	1:79:A:LEU:HD13	1:82:A:LEU:HD23	1	0.14
(1,644)	1:79:A:LEU:HD11	1:82:A:LEU:HD21	8	0.14
(1,644)	1:79:A:LEU:HD11	1:82:A:LEU:HD22	8	0.14
(1,644)	1:79:A:LEU:HD11	1:82:A:LEU:HD23	8	0.14
(1,644)	1:79:A:LEU:HD12	1:82:A:LEU:HD21	8	0.14
(1,644)	1:79:A:LEU:HD12	1:82:A:LEU:HD22	8	0.14
(1,644)	1:79:A:LEU:HD12	1:82:A:LEU:HD23	8	0.14
(1,644)	1:79:A:LEU:HD13	1:82:A:LEU:HD21	8	0.14
(1,644)	1:79:A:LEU:HD13	1:82:A:LEU:HD22	8	0.14
(1,644)	1:79:A:LEU:HD13	1:82:A:LEU:HD23	8	0.14
(1,523)	1:73:A:GLN:HE21	1:18:A:LYS:HE2	6	0.14
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG21	6	0.14
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG22	6	0.14
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG23	6	0.14
(1,491)	1:70:A:ASP:H	1:70:A:ASP:HB3	10	0.14
(1,469)	1:57:A:CYS:H	1:57:A:CYS:HB3	2	0.14
(1,447)	1:31:A:LYS:H	1:32:A:ILE:HB	4	0.14
(1,418)	1:33:A:ILE:HG21	1:65:A:ALA:HB1	10	0.14
(1,418)	1:33:A:ILE:HG21	1:65:A:ALA:HB2	10	0.14
(1,418)	1:33:A:ILE:HG21	1:65:A:ALA:HB3	10	0.14
(1,418)	1:33:A:ILE:HG22	1:65:A:ALA:HB1	10	0.14
(1,418)	1:33:A:ILE:HG22	1:65:A:ALA:HB2	10	0.14
(1,418)	1:33:A:ILE:HG22	1:65:A:ALA:HB3	10	0.14
(1,418)	1:33:A:ILE:HG23	1:65:A:ALA:HB1	10	0.14
(1,418)	1:33:A:ILE:HG23	1:65:A:ALA:HB2	10	0.14
(1,418)	1:33:A:ILE:HG23	1:65:A:ALA:HB3	10	0.14
(1,408)	1:84:A:GLU:HA	1:83:A:VAL:HG21	5	0.14
(1,408)	1:84:A:GLU:HA	1:83:A:VAL:HG22	5	0.14
(1,408)	1:84:A:GLU:HA	1:83:A:VAL:HG23	5	0.14
(1,365)	1:21:A:LEU:HA	1:24:A:LEU:HD11	10	0.14
(1,365)	1:21:A:LEU:HA	1:24:A:LEU:HD12	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,365)	1:21:A:LEU:HA	1:24:A:LEU:HD13	10	0.14
(1,350)	1:27:A:TYR:HE1	1:28:A:LEU:HB2	8	0.14
(1,350)	1:27:A:TYR:HE2	1:28:A:LEU:HB2	8	0.14
(1,348)	1:109:A:ILE:HA	1:16:A:VAL:HG11	10	0.14
(1,348)	1:109:A:ILE:HA	1:16:A:VAL:HG12	10	0.14
(1,348)	1:109:A:ILE:HA	1:16:A:VAL:HG13	10	0.14
(1,237)	1:51:A:ASP:H	1:51:A:ASP:HB3	2	0.14
(1,218)	1:72:A:LEU:HD21	1:78:A:GLY:HA2	10	0.14
(1,218)	1:72:A:LEU:HD22	1:78:A:GLY:HA2	10	0.14
(1,218)	1:72:A:LEU:HD23	1:78:A:GLY:HA2	10	0.14
(1,145)	1:16:A:VAL:H	1:16:A:VAL:HG21	4	0.14
(1,145)	1:16:A:VAL:H	1:16:A:VAL:HG22	4	0.14
(1,145)	1:16:A:VAL:H	1:16:A:VAL:HG23	4	0.14
(1,109)	1:71:A:TYR:HD1	1:68:A:LEU:HB2	10	0.14
(1,109)	1:71:A:TYR:HD2	1:68:A:LEU:HB2	10	0.14
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG21	1	0.14
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG22	1	0.14
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG23	1	0.14
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG21	1	0.14
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG22	1	0.14
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG23	1	0.14
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG21	1	0.14
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG22	1	0.14
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG23	1	0.14
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG21	2	0.14
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG22	2	0.14
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG23	2	0.14
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG21	2	0.14
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG22	2	0.14
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG23	2	0.14
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG21	2	0.14
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG22	2	0.14
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG23	2	0.14
(1,71)	1:95:A:LEU:HD21	1:86:A:ILE:HD11	1	0.14
(1,71)	1:95:A:LEU:HD21	1:86:A:ILE:HD12	1	0.14
(1,71)	1:95:A:LEU:HD21	1:86:A:ILE:HD13	1	0.14
(1,71)	1:95:A:LEU:HD22	1:86:A:ILE:HD11	1	0.14
(1,71)	1:95:A:LEU:HD22	1:86:A:ILE:HD12	1	0.14
(1,71)	1:95:A:LEU:HD22	1:86:A:ILE:HD13	1	0.14
(1,71)	1:95:A:LEU:HD23	1:86:A:ILE:HD11	1	0.14
(1,71)	1:95:A:LEU:HD23	1:86:A:ILE:HD12	1	0.14
(1,71)	1:95:A:LEU:HD23	1:86:A:ILE:HD13	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,65)	1:63:A:LYS:HE2	1:63:A:LYS:HD2	7	0.14
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD11	5	0.14
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD12	5	0.14
(1,53)	1:43:A:ALA:HB1	1:41:A:LEU:HD13	5	0.14
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD11	5	0.14
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD12	5	0.14
(1,53)	1:43:A:ALA:HB2	1:41:A:LEU:HD13	5	0.14
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD11	5	0.14
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD12	5	0.14
(1,53)	1:43:A:ALA:HB3	1:41:A:LEU:HD13	5	0.14
(1,24)	1:52:A:THR:H	1:52:A:THR:HG21	4	0.14
(1,24)	1:52:A:THR:H	1:52:A:THR:HG22	4	0.14
(1,24)	1:52:A:THR:H	1:52:A:THR:HG23	4	0.14
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG21	7	0.13
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG22	7	0.13
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG23	7	0.13
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG21	7	0.13
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG22	7	0.13
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG23	7	0.13
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG21	7	0.13
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG22	7	0.13
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG23	7	0.13
(1,1176)	1:32:A:ILE:H	1:32:A:ILE:HG13	5	0.13
(1,1176)	1:32:A:ILE:H	1:32:A:ILE:HG13	10	0.13
(1,1155)	1:71:A:TYR:HD1	1:68:A:LEU:HG	8	0.13
(1,1155)	1:71:A:TYR:HD2	1:68:A:LEU:HG	8	0.13
(1,1136)	1:48:A:SER:H	1:47:A:LEU:HD11	2	0.13
(1,1136)	1:48:A:SER:H	1:47:A:LEU:HD12	2	0.13
(1,1136)	1:48:A:SER:H	1:47:A:LEU:HD13	2	0.13
(1,1126)	1:53:A:ARG:H	1:53:A:ARG:HB3	1	0.13
(1,1118)	1:72:A:LEU:HA	1:46:A:ILE:HG21	7	0.13
(1,1118)	1:72:A:LEU:HA	1:46:A:ILE:HG22	7	0.13
(1,1118)	1:72:A:LEU:HA	1:46:A:ILE:HG23	7	0.13
(1,1083)	1:109:A:ILE:HG21	1:106:A:LEU:HA	3	0.13
(1,1083)	1:109:A:ILE:HG22	1:106:A:LEU:HA	3	0.13
(1,1083)	1:109:A:ILE:HG23	1:106:A:LEU:HA	3	0.13
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD11	3	0.13
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD12	3	0.13
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD13	3	0.13
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD11	3	0.13
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD12	3	0.13
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD13	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD11	3	0.13
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD12	3	0.13
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD13	3	0.13
(1,1049)	1:74:A:GLU:H	1:74:A:GLU:HG2	6	0.13
(1,1034)	1:79:A:LEU:H	1:79:A:LEU:HB3	10	0.13
(1,1031)	1:65:A:ALA:HA	1:69:A:LEU:HG	2	0.13
(1,998)	1:69:A:LEU:HA	1:82:A:LEU:HG	7	0.13
(1,994)	1:40:A:HIS:H	1:40:A:HIS:HB3	4	0.13
(1,964)	1:102:A:GLU:H	1:102:A:GLU:HB3	7	0.13
(1,956)	1:34:A:ALA:HB1	1:41:A:LEU:HD11	6	0.13
(1,956)	1:34:A:ALA:HB1	1:41:A:LEU:HD12	6	0.13
(1,956)	1:34:A:ALA:HB1	1:41:A:LEU:HD13	6	0.13
(1,956)	1:34:A:ALA:HB2	1:41:A:LEU:HD11	6	0.13
(1,956)	1:34:A:ALA:HB2	1:41:A:LEU:HD12	6	0.13
(1,956)	1:34:A:ALA:HB2	1:41:A:LEU:HD13	6	0.13
(1,956)	1:34:A:ALA:HB3	1:41:A:LEU:HD11	6	0.13
(1,956)	1:34:A:ALA:HB3	1:41:A:LEU:HD12	6	0.13
(1,956)	1:34:A:ALA:HB3	1:41:A:LEU:HD13	6	0.13
(1,956)	1:34:A:ALA:HB1	1:41:A:LEU:HD11	9	0.13
(1,956)	1:34:A:ALA:HB1	1:41:A:LEU:HD12	9	0.13
(1,956)	1:34:A:ALA:HB1	1:41:A:LEU:HD13	9	0.13
(1,956)	1:34:A:ALA:HB2	1:41:A:LEU:HD11	9	0.13
(1,956)	1:34:A:ALA:HB2	1:41:A:LEU:HD12	9	0.13
(1,956)	1:34:A:ALA:HB2	1:41:A:LEU:HD13	9	0.13
(1,956)	1:34:A:ALA:HB3	1:41:A:LEU:HD11	9	0.13
(1,956)	1:34:A:ALA:HB3	1:41:A:LEU:HD12	9	0.13
(1,956)	1:34:A:ALA:HB3	1:41:A:LEU:HD13	9	0.13
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD11	4	0.13
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD12	4	0.13
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD13	4	0.13
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD11	8	0.13
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD12	8	0.13
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD13	8	0.13
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD11	10	0.13
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD12	10	0.13
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD13	10	0.13
(1,935)	1:97:A:GLN:H	1:96:A:ILE:HG13	4	0.13
(1,930)	1:16:A:VAL:HG21	1:13:A:LEU:HA	6	0.13
(1,930)	1:16:A:VAL:HG22	1:13:A:LEU:HA	6	0.13
(1,930)	1:16:A:VAL:HG23	1:13:A:LEU:HA	6	0.13
(1,930)	1:16:A:VAL:HG21	1:13:A:LEU:HA	7	0.13
(1,930)	1:16:A:VAL:HG22	1:13:A:LEU:HA	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,930)	1:16:A:VAL:HG23	1:13:A:LEU:HA	7	0.13
(1,924)	1:87:A:ARG:HB2	1:84:A:GLU:HA	9	0.13
(1,877)	1:55:A:ILE:HG21	1:68:A:LEU:HB3	4	0.13
(1,877)	1:55:A:ILE:HG22	1:68:A:LEU:HB3	4	0.13
(1,877)	1:55:A:ILE:HG23	1:68:A:LEU:HB3	4	0.13
(1,877)	1:55:A:ILE:HG21	1:68:A:LEU:HB3	6	0.13
(1,877)	1:55:A:ILE:HG22	1:68:A:LEU:HB3	6	0.13
(1,877)	1:55:A:ILE:HG23	1:68:A:LEU:HB3	6	0.13
(1,705)	1:111:A:LEU:H	1:111:A:LEU:HB3	3	0.13
(1,705)	1:111:A:LEU:H	1:111:A:LEU:HB3	5	0.13
(1,669)	1:10:A:GLU:HG2	1:10:A:GLU:HA	9	0.13
(1,635)	1:32:A:ILE:H	1:31:A:LYS:HB2	9	0.13
(1,584)	1:79:A:LEU:HD21	1:69:A:LEU:HB2	4	0.13
(1,584)	1:79:A:LEU:HD22	1:69:A:LEU:HB2	4	0.13
(1,584)	1:79:A:LEU:HD23	1:69:A:LEU:HB2	4	0.13
(1,533)	1:79:A:LEU:HD11	1:80:A:ASP:HA	3	0.13
(1,533)	1:79:A:LEU:HD12	1:80:A:ASP:HA	3	0.13
(1,533)	1:79:A:LEU:HD13	1:80:A:ASP:HA	3	0.13
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG21	3	0.13
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG22	3	0.13
(1,522)	1:109:A:ILE:H	1:109:A:ILE:HG23	3	0.13
(1,469)	1:57:A:CYS:H	1:57:A:CYS:HB3	4	0.13
(1,469)	1:57:A:CYS:H	1:57:A:CYS:HB3	10	0.13
(1,452)	1:102:A:GLU:H	1:24:A:LEU:HD11	6	0.13
(1,452)	1:102:A:GLU:H	1:24:A:LEU:HD12	6	0.13
(1,452)	1:102:A:GLU:H	1:24:A:LEU:HD13	6	0.13
(1,413)	1:79:A:LEU:H	1:79:A:LEU:HD11	10	0.13
(1,413)	1:79:A:LEU:H	1:79:A:LEU:HD12	10	0.13
(1,413)	1:79:A:LEU:H	1:79:A:LEU:HD13	10	0.13
(1,408)	1:84:A:GLU:HA	1:83:A:VAL:HG21	2	0.13
(1,408)	1:84:A:GLU:HA	1:83:A:VAL:HG22	2	0.13
(1,408)	1:84:A:GLU:HA	1:83:A:VAL:HG23	2	0.13
(1,408)	1:84:A:GLU:HA	1:83:A:VAL:HG21	9	0.13
(1,408)	1:84:A:GLU:HA	1:83:A:VAL:HG22	9	0.13
(1,408)	1:84:A:GLU:HA	1:83:A:VAL:HG23	9	0.13
(1,351)	1:81:A:THR:HG21	1:46:A:ILE:HG21	3	0.13
(1,351)	1:81:A:THR:HG21	1:46:A:ILE:HG22	3	0.13
(1,351)	1:81:A:THR:HG21	1:46:A:ILE:HG23	3	0.13
(1,351)	1:81:A:THR:HG22	1:46:A:ILE:HG21	3	0.13
(1,351)	1:81:A:THR:HG22	1:46:A:ILE:HG22	3	0.13
(1,351)	1:81:A:THR:HG22	1:46:A:ILE:HG23	3	0.13
(1,351)	1:81:A:THR:HG23	1:46:A:ILE:HG21	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,351)	1:81:A:THR:HG23	1:46:A:ILE:HG22	3	0.13
(1,351)	1:81:A:THR:HG23	1:46:A:ILE:HG23	3	0.13
(1,348)	1:109:A:ILE:HA	1:16:A:VAL:HG11	4	0.13
(1,348)	1:109:A:ILE:HA	1:16:A:VAL:HG12	4	0.13
(1,348)	1:109:A:ILE:HA	1:16:A:VAL:HG13	4	0.13
(1,348)	1:109:A:ILE:HA	1:16:A:VAL:HG11	9	0.13
(1,348)	1:109:A:ILE:HA	1:16:A:VAL:HG12	9	0.13
(1,348)	1:109:A:ILE:HA	1:16:A:VAL:HG13	9	0.13
(1,246)	1:45:A:LYS:H	1:45:A:LYS:HG2	6	0.13
(1,186)	1:72:A:LEU:HG	1:46:A:ILE:HG12	7	0.13
(1,180)	1:98:A:LYS:H	1:99:A:ILE:HG12	2	0.13
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG21	7	0.13
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG22	7	0.13
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG23	7	0.13
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG21	7	0.13
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG22	7	0.13
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG23	7	0.13
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG21	7	0.13
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG22	7	0.13
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG23	7	0.13
(1,65)	1:63:A:LYS:HE2	1:63:A:LYS:HD2	8	0.13
(1,65)	1:63:A:LYS:HE2	1:63:A:LYS:HD2	10	0.13
(1,28)	1:102:A:GLU:HA	1:102:A:GLU:HG3	4	0.13
(1,1283)	1:47:A:LEU:HD11	1:71:A:TYR:HB2	7	0.12
(1,1283)	1:47:A:LEU:HD12	1:71:A:TYR:HB2	7	0.12
(1,1283)	1:47:A:LEU:HD13	1:71:A:TYR:HB2	7	0.12
(1,1185)	1:81:A:THR:HG21	1:44:A:LYS:HD2	3	0.12
(1,1185)	1:81:A:THR:HG22	1:44:A:LYS:HD2	3	0.12
(1,1185)	1:81:A:THR:HG23	1:44:A:LYS:HD2	3	0.12
(1,1118)	1:72:A:LEU:HA	1:46:A:ILE:HG21	3	0.12
(1,1118)	1:72:A:LEU:HA	1:46:A:ILE:HG22	3	0.12
(1,1118)	1:72:A:LEU:HA	1:46:A:ILE:HG23	3	0.12
(1,1108)	1:65:A:ALA:HA	1:35:A:GLU:HB2	7	0.12
(1,1108)	1:65:A:ALA:HA	1:35:A:GLU:HB2	10	0.12
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD11	2	0.12
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD12	2	0.12
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD13	2	0.12
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD11	2	0.12
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD12	2	0.12
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD13	2	0.12
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD11	2	0.12
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD12	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD13	2	0.12
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD11	4	0.12
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD12	4	0.12
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD13	4	0.12
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD11	4	0.12
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD12	4	0.12
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD13	4	0.12
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD11	4	0.12
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD12	4	0.12
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD13	4	0.12
(1,1061)	1:55:A:ILE:HD11	1:41:A:LEU:HD11	5	0.12
(1,1061)	1:55:A:ILE:HD11	1:41:A:LEU:HD12	5	0.12
(1,1061)	1:55:A:ILE:HD11	1:41:A:LEU:HD13	5	0.12
(1,1061)	1:55:A:ILE:HD12	1:41:A:LEU:HD11	5	0.12
(1,1061)	1:55:A:ILE:HD12	1:41:A:LEU:HD12	5	0.12
(1,1061)	1:55:A:ILE:HD12	1:41:A:LEU:HD13	5	0.12
(1,1061)	1:55:A:ILE:HD13	1:41:A:LEU:HD11	5	0.12
(1,1061)	1:55:A:ILE:HD13	1:41:A:LEU:HD12	5	0.12
(1,1061)	1:55:A:ILE:HD13	1:41:A:LEU:HD13	5	0.12
(1,1049)	1:74:A:GLU:H	1:74:A:GLU:HG2	3	0.12
(1,1038)	1:75:A:ASN:HA	1:76:A:PRO:HG2	9	0.12
(1,1034)	1:79:A:LEU:H	1:79:A:LEU:HB3	5	0.12
(1,994)	1:40:A:HIS:H	1:40:A:HIS:HB3	6	0.12
(1,956)	1:34:A:ALA:HB1	1:41:A:LEU:HD11	8	0.12
(1,956)	1:34:A:ALA:HB1	1:41:A:LEU:HD12	8	0.12
(1,956)	1:34:A:ALA:HB1	1:41:A:LEU:HD13	8	0.12
(1,956)	1:34:A:ALA:HB2	1:41:A:LEU:HD11	8	0.12
(1,956)	1:34:A:ALA:HB2	1:41:A:LEU:HD12	8	0.12
(1,956)	1:34:A:ALA:HB2	1:41:A:LEU:HD13	8	0.12
(1,956)	1:34:A:ALA:HB3	1:41:A:LEU:HD11	8	0.12
(1,956)	1:34:A:ALA:HB3	1:41:A:LEU:HD12	8	0.12
(1,956)	1:34:A:ALA:HB3	1:41:A:LEU:HD13	8	0.12
(1,930)	1:16:A:VAL:HG21	1:13:A:LEU:HA	10	0.12
(1,930)	1:16:A:VAL:HG22	1:13:A:LEU:HA	10	0.12
(1,930)	1:16:A:VAL:HG23	1:13:A:LEU:HA	10	0.12
(1,918)	1:49:A:ARG:HA	1:52:A:THR:HG21	4	0.12
(1,918)	1:49:A:ARG:HA	1:52:A:THR:HG22	4	0.12
(1,918)	1:49:A:ARG:HA	1:52:A:THR:HG23	4	0.12
(1,811)	1:47:A:LEU:H	1:46:A:ILE:HB	6	0.12
(1,772)	1:71:A:TYR:HE1	1:55:A:ILE:HB	1	0.12
(1,772)	1:71:A:TYR:HE2	1:55:A:ILE:HB	1	0.12
(1,764)	1:32:A:ILE:HG13	1:69:A:LEU:HD21	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,764)	1:32:A:ILE:HG13	1:69:A:LEU:HD22	10	0.12
(1,764)	1:32:A:ILE:HG13	1:69:A:LEU:HD23	10	0.12
(1,705)	1:111:A:LEU:H	1:111:A:LEU:HB3	6	0.12
(1,694)	1:36:A:ARG:H	1:36:A:ARG:HB3	1	0.12
(1,680)	1:21:A:LEU:H	1:21:A:LEU:HB3	4	0.12
(1,669)	1:10:A:GLU:HG2	1:10:A:GLU:HA	2	0.12
(1,669)	1:10:A:GLU:HG2	1:10:A:GLU:HA	6	0.12
(1,669)	1:10:A:GLU:HG2	1:10:A:GLU:HA	10	0.12
(1,619)	1:87:A:ARG:HA	1:96:A:ILE:HG21	7	0.12
(1,619)	1:87:A:ARG:HA	1:96:A:ILE:HG22	7	0.12
(1,619)	1:87:A:ARG:HA	1:96:A:ILE:HG23	7	0.12
(1,565)	1:44:A:LYS:H	1:44:A:LYS:HD2	2	0.12
(1,548)	1:46:A:ILE:HA	1:46:A:ILE:HD11	10	0.12
(1,548)	1:46:A:ILE:HA	1:46:A:ILE:HD12	10	0.12
(1,548)	1:46:A:ILE:HA	1:46:A:ILE:HD13	10	0.12
(1,546)	1:89:A:GLU:H	1:89:A:GLU:HB3	3	0.12
(1,533)	1:79:A:LEU:HD11	1:80:A:ASP:HA	10	0.12
(1,533)	1:79:A:LEU:HD12	1:80:A:ASP:HA	10	0.12
(1,533)	1:79:A:LEU:HD13	1:80:A:ASP:HA	10	0.12
(1,532)	1:46:A:ILE:HD11	1:46:A:ILE:HA	10	0.12
(1,532)	1:46:A:ILE:HD12	1:46:A:ILE:HA	10	0.12
(1,532)	1:46:A:ILE:HD13	1:46:A:ILE:HA	10	0.12
(1,523)	1:73:A:GLN:HE21	1:18:A:LYS:HE2	4	0.12
(1,491)	1:70:A:ASP:H	1:70:A:ASP:HB3	8	0.12
(1,470)	1:16:A:VAL:HG21	1:106:A:LEU:HB3	3	0.12
(1,470)	1:16:A:VAL:HG22	1:106:A:LEU:HB3	3	0.12
(1,470)	1:16:A:VAL:HG23	1:106:A:LEU:HB3	3	0.12
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD11	4	0.12
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD12	4	0.12
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD13	4	0.12
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD11	4	0.12
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD12	4	0.12
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD13	4	0.12
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD11	4	0.12
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD12	4	0.12
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD13	4	0.12
(1,381)	1:78:A:GLY:H	1:78:A:GLY:HA2	6	0.12
(1,361)	1:27:A:TYR:HD1	1:95:A:LEU:HD11	9	0.12
(1,361)	1:27:A:TYR:HD1	1:95:A:LEU:HD12	9	0.12
(1,361)	1:27:A:TYR:HD1	1:95:A:LEU:HD13	9	0.12
(1,361)	1:27:A:TYR:HD2	1:95:A:LEU:HD11	9	0.12
(1,361)	1:27:A:TYR:HD2	1:95:A:LEU:HD12	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,361)	1:27:A:TYR:HD2	1:95:A:LEU:HD13	9	0.12
(1,351)	1:81:A:THR:HG21	1:46:A:ILE:HG21	9	0.12
(1,351)	1:81:A:THR:HG21	1:46:A:ILE:HG22	9	0.12
(1,351)	1:81:A:THR:HG21	1:46:A:ILE:HG23	9	0.12
(1,351)	1:81:A:THR:HG22	1:46:A:ILE:HG21	9	0.12
(1,351)	1:81:A:THR:HG22	1:46:A:ILE:HG22	9	0.12
(1,351)	1:81:A:THR:HG22	1:46:A:ILE:HG23	9	0.12
(1,351)	1:81:A:THR:HG23	1:46:A:ILE:HG21	9	0.12
(1,351)	1:81:A:THR:HG23	1:46:A:ILE:HG22	9	0.12
(1,351)	1:81:A:THR:HG23	1:46:A:ILE:HG23	9	0.12
(1,319)	1:72:A:LEU:HD21	1:72:A:LEU:HA	3	0.12
(1,319)	1:72:A:LEU:HD22	1:72:A:LEU:HA	3	0.12
(1,319)	1:72:A:LEU:HD23	1:72:A:LEU:HA	3	0.12
(1,314)	1:25:A:ARG:HA	1:69:A:LEU:HG	10	0.12
(1,308)	1:104:A:LEU:HA	1:13:A:LEU:HB2	9	0.12
(1,308)	1:104:A:LEU:HA	1:13:A:LEU:HB2	10	0.12
(1,274)	1:115:A:LYS:H	1:114:A:LEU:HB3	1	0.12
(1,180)	1:98:A:LYS:H	1:99:A:ILE:HG12	10	0.12
(1,153)	1:114:A:LEU:HD11	1:115:A:LYS:HA	8	0.12
(1,153)	1:114:A:LEU:HD12	1:115:A:LYS:HA	8	0.12
(1,153)	1:114:A:LEU:HD13	1:115:A:LYS:HA	8	0.12
(1,132)	1:95:A:LEU:HD21	1:31:A:LYS:HB2	4	0.12
(1,132)	1:95:A:LEU:HD22	1:31:A:LYS:HB2	4	0.12
(1,132)	1:95:A:LEU:HD23	1:31:A:LYS:HB2	4	0.12
(1,132)	1:95:A:LEU:HD21	1:31:A:LYS:HB2	8	0.12
(1,132)	1:95:A:LEU:HD22	1:31:A:LYS:HB2	8	0.12
(1,132)	1:95:A:LEU:HD23	1:31:A:LYS:HB2	8	0.12
(1,109)	1:71:A:TYR:HD1	1:68:A:LEU:HB2	6	0.12
(1,109)	1:71:A:TYR:HD2	1:68:A:LEU:HB2	6	0.12
(1,71)	1:95:A:LEU:HD21	1:86:A:ILE:HD11	10	0.12
(1,71)	1:95:A:LEU:HD21	1:86:A:ILE:HD12	10	0.12
(1,71)	1:95:A:LEU:HD21	1:86:A:ILE:HD13	10	0.12
(1,71)	1:95:A:LEU:HD22	1:86:A:ILE:HD11	10	0.12
(1,71)	1:95:A:LEU:HD22	1:86:A:ILE:HD12	10	0.12
(1,71)	1:95:A:LEU:HD22	1:86:A:ILE:HD13	10	0.12
(1,71)	1:95:A:LEU:HD23	1:86:A:ILE:HD11	10	0.12
(1,71)	1:95:A:LEU:HD23	1:86:A:ILE:HD12	10	0.12
(1,71)	1:95:A:LEU:HD23	1:86:A:ILE:HD13	10	0.12
(1,42)	1:34:A:ALA:HB1	1:68:A:LEU:HB2	1	0.12
(1,42)	1:34:A:ALA:HB2	1:68:A:LEU:HB2	1	0.12
(1,42)	1:34:A:ALA:HB3	1:68:A:LEU:HB2	1	0.12
(1,1283)	1:47:A:LEU:HD11	1:71:A:TYR:HB2	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1283)	1:47:A:LEU:HD12	1:71:A:TYR:HB2	2	0.11
(1,1283)	1:47:A:LEU:HD13	1:71:A:TYR:HB2	2	0.11
(1,1247)	1:72:A:LEU:H	1:72:A:LEU:HG	7	0.11
(1,1207)	1:24:A:LEU:HD11	1:28:A:LEU:HG	5	0.11
(1,1207)	1:24:A:LEU:HD12	1:28:A:LEU:HG	5	0.11
(1,1207)	1:24:A:LEU:HD13	1:28:A:LEU:HG	5	0.11
(1,1198)	1:108:A:ASN:HD22	1:108:A:ASN:HB2	5	0.11
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG21	8	0.11
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG22	8	0.11
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG23	8	0.11
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG21	8	0.11
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG22	8	0.11
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG23	8	0.11
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG21	8	0.11
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG22	8	0.11
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG23	8	0.11
(1,1194)	1:64:A:ARG:HA	1:63:A:LYS:HD2	9	0.11
(1,1166)	1:14:A:THR:HG21	1:10:A:GLU:HB2	5	0.11
(1,1166)	1:14:A:THR:HG22	1:10:A:GLU:HB2	5	0.11
(1,1166)	1:14:A:THR:HG23	1:10:A:GLU:HB2	5	0.11
(1,1160)	1:20:A:ALA:HB1	1:24:A:LEU:HD11	7	0.11
(1,1160)	1:20:A:ALA:HB1	1:24:A:LEU:HD12	7	0.11
(1,1160)	1:20:A:ALA:HB1	1:24:A:LEU:HD13	7	0.11
(1,1160)	1:20:A:ALA:HB2	1:24:A:LEU:HD11	7	0.11
(1,1160)	1:20:A:ALA:HB2	1:24:A:LEU:HD12	7	0.11
(1,1160)	1:20:A:ALA:HB2	1:24:A:LEU:HD13	7	0.11
(1,1160)	1:20:A:ALA:HB3	1:24:A:LEU:HD11	7	0.11
(1,1160)	1:20:A:ALA:HB3	1:24:A:LEU:HD12	7	0.11
(1,1160)	1:20:A:ALA:HB3	1:24:A:LEU:HD13	7	0.11
(1,1160)	1:20:A:ALA:HB1	1:24:A:LEU:HD11	9	0.11
(1,1160)	1:20:A:ALA:HB1	1:24:A:LEU:HD12	9	0.11
(1,1160)	1:20:A:ALA:HB1	1:24:A:LEU:HD13	9	0.11
(1,1160)	1:20:A:ALA:HB2	1:24:A:LEU:HD11	9	0.11
(1,1160)	1:20:A:ALA:HB2	1:24:A:LEU:HD12	9	0.11
(1,1160)	1:20:A:ALA:HB2	1:24:A:LEU:HD13	9	0.11
(1,1160)	1:20:A:ALA:HB3	1:24:A:LEU:HD11	9	0.11
(1,1160)	1:20:A:ALA:HB3	1:24:A:LEU:HD12	9	0.11
(1,1160)	1:20:A:ALA:HB3	1:24:A:LEU:HD13	9	0.11
(1,1140)	1:46:A:ILE:HG21	1:47:A:LEU:HD11	1	0.11
(1,1140)	1:46:A:ILE:HG21	1:47:A:LEU:HD12	1	0.11
(1,1140)	1:46:A:ILE:HG21	1:47:A:LEU:HD13	1	0.11
(1,1140)	1:46:A:ILE:HG22	1:47:A:LEU:HD11	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1140)	1:46:A:ILE:HG22	1:47:A:LEU:HD12	1	0.11
(1,1140)	1:46:A:ILE:HG22	1:47:A:LEU:HD13	1	0.11
(1,1140)	1:46:A:ILE:HG23	1:47:A:LEU:HD11	1	0.11
(1,1140)	1:46:A:ILE:HG23	1:47:A:LEU:HD12	1	0.11
(1,1140)	1:46:A:ILE:HG23	1:47:A:LEU:HD13	1	0.11
(1,1137)	1:111:A:LEU:H	1:111:A:LEU:HA	6	0.11
(1,1126)	1:53:A:ARG:H	1:53:A:ARG:HB3	4	0.11
(1,1118)	1:72:A:LEU:HA	1:46:A:ILE:HG21	6	0.11
(1,1118)	1:72:A:LEU:HA	1:46:A:ILE:HG22	6	0.11
(1,1118)	1:72:A:LEU:HA	1:46:A:ILE:HG23	6	0.11
(1,1118)	1:72:A:LEU:HA	1:46:A:ILE:HG21	9	0.11
(1,1118)	1:72:A:LEU:HA	1:46:A:ILE:HG22	9	0.11
(1,1118)	1:72:A:LEU:HA	1:46:A:ILE:HG23	9	0.11
(1,1111)	1:38:A:PHE:HD1	1:52:A:THR:HG21	6	0.11
(1,1111)	1:38:A:PHE:HD1	1:52:A:THR:HG22	6	0.11
(1,1111)	1:38:A:PHE:HD1	1:52:A:THR:HG23	6	0.11
(1,1111)	1:38:A:PHE:HD2	1:52:A:THR:HG21	6	0.11
(1,1111)	1:38:A:PHE:HD2	1:52:A:THR:HG22	6	0.11
(1,1111)	1:38:A:PHE:HD2	1:52:A:THR:HG23	6	0.11
(1,1104)	1:45:A:LYS:HG2	1:42:A:ARG:HA	3	0.11
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD11	1	0.11
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD12	1	0.11
(1,1082)	1:52:A:THR:HG21	1:46:A:ILE:HD13	1	0.11
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD11	1	0.11
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD12	1	0.11
(1,1082)	1:52:A:THR:HG22	1:46:A:ILE:HD13	1	0.11
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD11	1	0.11
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD12	1	0.11
(1,1082)	1:52:A:THR:HG23	1:46:A:ILE:HD13	1	0.11
(1,1080)	1:75:A:ASN:H	1:75:A:ASN:HB3	8	0.11
(1,1005)	1:82:A:LEU:HD11	1:72:A:LEU:HD21	4	0.11
(1,1005)	1:82:A:LEU:HD11	1:72:A:LEU:HD22	4	0.11
(1,1005)	1:82:A:LEU:HD11	1:72:A:LEU:HD23	4	0.11
(1,1005)	1:82:A:LEU:HD12	1:72:A:LEU:HD21	4	0.11
(1,1005)	1:82:A:LEU:HD12	1:72:A:LEU:HD22	4	0.11
(1,1005)	1:82:A:LEU:HD12	1:72:A:LEU:HD23	4	0.11
(1,1005)	1:82:A:LEU:HD13	1:72:A:LEU:HD21	4	0.11
(1,1005)	1:82:A:LEU:HD13	1:72:A:LEU:HD22	4	0.11
(1,1005)	1:82:A:LEU:HD13	1:72:A:LEU:HD23	4	0.11
(1,964)	1:102:A:GLU:H	1:102:A:GLU:HB3	10	0.11
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD11	1	0.11
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD12	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,940)	1:111:A:LEU:H	1:111:A:LEU:HD13	1	0.11
(1,894)	1:107:A:ARG:H	1:106:A:LEU:H	5	0.11
(1,892)	1:95:A:LEU:HD11	1:86:A:ILE:HD11	7	0.11
(1,892)	1:95:A:LEU:HD11	1:86:A:ILE:HD12	7	0.11
(1,892)	1:95:A:LEU:HD11	1:86:A:ILE:HD13	7	0.11
(1,892)	1:95:A:LEU:HD12	1:86:A:ILE:HD11	7	0.11
(1,892)	1:95:A:LEU:HD12	1:86:A:ILE:HD12	7	0.11
(1,892)	1:95:A:LEU:HD12	1:86:A:ILE:HD13	7	0.11
(1,892)	1:95:A:LEU:HD13	1:86:A:ILE:HD11	7	0.11
(1,892)	1:95:A:LEU:HD13	1:86:A:ILE:HD12	7	0.11
(1,892)	1:95:A:LEU:HD13	1:86:A:ILE:HD13	7	0.11
(1,857)	1:111:A:LEU:HA	1:111:A:LEU:HG	7	0.11
(1,843)	1:96:A:ILE:HG12	1:95:A:LEU:HB2	9	0.11
(1,785)	1:112:A:GLU:H	1:112:A:GLU:HA	2	0.11
(1,785)	1:112:A:GLU:H	1:112:A:GLU:HA	10	0.11
(1,740)	1:47:A:LEU:HD11	1:46:A:ILE:HG21	1	0.11
(1,740)	1:47:A:LEU:HD11	1:46:A:ILE:HG22	1	0.11
(1,740)	1:47:A:LEU:HD11	1:46:A:ILE:HG23	1	0.11
(1,740)	1:47:A:LEU:HD12	1:46:A:ILE:HG21	1	0.11
(1,740)	1:47:A:LEU:HD12	1:46:A:ILE:HG22	1	0.11
(1,740)	1:47:A:LEU:HD12	1:46:A:ILE:HG23	1	0.11
(1,740)	1:47:A:LEU:HD13	1:46:A:ILE:HG21	1	0.11
(1,740)	1:47:A:LEU:HD13	1:46:A:ILE:HG22	1	0.11
(1,740)	1:47:A:LEU:HD13	1:46:A:ILE:HG23	1	0.11
(1,705)	1:111:A:LEU:H	1:111:A:LEU:HB3	8	0.11
(1,680)	1:21:A:LEU:H	1:21:A:LEU:HB3	1	0.11
(1,669)	1:10:A:GLU:HG2	1:10:A:GLU:HA	3	0.11
(1,647)	1:73:A:GLN:HE21	1:73:A:GLN:HG3	8	0.11
(1,619)	1:87:A:ARG:HA	1:96:A:ILE:HG21	3	0.11
(1,619)	1:87:A:ARG:HA	1:96:A:ILE:HG22	3	0.11
(1,619)	1:87:A:ARG:HA	1:96:A:ILE:HG23	3	0.11
(1,584)	1:79:A:LEU:HD21	1:69:A:LEU:HB2	5	0.11
(1,584)	1:79:A:LEU:HD22	1:69:A:LEU:HB2	5	0.11
(1,584)	1:79:A:LEU:HD23	1:69:A:LEU:HB2	5	0.11
(1,546)	1:89:A:GLU:H	1:89:A:GLU:HB3	4	0.11
(1,546)	1:89:A:GLU:H	1:89:A:GLU:HB3	10	0.11
(1,533)	1:79:A:LEU:HD11	1:80:A:ASP:HA	7	0.11
(1,533)	1:79:A:LEU:HD12	1:80:A:ASP:HA	7	0.11
(1,533)	1:79:A:LEU:HD13	1:80:A:ASP:HA	7	0.11
(1,378)	1:83:A:VAL:HB	1:82:A:LEU:HB2	7	0.11
(1,364)	1:14:A:THR:H	1:14:A:THR:HB	3	0.11
(1,348)	1:109:A:ILE:HA	1:16:A:VAL:HG11	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,348)	1:109:A:ILE:HA	1:16:A:VAL:HG12	7	0.11
(1,348)	1:109:A:ILE:HA	1:16:A:VAL:HG13	7	0.11
(1,314)	1:25:A:ARG:HA	1:69:A:LEU:HG	8	0.11
(1,279)	1:32:A:ILE:HD11	1:69:A:LEU:HD11	8	0.11
(1,279)	1:32:A:ILE:HD11	1:69:A:LEU:HD12	8	0.11
(1,279)	1:32:A:ILE:HD11	1:69:A:LEU:HD13	8	0.11
(1,279)	1:32:A:ILE:HD12	1:69:A:LEU:HD11	8	0.11
(1,279)	1:32:A:ILE:HD12	1:69:A:LEU:HD12	8	0.11
(1,279)	1:32:A:ILE:HD12	1:69:A:LEU:HD13	8	0.11
(1,279)	1:32:A:ILE:HD13	1:69:A:LEU:HD11	8	0.11
(1,279)	1:32:A:ILE:HD13	1:69:A:LEU:HD12	8	0.11
(1,279)	1:32:A:ILE:HD13	1:69:A:LEU:HD13	8	0.11
(1,197)	1:30:A:GLU:H	1:30:A:GLU:HA	7	0.11
(1,197)	1:30:A:GLU:H	1:30:A:GLU:HA	9	0.11
(1,115)	1:16:A:VAL:HG21	1:15:A:GLU:HB2	10	0.11
(1,115)	1:16:A:VAL:HG22	1:15:A:GLU:HB2	10	0.11
(1,115)	1:16:A:VAL:HG23	1:15:A:GLU:HB2	10	0.11
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG21	8	0.11
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG22	8	0.11
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG23	8	0.11
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG21	8	0.11
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG22	8	0.11
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG23	8	0.11
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG21	8	0.11
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG22	8	0.11
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG23	8	0.11
(1,71)	1:95:A:LEU:HD21	1:86:A:ILE:HD11	6	0.11
(1,71)	1:95:A:LEU:HD21	1:86:A:ILE:HD12	6	0.11
(1,71)	1:95:A:LEU:HD21	1:86:A:ILE:HD13	6	0.11
(1,71)	1:95:A:LEU:HD22	1:86:A:ILE:HD11	6	0.11
(1,71)	1:95:A:LEU:HD22	1:86:A:ILE:HD12	6	0.11
(1,71)	1:95:A:LEU:HD22	1:86:A:ILE:HD13	6	0.11
(1,71)	1:95:A:LEU:HD23	1:86:A:ILE:HD11	6	0.11
(1,71)	1:95:A:LEU:HD23	1:86:A:ILE:HD12	6	0.11
(1,71)	1:95:A:LEU:HD23	1:86:A:ILE:HD13	6	0.11
(1,37)	1:27:A:TYR:HE1	1:28:A:LEU:HD11	4	0.11
(1,37)	1:27:A:TYR:HE1	1:28:A:LEU:HD12	4	0.11
(1,37)	1:27:A:TYR:HE1	1:28:A:LEU:HD13	4	0.11
(1,37)	1:27:A:TYR:HE2	1:28:A:LEU:HD11	4	0.11
(1,37)	1:27:A:TYR:HE2	1:28:A:LEU:HD12	4	0.11
(1,37)	1:27:A:TYR:HE2	1:28:A:LEU:HD13	4	0.11
(1,30)	1:25:A:ARG:H	1:21:A:LEU:HB3	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:31:A:LYS:HB2	1:31:A:LYS:HD2	5	0.11
(1,2)	1:32:A:ILE:H	1:32:A:ILE:HG12	3	0.11
(1,1221)	1:108:A:ASN:HD21	1:108:A:ASN:HB3	6	0.1
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG21	10	0.1
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG22	10	0.1
(1,1196)	1:14:A:THR:HG21	1:16:A:VAL:HG23	10	0.1
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG21	10	0.1
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG22	10	0.1
(1,1196)	1:14:A:THR:HG22	1:16:A:VAL:HG23	10	0.1
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG21	10	0.1
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG22	10	0.1
(1,1196)	1:14:A:THR:HG23	1:16:A:VAL:HG23	10	0.1
(1,1192)	1:25:A:ARG:H	1:25:A:ARG:HB2	8	0.1
(1,1166)	1:14:A:THR:HG21	1:10:A:GLU:HB2	7	0.1
(1,1166)	1:14:A:THR:HG22	1:10:A:GLU:HB2	7	0.1
(1,1166)	1:14:A:THR:HG23	1:10:A:GLU:HB2	7	0.1
(1,1160)	1:20:A:ALA:HB1	1:24:A:LEU:HD11	1	0.1
(1,1160)	1:20:A:ALA:HB1	1:24:A:LEU:HD12	1	0.1
(1,1160)	1:20:A:ALA:HB1	1:24:A:LEU:HD13	1	0.1
(1,1160)	1:20:A:ALA:HB2	1:24:A:LEU:HD11	1	0.1
(1,1160)	1:20:A:ALA:HB2	1:24:A:LEU:HD12	1	0.1
(1,1160)	1:20:A:ALA:HB2	1:24:A:LEU:HD13	1	0.1
(1,1160)	1:20:A:ALA:HB3	1:24:A:LEU:HD11	1	0.1
(1,1160)	1:20:A:ALA:HB3	1:24:A:LEU:HD12	1	0.1
(1,1160)	1:20:A:ALA:HB3	1:24:A:LEU:HD13	1	0.1
(1,1158)	1:78:A:GLY:HA3	1:72:A:LEU:HD21	10	0.1
(1,1158)	1:78:A:GLY:HA3	1:72:A:LEU:HD22	10	0.1
(1,1158)	1:78:A:GLY:HA3	1:72:A:LEU:HD23	10	0.1
(1,1083)	1:109:A:ILE:HG21	1:106:A:LEU:HA	5	0.1
(1,1083)	1:109:A:ILE:HG22	1:106:A:LEU:HA	5	0.1
(1,1083)	1:109:A:ILE:HG23	1:106:A:LEU:HA	5	0.1
(1,1045)	1:55:A:ILE:HG21	1:71:A:TYR:HD1	8	0.1
(1,1045)	1:55:A:ILE:HG21	1:71:A:TYR:HD2	8	0.1
(1,1045)	1:55:A:ILE:HG22	1:71:A:TYR:HD1	8	0.1
(1,1045)	1:55:A:ILE:HG22	1:71:A:TYR:HD2	8	0.1
(1,1045)	1:55:A:ILE:HG23	1:71:A:TYR:HD1	8	0.1
(1,1045)	1:55:A:ILE:HG23	1:71:A:TYR:HD2	8	0.1
(1,1017)	1:36:A:ARG:HA	1:36:A:ARG:HG3	4	0.1
(1,992)	1:43:A:ALA:HB1	1:44:A:LYS:HD2	8	0.1
(1,992)	1:43:A:ALA:HB2	1:44:A:LYS:HD2	8	0.1
(1,992)	1:43:A:ALA:HB3	1:44:A:LYS:HD2	8	0.1
(1,868)	1:93:A:ASN:HD22	1:93:A:ASN:HB2	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,850)	1:73:A:GLN:HG2	1:79:A:LEU:HD11	4	0.1
(1,850)	1:73:A:GLN:HG2	1:79:A:LEU:HD12	4	0.1
(1,850)	1:73:A:GLN:HG2	1:79:A:LEU:HD13	4	0.1
(1,705)	1:111:A:LEU:H	1:111:A:LEU:HB3	4	0.1
(1,669)	1:10:A:GLU:HG2	1:10:A:GLU:HA	8	0.1
(1,584)	1:79:A:LEU:HD21	1:69:A:LEU:HB2	2	0.1
(1,584)	1:79:A:LEU:HD22	1:69:A:LEU:HB2	2	0.1
(1,584)	1:79:A:LEU:HD23	1:69:A:LEU:HB2	2	0.1
(1,565)	1:44:A:LYS:H	1:44:A:LYS:HD2	4	0.1
(1,513)	1:112:A:GLU:H	1:114:A:LEU:H	2	0.1
(1,476)	1:73:A:GLN:H	1:73:A:GLN:HG3	1	0.1
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD11	6	0.1
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD12	6	0.1
(1,463)	1:69:A:LEU:HD21	1:68:A:LEU:HD13	6	0.1
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD11	6	0.1
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD12	6	0.1
(1,463)	1:69:A:LEU:HD22	1:68:A:LEU:HD13	6	0.1
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD11	6	0.1
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD12	6	0.1
(1,463)	1:69:A:LEU:HD23	1:68:A:LEU:HD13	6	0.1
(1,391)	1:71:A:TYR:HD1	1:55:A:ILE:HG21	8	0.1
(1,391)	1:71:A:TYR:HD1	1:55:A:ILE:HG22	8	0.1
(1,391)	1:71:A:TYR:HD1	1:55:A:ILE:HG23	8	0.1
(1,391)	1:71:A:TYR:HD2	1:55:A:ILE:HG21	8	0.1
(1,391)	1:71:A:TYR:HD2	1:55:A:ILE:HG22	8	0.1
(1,391)	1:71:A:TYR:HD2	1:55:A:ILE:HG23	8	0.1
(1,361)	1:27:A:TYR:HD1	1:95:A:LEU:HD11	5	0.1
(1,361)	1:27:A:TYR:HD1	1:95:A:LEU:HD12	5	0.1
(1,361)	1:27:A:TYR:HD1	1:95:A:LEU:HD13	5	0.1
(1,361)	1:27:A:TYR:HD2	1:95:A:LEU:HD11	5	0.1
(1,361)	1:27:A:TYR:HD2	1:95:A:LEU:HD12	5	0.1
(1,361)	1:27:A:TYR:HD2	1:95:A:LEU:HD13	5	0.1
(1,348)	1:109:A:ILE:HA	1:16:A:VAL:HG11	1	0.1
(1,348)	1:109:A:ILE:HA	1:16:A:VAL:HG12	1	0.1
(1,348)	1:109:A:ILE:HA	1:16:A:VAL:HG13	1	0.1
(1,308)	1:104:A:LEU:HA	1:13:A:LEU:HB2	3	0.1
(1,274)	1:115:A:LYS:H	1:114:A:LEU:HB3	9	0.1
(1,269)	1:55:A:ILE:H	1:55:A:ILE:HB	8	0.1
(1,265)	1:73:A:GLN:H	1:71:A:TYR:HA	2	0.1
(1,145)	1:16:A:VAL:H	1:16:A:VAL:HG21	7	0.1
(1,145)	1:16:A:VAL:H	1:16:A:VAL:HG22	7	0.1
(1,145)	1:16:A:VAL:H	1:16:A:VAL:HG23	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,145)	1:16:A:VAL:H	1:16:A:VAL:HG21	10	0.1
(1,145)	1:16:A:VAL:H	1:16:A:VAL:HG22	10	0.1
(1,145)	1:16:A:VAL:H	1:16:A:VAL:HG23	10	0.1
(1,113)	1:69:A:LEU:HD21	1:34:A:ALA:HB1	10	0.1
(1,113)	1:69:A:LEU:HD21	1:34:A:ALA:HB2	10	0.1
(1,113)	1:69:A:LEU:HD21	1:34:A:ALA:HB3	10	0.1
(1,113)	1:69:A:LEU:HD22	1:34:A:ALA:HB1	10	0.1
(1,113)	1:69:A:LEU:HD22	1:34:A:ALA:HB2	10	0.1
(1,113)	1:69:A:LEU:HD22	1:34:A:ALA:HB3	10	0.1
(1,113)	1:69:A:LEU:HD23	1:34:A:ALA:HB1	10	0.1
(1,113)	1:69:A:LEU:HD23	1:34:A:ALA:HB2	10	0.1
(1,113)	1:69:A:LEU:HD23	1:34:A:ALA:HB3	10	0.1
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG21	10	0.1
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG22	10	0.1
(1,97)	1:16:A:VAL:HG21	1:14:A:THR:HG23	10	0.1
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG21	10	0.1
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG22	10	0.1
(1,97)	1:16:A:VAL:HG22	1:14:A:THR:HG23	10	0.1
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG21	10	0.1
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG22	10	0.1
(1,97)	1:16:A:VAL:HG23	1:14:A:THR:HG23	10	0.1
(1,17)	1:31:A:LYS:HB2	1:31:A:LYS:HD2	2	0.1
(1,17)	1:31:A:LYS:HB2	1:31:A:LYS:HD2	6	0.1
(1,17)	1:31:A:LYS:HB2	1:31:A:LYS:HD2	8	0.1
(1,2)	1:32:A:ILE:H	1:32:A:ILE:HG12	1	0.1

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

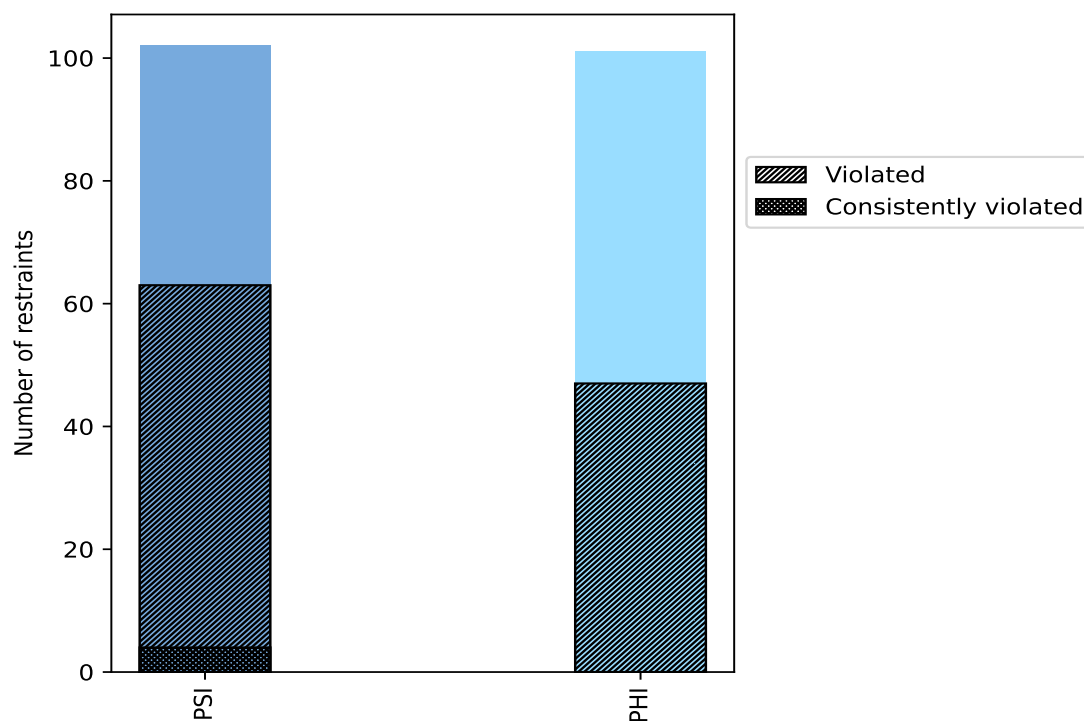
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	102	50.2	63	61.8	31.0	4	3.9	2.0
PHI	101	49.8	47	46.5	23.2	0	0.0	0.0
Total	203	100.0	110	54.2	54.2	4	2.0	2.0

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

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



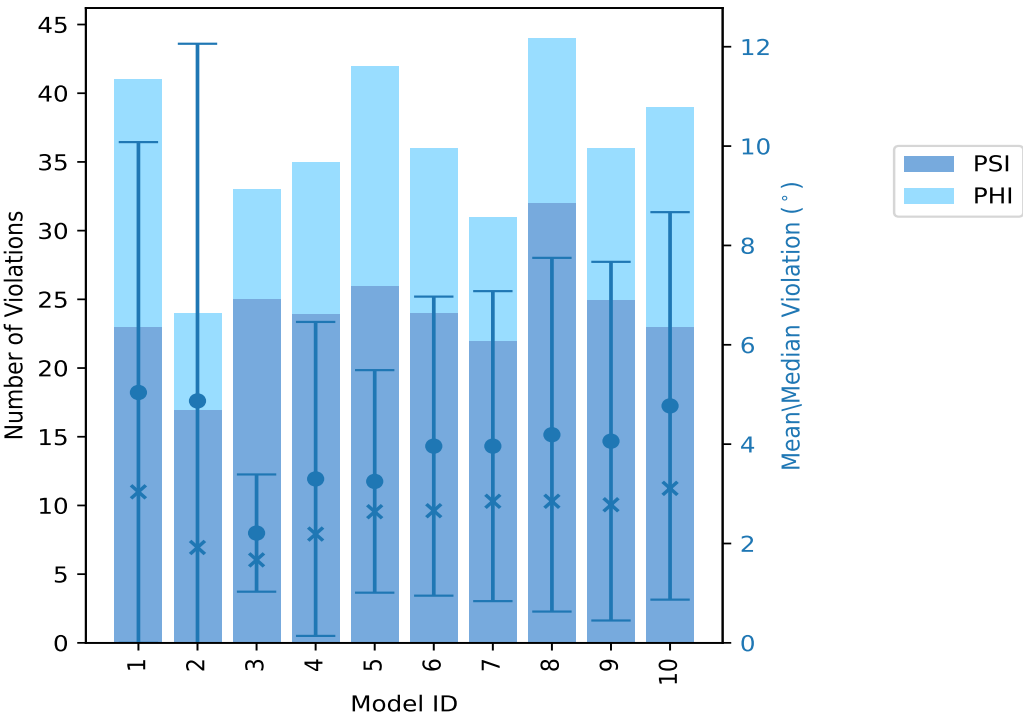
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	23	18	41	5.04	18.83	5.04	3.04
2	17	7	24	4.87	28.36	7.19	1.92
3	25	8	33	2.21	5.39	1.18	1.67
4	24	11	35	3.3	14.89	3.16	2.19
5	26	16	42	3.25	9.56	2.24	2.64
6	24	12	36	3.96	12.07	3.01	2.66
7	22	9	31	3.96	12.17	3.12	2.85
8	32	12	44	4.19	16.46	3.56	2.85
9	25	11	36	4.06	16.39	3.61	2.78
10	23	16	39	4.77	14.25	3.9	3.11

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

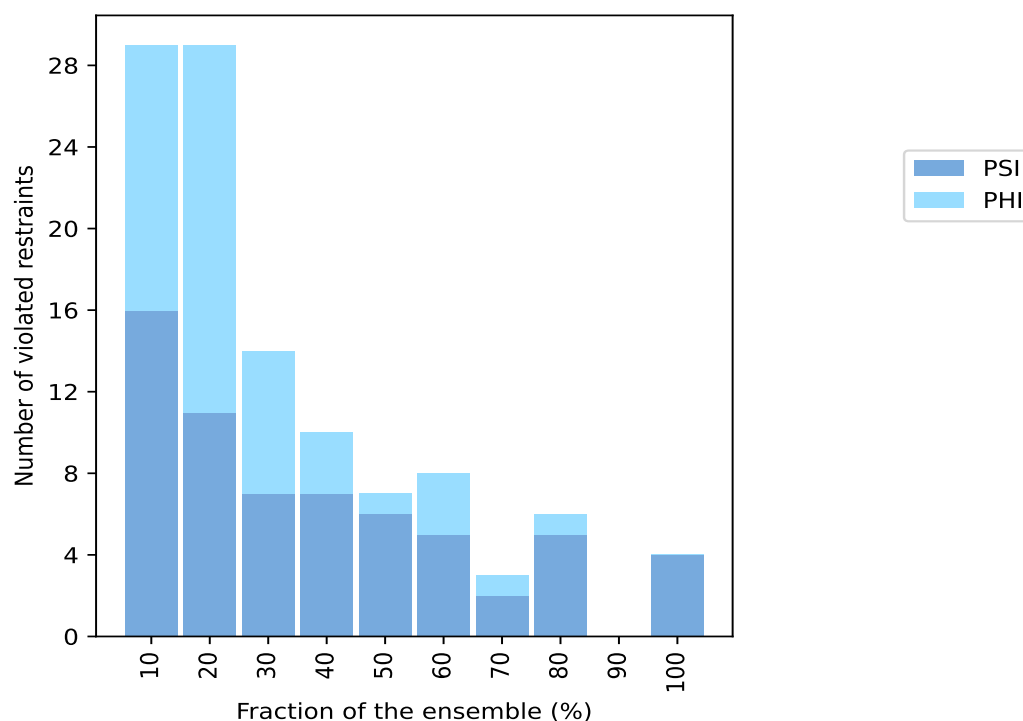
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
16	13	29	1	10.0
11	18	29	2	20.0
7	7	14	3	30.0
7	3	10	4	40.0
6	1	7	5	50.0
5	3	8	6	60.0
2	1	3	7	70.0
5	1	6	8	80.0
0	0	0	9	90.0
4	0	4	10	100.0

¹ Number of models with violations

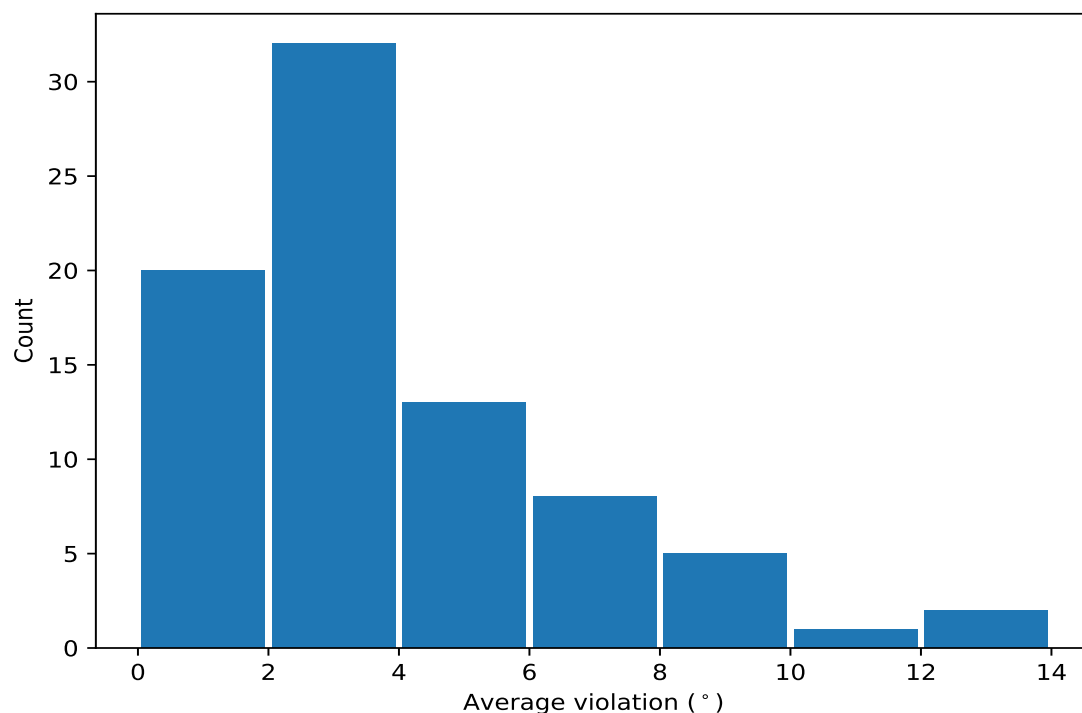
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle 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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,47)	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	1:34:A:ALA:N	10	7.73	4.67	6.02
(1,129)	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	1:76:A:PRO:N	10	5.98	4.01	5.09
(1,13)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:LYS:N	10	4.32	1.37	4.2
(1,69)	1:44:A:LYS:N	1:44:A:LYS:CA	1:44:A:LYS:C	1:45:A:LYS:N	10	3.31	1.55	3.1
(1,157)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:LYS:N	8	6.18	1.8	5.95
(1,53)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:HIS:N	8	5.41	2.98	5.12
(1,9)	1:14:A:THR:N	1:14:A:THR:CA	1:14:A:THR:C	1:15:A:GLU:N	8	5.34	7.87	2.41
(1,48)	1:33:A:ILE:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	8	5.26	4.64	3.38
(1,95)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:THR:N	8	3.64	2.0	3.48
(1,123)	1:72:A:LEU:N	1:72:A:LEU:CA	1:72:A:LEU:C	1:73:A:GLN:N	8	3.18	2.9	1.88
(1,94)	1:57:A:CYS:C	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	7	4.87	3.45	2.83
(1,195)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:LYS:N	7	2.25	0.79	2.45
(1,71)	1:45:A:LYS:N	1:45:A:LYS:CA	1:45:A:LYS:C	1:46:A:ILE:N	7	1.94	0.69	1.92

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,158)	1:89:A:GLU:C	1:90:A:LYS:N	1:90:A:LYS:CA	1:90:A:LYS:C	6	6.34	3.93	6.16
(1,125)	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	1:74:A:GLU:N	6	6.05	6.2	2.13
(1,54)	1:36:A:ARG:C	1:37:A:HIS:N	1:37:A:HIS:CA	1:37:A:HIS:C	6	5.85	4.33	4.38
(1,155)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:GLU:N	6	4.65	3.59	3.62
(1,130)	1:75:A:ASN:C	1:76:A:PRO:N	1:76:A:PRO:CA	1:76:A:PRO:C	6	3.69	2.04	3.69
(1,163)	1:93:A:ASN:N	1:93:A:ASN:CA	1:93:A:ASN:C	1:94:A:PHE:N	6	3.21	1.41	2.82
(1,7)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:THR:N	6	2.82	0.97	2.94
(1,67)	1:43:A:ALA:N	1:43:A:ALA:CA	1:43:A:ALA:C	1:44:A:LYS:N	6	1.5	0.44	1.37
(1,93)	1:57:A:CYS:N	1:57:A:CYS:CA	1:57:A:CYS:C	1:58:A:ARG:N	5	6.17	3.45	6.91
(1,55)	1:37:A:HIS:N	1:37:A:HIS:CA	1:37:A:HIS:C	1:38:A:PHE:N	5	4.93	6.81	1.75
(1,127)	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	1:75:A:ASN:N	5	4.48	3.38	2.94
(1,154)	1:87:A:ARG:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	5	3.92	2.48	3.35
(1,189)	1:106:A:LEU:N	1:106:A:LEU:CA	1:106:A:LEU:C	1:107:A:ARG:N	5	2.71	0.47	2.87
(1,61)	1:40:A:HIS:N	1:40:A:HIS:CA	1:40:A:HIS:C	1:41:A:LEU:N	5	2.7	0.6	2.91
(1,203)	1:113:A:HIS:N	1:113:A:HIS:CA	1:113:A:HIS:C	1:114:A:LEU:N	5	2.03	0.84	1.88
(1,8)	1:13:A:LEU:C	1:14:A:THR:N	1:14:A:THR:CA	1:14:A:THR:C	4	9.03	11.2	3.22
(1,128)	1:74:A:GLU:C	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	4	4.31	3.41	2.96
(1,45)	1:32:A:ILE:N	1:32:A:ILE:CA	1:32:A:ILE:C	1:33:A:ILE:N	4	3.33	2.12	3.26
(1,135)	1:78:A:GLY:N	1:78:A:GLY:CA	1:78:A:GLY:C	1:79:A:LEU:N	4	3.23	1.5	3.2
(1,153)	1:87:A:ARG:N	1:87:A:ARG:CA	1:87:A:ARG:C	1:88:A:ARG:N	4	2.9	2.32	1.9
(1,121)	1:71:A:TYR:N	1:71:A:TYR:CA	1:71:A:TYR:C	1:72:A:LEU:N	4	2.85	0.39	2.93
(1,1)	1:10:A:GLU:N	1:10:A:GLU:CA	1:10:A:GLU:C	1:11:A:GLU:N	4	2.73	1.52	2.63
(1,2)	1:10:A:GLU:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	4	2.07	0.7	2.22
(1,105)	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1:64:A:ARG:N	4	1.69	0.5	1.56
(1,43)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:ILE:N	4	1.49	0.37	1.43
(1,131)	1:76:A:PRO:N	1:76:A:PRO:CA	1:76:A:PRO:C	1:77:A:LYS:N	3	7.55	5.89	3.45
(1,56)	1:37:A:HIS:C	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	3	6.89	7.89	1.59
(1,159)	1:90:A:LYS:N	1:90:A:LYS:CA	1:90:A:LYS:C	1:91:A:THR:N	3	6.72	3.13	4.53
(1,156)	1:88:A:ARG:C	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	3	5.34	1.82	5.47
(1,160)	1:90:A:LYS:C	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	3	4.71	3.7	3.06
(1,87)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:ILE:N	3	3.83	1.44	4.2
(1,46)	1:32:A:ILE:C	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	3	3.04	1.33	3.68
(1,84)	1:52:A:THR:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	3	2.62	0.83	2.25
(1,99)	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	1:61:A:SER:N	3	2.26	0.45	2.35
(1,151)	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	1:87:A:ARG:N	3	2.25	0.53	2.56
(1,137)	1:79:A:LEU:N	1:79:A:LEU:CA	1:79:A:LEU:C	1:80:A:ASP:N	3	1.88	0.89	1.3
(1,133)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:GLY:N	3	1.85	0.76	1.32
(1,42)	1:30:A:GLU:C	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	3	1.65	0.18	1.66
(1,6)	1:12:A:ASP:C	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	3	1.22	0.13	1.16
(1,77)	1:49:A:ARG:N	1:49:A:ARG:CA	1:49:A:ARG:C	1:50:A:GLU:N	2	13.48	1.41	13.48
(1,126)	1:73:A:GLN:C	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	2	13.41	1.12	13.41
(1,78)	1:49:A:ARG:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	2	11.66	0.19	11.66
(1,76)	1:48:A:SER:C	1:49:A:ARG:N	1:49:A:ARG:CA	1:49:A:ARG:C	2	9.45	0.1	9.45
(1,132)	1:76:A:PRO:C	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	2	9.38	7.01	9.38
(1,124)	1:72:A:LEU:C	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	2	9.21	2.17	9.21
(1,75)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:ARG:N	2	8.18	0.3	8.18
(1,101)	1:61:A:SER:N	1:61:A:SER:CA	1:61:A:SER:C	1:62:A:ARG:N	2	3.55	1.27	3.55
(1,97)	1:59:A:THR:N	1:59:A:THR:CA	1:59:A:THR:C	1:60:A:SER:N	2	3.52	0.74	3.52
(1,89)	1:55:A:ILE:N	1:55:A:ILE:CA	1:55:A:ILE:C	1:56:A:SER:N	2	2.9	0.29	2.9
(1,91)	1:56:A:SER:N	1:56:A:SER:CA	1:56:A:SER:C	1:57:A:CYS:N	2	2.59	0.02	2.59
(1,14)	1:16:A:VAL:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	2	2.47	0.03	2.47

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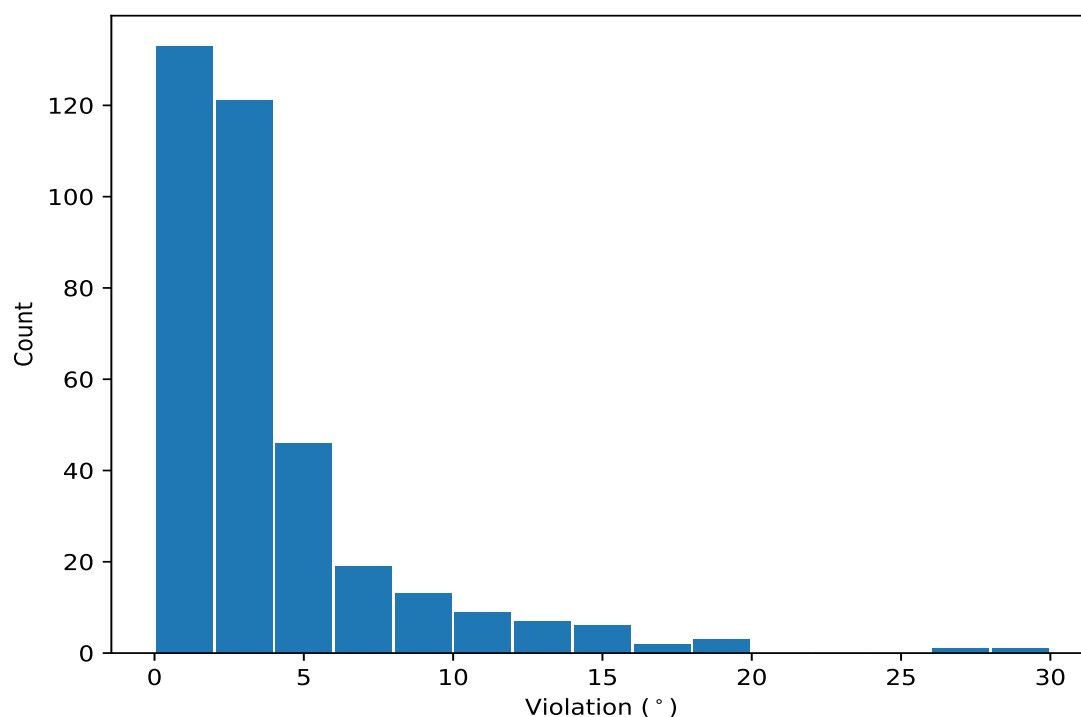
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,152)	1:86:A:ILE:C	1:87:A:ARG:N	1:87:A:ARG:CA	1:87:A:ARG:C	2	2.4	1.02	2.4
(1,72)	1:46:A:ILE:C	1:47:A:LEU:N	1:47:A:LEU:CA	1:47:A:LEU:C	2	2.33	0.32	2.33
(1,88)	1:54:A:GLU:C	1:55:A:ILE:N	1:55:A:ILE:CA	1:55:A:ILE:C	2	2.2	0.23	2.2
(1,96)	1:58:A:ARG:C	1:59:A:THR:N	1:59:A:THR:CA	1:59:A:THR:C	2	2.18	1.0	2.18
(1,150)	1:85:A:SER:C	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	2	2.06	0.71	2.06
(1,74)	1:47:A:LEU:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	2	1.86	0.57	1.86
(1,102)	1:61:A:SER:C	1:62:A:ARG:N	1:62:A:ARG:CA	1:62:A:ARG:C	2	1.8	0.68	1.8
(1,161)	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1:92:A:GLN:N	2	1.75	0.59	1.75
(1,62)	1:40:A:HIS:C	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:C	2	1.74	0.67	1.74
(1,40)	1:29:A:CYS:C	1:30:A:GLU:N	1:30:A:GLU:CA	1:30:A:GLU:C	2	1.56	0.44	1.56
(1,167)	1:95:A:LEU:N	1:95:A:LEU:CA	1:95:A:LEU:C	1:96:A:ILE:N	2	1.5	0.28	1.5
(1,92)	1:56:A:SER:C	1:57:A:CYS:N	1:57:A:CYS:CA	1:57:A:CYS:C	2	1.5	0.33	1.5
(1,63)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:C	1:42:A:ARG:N	2	1.45	0.44	1.45
(1,58)	1:38:A:PHE:C	1:39:A:ASP:N	1:39:A:ASP:CA	1:39:A:ASP:C	2	1.43	0.26	1.43
(1,103)	1:62:A:ARG:N	1:62:A:ARG:CA	1:62:A:ARG:C	1:63:A:LYS:N	2	1.38	0.29	1.38
(1,98)	1:59:A:THR:C	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	2	1.33	0.12	1.33
(1,117)	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	1:70:A:ASP:N	2	1.21	0.11	1.21

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 (°)
(1,8)	1:13:A:LEU:C	1:14:A:THR:N	1:14:A:THR:CA	1:14:A:THR:C	2	28.36
(1,9)	1:14:A:THR:N	1:14:A:THR:CA	1:14:A:THR:C	1:15:A:GLU:N	2	26.08
(1,47)	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	1:34:A:ALA:N	1	18.83
(1,55)	1:37:A:HIS:N	1:37:A:HIS:CA	1:37:A:HIS:C	1:38:A:PHE:N	1	18.55
(1,56)	1:37:A:HIS:C	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	1	18.04
(1,125)	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	1:74:A:GLU:N	8	16.46
(1,132)	1:76:A:PRO:C	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	9	16.39
(1,131)	1:76:A:PRO:N	1:76:A:PRO:CA	1:76:A:PRO:C	1:77:A:LYS:N	9	15.88
(1,54)	1:36:A:ARG:C	1:37:A:HIS:N	1:37:A:HIS:CA	1:37:A:HIS:C	1	14.92
(1,77)	1:49:A:ARG:N	1:49:A:ARG:CA	1:49:A:ARG:C	1:50:A:GLU:N	4	14.89
(1,48)	1:33:A:ILE:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	1	14.7
(1,126)	1:73:A:GLN:C	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	8	14.53
(1,129)	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	1:76:A:PRO:N	10	14.25
(1,47)	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	1:34:A:ALA:N	10	13.84
(1,125)	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	1:74:A:GLU:N	10	12.9
(1,126)	1:73:A:GLN:C	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	10	12.29
(1,155)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:GLU:N	2	12.26
(1,158)	1:89:A:GLU:C	1:90:A:LYS:N	1:90:A:LYS:CA	1:90:A:LYS:C	7	12.17
(1,129)	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	1:76:A:PRO:N	8	12.1
(1,77)	1:49:A:ARG:N	1:49:A:ARG:CA	1:49:A:ARG:C	1:50:A:GLU:N	6	12.07
(1,78)	1:49:A:ARG:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	6	11.85
(1,78)	1:49:A:ARG:C	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	4	11.46
(1,124)	1:72:A:LEU:C	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	10	11.38
(1,48)	1:33:A:ILE:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	10	11.17
(1,159)	1:90:A:LYS:N	1:90:A:LYS:CA	1:90:A:LYS:C	1:91:A:THR:N	7	11.15
(1,53)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:HIS:N	1	10.96
(1,127)	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	1:75:A:ASN:N	9	10.78
(1,94)	1:57:A:CYS:C	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	8	10.14
(1,128)	1:74:A:GLU:C	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	9	10.09
(1,123)	1:72:A:LEU:N	1:72:A:LEU:CA	1:72:A:LEU:C	1:73:A:GLN:N	10	9.91
(1,160)	1:90:A:LYS:C	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	7	9.83
(1,93)	1:57:A:CYS:N	1:57:A:CYS:CA	1:57:A:CYS:C	1:58:A:ARG:N	1	9.83
(1,93)	1:57:A:CYS:N	1:57:A:CYS:CA	1:57:A:CYS:C	1:58:A:ARG:N	8	9.77
(1,157)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:LYS:N	7	9.71
(1,158)	1:89:A:GLU:C	1:90:A:LYS:N	1:90:A:LYS:CA	1:90:A:LYS:C	5	9.56
(1,76)	1:48:A:SER:C	1:49:A:ARG:N	1:49:A:ARG:CA	1:49:A:ARG:C	6	9.55
(1,76)	1:48:A:SER:C	1:49:A:ARG:N	1:49:A:ARG:CA	1:49:A:ARG:C	4	9.35
(1,154)	1:87:A:ARG:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	5	8.67
(1,47)	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	1:34:A:ALA:N	6	8.52
(1,75)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:ARG:N	4	8.47
(1,94)	1:57:A:CYS:C	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1	8.28
(1,158)	1:89:A:GLU:C	1:90:A:LYS:N	1:90:A:LYS:CA	1:90:A:LYS:C	6	8.24
(1,157)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:LYS:N	10	7.96
(1,75)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:ARG:N	6	7.88
(1,94)	1:57:A:CYS:C	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	7	7.85
(1,53)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:HIS:N	8	7.58
(1,156)	1:88:A:ARG:C	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	2	7.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,129)	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	1:76:A:PRO:N	5	7.46
(1,53)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:HIS:N	6	7.32
(1,124)	1:72:A:LEU:C	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	8	7.04
(1,93)	1:57:A:CYS:N	1:57:A:CYS:CA	1:57:A:CYS:C	1:58:A:ARG:N	7	6.91
(1,95)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:THR:N	1	6.8
(1,153)	1:87:A:ARG:N	1:87:A:ARG:CA	1:87:A:ARG:C	1:88:A:ARG:N	5	6.78
(1,47)	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	1:34:A:ALA:N	7	6.7
(1,54)	1:36:A:ARG:C	1:37:A:HIS:N	1:37:A:HIS:CA	1:37:A:HIS:C	8	6.58
(1,157)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:LYS:N	4	6.55
(1,130)	1:75:A:ASN:C	1:76:A:PRO:N	1:76:A:PRO:CA	1:76:A:PRO:C	10	6.47
(1,53)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:HIS:N	10	6.35
(1,13)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:LYS:N	9	6.19
(1,157)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:LYS:N	6	6.16
(1,47)	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	1:34:A:ALA:N	4	6.06
(1,47)	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	1:34:A:ALA:N	5	5.98
(1,95)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:THR:N	8	5.97
(1,69)	1:44:A:LYS:N	1:44:A:LYS:CA	1:44:A:LYS:C	1:45:A:LYS:N	8	5.96
(1,13)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:LYS:N	10	5.86
(1,163)	1:93:A:ASN:N	1:93:A:ASN:CA	1:93:A:ASN:C	1:94:A:PHE:N	5	5.79
(1,130)	1:75:A:ASN:C	1:76:A:PRO:N	1:76:A:PRO:CA	1:76:A:PRO:C	5	5.78
(1,123)	1:72:A:LEU:N	1:72:A:LEU:CA	1:72:A:LEU:C	1:73:A:GLN:N	8	5.76
(1,157)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:LYS:N	5	5.74
(1,69)	1:44:A:LYS:N	1:44:A:LYS:CA	1:44:A:LYS:C	1:45:A:LYS:N	9	5.67
(1,45)	1:32:A:ILE:N	1:32:A:ILE:CA	1:32:A:ILE:C	1:33:A:ILE:N	1	5.66
(1,13)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:LYS:N	8	5.61
(1,156)	1:88:A:ARG:C	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	5	5.47
(1,129)	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	1:76:A:PRO:N	1	5.44
(1,129)	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	1:76:A:PRO:N	3	5.39
(1,135)	1:78:A:GLY:N	1:78:A:GLY:CA	1:78:A:GLY:C	1:79:A:LEU:N	9	5.37
(1,87)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:ILE:N	6	5.37
(1,45)	1:32:A:ILE:N	1:32:A:ILE:CA	1:32:A:ILE:C	1:33:A:ILE:N	10	5.23
(1,13)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:LYS:N	5	5.19
(1,47)	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	1:34:A:ALA:N	8	5.12
(1,127)	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	1:75:A:ASN:N	10	5.08
(1,157)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:LYS:N	2	5.07
(1,54)	1:36:A:ARG:C	1:37:A:HIS:N	1:37:A:HIS:CA	1:37:A:HIS:C	10	5.06
(1,47)	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	1:34:A:ALA:N	2	4.88
(1,101)	1:61:A:SER:N	1:61:A:SER:CA	1:61:A:SER:C	1:62:A:ARG:N	3	4.82
(1,129)	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	1:76:A:PRO:N	6	4.79
(1,47)	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	1:34:A:ALA:N	9	4.76
(1,95)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:THR:N	5	4.75
(1,155)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:GLU:N	5	4.71
(1,1)	1:10:A:GLU:N	1:10:A:GLU:CA	1:10:A:GLU:C	1:11:A:GLU:N	8	4.62
(1,48)	1:33:A:ILE:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	6	4.6
(1,13)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:LYS:N	1	4.6
(1,159)	1:90:A:LYS:N	1:90:A:LYS:CA	1:90:A:LYS:C	1:91:A:THR:N	6	4.53
(1,159)	1:90:A:LYS:N	1:90:A:LYS:CA	1:90:A:LYS:C	1:91:A:THR:N	1	4.48
(1,157)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:LYS:N	1	4.47
(1,155)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:GLU:N	9	4.41
(1,130)	1:75:A:ASN:C	1:76:A:PRO:N	1:76:A:PRO:CA	1:76:A:PRO:C	9	4.4
(1,95)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:THR:N	7	4.37

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,97)	1:59:A:THR:N	1:59:A:THR:CA	1:59:A:THR:C	1:60:A:SER:N	7	4.27
(1,46)	1:32:A:ILE:C	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	10	4.24
(1,69)	1:44:A:LYS:N	1:44:A:LYS:CA	1:44:A:LYS:C	1:45:A:LYS:N	10	4.23
(1,87)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:ILE:N	4	4.2
(1,48)	1:33:A:ILE:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	7	4.17
(1,163)	1:93:A:ASN:N	1:93:A:ASN:CA	1:93:A:ASN:C	1:94:A:PHE:N	1	4.09
(1,158)	1:89:A:GLU:C	1:90:A:LYS:N	1:90:A:LYS:CA	1:90:A:LYS:C	1	4.09
(1,7)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:THR:N	8	4.06
(1,129)	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	1:76:A:PRO:N	7	4.03
(1,100)	1:60:A:SER:C	1:61:A:SER:N	1:61:A:SER:CA	1:61:A:SER:C	3	3.99
(1,8)	1:13:A:LEU:C	1:14:A:THR:N	1:14:A:THR:CA	1:14:A:THR:C	5	3.93
(1,53)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:HIS:N	5	3.88
(1,13)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:LYS:N	6	3.81
(1,1)	1:10:A:GLU:N	1:10:A:GLU:CA	1:10:A:GLU:C	1:11:A:GLU:N	9	3.81
(1,69)	1:44:A:LYS:N	1:44:A:LYS:CA	1:44:A:LYS:C	1:45:A:LYS:N	1	3.79
(1,7)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:THR:N	10	3.78
(1,157)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:LYS:N	3	3.77
(1,84)	1:52:A:THR:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	8	3.77
(1,9)	1:14:A:THR:N	1:14:A:THR:CA	1:14:A:THR:C	1:15:A:GLU:N	3	3.72
(1,54)	1:36:A:ARG:C	1:37:A:HIS:N	1:37:A:HIS:CA	1:37:A:HIS:C	6	3.71
(1,154)	1:87:A:ARG:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	7	3.69
(1,13)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:LYS:N	2	3.69
(1,46)	1:32:A:ILE:C	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	1	3.68
(1,13)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:LYS:N	3	3.54
(1,203)	1:113:A:HIS:N	1:113:A:HIS:CA	1:113:A:HIS:C	1:114:A:LEU:N	4	3.49
(1,135)	1:78:A:GLY:N	1:78:A:GLY:CA	1:78:A:GLY:C	1:79:A:LEU:N	10	3.47
(1,131)	1:76:A:PRO:N	1:76:A:PRO:CA	1:76:A:PRO:C	1:77:A:LYS:N	10	3.45
(1,152)	1:86:A:ILE:C	1:87:A:ARG:N	1:87:A:ARG:CA	1:87:A:ARG:C	5	3.41
(1,57)	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	1:39:A:ASP:N	9	3.4
(1,163)	1:93:A:ASN:N	1:93:A:ASN:CA	1:93:A:ASN:C	1:94:A:PHE:N	3	3.39
(1,154)	1:87:A:ARG:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1	3.35
(1,61)	1:40:A:HIS:N	1:40:A:HIS:CA	1:40:A:HIS:C	1:41:A:LEU:N	9	3.33
(1,189)	1:106:A:LEU:N	1:106:A:LEU:CA	1:106:A:LEU:C	1:107:A:ARG:N	3	3.31
(1,131)	1:76:A:PRO:N	1:76:A:PRO:CA	1:76:A:PRO:C	1:77:A:LYS:N	5	3.31
(1,121)	1:71:A:TYR:N	1:71:A:TYR:CA	1:71:A:TYR:C	1:72:A:LEU:N	6	3.31
(1,13)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:LYS:N	7	3.21
(1,195)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:LYS:N	9	3.2
(1,89)	1:55:A:ILE:N	1:55:A:ILE:CA	1:55:A:ILE:C	1:56:A:SER:N	8	3.19
(1,9)	1:14:A:THR:N	1:14:A:THR:CA	1:14:A:THR:C	1:15:A:GLU:N	9	3.19
(1,96)	1:58:A:ARG:C	1:59:A:THR:N	1:59:A:THR:CA	1:59:A:THR:C	5	3.18
(1,69)	1:44:A:LYS:N	1:44:A:LYS:CA	1:44:A:LYS:C	1:45:A:LYS:N	6	3.14
(1,137)	1:79:A:LEU:N	1:79:A:LEU:CA	1:79:A:LEU:C	1:80:A:ASP:N	9	3.13
(1,61)	1:40:A:HIS:N	1:40:A:HIS:CA	1:40:A:HIS:C	1:41:A:LEU:N	4	3.12
(1,128)	1:74:A:GLU:C	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	10	3.11
(1,160)	1:90:A:LYS:C	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1	3.06
(1,69)	1:44:A:LYS:N	1:44:A:LYS:CA	1:44:A:LYS:C	1:45:A:LYS:N	5	3.06
(1,54)	1:36:A:ARG:C	1:37:A:HIS:N	1:37:A:HIS:CA	1:37:A:HIS:C	9	3.06
(1,156)	1:88:A:ARG:C	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1	3.04
(1,7)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:THR:N	2	3.02
(1,189)	1:106:A:LEU:N	1:106:A:LEU:CA	1:106:A:LEU:C	1:107:A:ARG:N	6	3.01
(1,53)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:HIS:N	4	2.99

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,158)	1:89:A:GLU:C	1:90:A:LYS:N	1:90:A:LYS:CA	1:90:A:LYS:C	4	2.98
(1,130)	1:75:A:ASN:C	1:76:A:PRO:N	1:76:A:PRO:CA	1:76:A:PRO:C	8	2.97
(1,121)	1:71:A:TYR:N	1:71:A:TYR:CA	1:71:A:TYR:C	1:72:A:LEU:N	10	2.96
(1,195)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:LYS:N	10	2.95
(1,127)	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	1:75:A:ASN:N	8	2.94
(1,71)	1:45:A:LYS:N	1:45:A:LYS:CA	1:45:A:LYS:C	1:46:A:ILE:N	7	2.94
(1,135)	1:78:A:GLY:N	1:78:A:GLY:CA	1:78:A:GLY:C	1:79:A:LEU:N	8	2.93
(1,133)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:GLY:N	8	2.92
(1,129)	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	1:76:A:PRO:N	4	2.92
(1,61)	1:40:A:HIS:N	1:40:A:HIS:CA	1:40:A:HIS:C	1:41:A:LEU:N	2	2.91
(1,195)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:LYS:N	6	2.9
(1,121)	1:71:A:TYR:N	1:71:A:TYR:CA	1:71:A:TYR:C	1:72:A:LEU:N	8	2.9
(1,189)	1:106:A:LEU:N	1:106:A:LEU:CA	1:106:A:LEU:C	1:107:A:ARG:N	7	2.87
(1,7)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:THR:N	7	2.85
(1,94)	1:57:A:CYS:C	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	9	2.83
(1,164)	1:93:A:ASN:C	1:94:A:PHE:N	1:94:A:PHE:CA	1:94:A:PHE:C	5	2.82
(1,155)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:GLU:N	1	2.82
(1,53)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:HIS:N	3	2.82
(1,128)	1:74:A:GLU:C	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	8	2.8
(1,2)	1:10:A:GLU:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	1	2.8
(1,97)	1:59:A:THR:N	1:59:A:THR:CA	1:59:A:THR:C	1:60:A:SER:N	8	2.78
(1,150)	1:85:A:SER:C	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	5	2.77
(1,99)	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	1:61:A:SER:N	8	2.76
(1,93)	1:57:A:CYS:N	1:57:A:CYS:CA	1:57:A:CYS:C	1:58:A:ARG:N	9	2.74
(1,49)	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	1:35:A:GLU:N	10	2.73
(1,151)	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	1:87:A:ARG:N	5	2.68
(1,71)	1:45:A:LYS:N	1:45:A:LYS:CA	1:45:A:LYS:C	1:46:A:ILE:N	4	2.67
(1,141)	1:81:A:THR:N	1:81:A:THR:CA	1:81:A:THR:C	1:82:A:LEU:N	9	2.65
(1,72)	1:46:A:ILE:C	1:47:A:LEU:N	1:47:A:LEU:CA	1:47:A:LEU:C	4	2.65
(1,47)	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	1:34:A:ALA:N	3	2.63
(1,153)	1:87:A:ARG:N	1:87:A:ARG:CA	1:87:A:ARG:C	1:88:A:ARG:N	9	2.62
(1,2)	1:10:A:GLU:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	9	2.62
(1,108)	1:64:A:ARG:C	1:65:A:ALA:N	1:65:A:ALA:CA	1:65:A:ALA:C	3	2.61
(1,91)	1:56:A:SER:N	1:56:A:SER:CA	1:56:A:SER:C	1:57:A:CYS:N	7	2.61
(1,89)	1:55:A:ILE:N	1:55:A:ILE:CA	1:55:A:ILE:C	1:56:A:SER:N	7	2.6
(1,48)	1:33:A:ILE:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	5	2.6
(1,23)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:GLU:N	8	2.6
(1,95)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:THR:N	3	2.58
(1,91)	1:56:A:SER:N	1:56:A:SER:CA	1:56:A:SER:C	1:57:A:CYS:N	8	2.57
(1,151)	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	1:87:A:ARG:N	1	2.56
(1,8)	1:13:A:LEU:C	1:14:A:THR:N	1:14:A:THR:CA	1:14:A:THR:C	4	2.52
(1,61)	1:40:A:HIS:N	1:40:A:HIS:CA	1:40:A:HIS:C	1:41:A:LEU:N	7	2.5
(1,14)	1:16:A:VAL:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	10	2.5
(1,9)	1:14:A:THR:N	1:14:A:THR:CA	1:14:A:THR:C	1:15:A:GLU:N	1	2.5
(1,83)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:ARG:N	1	2.49
(1,102)	1:61:A:SER:C	1:62:A:ARG:N	1:62:A:ARG:CA	1:62:A:ARG:C	3	2.48
(1,195)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:LYS:N	2	2.45
(1,69)	1:44:A:LYS:N	1:44:A:LYS:CA	1:44:A:LYS:C	1:45:A:LYS:N	2	2.45
(1,14)	1:16:A:VAL:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	8	2.44
(1,88)	1:54:A:GLU:C	1:55:A:ILE:N	1:55:A:ILE:CA	1:55:A:ILE:C	6	2.43
(1,74)	1:47:A:LEU:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	6	2.43

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,105)	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1:64:A:ARG:N	6	2.42
(1,71)	1:45:A:LYS:N	1:45:A:LYS:CA	1:45:A:LYS:C	1:46:A:ILE:N	9	2.42
(1,62)	1:40:A:HIS:C	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:C	8	2.41
(1,155)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:GLU:N	7	2.37
(1,132)	1:76:A:PRO:C	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	5	2.37
(1,189)	1:106:A:LEU:N	1:106:A:LEU:CA	1:106:A:LEU:C	1:107:A:ARG:N	10	2.36
(1,99)	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	1:61:A:SER:N	3	2.35
(1,161)	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1:92:A:GLN:N	9	2.34
(1,203)	1:113:A:HIS:N	1:113:A:HIS:CA	1:113:A:HIS:C	1:114:A:LEU:N	8	2.32
(1,9)	1:14:A:THR:N	1:14:A:THR:CA	1:14:A:THR:C	1:15:A:GLU:N	8	2.32
(1,101)	1:61:A:SER:N	1:61:A:SER:CA	1:61:A:SER:C	1:62:A:ARG:N	5	2.28
(1,95)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:THR:N	6	2.28
(1,69)	1:44:A:LYS:N	1:44:A:LYS:CA	1:44:A:LYS:C	1:45:A:LYS:N	7	2.28
(1,129)	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	1:76:A:PRO:N	9	2.27
(1,163)	1:93:A:ASN:N	1:93:A:ASN:CA	1:93:A:ASN:C	1:94:A:PHE:N	8	2.25
(1,84)	1:52:A:THR:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	4	2.25
(1,125)	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	1:74:A:GLU:N	9	2.23
(1,121)	1:71:A:TYR:N	1:71:A:TYR:CA	1:71:A:TYR:C	1:72:A:LEU:N	4	2.23
(1,127)	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	1:75:A:ASN:N	5	2.2
(1,67)	1:43:A:ALA:N	1:43:A:ALA:CA	1:43:A:ALA:C	1:44:A:LYS:N	4	2.19
(1,123)	1:72:A:LEU:N	1:72:A:LEU:CA	1:72:A:LEU:C	1:73:A:GLN:N	9	2.13
(1,123)	1:72:A:LEU:N	1:72:A:LEU:CA	1:72:A:LEU:C	1:73:A:GLN:N	7	2.08
(1,43)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:ILE:N	2	2.06
(1,125)	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	1:74:A:GLU:N	4	2.04
(1,189)	1:106:A:LEU:N	1:106:A:LEU:CA	1:106:A:LEU:C	1:107:A:ARG:N	5	2.01
(1,72)	1:46:A:ILE:C	1:47:A:LEU:N	1:47:A:LEU:CA	1:47:A:LEU:C	6	2.01
(1,18)	1:18:A:LYS:C	1:19:A:ASP:N	1:19:A:ASP:CA	1:19:A:ASP:C	10	2.01
(1,40)	1:29:A:CYS:C	1:30:A:GLU:N	1:30:A:GLU:CA	1:30:A:GLU:C	1	2.0
(1,88)	1:54:A:GLU:C	1:55:A:ILE:N	1:55:A:ILE:CA	1:55:A:ILE:C	4	1.97
(1,67)	1:43:A:ALA:N	1:43:A:ALA:CA	1:43:A:ALA:C	1:44:A:LYS:N	10	1.96
(1,195)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:LYS:N	1	1.95
(1,154)	1:87:A:ARG:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	6	1.95
(1,7)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:THR:N	4	1.95
(1,55)	1:37:A:HIS:N	1:37:A:HIS:CA	1:37:A:HIS:C	1:38:A:PHE:N	5	1.93
(1,154)	1:87:A:ARG:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	10	1.92
(1,71)	1:45:A:LYS:N	1:45:A:LYS:CA	1:45:A:LYS:C	1:46:A:ILE:N	1	1.92
(1,87)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:ILE:N	3	1.91
(1,163)	1:93:A:ASN:N	1:93:A:ASN:CA	1:93:A:ASN:C	1:94:A:PHE:N	9	1.9
(1,63)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:C	1:42:A:ARG:N	6	1.89
(1,203)	1:113:A:HIS:N	1:113:A:HIS:CA	1:113:A:HIS:C	1:114:A:LEU:N	1	1.88
(1,105)	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1:64:A:ARG:N	10	1.88
(1,136)	1:78:A:GLY:C	1:79:A:LEU:N	1:79:A:LEU:CA	1:79:A:LEU:C	9	1.87
(1,59)	1:39:A:ASP:N	1:39:A:ASP:CA	1:39:A:ASP:C	1:40:A:HIS:N	1	1.87
(1,42)	1:30:A:GLU:C	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	5	1.87
(1,163)	1:93:A:ASN:N	1:93:A:ASN:CA	1:93:A:ASN:C	1:94:A:PHE:N	6	1.86
(1,84)	1:52:A:THR:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	6	1.84
(1,9)	1:14:A:THR:N	1:14:A:THR:CA	1:14:A:THR:C	1:15:A:GLU:N	10	1.84
(1,92)	1:56:A:SER:C	1:57:A:CYS:N	1:57:A:CYS:CA	1:57:A:CYS:C	9	1.82
(1,2)	1:10:A:GLU:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	10	1.81
(1,167)	1:95:A:LEU:N	1:95:A:LEU:CA	1:95:A:LEU:C	1:96:A:ILE:N	9	1.78
(1,94)	1:57:A:CYS:C	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	2	1.78

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,104)	1:62:A:ARG:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	7	1.77
(1,54)	1:36:A:ARG:C	1:37:A:HIS:N	1:37:A:HIS:CA	1:37:A:HIS:C	7	1.76
(1,55)	1:37:A:HIS:N	1:37:A:HIS:CA	1:37:A:HIS:C	1:38:A:PHE:N	4	1.75
(1,48)	1:33:A:ILE:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	8	1.75
(1,94)	1:57:A:CYS:C	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	6	1.72
(1,48)	1:33:A:ILE:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	4	1.72
(1,34)	1:26:A:VAL:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	10	1.71
(1,142)	1:81:A:THR:C	1:82:A:LEU:N	1:82:A:LEU:CA	1:82:A:LEU:C	8	1.7
(1,58)	1:38:A:PHE:C	1:39:A:ASP:N	1:39:A:ASP:CA	1:39:A:ASP:C	1	1.69
(1,103)	1:62:A:ARG:N	1:62:A:ARG:CA	1:62:A:ARG:C	1:63:A:LYS:N	3	1.68
(1,99)	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	1:61:A:SER:N	1	1.68
(1,9)	1:14:A:THR:N	1:14:A:THR:CA	1:14:A:THR:C	1:15:A:GLU:N	6	1.68
(1,123)	1:72:A:LEU:N	1:72:A:LEU:CA	1:72:A:LEU:C	1:73:A:GLN:N	3	1.67
(1,42)	1:30:A:GLU:C	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	3	1.66
(1,61)	1:40:A:HIS:N	1:40:A:HIS:CA	1:40:A:HIS:C	1:41:A:LEU:N	3	1.64
(1,123)	1:72:A:LEU:N	1:72:A:LEU:CA	1:72:A:LEU:C	1:73:A:GLN:N	2	1.6
(1,125)	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	1:74:A:GLU:N	3	1.59
(1,93)	1:57:A:CYS:N	1:57:A:CYS:CA	1:57:A:CYS:C	1:58:A:ARG:N	10	1.59
(1,56)	1:37:A:HIS:C	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	9	1.59
(1,67)	1:43:A:ALA:N	1:43:A:ALA:CA	1:43:A:ALA:C	1:44:A:LYS:N	6	1.53
(1,94)	1:57:A:CYS:C	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	10	1.52
(1,13)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:LYS:N	4	1.52
(1,43)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:ILE:N	9	1.51
(1,151)	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	1:87:A:ARG:N	6	1.5
(1,98)	1:59:A:THR:C	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	1	1.45
(1,21)	1:20:A:ALA:N	1:20:A:ALA:CA	1:20:A:ALA:C	1:21:A:LEU:N	10	1.45
(1,1)	1:10:A:GLU:N	1:10:A:GLU:CA	1:10:A:GLU:C	1:11:A:GLU:N	4	1.45
(1,31)	1:25:A:ARG:N	1:25:A:ARG:CA	1:25:A:ARG:C	1:26:A:VAL:N	6	1.44
(1,42)	1:30:A:GLU:C	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	2	1.42
(1,162)	1:92:A:GLN:C	1:93:A:ASN:N	1:93:A:ASN:CA	1:93:A:ASN:C	8	1.41
(1,203)	1:113:A:HIS:N	1:113:A:HIS:CA	1:113:A:HIS:C	1:114:A:LEU:N	9	1.4
(1,127)	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	1:75:A:ASN:N	2	1.4
(1,53)	1:36:A:ARG:N	1:36:A:ARG:CA	1:36:A:ARG:C	1:37:A:HIS:N	2	1.4
(1,6)	1:12:A:ASP:C	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	2	1.4
(1,86)	1:53:A:ARG:C	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	4	1.39
(1,48)	1:33:A:ILE:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	2	1.39
(1,152)	1:86:A:ILE:C	1:87:A:ARG:N	1:87:A:ARG:CA	1:87:A:ARG:C	1	1.38
(1,113)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:LEU:N	3	1.38
(1,95)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:THR:N	4	1.36
(1,9)	1:14:A:THR:N	1:14:A:THR:CA	1:14:A:THR:C	1:15:A:GLU:N	7	1.36
(1,155)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:GLU:N	8	1.35
(1,150)	1:85:A:SER:C	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	2	1.35
(1,69)	1:44:A:LYS:N	1:44:A:LYS:CA	1:44:A:LYS:C	1:45:A:LYS:N	4	1.35
(1,43)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:ILE:N	8	1.35
(1,32)	1:25:A:ARG:C	1:26:A:VAL:N	1:26:A:VAL:CA	1:26:A:VAL:C	10	1.34
(1,133)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:GLY:N	5	1.32
(1,117)	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	1:70:A:ASP:N	6	1.32
(1,90)	1:55:A:ILE:C	1:56:A:SER:N	1:56:A:SER:CA	1:56:A:SER:C	9	1.32
(1,8)	1:13:A:LEU:C	1:14:A:THR:N	1:14:A:THR:CA	1:14:A:THR:C	1	1.32
(1,71)	1:45:A:LYS:N	1:45:A:LYS:CA	1:45:A:LYS:C	1:46:A:ILE:N	2	1.31
(1,137)	1:79:A:LEU:N	1:79:A:LEU:CA	1:79:A:LEU:C	1:80:A:ASP:N	8	1.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,133)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:GLY:N	3	1.3
(1,197)	1:110:A:LYS:N	1:110:A:LYS:CA	1:110:A:LYS:C	1:111:A:LEU:N	5	1.29
(1,130)	1:75:A:ASN:C	1:76:A:PRO:N	1:76:A:PRO:CA	1:76:A:PRO:C	3	1.29
(1,74)	1:47:A:LEU:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	4	1.29
(1,7)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:THR:N	5	1.29
(1,45)	1:32:A:ILE:N	1:32:A:ILE:CA	1:32:A:ILE:C	1:33:A:ILE:N	6	1.28
(1,81)	1:51:A:ASP:N	1:51:A:ASP:CA	1:51:A:ASP:C	1:52:A:THR:N	8	1.25
(1,71)	1:45:A:LYS:N	1:45:A:LYS:CA	1:45:A:LYS:C	1:46:A:ILE:N	8	1.25
(1,55)	1:37:A:HIS:N	1:37:A:HIS:CA	1:37:A:HIS:C	1:38:A:PHE:N	3	1.25
(1,167)	1:95:A:LEU:N	1:95:A:LEU:CA	1:95:A:LEU:C	1:96:A:ILE:N	5	1.23
(1,160)	1:90:A:LYS:C	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	6	1.23
(1,128)	1:74:A:GLU:C	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	5	1.23
(1,105)	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1:64:A:ARG:N	4	1.23
(1,196)	1:109:A:ILE:C	1:110:A:LYS:N	1:110:A:LYS:CA	1:110:A:LYS:C	5	1.22
(1,195)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:LYS:N	7	1.22
(1,130)	1:75:A:ASN:C	1:76:A:PRO:N	1:76:A:PRO:CA	1:76:A:PRO:C	1	1.22
(1,105)	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1:64:A:ARG:N	8	1.22
(1,65)	1:42:A:ARG:N	1:42:A:ARG:CA	1:42:A:ARG:C	1:43:A:ALA:N	7	1.22
(1,98)	1:59:A:THR:C	1:60:A:SER:N	1:60:A:SER:CA	1:60:A:SER:C	3	1.21
(1,67)	1:43:A:ALA:N	1:43:A:ALA:CA	1:43:A:ALA:C	1:44:A:LYS:N	8	1.21
(1,137)	1:79:A:LEU:N	1:79:A:LEU:CA	1:79:A:LEU:C	1:80:A:ASP:N	10	1.2
(1,153)	1:87:A:ARG:N	1:87:A:ARG:CA	1:87:A:ARG:C	1:88:A:ARG:N	4	1.19
(1,96)	1:58:A:ARG:C	1:59:A:THR:N	1:59:A:THR:CA	1:59:A:THR:C	3	1.19
(1,55)	1:37:A:HIS:N	1:37:A:HIS:CA	1:37:A:HIS:C	1:38:A:PHE:N	8	1.19
(1,46)	1:32:A:ILE:C	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	7	1.19
(1,69)	1:44:A:LYS:N	1:44:A:LYS:CA	1:44:A:LYS:C	1:45:A:LYS:N	3	1.18
(1,92)	1:56:A:SER:C	1:57:A:CYS:N	1:57:A:CYS:CA	1:57:A:CYS:C	7	1.17
(1,58)	1:38:A:PHE:C	1:39:A:ASP:N	1:39:A:ASP:CA	1:39:A:ASP:C	10	1.17
(1,161)	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	1:92:A:GLN:N	5	1.16
(1,135)	1:78:A:GLY:N	1:78:A:GLY:CA	1:78:A:GLY:C	1:79:A:LEU:N	3	1.16
(1,6)	1:12:A:ASP:C	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	4	1.16
(1,45)	1:32:A:ILE:N	1:32:A:ILE:CA	1:32:A:ILE:C	1:33:A:ILE:N	8	1.15
(1,123)	1:72:A:LEU:N	1:72:A:LEU:CA	1:72:A:LEU:C	1:73:A:GLN:N	5	1.14
(1,102)	1:61:A:SER:C	1:62:A:ARG:N	1:62:A:ARG:CA	1:62:A:ARG:C	5	1.13
(1,40)	1:29:A:CYS:C	1:30:A:GLU:N	1:30:A:GLU:CA	1:30:A:GLU:C	9	1.13
(1,129)	1:75:A:ASN:N	1:75:A:ASN:CA	1:75:A:ASN:C	1:76:A:PRO:N	2	1.12
(1,123)	1:72:A:LEU:N	1:72:A:LEU:CA	1:72:A:LEU:C	1:73:A:GLN:N	6	1.12
(1,67)	1:43:A:ALA:N	1:43:A:ALA:CA	1:43:A:ALA:C	1:44:A:LYS:N	3	1.11
(1,195)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:LYS:N	3	1.1
(1,169)	1:96:A:ILE:N	1:96:A:ILE:CA	1:96:A:ILE:C	1:97:A:GLN:N	5	1.1
(1,117)	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	1:70:A:ASP:N	4	1.1
(1,103)	1:62:A:ARG:N	1:62:A:ARG:CA	1:62:A:ARG:C	1:63:A:LYS:N	4	1.09
(1,71)	1:45:A:LYS:N	1:45:A:LYS:CA	1:45:A:LYS:C	1:46:A:ILE:N	3	1.09
(1,6)	1:12:A:ASP:C	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1	1.09
(1,125)	1:73:A:GLN:N	1:73:A:GLN:CA	1:73:A:GLN:C	1:74:A:GLU:N	1	1.08
(1,203)	1:113:A:HIS:N	1:113:A:HIS:CA	1:113:A:HIS:C	1:114:A:LEU:N	3	1.07
(1,62)	1:40:A:HIS:C	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:C	1	1.07
(1,2)	1:10:A:GLU:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	3	1.05
(1,95)	1:58:A:ARG:N	1:58:A:ARG:CA	1:58:A:ARG:C	1:59:A:THR:N	2	1.04
(1,79)	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	1:51:A:ASP:N	4	1.04
(1,43)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:ILE:N	7	1.04

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,67)	1:43:A:ALA:N	1:43:A:ALA:CA	1:43:A:ALA:C	1:44:A:LYS:N	5	1.03
(1,56)	1:37:A:HIS:C	1:38:A:PHE:N	1:38:A:PHE:CA	1:38:A:PHE:C	5	1.03
(1,1)	1:10:A:GLU:N	1:10:A:GLU:CA	1:10:A:GLU:C	1:11:A:GLU:N	5	1.03
(1,158)	1:89:A:GLU:C	1:90:A:LYS:N	1:90:A:LYS:CA	1:90:A:LYS:C	10	1.02
(1,153)	1:87:A:ARG:N	1:87:A:ARG:CA	1:87:A:ARG:C	1:88:A:ARG:N	2	1.02
(1,35)	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	1:28:A:LEU:N	7	1.02
(1,107)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:ALA:N	1	1.01
(1,63)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:C	1:42:A:ARG:N	5	1.01