



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 02:21 AM UTC

PDB ID : 7P27 / pdb_00007p27
BMRB ID : 27158
Title : NMR solution structure of Chikungunya virus macro domain
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Deposited on : 2021-07-04

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<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

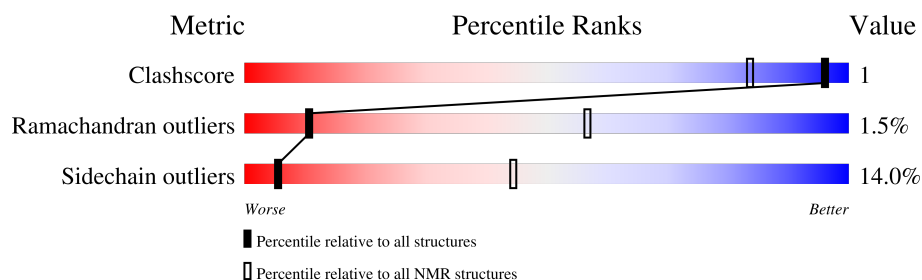
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 80%.

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	168	

2 Ensemble composition and analysis

This entry contains 21 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:3-A:160 (158)	0.67	1

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

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

The models can be grouped into 2 clusters and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2444 atoms, of which 1216 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Polypeptide P1234.

Mol	Chain	Residues	Atoms						Trace
1	A	160	Total	C	H	N	O	S	0
			2444	765	1216	215	240	8	

There are 8 discrepancies between the modelled and reference sequences:

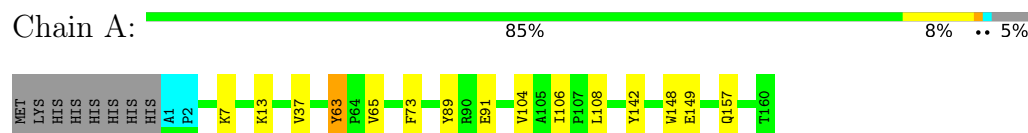
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP Q8JUX6
A	-6	LYS	-	expression tag	UNP Q8JUX6
A	-5	HIS	-	expression tag	UNP Q8JUX6
A	-4	HIS	-	expression tag	UNP Q8JUX6
A	-3	HIS	-	expression tag	UNP Q8JUX6
A	-2	HIS	-	expression tag	UNP Q8JUX6
A	-1	HIS	-	expression tag	UNP Q8JUX6
A	0	HIS	-	expression tag	UNP Q8JUX6

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: Polyprotein P1234

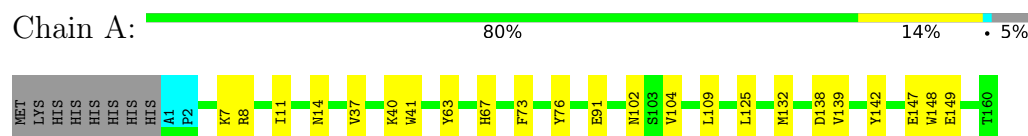


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

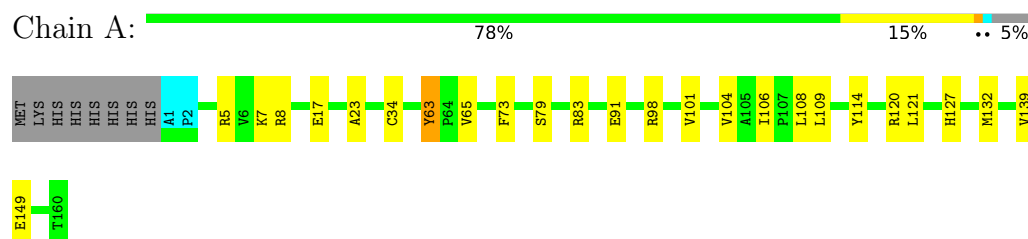
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Polyprotein P1234



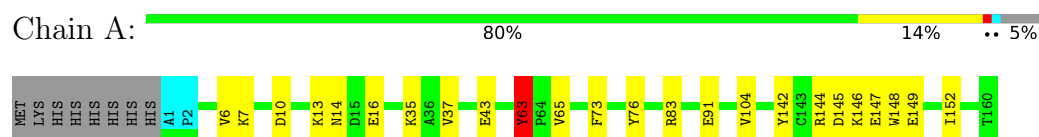
4.2.2 Score per residue for model 2

- Molecule 1: Polyprotein P1234



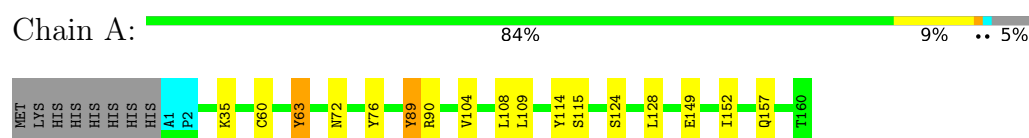
4.2.3 Score per residue for model 3

- Molecule 1: Polyprotein P1234



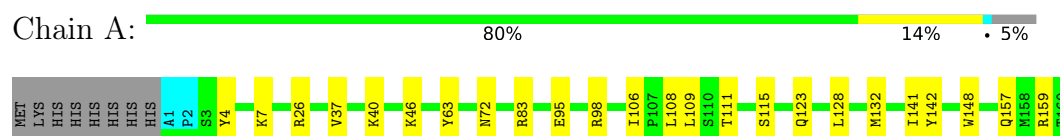
4.2.4 Score per residue for model 4

- Molecule 1: Polyprotein P1234



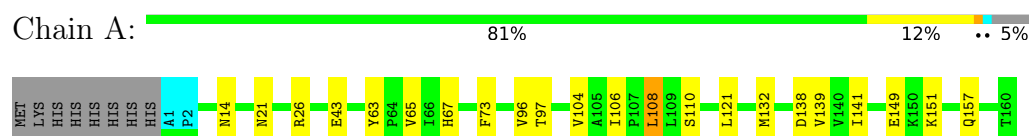
4.2.5 Score per residue for model 5

- Molecule 1: Polyprotein P1234



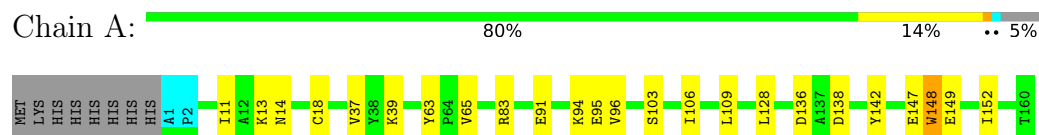
4.2.6 Score per residue for model 6

- Molecule 1: Polyprotein P1234



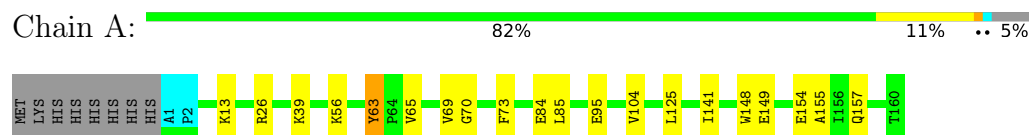
4.2.7 Score per residue for model 7

- Molecule 1: Polyprotein P1234



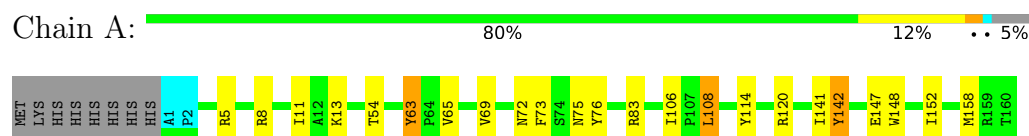
4.2.8 Score per residue for model 8

- Molecule 1: Polyprotein P1234



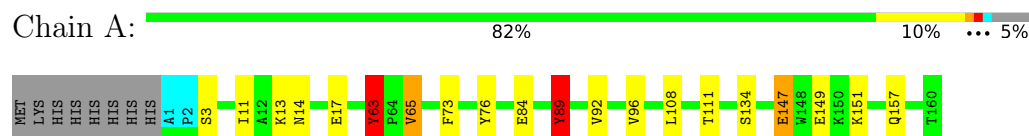
4.2.9 Score per residue for model 9

- Molecule 1: Polyprotein P1234



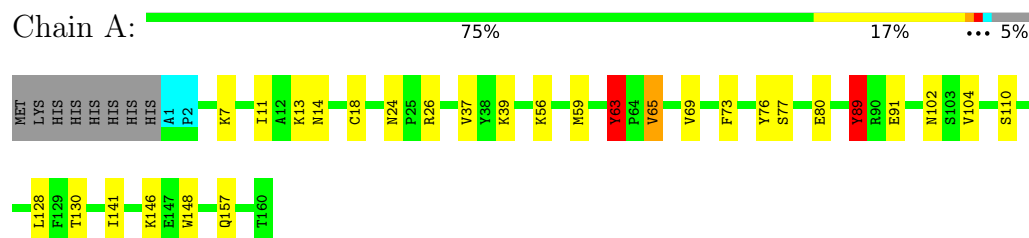
4.2.10 Score per residue for model 10

- Molecule 1: Polyprotein P1234



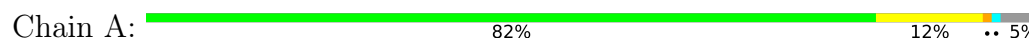
4.2.11 Score per residue for model 11

- Molecule 1: Polyprotein P1234



4.2.12 Score per residue for model 12

- Molecule 1: Polyprotein P1234

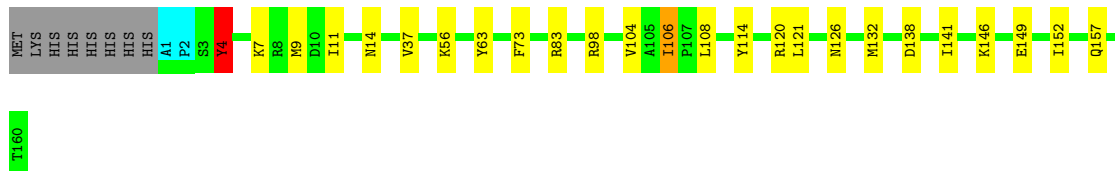




4.2.13 Score per residue for model 13

- Molecule 1: Polyprotein P1234

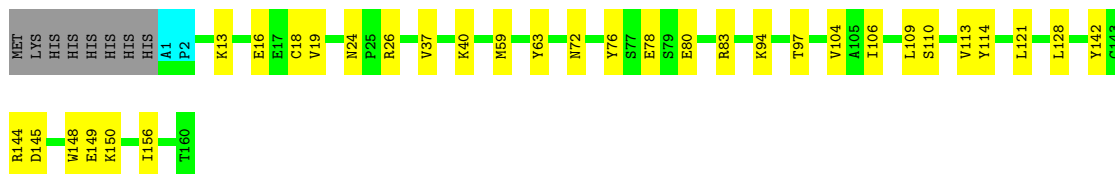
Chain A: 79% 14% ... 5%



4.2.14 Score per residue for model 14

- Molecule 1: Polyprotein P1234

Chain A: 75% 19% • 5%



4.2.15 Score per residue for model 15

- Molecule 1: Polyprotein P1234

Chain A: 81% 11% • 5%



4.2.16 Score per residue for model 16

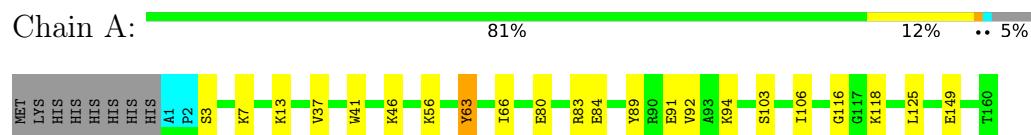
- Molecule 1: Polyprotein P1234

Chain A: 80% 13% • 5%



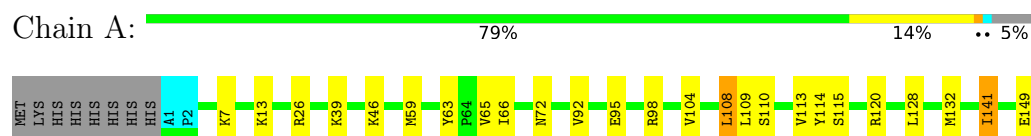
4.2.17 Score per residue for model 17

- Molecule 1: Polyprotein P1234



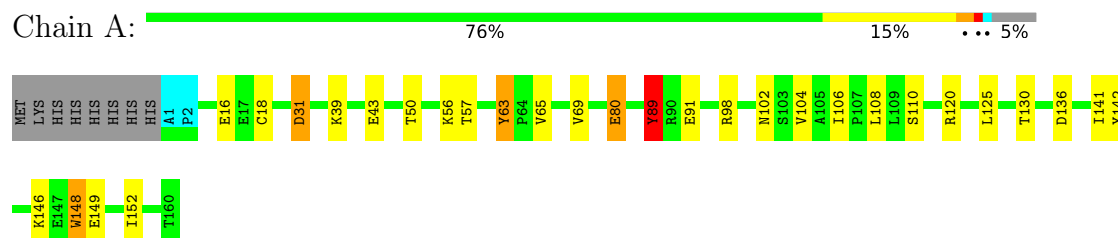
4.2.18 Score per residue for model 18

- Molecule 1: Polyprotein P1234



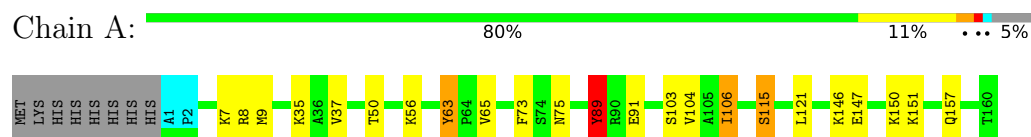
4.2.19 Score per residue for model 19

- Molecule 1: Polyprotein P1234



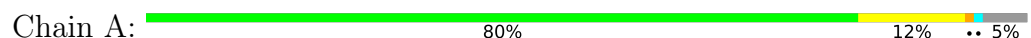
4.2.20 Score per residue for model 20

- Molecule 1: Polyprotein P1234



4.2.21 Score per residue for model 21

- Molecule 1: Polyprotein P1234



MET	LYS	HIS	HIS	HIS	HIS	HIS	HIS	A1	P2	I11	A12	K13	N24	E43	S44	F45	K56	T57	Y63	P64	V65	Y76	E80	Y89	R90	E91	K94	N102	I106	L128	F129	T130	Y142	E147	M148	E149	R159	T160
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5 Refinement protocol and experimental data overview

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

Of the 21 calculated structures, 21 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
DYANA	structure calculation	
Amber	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	1670
Number of shifts mapped to atoms	1670
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

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	0.60±0.01	0±0/1238 (0.0± 0.0%)	1.16±0.02	2±1/1674 (0.1± 0.1%)
All	All	0.60	0/25998 (0.0%)	1.16	32/35154 (0.1%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.0±0.8
All	All	0	21

There are no bond-length outliers.

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	67	HIS	ND1-CE1-NE2	9.47	117.87	108.40	1	1
1	A	67	HIS	CB-CG-CD2	-7.83	121.02	131.20	1	1
1	A	67	HIS	ND1-CG-CD2	7.06	113.16	106.10	1	1
1	A	67	HIS	CG-ND1-CE1	-6.68	97.94	109.30	1	1
1	A	106	ILE	CB-CA-C	6.47	116.70	110.16	14	13
1	A	31	ASP	CA-CB-CG	5.85	118.45	112.60	19	1
1	A	80	GLU	CA-C-N	5.68	127.23	120.14	19	4
1	A	80	GLU	C-N-CA	5.68	127.23	120.14	19	4
1	A	145	ASP	CA-CB-CG	-5.51	107.08	112.60	3	2
1	A	127	HIS	CB-CG-CD2	-5.20	124.44	131.20	2	1
1	A	45	PHE	CA-CB-CG	5.18	118.98	113.80	21	1
1	A	37	VAL	CA-C-N	5.13	127.16	120.28	16	1
1	A	37	VAL	C-N-CA	5.13	127.16	120.28	16	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	76	TYR	Sidechain	6
1	A	89	TYR	Sidechain	5
1	A	109	LEU	Peptide	4
1	A	8	ARG	Sidechain	2
1	A	4	TYR	Sidechain	2
1	A	120	ARG	Sidechain	1
1	A	159	ARG	Sidechain	1

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1216	1204	1204	2±1
All	All	25536	25284	25284	44

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:TYR:CE2	1:A:65:VAL:HG22	0.67	2.23	3	3
1:A:70:GLY:CA	1:A:85:LEU:HD13	0.60	2.27	8	1
1:A:132:MET:HG2	1:A:139:VAL:HG11	0.57	1.75	6	2
1:A:4:TYR:CD1	1:A:132:MET:HE1	0.57	2.34	5	1
1:A:23:ALA:HB2	1:A:34:CYS:SG	0.55	2.42	2	1
1:A:89:TYR:C	1:A:89:TYR:CD1	0.53	2.87	19	4
1:A:89:TYR:C	1:A:89:TYR:CD2	0.52	2.87	20	3
1:A:50:THR:HG23	1:A:69:VAL:CG2	0.52	2.34	19	1
1:A:66:ILE:HG21	1:A:92:VAL:HG23	0.52	1.81	18	1
1:A:89:TYR:CZ	1:A:130:THR:HG22	0.49	2.43	19	2
1:A:148:TRP:CZ3	1:A:152:ILE:HD11	0.46	2.46	7	3
1:A:70:GLY:HA3	1:A:85:LEU:HD13	0.46	1.86	8	1
1:A:128:LEU:HD13	1:A:128:LEU:C	0.46	2.36	15	1
1:A:108:LEU:HD21	1:A:141:ILE:HG23	0.46	1.87	18	2
1:A:96:VAL:HG13	1:A:104:VAL:HG11	0.45	1.87	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:LEU:HD21	1:A:155:ALA:HB1	0.45	1.87	8	1
1:A:70:GLY:HA2	1:A:85:LEU:HD13	0.45	1.87	8	1
1:A:142:TYR:C	1:A:142:TYR:CD2	0.45	2.95	9	1
1:A:105:ALA:HB1	1:A:142:TYR:CE1	0.44	2.47	12	1
1:A:116:GLY:O	1:A:118:LYS:CE	0.43	2.67	17	1
1:A:40:LYS:HB3	1:A:41:TRP:CD1	0.42	2.49	1	1
1:A:108:LEU:HD12	1:A:111:THR:CG2	0.42	2.44	10	1
1:A:4:TYR:CE1	1:A:141:ILE:HD13	0.42	2.49	13	1
1:A:21:ASN:HD21	1:A:67:HIS:CG	0.41	2.33	6	1
1:A:66:ILE:CG2	1:A:92:VAL:HG22	0.41	2.45	17	1
1:A:121:LEU:C	1:A:121:LEU:HD13	0.41	2.40	14	1
1:A:108:LEU:HD22	1:A:148:TRP:CZ3	0.41	2.51	9	1
1:A:17:GLU:O	1:A:101:VAL:HG11	0.41	2.16	2	1
1:A:66:ILE:CG2	1:A:92:VAL:HG23	0.41	2.46	18	1
1:A:66:ILE:N	1:A:66:ILE:HD12	0.41	2.31	15	1
1:A:147:GLU:OE2	1:A:151:LYS:NZ	0.40	2.53	10	1
1:A:18:CYS:HB3	1:A:104:VAL:HG23	0.40	1.93	14	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	157/168 (93%)	145±2 (92±1%)	10±2 (6±1%)	2±1 (1±1%)	11	57
All	All	3297/3528 (93%)	3041 (92%)	208 (6%)	48 (1%)	11	57

All 5 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	63	TYR	21
1	A	73	PHE	11
1	A	14	ASN	6
1	A	115	SER	6
1	A	110	SER	4

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	132/141 (94%)	113±4 (86±3%)	19±4 (14±3%)	5	44
All	All	2772/2961 (94%)	2383 (86%)	389 (14%)	5	44

All 96 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	149	GLU	15
1	A	104	VAL	13
1	A	65	VAL	13
1	A	63	TYR	12
1	A	13	LYS	12
1	A	7	LYS	11
1	A	91	GLU	11
1	A	148	TRP	11
1	A	157	GLN	11
1	A	37	VAL	10
1	A	142	TYR	10
1	A	83	ARG	10
1	A	108	LEU	9
1	A	11	ILE	8
1	A	147	GLU	8
1	A	114	TYR	8
1	A	128	LEU	8
1	A	56	LYS	8
1	A	89	TYR	7
1	A	26	ARG	7
1	A	141	ILE	7
1	A	102	ASN	6
1	A	120	ARG	6
1	A	39	LYS	6
1	A	98	ARG	5
1	A	121	LEU	5
1	A	146	LYS	5
1	A	72	ASN	5
1	A	80	GLU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	109	LEU	4
1	A	125	LEU	4
1	A	138	ASP	4
1	A	43	GLU	4
1	A	95	GLU	4
1	A	18	CYS	4
1	A	94	LYS	4
1	A	106	ILE	4
1	A	59	MET	4
1	A	5	ARG	3
1	A	132	MET	3
1	A	16	GLU	3
1	A	35	LYS	3
1	A	152	ILE	3
1	A	40	LYS	3
1	A	46	LYS	3
1	A	103	SER	3
1	A	69	VAL	3
1	A	84	GLU	3
1	A	75	ASN	3
1	A	3	SER	3
1	A	24	ASN	3
1	A	113	VAL	3
1	A	8	ARG	2
1	A	79	SER	2
1	A	144	ARG	2
1	A	76	TYR	2
1	A	123	GLN	2
1	A	159	ARG	2
1	A	97	THR	2
1	A	151	LYS	2
1	A	96	VAL	2
1	A	136	ASP	2
1	A	110	SER	2
1	A	9	MET	2
1	A	19	VAL	2
1	A	150	LYS	2
1	A	57	THR	2
1	A	139	VAL	1
1	A	6	VAL	1
1	A	10	ASP	1
1	A	60	CYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	90	ARG	1
1	A	124	SER	1
1	A	111	THR	1
1	A	154	GLU	1
1	A	54	THR	1
1	A	158	MET	1
1	A	17	GLU	1
1	A	92	VAL	1
1	A	134	SER	1
1	A	77	SER	1
1	A	82	ASP	1
1	A	118	LYS	1
1	A	4	TYR	1
1	A	14	ASN	1
1	A	126	ASN	1
1	A	78	GLU	1
1	A	145	ASP	1
1	A	156	ILE	1
1	A	33	VAL	1
1	A	153	SER	1
1	A	41	TRP	1
1	A	31	ASP	1
1	A	50	THR	1
1	A	115	SER	1
1	A	130	THR	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 80% 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	1670
Number of shifts mapped to atoms	1670
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	152	-0.02 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	143	0.12 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	146	0.04 ± 0.13	None needed (< 0.5 ppm)
^{15}N	137	0.28 ± 0.28	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 80%, i.e. 1661 atoms were assigned a chemical shift out of a possible 2080. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	731/787 (93%)	299/320 (93%)	296/316 (94%)	136/151 (90%)
Sidechain	930/1162 (80%)	625/754 (83%)	305/359 (85%)	0/49 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	0/131 (0%)	0/63 (0%)	0/64 (0%)	0/4 (0%)
Overall	1661/2080 (80%)	924/1137 (81%)	601/739 (81%)	136/204 (67%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1670 atoms were assigned a chemical shift out of a possible 2101. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	736/795 (93%)	301/323 (93%)	298/320 (93%)	137/152 (90%)
Sidechain	934/1175 (79%)	628/763 (82%)	306/363 (84%)	0/49 (0%)
Aromatic	0/131 (0%)	0/63 (0%)	0/64 (0%)	0/4 (0%)
Overall	1670/2101 (79%)	929/1149 (81%)	604/747 (81%)	137/205 (67%)

7.1.4 Statistically unusual chemical shifts ⓘ

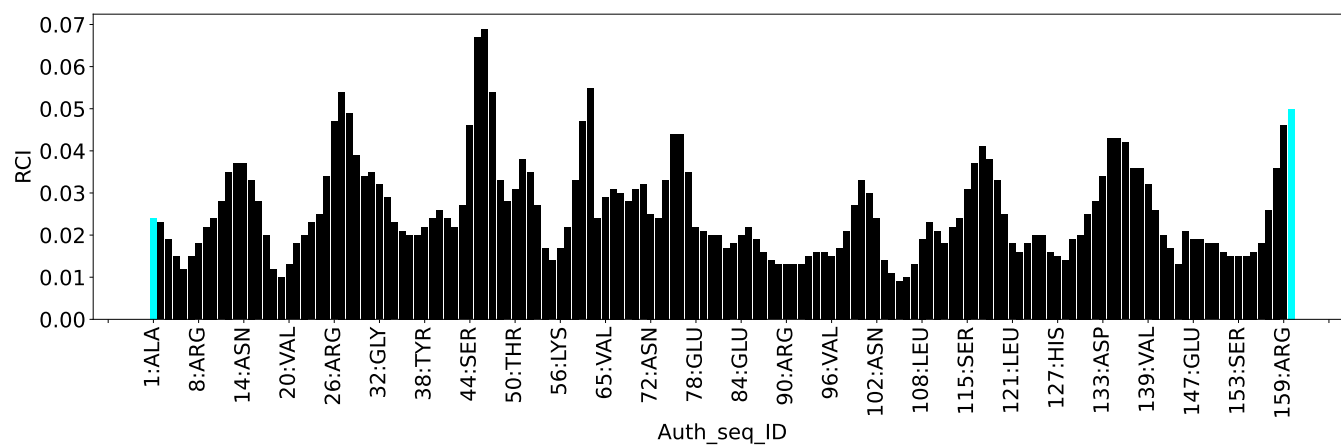
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	40	LYS	HG3	-0.63	0.04 – 2.67	-7.5
1	A	40	LYS	HG2	-0.38	0.13 – 2.61	-7.1
1	A	159	ARG	HD2	1.97	1.97 – 4.26	-5.0

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2905
Intra-residue ($ i-j =0$)	1069
Sequential ($ i-j =1$)	826
Medium range ($ i-j >1$ and $ i-j <5$)	370
Long range ($ i-j \geq 5$)	522
Inter-chain	0
Hydrogen bond restraints	118
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	17.3
Number of long range restraints per residue ¹	3.2

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)	15.1	0.2
0.2-0.5 (Medium)	25.4	0.5
>0.5 (Large)	43.5	3.83

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis

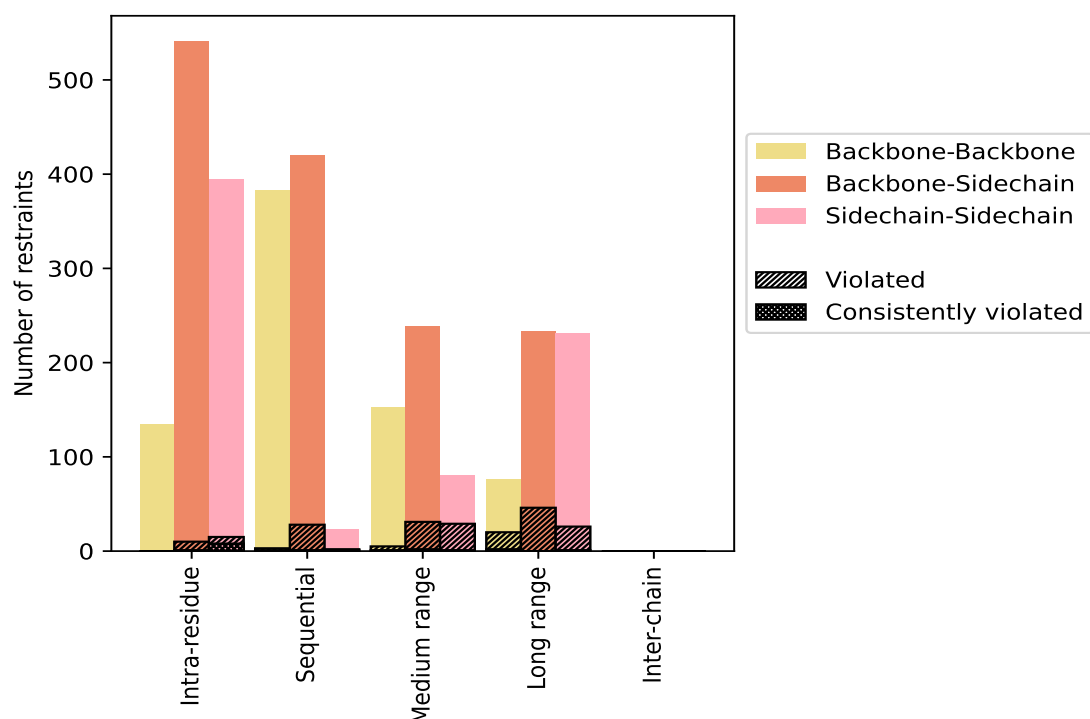
9.1 Summary of distance violations

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)	1069	36.8	25	2.3	0.9	9	0.8	0.3
Backbone-Backbone	134	4.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	541	18.6	10	1.8	0.3	1	0.2	0.0
Sidechain-Sidechain	394	13.6	15	3.8	0.5	8	2.0	0.3
Sequential (i-j =1)	826	28.4	33	4.0	1.1	3	0.4	0.1
Backbone-Backbone	383	13.2	3	0.8	0.1	1	0.3	0.0
Backbone-Sidechain	420	14.5	28	6.7	1.0	1	0.2	0.0
Sidechain-Sidechain	23	0.8	2	8.7	0.1	1	4.3	0.0
Medium range (i-j >1 & i-j <5)	370	12.7	57	15.4	2.0	4	1.1	0.1
Backbone-Backbone	152	5.2	5	3.3	0.2	1	0.7	0.0
Backbone-Sidechain	138	4.8	23	16.7	0.8	2	1.4	0.1
Sidechain-Sidechain	80	2.8	29	36.2	1.0	1	1.2	0.0
Long range (i-j ≥5)	522	18.0	90	17.2	3.1	3	0.6	0.1
Backbone-Backbone	76	2.6	20	26.3	0.7	2	2.6	0.1
Backbone-Sidechain	215	7.4	44	20.5	1.5	0	0.0	0.0
Sidechain-Sidechain	231	8.0	26	11.3	0.9	1	0.4	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	118	4.1	10	8.5	0.3	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2905	100.0	215	7.4	7.4	19	0.7	0.7
Backbone-Backbone	745	25.6	28	3.8	1.0	4	0.5	0.1
Backbone-Sidechain	1432	49.3	115	8.0	4.0	4	0.3	0.1
Sidechain-Sidechain	728	25.1	72	9.9	2.5	11	1.5	0.4

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	12	11	20	25	0	68	0.65	1.89	0.46	0.5
2	14	13	26	29	0	82	0.67	2.0	0.53	0.51
3	14	10	22	32	0	78	0.65	2.3	0.43	0.58
4	15	15	26	33	0	89	0.69	2.54	0.53	0.62
5	16	13	23	31	0	83	0.6	2.45	0.46	0.45
6	13	13	19	35	0	80	0.62	2.43	0.45	0.54
7	13	13	25	37	0	88	0.67	2.6	0.5	0.57
8	15	11	27	34	0	87	0.69	2.65	0.54	0.51
9	17	12	23	36	0	88	0.62	2.26	0.49	0.46
10	14	13	27	31	0	85	0.61	2.05	0.47	0.47

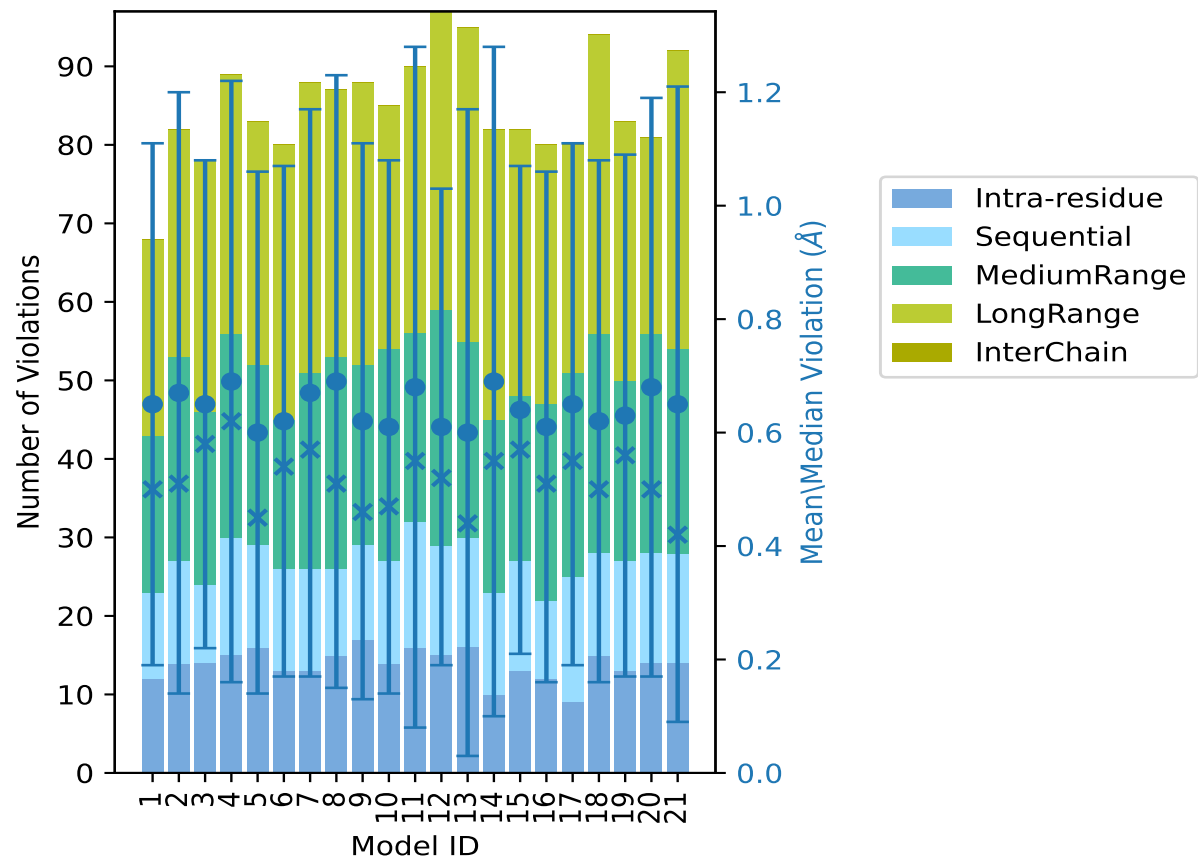
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	16	16	24	34	0	90	0.68	3.67	0.6	0.55
12	15	14	30	38	0	97	0.61	1.64	0.42	0.52
13	16	14	25	40	0	95	0.6	3.83	0.57	0.44
14	10	13	22	37	0	82	0.69	3.6	0.59	0.55
15	13	14	21	34	0	82	0.64	1.84	0.43	0.57
16	12	10	25	33	0	80	0.61	2.58	0.45	0.51
17	9	16	26	29	0	80	0.65	1.84	0.46	0.55
18	15	13	28	38	0	94	0.62	2.48	0.46	0.5
19	13	14	23	33	0	83	0.63	2.49	0.46	0.56
20	14	14	28	25	0	81	0.68	2.52	0.51	0.5
21	14	14	26	38	0	92	0.65	3.27	0.56	0.42

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

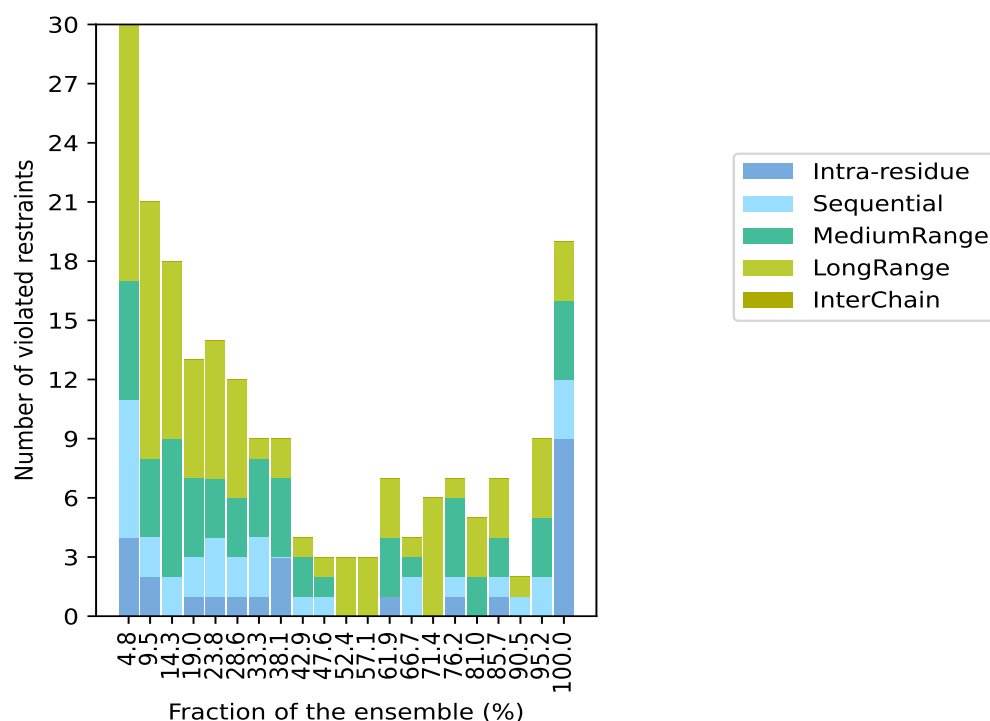
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2582(IR:1044, SQ:793, MR:313, LR:432, IC:0) restraints are 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	%
4	7	6	13	0	30	1	4.8
2	2	4	13	0	21	2	9.5
0	2	7	9	0	18	3	14.3
1	2	4	6	0	13	4	19.0
1	3	3	7	0	14	5	23.8
1	2	3	6	0	12	6	28.6
1	3	4	1	0	9	7	33.3
3	0	4	2	0	9	8	38.1
0	1	2	1	0	4	9	42.9
0	1	1	1	0	3	10	47.6
0	0	0	3	0	3	11	52.4
0	0	0	3	0	3	12	57.1
1	0	3	3	0	7	13	61.9
0	2	1	1	0	4	14	66.7
0	0	0	6	0	6	15	71.4
1	1	4	1	0	7	16	76.2
0	0	2	3	0	5	17	81.0
1	1	2	3	0	7	18	85.7
0	1	0	1	0	2	19	90.5
0	2	3	4	0	9	20	95.2
9	3	4	3	0	19	21	100.0

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

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

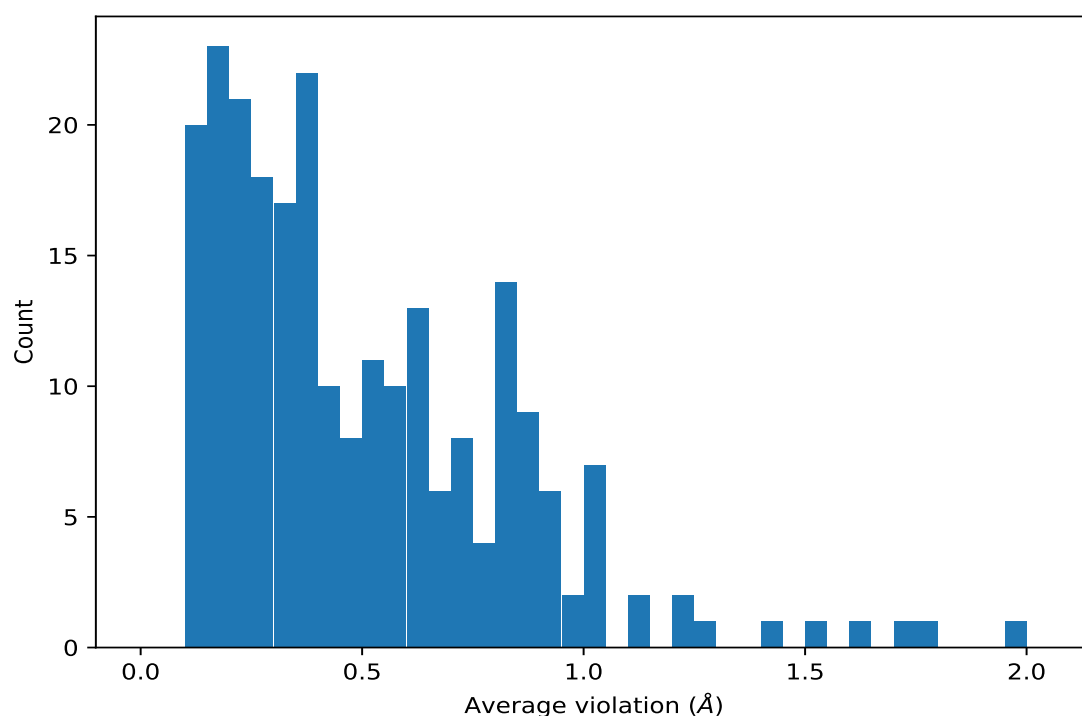
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	21	1.97	0.75	1.69
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	21	1.61	0.0	1.61
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	21	1.54	0.01	1.54
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	21	1.42	0.01	1.42
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	21	1.25	0.49	1.21
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	21	1.11	0.0	1.11
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	21	1.02	0.01	1.01
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	21	1.0	0.4	0.97
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	21	0.99	0.17	1.02
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	21	0.92	0.21	0.9
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	21	0.86	0.18	0.86
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	21	0.85	0.0	0.85
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	21	0.81	0.01	0.81
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	21	0.71	0.01	0.71
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	21	0.7	0.21	0.71
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	21	0.65	0.16	0.69

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	21	0.39	0.02	0.4
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	21	0.35	0.15	0.32
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	21	0.3	0.15	0.22
(2,140)	1:25:A:PRO:HG2	1:52:A:VAL:HA	20	0.91	0.48	0.8
(1,405)	1:76:A:TYR:HB2	1:81:A:GLY:HA3	20	0.84	0.31	0.78
(1,451)	1:87:A:ALA:HA	1:90:A:ARG:HG2	20	0.78	0.19	0.78
(1,498)	1:94:A:LYS:HB2	1:95:A:GLU:HA	20	0.74	0.18	0.78
(1,452)	1:87:A:ALA:HA	1:91:A:GLU:HG2	20	0.7	0.41	0.54
(2,45)	1:8:A:ARG:HB2	1:149:A:GLU:HA	20	0.67	0.21	0.66
(5,394)	1:61:A:GLY:HA3	1:63:A:TYR:H	20	0.58	0.14	0.58
(1,150)	1:25:A:PRO:HB3	1:50:A:THR:HA	20	0.39	0.15	0.44
(1,423)	1:82:A:ASP:HB2	1:83:A:ARG:HA	20	0.23	0.06	0.24
(1,60)	1:8:A:ARG:HB2	1:146:A:LYS:HA	19	0.63	0.21	0.64
(5,500)	1:83:A:ARG:HG2	1:84:A:GLU:H	19	0.53	0.24	0.5
(1,221)	1:35:A:LYS:HE3	1:39:A:LYS:HE2	18	1.75	1.12	1.6
(2,562)	1:147:A:GLU:HG2	1:150:A:LYS:HG3	18	1.22	0.74	1.06
(1,380)	1:66:A:ILE:HA	1:95:A:GLU:HG2	18	0.92	0.29	0.94
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG11	18	0.8	0.21	0.84
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG12	18	0.8	0.21	0.84
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG13	18	0.8	0.21	0.84
(4,41)	1:41:A:TRP:HH2	1:60:A:CYS:HB3	18	0.66	0.32	0.7
(5,586)	1:94:A:LYS:H	1:94:A:LYS:HG3	18	0.6	0.06	0.6
(2,585)	1:157:A:GLN:HG3	1:158:A:MET:HA	18	0.25	0.05	0.26
(1,644)	1:120:A:ARG:HB3	1:124:A:SER:HB3	17	1.03	0.64	0.88
(1,650)	1:121:A:LEU:HA	1:125:A:LEU:HB3	17	0.93	0.38	1.06
(2,12)	1:4:A:TYR:HB3	1:156:A:ILE:HA	17	0.79	0.37	0.88
(1,166)	1:27:A:GLY:HA2	1:45:A:PHE:HA	17	0.43	0.13	0.45
(6,4)	1:6:A:VAL:HG11	1:143:A:CYS:H	17	0.37	0.17	0.29
(6,4)	1:6:A:VAL:HG12	1:143:A:CYS:H	17	0.37	0.17	0.29
(6,4)	1:6:A:VAL:HG13	1:143:A:CYS:H	17	0.37	0.17	0.29
(1,187)	1:29:A:PRO:HG2	1:35:A:LYS:HE3	16	1.21	0.6	1.16
(1,418)	1:80:A:GLU:HA	1:83:A:ARG:HG3	16	0.59	0.21	0.55
(2,173)	1:35:A:LYS:HG2	1:38:A:TYR:HB2	16	0.55	0.18	0.56
(1,508)	1:94:A:LYS:HE2	1:98:A:ARG:HD3	16	0.49	0.17	0.49
(1,508)	1:94:A:LYS:HE3	1:98:A:ARG:HD3	16	0.49	0.17	0.49
(6,7)	1:9:A:MET:HB2	1:13:A:LYS:H	16	0.43	0.19	0.43
(1,110)	1:14:A:ASN:HA	1:15:A:ASP:HB2	16	0.21	0.05	0.21
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE2	16	0.17	0.02	0.17
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE3	16	0.17	0.02	0.17
(4,42)	1:41:A:TRP:HH2	1:63:A:TYR:HB2	15	1.71	0.43	1.79
(1,601)	1:111:A:THR:HA	1:120:A:ARG:HD2	15	0.93	0.51	0.83
(4,93)	1:143:A:CYS:HB2	1:148:A:TRP:HZ3	15	0.86	0.45	0.81

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG11	15	0.52	0.18	0.55
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG12	15	0.52	0.18	0.55
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG13	15	0.52	0.18	0.55
(1,34)	1:7:A:LYS:HA	1:149:A:GLU:HG2	15	0.49	0.25	0.43
(5,50)	1:8:A:ARG:HG2	1:149:A:GLU:H	15	0.35	0.18	0.32
(1,481)	1:91:A:GLU:HG2	1:94:A:LYS:HE3	14	0.84	0.62	0.68
(5,188)	1:27:A:GLY:HA3	1:48:A:SER:H	14	0.38	0.21	0.32
(5,37)	1:7:A:LYS:HB2	1:8:A:ARG:H	14	0.19	0.06	0.18
(1,606)	1:113:A:VAL:HB	1:114:A:TYR:HA	14	0.12	0.01	0.12
(1,630)	1:118:A:LYS:HD2	1:120:A:ARG:HD3	13	0.86	0.59	0.74
(6,71)	1:60:A:CYS:HB2	1:63:A:TYR:H	13	0.6	0.44	0.36
(5,548)	1:89:A:TYR:HB2	1:131:A:ALA:H	13	0.5	0.26	0.5
(3,29)	1:41:A:TRP:HD1	1:60:A:CYS:HB3	13	0.45	0.23	0.36
(1,39)	1:7:A:LYS:HB2	1:9:A:MET:HB2	13	0.37	0.25	0.32
(1,118)	1:18:A:CYS:HB3	1:101:A:VAL:HB	13	0.31	0.15	0.27
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	13	0.28	0.05	0.28
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	13	0.28	0.05	0.28
(2,452)	1:108:A:LEU:HG	1:143:A:CYS:HB2	12	0.69	0.23	0.72
(5,153)	1:21:A:ASN:HB3	1:68:A:ALA:H	12	0.62	0.29	0.5
(2,206)	1:48:A:SER:HA	1:56:A:LYS:HE2	12	0.55	0.27	0.44
(1,311)	1:50:A:THR:HB	1:56:A:LYS:HD3	11	0.64	0.36	0.67
(1,89)	1:12:A:ALA:HB1	1:40:A:LYS:HB3	11	0.32	0.13	0.34
(1,89)	1:12:A:ALA:HB2	1:40:A:LYS:HB3	11	0.32	0.13	0.34
(1,89)	1:12:A:ALA:HB3	1:40:A:LYS:HB3	11	0.32	0.13	0.34
(5,113)	1:17:A:GLU:H	1:103:A:SER:H	11	0.14	0.02	0.13
(1,632)	1:118:A:LYS:HD3	1:120:A:ARG:HD3	10	1.0	0.63	0.97
(1,155)	1:25:A:PRO:HG3	1:51:A:PRO:HA	10	0.3	0.12	0.29
(1,767)	1:149:A:GLU:HG3	1:150:A:LYS:HA	10	0.26	0.12	0.26
(1,575)	1:107:A:PRO:HA	1:108:A:LEU:HB3	9	0.75	0.09	0.8
(2,393)	1:96:A:VAL:HG21	1:137:A:ALA:HA	9	0.38	0.21	0.26
(2,393)	1:96:A:VAL:HG22	1:137:A:ALA:HA	9	0.38	0.21	0.26
(2,393)	1:96:A:VAL:HG23	1:137:A:ALA:HA	9	0.38	0.21	0.26
(1,829)	1:156:A:ILE:HA	1:159:A:ARG:HG2	9	0.33	0.09	0.32
(1,396)	1:73:A:PHE:HA	1:76:A:TYR:HA	9	0.15	0.02	0.14
(1,460)	1:89:A:TYR:HB3	1:128:A:LEU:HA	8	1.01	0.5	0.96
(1,216)	1:35:A:LYS:HG3	1:39:A:LYS:HB2	8	0.65	0.55	0.46
(2,577)	1:153:A:SER:HA	1:157:A:GLN:HG3	8	0.58	0.52	0.26
(2,357)	1:91:A:GLU:HG3	1:94:A:LYS:HG3	8	0.52	0.27	0.45
(1,343)	1:56:A:LYS:HB3	1:56:A:LYS:HE2	8	0.42	0.15	0.48
(1,343)	1:56:A:LYS:HB3	1:56:A:LYS:HE3	8	0.42	0.15	0.48
(1,32)	1:7:A:LYS:HA	1:7:A:LYS:HE3	8	0.32	0.21	0.2
(5,256)	1:40:A:LYS:H	1:40:A:LYS:HD3	8	0.27	0.12	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,44)	1:7:A:LYS:HB3	1:9:A:MET:HB2	8	0.27	0.12	0.24
(2,388)	1:96:A:VAL:HG21	1:101:A:VAL:HA	8	0.21	0.12	0.14
(2,388)	1:96:A:VAL:HG22	1:101:A:VAL:HA	8	0.21	0.12	0.14
(2,388)	1:96:A:VAL:HG23	1:101:A:VAL:HA	8	0.21	0.12	0.14
(1,220)	1:35:A:LYS:HE2	1:39:A:LYS:HG2	7	1.02	0.54	1.17
(1,757)	1:147:A:GLU:HA	1:150:A:LYS:HG2	7	0.31	0.1	0.31
(6,105)	1:96:A:VAL:HG21	1:101:A:VAL:H	7	0.27	0.13	0.21
(6,105)	1:96:A:VAL:HG22	1:101:A:VAL:H	7	0.27	0.13	0.21
(6,105)	1:96:A:VAL:HG23	1:101:A:VAL:H	7	0.27	0.13	0.21
(5,68)	1:10:A:ASP:HB3	1:11:A:ILE:H	7	0.26	0.1	0.24
(2,315)	1:80:A:GLU:HA	1:83:A:ARG:HD2	7	0.26	0.07	0.26
(6,8)	1:11:A:ILE:HG12	1:14:A:ASN:H	7	0.25	0.08	0.24
(1,712)	1:136:A:ASP:HB3	1:137:A:ALA:HA	7	0.24	0.02	0.24
(1,209)	1:35:A:LYS:HB3	1:35:A:LYS:HD2	7	0.21	0.06	0.19
(1,209)	1:35:A:LYS:HB3	1:35:A:LYS:HD3	7	0.21	0.06	0.19
(1,845)	1:158:A:MET:HB2	1:159:A:ARG:HA	7	0.13	0.02	0.12
(1,301)	1:48:A:SER:HA	1:56:A:LYS:HD3	6	1.03	0.47	1.17
(2,449)	1:108:A:LEU:HA	1:125:A:LEU:HD21	6	0.8	0.4	0.86
(2,449)	1:108:A:LEU:HA	1:125:A:LEU:HD22	6	0.8	0.4	0.86
(2,449)	1:108:A:LEU:HA	1:125:A:LEU:HD23	6	0.8	0.4	0.86
(1,476)	1:91:A:GLU:HA	1:94:A:LYS:HB2	6	0.72	0.54	0.66
(1,359)	1:59:A:MET:HG3	1:64:A:PRO:HA	6	0.54	0.23	0.56
(1,414)	1:79:A:SER:HB2	1:80:A:GLU:HA	6	0.54	0.16	0.59
(3,63)	1:121:A:LEU:HD21	1:148:A:TRP:HD1	6	0.49	0.28	0.4
(3,63)	1:121:A:LEU:HD22	1:148:A:TRP:HD1	6	0.49	0.28	0.4
(3,63)	1:121:A:LEU:HD23	1:148:A:TRP:HD1	6	0.49	0.28	0.4
(1,420)	1:81:A:GLY:HA3	1:84:A:GLU:HB2	6	0.39	0.28	0.26
(1,420)	1:81:A:GLY:HA3	1:84:A:GLU:HB3	6	0.39	0.28	0.26
(2,141)	1:25:A:PRO:HG2	1:52:A:VAL:HG11	6	0.38	0.18	0.36
(2,141)	1:25:A:PRO:HG2	1:52:A:VAL:HG12	6	0.38	0.18	0.36
(2,141)	1:25:A:PRO:HG2	1:52:A:VAL:HG13	6	0.38	0.18	0.36
(1,828)	1:156:A:ILE:HA	1:159:A:ARG:HB2	6	0.36	0.13	0.36
(5,861)	1:141:A:ILE:H	1:141:A:ILE:HB	6	0.19	0.06	0.17
(1,466)	1:90:A:ARG:HA	1:131:A:ALA:HA	6	0.15	0.04	0.15
(2,341)	1:88:A:ALA:HA	1:89:A:TYR:HB3	6	0.14	0.01	0.14
(2,194)	1:44:A:SER:HB3	1:60:A:CYS:HB3	5	0.99	0.62	1.33
(1,479)	1:91:A:GLU:HG2	1:94:A:LYS:HG3	5	0.91	0.16	0.89
(2,329)	1:85:A:LEU:HG	1:109:A:LEU:HD21	5	0.87	0.29	0.78
(2,329)	1:85:A:LEU:HG	1:109:A:LEU:HD22	5	0.87	0.29	0.78
(2,329)	1:85:A:LEU:HG	1:109:A:LEU:HD23	5	0.87	0.29	0.78
(3,64)	1:121:A:LEU:HD21	1:148:A:TRP:HZ3	5	0.8	0.32	0.78
(3,64)	1:121:A:LEU:HD22	1:148:A:TRP:HZ3	5	0.8	0.32	0.78

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,64)	1:121:A:LEU:HD23	1:148:A:TRP:HZ3	5	0.8	0.32	0.78
(2,561)	1:147:A:GLU:HB2	1:151:A:LYS:HD2	5	0.78	0.34	0.78
(5,52)	1:8:A:ARG:HD3	1:149:A:GLU:H	5	0.69	0.16	0.75
(1,760)	1:147:A:GLU:HG2	1:150:A:LYS:HD2	5	0.61	0.15	0.55
(1,760)	1:147:A:GLU:HG3	1:150:A:LYS:HD2	5	0.61	0.15	0.55
(4,49)	1:58:A:VAL:HG21	1:67:A:HIS:HE1	5	0.55	0.12	0.51
(4,49)	1:58:A:VAL:HG22	1:67:A:HIS:HE1	5	0.55	0.12	0.51
(4,49)	1:58:A:VAL:HG23	1:67:A:HIS:HE1	5	0.55	0.12	0.51
(1,52)	1:7:A:LYS:HD3	1:140:A:VAL:HG21	5	0.23	0.07	0.22
(1,52)	1:7:A:LYS:HD3	1:140:A:VAL:HG22	5	0.23	0.07	0.22
(1,52)	1:7:A:LYS:HD3	1:140:A:VAL:HG23	5	0.23	0.07	0.22
(5,119)	1:17:A:GLU:HG3	1:18:A:CYS:H	5	0.23	0.07	0.24
(5,560)	1:90:A:ARG:HG3	1:91:A:GLU:H	5	0.22	0.1	0.2
(1,497)	1:94:A:LYS:HB2	1:94:A:LYS:HE2	5	0.17	0.05	0.15
(1,497)	1:94:A:LYS:HB2	1:94:A:LYS:HE3	5	0.17	0.05	0.15
(5,339)	1:54:A:THR:H	1:88:A:ALA:HA	5	0.17	0.05	0.18
(5,547)	1:89:A:TYR:HB2	1:90:A:ARG:H	5	0.14	0.02	0.14
(1,620)	1:118:A:LYS:HB2	1:120:A:ARG:HD3	4	0.86	0.6	0.86
(1,628)	1:118:A:LYS:HG3	1:119:A:ASP:HA	4	0.82	0.32	0.98
(2,514)	1:125:A:LEU:HG	1:152:A:ILE:HG13	4	0.8	0.16	0.82
(1,480)	1:91:A:GLU:HG2	1:94:A:LYS:HD2	4	0.55	0.36	0.5
(6,106)	1:96:A:VAL:HG21	1:136:A:ASP:H	4	0.4	0.1	0.44
(6,106)	1:96:A:VAL:HG22	1:136:A:ASP:H	4	0.4	0.1	0.44
(6,106)	1:96:A:VAL:HG23	1:136:A:ASP:H	4	0.4	0.1	0.44
(2,51)	1:10:A:ASP:HB2	1:13:A:LYS:HG2	4	0.4	0.15	0.35
(2,83)	1:17:A:GLU:HG2	1:101:A:VAL:HA	4	0.34	0.16	0.3
(1,640)	1:120:A:ARG:HB2	1:120:A:ARG:HD2	4	0.28	0.05	0.28
(1,640)	1:120:A:ARG:HB2	1:120:A:ARG:HD3	4	0.28	0.05	0.28
(1,848)	1:158:A:MET:HG3	1:159:A:ARG:HA	4	0.26	0.11	0.22
(7,117)	1:159:A:ARG:H	1:155:A:ALA:O	4	0.24	0.15	0.18
(2,515)	1:125:A:LEU:HG	1:155:A:ALA:HA	4	0.19	0.03	0.18
(1,679)	1:125:A:LEU:HG	1:152:A:ILE:HA	4	0.16	0.04	0.16
(5,35)	1:7:A:LYS:H	1:143:A:CYS:H	4	0.15	0.04	0.15
(5,391)	1:60:A:CYS:H	1:63:A:TYR:H	4	0.13	0.02	0.14
(2,330)	1:85:A:LEU:HD11	1:109:A:LEU:HB3	3	0.61	0.15	0.55
(2,330)	1:85:A:LEU:HD12	1:109:A:LEU:HB3	3	0.61	0.15	0.55
(2,330)	1:85:A:LEU:HD13	1:109:A:LEU:HB3	3	0.61	0.15	0.55
(1,504)	1:94:A:LYS:HG2	1:95:A:GLU:HA	3	0.58	0.02	0.58
(2,10)	1:4:A:TYR:HB3	1:139:A:VAL:HB	3	0.46	0.22	0.59
(2,358)	1:91:A:GLU:HG3	1:94:A:LYS:HD2	3	0.43	0.14	0.51
(2,366)	1:92:A:VAL:HG21	1:109:A:LEU:HG	3	0.36	0.07	0.4
(2,366)	1:92:A:VAL:HG22	1:109:A:LEU:HG	3	0.36	0.07	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,366)	1:92:A:VAL:HG23	1:109:A:LEU:HG	3	0.36	0.07	0.4
(2,529)	1:128:A:LEU:HD11	1:132:A:MET:HG3	3	0.33	0.19	0.25
(2,529)	1:128:A:LEU:HD12	1:132:A:MET:HG3	3	0.33	0.19	0.25
(2,529)	1:128:A:LEU:HD13	1:132:A:MET:HG3	3	0.33	0.19	0.25
(2,560)	1:147:A:GLU:HA	1:150:A:LYS:HE2	3	0.32	0.08	0.29
(1,830)	1:156:A:ILE:HA	1:159:A:ARG:HD2	3	0.28	0.04	0.28
(5,696)	1:109:A:LEU:HA	1:111:A:THR:H	3	0.26	0.08	0.32
(3,6)	1:4:A:TYR:HD1	1:159:A:ARG:HB3	3	0.24	0.04	0.26
(3,6)	1:4:A:TYR:HD2	1:159:A:ARG:HB3	3	0.24	0.04	0.26
(1,634)	1:119:A:ASP:HA	1:120:A:ARG:HG3	3	0.24	0.11	0.2
(2,86)	1:18:A:CYS:HA	1:64:A:PRO:HB2	3	0.21	0.01	0.21
(6,56)	1:48:A:SER:H	1:58:A:VAL:HG21	3	0.2	0.04	0.19
(6,56)	1:48:A:SER:H	1:58:A:VAL:HG22	3	0.2	0.04	0.19
(6,56)	1:48:A:SER:H	1:58:A:VAL:HG23	3	0.2	0.04	0.19
(2,528)	1:128:A:LEU:HD11	1:132:A:MET:HB3	3	0.16	0.01	0.15
(2,528)	1:128:A:LEU:HD12	1:132:A:MET:HB3	3	0.16	0.01	0.15
(2,528)	1:128:A:LEU:HD13	1:132:A:MET:HB3	3	0.16	0.01	0.15
(5,747)	1:121:A:LEU:HB2	1:123:A:GLN:H	3	0.14	0.03	0.13
(7,100)	1:140:A:VAL:N	1:104:A:VAL:O	3	0.14	0.03	0.12
(5,681)	1:106:A:ILE:HB	1:140:A:VAL:H	3	0.13	0.02	0.12
(1,117)	1:18:A:CYS:HA	1:63:A:TYR:HA	3	0.12	0.01	0.11
(5,131)	1:19:A:VAL:H	1:65:A:VAL:HA	3	0.11	0.02	0.1
(6,93)	1:89:A:TYR:H	1:127:A:HIS:HB3	2	1.14	0.3	1.14
(1,218)	1:35:A:LYS:HD2	1:38:A:TYR:HB2	2	0.87	0.05	0.87
(1,70)	1:9:A:MET:HB3	1:13:A:LYS:HD2	2	0.74	0.64	0.74
(1,70)	1:9:A:MET:HB3	1:13:A:LYS:HD3	2	0.74	0.64	0.74
(2,299)	1:72:A:ASN:HB3	1:75:A:ASN:HB2	2	0.72	0.5	0.72
(1,28)	1:6:A:VAL:HG21	1:153:A:SER:HA	2	0.63	0.1	0.63
(1,28)	1:6:A:VAL:HG22	1:153:A:SER:HA	2	0.63	0.1	0.63
(1,28)	1:6:A:VAL:HG23	1:153:A:SER:HA	2	0.63	0.1	0.63
(2,490)	1:121:A:LEU:HD21	1:125:A:LEU:HB3	2	0.52	0.19	0.52
(2,490)	1:121:A:LEU:HD22	1:125:A:LEU:HB3	2	0.52	0.19	0.52
(2,490)	1:121:A:LEU:HD23	1:125:A:LEU:HB3	2	0.52	0.19	0.52
(7,31)	1:74:A:SER:H	1:72:A:ASN:O	2	0.44	0.18	0.44
(1,407)	1:77:A:SER:HB3	1:78:A:GLU:HA	2	0.38	0.01	0.38
(2,207)	1:48:A:SER:HA	1:58:A:VAL:HG21	2	0.33	0.05	0.33
(2,207)	1:48:A:SER:HA	1:58:A:VAL:HG22	2	0.33	0.05	0.33
(2,207)	1:48:A:SER:HA	1:58:A:VAL:HG23	2	0.33	0.05	0.33
(2,415)	1:102:A:ASN:HB3	1:137:A:ALA:HA	2	0.29	0.01	0.29
(6,92)	1:89:A:TYR:H	1:109:A:LEU:HD21	2	0.18	0.06	0.18
(6,92)	1:89:A:TYR:H	1:109:A:LEU:HD22	2	0.18	0.06	0.18
(6,92)	1:89:A:TYR:H	1:109:A:LEU:HD23	2	0.18	0.06	0.18

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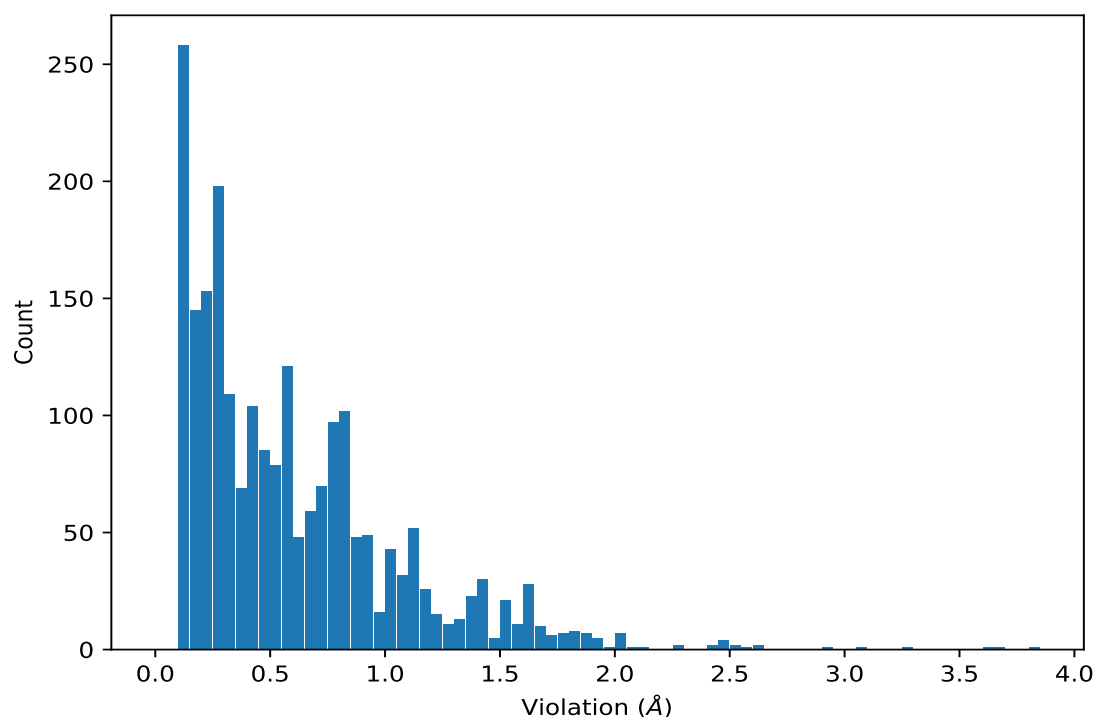
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(5,429)	1:69:A:VAL:H	1:69:A:VAL:HB	2	0.16	0.03	0.16
(7,106)	1:152:A:ILE:N	1:148:A:TRP:O	2	0.16	0.05	0.16
(5,138)	1:20:A:VAL:H	1:105:A:ALA:H	2	0.16	0.01	0.16
(5,312)	1:50:A:THR:H	1:50:A:THR:HB	2	0.15	0.0	0.15
(5,165)	1:23:A:ALA:H	1:69:A:VAL:HA	2	0.15	0.03	0.15
(2,493)	1:121:A:LEU:HD21	1:148:A:TRP:HA	2	0.14	0.02	0.14
(2,493)	1:121:A:LEU:HD22	1:148:A:TRP:HA	2	0.14	0.02	0.14
(2,493)	1:121:A:LEU:HD23	1:148:A:TRP:HA	2	0.14	0.02	0.14
(5,338)	1:54:A:THR:H	1:69:A:VAL:HB	2	0.14	0.02	0.14
(5,58)	1:9:A:MET:H	1:143:A:CYS:H	2	0.12	0.01	0.12
(5,116)	1:17:A:GLU:HB2	1:103:A:SER:H	2	0.12	0.01	0.12
(1,355)	1:58:A:VAL:HB	1:59:A:MET:HA	2	0.12	0.0	0.12
(1,126)	1:20:A:VAL:HA	1:66:A:ILE:HA	2	0.11	0.01	0.11
(5,133)	1:19:A:VAL:HA	1:105:A:ALA:H	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

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)
(1,221)	1:35:A:LYS:HE3	1:39:A:LYS:HE2	13	3.83
(1,221)	1:35:A:LYS:HE3	1:39:A:LYS:HE2	11	3.67
(1,221)	1:35:A:LYS:HE3	1:39:A:LYS:HE2	14	3.6
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	21	3.27
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	11	3.06
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	14	2.94
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	8	2.65
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	7	2.6
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	16	2.58
(2,562)	1:147:A:GLU:HG2	1:150:A:LYS:HG3	4	2.54
(1,221)	1:35:A:LYS:HE3	1:39:A:LYS:HE2	20	2.52
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	19	2.49
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	13	2.48
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	18	2.48
(1,221)	1:35:A:LYS:HE3	1:39:A:LYS:HE2	5	2.45
(2,562)	1:147:A:GLU:HG2	1:150:A:LYS:HG3	13	2.44
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	6	2.43
(1,221)	1:35:A:LYS:HE3	1:39:A:LYS:HE2	3	2.3
(2,562)	1:147:A:GLU:HG2	1:150:A:LYS:HG3	9	2.26
(1,221)	1:35:A:LYS:HE3	1:39:A:LYS:HE2	21	2.14
(1,221)	1:35:A:LYS:HE3	1:39:A:LYS:HE2	4	2.07
(1,481)	1:91:A:GLU:HG2	1:94:A:LYS:HE3	10	2.05
(2,562)	1:147:A:GLU:HG2	1:150:A:LYS:HG3	20	2.04
(1,644)	1:120:A:ARG:HB3	1:124:A:SER:HB3	7	2.04
(4,42)	1:41:A:TRP:HH2	1:63:A:TYR:HB2	10	2.01
(2,140)	1:25:A:PRO:HG2	1:52:A:VAL:HA	2	2.0
(1,187)	1:29:A:PRO:HG2	1:35:A:LYS:HE3	2	2.0
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	8	2.0
(4,42)	1:41:A:TRP:HH2	1:63:A:TYR:HB2	7	1.97
(4,42)	1:41:A:TRP:HH2	1:63:A:TYR:HB2	4	1.95
(4,42)	1:41:A:TRP:HH2	1:63:A:TYR:HB2	11	1.95
(4,42)	1:41:A:TRP:HH2	1:63:A:TYR:HB2	18	1.93
(1,187)	1:29:A:PRO:HG2	1:35:A:LYS:HE3	6	1.93
(1,644)	1:120:A:ARG:HB3	1:124:A:SER:HB3	8	1.91
(1,187)	1:29:A:PRO:HG2	1:35:A:LYS:HE3	10	1.9
(4,42)	1:41:A:TRP:HH2	1:63:A:TYR:HB2	1	1.89
(4,42)	1:41:A:TRP:HH2	1:63:A:TYR:HB2	21	1.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,644)	1:120:A:ARG:HB3	1:124:A:SER:HB3	2	1.89
(1,632)	1:118:A:LYS:HD3	1:120:A:ARG:HD3	21	1.87
(2,562)	1:147:A:GLU:HG2	1:150:A:LYS:HG3	7	1.85
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	14	1.85
(1,644)	1:120:A:ARG:HB3	1:124:A:SER:HB3	15	1.84
(1,632)	1:118:A:LYS:HD3	1:120:A:ARG:HD3	17	1.84
(1,221)	1:35:A:LYS:HE3	1:39:A:LYS:HE2	2	1.84
(1,630)	1:118:A:LYS:HD2	1:120:A:ARG:HD3	19	1.83
(1,187)	1:29:A:PRO:HG2	1:35:A:LYS:HE3	4	1.83
(1,187)	1:29:A:PRO:HG2	1:35:A:LYS:HE3	17	1.82
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	2	1.8
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	9	1.8
(4,42)	1:41:A:TRP:HH2	1:63:A:TYR:HB2	20	1.79
(1,630)	1:118:A:LYS:HD2	1:120:A:ARG:HD3	2	1.79
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	17	1.77
(1,630)	1:118:A:LYS:HD2	1:120:A:ARG:HD3	18	1.76
(1,481)	1:91:A:GLU:HG2	1:94:A:LYS:HE3	14	1.76
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	2	1.76
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	20	1.75
(4,42)	1:41:A:TRP:HH2	1:63:A:TYR:HB2	2	1.74
(4,42)	1:41:A:TRP:HH2	1:63:A:TYR:HB2	9	1.74
(2,194)	1:44:A:SER:HB3	1:60:A:CYS:HB3	15	1.73
(1,601)	1:111:A:THR:HA	1:120:A:ARG:HD2	9	1.72
(1,187)	1:29:A:PRO:HG2	1:35:A:LYS:HE3	1	1.72
(2,140)	1:25:A:PRO:HG2	1:52:A:VAL:HA	7	1.71
(4,42)	1:41:A:TRP:HH2	1:63:A:TYR:HB2	19	1.69
(1,220)	1:35:A:LYS:HE2	1:39:A:LYS:HG2	19	1.69
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	5	1.69
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	8	1.68
(4,42)	1:41:A:TRP:HH2	1:63:A:TYR:HB2	8	1.67
(2,562)	1:147:A:GLU:HG2	1:150:A:LYS:HG3	1	1.67
(1,601)	1:111:A:THR:HA	1:120:A:ARG:HD2	8	1.67
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	7	1.67
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	21	1.67
(1,301)	1:48:A:SER:HA	1:56:A:LYS:HD3	14	1.66
(1,632)	1:118:A:LYS:HD3	1:120:A:ARG:HD3	8	1.65
(4,42)	1:41:A:TRP:HH2	1:63:A:TYR:HB2	12	1.64
(2,140)	1:25:A:PRO:HG2	1:52:A:VAL:HA	11	1.63
(1,460)	1:89:A:TYR:HB3	1:128:A:LEU:HA	21	1.63
(4,42)	1:41:A:TRP:HH2	1:63:A:TYR:HB2	3	1.62
(1,216)	1:35:A:LYS:HG3	1:39:A:LYS:HB2	20	1.62
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	1	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	2	1.61
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	3	1.61
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	4	1.61
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	5	1.61
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	7	1.61
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	8	1.61
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	12	1.61
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	13	1.61
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	14	1.61
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	15	1.61
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	16	1.61
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	18	1.61
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	19	1.61
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	20	1.61
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	21	1.61
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	6	1.6
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	9	1.6
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	10	1.6
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	11	1.6
(4,105)	1:148:A:TRP:HD1	1:148:A:TRP:HH2	17	1.6
(1,601)	1:111:A:THR:HA	1:120:A:ARG:HD2	11	1.6
(1,460)	1:89:A:TYR:HB3	1:128:A:LEU:HA	4	1.59
(1,220)	1:35:A:LYS:HE2	1:39:A:LYS:HG2	8	1.59
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	4	1.55
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	8	1.55
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	9	1.55
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	11	1.55
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	12	1.55
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	13	1.55
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	16	1.55
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	18	1.55
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	19	1.55
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	1	1.54
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	2	1.54
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	3	1.54
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	5	1.54
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	6	1.54
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	7	1.54
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	10	1.54
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	14	1.54
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	17	1.54
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	20	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	21	1.54
(2,562)	1:147:A:GLU:HG2	1:150:A:LYS:HG3	17	1.54
(1,644)	1:120:A:ARG:HB3	1:124:A:SER:HB3	1	1.54
(1,644)	1:120:A:ARG:HB3	1:124:A:SER:HB3	4	1.54
(4,31)	1:41:A:TRP:HE3	1:41:A:TRP:HE1	15	1.53
(2,577)	1:153:A:SER:HA	1:157:A:GLN:HG3	16	1.52
(1,460)	1:89:A:TYR:HB3	1:128:A:LEU:HA	11	1.52
(1,216)	1:35:A:LYS:HG3	1:39:A:LYS:HB2	3	1.52
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	12	1.51
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	10	1.51
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	15	1.5
(2,12)	1:4:A:TYR:HB3	1:156:A:ILE:HA	5	1.49
(1,405)	1:76:A:TYR:HB2	1:81:A:GLY:HA3	4	1.49
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	4	1.49
(1,620)	1:118:A:LYS:HB2	1:120:A:ARG:HD3	18	1.48
(1,187)	1:29:A:PRO:HG2	1:35:A:LYS:HE3	9	1.48
(6,93)	1:89:A:TYR:H	1:127:A:HIS:HB3	15	1.44
(1,620)	1:118:A:LYS:HB2	1:120:A:ARG:HD3	20	1.44
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	1	1.43
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	7	1.43
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	14	1.43
(2,329)	1:85:A:LEU:HG	1:109:A:LEU:HD21	12	1.43
(2,329)	1:85:A:LEU:HG	1:109:A:LEU:HD22	12	1.43
(2,329)	1:85:A:LEU:HG	1:109:A:LEU:HD23	12	1.43
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	2	1.43
(6,71)	1:60:A:CYS:HB2	1:63:A:TYR:H	20	1.42
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	3	1.42
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	4	1.42
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	8	1.42
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	9	1.42
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	10	1.42
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	11	1.42
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	12	1.42
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	13	1.42
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	16	1.42
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	17	1.42
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	18	1.42
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	19	1.42
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	20	1.42
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	21	1.42
(1,405)	1:76:A:TYR:HB2	1:81:A:GLY:HA3	14	1.42
(4,93)	1:143:A:CYS:HB2	1:148:A:TRP:HZ3	21	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	2	1.41
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	5	1.41
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	6	1.41
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	17	1.41
(4,93)	1:143:A:CYS:HB2	1:148:A:TRP:HZ3	10	1.4
(2,561)	1:147:A:GLU:HB2	1:151:A:LYS:HD2	8	1.4
(2,449)	1:108:A:LEU:HA	1:125:A:LEU:HD21	8	1.4
(2,449)	1:108:A:LEU:HA	1:125:A:LEU:HD22	8	1.4
(2,449)	1:108:A:LEU:HA	1:125:A:LEU:HD23	8	1.4
(2,194)	1:44:A:SER:HB3	1:60:A:CYS:HB3	21	1.4
(1,650)	1:121:A:LEU:HA	1:125:A:LEU:HB3	1	1.4
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	11	1.39
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	12	1.39
(1,481)	1:91:A:GLU:HG2	1:94:A:LYS:HE3	4	1.38
(1,70)	1:9:A:MET:HB3	1:13:A:LYS:HD2	9	1.38
(1,70)	1:9:A:MET:HB3	1:13:A:LYS:HD3	9	1.38
(4,93)	1:143:A:CYS:HB2	1:148:A:TRP:HZ3	9	1.37
(4,26)	1:41:A:TRP:HD1	1:41:A:TRP:HE3	15	1.37
(1,311)	1:50:A:THR:HB	1:56:A:LYS:HD3	12	1.37
(1,221)	1:35:A:LYS:HE3	1:39:A:LYS:HE2	17	1.37
(2,577)	1:153:A:SER:HA	1:157:A:GLN:HG3	3	1.36
(1,481)	1:91:A:GLU:HG2	1:94:A:LYS:HE3	12	1.36
(1,476)	1:91:A:GLU:HA	1:94:A:LYS:HB2	21	1.36
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	12	1.36
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	5	1.35
(1,380)	1:66:A:ILE:HA	1:95:A:GLU:HG2	20	1.35
(1,221)	1:35:A:LYS:HE3	1:39:A:LYS:HE2	16	1.35
(4,93)	1:143:A:CYS:HB2	1:148:A:TRP:HZ3	16	1.34
(1,650)	1:121:A:LEU:HA	1:125:A:LEU:HB3	20	1.34
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	1	1.34
(4,93)	1:143:A:CYS:HB2	1:148:A:TRP:HZ3	1	1.33
(2,194)	1:44:A:SER:HB3	1:60:A:CYS:HB3	6	1.33
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	9	1.33
(1,601)	1:111:A:THR:HA	1:120:A:ARG:HD2	4	1.32
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	18	1.32
(1,380)	1:66:A:ILE:HA	1:95:A:GLU:HG2	17	1.32
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	10	1.31
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	7	1.31
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	21	1.3
(1,632)	1:118:A:LYS:HD3	1:120:A:ARG:HD3	7	1.3
(4,93)	1:143:A:CYS:HB2	1:148:A:TRP:HZ3	8	1.29
(2,140)	1:25:A:PRO:HG2	1:52:A:VAL:HA	13	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	1:4:A:TYR:HB3	1:156:A:ILE:HA	8	1.28
(1,650)	1:121:A:LEU:HA	1:125:A:LEU:HB3	11	1.28
(1,476)	1:91:A:GLU:HA	1:94:A:LYS:HB2	14	1.28
(1,380)	1:66:A:ILE:HA	1:95:A:GLU:HG2	15	1.28
(1,632)	1:118:A:LYS:HD3	1:120:A:ARG:HD3	20	1.27
(1,481)	1:91:A:GLU:HG2	1:94:A:LYS:HE3	8	1.27
(1,452)	1:87:A:ALA:HA	1:91:A:GLU:HG2	8	1.27
(1,220)	1:35:A:LYS:HE2	1:39:A:LYS:HG2	7	1.27
(6,71)	1:60:A:CYS:HB2	1:63:A:TYR:H	14	1.26
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	20	1.24
(1,644)	1:120:A:ARG:HB3	1:124:A:SER:HB3	12	1.24
(1,452)	1:87:A:ALA:HA	1:91:A:GLU:HG2	18	1.23
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	19	1.22
(3,64)	1:121:A:LEU:HD21	1:148:A:TRP:HZ3	4	1.22
(3,64)	1:121:A:LEU:HD22	1:148:A:TRP:HZ3	4	1.22
(3,64)	1:121:A:LEU:HD23	1:148:A:TRP:HZ3	4	1.22
(2,299)	1:72:A:ASN:HB3	1:75:A:ASN:HB2	11	1.22
(2,140)	1:25:A:PRO:HG2	1:52:A:VAL:HA	6	1.22
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	4	1.22
(1,452)	1:87:A:ALA:HA	1:91:A:GLU:HG2	9	1.22
(1,452)	1:87:A:ALA:HA	1:91:A:GLU:HG2	10	1.22
(1,301)	1:48:A:SER:HA	1:56:A:LYS:HD3	4	1.22
(1,601)	1:111:A:THR:HA	1:120:A:ARG:HD2	5	1.21
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	13	1.21
(2,357)	1:91:A:GLU:HG3	1:94:A:LYS:HG3	10	1.2
(1,601)	1:111:A:THR:HA	1:120:A:ARG:HD2	12	1.2
(1,405)	1:76:A:TYR:HB2	1:81:A:GLY:HA3	10	1.2
(4,41)	1:41:A:TRP:HH2	1:60:A:CYS:HB3	6	1.19
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	15	1.19
(2,12)	1:4:A:TYR:HB3	1:156:A:ILE:HA	18	1.19
(1,601)	1:111:A:THR:HA	1:120:A:ARG:HD2	13	1.19
(1,451)	1:87:A:ALA:HA	1:90:A:ARG:HG2	21	1.19
(1,405)	1:76:A:TYR:HB2	1:81:A:GLY:HA3	3	1.19
(1,380)	1:66:A:ILE:HA	1:95:A:GLU:HG2	1	1.19
(1,187)	1:29:A:PRO:HG2	1:35:A:LYS:HE3	18	1.19
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	16	1.19
(1,452)	1:87:A:ALA:HA	1:91:A:GLU:HG2	4	1.18
(1,301)	1:48:A:SER:HA	1:56:A:LYS:HD3	5	1.18
(6,71)	1:60:A:CYS:HB2	1:63:A:TYR:H	3	1.17
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	12	1.17
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	9	1.17
(1,630)	1:118:A:LYS:HD2	1:120:A:ARG:HD3	7	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,311)	1:50:A:THR:HB	1:56:A:LYS:HD3	11	1.17
(1,301)	1:48:A:SER:HA	1:56:A:LYS:HD3	15	1.17
(1,220)	1:35:A:LYS:HE2	1:39:A:LYS:HG2	18	1.17
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG11	16	1.16
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG12	16	1.16
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG13	16	1.16
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	4	1.16
(2,140)	1:25:A:PRO:HG2	1:52:A:VAL:HA	16	1.16
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	6	1.15
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	5	1.15
(1,650)	1:121:A:LEU:HA	1:125:A:LEU:HB3	2	1.15
(1,650)	1:121:A:LEU:HA	1:125:A:LEU:HB3	4	1.15
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	14	1.15
(1,452)	1:87:A:ALA:HA	1:91:A:GLU:HG2	5	1.15
(6,71)	1:60:A:CYS:HB2	1:63:A:TYR:H	4	1.14
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	8	1.14
(5,153)	1:21:A:ASN:HB3	1:68:A:ALA:H	15	1.14
(2,562)	1:147:A:GLU:HG2	1:150:A:LYS:HG3	3	1.14
(2,140)	1:25:A:PRO:HG2	1:52:A:VAL:HA	15	1.14
(2,12)	1:4:A:TYR:HB3	1:156:A:ILE:HA	7	1.14
(1,479)	1:91:A:GLU:HG2	1:94:A:LYS:HG3	12	1.14
(1,460)	1:89:A:TYR:HB3	1:128:A:LEU:HA	10	1.14
(1,650)	1:121:A:LEU:HA	1:125:A:LEU:HB3	5	1.13
(1,644)	1:120:A:ARG:HB3	1:124:A:SER:HB3	14	1.13
(1,452)	1:87:A:ALA:HA	1:91:A:GLU:HG2	6	1.13
(1,187)	1:29:A:PRO:HG2	1:35:A:LYS:HE3	21	1.13
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	8	1.12
(2,12)	1:4:A:TYR:HB3	1:156:A:ILE:HA	19	1.12
(1,650)	1:121:A:LEU:HA	1:125:A:LEU:HB3	17	1.12
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	4	1.11
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	3	1.11
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	4	1.11
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	5	1.11
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	6	1.11
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	7	1.11
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	8	1.11
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	9	1.11
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	10	1.11
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	13	1.11
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	14	1.11
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	15	1.11
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	16	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	19	1.11
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	20	1.11
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	21	1.11
(2,140)	1:25:A:PRO:HG2	1:52:A:VAL:HA	5	1.11
(1,650)	1:121:A:LEU:HA	1:125:A:LEU:HB3	12	1.11
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	13	1.11
(1,476)	1:91:A:GLU:HA	1:94:A:LYS:HB2	17	1.11
(1,451)	1:87:A:ALA:HA	1:90:A:ARG:HG2	11	1.11
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	13	1.1
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	1	1.1
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	2	1.1
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	11	1.1
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	12	1.1
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	17	1.1
(4,103)	1:148:A:TRP:HD1	1:148:A:TRP:HZ3	18	1.1
(2,45)	1:8:A:ARG:HB2	1:149:A:GLU:HA	2	1.1
(1,380)	1:66:A:ILE:HA	1:95:A:GLU:HG2	2	1.1
(1,187)	1:29:A:PRO:HG2	1:35:A:LYS:HE3	15	1.1
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	7	1.09
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	11	1.09
(2,562)	1:147:A:GLU:HG2	1:150:A:LYS:HG3	18	1.09
(4,41)	1:41:A:TRP:HH2	1:60:A:CYS:HB3	5	1.08
(2,206)	1:48:A:SER:HA	1:56:A:LYS:HE2	11	1.08
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	1	1.08
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	8	1.08
(1,480)	1:91:A:GLU:HG2	1:94:A:LYS:HD2	21	1.08
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	17	1.07
(4,41)	1:41:A:TRP:HH2	1:60:A:CYS:HB3	17	1.07
(1,380)	1:66:A:ILE:HA	1:95:A:GLU:HG2	11	1.07
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	15	1.07
(1,39)	1:7:A:LYS:HB2	1:9:A:MET:HB2	9	1.07
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG11	14	1.06
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG12	14	1.06
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG13	14	1.06
(5,548)	1:89:A:TYR:HB2	1:131:A:ALA:H	9	1.06
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	18	1.06
(2,452)	1:108:A:LEU:HG	1:143:A:CYS:HB2	17	1.06
(2,449)	1:108:A:LEU:HA	1:125:A:LEU:HD21	19	1.06
(2,449)	1:108:A:LEU:HA	1:125:A:LEU:HD22	19	1.06
(2,449)	1:108:A:LEU:HA	1:125:A:LEU:HD23	19	1.06
(2,22)	1:5:A:ARG:HD3	1:140:A:VAL:HG21	12	1.06
(2,22)	1:5:A:ARG:HD3	1:140:A:VAL:HG22	12	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,22)	1:5:A:ARG:HD3	1:140:A:VAL:HG23	12	1.06
(1,650)	1:121:A:LEU:HA	1:125:A:LEU:HB3	6	1.06
(1,380)	1:66:A:ILE:HA	1:95:A:GLU:HG2	6	1.06
(1,380)	1:66:A:ILE:HA	1:95:A:GLU:HG2	10	1.06
(2,449)	1:108:A:LEU:HA	1:125:A:LEU:HD21	18	1.05
(2,449)	1:108:A:LEU:HA	1:125:A:LEU:HD22	18	1.05
(2,449)	1:108:A:LEU:HA	1:125:A:LEU:HD23	18	1.05
(1,628)	1:118:A:LYS:HG3	1:119:A:ASP:HA	8	1.05
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	16	1.04
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	19	1.04
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG11	11	1.03
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG12	11	1.03
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG13	11	1.03
(5,188)	1:27:A:GLY:HA3	1:48:A:SER:H	6	1.03
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	3	1.03
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	9	1.03
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	10	1.03
(1,405)	1:76:A:TYR:HB2	1:81:A:GLY:HA3	9	1.03
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	10	1.02
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	1	1.02
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	5	1.02
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	7	1.02
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	11	1.02
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	15	1.02
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	17	1.02
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	19	1.02
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	21	1.02
(2,562)	1:147:A:GLU:HG2	1:150:A:LYS:HG3	2	1.02
(2,12)	1:4:A:TYR:HB3	1:156:A:ILE:HA	20	1.02
(1,630)	1:118:A:LYS:HD2	1:120:A:ARG:HD3	9	1.02
(1,452)	1:87:A:ALA:HA	1:91:A:GLU:HG2	13	1.02
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	14	1.01
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	9	1.01
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	2	1.01
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	3	1.01
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	4	1.01
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	6	1.01
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	8	1.01
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	12	1.01
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	13	1.01
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	14	1.01
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	16	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	18	1.01
(4,101)	1:148:A:TRP:HD1	1:148:A:TRP:HE3	20	1.01
(1,479)	1:91:A:GLU:HG2	1:94:A:LYS:HG3	4	1.01
(1,418)	1:80:A:GLU:HA	1:83:A:ARG:HG3	15	1.01
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	15	1.0
(5,153)	1:21:A:ASN:HB3	1:68:A:ALA:H	19	1.0
(1,650)	1:121:A:LEU:HA	1:125:A:LEU:HB3	21	1.0
(1,628)	1:118:A:LYS:HG3	1:119:A:ASP:HA	21	1.0
(1,451)	1:87:A:ALA:HA	1:90:A:ARG:HG2	2	1.0
(1,481)	1:91:A:GLU:HG2	1:94:A:LYS:HE3	21	0.99
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	3	0.99
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	10	0.98
(1,405)	1:76:A:TYR:HB2	1:81:A:GLY:HA3	16	0.98
(1,380)	1:66:A:ILE:HA	1:95:A:GLU:HG2	3	0.98
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	21	0.97
(3,64)	1:121:A:LEU:HD21	1:148:A:TRP:HZ3	18	0.97
(3,64)	1:121:A:LEU:HD22	1:148:A:TRP:HZ3	18	0.97
(3,64)	1:121:A:LEU:HD23	1:148:A:TRP:HZ3	18	0.97
(2,514)	1:125:A:LEU:HG	1:152:A:ILE:HG13	9	0.97
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	9	0.97
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	17	0.96
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	18	0.96
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	17	0.96
(4,41)	1:41:A:TRP:HH2	1:60:A:CYS:HB3	13	0.96
(1,34)	1:7:A:LYS:HA	1:149:A:GLU:HG2	13	0.96
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG11	18	0.95
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG12	18	0.95
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG13	18	0.95
(4,41)	1:41:A:TRP:HH2	1:60:A:CYS:HB3	15	0.95
(1,628)	1:118:A:LYS:HG3	1:119:A:ASP:HA	17	0.95
(1,221)	1:35:A:LYS:HE3	1:39:A:LYS:HE2	1	0.95
(1,34)	1:7:A:LYS:HA	1:149:A:GLU:HG2	21	0.95
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG11	13	0.94
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG12	13	0.94
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG13	13	0.94
(2,514)	1:125:A:LEU:HG	1:152:A:ILE:HG13	8	0.94
(2,12)	1:4:A:TYR:HB3	1:156:A:ILE:HA	12	0.94
(1,650)	1:121:A:LEU:HA	1:125:A:LEU:HB3	13	0.94
(1,650)	1:121:A:LEU:HA	1:125:A:LEU:HB3	16	0.94
(1,420)	1:81:A:GLY:HA3	1:84:A:GLU:HB2	4	0.94
(1,420)	1:81:A:GLY:HA3	1:84:A:GLU:HB3	4	0.94
(1,418)	1:80:A:GLU:HA	1:83:A:ARG:HG3	19	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,405)	1:76:A:TYR:HB2	1:81:A:GLY:HA3	11	0.94
(1,60)	1:8:A:ARG:HB2	1:146:A:LYS:HA	11	0.94
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	10	0.93
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	3	0.93
(2,452)	1:108:A:LEU:HG	1:143:A:CYS:HB2	14	0.93
(2,45)	1:8:A:ARG:HB2	1:149:A:GLU:HA	13	0.93
(1,33)	1:7:A:LYS:HA	1:8:A:ARG:HB2	17	0.93
(5,548)	1:89:A:TYR:HB2	1:131:A:ALA:H	18	0.92
(1,405)	1:76:A:TYR:HB2	1:81:A:GLY:HA3	2	0.92
(1,218)	1:35:A:LYS:HD2	1:38:A:TYR:HB2	20	0.92
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	19	0.91
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	12	0.91
(3,63)	1:121:A:LEU:HD21	1:148:A:TRP:HD1	16	0.91
(3,63)	1:121:A:LEU:HD22	1:148:A:TRP:HD1	16	0.91
(3,63)	1:121:A:LEU:HD23	1:148:A:TRP:HD1	16	0.91
(2,562)	1:147:A:GLU:HG2	1:150:A:LYS:HG3	12	0.91
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	16	0.91
(1,451)	1:87:A:ALA:HA	1:90:A:ARG:HG2	4	0.91
(1,359)	1:59:A:MET:HG3	1:64:A:PRO:HA	17	0.91
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	6	0.91
(1,60)	1:8:A:ARG:HB2	1:146:A:LYS:HA	21	0.91
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG11	1	0.9
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG12	1	0.9
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG13	1	0.9
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	5	0.9
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	7	0.9
(4,41)	1:41:A:TRP:HH2	1:60:A:CYS:HB3	12	0.9
(2,45)	1:8:A:ARG:HB2	1:149:A:GLU:HA	5	0.9
(2,12)	1:4:A:TYR:HB3	1:156:A:ILE:HA	10	0.9
(1,760)	1:147:A:GLU:HG2	1:150:A:LYS:HD2	12	0.9
(1,760)	1:147:A:GLU:HG3	1:150:A:LYS:HD2	12	0.9
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	20	0.9
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG11	20	0.89
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG12	20	0.89
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG13	20	0.89
(5,500)	1:83:A:ARG:HG2	1:84:A:GLU:H	3	0.89
(5,500)	1:83:A:ARG:HG2	1:84:A:GLU:H	7	0.89
(5,500)	1:83:A:ARG:HG2	1:84:A:GLU:H	16	0.89
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	21	0.89
(1,479)	1:91:A:GLU:HG2	1:94:A:LYS:HG3	8	0.89
(1,380)	1:66:A:ILE:HA	1:95:A:GLU:HG2	21	0.89
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	5	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	15	0.88
(2,140)	1:25:A:PRO:HG2	1:52:A:VAL:HA	12	0.88
(2,45)	1:8:A:ARG:HB2	1:149:A:GLU:HA	6	0.88
(2,12)	1:4:A:TYR:HB3	1:156:A:ILE:HA	1	0.88
(1,644)	1:120:A:ARG:HB3	1:124:A:SER:HB3	3	0.88
(1,630)	1:118:A:LYS:HD2	1:120:A:ARG:HD3	11	0.88
(1,451)	1:87:A:ALA:HA	1:90:A:ARG:HG2	20	0.88
(1,380)	1:66:A:ILE:HA	1:95:A:GLU:HG2	19	0.88
(1,60)	1:8:A:ARG:HB2	1:146:A:LYS:HA	4	0.88
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG11	8	0.87
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG12	8	0.87
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG13	8	0.87
(5,153)	1:21:A:ASN:HB3	1:68:A:ALA:H	5	0.87
(5,52)	1:8:A:ARG:HD3	1:149:A:GLU:H	11	0.87
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	12	0.87
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	13	0.87
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	3	0.87
(2,206)	1:48:A:SER:HA	1:56:A:LYS:HE2	10	0.87
(1,498)	1:94:A:LYS:HB2	1:95:A:GLU:HA	6	0.87
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG11	3	0.86
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG12	3	0.86
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG13	3	0.86
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	10	0.86
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	11	0.86
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	9	0.86
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	11	0.86
(4,93)	1:143:A:CYS:HB2	1:148:A:TRP:HZ3	15	0.86
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	20	0.86
(2,562)	1:147:A:GLU:HG2	1:150:A:LYS:HG3	11	0.86
(2,452)	1:108:A:LEU:HG	1:143:A:CYS:HB2	15	0.86
(1,650)	1:121:A:LEU:HA	1:125:A:LEU:HB3	7	0.86
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	5	0.86
(1,498)	1:94:A:LYS:HB2	1:95:A:GLU:HA	11	0.86
(1,405)	1:76:A:TYR:HB2	1:81:A:GLY:HA3	18	0.86
(1,380)	1:66:A:ILE:HA	1:95:A:GLU:HG2	9	0.86
(1,301)	1:48:A:SER:HA	1:56:A:LYS:HD3	11	0.86
(1,221)	1:35:A:LYS:HE3	1:39:A:LYS:HE2	9	0.86
(1,220)	1:35:A:LYS:HE2	1:39:A:LYS:HG2	21	0.86
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	1	0.85
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	2	0.85
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	6	0.85
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	7	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	8	0.85
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	9	0.85
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	10	0.85
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	11	0.85
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	13	0.85
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	14	0.85
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	15	0.85
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	16	0.85
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	17	0.85
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	18	0.85
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	19	0.85
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	20	0.85
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	21	0.85
(1,650)	1:121:A:LEU:HA	1:125:A:LEU:HB3	15	0.85
(1,575)	1:107:A:PRO:HA	1:108:A:LEU:HB3	2	0.85
(1,498)	1:94:A:LYS:HB2	1:95:A:GLU:HA	9	0.85
(1,479)	1:91:A:GLU:HG2	1:94:A:LYS:HG3	18	0.85
(1,187)	1:29:A:PRO:HG2	1:35:A:LYS:HE3	7	0.85
(5,153)	1:21:A:ASN:HB3	1:68:A:ALA:H	13	0.84
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	3	0.84
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	4	0.84
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	5	0.84
(4,106)	1:148:A:TRP:HE3	1:148:A:TRP:HE1	12	0.84
(4,41)	1:41:A:TRP:HH2	1:60:A:CYS:HB3	8	0.84
(4,41)	1:41:A:TRP:HH2	1:60:A:CYS:HB3	18	0.84
(1,575)	1:107:A:PRO:HA	1:108:A:LEU:HB3	15	0.84
(1,481)	1:91:A:GLU:HG2	1:94:A:LYS:HE3	18	0.84
(1,418)	1:80:A:GLU:HA	1:83:A:ARG:HG3	11	0.84
(1,187)	1:29:A:PRO:HG2	1:35:A:LYS:HE3	19	0.84
(1,60)	1:8:A:ARG:HB2	1:146:A:LYS:HA	6	0.84
(6,93)	1:89:A:TYR:H	1:127:A:HIS:HB3	21	0.83
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	11	0.83
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	18	0.83
(2,173)	1:35:A:LYS:HG2	1:38:A:TYR:HB2	17	0.83
(1,601)	1:111:A:THR:HA	1:120:A:ARG:HD2	7	0.83
(1,575)	1:107:A:PRO:HA	1:108:A:LEU:HB3	20	0.83
(1,498)	1:94:A:LYS:HB2	1:95:A:GLU:HA	5	0.83
(1,498)	1:94:A:LYS:HB2	1:95:A:GLU:HA	7	0.83
(1,498)	1:94:A:LYS:HB2	1:95:A:GLU:HA	20	0.83
(1,380)	1:66:A:ILE:HA	1:95:A:GLU:HG2	16	0.83
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG11	2	0.82
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG12	2	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG13	2	0.82
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	2	0.82
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	20	0.82
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	14	0.82
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	7	0.82
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	15	0.82
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	14	0.82
(3,29)	1:41:A:TRP:HD1	1:60:A:CYS:HB3	12	0.82
(2,329)	1:85:A:LEU:HG	1:109:A:LEU:HD21	17	0.82
(2,329)	1:85:A:LEU:HG	1:109:A:LEU:HD22	17	0.82
(2,329)	1:85:A:LEU:HG	1:109:A:LEU:HD23	17	0.82
(2,140)	1:25:A:PRO:HG2	1:52:A:VAL:HA	4	0.82
(1,498)	1:94:A:LYS:HB2	1:95:A:GLU:HA	1	0.82
(1,498)	1:94:A:LYS:HB2	1:95:A:GLU:HA	12	0.82
(1,451)	1:87:A:ALA:HA	1:90:A:ARG:HG2	19	0.82
(1,418)	1:80:A:GLU:HA	1:83:A:ARG:HG3	5	0.82
(1,218)	1:35:A:LYS:HD2	1:38:A:TYR:HB2	3	0.82
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	4	0.82
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG11	17	0.82
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG12	17	0.82
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG13	17	0.82
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	9	0.81
(5,52)	1:8:A:ARG:HD3	1:149:A:GLU:H	19	0.81
(4,93)	1:143:A:CYS:HB2	1:148:A:TRP:HZ3	14	0.81
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	3	0.81
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	4	0.81
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	5	0.81
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	7	0.81
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	8	0.81
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	9	0.81
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	10	0.81
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	11	0.81
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	12	0.81
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	16	0.81
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	19	0.81
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	20	0.81
(2,452)	1:108:A:LEU:HG	1:143:A:CYS:HB2	20	0.81
(2,330)	1:85:A:LEU:HD11	1:109:A:LEU:HB3	3	0.81
(2,330)	1:85:A:LEU:HD12	1:109:A:LEU:HB3	3	0.81
(2,330)	1:85:A:LEU:HD13	1:109:A:LEU:HB3	3	0.81
(1,575)	1:107:A:PRO:HA	1:108:A:LEU:HB3	4	0.81
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	21	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	2	0.8
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	6	0.8
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	13	0.8
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	14	0.8
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	18	0.8
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	21	0.8
(3,63)	1:121:A:LEU:HD21	1:148:A:TRP:HD1	21	0.8
(3,63)	1:121:A:LEU:HD22	1:148:A:TRP:HD1	21	0.8
(3,63)	1:121:A:LEU:HD23	1:148:A:TRP:HD1	21	0.8
(1,575)	1:107:A:PRO:HA	1:108:A:LEU:HB3	6	0.8
(1,498)	1:94:A:LYS:HB2	1:95:A:GLU:HA	16	0.8
(1,451)	1:87:A:ALA:HA	1:90:A:ARG:HG2	5	0.8
(1,451)	1:87:A:ALA:HA	1:90:A:ARG:HG2	9	0.8
(1,60)	1:8:A:ARG:HB2	1:146:A:LYS:HA	20	0.8
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG11	12	0.79
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG12	12	0.79
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG13	12	0.79
(5,394)	1:61:A:GLY:HA3	1:63:A:TYR:H	18	0.79
(5,153)	1:21:A:ASN:HB3	1:68:A:ALA:H	16	0.79
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	2	0.79
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	16	0.79
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	17	0.79
(2,561)	1:147:A:GLU:HB2	1:151:A:LYS:HD2	10	0.79
(2,173)	1:35:A:LYS:HG2	1:38:A:TYR:HB2	2	0.79
(1,498)	1:94:A:LYS:HB2	1:95:A:GLU:HA	2	0.79
(1,405)	1:76:A:TYR:HB2	1:81:A:GLY:HA3	13	0.79
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG11	12	0.79
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG12	12	0.79
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG13	12	0.79
(6,7)	1:9:A:MET:HB2	1:13:A:LYS:H	2	0.78
(6,4)	1:6:A:VAL:HG11	1:143:A:CYS:H	11	0.78
(6,4)	1:6:A:VAL:HG12	1:143:A:CYS:H	11	0.78
(6,4)	1:6:A:VAL:HG13	1:143:A:CYS:H	11	0.78
(5,500)	1:83:A:ARG:HG2	1:84:A:GLU:H	9	0.78
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	1	0.78
(4,30)	1:41:A:TRP:HD1	1:41:A:TRP:HH2	1	0.78
(3,64)	1:121:A:LEU:HD21	1:148:A:TRP:HZ3	6	0.78
(3,64)	1:121:A:LEU:HD22	1:148:A:TRP:HZ3	6	0.78
(3,64)	1:121:A:LEU:HD23	1:148:A:TRP:HZ3	6	0.78
(3,64)	1:121:A:LEU:HD21	1:148:A:TRP:HZ3	13	0.78
(3,64)	1:121:A:LEU:HD22	1:148:A:TRP:HZ3	13	0.78
(3,64)	1:121:A:LEU:HD23	1:148:A:TRP:HZ3	13	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,29)	1:41:A:TRP:HD1	1:60:A:CYS:HB3	8	0.78
(2,561)	1:147:A:GLU:HB2	1:151:A:LYS:HD2	9	0.78
(2,329)	1:85:A:LEU:HG	1:109:A:LEU:HD21	20	0.78
(2,329)	1:85:A:LEU:HG	1:109:A:LEU:HD22	20	0.78
(2,329)	1:85:A:LEU:HG	1:109:A:LEU:HD23	20	0.78
(2,140)	1:25:A:PRO:HG2	1:52:A:VAL:HA	3	0.78
(2,45)	1:8:A:ARG:HB2	1:149:A:GLU:HA	4	0.78
(2,45)	1:8:A:ARG:HB2	1:149:A:GLU:HA	11	0.78
(1,601)	1:111:A:THR:HA	1:120:A:ARG:HD2	19	0.78
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	2	0.78
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	15	0.78
(1,508)	1:94:A:LYS:HE2	1:98:A:ARG:HD3	14	0.78
(1,508)	1:94:A:LYS:HE3	1:98:A:ARG:HD3	14	0.78
(1,460)	1:89:A:TYR:HB3	1:128:A:LEU:HA	15	0.78
(1,451)	1:87:A:ALA:HA	1:90:A:ARG:HG2	10	0.78
(1,451)	1:87:A:ALA:HA	1:90:A:ARG:HG2	12	0.78
(1,150)	1:25:A:PRO:HB3	1:50:A:THR:HA	21	0.78
(1,60)	1:8:A:ARG:HB2	1:146:A:LYS:HA	5	0.78
(1,34)	1:7:A:LYS:HA	1:149:A:GLU:HG2	12	0.78
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG11	17	0.77
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG12	17	0.77
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG13	17	0.77
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	17	0.77
(5,394)	1:61:A:GLY:HA3	1:63:A:TYR:H	10	0.77
(5,394)	1:61:A:GLY:HA3	1:63:A:TYR:H	12	0.77
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	3	0.77
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	15	0.77
(2,452)	1:108:A:LEU:HG	1:143:A:CYS:HB2	3	0.77
(2,140)	1:25:A:PRO:HG2	1:52:A:VAL:HA	19	0.77
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	19	0.77
(1,498)	1:94:A:LYS:HB2	1:95:A:GLU:HA	4	0.77
(1,498)	1:94:A:LYS:HB2	1:95:A:GLU:HA	19	0.77
(1,452)	1:87:A:ALA:HA	1:91:A:GLU:HG2	19	0.77
(1,451)	1:87:A:ALA:HA	1:90:A:ARG:HG2	8	0.77
(1,405)	1:76:A:TYR:HB2	1:81:A:GLY:HA3	1	0.77
(1,405)	1:76:A:TYR:HB2	1:81:A:GLY:HA3	19	0.77
(1,311)	1:50:A:THR:HB	1:56:A:LYS:HD3	7	0.77
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	20	0.77
(1,60)	1:8:A:ARG:HB2	1:146:A:LYS:HA	19	0.77
(6,7)	1:9:A:MET:HB2	1:13:A:LYS:H	4	0.76
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	16	0.76
(4,93)	1:143:A:CYS:HB2	1:148:A:TRP:HZ3	3	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,49)	1:58:A:VAL:HG21	1:67:A:HIS:HE1	14	0.76
(4,49)	1:58:A:VAL:HG22	1:67:A:HIS:HE1	14	0.76
(4,49)	1:58:A:VAL:HG23	1:67:A:HIS:HE1	14	0.76
(2,452)	1:108:A:LEU:HG	1:143:A:CYS:HB2	7	0.76
(2,206)	1:48:A:SER:HA	1:56:A:LYS:HE2	13	0.76
(1,498)	1:94:A:LYS:HB2	1:95:A:GLU:HA	10	0.76
(1,498)	1:94:A:LYS:HB2	1:95:A:GLU:HA	13	0.76
(1,498)	1:94:A:LYS:HB2	1:95:A:GLU:HA	18	0.76
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	8	0.75
(5,394)	1:61:A:GLY:HA3	1:63:A:TYR:H	16	0.75
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	13	0.75
(5,52)	1:8:A:ARG:HD3	1:149:A:GLU:H	16	0.75
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	7	0.75
(2,329)	1:85:A:LEU:HG	1:109:A:LEU:HD21	13	0.75
(2,329)	1:85:A:LEU:HG	1:109:A:LEU:HD22	13	0.75
(2,329)	1:85:A:LEU:HG	1:109:A:LEU:HD23	13	0.75
(2,206)	1:48:A:SER:HA	1:56:A:LYS:HE2	19	0.75
(2,173)	1:35:A:LYS:HG2	1:38:A:TYR:HB2	4	0.75
(2,140)	1:25:A:PRO:HG2	1:52:A:VAL:HA	1	0.75
(2,140)	1:25:A:PRO:HG2	1:52:A:VAL:HA	18	0.75
(2,45)	1:8:A:ARG:HB2	1:149:A:GLU:HA	7	0.75
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	17	0.75
(1,508)	1:94:A:LYS:HE2	1:98:A:ARG:HD3	10	0.75
(1,508)	1:94:A:LYS:HE3	1:98:A:ARG:HD3	10	0.75
(1,498)	1:94:A:LYS:HB2	1:95:A:GLU:HA	3	0.75
(1,498)	1:94:A:LYS:HB2	1:95:A:GLU:HA	15	0.75
(1,451)	1:87:A:ALA:HA	1:90:A:ARG:HG2	16	0.75
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	14	0.74
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	21	0.74
(5,394)	1:61:A:GLY:HA3	1:63:A:TYR:H	4	0.74
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	2	0.74
(2,562)	1:147:A:GLU:HG2	1:150:A:LYS:HG3	6	0.74
(2,206)	1:48:A:SER:HA	1:56:A:LYS:HE2	14	0.74
(1,644)	1:120:A:ARG:HB3	1:124:A:SER:HB3	6	0.74
(1,644)	1:120:A:ARG:HB3	1:124:A:SER:HB3	17	0.74
(1,630)	1:118:A:LYS:HD2	1:120:A:ARG:HD3	12	0.74
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	3	0.74
(1,451)	1:87:A:ALA:HA	1:90:A:ARG:HG2	3	0.74
(1,451)	1:87:A:ALA:HA	1:90:A:ARG:HG2	7	0.74
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG11	15	0.73
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG12	15	0.73
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG13	15	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	1	0.73
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	11	0.73
(3,29)	1:41:A:TRP:HD1	1:60:A:CYS:HB3	18	0.73
(1,575)	1:107:A:PRO:HA	1:108:A:LEU:HB3	18	0.73
(1,498)	1:94:A:LYS:HB2	1:95:A:GLU:HA	8	0.73
(1,405)	1:76:A:TYR:HB2	1:81:A:GLY:HA3	6	0.73
(1,34)	1:7:A:LYS:HA	1:149:A:GLU:HG2	19	0.73
(1,32)	1:7:A:LYS:HA	1:7:A:LYS:HE3	15	0.73
(1,28)	1:6:A:VAL:HG21	1:153:A:SER:HA	7	0.73
(1,28)	1:6:A:VAL:HG22	1:153:A:SER:HA	7	0.73
(1,28)	1:6:A:VAL:HG23	1:153:A:SER:HA	7	0.73
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	7	0.72
(5,500)	1:83:A:ARG:HG2	1:84:A:GLU:H	6	0.72
(5,50)	1:8:A:ARG:HG2	1:149:A:GLU:H	12	0.72
(2,490)	1:121:A:LEU:HD21	1:125:A:LEU:HB3	15	0.72
(2,490)	1:121:A:LEU:HD22	1:125:A:LEU:HB3	15	0.72
(2,490)	1:121:A:LEU:HD23	1:125:A:LEU:HB3	15	0.72
(1,460)	1:89:A:TYR:HB3	1:128:A:LEU:HA	19	0.72
(1,405)	1:76:A:TYR:HB2	1:81:A:GLY:HA3	7	0.72
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	1	0.72
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG11	19	0.71
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG12	19	0.71
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG13	19	0.71
(5,500)	1:83:A:ARG:HG2	1:84:A:GLU:H	13	0.71
(5,394)	1:61:A:GLY:HA3	1:63:A:TYR:H	7	0.71
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	1	0.71
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	14	0.71
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	18	0.71
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	3	0.71
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	4	0.71
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	5	0.71
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	7	0.71
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	8	0.71
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	9	0.71
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	10	0.71
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	11	0.71
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	12	0.71
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	13	0.71
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	14	0.71
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	16	0.71
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	17	0.71
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	18	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	19	0.71
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	20	0.71
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	21	0.71
(2,393)	1:96:A:VAL:HG21	1:137:A:ALA:HA	18	0.71
(2,393)	1:96:A:VAL:HG22	1:137:A:ALA:HA	18	0.71
(2,393)	1:96:A:VAL:HG23	1:137:A:ALA:HA	18	0.71
(2,173)	1:35:A:LYS:HG2	1:38:A:TYR:HB2	6	0.71
(1,451)	1:87:A:ALA:HA	1:90:A:ARG:HG2	18	0.71
(1,418)	1:80:A:GLU:HA	1:83:A:ARG:HG3	16	0.71
(1,311)	1:50:A:THR:HB	1:56:A:LYS:HD3	2	0.71
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG11	14	0.71
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG12	14	0.71
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG13	14	0.71
(5,190)	1:27:A:GLY:HA2	1:49:A:ALA:H	6	0.7
(4,41)	1:41:A:TRP:HH2	1:60:A:CYS:HB3	16	0.7
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	1	0.7
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	2	0.7
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	6	0.7
(1,60)	1:8:A:ARG:HB2	1:146:A:LYS:HA	3	0.7
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG11	4	0.69
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG12	4	0.69
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG13	4	0.69
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	18	0.69
(4,93)	1:143:A:CYS:HB2	1:148:A:TRP:HZ3	4	0.69
(4,41)	1:41:A:TRP:HH2	1:60:A:CYS:HB3	2	0.69
(4,28)	1:41:A:TRP:HD1	1:41:A:TRP:HZ3	15	0.69
(2,514)	1:125:A:LEU:HG	1:152:A:ILE:HG13	19	0.69
(2,452)	1:108:A:LEU:HG	1:143:A:CYS:HB2	21	0.69
(2,45)	1:8:A:ARG:HB2	1:149:A:GLU:HA	15	0.69
(2,45)	1:8:A:ARG:HB2	1:149:A:GLU:HA	18	0.69
(1,480)	1:91:A:GLU:HG2	1:94:A:LYS:HD2	14	0.69
(1,380)	1:66:A:ILE:HA	1:95:A:GLU:HG2	4	0.69
(1,380)	1:66:A:ILE:HA	1:95:A:GLU:HG2	13	0.69
(5,548)	1:89:A:TYR:HB2	1:131:A:ALA:H	6	0.68
(5,500)	1:83:A:ARG:HG2	1:84:A:GLU:H	20	0.68
(1,451)	1:87:A:ALA:HA	1:90:A:ARG:HG2	1	0.68
(1,311)	1:50:A:THR:HB	1:56:A:LYS:HD3	3	0.68
(1,221)	1:35:A:LYS:HE3	1:39:A:LYS:HE2	18	0.68
(1,118)	1:18:A:CYS:HB3	1:101:A:VAL:HB	6	0.68
(6,16)	1:19:A:VAL:HG11	1:106:A:ILE:H	17	0.67
(6,16)	1:19:A:VAL:HG12	1:106:A:ILE:H	17	0.67
(6,16)	1:19:A:VAL:HG13	1:106:A:ILE:H	17	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	3	0.67
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	9	0.67
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	12	0.67
(2,45)	1:8:A:ARG:HB2	1:149:A:GLU:HA	19	0.67
(1,508)	1:94:A:LYS:HE2	1:98:A:ARG:HD3	4	0.67
(1,508)	1:94:A:LYS:HE3	1:98:A:ARG:HD3	4	0.67
(1,311)	1:50:A:THR:HB	1:56:A:LYS:HD3	14	0.67
(1,60)	1:8:A:ARG:HB2	1:146:A:LYS:HA	18	0.67
(5,394)	1:61:A:GLY:HA3	1:63:A:TYR:H	11	0.66
(5,50)	1:8:A:ARG:HG2	1:149:A:GLU:H	13	0.66
(2,449)	1:108:A:LEU:HA	1:125:A:LEU:HD21	9	0.66
(2,449)	1:108:A:LEU:HA	1:125:A:LEU:HD22	9	0.66
(2,449)	1:108:A:LEU:HA	1:125:A:LEU:HD23	9	0.66
(2,393)	1:96:A:VAL:HG21	1:137:A:ALA:HA	5	0.66
(2,393)	1:96:A:VAL:HG22	1:137:A:ALA:HA	5	0.66
(2,393)	1:96:A:VAL:HG23	1:137:A:ALA:HA	5	0.66
(2,45)	1:8:A:ARG:HB2	1:149:A:GLU:HA	8	0.66
(1,632)	1:118:A:LYS:HD3	1:120:A:ARG:HD3	2	0.66
(1,575)	1:107:A:PRO:HA	1:108:A:LEU:HB3	5	0.66
(1,479)	1:91:A:GLU:HG2	1:94:A:LYS:HG3	10	0.66
(1,414)	1:79:A:SER:HB2	1:80:A:GLU:HA	17	0.66
(1,39)	1:7:A:LYS:HB2	1:9:A:MET:HB2	12	0.66
(5,586)	1:94:A:LYS:H	1:94:A:LYS:HG3	4	0.65
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	5	0.65
(3,29)	1:41:A:TRP:HD1	1:60:A:CYS:HB3	11	0.65
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	6	0.65
(1,451)	1:87:A:ALA:HA	1:90:A:ARG:HG2	14	0.65
(1,405)	1:76:A:TYR:HB2	1:81:A:GLY:HA3	15	0.65
(1,213)	1:35:A:LYS:HG2	1:39:A:LYS:HG2	3	0.65
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	19	0.65
(5,586)	1:94:A:LYS:H	1:94:A:LYS:HG3	5	0.64
(2,452)	1:108:A:LEU:HG	1:143:A:CYS:HB2	13	0.64
(2,45)	1:8:A:ARG:HB2	1:149:A:GLU:HA	14	0.64
(2,10)	1:4:A:TYR:HB3	1:139:A:VAL:HB	21	0.64
(1,630)	1:118:A:LYS:HD2	1:120:A:ARG:HD3	5	0.64
(1,601)	1:111:A:THR:HA	1:120:A:ARG:HD2	2	0.64
(1,414)	1:79:A:SER:HB2	1:80:A:GLU:HA	20	0.64
(1,166)	1:27:A:GLY:HA2	1:45:A:PHE:HA	2	0.64
(1,60)	1:8:A:ARG:HB2	1:146:A:LYS:HA	13	0.64
(5,586)	1:94:A:LYS:H	1:94:A:LYS:HG3	2	0.63
(5,586)	1:94:A:LYS:H	1:94:A:LYS:HG3	8	0.63
(5,586)	1:94:A:LYS:H	1:94:A:LYS:HG3	9	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,586)	1:94:A:LYS:H	1:94:A:LYS:HG3	13	0.63
(5,500)	1:83:A:ARG:HG2	1:84:A:GLU:H	17	0.63
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	1	0.63
(2,452)	1:108:A:LEU:HG	1:143:A:CYS:HB2	16	0.63
(2,173)	1:35:A:LYS:HG2	1:38:A:TYR:HB2	1	0.63
(2,141)	1:25:A:PRO:HG2	1:52:A:VAL:HG11	12	0.63
(2,141)	1:25:A:PRO:HG2	1:52:A:VAL:HG12	12	0.63
(2,141)	1:25:A:PRO:HG2	1:52:A:VAL:HG13	12	0.63
(2,51)	1:10:A:ASP:HB2	1:13:A:LYS:HG2	4	0.63
(2,45)	1:8:A:ARG:HB2	1:149:A:GLU:HA	21	0.63
(1,575)	1:107:A:PRO:HA	1:108:A:LEU:HB3	12	0.63
(1,508)	1:94:A:LYS:HE2	1:98:A:ARG:HD3	11	0.63
(1,508)	1:94:A:LYS:HE3	1:98:A:ARG:HD3	11	0.63
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG11	2	0.63
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG12	2	0.63
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG13	2	0.63
(7,31)	1:74:A:SER:H	1:72:A:ASN:O	12	0.62
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	4	0.62
(5,586)	1:94:A:LYS:H	1:94:A:LYS:HG3	19	0.62
(5,548)	1:89:A:TYR:HB2	1:131:A:ALA:H	8	0.62
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	6	0.62
(2,393)	1:96:A:VAL:HG21	1:137:A:ALA:HA	13	0.62
(2,393)	1:96:A:VAL:HG22	1:137:A:ALA:HA	13	0.62
(2,393)	1:96:A:VAL:HG23	1:137:A:ALA:HA	13	0.62
(2,12)	1:4:A:TYR:HB3	1:156:A:ILE:HA	16	0.62
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	11	0.62
(1,60)	1:8:A:ARG:HB2	1:146:A:LYS:HA	14	0.62
(1,60)	1:8:A:ARG:HB2	1:146:A:LYS:HA	16	0.62
(5,586)	1:94:A:LYS:H	1:94:A:LYS:HG3	15	0.61
(5,586)	1:94:A:LYS:H	1:94:A:LYS:HG3	16	0.61
(4,93)	1:143:A:CYS:HB2	1:148:A:TRP:HZ3	7	0.61
(2,577)	1:153:A:SER:HA	1:157:A:GLN:HG3	15	0.61
(2,173)	1:35:A:LYS:HG2	1:38:A:TYR:HB2	13	0.61
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	7	0.61
(1,575)	1:107:A:PRO:HA	1:108:A:LEU:HB3	13	0.61
(1,405)	1:76:A:TYR:HB2	1:81:A:GLY:HA3	17	0.61
(5,586)	1:94:A:LYS:H	1:94:A:LYS:HG3	7	0.6
(5,586)	1:94:A:LYS:H	1:94:A:LYS:HG3	11	0.6
(5,586)	1:94:A:LYS:H	1:94:A:LYS:HG3	18	0.6
(5,394)	1:61:A:GLY:HA3	1:63:A:TYR:H	13	0.6
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	20	0.6
(4,49)	1:58:A:VAL:HG21	1:67:A:HIS:HE1	11	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,49)	1:58:A:VAL:HG22	1:67:A:HIS:HE1	11	0.6
(4,49)	1:58:A:VAL:HG23	1:67:A:HIS:HE1	11	0.6
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	1	0.6
(2,357)	1:91:A:GLU:HG3	1:94:A:LYS:HG3	7	0.6
(2,173)	1:35:A:LYS:HG2	1:38:A:TYR:HB2	7	0.6
(2,45)	1:8:A:ARG:HB2	1:149:A:GLU:HA	10	0.6
(2,45)	1:8:A:ARG:HB2	1:149:A:GLU:HA	16	0.6
(1,644)	1:120:A:ARG:HB3	1:124:A:SER:HB3	16	0.6
(1,601)	1:111:A:THR:HA	1:120:A:ARG:HD2	15	0.6
(1,504)	1:94:A:LYS:HG2	1:95:A:GLU:HA	14	0.6
(1,414)	1:79:A:SER:HB2	1:80:A:GLU:HA	13	0.6
(1,359)	1:59:A:MET:HG3	1:64:A:PRO:HA	14	0.6
(1,221)	1:35:A:LYS:HE3	1:39:A:LYS:HE2	19	0.6
(1,60)	1:8:A:ARG:HB2	1:146:A:LYS:HA	8	0.6
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG11	18	0.6
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG12	18	0.6
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG13	18	0.6
(1,34)	1:7:A:LYS:HA	1:149:A:GLU:HG2	10	0.6
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	10	0.59
(5,586)	1:94:A:LYS:H	1:94:A:LYS:HG3	1	0.59
(5,586)	1:94:A:LYS:H	1:94:A:LYS:HG3	3	0.59
(5,586)	1:94:A:LYS:H	1:94:A:LYS:HG3	12	0.59
(5,394)	1:61:A:GLY:HA3	1:63:A:TYR:H	14	0.59
(5,394)	1:61:A:GLY:HA3	1:63:A:TYR:H	19	0.59
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	16	0.59
(3,29)	1:41:A:TRP:HD1	1:60:A:CYS:HB3	7	0.59
(2,529)	1:128:A:LEU:HD11	1:132:A:MET:HG3	10	0.59
(2,529)	1:128:A:LEU:HD12	1:132:A:MET:HG3	10	0.59
(2,529)	1:128:A:LEU:HD13	1:132:A:MET:HG3	10	0.59
(2,329)	1:85:A:LEU:HG	1:109:A:LEU:HD21	6	0.59
(2,329)	1:85:A:LEU:HG	1:109:A:LEU:HD22	6	0.59
(2,329)	1:85:A:LEU:HG	1:109:A:LEU:HD23	6	0.59
(2,173)	1:35:A:LYS:HG2	1:38:A:TYR:HB2	5	0.59
(2,83)	1:17:A:GLU:HG2	1:101:A:VAL:HA	15	0.59
(2,10)	1:4:A:TYR:HB3	1:139:A:VAL:HB	3	0.59
(1,828)	1:156:A:ILE:HA	1:159:A:ARG:HB2	17	0.59
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	12	0.59
(1,380)	1:66:A:ILE:HA	1:95:A:GLU:HG2	14	0.59
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	18	0.59
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	3	0.58
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	21	0.58
(5,394)	1:61:A:GLY:HA3	1:63:A:TYR:H	8	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,188)	1:27:A:GLY:HA3	1:48:A:SER:H	15	0.58
(2,514)	1:125:A:LEU:HG	1:152:A:ILE:HG13	7	0.58
(1,522)	1:97:A:THR:HA	1:100:A:GLY:HA3	12	0.58
(1,508)	1:94:A:LYS:HE2	1:98:A:ARG:HD3	3	0.58
(1,508)	1:94:A:LYS:HE3	1:98:A:ARG:HD3	3	0.58
(1,504)	1:94:A:LYS:HG2	1:95:A:GLU:HA	21	0.58
(1,414)	1:79:A:SER:HB2	1:80:A:GLU:HA	7	0.58
(1,405)	1:76:A:TYR:HB2	1:81:A:GLY:HA3	20	0.58
(1,155)	1:25:A:PRO:HG3	1:51:A:PRO:HA	12	0.58
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG11	3	0.58
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG12	3	0.58
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG13	3	0.58
(6,7)	1:9:A:MET:HB2	1:13:A:LYS:H	7	0.57
(6,7)	1:9:A:MET:HB2	1:13:A:LYS:H	15	0.57
(6,4)	1:6:A:VAL:HG11	1:143:A:CYS:H	3	0.57
(6,4)	1:6:A:VAL:HG12	1:143:A:CYS:H	3	0.57
(6,4)	1:6:A:VAL:HG13	1:143:A:CYS:H	3	0.57
(5,586)	1:94:A:LYS:H	1:94:A:LYS:HG3	6	0.57
(5,586)	1:94:A:LYS:H	1:94:A:LYS:HG3	20	0.57
(5,52)	1:8:A:ARG:HD3	1:149:A:GLU:H	14	0.57
(2,140)	1:25:A:PRO:HG2	1:52:A:VAL:HA	8	0.57
(1,760)	1:147:A:GLU:HG2	1:150:A:LYS:HD2	3	0.57
(1,760)	1:147:A:GLU:HG3	1:150:A:LYS:HD2	3	0.57
(1,508)	1:94:A:LYS:HE2	1:98:A:ARG:HD3	19	0.57
(1,508)	1:94:A:LYS:HE3	1:98:A:ARG:HD3	19	0.57
(1,452)	1:87:A:ALA:HA	1:91:A:GLU:HG2	12	0.57
(1,420)	1:81:A:GLY:HA3	1:84:A:GLU:HB2	14	0.57
(1,420)	1:81:A:GLY:HA3	1:84:A:GLU:HB3	14	0.57
(1,418)	1:80:A:GLU:HA	1:83:A:ARG:HG3	7	0.57
(1,414)	1:79:A:SER:HB2	1:80:A:GLU:HA	11	0.57
(1,359)	1:59:A:MET:HG3	1:64:A:PRO:HA	6	0.57
(1,166)	1:27:A:GLY:HA2	1:45:A:PHE:HA	4	0.57
(1,166)	1:27:A:GLY:HA2	1:45:A:PHE:HA	18	0.57
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	19	0.56
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	10	0.56
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	19	0.56
(2,562)	1:147:A:GLU:HG2	1:150:A:LYS:HG3	21	0.56
(2,45)	1:8:A:ARG:HB2	1:149:A:GLU:HA	20	0.56
(2,12)	1:4:A:TYR:HB3	1:156:A:ILE:HA	11	0.56
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	5	0.56
(1,504)	1:94:A:LYS:HG2	1:95:A:GLU:HA	17	0.56
(1,451)	1:87:A:ALA:HA	1:90:A:ARG:HG2	6	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,359)	1:59:A:MET:HG3	1:64:A:PRO:HA	10	0.56
(1,343)	1:56:A:LYS:HB3	1:56:A:LYS:HE2	8	0.56
(1,343)	1:56:A:LYS:HB3	1:56:A:LYS:HE3	8	0.56
(1,343)	1:56:A:LYS:HB3	1:56:A:LYS:HE2	18	0.56
(1,343)	1:56:A:LYS:HB3	1:56:A:LYS:HE3	18	0.56
(1,166)	1:27:A:GLY:HA2	1:45:A:PHE:HA	3	0.56
(1,166)	1:27:A:GLY:HA2	1:45:A:PHE:HA	17	0.56
(1,118)	1:18:A:CYS:HB3	1:101:A:VAL:HB	7	0.56
(1,89)	1:12:A:ALA:HB1	1:40:A:LYS:HB3	6	0.56
(1,89)	1:12:A:ALA:HB2	1:40:A:LYS:HB3	6	0.56
(1,89)	1:12:A:ALA:HB3	1:40:A:LYS:HB3	6	0.56
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG11	9	0.56
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG12	9	0.56
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG13	9	0.56
(6,7)	1:9:A:MET:HB2	1:13:A:LYS:H	16	0.55
(5,697)	1:109:A:LEU:HG	1:110:A:SER:H	7	0.55
(5,394)	1:61:A:GLY:HA3	1:63:A:TYR:H	3	0.55
(2,330)	1:85:A:LEU:HD11	1:109:A:LEU:HB3	19	0.55
(2,330)	1:85:A:LEU:HD12	1:109:A:LEU:HB3	19	0.55
(2,330)	1:85:A:LEU:HD13	1:109:A:LEU:HB3	19	0.55
(1,760)	1:147:A:GLU:HG2	1:150:A:LYS:HD2	13	0.55
(1,760)	1:147:A:GLU:HG3	1:150:A:LYS:HD2	13	0.55
(1,632)	1:118:A:LYS:HD3	1:120:A:ARG:HD3	19	0.55
(1,508)	1:94:A:LYS:HE2	1:98:A:ARG:HD3	7	0.55
(1,508)	1:94:A:LYS:HE3	1:98:A:ARG:HD3	7	0.55
(1,418)	1:80:A:GLU:HA	1:83:A:ARG:HG3	8	0.55
(1,418)	1:80:A:GLU:HA	1:83:A:ARG:HG3	17	0.55
(1,187)	1:29:A:PRO:HG2	1:35:A:LYS:HE3	8	0.55
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG11	15	0.55
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG12	15	0.55
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG13	15	0.55
(6,4)	1:6:A:VAL:HG11	1:143:A:CYS:H	6	0.54
(6,4)	1:6:A:VAL:HG12	1:143:A:CYS:H	6	0.54
(6,4)	1:6:A:VAL:HG13	1:143:A:CYS:H	6	0.54
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	20	0.54
(5,548)	1:89:A:TYR:HB2	1:131:A:ALA:H	5	0.54
(5,256)	1:40:A:LYS:H	1:40:A:LYS:HD3	5	0.54
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	13	0.54
(2,358)	1:91:A:GLU:HG3	1:94:A:LYS:HD2	17	0.54
(2,173)	1:35:A:LYS:HG2	1:38:A:TYR:HB2	9	0.54
(2,173)	1:35:A:LYS:HG2	1:38:A:TYR:HB2	12	0.54
(2,141)	1:25:A:PRO:HG2	1:52:A:VAL:HG11	7	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,141)	1:25:A:PRO:HG2	1:52:A:VAL:HG12	7	0.54
(2,141)	1:25:A:PRO:HG2	1:52:A:VAL:HG13	7	0.54
(1,760)	1:147:A:GLU:HG2	1:150:A:LYS:HD2	6	0.54
(1,760)	1:147:A:GLU:HG3	1:150:A:LYS:HD2	6	0.54
(1,418)	1:80:A:GLU:HA	1:83:A:ARG:HG3	3	0.54
(1,216)	1:35:A:LYS:HG3	1:39:A:LYS:HB2	15	0.54
(1,166)	1:27:A:GLY:HA2	1:45:A:PHE:HA	11	0.54
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG11	13	0.54
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG12	13	0.54
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG13	13	0.54
(5,500)	1:83:A:ARG:HG2	1:84:A:GLU:H	21	0.53
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	4	0.53
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	19	0.53
(2,12)	1:4:A:TYR:HB3	1:156:A:ILE:HA	9	0.53
(1,343)	1:56:A:LYS:HB3	1:56:A:LYS:HE2	6	0.53
(1,343)	1:56:A:LYS:HB3	1:56:A:LYS:HE3	6	0.53
(1,216)	1:35:A:LYS:HG3	1:39:A:LYS:HB2	10	0.53
(1,28)	1:6:A:VAL:HG21	1:153:A:SER:HA	14	0.53
(1,28)	1:6:A:VAL:HG22	1:153:A:SER:HA	14	0.53
(1,28)	1:6:A:VAL:HG23	1:153:A:SER:HA	14	0.53
(6,7)	1:9:A:MET:HB2	1:13:A:LYS:H	3	0.52
(6,4)	1:6:A:VAL:HG11	1:143:A:CYS:H	10	0.52
(6,4)	1:6:A:VAL:HG12	1:143:A:CYS:H	10	0.52
(6,4)	1:6:A:VAL:HG13	1:143:A:CYS:H	10	0.52
(6,4)	1:6:A:VAL:HG11	1:143:A:CYS:H	12	0.52
(6,4)	1:6:A:VAL:HG12	1:143:A:CYS:H	12	0.52
(6,4)	1:6:A:VAL:HG13	1:143:A:CYS:H	12	0.52
(2,45)	1:8:A:ARG:HB2	1:149:A:GLU:HA	1	0.52
(1,508)	1:94:A:LYS:HE2	1:98:A:ARG:HD3	15	0.52
(1,508)	1:94:A:LYS:HE3	1:98:A:ARG:HD3	15	0.52
(1,452)	1:87:A:ALA:HA	1:91:A:GLU:HG2	2	0.52
(1,343)	1:56:A:LYS:HB3	1:56:A:LYS:HE2	20	0.52
(1,343)	1:56:A:LYS:HB3	1:56:A:LYS:HE3	20	0.52
(1,150)	1:25:A:PRO:HB3	1:50:A:THR:HA	2	0.52
(1,39)	1:7:A:LYS:HB2	1:9:A:MET:HB2	17	0.52
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG11	10	0.51
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG12	10	0.51
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG13	10	0.51
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	17	0.51
(5,394)	1:61:A:GLY:HA3	1:63:A:TYR:H	21	0.51
(5,153)	1:21:A:ASN:HB3	1:68:A:ALA:H	17	0.51
(4,49)	1:58:A:VAL:HG21	1:67:A:HIS:HE1	15	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,49)	1:58:A:VAL:HG22	1:67:A:HIS:HE1	15	0.51
(4,49)	1:58:A:VAL:HG23	1:67:A:HIS:HE1	15	0.51
(2,452)	1:108:A:LEU:HG	1:143:A:CYS:HB2	8	0.51
(2,358)	1:91:A:GLU:HG3	1:94:A:LYS:HD2	14	0.51
(2,173)	1:35:A:LYS:HG2	1:38:A:TYR:HB2	16	0.51
(2,140)	1:25:A:PRO:HG2	1:52:A:VAL:HA	14	0.51
(2,45)	1:8:A:ARG:HB2	1:149:A:GLU:HA	9	0.51
(1,481)	1:91:A:GLU:HG2	1:94:A:LYS:HE3	11	0.51
(1,311)	1:50:A:THR:HB	1:56:A:LYS:HD3	6	0.51
(1,150)	1:25:A:PRO:HB3	1:50:A:THR:HA	16	0.51
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG11	1	0.51
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG12	1	0.51
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG13	1	0.51
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	15	0.5
(5,548)	1:89:A:TYR:HB2	1:131:A:ALA:H	2	0.5
(5,548)	1:89:A:TYR:HB2	1:131:A:ALA:H	7	0.5
(5,500)	1:83:A:ARG:HG2	1:84:A:GLU:H	14	0.5
(5,394)	1:61:A:GLY:HA3	1:63:A:TYR:H	1	0.5
(5,394)	1:61:A:GLY:HA3	1:63:A:TYR:H	20	0.5
(2,173)	1:35:A:LYS:HG2	1:38:A:TYR:HB2	14	0.5
(1,760)	1:147:A:GLU:HG2	1:150:A:LYS:HD2	20	0.5
(1,760)	1:147:A:GLU:HG3	1:150:A:LYS:HD2	20	0.5
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	18	0.5
(1,452)	1:87:A:ALA:HA	1:91:A:GLU:HG2	20	0.5
(1,150)	1:25:A:PRO:HB3	1:50:A:THR:HA	4	0.5
(1,32)	1:7:A:LYS:HA	1:7:A:LYS:HE3	5	0.5
(7,117)	1:159:A:ARG:H	1:155:A:ALA:O	17	0.49
(6,4)	1:6:A:VAL:HG11	1:143:A:CYS:H	18	0.49
(6,4)	1:6:A:VAL:HG12	1:143:A:CYS:H	18	0.49
(6,4)	1:6:A:VAL:HG13	1:143:A:CYS:H	18	0.49
(5,394)	1:61:A:GLY:HA3	1:63:A:TYR:H	5	0.49
(5,394)	1:61:A:GLY:HA3	1:63:A:TYR:H	9	0.49
(2,357)	1:91:A:GLU:HG3	1:94:A:LYS:HG3	11	0.49
(1,829)	1:156:A:ILE:HA	1:159:A:ARG:HG2	8	0.49
(1,644)	1:120:A:ARG:HB3	1:124:A:SER:HB3	10	0.49
(1,601)	1:111:A:THR:HA	1:120:A:ARG:HD2	20	0.49
(1,166)	1:27:A:GLY:HA2	1:45:A:PHE:HA	10	0.49
(1,150)	1:25:A:PRO:HB3	1:50:A:THR:HA	3	0.49
(1,34)	1:7:A:LYS:HA	1:149:A:GLU:HG2	6	0.49
(6,106)	1:96:A:VAL:HG21	1:136:A:ASP:H	18	0.48
(6,106)	1:96:A:VAL:HG22	1:136:A:ASP:H	18	0.48
(6,106)	1:96:A:VAL:HG23	1:136:A:ASP:H	18	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG11	7	0.48
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG12	7	0.48
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG13	7	0.48
(5,153)	1:21:A:ASN:HB3	1:68:A:ALA:H	3	0.48
(5,153)	1:21:A:ASN:HB3	1:68:A:ALA:H	6	0.48
(2,561)	1:147:A:GLU:HB2	1:151:A:LYS:HD2	5	0.48
(2,357)	1:91:A:GLU:HG3	1:94:A:LYS:HG3	1	0.48
(2,173)	1:35:A:LYS:HG2	1:38:A:TYR:HB2	8	0.48
(1,418)	1:80:A:GLU:HA	1:83:A:ARG:HG3	9	0.48
(1,166)	1:27:A:GLY:HA2	1:45:A:PHE:HA	20	0.48
(1,150)	1:25:A:PRO:HB3	1:50:A:THR:HA	18	0.48
(1,150)	1:25:A:PRO:HB3	1:50:A:THR:HA	20	0.48
(1,60)	1:8:A:ARG:HB2	1:146:A:LYS:HA	15	0.48
(1,32)	1:7:A:LYS:HA	1:7:A:LYS:HE3	18	0.48
(6,106)	1:96:A:VAL:HG21	1:136:A:ASP:H	20	0.47
(6,106)	1:96:A:VAL:HG22	1:136:A:ASP:H	20	0.47
(6,106)	1:96:A:VAL:HG23	1:136:A:ASP:H	20	0.47
(6,105)	1:96:A:VAL:HG21	1:101:A:VAL:H	18	0.47
(6,105)	1:96:A:VAL:HG22	1:101:A:VAL:H	18	0.47
(6,105)	1:96:A:VAL:HG23	1:101:A:VAL:H	18	0.47
(5,50)	1:8:A:ARG:HG2	1:149:A:GLU:H	4	0.47
(5,50)	1:8:A:ARG:HG2	1:149:A:GLU:H	21	0.47
(4,49)	1:58:A:VAL:HG21	1:67:A:HIS:HE1	8	0.47
(4,49)	1:58:A:VAL:HG22	1:67:A:HIS:HE1	8	0.47
(4,49)	1:58:A:VAL:HG23	1:67:A:HIS:HE1	8	0.47
(2,330)	1:85:A:LEU:HD11	1:109:A:LEU:HB3	16	0.47
(2,330)	1:85:A:LEU:HD12	1:109:A:LEU:HB3	16	0.47
(2,330)	1:85:A:LEU:HD13	1:109:A:LEU:HB3	16	0.47
(2,206)	1:48:A:SER:HA	1:56:A:LYS:HE2	9	0.47
(1,418)	1:80:A:GLU:HA	1:83:A:ARG:HG3	2	0.47
(1,359)	1:59:A:MET:HG3	1:64:A:PRO:HA	7	0.47
(1,221)	1:35:A:LYS:HE3	1:39:A:LYS:HE2	10	0.47
(1,44)	1:7:A:LYS:HB3	1:9:A:MET:HB2	9	0.47
(6,105)	1:96:A:VAL:HG21	1:101:A:VAL:H	13	0.46
(6,105)	1:96:A:VAL:HG22	1:101:A:VAL:H	13	0.46
(6,105)	1:96:A:VAL:HG23	1:101:A:VAL:H	13	0.46
(6,71)	1:60:A:CYS:HB2	1:63:A:TYR:H	11	0.46
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	1	0.46
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	20	0.46
(5,330)	1:53:A:GLY:HA3	1:88:A:ALA:H	16	0.46
(5,188)	1:27:A:GLY:HA3	1:48:A:SER:H	17	0.46
(4,41)	1:41:A:TRP:HH2	1:60:A:CYS:HB3	9	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	1:4:A:TYR:HB3	1:156:A:ILE:HA	14	0.46
(1,767)	1:149:A:GLU:HG3	1:150:A:LYS:HA	7	0.46
(1,757)	1:147:A:GLU:HA	1:150:A:LYS:HG2	12	0.46
(1,508)	1:94:A:LYS:HE2	1:98:A:ARG:HD3	18	0.46
(1,508)	1:94:A:LYS:HE3	1:98:A:ARG:HD3	18	0.46
(1,452)	1:87:A:ALA:HA	1:91:A:GLU:HG2	21	0.46
(1,418)	1:80:A:GLU:HA	1:83:A:ARG:HG3	6	0.46
(1,221)	1:35:A:LYS:HE3	1:39:A:LYS:HE2	12	0.46
(1,150)	1:25:A:PRO:HB3	1:50:A:THR:HA	5	0.46
(1,60)	1:8:A:ARG:HB2	1:146:A:LYS:HA	12	0.46
(6,7)	1:9:A:MET:HB2	1:13:A:LYS:H	8	0.45
(6,7)	1:9:A:MET:HB2	1:13:A:LYS:H	19	0.45
(5,394)	1:61:A:GLY:HA3	1:63:A:TYR:H	15	0.45
(5,153)	1:21:A:ASN:HB3	1:68:A:ALA:H	11	0.45
(5,52)	1:8:A:ARG:HD3	1:149:A:GLU:H	3	0.45
(3,19)	1:38:A:TYR:HD1	1:39:A:LYS:HG3	10	0.45
(3,19)	1:38:A:TYR:HD2	1:39:A:LYS:HG3	10	0.45
(2,561)	1:147:A:GLU:HB2	1:151:A:LYS:HD2	14	0.45
(1,451)	1:87:A:ALA:HA	1:90:A:ARG:HG2	13	0.45
(1,166)	1:27:A:GLY:HA2	1:45:A:PHE:HA	19	0.45
(1,150)	1:25:A:PRO:HB3	1:50:A:THR:HA	14	0.45
(1,89)	1:12:A:ALA:HB1	1:40:A:LYS:HB3	5	0.45
(1,89)	1:12:A:ALA:HB2	1:40:A:LYS:HB3	5	0.45
(1,89)	1:12:A:ALA:HB3	1:40:A:LYS:HB3	5	0.45
(1,60)	1:8:A:ARG:HB2	1:146:A:LYS:HA	7	0.45
(1,44)	1:7:A:LYS:HB3	1:9:A:MET:HB2	5	0.45
(1,34)	1:7:A:LYS:HA	1:149:A:GLU:HG2	18	0.45
(6,4)	1:6:A:VAL:HG11	1:143:A:CYS:H	16	0.44
(6,4)	1:6:A:VAL:HG12	1:143:A:CYS:H	16	0.44
(6,4)	1:6:A:VAL:HG13	1:143:A:CYS:H	16	0.44
(5,548)	1:89:A:TYR:HB2	1:131:A:ALA:H	1	0.44
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	10	0.44
(5,188)	1:27:A:GLY:HA3	1:48:A:SER:H	13	0.44
(5,50)	1:8:A:ARG:HG2	1:149:A:GLU:H	5	0.44
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	8	0.44
(3,63)	1:121:A:LEU:HD21	1:148:A:TRP:HD1	1	0.44
(3,63)	1:121:A:LEU:HD22	1:148:A:TRP:HD1	1	0.44
(3,63)	1:121:A:LEU:HD23	1:148:A:TRP:HD1	1	0.44
(3,29)	1:41:A:TRP:HD1	1:60:A:CYS:HB3	16	0.44
(2,388)	1:96:A:VAL:HG21	1:101:A:VAL:HA	13	0.44
(2,388)	1:96:A:VAL:HG22	1:101:A:VAL:HA	13	0.44
(2,388)	1:96:A:VAL:HG23	1:101:A:VAL:HA	13	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,140)	1:25:A:PRO:HG2	1:52:A:VAL:HA	10	0.44
(1,848)	1:158:A:MET:HG3	1:159:A:ARG:HA	19	0.44
(1,452)	1:87:A:ALA:HA	1:91:A:GLU:HG2	3	0.44
(1,418)	1:80:A:GLU:HA	1:83:A:ARG:HG3	10	0.44
(1,418)	1:80:A:GLU:HA	1:83:A:ARG:HG3	20	0.44
(1,380)	1:66:A:ILE:HA	1:95:A:GLU:HG2	12	0.44
(1,150)	1:25:A:PRO:HB3	1:50:A:THR:HA	1	0.44
(1,118)	1:18:A:CYS:HB3	1:101:A:VAL:HB	12	0.44
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG11	11	0.44
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG12	11	0.44
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG13	11	0.44
(5,50)	1:8:A:ARG:HG2	1:149:A:GLU:H	15	0.43
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	21	0.43
(4,49)	1:58:A:VAL:HG21	1:67:A:HIS:HE1	19	0.43
(4,49)	1:58:A:VAL:HG22	1:67:A:HIS:HE1	19	0.43
(4,49)	1:58:A:VAL:HG23	1:67:A:HIS:HE1	19	0.43
(2,562)	1:147:A:GLU:HG2	1:150:A:LYS:HG3	8	0.43
(2,560)	1:147:A:GLU:HA	1:150:A:LYS:HE2	2	0.43
(2,452)	1:108:A:LEU:HG	1:143:A:CYS:HB2	4	0.43
(2,357)	1:91:A:GLU:HG3	1:94:A:LYS:HG3	20	0.43
(2,141)	1:25:A:PRO:HG2	1:52:A:VAL:HG11	2	0.43
(2,141)	1:25:A:PRO:HG2	1:52:A:VAL:HG12	2	0.43
(2,141)	1:25:A:PRO:HG2	1:52:A:VAL:HG13	2	0.43
(2,12)	1:4:A:TYR:HB3	1:156:A:ILE:HA	6	0.43
(1,405)	1:76:A:TYR:HB2	1:81:A:GLY:HA3	5	0.43
(1,343)	1:56:A:LYS:HB3	1:56:A:LYS:HE2	3	0.43
(1,343)	1:56:A:LYS:HB3	1:56:A:LYS:HE3	3	0.43
(1,150)	1:25:A:PRO:HB3	1:50:A:THR:HA	10	0.43
(1,39)	1:7:A:LYS:HB2	1:9:A:MET:HB2	11	0.43
(1,34)	1:7:A:LYS:HA	1:149:A:GLU:HG2	16	0.43
(6,106)	1:96:A:VAL:HG21	1:136:A:ASP:H	15	0.42
(6,106)	1:96:A:VAL:HG22	1:136:A:ASP:H	15	0.42
(6,106)	1:96:A:VAL:HG23	1:136:A:ASP:H	15	0.42
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	6	0.42
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	15	0.42
(5,50)	1:8:A:ARG:HG2	1:149:A:GLU:H	6	0.42
(2,206)	1:48:A:SER:HA	1:56:A:LYS:HE2	7	0.42
(2,206)	1:48:A:SER:HA	1:56:A:LYS:HE2	12	0.42
(2,51)	1:10:A:ASP:HB2	1:13:A:LYS:HG2	1	0.42
(1,508)	1:94:A:LYS:HE2	1:98:A:ARG:HD3	5	0.42
(1,508)	1:94:A:LYS:HE3	1:98:A:ARG:HD3	5	0.42
(1,89)	1:12:A:ALA:HB1	1:40:A:LYS:HB3	15	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:12:A:ALA:HB2	1:40:A:LYS:HB3	15	0.42
(1,89)	1:12:A:ALA:HB3	1:40:A:LYS:HB3	15	0.42
(5,500)	1:83:A:ARG:HG2	1:84:A:GLU:H	18	0.41
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	17	0.41
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	20	0.41
(4,41)	1:41:A:TRP:HH2	1:60:A:CYS:HB3	14	0.41
(2,562)	1:147:A:GLU:HG2	1:150:A:LYS:HG3	19	0.41
(2,366)	1:92:A:VAL:HG21	1:109:A:LEU:HG	21	0.41
(2,366)	1:92:A:VAL:HG22	1:109:A:LEU:HG	21	0.41
(2,366)	1:92:A:VAL:HG23	1:109:A:LEU:HG	21	0.41
(2,12)	1:4:A:TYR:HB3	1:156:A:ILE:HA	13	0.41
(1,829)	1:156:A:ILE:HA	1:159:A:ARG:HG2	21	0.41
(1,828)	1:156:A:ILE:HA	1:159:A:ARG:HB2	4	0.41
(1,828)	1:156:A:ILE:HA	1:159:A:ARG:HB2	5	0.41
(1,767)	1:149:A:GLU:HG3	1:150:A:LYS:HA	17	0.41
(1,757)	1:147:A:GLU:HA	1:150:A:LYS:HG2	8	0.41
(1,460)	1:89:A:TYR:HB3	1:128:A:LEU:HA	20	0.41
(1,405)	1:76:A:TYR:HB2	1:81:A:GLY:HA3	8	0.41
(1,311)	1:50:A:THR:HB	1:56:A:LYS:HD3	13	0.41
(1,166)	1:27:A:GLY:HA2	1:45:A:PHE:HA	14	0.41
(1,89)	1:12:A:ALA:HB1	1:40:A:LYS:HB3	16	0.41
(1,89)	1:12:A:ALA:HB2	1:40:A:LYS:HB3	16	0.41
(1,89)	1:12:A:ALA:HB3	1:40:A:LYS:HB3	16	0.41
(6,7)	1:9:A:MET:HB2	1:13:A:LYS:H	5	0.4
(6,7)	1:9:A:MET:HB2	1:13:A:LYS:H	21	0.4
(5,560)	1:90:A:ARG:HG3	1:91:A:GLU:H	12	0.4
(5,500)	1:83:A:ARG:HG2	1:84:A:GLU:H	12	0.4
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	1	0.4
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	3	0.4
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	5	0.4
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	9	0.4
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	11	0.4
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	12	0.4
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	16	0.4
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	6	0.4
(4,93)	1:143:A:CYS:HB2	1:148:A:TRP:HZ3	19	0.4
(4,41)	1:41:A:TRP:HH2	1:60:A:CYS:HB3	3	0.4
(2,366)	1:92:A:VAL:HG21	1:109:A:LEU:HG	9	0.4
(2,366)	1:92:A:VAL:HG22	1:109:A:LEU:HG	9	0.4
(2,366)	1:92:A:VAL:HG23	1:109:A:LEU:HG	9	0.4
(1,481)	1:91:A:GLU:HG2	1:94:A:LYS:HE3	16	0.4
(1,451)	1:87:A:ALA:HA	1:90:A:ARG:HG2	15	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,216)	1:35:A:LYS:HG3	1:39:A:LYS:HB2	21	0.4
(1,187)	1:29:A:PRO:HG2	1:35:A:LYS:HE3	14	0.4
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG11	20	0.4
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG12	20	0.4
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG13	20	0.4
(6,71)	1:60:A:CYS:HB2	1:63:A:TYR:H	12	0.39
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	2	0.39
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	2	0.39
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	7	0.39
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	8	0.39
(5,188)	1:27:A:GLY:HA3	1:48:A:SER:H	10	0.39
(5,68)	1:10:A:ASP:HB3	1:11:A:ILE:H	1	0.39
(2,388)	1:96:A:VAL:HG21	1:101:A:VAL:HA	18	0.39
(2,388)	1:96:A:VAL:HG22	1:101:A:VAL:HA	18	0.39
(2,388)	1:96:A:VAL:HG23	1:101:A:VAL:HA	18	0.39
(2,83)	1:17:A:GLU:HG2	1:101:A:VAL:HA	17	0.39
(1,644)	1:120:A:ARG:HB3	1:124:A:SER:HB3	21	0.39
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	13	0.39
(1,508)	1:94:A:LYS:HE2	1:98:A:ARG:HD3	20	0.39
(1,508)	1:94:A:LYS:HE3	1:98:A:ARG:HD3	20	0.39
(1,481)	1:91:A:GLU:HG2	1:94:A:LYS:HE3	2	0.39
(1,407)	1:77:A:SER:HB3	1:78:A:GLU:HA	12	0.39
(1,150)	1:25:A:PRO:HB3	1:50:A:THR:HA	8	0.39
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	20	0.39
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	20	0.39
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	13	0.38
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	14	0.38
(5,500)	1:83:A:ARG:HG2	1:84:A:GLU:H	8	0.38
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	13	0.38
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	19	0.38
(2,357)	1:91:A:GLU:HG3	1:94:A:LYS:HG3	16	0.38
(2,207)	1:48:A:SER:HA	1:58:A:VAL:HG21	21	0.38
(2,207)	1:48:A:SER:HA	1:58:A:VAL:HG22	21	0.38
(2,207)	1:48:A:SER:HA	1:58:A:VAL:HG23	21	0.38
(1,829)	1:156:A:ILE:HA	1:159:A:ARG:HG2	12	0.38
(1,634)	1:119:A:ASP:HA	1:120:A:ARG:HG3	4	0.38
(1,407)	1:77:A:SER:HB3	1:78:A:GLU:HA	6	0.38
(1,155)	1:25:A:PRO:HG3	1:51:A:PRO:HA	15	0.38
(1,89)	1:12:A:ALA:HB1	1:40:A:LYS:HB3	17	0.38
(1,89)	1:12:A:ALA:HB2	1:40:A:LYS:HB3	17	0.38
(1,89)	1:12:A:ALA:HB3	1:40:A:LYS:HB3	17	0.38
(6,8)	1:11:A:ILE:HG12	1:14:A:ASN:H	16	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	18	0.37
(5,500)	1:83:A:ARG:HG2	1:84:A:GLU:H	5	0.37
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	4	0.37
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	6	0.37
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	14	0.37
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	21	0.37
(4,93)	1:143:A:CYS:HB2	1:148:A:TRP:HZ3	17	0.37
(3,63)	1:121:A:LEU:HD21	1:148:A:TRP:HD1	19	0.37
(3,63)	1:121:A:LEU:HD22	1:148:A:TRP:HD1	19	0.37
(3,63)	1:121:A:LEU:HD23	1:148:A:TRP:HD1	19	0.37
(2,45)	1:8:A:ARG:HB2	1:149:A:GLU:HA	12	0.37
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	4	0.37
(1,508)	1:94:A:LYS:HE2	1:98:A:ARG:HD3	12	0.37
(1,508)	1:94:A:LYS:HE3	1:98:A:ARG:HD3	12	0.37
(1,418)	1:80:A:GLU:HA	1:83:A:ARG:HG3	18	0.37
(1,166)	1:27:A:GLY:HA2	1:45:A:PHE:HA	8	0.37
(1,60)	1:8:A:ARG:HB2	1:146:A:LYS:HA	9	0.37
(1,39)	1:7:A:LYS:HB2	1:9:A:MET:HB2	3	0.37
(6,71)	1:60:A:CYS:HB2	1:63:A:TYR:H	18	0.36
(5,746)	1:121:A:LEU:HB2	1:122:A:THR:H	5	0.36
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	6	0.36
(5,586)	1:94:A:LYS:H	1:94:A:LYS:HG3	10	0.36
(5,188)	1:27:A:GLY:HA3	1:48:A:SER:H	2	0.36
(5,68)	1:10:A:ASP:HB3	1:11:A:ILE:H	4	0.36
(4,41)	1:41:A:TRP:HH2	1:60:A:CYS:HB3	10	0.36
(3,29)	1:41:A:TRP:HD1	1:60:A:CYS:HB3	19	0.36
(2,173)	1:35:A:LYS:HG2	1:38:A:TYR:HB2	11	0.36
(1,630)	1:118:A:LYS:HD2	1:120:A:ARG:HD3	17	0.36
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	14	0.36
(1,220)	1:35:A:LYS:HE2	1:39:A:LYS:HG2	6	0.36
(1,150)	1:25:A:PRO:HB3	1:50:A:THR:HA	9	0.36
(1,34)	1:7:A:LYS:HA	1:149:A:GLU:HG2	3	0.36
(5,500)	1:83:A:ARG:HG2	1:84:A:GLU:H	1	0.35
(5,394)	1:61:A:GLY:HA3	1:63:A:TYR:H	17	0.35
(5,337)	1:54:A:THR:H	1:69:A:VAL:H	12	0.35
(5,256)	1:40:A:LYS:H	1:40:A:LYS:HD3	11	0.35
(5,192)	1:28:A:LEU:H	1:28:A:LEU:HB3	18	0.35
(5,68)	1:10:A:ASP:HB3	1:11:A:ILE:H	2	0.35
(4,41)	1:41:A:TRP:HH2	1:60:A:CYS:HB3	1	0.35
(3,29)	1:41:A:TRP:HD1	1:60:A:CYS:HB3	10	0.35
(2,585)	1:157:A:GLN:HG3	1:158:A:MET:HA	10	0.35
(2,393)	1:96:A:VAL:HG21	1:137:A:ALA:HA	15	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,393)	1:96:A:VAL:HG22	1:137:A:ALA:HA	15	0.35
(2,393)	1:96:A:VAL:HG23	1:137:A:ALA:HA	15	0.35
(2,356)	1:91:A:GLU:HA	1:94:A:LYS:HE3	10	0.35
(2,206)	1:48:A:SER:HA	1:56:A:LYS:HE2	6	0.35
(2,140)	1:25:A:PRO:HG2	1:52:A:VAL:HA	9	0.35
(1,640)	1:120:A:ARG:HB2	1:120:A:ARG:HD2	9	0.35
(1,640)	1:120:A:ARG:HB2	1:120:A:ARG:HD3	9	0.35
(1,632)	1:118:A:LYS:HD3	1:120:A:ARG:HD3	18	0.35
(1,452)	1:87:A:ALA:HA	1:91:A:GLU:HG2	1	0.35
(1,343)	1:56:A:LYS:HB3	1:56:A:LYS:HE2	21	0.35
(1,343)	1:56:A:LYS:HB3	1:56:A:LYS:HE3	21	0.35
(1,221)	1:35:A:LYS:HE3	1:39:A:LYS:HE2	7	0.35
(1,166)	1:27:A:GLY:HA2	1:45:A:PHE:HA	7	0.35
(1,155)	1:25:A:PRO:HG3	1:51:A:PRO:HA	3	0.35
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	6	0.35
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	6	0.35
(1,60)	1:8:A:ARG:HB2	1:146:A:LYS:HA	1	0.35
(6,8)	1:11:A:ILE:HG12	1:14:A:ASN:H	14	0.34
(5,500)	1:83:A:ARG:HG2	1:84:A:GLU:H	4	0.34
(5,153)	1:21:A:ASN:HB3	1:68:A:ALA:H	14	0.34
(2,315)	1:80:A:GLU:HA	1:83:A:ARG:HD2	5	0.34
(2,315)	1:80:A:GLU:HA	1:83:A:ARG:HD2	15	0.34
(1,632)	1:118:A:LYS:HD3	1:120:A:ARG:HD3	9	0.34
(1,601)	1:111:A:THR:HA	1:120:A:ARG:HD2	18	0.34
(1,420)	1:81:A:GLY:HA3	1:84:A:GLU:HB2	10	0.34
(1,420)	1:81:A:GLY:HA3	1:84:A:GLU:HB3	10	0.34
(1,89)	1:12:A:ALA:HB1	1:40:A:LYS:HB3	21	0.34
(1,89)	1:12:A:ALA:HB2	1:40:A:LYS:HB3	21	0.34
(1,89)	1:12:A:ALA:HB3	1:40:A:LYS:HB3	21	0.34
(1,34)	1:7:A:LYS:HA	1:149:A:GLU:HG2	11	0.34
(5,188)	1:27:A:GLY:HA3	1:48:A:SER:H	7	0.33
(5,119)	1:17:A:GLU:HG3	1:18:A:CYS:H	3	0.33
(2,490)	1:121:A:LEU:HD21	1:125:A:LEU:HB3	17	0.33
(2,490)	1:121:A:LEU:HD22	1:125:A:LEU:HB3	17	0.33
(2,490)	1:121:A:LEU:HD23	1:125:A:LEU:HB3	17	0.33
(1,830)	1:156:A:ILE:HA	1:159:A:ARG:HD2	2	0.33
(1,829)	1:156:A:ILE:HA	1:159:A:ARG:HG2	3	0.33
(1,767)	1:149:A:GLU:HG3	1:150:A:LYS:HA	4	0.33
(1,757)	1:147:A:GLU:HA	1:150:A:LYS:HG2	2	0.33
(1,630)	1:118:A:LYS:HD2	1:120:A:ARG:HD3	8	0.33
(1,311)	1:50:A:THR:HB	1:56:A:LYS:HD3	21	0.33
(1,39)	1:7:A:LYS:HB2	1:9:A:MET:HB2	18	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG11	6	0.32
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG12	6	0.32
(6,18)	1:20:A:VAL:H	1:104:A:VAL:HG13	6	0.32
(6,4)	1:6:A:VAL:HG11	1:143:A:CYS:H	13	0.32
(6,4)	1:6:A:VAL:HG12	1:143:A:CYS:H	13	0.32
(6,4)	1:6:A:VAL:HG13	1:143:A:CYS:H	13	0.32
(5,696)	1:109:A:LEU:HA	1:111:A:THR:H	5	0.32
(5,696)	1:109:A:LEU:HA	1:111:A:THR:H	12	0.32
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	7	0.32
(5,548)	1:89:A:TYR:HB2	1:131:A:ALA:H	16	0.32
(5,50)	1:8:A:ARG:HG2	1:149:A:GLU:H	8	0.32
(2,585)	1:157:A:GLN:HG3	1:158:A:MET:HA	4	0.32
(2,562)	1:147:A:GLU:HG2	1:150:A:LYS:HG3	14	0.32
(2,449)	1:108:A:LEU:HA	1:125:A:LEU:HD21	13	0.32
(2,449)	1:108:A:LEU:HA	1:125:A:LEU:HD22	13	0.32
(2,449)	1:108:A:LEU:HA	1:125:A:LEU:HD23	13	0.32
(2,357)	1:91:A:GLU:HG3	1:94:A:LYS:HG3	2	0.32
(2,12)	1:4:A:TYR:HB3	1:156:A:ILE:HA	17	0.32
(1,829)	1:156:A:ILE:HA	1:159:A:ARG:HG2	7	0.32
(1,767)	1:149:A:GLU:HG3	1:150:A:LYS:HA	18	0.32
(1,644)	1:120:A:ARG:HB3	1:124:A:SER:HB3	19	0.32
(1,423)	1:82:A:ASP:HB2	1:83:A:ARG:HA	3	0.32
(1,166)	1:27:A:GLY:HA2	1:45:A:PHE:HA	16	0.32
(1,155)	1:25:A:PRO:HG3	1:51:A:PRO:HA	21	0.32
(1,150)	1:25:A:PRO:HB3	1:50:A:THR:HA	11	0.32
(1,118)	1:18:A:CYS:HB3	1:101:A:VAL:HB	21	0.32
(1,52)	1:7:A:LYS:HD3	1:140:A:VAL:HG21	21	0.32
(1,52)	1:7:A:LYS:HD3	1:140:A:VAL:HG22	21	0.32
(1,52)	1:7:A:LYS:HD3	1:140:A:VAL:HG23	21	0.32
(1,39)	1:7:A:LYS:HB2	1:9:A:MET:HB2	20	0.32
(6,71)	1:60:A:CYS:HB2	1:63:A:TYR:H	8	0.31
(6,71)	1:60:A:CYS:HB2	1:63:A:TYR:H	10	0.31
(6,7)	1:9:A:MET:HB2	1:13:A:LYS:H	13	0.31
(5,188)	1:27:A:GLY:HA3	1:48:A:SER:H	16	0.31
(5,37)	1:7:A:LYS:HB2	1:8:A:ARG:H	12	0.31
(2,585)	1:157:A:GLN:HG3	1:158:A:MET:HA	19	0.31
(2,449)	1:108:A:LEU:HA	1:125:A:LEU:HD21	7	0.31
(2,449)	1:108:A:LEU:HA	1:125:A:LEU:HD22	7	0.31
(2,449)	1:108:A:LEU:HA	1:125:A:LEU:HD23	7	0.31
(2,206)	1:48:A:SER:HA	1:56:A:LYS:HE2	4	0.31
(1,829)	1:156:A:ILE:HA	1:159:A:ARG:HG2	13	0.31
(1,767)	1:149:A:GLU:HG3	1:150:A:LYS:HA	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,757)	1:147:A:GLU:HA	1:150:A:LYS:HG2	13	0.31
(1,630)	1:118:A:LYS:HD2	1:120:A:ARG:HD3	4	0.31
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	9	0.31
(1,508)	1:94:A:LYS:HE2	1:98:A:ARG:HD3	9	0.31
(1,508)	1:94:A:LYS:HE3	1:98:A:ARG:HD3	9	0.31
(1,460)	1:89:A:TYR:HB3	1:128:A:LEU:HA	9	0.31
(1,452)	1:87:A:ALA:HA	1:91:A:GLU:HG2	17	0.31
(1,423)	1:82:A:ASP:HB2	1:83:A:ARG:HA	9	0.31
(1,423)	1:82:A:ASP:HB2	1:83:A:ARG:HA	18	0.31
(1,423)	1:82:A:ASP:HB2	1:83:A:ARG:HA	21	0.31
(1,209)	1:35:A:LYS:HB3	1:35:A:LYS:HD2	4	0.31
(1,209)	1:35:A:LYS:HB3	1:35:A:LYS:HD3	4	0.31
(1,166)	1:27:A:GLY:HA2	1:45:A:PHE:HA	9	0.31
(1,155)	1:25:A:PRO:HG3	1:51:A:PRO:HA	13	0.31
(1,150)	1:25:A:PRO:HB3	1:50:A:THR:HA	7	0.31
(6,71)	1:60:A:CYS:HB2	1:63:A:TYR:H	19	0.3
(5,548)	1:89:A:TYR:HB2	1:131:A:ALA:H	14	0.3
(5,188)	1:27:A:GLY:HA3	1:48:A:SER:H	14	0.3
(5,153)	1:21:A:ASN:HB3	1:68:A:ALA:H	7	0.3
(5,50)	1:8:A:ARG:HG2	1:149:A:GLU:H	11	0.3
(4,92)	1:129:A:PHE:HZ	1:159:A:ARG:HD2	3	0.3
(3,29)	1:41:A:TRP:HD1	1:60:A:CYS:HB3	20	0.3
(2,585)	1:157:A:GLN:HG3	1:158:A:MET:HA	6	0.3
(2,585)	1:157:A:GLN:HG3	1:158:A:MET:HA	11	0.3
(2,491)	1:121:A:LEU:HD21	1:125:A:LEU:HG	17	0.3
(2,491)	1:121:A:LEU:HD22	1:125:A:LEU:HG	17	0.3
(2,491)	1:121:A:LEU:HD23	1:125:A:LEU:HG	17	0.3
(2,415)	1:102:A:ASN:HB3	1:137:A:ALA:HA	10	0.3
(2,173)	1:35:A:LYS:HG2	1:38:A:TYR:HB2	15	0.3
(1,828)	1:156:A:ILE:HA	1:159:A:ARG:HB2	9	0.3
(1,640)	1:120:A:ARG:HB2	1:120:A:ARG:HD2	11	0.3
(1,640)	1:120:A:ARG:HB2	1:120:A:ARG:HD3	11	0.3
(1,508)	1:94:A:LYS:HE2	1:98:A:ARG:HD3	21	0.3
(1,508)	1:94:A:LYS:HE3	1:98:A:ARG:HD3	21	0.3
(1,480)	1:91:A:GLU:HG2	1:94:A:LYS:HD2	10	0.3
(1,380)	1:66:A:ILE:HA	1:95:A:GLU:HG2	8	0.3
(1,118)	1:18:A:CYS:HB3	1:101:A:VAL:HB	20	0.3
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	1	0.3
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	1	0.3
(7,17)	1:46:A:LYS:H	1:43:A:GLU:O	5	0.29
(6,7)	1:9:A:MET:HB2	1:13:A:LYS:H	1	0.29
(6,4)	1:6:A:VAL:HG11	1:143:A:CYS:H	20	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(6,4)	1:6:A:VAL:HG12	1:143:A:CYS:H	20	0.29
(6,4)	1:6:A:VAL:HG13	1:143:A:CYS:H	20	0.29
(5,256)	1:40:A:LYS:H	1:40:A:LYS:HD3	9	0.29
(5,37)	1:7:A:LYS:HB2	1:8:A:ARG:H	20	0.29
(2,585)	1:157:A:GLN:HG3	1:158:A:MET:HA	20	0.29
(2,560)	1:147:A:GLU:HA	1:150:A:LYS:HE2	8	0.29
(2,357)	1:91:A:GLU:HG3	1:94:A:LYS:HG3	3	0.29
(2,315)	1:80:A:GLU:HA	1:83:A:ARG:HD2	9	0.29
(1,829)	1:156:A:ILE:HA	1:159:A:ARG:HG2	16	0.29
(1,620)	1:118:A:LYS:HB2	1:120:A:ARG:HD3	12	0.29
(1,423)	1:82:A:ASP:HB2	1:83:A:ARG:HA	1	0.29
(1,405)	1:76:A:TYR:HB2	1:81:A:GLY:HA3	12	0.29
(1,166)	1:27:A:GLY:HA2	1:45:A:PHE:HA	1	0.29
(1,110)	1:14:A:ASN:HA	1:15:A:ASP:HB2	2	0.29
(1,110)	1:14:A:ASN:HA	1:15:A:ASP:HB2	15	0.29
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	13	0.29
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	13	0.29
(1,34)	1:7:A:LYS:HA	1:149:A:GLU:HG2	8	0.29
(1,34)	1:7:A:LYS:HA	1:149:A:GLU:HG2	20	0.29
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	12	0.28
(5,548)	1:89:A:TYR:HB2	1:131:A:ALA:H	17	0.28
(5,188)	1:27:A:GLY:HA3	1:48:A:SER:H	18	0.28
(3,63)	1:121:A:LEU:HD21	1:148:A:TRP:HD1	9	0.28
(3,63)	1:121:A:LEU:HD22	1:148:A:TRP:HD1	9	0.28
(3,63)	1:121:A:LEU:HD23	1:148:A:TRP:HD1	9	0.28
(3,29)	1:41:A:TRP:HD1	1:60:A:CYS:HB3	4	0.28
(3,6)	1:4:A:TYR:HD1	1:159:A:ARG:HB3	14	0.28
(3,6)	1:4:A:TYR:HD2	1:159:A:ARG:HB3	14	0.28
(2,585)	1:157:A:GLN:HG3	1:158:A:MET:HA	2	0.28
(2,585)	1:157:A:GLN:HG3	1:158:A:MET:HA	9	0.28
(2,497)	1:121:A:LEU:HD21	1:152:A:ILE:HA	10	0.28
(2,497)	1:121:A:LEU:HD22	1:152:A:ILE:HA	10	0.28
(2,497)	1:121:A:LEU:HD23	1:152:A:ILE:HA	10	0.28
(2,415)	1:102:A:ASN:HB3	1:137:A:ALA:HA	7	0.28
(2,207)	1:48:A:SER:HA	1:58:A:VAL:HG21	11	0.28
(2,207)	1:48:A:SER:HA	1:58:A:VAL:HG22	11	0.28
(2,207)	1:48:A:SER:HA	1:58:A:VAL:HG23	11	0.28
(2,141)	1:25:A:PRO:HG2	1:52:A:VAL:HG11	13	0.28
(2,141)	1:25:A:PRO:HG2	1:52:A:VAL:HG12	13	0.28
(2,141)	1:25:A:PRO:HG2	1:52:A:VAL:HG13	13	0.28
(2,51)	1:10:A:ASP:HB2	1:13:A:LYS:HG2	19	0.28
(1,830)	1:156:A:ILE:HA	1:159:A:ARG:HD2	16	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,712)	1:136:A:ASP:HB3	1:137:A:ALA:HA	11	0.28
(1,423)	1:82:A:ASP:HB2	1:83:A:ARG:HA	19	0.28
(1,343)	1:56:A:LYS:HB3	1:56:A:LYS:HE2	2	0.28
(1,343)	1:56:A:LYS:HB3	1:56:A:LYS:HE3	2	0.28
(1,187)	1:29:A:PRO:HG2	1:35:A:LYS:HE3	12	0.28
(1,118)	1:18:A:CYS:HB3	1:101:A:VAL:HB	14	0.28
(1,110)	1:14:A:ASN:HA	1:15:A:ASP:HB2	11	0.28
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	5	0.28
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	5	0.28
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	7	0.28
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	7	0.28
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	14	0.28
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	14	0.28
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	16	0.28
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	16	0.28
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	21	0.28
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	21	0.28
(1,52)	1:7:A:LYS:HD3	1:140:A:VAL:HG21	10	0.28
(1,52)	1:7:A:LYS:HD3	1:140:A:VAL:HG22	10	0.28
(1,52)	1:7:A:LYS:HD3	1:140:A:VAL:HG23	10	0.28
(1,44)	1:7:A:LYS:HB3	1:9:A:MET:HB2	18	0.28
(1,39)	1:7:A:LYS:HB2	1:9:A:MET:HB2	16	0.28
(1,34)	1:7:A:LYS:HA	1:149:A:GLU:HG2	14	0.28
(6,105)	1:96:A:VAL:HG21	1:101:A:VAL:H	5	0.27
(6,105)	1:96:A:VAL:HG22	1:101:A:VAL:H	5	0.27
(6,105)	1:96:A:VAL:HG23	1:101:A:VAL:H	5	0.27
(6,71)	1:60:A:CYS:HB2	1:63:A:TYR:H	21	0.27
(6,4)	1:6:A:VAL:HG11	1:143:A:CYS:H	14	0.27
(6,4)	1:6:A:VAL:HG12	1:143:A:CYS:H	14	0.27
(6,4)	1:6:A:VAL:HG13	1:143:A:CYS:H	14	0.27
(5,861)	1:141:A:ILE:H	1:141:A:ILE:HB	11	0.27
(5,500)	1:83:A:ARG:HG2	1:84:A:GLU:H	11	0.27
(5,394)	1:61:A:GLY:HA3	1:63:A:TYR:H	6	0.27
(2,585)	1:157:A:GLN:HG3	1:158:A:MET:HA	14	0.27
(2,577)	1:153:A:SER:HA	1:157:A:GLN:HG3	4	0.27
(2,334)	1:86:A:ALA:HB1	1:127:A:HIS:HB3	21	0.27
(2,334)	1:86:A:ALA:HB2	1:127:A:HIS:HB3	21	0.27
(2,334)	1:86:A:ALA:HB3	1:127:A:HIS:HB3	21	0.27
(2,141)	1:25:A:PRO:HG2	1:52:A:VAL:HG11	16	0.27
(2,141)	1:25:A:PRO:HG2	1:52:A:VAL:HG12	16	0.27
(2,141)	1:25:A:PRO:HG2	1:52:A:VAL:HG13	16	0.27
(1,828)	1:156:A:ILE:HA	1:159:A:ARG:HB2	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,757)	1:147:A:GLU:HA	1:150:A:LYS:HG2	4	0.27
(1,650)	1:121:A:LEU:HA	1:125:A:LEU:HB3	8	0.27
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	1	0.27
(1,497)	1:94:A:LYS:HB2	1:94:A:LYS:HE2	5	0.27
(1,497)	1:94:A:LYS:HB2	1:94:A:LYS:HE3	5	0.27
(1,452)	1:87:A:ALA:HA	1:91:A:GLU:HG2	7	0.27
(1,423)	1:82:A:ASP:HB2	1:83:A:ARG:HA	8	0.27
(1,209)	1:35:A:LYS:HB3	1:35:A:LYS:HD2	2	0.27
(1,209)	1:35:A:LYS:HB3	1:35:A:LYS:HD3	2	0.27
(1,187)	1:29:A:PRO:HG2	1:35:A:LYS:HE3	13	0.27
(1,155)	1:25:A:PRO:HG3	1:51:A:PRO:HA	14	0.27
(1,118)	1:18:A:CYS:HB3	1:101:A:VAL:HB	9	0.27
(1,44)	1:7:A:LYS:HB3	1:9:A:MET:HB2	2	0.27
(6,71)	1:60:A:CYS:HB2	1:63:A:TYR:H	16	0.26
(6,56)	1:48:A:SER:H	1:58:A:VAL:HG21	11	0.26
(6,56)	1:48:A:SER:H	1:58:A:VAL:HG22	11	0.26
(6,56)	1:48:A:SER:H	1:58:A:VAL:HG23	11	0.26
(6,8)	1:11:A:ILE:HG12	1:14:A:ASN:H	12	0.26
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	9	0.26
(5,560)	1:90:A:ARG:HG3	1:91:A:GLU:H	21	0.26
(5,442)	1:73:A:PHE:H	1:115:A:SER:HA	12	0.26
(5,119)	1:17:A:GLU:HG3	1:18:A:CYS:H	10	0.26
(5,50)	1:8:A:ARG:HG2	1:149:A:GLU:H	7	0.26
(5,37)	1:7:A:LYS:HB2	1:8:A:ARG:H	17	0.26
(4,41)	1:41:A:TRP:HH2	1:60:A:CYS:HB3	20	0.26
(3,64)	1:121:A:LEU:HD21	1:148:A:TRP:HZ3	5	0.26
(3,64)	1:121:A:LEU:HD22	1:148:A:TRP:HZ3	5	0.26
(3,64)	1:121:A:LEU:HD23	1:148:A:TRP:HZ3	5	0.26
(3,6)	1:4:A:TYR:HD1	1:159:A:ARG:HB3	5	0.26
(3,6)	1:4:A:TYR:HD2	1:159:A:ARG:HB3	5	0.26
(2,393)	1:96:A:VAL:HG21	1:137:A:ALA:HA	8	0.26
(2,393)	1:96:A:VAL:HG22	1:137:A:ALA:HA	8	0.26
(2,393)	1:96:A:VAL:HG23	1:137:A:ALA:HA	8	0.26
(2,393)	1:96:A:VAL:HG21	1:137:A:ALA:HA	9	0.26
(2,393)	1:96:A:VAL:HG22	1:137:A:ALA:HA	9	0.26
(2,393)	1:96:A:VAL:HG23	1:137:A:ALA:HA	9	0.26
(2,366)	1:92:A:VAL:HG21	1:109:A:LEU:HG	18	0.26
(2,366)	1:92:A:VAL:HG22	1:109:A:LEU:HG	18	0.26
(2,366)	1:92:A:VAL:HG23	1:109:A:LEU:HG	18	0.26
(2,315)	1:80:A:GLU:HA	1:83:A:ARG:HD2	8	0.26
(1,829)	1:156:A:ILE:HA	1:159:A:ARG:HG2	19	0.26
(1,712)	1:136:A:ASP:HB3	1:137:A:ALA:HA	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,712)	1:136:A:ASP:HB3	1:137:A:ALA:HA	12	0.26
(1,628)	1:118:A:LYS:HG3	1:119:A:ASP:HA	18	0.26
(1,508)	1:94:A:LYS:HE2	1:98:A:ARG:HD3	1	0.26
(1,508)	1:94:A:LYS:HE3	1:98:A:ARG:HD3	1	0.26
(1,481)	1:91:A:GLU:HG2	1:94:A:LYS:HE3	7	0.26
(1,423)	1:82:A:ASP:HB2	1:83:A:ARG:HA	4	0.26
(1,311)	1:50:A:THR:HB	1:56:A:LYS:HD3	4	0.26
(1,209)	1:35:A:LYS:HB3	1:35:A:LYS:HD2	10	0.26
(1,209)	1:35:A:LYS:HB3	1:35:A:LYS:HD3	10	0.26
(1,150)	1:25:A:PRO:HB3	1:50:A:THR:HA	12	0.26
(1,110)	1:14:A:ASN:HA	1:15:A:ASP:HB2	6	0.26
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	10	0.26
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	10	0.26
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG11	5	0.26
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG12	5	0.26
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG13	5	0.26
(7,31)	1:74:A:SER:H	1:72:A:ASN:O	21	0.25
(6,4)	1:6:A:VAL:HG11	1:143:A:CYS:H	9	0.25
(6,4)	1:6:A:VAL:HG12	1:143:A:CYS:H	9	0.25
(6,4)	1:6:A:VAL:HG13	1:143:A:CYS:H	9	0.25
(5,861)	1:141:A:ILE:H	1:141:A:ILE:HB	8	0.25
(5,339)	1:54:A:THR:H	1:88:A:ALA:HA	4	0.25
(5,188)	1:27:A:GLY:HA3	1:48:A:SER:H	4	0.25
(5,37)	1:7:A:LYS:HB2	1:8:A:ARG:H	15	0.25
(2,585)	1:157:A:GLN:HG3	1:158:A:MET:HA	5	0.25
(2,529)	1:128:A:LEU:HD11	1:132:A:MET:HG3	16	0.25
(2,529)	1:128:A:LEU:HD12	1:132:A:MET:HG3	16	0.25
(2,529)	1:128:A:LEU:HD13	1:132:A:MET:HG3	16	0.25
(2,388)	1:96:A:VAL:HG21	1:101:A:VAL:HA	5	0.25
(2,388)	1:96:A:VAL:HG22	1:101:A:VAL:HA	5	0.25
(2,388)	1:96:A:VAL:HG23	1:101:A:VAL:HA	5	0.25
(2,206)	1:48:A:SER:HA	1:56:A:LYS:HE2	5	0.25
(2,194)	1:44:A:SER:HB3	1:60:A:CYS:HB3	2	0.25
(2,51)	1:10:A:ASP:HB2	1:13:A:LYS:HG2	13	0.25
(1,640)	1:120:A:ARG:HB2	1:120:A:ARG:HD2	13	0.25
(1,640)	1:120:A:ARG:HB2	1:120:A:ARG:HD3	13	0.25
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	2	0.25
(1,452)	1:87:A:ALA:HA	1:91:A:GLU:HG2	15	0.25
(1,379)	1:66:A:ILE:HA	1:95:A:GLU:HB2	17	0.25
(1,379)	1:66:A:ILE:HA	1:95:A:GLU:HB3	17	0.25
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	9	0.25
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG11	16	0.25
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG12	16	0.25
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG13	16	0.25
(6,92)	1:89:A:TYR:H	1:109:A:LEU:HD21	12	0.24
(6,92)	1:89:A:TYR:H	1:109:A:LEU:HD22	12	0.24
(6,92)	1:89:A:TYR:H	1:109:A:LEU:HD23	12	0.24
(6,8)	1:11:A:ILE:HG12	1:14:A:ASN:H	6	0.24
(6,7)	1:9:A:MET:HB2	1:13:A:LYS:H	14	0.24
(6,4)	1:6:A:VAL:HG11	1:143:A:CYS:H	17	0.24
(6,4)	1:6:A:VAL:HG12	1:143:A:CYS:H	17	0.24
(6,4)	1:6:A:VAL:HG13	1:143:A:CYS:H	17	0.24
(5,256)	1:40:A:LYS:H	1:40:A:LYS:HD3	15	0.24
(5,188)	1:27:A:GLY:HA3	1:48:A:SER:H	1	0.24
(5,119)	1:17:A:GLU:HG3	1:18:A:CYS:H	11	0.24
(5,68)	1:10:A:ASP:HB3	1:11:A:ILE:H	19	0.24
(2,577)	1:153:A:SER:HA	1:157:A:GLN:HG3	13	0.24
(2,577)	1:153:A:SER:HA	1:157:A:GLN:HG3	18	0.24
(2,315)	1:80:A:GLU:HA	1:83:A:ARG:HD2	20	0.24
(2,194)	1:44:A:SER:HB3	1:60:A:CYS:HB3	7	0.24
(2,140)	1:25:A:PRO:HG2	1:52:A:VAL:HA	21	0.24
(1,830)	1:156:A:ILE:HA	1:159:A:ARG:HD2	11	0.24
(1,712)	1:136:A:ASP:HB3	1:137:A:ALA:HA	13	0.24
(1,630)	1:118:A:LYS:HD2	1:120:A:ARG:HD3	21	0.24
(1,508)	1:94:A:LYS:HE2	1:98:A:ARG:HD3	16	0.24
(1,508)	1:94:A:LYS:HE3	1:98:A:ARG:HD3	16	0.24
(1,423)	1:82:A:ASP:HB2	1:83:A:ARG:HA	6	0.24
(1,423)	1:82:A:ASP:HB2	1:83:A:ARG:HA	17	0.24
(1,153)	1:25:A:PRO:HG2	1:52:A:VAL:HB	10	0.24
(1,118)	1:18:A:CYS:HB3	1:101:A:VAL:HB	11	0.24
(1,118)	1:18:A:CYS:HB3	1:101:A:VAL:HB	18	0.24
(1,110)	1:14:A:ASN:HA	1:15:A:ASP:HB2	10	0.24
(7,117)	1:159:A:ARG:H	1:155:A:ALA:O	10	0.23
(6,7)	1:9:A:MET:HB2	1:13:A:LYS:H	20	0.23
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	11	0.23
(2,585)	1:157:A:GLN:HG3	1:158:A:MET:HA	12	0.23
(2,560)	1:147:A:GLU:HA	1:150:A:LYS:HE2	13	0.23
(2,515)	1:125:A:LEU:HG	1:155:A:ALA:HA	2	0.23
(2,358)	1:91:A:GLU:HG3	1:94:A:LYS:HD2	10	0.23
(2,299)	1:72:A:ASN:HB3	1:75:A:ASN:HB2	21	0.23
(2,86)	1:18:A:CYS:HA	1:64:A:PRO:HB2	21	0.23
(1,848)	1:158:A:MET:HG3	1:159:A:ARG:HA	12	0.23
(1,757)	1:147:A:GLU:HA	1:150:A:LYS:HG2	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,640)	1:120:A:ARG:HB2	1:120:A:ARG:HD2	4	0.23
(1,640)	1:120:A:ARG:HB2	1:120:A:ARG:HD3	4	0.23
(1,423)	1:82:A:ASP:HB2	1:83:A:ARG:HA	14	0.23
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE2	10	0.23
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE3	10	0.23
(1,216)	1:35:A:LYS:HG3	1:39:A:LYS:HB2	12	0.23
(1,166)	1:27:A:GLY:HA2	1:45:A:PHE:HA	12	0.23
(1,155)	1:25:A:PRO:HG3	1:51:A:PRO:HA	2	0.23
(1,155)	1:25:A:PRO:HG3	1:51:A:PRO:HA	17	0.23
(1,110)	1:14:A:ASN:HA	1:15:A:ASP:HB2	4	0.23
(1,110)	1:14:A:ASN:HA	1:15:A:ASP:HB2	5	0.23
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	8	0.23
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	8	0.23
(1,89)	1:12:A:ALA:HB1	1:40:A:LYS:HB3	20	0.23
(1,89)	1:12:A:ALA:HB2	1:40:A:LYS:HB3	20	0.23
(1,89)	1:12:A:ALA:HB3	1:40:A:LYS:HB3	20	0.23
(1,39)	1:7:A:LYS:HB2	1:9:A:MET:HB2	13	0.23
(6,106)	1:96:A:VAL:HG21	1:136:A:ASP:H	14	0.22
(6,106)	1:96:A:VAL:HG22	1:136:A:ASP:H	14	0.22
(6,106)	1:96:A:VAL:HG23	1:136:A:ASP:H	14	0.22
(6,4)	1:6:A:VAL:HG11	1:143:A:CYS:H	8	0.22
(6,4)	1:6:A:VAL:HG12	1:143:A:CYS:H	8	0.22
(6,4)	1:6:A:VAL:HG13	1:143:A:CYS:H	8	0.22
(6,4)	1:6:A:VAL:HG11	1:143:A:CYS:H	19	0.22
(6,4)	1:6:A:VAL:HG12	1:143:A:CYS:H	19	0.22
(6,4)	1:6:A:VAL:HG13	1:143:A:CYS:H	19	0.22
(5,903)	1:149:A:GLU:HG2	1:153:A:SER:H	20	0.22
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	2	0.22
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	5	0.22
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	15	0.22
(5,548)	1:89:A:TYR:HB2	1:131:A:ALA:H	13	0.22
(5,256)	1:40:A:LYS:H	1:40:A:LYS:HD3	3	0.22
(5,256)	1:40:A:LYS:H	1:40:A:LYS:HD3	19	0.22
(5,50)	1:8:A:ARG:HG2	1:149:A:GLU:H	17	0.22
(2,585)	1:157:A:GLN:HG3	1:158:A:MET:HA	8	0.22
(2,585)	1:157:A:GLN:HG3	1:158:A:MET:HA	13	0.22
(2,585)	1:157:A:GLN:HG3	1:158:A:MET:HA	17	0.22
(2,456)	1:108:A:LEU:HD21	1:121:A:LEU:HA	18	0.22
(2,456)	1:108:A:LEU:HD22	1:121:A:LEU:HA	18	0.22
(2,456)	1:108:A:LEU:HD23	1:121:A:LEU:HA	18	0.22
(1,848)	1:158:A:MET:HG3	1:159:A:ARG:HA	8	0.22
(1,767)	1:149:A:GLU:HG3	1:150:A:LYS:HA	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,712)	1:136:A:ASP:HB3	1:137:A:ALA:HA	4	0.22
(1,712)	1:136:A:ASP:HB3	1:137:A:ALA:HA	5	0.22
(1,712)	1:136:A:ASP:HB3	1:137:A:ALA:HA	17	0.22
(1,620)	1:118:A:LYS:HB2	1:120:A:ARG:HD3	7	0.22
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	10	0.22
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	11	0.22
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	16	0.22
(1,601)	1:111:A:THR:HA	1:120:A:ARG:HD2	6	0.22
(1,476)	1:91:A:GLU:HA	1:94:A:LYS:HB2	7	0.22
(1,466)	1:90:A:ARG:HA	1:131:A:ALA:HA	21	0.22
(1,423)	1:82:A:ASP:HB2	1:83:A:ARG:HA	20	0.22
(1,150)	1:25:A:PRO:HB3	1:50:A:THR:HA	17	0.22
(1,118)	1:18:A:CYS:HB3	1:101:A:VAL:HB	17	0.22
(1,52)	1:7:A:LYS:HD3	1:140:A:VAL:HG21	8	0.22
(1,52)	1:7:A:LYS:HD3	1:140:A:VAL:HG22	8	0.22
(1,52)	1:7:A:LYS:HD3	1:140:A:VAL:HG23	8	0.22
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG11	7	0.22
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG12	7	0.22
(1,50)	1:7:A:LYS:HG3	1:140:A:VAL:HG13	7	0.22
(7,106)	1:152:A:ILE:N	1:148:A:TRP:O	2	0.21
(7,93)	1:134:A:SER:H	1:131:A:ALA:O	12	0.21
(6,105)	1:96:A:VAL:HG21	1:101:A:VAL:H	4	0.21
(6,105)	1:96:A:VAL:HG22	1:101:A:VAL:H	4	0.21
(6,105)	1:96:A:VAL:HG23	1:101:A:VAL:H	4	0.21
(6,8)	1:11:A:ILE:HG12	1:14:A:ASN:H	20	0.21
(6,4)	1:6:A:VAL:HG11	1:143:A:CYS:H	5	0.21
(6,4)	1:6:A:VAL:HG12	1:143:A:CYS:H	5	0.21
(6,4)	1:6:A:VAL:HG13	1:143:A:CYS:H	5	0.21
(5,37)	1:7:A:LYS:HB2	1:8:A:ARG:H	16	0.21
(4,21)	1:41:A:TRP:HA	1:41:A:TRP:HE3	15	0.21
(2,315)	1:80:A:GLU:HA	1:83:A:ARG:HD2	19	0.21
(2,86)	1:18:A:CYS:HA	1:64:A:PRO:HB2	13	0.21
(2,83)	1:17:A:GLU:HG2	1:101:A:VAL:HA	5	0.21
(1,679)	1:125:A:LEU:HG	1:152:A:ILE:HA	8	0.21
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	20	0.21
(1,498)	1:94:A:LYS:HB2	1:95:A:GLU:HA	17	0.21
(1,423)	1:82:A:ASP:HB2	1:83:A:ARG:HA	10	0.21
(1,155)	1:25:A:PRO:HG3	1:51:A:PRO:HA	16	0.21
(1,150)	1:25:A:PRO:HB3	1:50:A:THR:HA	15	0.21
(1,110)	1:14:A:ASN:HA	1:15:A:ASP:HB2	14	0.21
(1,110)	1:14:A:ASN:HA	1:15:A:ASP:HB2	19	0.21
(1,89)	1:12:A:ALA:HB1	1:40:A:LYS:HB3	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:12:A:ALA:HB2	1:40:A:LYS:HB3	1	0.21
(1,89)	1:12:A:ALA:HB3	1:40:A:LYS:HB3	1	0.21
(1,32)	1:7:A:LYS:HA	1:7:A:LYS:HE3	7	0.21
(6,7)	1:9:A:MET:HB2	1:13:A:LYS:H	12	0.2
(5,560)	1:90:A:ARG:HG3	1:91:A:GLU:H	11	0.2
(5,153)	1:21:A:ASN:HB3	1:68:A:ALA:H	9	0.2
(5,119)	1:17:A:GLU:HG3	1:18:A:CYS:H	5	0.2
(5,68)	1:10:A:ASP:HB3	1:11:A:ILE:H	18	0.2
(5,35)	1:7:A:LYS:H	1:143:A:CYS:H	18	0.2
(4,41)	1:41:A:TRP:HH2	1:60:A:CYS:HB3	7	0.2
(4,41)	1:41:A:TRP:HH2	1:60:A:CYS:HB3	11	0.2
(2,585)	1:157:A:GLN:HG3	1:158:A:MET:HA	1	0.2
(2,585)	1:157:A:GLN:HG3	1:158:A:MET:HA	18	0.2
(2,577)	1:153:A:SER:HA	1:157:A:GLN:HG3	8	0.2
(2,515)	1:125:A:LEU:HG	1:155:A:ALA:HA	11	0.2
(2,393)	1:96:A:VAL:HG21	1:137:A:ALA:HA	16	0.2
(2,393)	1:96:A:VAL:HG22	1:137:A:ALA:HA	16	0.2
(2,393)	1:96:A:VAL:HG23	1:137:A:ALA:HA	16	0.2
(2,86)	1:18:A:CYS:HA	1:64:A:PRO:HB2	6	0.2
(1,634)	1:119:A:ASP:HA	1:120:A:ARG:HG3	11	0.2
(1,498)	1:94:A:LYS:HB2	1:95:A:GLU:HA	14	0.2
(1,481)	1:91:A:GLU:HG2	1:94:A:LYS:HE3	15	0.2
(1,418)	1:80:A:GLU:HA	1:83:A:ARG:HG3	12	0.2
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE2	9	0.2
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE3	9	0.2
(1,110)	1:14:A:ASN:HA	1:15:A:ASP:HB2	18	0.2
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE2	4	0.2
(1,102)	1:13:A:LYS:HB3	1:13:A:LYS:HE3	4	0.2
(1,44)	1:7:A:LYS:HB3	1:9:A:MET:HB2	17	0.2
(1,34)	1:7:A:LYS:HA	1:149:A:GLU:HG2	15	0.2
(6,56)	1:48:A:SER:H	1:58:A:VAL:HG21	7	0.19
(6,56)	1:48:A:SER:H	1:58:A:VAL:HG22	7	0.19
(6,56)	1:48:A:SER:H	1:58:A:VAL:HG23	7	0.19
(6,8)	1:11:A:ILE:HG12	1:14:A:ASN:H	8	0.19
(5,861)	1:141:A:ILE:H	1:141:A:ILE:HB	9	0.19
(5,747)	1:121:A:LEU:HB2	1:123:A:GLN:H	18	0.19
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	13	0.19
(5,429)	1:69:A:VAL:H	1:69:A:VAL:HB	12	0.19
(5,339)	1:54:A:THR:H	1:88:A:ALA:HA	18	0.19
(5,256)	1:40:A:LYS:H	1:40:A:LYS:HD3	21	0.19
(5,113)	1:17:A:GLU:H	1:103:A:SER:H	16	0.19
(5,68)	1:10:A:ASP:HB3	1:11:A:ILE:H	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,38)	1:7:A:LYS:HB2	1:9:A:MET:H	4	0.19
(5,37)	1:7:A:LYS:HB2	1:8:A:ARG:H	21	0.19
(4,42)	1:41:A:TRP:HH2	1:63:A:TYR:HB2	13	0.19
(3,29)	1:41:A:TRP:HD1	1:60:A:CYS:HB3	3	0.19
(3,29)	1:41:A:TRP:HD1	1:60:A:CYS:HB3	21	0.19
(2,393)	1:96:A:VAL:HG21	1:137:A:ALA:HA	21	0.19
(2,393)	1:96:A:VAL:HG22	1:137:A:ALA:HA	21	0.19
(2,393)	1:96:A:VAL:HG23	1:137:A:ALA:HA	21	0.19
(1,828)	1:156:A:ILE:HA	1:159:A:ARG:HB2	6	0.19
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	17	0.19
(1,476)	1:91:A:GLU:HA	1:94:A:LYS:HB2	1	0.19
(1,414)	1:79:A:SER:HB2	1:80:A:GLU:HA	15	0.19
(1,396)	1:73:A:PHE:HA	1:76:A:TYR:HA	21	0.19
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE2	20	0.19
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE3	20	0.19
(1,216)	1:35:A:LYS:HG3	1:39:A:LYS:HB2	11	0.19
(1,209)	1:35:A:LYS:HB3	1:35:A:LYS:HD2	5	0.19
(1,209)	1:35:A:LYS:HB3	1:35:A:LYS:HD3	5	0.19
(1,118)	1:18:A:CYS:HB3	1:101:A:VAL:HB	13	0.19
(1,110)	1:14:A:ASN:HA	1:15:A:ASP:HB2	13	0.19
(1,89)	1:12:A:ALA:HB1	1:40:A:LYS:HB3	2	0.19
(1,89)	1:12:A:ALA:HB2	1:40:A:LYS:HB3	2	0.19
(1,89)	1:12:A:ALA:HB3	1:40:A:LYS:HB3	2	0.19
(1,44)	1:7:A:LYS:HB3	1:9:A:MET:HB2	19	0.19
(7,100)	1:140:A:VAL:N	1:104:A:VAL:O	18	0.18
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	4	0.18
(5,339)	1:54:A:THR:H	1:88:A:ALA:HA	8	0.18
(5,188)	1:27:A:GLY:HA3	1:48:A:SER:H	9	0.18
(5,188)	1:27:A:GLY:HA3	1:48:A:SER:H	11	0.18
(5,50)	1:8:A:ARG:HG2	1:149:A:GLU:H	1	0.18
(5,37)	1:7:A:LYS:HB2	1:8:A:ARG:H	3	0.18
(5,37)	1:7:A:LYS:HB2	1:8:A:ARG:H	9	0.18
(5,37)	1:7:A:LYS:HB2	1:8:A:ARG:H	18	0.18
(3,6)	1:4:A:TYR:HD1	1:159:A:ARG:HB3	3	0.18
(3,6)	1:4:A:TYR:HD2	1:159:A:ARG:HB3	3	0.18
(2,577)	1:153:A:SER:HA	1:157:A:GLN:HG3	21	0.18
(2,83)	1:17:A:GLU:HG2	1:101:A:VAL:HA	3	0.18
(1,679)	1:125:A:LEU:HG	1:152:A:ILE:HA	19	0.18
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	8	0.18
(1,497)	1:94:A:LYS:HB2	1:94:A:LYS:HE2	13	0.18
(1,497)	1:94:A:LYS:HB2	1:94:A:LYS:HE3	13	0.18
(1,423)	1:82:A:ASP:HB2	1:83:A:ARG:HA	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,423)	1:82:A:ASP:HB2	1:83:A:ARG:HA	11	0.18
(1,423)	1:82:A:ASP:HB2	1:83:A:ARG:HA	15	0.18
(1,420)	1:81:A:GLY:HA3	1:84:A:GLU:HB2	1	0.18
(1,420)	1:81:A:GLY:HA3	1:84:A:GLU:HB3	1	0.18
(1,396)	1:73:A:PHE:HA	1:76:A:TYR:HA	19	0.18
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE2	2	0.18
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE3	2	0.18
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE2	7	0.18
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE3	7	0.18
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE2	16	0.18
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE3	16	0.18
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE2	21	0.18
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE3	21	0.18
(1,220)	1:35:A:LYS:HE2	1:39:A:LYS:HG2	15	0.18
(1,209)	1:35:A:LYS:HB3	1:35:A:LYS:HD2	21	0.18
(1,209)	1:35:A:LYS:HB3	1:35:A:LYS:HD3	21	0.18
(1,166)	1:27:A:GLY:HA2	1:45:A:PHE:HA	6	0.18
(1,110)	1:14:A:ASN:HA	1:15:A:ASP:HB2	1	0.18
(1,89)	1:12:A:ALA:HB1	1:40:A:LYS:HB3	8	0.18
(1,89)	1:12:A:ALA:HB2	1:40:A:LYS:HB3	8	0.18
(1,89)	1:12:A:ALA:HB3	1:40:A:LYS:HB3	8	0.18
(1,52)	1:7:A:LYS:HD3	1:140:A:VAL:HG21	6	0.18
(1,52)	1:7:A:LYS:HD3	1:140:A:VAL:HG22	6	0.18
(1,52)	1:7:A:LYS:HD3	1:140:A:VAL:HG23	6	0.18
(1,44)	1:7:A:LYS:HB3	1:9:A:MET:HB2	6	0.18
(1,32)	1:7:A:LYS:HA	1:7:A:LYS:HE3	11	0.18
(1,32)	1:7:A:LYS:HA	1:7:A:LYS:HE3	20	0.18
(6,105)	1:96:A:VAL:HG21	1:101:A:VAL:H	8	0.17
(6,105)	1:96:A:VAL:HG22	1:101:A:VAL:H	8	0.17
(6,105)	1:96:A:VAL:HG23	1:101:A:VAL:H	8	0.17
(6,4)	1:6:A:VAL:HG11	1:143:A:CYS:H	4	0.17
(6,4)	1:6:A:VAL:HG12	1:143:A:CYS:H	4	0.17
(6,4)	1:6:A:VAL:HG13	1:143:A:CYS:H	4	0.17
(6,4)	1:6:A:VAL:HG11	1:143:A:CYS:H	21	0.17
(6,4)	1:6:A:VAL:HG12	1:143:A:CYS:H	21	0.17
(6,4)	1:6:A:VAL:HG13	1:143:A:CYS:H	21	0.17
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	16	0.17
(5,500)	1:83:A:ARG:HG2	1:84:A:GLU:H	2	0.17
(5,165)	1:23:A:ALA:H	1:69:A:VAL:HA	7	0.17
(2,585)	1:157:A:GLN:HG3	1:158:A:MET:HA	7	0.17
(2,528)	1:128:A:LEU:HD11	1:132:A:MET:HB3	12	0.17
(2,528)	1:128:A:LEU:HD12	1:132:A:MET:HB3	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,528)	1:128:A:LEU:HD13	1:132:A:MET:HB3	12	0.17
(2,515)	1:125:A:LEU:HG	1:155:A:ALA:HA	9	0.17
(2,452)	1:108:A:LEU:HG	1:143:A:CYS:HB2	9	0.17
(1,845)	1:158:A:MET:HB2	1:159:A:ARG:HA	17	0.17
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	3	0.17
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	15	0.17
(1,601)	1:111:A:THR:HA	1:120:A:ARG:HD2	17	0.17
(1,466)	1:90:A:ARG:HA	1:131:A:ALA:HA	15	0.17
(1,466)	1:90:A:ARG:HA	1:131:A:ALA:HA	19	0.17
(1,423)	1:82:A:ASP:HB2	1:83:A:ARG:HA	7	0.17
(1,423)	1:82:A:ASP:HB2	1:83:A:ARG:HA	13	0.17
(1,423)	1:82:A:ASP:HB2	1:83:A:ARG:HA	16	0.17
(1,420)	1:81:A:GLY:HA3	1:84:A:GLU:HB2	2	0.17
(1,420)	1:81:A:GLY:HA3	1:84:A:GLU:HB3	2	0.17
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE2	18	0.17
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE3	18	0.17
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE2	19	0.17
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE3	19	0.17
(1,216)	1:35:A:LYS:HG3	1:39:A:LYS:HB2	14	0.17
(1,209)	1:35:A:LYS:HB3	1:35:A:LYS:HD2	12	0.17
(1,209)	1:35:A:LYS:HB3	1:35:A:LYS:HD3	12	0.17
(1,39)	1:7:A:LYS:HB2	1:9:A:MET:HB2	10	0.17
(6,105)	1:96:A:VAL:HG21	1:101:A:VAL:H	9	0.16
(6,105)	1:96:A:VAL:HG22	1:101:A:VAL:H	9	0.16
(6,105)	1:96:A:VAL:HG23	1:101:A:VAL:H	9	0.16
(6,105)	1:96:A:VAL:HG21	1:101:A:VAL:H	14	0.16
(6,105)	1:96:A:VAL:HG22	1:101:A:VAL:H	14	0.16
(6,105)	1:96:A:VAL:HG23	1:101:A:VAL:H	14	0.16
(6,56)	1:48:A:SER:H	1:58:A:VAL:HG21	21	0.16
(6,56)	1:48:A:SER:H	1:58:A:VAL:HG22	21	0.16
(6,56)	1:48:A:SER:H	1:58:A:VAL:HG23	21	0.16
(5,547)	1:89:A:TYR:HB2	1:90:A:ARG:H	10	0.16
(5,138)	1:20:A:VAL:H	1:105:A:ALA:H	14	0.16
(5,113)	1:17:A:GLU:H	1:103:A:SER:H	1	0.16
(5,35)	1:7:A:LYS:H	1:143:A:CYS:H	5	0.16
(2,140)	1:25:A:PRO:HG2	1:52:A:VAL:HA	20	0.16
(2,10)	1:4:A:TYR:HB3	1:139:A:VAL:HB	14	0.16
(1,757)	1:147:A:GLU:HA	1:150:A:LYS:HG2	9	0.16
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	6	0.16
(1,420)	1:81:A:GLY:HA3	1:84:A:GLU:HB2	13	0.16
(1,420)	1:81:A:GLY:HA3	1:84:A:GLU:HB3	13	0.16
(1,396)	1:73:A:PHE:HA	1:76:A:TYR:HA	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE2	12	0.16
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE3	12	0.16
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE2	13	0.16
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE3	13	0.16
(1,118)	1:18:A:CYS:HB3	1:101:A:VAL:HB	2	0.16
(1,110)	1:14:A:ASN:HA	1:15:A:ASP:HB2	7	0.16
(1,60)	1:8:A:ARG:HB2	1:146:A:LYS:HA	10	0.16
(7,105)	1:152:A:ILE:H	1:148:A:TRP:O	2	0.15
(5,861)	1:141:A:ILE:H	1:141:A:ILE:HB	12	0.15
(5,681)	1:106:A:ILE:HB	1:140:A:VAL:H	17	0.15
(5,560)	1:90:A:ARG:HG3	1:91:A:GLU:H	4	0.15
(5,547)	1:89:A:TYR:HB2	1:90:A:ARG:H	19	0.15
(5,391)	1:60:A:CYS:H	1:63:A:TYR:H	15	0.15
(5,341)	1:54:A:THR:HB	1:55:A:ALA:H	19	0.15
(5,338)	1:54:A:THR:H	1:69:A:VAL:HB	11	0.15
(5,312)	1:50:A:THR:H	1:50:A:THR:HB	9	0.15
(5,312)	1:50:A:THR:H	1:50:A:THR:HB	13	0.15
(5,138)	1:20:A:VAL:H	1:105:A:ALA:H	16	0.15
(5,113)	1:17:A:GLU:H	1:103:A:SER:H	6	0.15
(5,113)	1:17:A:GLU:H	1:103:A:SER:H	15	0.15
(5,50)	1:8:A:ARG:HG2	1:149:A:GLU:H	19	0.15
(5,37)	1:7:A:LYS:HB2	1:8:A:ARG:H	2	0.15
(5,37)	1:7:A:LYS:HB2	1:8:A:ARG:H	14	0.15
(2,585)	1:157:A:GLN:HG3	1:158:A:MET:HA	21	0.15
(2,528)	1:128:A:LEU:HD11	1:132:A:MET:HB3	8	0.15
(2,528)	1:128:A:LEU:HD12	1:132:A:MET:HB3	8	0.15
(2,528)	1:128:A:LEU:HD13	1:132:A:MET:HB3	8	0.15
(2,528)	1:128:A:LEU:HD11	1:132:A:MET:HB3	13	0.15
(2,528)	1:128:A:LEU:HD12	1:132:A:MET:HB3	13	0.15
(2,528)	1:128:A:LEU:HD13	1:132:A:MET:HB3	13	0.15
(2,493)	1:121:A:LEU:HD21	1:148:A:TRP:HA	16	0.15
(2,493)	1:121:A:LEU:HD22	1:148:A:TRP:HA	16	0.15
(2,493)	1:121:A:LEU:HD23	1:148:A:TRP:HA	16	0.15
(2,341)	1:88:A:ALA:HA	1:89:A:TYR:HB3	3	0.15
(2,341)	1:88:A:ALA:HA	1:89:A:TYR:HB3	14	0.15
(2,12)	1:4:A:TYR:HB3	1:156:A:ILE:HA	4	0.15
(1,845)	1:158:A:MET:HB2	1:159:A:ARG:HA	1	0.15
(1,767)	1:149:A:GLU:HG3	1:150:A:LYS:HA	8	0.15
(1,644)	1:120:A:ARG:HB3	1:124:A:SER:HB3	18	0.15
(1,632)	1:118:A:LYS:HD3	1:120:A:ARG:HD3	11	0.15
(1,623)	1:118:A:LYS:HB3	1:118:A:LYS:HE2	18	0.15
(1,623)	1:118:A:LYS:HB3	1:118:A:LYS:HE3	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	21	0.15
(1,497)	1:94:A:LYS:HB2	1:94:A:LYS:HE2	4	0.15
(1,497)	1:94:A:LYS:HB2	1:94:A:LYS:HE3	4	0.15
(1,481)	1:91:A:GLU:HG2	1:94:A:LYS:HE3	13	0.15
(1,480)	1:91:A:GLU:HG2	1:94:A:LYS:HD2	17	0.15
(1,423)	1:82:A:ASP:HB2	1:83:A:ARG:HA	5	0.15
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE2	3	0.15
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE3	3	0.15
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE2	4	0.15
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE3	4	0.15
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE2	8	0.15
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE3	8	0.15
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE2	11	0.15
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE3	11	0.15
(1,150)	1:25:A:PRO:HB3	1:50:A:THR:HA	13	0.15
(1,34)	1:7:A:LYS:HA	1:149:A:GLU:HG2	4	0.15
(1,32)	1:7:A:LYS:HA	1:7:A:LYS:HE3	2	0.15
(7,99)	1:140:A:VAL:H	1:104:A:VAL:O	18	0.14
(5,696)	1:109:A:LEU:HA	1:111:A:THR:H	7	0.14
(5,548)	1:89:A:TYR:HB2	1:131:A:ALA:H	3	0.14
(5,547)	1:89:A:TYR:HB2	1:90:A:ARG:H	15	0.14
(5,391)	1:60:A:CYS:H	1:63:A:TYR:H	5	0.14
(5,256)	1:40:A:LYS:H	1:40:A:LYS:HD3	10	0.14
(5,131)	1:19:A:VAL:H	1:65:A:VAL:HA	21	0.14
(5,113)	1:17:A:GLU:H	1:103:A:SER:H	2	0.14
(5,35)	1:7:A:LYS:H	1:143:A:CYS:H	3	0.14
(4,93)	1:143:A:CYS:HB2	1:148:A:TRP:HZ3	6	0.14
(3,63)	1:121:A:LEU:HD21	1:148:A:TRP:HD1	7	0.14
(3,63)	1:121:A:LEU:HD22	1:148:A:TRP:HD1	7	0.14
(3,63)	1:121:A:LEU:HD23	1:148:A:TRP:HD1	7	0.14
(3,29)	1:41:A:TRP:HD1	1:60:A:CYS:HB3	1	0.14
(2,529)	1:128:A:LEU:HD11	1:132:A:MET:HG3	17	0.14
(2,529)	1:128:A:LEU:HD12	1:132:A:MET:HG3	17	0.14
(2,529)	1:128:A:LEU:HD13	1:132:A:MET:HG3	17	0.14
(2,515)	1:125:A:LEU:HG	1:155:A:ALA:HA	19	0.14
(2,388)	1:96:A:VAL:HG21	1:101:A:VAL:HA	4	0.14
(2,388)	1:96:A:VAL:HG22	1:101:A:VAL:HA	4	0.14
(2,388)	1:96:A:VAL:HG23	1:101:A:VAL:HA	4	0.14
(2,388)	1:96:A:VAL:HG21	1:101:A:VAL:HA	9	0.14
(2,388)	1:96:A:VAL:HG22	1:101:A:VAL:HA	9	0.14
(2,388)	1:96:A:VAL:HG23	1:101:A:VAL:HA	9	0.14
(2,341)	1:88:A:ALA:HA	1:89:A:TYR:HB3	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,331)	1:85:A:LEU:HD11	1:110:A:SER:HA	12	0.14
(2,331)	1:85:A:LEU:HD12	1:110:A:SER:HA	12	0.14
(2,331)	1:85:A:LEU:HD13	1:110:A:SER:HA	12	0.14
(2,315)	1:80:A:GLU:HA	1:83:A:ARG:HD2	18	0.14
(1,848)	1:158:A:MET:HG3	1:159:A:ARG:HA	6	0.14
(1,845)	1:158:A:MET:HB2	1:159:A:ARG:HA	7	0.14
(1,829)	1:156:A:ILE:HA	1:159:A:ARG:HG2	2	0.14
(1,767)	1:149:A:GLU:HG3	1:150:A:LYS:HA	13	0.14
(1,767)	1:149:A:GLU:HG3	1:150:A:LYS:HA	21	0.14
(1,650)	1:121:A:LEU:HA	1:125:A:LEU:HB3	19	0.14
(1,610)	1:115:A:SER:HA	1:116:A:GLY:HA3	19	0.14
(1,497)	1:94:A:LYS:HB2	1:94:A:LYS:HE2	8	0.14
(1,497)	1:94:A:LYS:HB2	1:94:A:LYS:HE3	8	0.14
(1,476)	1:91:A:GLU:HA	1:94:A:LYS:HB2	20	0.14
(1,396)	1:73:A:PHE:HA	1:76:A:TYR:HA	6	0.14
(1,396)	1:73:A:PHE:HA	1:76:A:TYR:HA	9	0.14
(1,396)	1:73:A:PHE:HA	1:76:A:TYR:HA	13	0.14
(1,396)	1:73:A:PHE:HA	1:76:A:TYR:HA	16	0.14
(1,396)	1:73:A:PHE:HA	1:76:A:TYR:HA	18	0.14
(1,359)	1:59:A:MET:HG3	1:64:A:PRO:HA	4	0.14
(1,150)	1:25:A:PRO:HB3	1:50:A:THR:HA	19	0.14
(1,110)	1:14:A:ASN:HA	1:15:A:ASP:HB2	20	0.14
(1,52)	1:7:A:LYS:HD3	1:140:A:VAL:HG21	4	0.14
(1,52)	1:7:A:LYS:HD3	1:140:A:VAL:HG22	4	0.14
(1,52)	1:7:A:LYS:HD3	1:140:A:VAL:HG23	4	0.14
(1,39)	1:7:A:LYS:HB2	1:9:A:MET:HB2	5	0.14
(7,29)	1:73:A:PHE:H	1:70:A:GLY:O	7	0.13
(6,71)	1:60:A:CYS:HB2	1:63:A:TYR:H	13	0.13
(6,8)	1:11:A:ILE:HG12	1:14:A:ASN:H	4	0.13
(6,7)	1:9:A:MET:HB2	1:13:A:LYS:H	11	0.13
(5,861)	1:141:A:ILE:H	1:141:A:ILE:HB	5	0.13
(5,747)	1:121:A:LEU:HB2	1:123:A:GLN:H	14	0.13
(5,547)	1:89:A:TYR:HB2	1:90:A:ARG:H	20	0.13
(5,429)	1:69:A:VAL:H	1:69:A:VAL:HB	11	0.13
(5,391)	1:60:A:CYS:H	1:63:A:TYR:H	11	0.13
(5,362)	1:56:A:LYS:HG2	1:57:A:THR:H	21	0.13
(5,116)	1:17:A:GLU:HB2	1:103:A:SER:H	16	0.13
(5,113)	1:17:A:GLU:H	1:103:A:SER:H	13	0.13
(5,58)	1:9:A:MET:H	1:143:A:CYS:H	12	0.13
(5,37)	1:7:A:LYS:HB2	1:8:A:ARG:H	6	0.13
(4,93)	1:143:A:CYS:HB2	1:148:A:TRP:HZ3	13	0.13
(2,393)	1:96:A:VAL:HG21	1:137:A:ALA:HA	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,393)	1:96:A:VAL:HG22	1:137:A:ALA:HA	19	0.13
(2,393)	1:96:A:VAL:HG23	1:137:A:ALA:HA	19	0.13
(2,388)	1:96:A:VAL:HG21	1:101:A:VAL:HA	21	0.13
(2,388)	1:96:A:VAL:HG22	1:101:A:VAL:HA	21	0.13
(2,388)	1:96:A:VAL:HG23	1:101:A:VAL:HA	21	0.13
(2,341)	1:88:A:ALA:HA	1:89:A:TYR:HB3	16	0.13
(2,206)	1:48:A:SER:HA	1:56:A:LYS:HE2	2	0.13
(1,686)	1:127:A:HIS:HA	1:130:A:THR:HB	4	0.13
(1,679)	1:125:A:LEU:HG	1:152:A:ILE:HA	18	0.13
(1,634)	1:119:A:ASP:HA	1:120:A:ARG:HG3	9	0.13
(1,630)	1:118:A:LYS:HD2	1:120:A:ARG:HD3	13	0.13
(1,606)	1:113:A:VAL:HB	1:114:A:TYR:HA	2	0.13
(1,606)	1:113:A:VAL:HB	1:114:A:TYR:HA	21	0.13
(1,481)	1:91:A:GLU:HG2	1:94:A:LYS:HE3	3	0.13
(1,466)	1:90:A:ARG:HA	1:131:A:ALA:HA	4	0.13
(1,396)	1:73:A:PHE:HA	1:76:A:TYR:HA	20	0.13
(1,343)	1:56:A:LYS:HB3	1:56:A:LYS:HE2	13	0.13
(1,343)	1:56:A:LYS:HB3	1:56:A:LYS:HE3	13	0.13
(1,311)	1:50:A:THR:HB	1:56:A:LYS:HD3	5	0.13
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE2	1	0.13
(1,292)	1:46:A:LYS:HB3	1:46:A:LYS:HE3	1	0.13
(1,118)	1:18:A:CYS:HB3	1:101:A:VAL:HB	10	0.13
(1,117)	1:18:A:CYS:HA	1:63:A:TYR:HA	5	0.13
(1,110)	1:14:A:ASN:HA	1:15:A:ASP:HB2	3	0.13
(1,44)	1:7:A:LYS:HB3	1:9:A:MET:HB2	20	0.13
(1,39)	1:7:A:LYS:HB2	1:9:A:MET:HB2	1	0.13
(7,117)	1:159:A:ARG:H	1:155:A:ALA:O	1	0.12
(7,100)	1:140:A:VAL:N	1:104:A:VAL:O	10	0.12
(7,100)	1:140:A:VAL:N	1:104:A:VAL:O	13	0.12
(5,861)	1:141:A:ILE:H	1:141:A:ILE:HB	19	0.12
(5,681)	1:106:A:ILE:HB	1:140:A:VAL:H	18	0.12
(5,338)	1:54:A:THR:H	1:69:A:VAL:HB	12	0.12
(5,165)	1:23:A:ALA:H	1:69:A:VAL:HA	13	0.12
(5,113)	1:17:A:GLU:H	1:103:A:SER:H	7	0.12
(5,113)	1:17:A:GLU:H	1:103:A:SER:H	8	0.12
(5,113)	1:17:A:GLU:H	1:103:A:SER:H	10	0.12
(5,68)	1:10:A:ASP:HB3	1:11:A:ILE:H	11	0.12
(5,58)	1:9:A:MET:H	1:143:A:CYS:H	5	0.12
(5,37)	1:7:A:LYS:HB2	1:8:A:ARG:H	10	0.12
(2,562)	1:147:A:GLU:HG2	1:150:A:LYS:HG3	10	0.12
(2,493)	1:121:A:LEU:HD21	1:148:A:TRP:HA	21	0.12
(2,493)	1:121:A:LEU:HD22	1:148:A:TRP:HA	21	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,493)	1:121:A:LEU:HD23	1:148:A:TRP:HA	21	0.12
(2,341)	1:88:A:ALA:HA	1:89:A:TYR:HB3	5	0.12
(2,341)	1:88:A:ALA:HA	1:89:A:TYR:HB3	13	0.12
(1,845)	1:158:A:MET:HB2	1:159:A:ARG:HA	10	0.12
(1,845)	1:158:A:MET:HB2	1:159:A:ARG:HA	21	0.12
(1,650)	1:121:A:LEU:HA	1:125:A:LEU:HB3	18	0.12
(1,606)	1:113:A:VAL:HB	1:114:A:TYR:HA	1	0.12
(1,606)	1:113:A:VAL:HB	1:114:A:TYR:HA	6	0.12
(1,606)	1:113:A:VAL:HB	1:114:A:TYR:HA	9	0.12
(1,606)	1:113:A:VAL:HB	1:114:A:TYR:HA	15	0.12
(1,606)	1:113:A:VAL:HB	1:114:A:TYR:HA	17	0.12
(1,606)	1:113:A:VAL:HB	1:114:A:TYR:HA	19	0.12
(1,452)	1:87:A:ALA:HA	1:91:A:GLU:HG2	11	0.12
(1,355)	1:58:A:VAL:HB	1:59:A:MET:HA	5	0.12
(1,327)	1:53:A:GLY:HA3	1:84:A:GLU:HA	2	0.12
(1,301)	1:48:A:SER:HA	1:56:A:LYS:HD3	13	0.12
(1,209)	1:35:A:LYS:HB3	1:35:A:LYS:HD2	6	0.12
(1,209)	1:35:A:LYS:HB3	1:35:A:LYS:HD3	6	0.12
(1,126)	1:20:A:VAL:HA	1:66:A:ILE:HA	18	0.12
(1,110)	1:14:A:ASN:HA	1:15:A:ASP:HB2	16	0.12
(1,89)	1:12:A:ALA:HB1	1:40:A:LYS:HB3	12	0.12
(1,89)	1:12:A:ALA:HB2	1:40:A:LYS:HB3	12	0.12
(1,89)	1:12:A:ALA:HB3	1:40:A:LYS:HB3	12	0.12
(1,39)	1:7:A:LYS:HB2	1:9:A:MET:HB2	15	0.12
(7,117)	1:159:A:ARG:H	1:155:A:ALA:O	4	0.11
(7,106)	1:152:A:ILE:N	1:148:A:TRP:O	10	0.11
(6,92)	1:89:A:TYR:H	1:109:A:LEU:HD21	5	0.11
(6,92)	1:89:A:TYR:H	1:109:A:LEU:HD22	5	0.11
(6,92)	1:89:A:TYR:H	1:109:A:LEU:HD23	5	0.11
(5,981)	1:159:A:ARG:H	1:159:A:ARG:HG2	18	0.11
(5,981)	1:159:A:ARG:H	1:159:A:ARG:HG3	18	0.11
(5,747)	1:121:A:LEU:HB2	1:123:A:GLN:H	9	0.11
(5,681)	1:106:A:ILE:HB	1:140:A:VAL:H	9	0.11
(5,627)	1:98:A:ARG:HB3	1:100:A:GLY:H	8	0.11
(5,560)	1:90:A:ARG:HG3	1:91:A:GLU:H	20	0.11
(5,547)	1:89:A:TYR:HB2	1:90:A:ARG:H	11	0.11
(5,339)	1:54:A:THR:H	1:88:A:ALA:HA	12	0.11
(5,339)	1:54:A:THR:H	1:88:A:ALA:HA	21	0.11
(5,181)	1:26:A:ARG:H	1:49:A:ALA:HA	2	0.11
(5,133)	1:19:A:VAL:HA	1:105:A:ALA:H	5	0.11
(5,119)	1:17:A:GLU:HG3	1:18:A:CYS:H	14	0.11
(5,116)	1:17:A:GLU:HB2	1:103:A:SER:H	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,113)	1:17:A:GLU:H	1:103:A:SER:H	3	0.11
(5,50)	1:8:A:ARG:HG2	1:149:A:GLU:H	10	0.11
(4,18)	1:40:A:LYS:HB2	1:41:A:TRP:HZ2	17	0.11
(2,388)	1:96:A:VAL:HG21	1:101:A:VAL:HA	8	0.11
(2,388)	1:96:A:VAL:HG22	1:101:A:VAL:HA	8	0.11
(2,388)	1:96:A:VAL:HG23	1:101:A:VAL:HA	8	0.11
(2,388)	1:96:A:VAL:HG21	1:101:A:VAL:HA	14	0.11
(2,388)	1:96:A:VAL:HG22	1:101:A:VAL:HA	14	0.11
(2,388)	1:96:A:VAL:HG23	1:101:A:VAL:HA	14	0.11
(2,376)	1:94:A:LYS:HB3	1:97:A:THR:HB	2	0.11
(2,173)	1:35:A:LYS:HG2	1:38:A:TYR:HB2	18	0.11
(2,45)	1:8:A:ARG:HB2	1:149:A:GLU:HA	3	0.11
(1,845)	1:158:A:MET:HB2	1:159:A:ARG:HA	9	0.11
(1,845)	1:158:A:MET:HB2	1:159:A:ARG:HA	15	0.11
(1,788)	1:151:A:LYS:HA	1:154:A:GLU:HB2	18	0.11
(1,788)	1:151:A:LYS:HA	1:154:A:GLU:HB3	18	0.11
(1,767)	1:149:A:GLU:HG3	1:150:A:LYS:HA	15	0.11
(1,679)	1:125:A:LEU:HG	1:152:A:ILE:HA	9	0.11
(1,644)	1:120:A:ARG:HB3	1:124:A:SER:HB3	20	0.11
(1,606)	1:113:A:VAL:HB	1:114:A:TYR:HA	4	0.11
(1,606)	1:113:A:VAL:HB	1:114:A:TYR:HA	10	0.11
(1,606)	1:113:A:VAL:HB	1:114:A:TYR:HA	11	0.11
(1,606)	1:113:A:VAL:HB	1:114:A:TYR:HA	16	0.11
(1,497)	1:94:A:LYS:HB2	1:94:A:LYS:HE2	12	0.11
(1,497)	1:94:A:LYS:HB2	1:94:A:LYS:HE3	12	0.11
(1,466)	1:90:A:ARG:HA	1:131:A:ALA:HA	10	0.11
(1,466)	1:90:A:ARG:HA	1:131:A:ALA:HA	11	0.11
(1,452)	1:87:A:ALA:HA	1:91:A:GLU:HG2	16	0.11
(1,355)	1:58:A:VAL:HB	1:59:A:MET:HA	15	0.11
(1,117)	1:18:A:CYS:HA	1:63:A:TYR:HA	1	0.11
(1,117)	1:18:A:CYS:HA	1:63:A:TYR:HA	15	0.11
(1,32)	1:7:A:LYS:HA	1:7:A:LYS:HE3	9	0.11
(1,23)	1:6:A:VAL:HA	1:142:A:TYR:HA	6	0.11
(7,118)	1:159:A:ARG:N	1:155:A:ALA:O	17	0.1
(5,500)	1:83:A:ARG:HG2	1:84:A:GLU:H	19	0.1
(5,391)	1:60:A:CYS:H	1:63:A:TYR:H	17	0.1
(5,133)	1:19:A:VAL:HA	1:105:A:ALA:H	6	0.1
(5,131)	1:19:A:VAL:H	1:65:A:VAL:HA	3	0.1
(5,131)	1:19:A:VAL:H	1:65:A:VAL:HA	12	0.1
(5,113)	1:17:A:GLU:H	1:103:A:SER:H	12	0.1
(5,50)	1:8:A:ARG:HG2	1:149:A:GLU:H	18	0.1
(5,37)	1:7:A:LYS:HB2	1:8:A:ARG:H	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,35)	1:7:A:LYS:H	1:143:A:CYS:H	2	0.1
(4,95)	1:148:A:TRP:H	1:148:A:TRP:HE3	3	0.1
(2,141)	1:25:A:PRO:HG2	1:52:A:VAL:HG11	15	0.1
(2,141)	1:25:A:PRO:HG2	1:52:A:VAL:HG12	15	0.1
(2,141)	1:25:A:PRO:HG2	1:52:A:VAL:HG13	15	0.1
(1,811)	1:153:A:SER:HA	1:154:A:GLU:HA	8	0.1
(1,606)	1:113:A:VAL:HB	1:114:A:TYR:HA	12	0.1
(1,606)	1:113:A:VAL:HB	1:114:A:TYR:HA	20	0.1
(1,155)	1:25:A:PRO:HG3	1:51:A:PRO:HA	9	0.1
(1,126)	1:20:A:VAL:HA	1:66:A:ILE:HA	21	0.1
(1,87)	1:12:A:ALA:HA	1:13:A:LYS:HA	19	0.1
(1,70)	1:9:A:MET:HB3	1:13:A:LYS:HD2	16	0.1
(1,70)	1:9:A:MET:HB3	1:13:A:LYS:HD3	16	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found