



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2KCR / pdb_00002ker
BMRB ID : 16094
Title : Solution structure of anntoxin
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Deposited on : 2008-12-29

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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

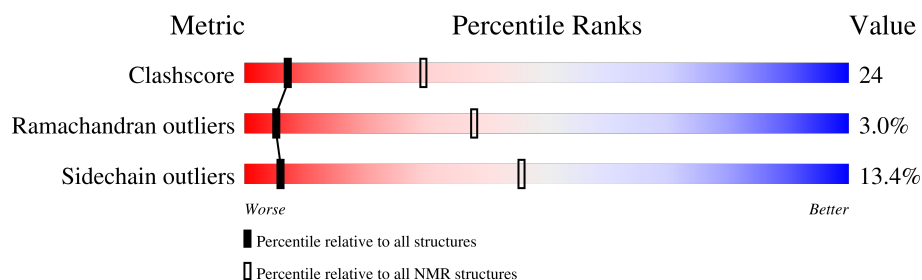
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 46%.

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	61	38% 28% 7% 28%

2 Ensemble composition and analysis

This entry contains 10 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:4-A:11, A:19-A:37, A:45-A:61 (44)	0.77	5

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 2 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 915 atoms, of which 437 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called anntoxin.

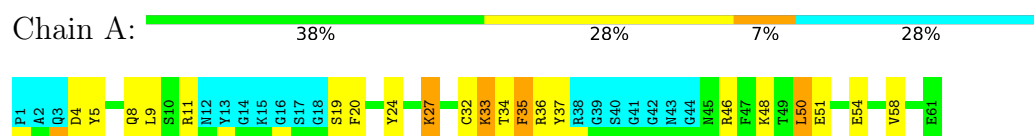
Mol	Chain	Residues	Atoms						Trace
1	A	61	Total	C	H	N	O	S	0
			915	290	437	86	98	4	

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: anntoxin

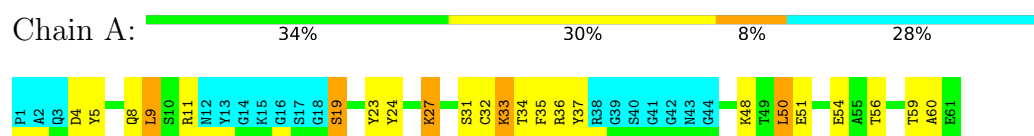


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

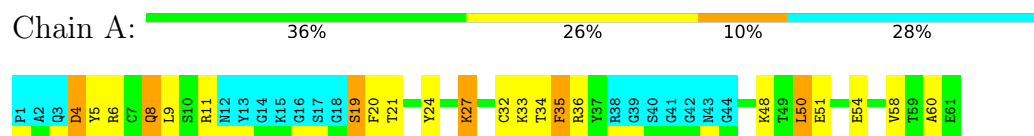
4.2.1 Score per residue for model 1

- Molecule 1: anntoxin



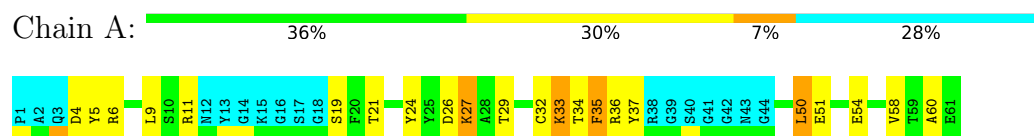
4.2.2 Score per residue for model 2

- Molecule 1: anntoxin



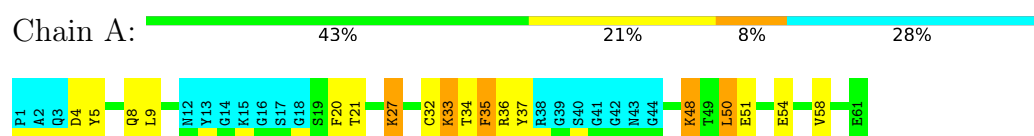
4.2.3 Score per residue for model 3

- Molecule 1: anntoxin



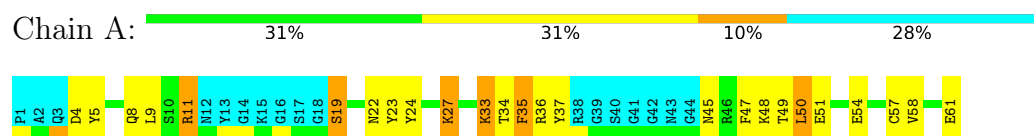
4.2.4 Score per residue for model 4

- Molecule 1: anntoxin



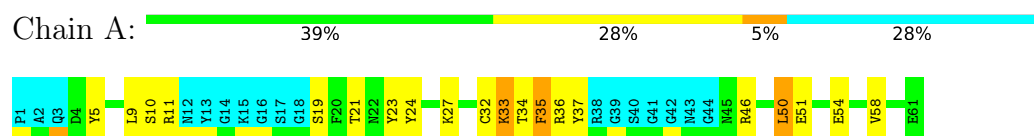
4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: anntoxin



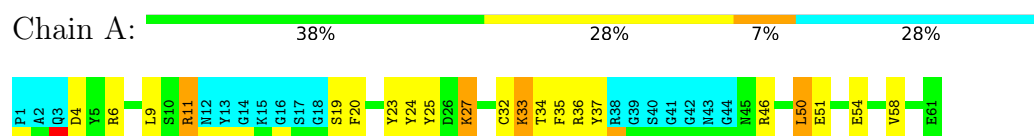
4.2.6 Score per residue for model 6

- Molecule 1: anntoxin



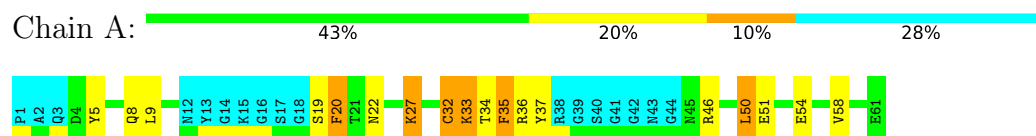
4.2.7 Score per residue for model 7

- Molecule 1: anntoxin



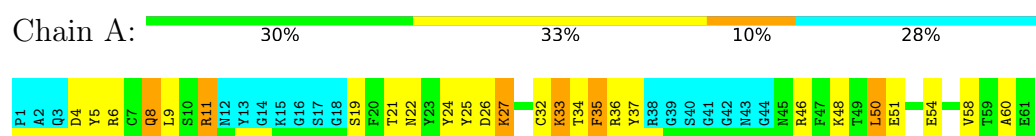
4.2.8 Score per residue for model 8

- Molecule 1: anntoxin



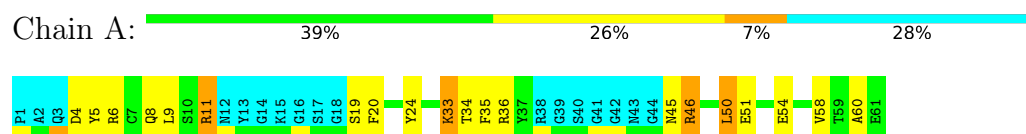
4.2.9 Score per residue for model 9

- Molecule 1: anntoxin



4.2.10 Score per residue for model 10

- Molecule 1: anntoxin



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	336
Number of shifts mapped to atoms	336
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	46%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	369	337	337	17±3
All	All	3690	3370	3370	167

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 24.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:GLN:HA	1:A:27:LYS:HE3	0.75	1.55	5	3
1:A:33:LYS:HG3	1:A:34:THR:H	0.72	1.44	7	7
1:A:33:LYS:HA	1:A:33:LYS:HE3	0.68	1.64	10	6
1:A:11:ARG:HB3	1:A:24:TYR:CD2	0.67	2.24	6	5
1:A:19:SER:HB2	1:A:36:ARG:HD2	0.65	1.68	9	7
1:A:32:CYS:HB2	1:A:50:LEU:HD23	0.64	1.70	6	7
1:A:8:GLN:HG3	1:A:9:LEU:H	0.62	1.55	10	3
1:A:5:TYR:O	1:A:9:LEU:HG	0.60	1.97	9	6
1:A:54:GLU:O	1:A:58:VAL:HB	0.60	1.97	9	9
1:A:5:TYR:HB3	1:A:9:LEU:HG	0.59	1.73	6	2
1:A:50:LEU:O	1:A:50:LEU:HD22	0.59	1.98	8	7
1:A:51:GLU:HA	1:A:54:GLU:HG2	0.56	1.76	7	8
1:A:56:THR:O	1:A:60:ALA:HB3	0.56	2.00	1	1
1:A:20:PHE:O	1:A:36:ARG:HD3	0.56	2.01	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:LYS:HB3	1:A:27:LYS:HZ3	0.55	1.61	8	1
1:A:33:LYS:HG3	1:A:34:THR:N	0.54	2.18	8	9
1:A:23:TYR:HA	1:A:34:THR:HA	0.53	1.79	6	3
1:A:50:LEU:HD22	1:A:50:LEU:O	0.53	2.04	9	3
1:A:19:SER:CB	1:A:36:ARG:HD2	0.52	2.33	9	2
1:A:33:LYS:HE2	1:A:34:THR:H	0.52	1.64	6	2
1:A:8:GLN:HB3	1:A:27:LYS:HE3	0.52	1.79	2	1
1:A:21:THR:HA	1:A:35:PHE:O	0.52	2.05	3	4
1:A:4:ASP:HB3	1:A:6:ARG:HG2	0.52	1.81	2	4
1:A:6:ARG:HA	1:A:9:LEU:HD21	0.51	1.80	7	1
1:A:50:LEU:HD13	1:A:51:GLU:N	0.51	2.20	5	7
1:A:26:ASP:HB3	1:A:29:THR:HG22	0.51	1.82	3	1
1:A:50:LEU:C	1:A:50:LEU:HD13	0.50	2.32	10	4
1:A:11:ARG:HB2	1:A:24:TYR:CD2	0.50	2.42	5	1
1:A:36:ARG:O	1:A:37:TYR:HB3	0.49	2.07	3	1
1:A:4:ASP:CG	1:A:5:TYR:H	0.49	2.16	5	3
1:A:20:PHE:O	1:A:36:ARG:HA	0.49	2.07	4	3
1:A:35:PHE:CE2	1:A:37:TYR:HA	0.48	2.43	8	4
1:A:11:ARG:CB	1:A:24:TYR:CD2	0.48	2.96	9	3
1:A:8:GLN:CB	1:A:27:LYS:HE3	0.48	2.38	2	1
1:A:23:TYR:CE1	1:A:49:THR:HA	0.48	2.43	5	1
1:A:23:TYR:CD1	1:A:49:THR:HA	0.47	2.45	5	1
1:A:5:TYR:HA	1:A:8:GLN:HG2	0.47	1.85	8	1
1:A:22:ASN:HB3	1:A:47:PHE:O	0.46	2.10	5	1
1:A:50:LEU:HD13	1:A:50:LEU:C	0.45	2.35	3	6
1:A:25:TYR:CE2	1:A:27:LYS:HE2	0.45	2.46	7	1
1:A:4:ASP:CG	1:A:5:TYR:N	0.45	2.75	9	4
1:A:24:TYR:CD1	1:A:35:PHE:HB3	0.44	2.47	2	1
1:A:11:ARG:HB3	1:A:24:TYR:HD2	0.44	1.71	10	2
1:A:45:ASN:O	1:A:46:ARG:HB3	0.43	2.13	10	1
1:A:37:TYR:CE1	1:A:46:ARG:HB2	0.43	2.48	9	1
1:A:27:LYS:HB3	1:A:27:LYS:NZ	0.43	2.29	2	2
1:A:48:LYS:N	1:A:48:LYS:HD3	0.42	2.30	5	1
1:A:33:LYS:CG	1:A:34:THR:H	0.42	2.24	4	3
1:A:48:LYS:N	1:A:48:LYS:CD	0.42	2.83	4	1
1:A:8:GLN:HB2	1:A:9:LEU:H	0.42	1.50	1	1
1:A:57:CYS:O	1:A:61:GLU:HG2	0.42	2.15	5	1
1:A:25:TYR:HE1	1:A:27:LYS:HE2	0.41	1.75	9	1
1:A:23:TYR:CD2	1:A:34:THR:HG23	0.41	2.51	6	1
1:A:9:LEU:HD13	1:A:45:ASN:HB3	0.41	1.93	5	1
1:A:27:LYS:NZ	1:A:27:LYS:HB3	0.40	2.31	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:TYR:CE1	1:A:27:LYS:HE2	0.40	2.52	9	1
1:A:37:TYR:CD1	1:A:46:ARG:HD3	0.40	2.51	8	1
1:A:24:TYR:CE2	1:A:26:ASP:HB2	0.40	2.52	9	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	43/61 (70%)	34±1 (80±3%)	7±2 (17±4%)	1±1 (3±3%)	5	38
All	All	430/610 (70%)	344 (80%)	73 (17%)	13 (3%)	5	38

All 7 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	19	SER	4
1	A	46	ARG	3
1	A	8	GLN	2
1	A	9	LEU	1
1	A	4	ASP	1
1	A	20	PHE	1
1	A	10	SER	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	41/50 (82%)	36±1 (87±3%)	6±1 (13±3%)	6	46
All	All	410/500 (82%)	355 (87%)	55 (13%)	6	46

All 12 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	35	PHE	10
1	A	50	LEU	10
1	A	27	LYS	9
1	A	33	LYS	9
1	A	48	LYS	4
1	A	11	ARG	4
1	A	20	PHE	2
1	A	32	CYS	2
1	A	22	ASN	2
1	A	31	SER	1
1	A	59	THR	1
1	A	21	THR	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 46% for the well-defined parts and 44% 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	336
Number of shifts mapped to atoms	336
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

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 46%, i.e. 271 atoms were assigned a chemical shift out of a possible 595. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	86/220 (39%)	86/88 (98%)	0/88 (0%)	0/44 (0%)
Sidechain	165/300 (55%)	165/190 (87%)	0/92 (0%)	0/18 (0%)
Aromatic	20/75 (27%)	20/35 (57%)	0/40 (0%)	0/0 (—%)
Overall	271/595 (46%)	271/313 (87%)	0/220 (0%)	0/62 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 44%, i.e. 336 atoms were assigned a chemical shift out of a possible 771. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	117/310 (38%)	117/128 (91%)	0/122 (0%)	0/60 (0%)
Sidechain	199/377 (53%)	199/238 (84%)	0/114 (0%)	0/25 (0%)
Aromatic	20/84 (24%)	20/39 (51%)	0/45 (0%)	0/0 (—%)
Overall	336/771 (44%)	336/405 (83%)	0/281 (0%)	0/85 (0%)

7.1.4 Statistically unusual chemical shifts ⓘ

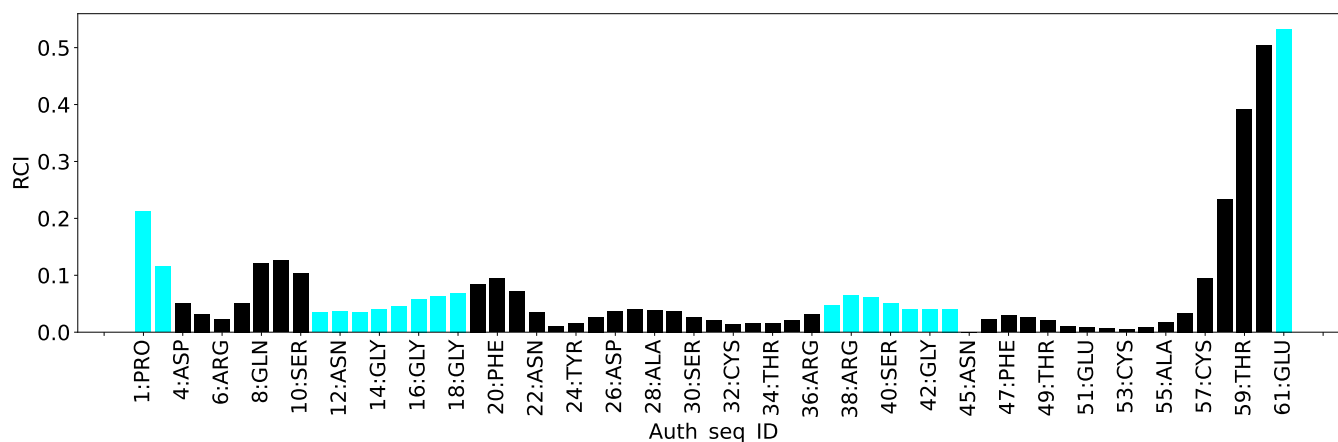
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	11	ARG	HG3	-0.42	0.15 – 2.94	-7.0
1	A	11	ARG	HG2	-0.02	0.26 – 2.87	-6.1
1	A	11	ARG	HD3	1.64	1.81 – 4.39	-5.7
1	A	53	CYS	HA	1.89	1.97 – 7.35	-5.2

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	577
Intra-residue ($ i-j =0$)	283
Sequential ($ i-j =1$)	154
Medium range ($ i-j >1$ and $ i-j <5$)	40
Long range ($ i-j \geq 5$)	66
Inter-chain	0
Hydrogen bond restraints	34
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	9.5
Number of long range restraints per residue ¹	1.3

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)	85.1	0.2
0.2-0.5 (Medium)	123.8	0.5
>0.5 (Large)	131.6	5.66

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 ⓘ

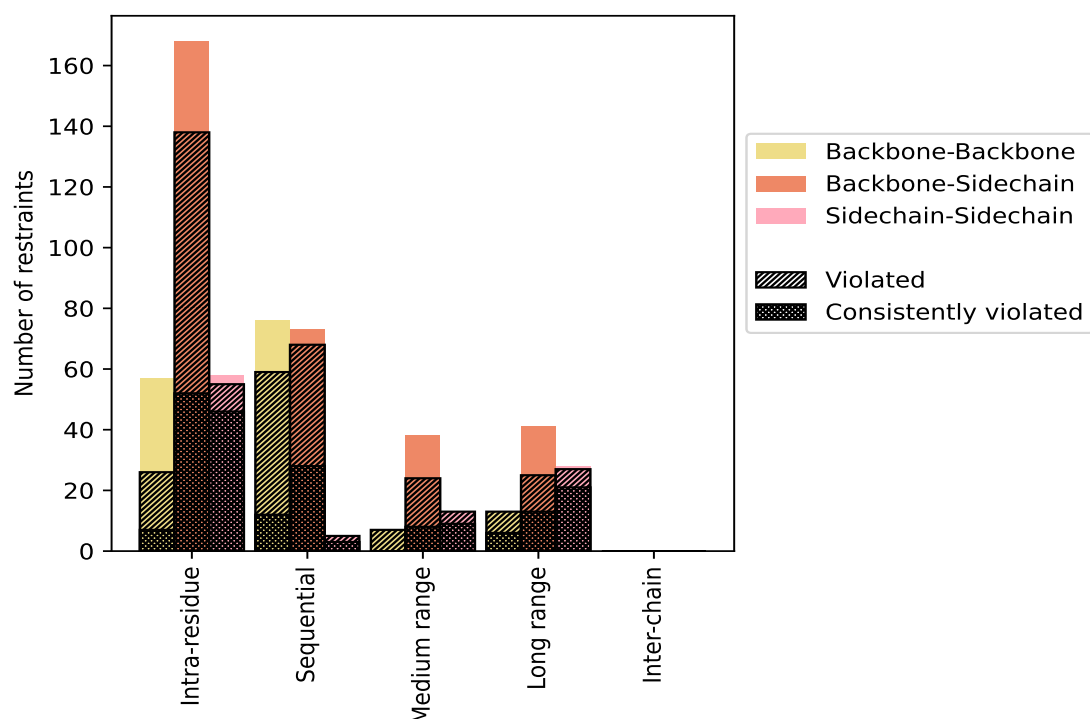
9.1 Summary of distance violations ⓘ

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)	283	49.0	219	77.4	38.0	105	37.1	18.2
Backbone-Backbone	57	9.9	26	45.6	4.5	7	12.3	1.2
Backbone-Sidechain	168	29.1	138	82.1	23.9	52	31.0	9.0
Sidechain-Sidechain	58	10.1	55	94.8	9.5	46	79.3	8.0
Sequential (i-j =1)	154	26.7	132	85.7	22.9	43	27.9	7.5
Backbone-Backbone	76	13.2	59	77.6	10.2	12	15.8	2.1
Backbone-Sidechain	73	12.7	68	93.2	11.8	28	38.4	4.9
Sidechain-Sidechain	5	0.9	5	100.0	0.9	3	60.0	0.5
Medium range (i-j >1 & i-j <5)	40	6.9	40	100.0	6.9	16	40.0	2.8
Backbone-Backbone	7	1.2	7	100.0	1.2	0	0.0	0.0
Backbone-Sidechain	20	3.5	20	100.0	3.5	7	35.0	1.2
Sidechain-Sidechain	13	2.3	13	100.0	2.3	9	69.2	1.6
Long range (i-j ≥5)	66	11.4	65	98.5	11.3	40	60.6	6.9
Backbone-Backbone	13	2.3	13	100.0	2.3	6	46.2	1.0
Backbone-Sidechain	25	4.3	25	100.0	4.3	13	52.0	2.3
Sidechain-Sidechain	28	4.9	27	96.4	4.7	21	75.0	3.6
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	34	5.9	4	11.8	0.7	1	2.9	0.2
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	577	100.0	460	79.7	79.7	205	35.5	35.5
Backbone-Backbone	153	26.5	105	68.6	18.2	25	16.3	4.3
Backbone-Sidechain	320	55.5	255	79.7	44.2	101	31.6	17.5
Sidechain-Sidechain	104	18.0	100	96.2	17.3	79	76.0	13.7

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

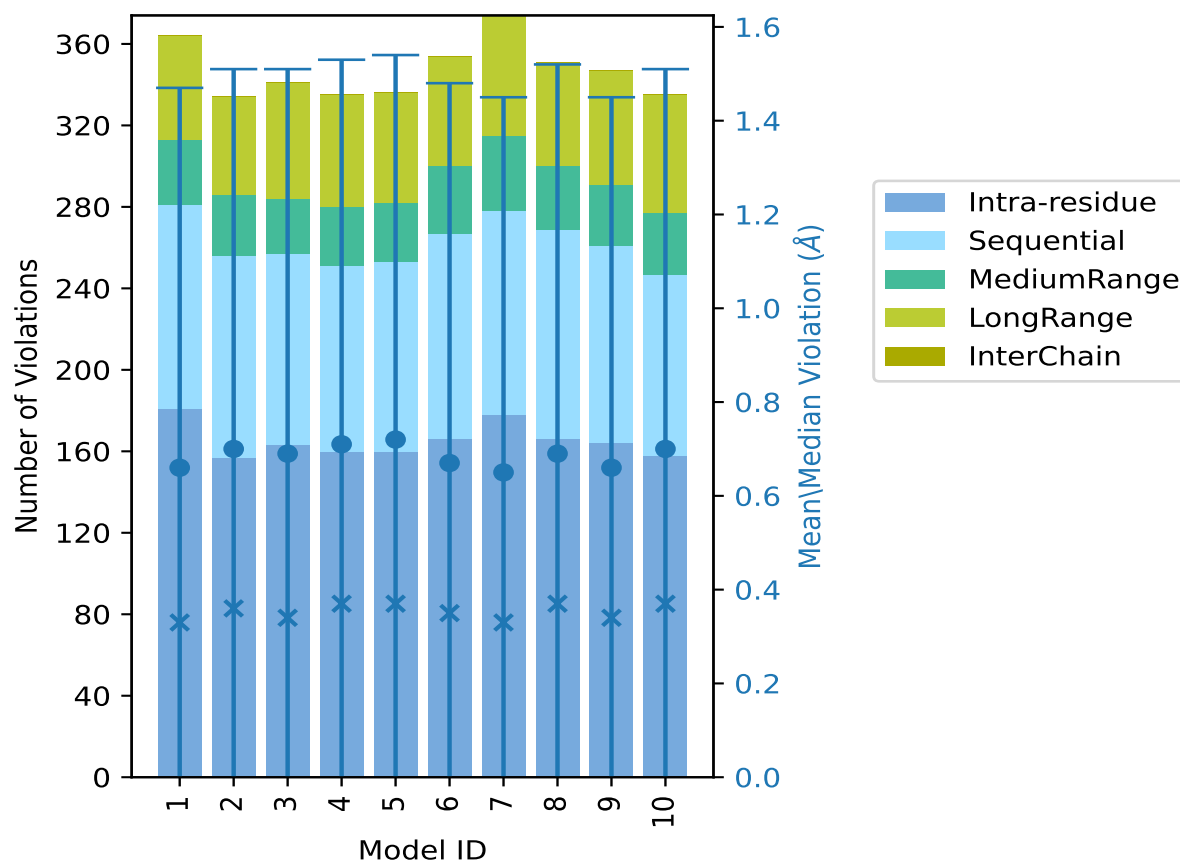
9.2 Distance violation statistics for each model [i](#)

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	181	100	32	51	0	364	0.66	5.33	0.81	0.33
2	157	99	30	48	0	334	0.7	4.96	0.81	0.36
3	163	94	27	57	0	341	0.69	5.29	0.82	0.34
4	160	91	29	55	0	335	0.71	5.13	0.82	0.37
5	160	93	29	54	0	336	0.72	4.64	0.82	0.37
6	166	101	33	54	0	354	0.67	5.66	0.81	0.35
7	178	100	37	59	0	374	0.65	5.08	0.8	0.33
8	166	103	31	51	0	351	0.69	5.35	0.83	0.37
9	164	97	30	56	0	347	0.66	5.07	0.79	0.34
10	158	89	30	58	0	335	0.7	4.72	0.81	0.37

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

9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 87(IR:64, SQ:22, MR:0, LR:1, 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	%
21	7	3	1	0	32	1	10.0
3	4	2	2	0	11	2	20.0
9	9	3	2	0	23	3	30.0

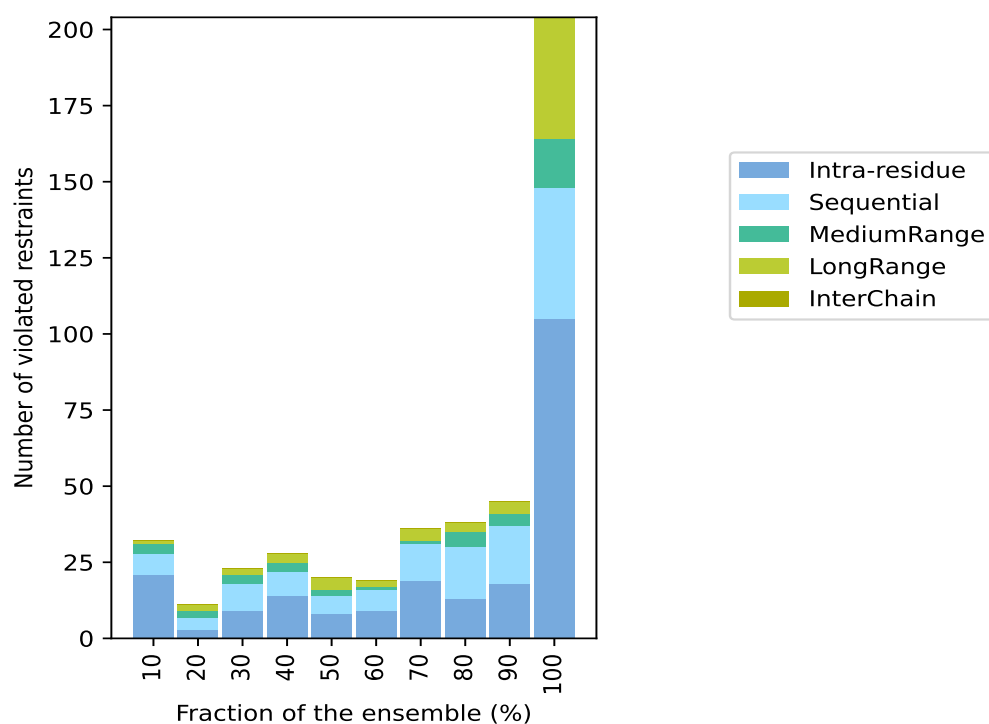
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
14	8	3	3	0	28	4	40.0
8	6	2	4	0	20	5	50.0
9	7	1	2	0	19	6	60.0
19	12	1	4	0	36	7	70.0
13	17	5	3	0	38	8	80.0
18	19	4	4	0	45	9	90.0
105	43	16	40	0	204	10	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶ Number of models with violations

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

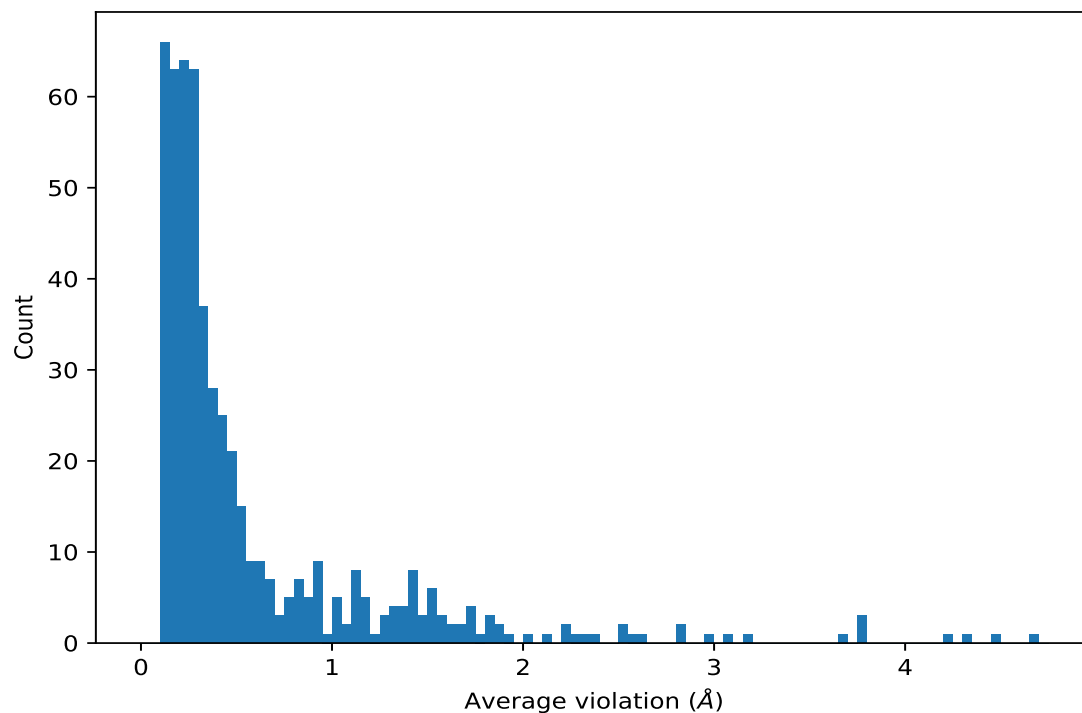


9.4 Most violated distance restraints in the ensemble [i](#)

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)
(1,109)	1:24:A:TYR:HE1	1:11:A:ARG:HG3	10	4.68	0.76	5.04
(1,98)	1:24:A:TYR:HD1	1:11:A:ARG:HD3	10	4.48	0.4	4.44
(1,112)	1:24:A:TYR:HE1	1:26:A:ASP:HA	10	4.31	0.31	4.42
(1,110)	1:24:A:TYR:HE1	1:11:A:ARG:HG2	10	4.22	0.27	4.31
(1,100)	1:24:A:TYR:HD1	1:11:A:ARG:HG3	10	3.8	0.62	4.06
(1,104)	1:24:A:TYR:HD1	1:25:A:TYR:HA	10	3.79	0.09	3.77
(1,107)	1:24:A:TYR:HE1	1:11:A:ARG:HD3	10	3.76	0.52	3.62
(1,101)	1:24:A:TYR:HD1	1:11:A:ARG:HG2	10	3.68	0.21	3.62
(1,99)	1:24:A:TYR:HD1	1:11:A:ARG:HD2	10	3.18	0.27	3.21
(1,108)	1:24:A:TYR:HE1	1:11:A:ARG:HD2	10	3.07	0.36	3.11
(1,59)	1:16:A:GLY:HA2	1:15:A:LYS:HA	10	2.96	0.11	2.97
(1,120)	1:26:A:ASP:HB2	1:32:A:CYS:HA	10	2.81	0.17	2.76
(1,63)	1:18:A:GLY:HA3	1:18:A:GLY:HA2	10	2.81	0.0	2.81
(1,106)	1:24:A:TYR:HE1	1:11:A:ARG:HB2	10	2.61	0.3	2.55
(1,60)	1:17:A:SER:HA	1:17:A:SER:HB3	10	2.59	0.03	2.58

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,121)	1:27:A:LYS:HA	1:27:A:LYS:HB3	10	2.53	0.08	2.56
(1,96)	1:24:A:TYR:HD1	1:11:A:ARG:HA	10	2.51	0.39	2.56
(1,92)	1:24:A:TYR:HA	1:25:A:TYR:HB3	10	2.36	0.06	2.36
(1,52)	1:13:A:TYR:HA	1:14:A:GLY:HA2	10	2.34	0.21	2.3
(1,89)	1:24:A:TYR:HA	1:11:A:ARG:HA	10	2.3	0.19	2.36
(1,70)	1:19:A:SER:HB3	1:36:A:ARG:HD3	10	2.24	0.33	2.26
(1,68)	1:19:A:SER:HA	1:36:A:ARG:HD3	10	2.22	0.13	2.23
(1,62)	1:17:A:SER:HA	1:18:A:GLY:HA2	10	2.12	0.07	2.08
(1,77)	1:22:A:ASN:HA	1:22:A:ASN:HB3	10	2.03	0.08	2.04
(1,91)	1:24:A:TYR:HA	1:24:A:TYR:HB3	10	1.92	0.03	1.93
(1,128)	1:27:A:LYS:HE3	1:27:A:LYS:HG3	10	1.9	0.18	1.97
(1,53)	1:13:A:TYR:HB3	1:13:A:TYR:HA	10	1.85	0.05	1.83
(1,25)	1:9:A:LEU:HD11	1:9:A:LEU:HA	10	1.82	0.02	1.83
(1,25)	1:9:A:LEU:HD12	1:9:A:LEU:HA	10	1.82	0.02	1.83
(1,25)	1:9:A:LEU:HD13	1:9:A:LEU:HA	10	1.82	0.02	1.83
(1,97)	1:24:A:TYR:HD1	1:11:A:ARG:HB2	10	1.76	0.31	1.74
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG11	10	1.73	0.15	1.78
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG12	10	1.73	0.15	1.78
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG13	10	1.73	0.15	1.78
(1,113)	1:24:A:TYR:HE1	1:26:A:ASP:HB2	10	1.71	0.28	1.62
(1,39)	1:11:A:ARG:HD3	1:11:A:ARG:HD2	10	1.68	0.0	1.68
(1,111)	1:24:A:TYR:HE1	1:24:A:TYR:HD1	10	1.68	0.0	1.68
(1,76)	1:22:A:ASN:HA	1:21:A:THR:HB	10	1.64	0.05	1.63
(1,123)	1:27:A:LYS:HA	1:27:A:LYS:HE3	10	1.62	0.51	1.78
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG11	10	1.58	0.27	1.58
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG12	10	1.58	0.27	1.58
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG13	10	1.58	0.27	1.58
(1,184)	1:37:A:TYR:HB2	1:46:A:ARG:HB3	10	1.54	0.1	1.57
(1,20)	1:7:A:CYS:HB2	1:3:A:GLN:HG3	10	1.54	0.56	1.52
(1,58)	1:16:A:GLY:HA3	1:16:A:GLY:HA2	10	1.54	0.01	1.54
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD11	10	1.5	1.01	1.51
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD12	10	1.5	1.01	1.51
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD13	10	1.5	1.01	1.51
(1,37)	1:11:A:ARG:HD3	1:11:A:ARG:HA	10	1.48	0.32	1.68
(1,105)	1:24:A:TYR:HE1	1:11:A:ARG:HB3	10	1.48	0.3	1.48
(1,103)	1:24:A:TYR:HD1	1:24:A:TYR:HB3	10	1.48	0.02	1.47
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG21	10	1.45	0.11	1.47
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG22	10	1.45	0.11	1.47
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG23	10	1.45	0.11	1.47
(1,69)	1:19:A:SER:HB3	1:19:A:SER:HB2	10	1.43	0.0	1.43
(1,390)	1:27:A:LYS:H	1:27:A:LYS:HE3	10	1.43	0.14	1.48
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG11	10	1.42	0.02	1.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG12	10	1.42	0.02	1.42
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG13	10	1.42	0.02	1.42
(1,67)	1:19:A:SER:HA	1:36:A:ARG:HB3	10	1.39	0.24	1.4
(1,254)	1:58:A:VAL:HG11	1:54:A:GLU:HB3	10	1.38	0.1	1.41
(1,254)	1:58:A:VAL:HG12	1:54:A:GLU:HB3	10	1.38	0.1	1.41
(1,254)	1:58:A:VAL:HG13	1:54:A:GLU:HB3	10	1.38	0.1	1.41
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG21	10	1.33	0.1	1.32
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG22	10	1.33	0.1	1.32
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG23	10	1.33	0.1	1.32
(1,247)	1:57:A:CYS:HA	1:3:A:GLN:HG3	10	1.31	0.49	1.51
(1,79)	1:22:A:ASN:HB2	1:22:A:ASN:HB3	10	1.27	0.0	1.27
(1,286)	1:7:A:CYS:H	1:8:A:GLN:HG3	10	1.27	0.3	1.26
(1,241)	1:55:A:ALA:HA	1:54:A:GLU:HG3	10	1.26	0.04	1.25
(1,139)	1:32:A:CYS:HB3	1:23:A:TYR:HB3	10	1.23	0.16	1.19
(1,339)	1:16:A:GLY:H	1:38:A:ARG:HG3	10	1.2	0.53	1.23
(1,95)	1:24:A:TYR:HB3	1:11:A:ARG:HB2	10	1.19	0.35	1.1
(1,54)	1:14:A:GLY:HA3	1:14:A:GLY:HA2	10	1.18	0.01	1.17
(1,152)	1:34:A:THR:HA	1:33:A:LYS:HE3	10	1.17	0.46	0.98
(1,163)	1:35:A:PHE:HD1	1:34:A:THR:HA	10	1.17	0.1	1.15
(1,197)	1:47:A:PHE:HB3	1:23:A:TYR:HB3	10	1.14	0.19	1.11
(1,86)	1:23:A:TYR:HD1	1:48:A:LYS:HA	10	1.14	0.16	1.18
(1,393)	1:28:A:ALA:H	1:28:A:ALA:HB3	10	1.12	0.02	1.12
(1,66)	1:19:A:SER:HA	1:36:A:ARG:HA	10	1.11	0.16	1.12
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD21	10	1.11	0.12	1.1
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD22	10	1.11	0.12	1.1
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD23	10	1.11	0.12	1.1
(1,22)	1:8:A:GLN:HA	1:27:A:LYS:HE3	10	1.1	0.48	1.14
(1,294)	1:9:A:LEU:H	1:8:A:GLN:HG3	10	1.07	0.39	1.27
(1,509)	1:54:A:GLU:H	1:54:A:GLU:HG3	10	1.06	0.04	1.07
(1,145)	1:33:A:LYS:HA	1:33:A:LYS:HE3	10	1.03	0.47	1.08
(1,215)	1:50:A:LEU:HD21	1:54:A:GLU:HG3	10	1.03	0.07	1.05
(1,215)	1:50:A:LEU:HD22	1:54:A:GLU:HG3	10	1.03	0.07	1.05
(1,215)	1:50:A:LEU:HD23	1:54:A:GLU:HG3	10	1.03	0.07	1.05
(1,378)	1:25:A:TYR:H	1:24:A:TYR:HB3	10	1.03	0.06	1.04
(1,40)	1:11:A:ARG:HD3	1:11:A:ARG:HG3	10	0.97	0.01	0.97
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD11	10	0.94	0.28	1.05
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD12	10	0.94	0.28	1.05
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD13	10	0.94	0.28	1.05
(1,534)	1:59:A:THR:H	1:59:A:THR:HG21	10	0.94	0.26	1.03
(1,534)	1:59:A:THR:H	1:59:A:THR:HG22	10	0.94	0.26	1.03
(1,534)	1:59:A:THR:H	1:59:A:THR:HG23	10	0.94	0.26	1.03
(1,35)	1:11:A:ARG:HB2	1:11:A:ARG:HB3	10	0.92	0.0	0.92

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,265)	1:3:A:GLN:H	1:3:A:GLN:HG3	10	0.9	0.41	0.84
(1,38)	1:11:A:ARG:HD3	1:11:A:ARG:HB2	10	0.9	0.22	1.0
(1,48)	1:12:A:ASN:HA	1:12:A:ASN:HB3	10	0.89	0.23	1.01
(1,87)	1:23:A:TYR:HD1	1:49:A:THR:HA	10	0.86	0.21	0.9
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD11	10	0.86	0.25	0.82
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD12	10	0.86	0.25	0.82
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD13	10	0.86	0.25	0.82
(1,72)	1:20:A:PHE:HA	1:20:A:PHE:HB3	10	0.85	0.17	0.94
(1,82)	1:23:A:TYR:HA	1:34:A:THR:HB	10	0.85	0.03	0.86
(1,85)	1:23:A:TYR:HD1	1:23:A:TYR:HB3	10	0.85	0.01	0.85
(1,309)	1:12:A:ASN:H	1:11:A:ARG:HB2	10	0.84	0.25	0.83
(1,36)	1:11:A:ARG:HB2	1:11:A:ARG:HG2	10	0.84	0.13	0.92
(1,50)	1:12:A:ASN:HB3	1:12:A:ASN:HB2	10	0.82	0.01	0.82
(1,124)	1:27:A:LYS:HA	1:27:A:LYS:HG3	10	0.8	0.06	0.8
(1,176)	1:36:A:ARG:HD3	1:36:A:ARG:HA	10	0.79	0.09	0.78
(1,149)	1:33:A:LYS:HE3	1:33:A:LYS:HG3	10	0.78	0.26	0.6
(1,114)	1:25:A:TYR:HA	1:32:A:CYS:HA	10	0.77	0.04	0.76
(1,11)	1:5:A:TYR:HB3	1:8:A:GLN:HG3	10	0.77	0.29	0.84
(1,90)	1:24:A:TYR:HA	1:23:A:TYR:HA	10	0.76	0.01	0.77
(1,318)	1:13:A:TYR:H	1:12:A:ASN:HB3	10	0.72	0.28	0.84
(1,119)	1:26:A:ASP:HB2	1:26:A:ASP:HB3	10	0.72	0.0	0.72
(1,75)	1:21:A:THR:HB	1:21:A:THR:HA	10	0.7	0.01	0.7
(1,211)	1:49:A:THR:HG21	1:49:A:THR:HA	10	0.67	0.03	0.66
(1,211)	1:49:A:THR:HG22	1:49:A:THR:HA	10	0.67	0.03	0.66
(1,211)	1:49:A:THR:HG23	1:49:A:THR:HA	10	0.67	0.03	0.66
(1,116)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	10	0.65	0.0	0.65
(1,191)	1:46:A:ARG:HA	1:46:A:ARG:HB3	10	0.64	0.01	0.65
(1,56)	1:15:A:LYS:HA	1:15:A:LYS:HB2	10	0.62	0.12	0.7
(1,84)	1:23:A:TYR:HD1	1:22:A:ASN:HA	10	0.62	0.16	0.6
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG21	10	0.62	0.08	0.64
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG22	10	0.62	0.08	0.64
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG23	10	0.62	0.08	0.64
(1,240)	1:54:A:GLU:HG3	1:54:A:GLU:HB3	10	0.62	0.0	0.62
(1,51)	1:13:A:TYR:HA	1:13:A:TYR:HB2	10	0.61	0.09	0.57
(1,71)	1:19:A:SER:HB2	1:36:A:ARG:HD3	10	0.59	0.14	0.6
(1,41)	1:11:A:ARG:HD3	1:11:A:ARG:HG2	10	0.58	0.11	0.63
(1,118)	1:26:A:ASP:HA	1:26:A:ASP:HB2	10	0.58	0.04	0.59
(1,46)	1:11:A:ARG:HG3	1:11:A:ARG:HB2	10	0.57	0.08	0.57
(1,127)	1:27:A:LYS:HE3	1:27:A:LYS:HB3	10	0.57	0.26	0.49
(1,323)	1:13:A:TYR:H	1:14:A:GLY:H	10	0.57	0.29	0.64
(1,352)	1:19:A:SER:H	1:18:A:GLY:HA2	10	0.56	0.12	0.55
(1,117)	1:26:A:ASP:HA	1:26:A:ASP:HB3	10	0.56	0.01	0.56

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,44)	1:11:A:ARG:HD2	1:11:A:ARG:HG2	10	0.54	0.02	0.55
(1,411)	1:32:A:CYS:H	1:31:A:SER:HB3	10	0.54	0.14	0.55
(1,3)	1:1:A:PRO:HD3	1:1:A:PRO:HG3	10	0.52	0.01	0.52
(1,122)	1:27:A:LYS:HA	1:27:A:LYS:HB2	10	0.52	0.08	0.48
(1,472)	1:49:A:THR:H	1:52:A:ASP:HB3	10	0.52	0.21	0.53
(1,47)	1:11:A:ARG:HG3	1:11:A:ARG:HG2	10	0.52	0.0	0.52
(1,78)	1:22:A:ASN:HA	1:22:A:ASN:HB2	10	0.52	0.03	0.54
(1,452)	1:42:A:GLY:H	1:41:A:GLY:HA3	10	0.52	0.15	0.51
(1,361)	1:21:A:THR:H	1:20:A:PHE:HB3	10	0.51	0.3	0.57
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG21	10	0.51	0.03	0.52
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG22	10	0.51	0.03	0.52
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG23	10	0.51	0.03	0.52
(1,196)	1:47:A:PHE:HA	1:48:A:LYS:HD3	10	0.5	0.21	0.48
(1,319)	1:13:A:TYR:H	1:12:A:ASN:HB2	10	0.49	0.09	0.48
(1,331)	1:15:A:LYS:H	1:15:A:LYS:HG3	10	0.49	0.17	0.45
(1,43)	1:11:A:ARG:HD2	1:11:A:ARG:HG3	10	0.49	0.08	0.46
(1,341)	1:17:A:SER:H	1:16:A:GLY:HA2	10	0.48	0.16	0.41
(1,81)	1:23:A:TYR:HA	1:23:A:TYR:HB3	10	0.47	0.02	0.48
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG11	10	0.46	0.04	0.48
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG12	10	0.46	0.04	0.48
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG13	10	0.46	0.04	0.48
(1,404)	1:30:A:SER:H	1:29:A:THR:HG21	10	0.46	0.09	0.44
(1,404)	1:30:A:SER:H	1:29:A:THR:HG22	10	0.46	0.09	0.44
(1,404)	1:30:A:SER:H	1:29:A:THR:HG23	10	0.46	0.09	0.44
(1,356)	1:20:A:PHE:H	1:19:A:SER:HB2	10	0.45	0.35	0.3
(1,213)	1:50:A:LEU:HD11	1:51:A:GLU:HG2	10	0.45	0.14	0.4
(1,213)	1:50:A:LEU:HD12	1:51:A:GLU:HG2	10	0.45	0.14	0.4
(1,213)	1:50:A:LEU:HD13	1:51:A:GLU:HG2	10	0.45	0.14	0.4
(1,143)	1:33:A:LYS:HA	1:33:A:LYS:HB3	10	0.44	0.06	0.46
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB1	10	0.44	0.11	0.43
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB2	10	0.44	0.11	0.43
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB3	10	0.44	0.11	0.43
(1,57)	1:15:A:LYS:HA	1:15:A:LYS:HG2	10	0.43	0.11	0.45
(1,18)	1:7:A:CYS:HA	1:57:A:CYS:HB2	10	0.43	0.2	0.36
(1,359)	1:20:A:PHE:H	1:20:A:PHE:HB2	10	0.42	0.15	0.47
(1,448)	1:41:A:GLY:H	1:40:A:SER:H	10	0.42	0.21	0.37
(1,26)	1:9:A:LEU:HD11	1:45:A:ASN:HB2	10	0.41	0.24	0.44
(1,26)	1:9:A:LEU:HD12	1:45:A:ASN:HB2	10	0.41	0.24	0.44
(1,26)	1:9:A:LEU:HD13	1:45:A:ASN:HB2	10	0.41	0.24	0.44
(1,4)	1:1:A:PRO:HD2	1:1:A:PRO:HG3	10	0.41	0.13	0.34
(1,1)	1:1:A:PRO:HB3	1:1:A:PRO:HD2	10	0.4	0.06	0.42
(1,345)	1:17:A:SER:H	1:38:A:ARG:HA	10	0.4	0.23	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,204)	1:48:A:LYS:HA	1:48:A:LYS:HD2	10	0.39	0.08	0.42
(1,115)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	10	0.39	0.0	0.39
(1,244)	1:55:A:ALA:HB1	1:56:A:THR:HB	10	0.39	0.07	0.38
(1,244)	1:55:A:ALA:HB2	1:56:A:THR:HB	10	0.39	0.07	0.38
(1,244)	1:55:A:ALA:HB3	1:56:A:THR:HB	10	0.39	0.07	0.38
(1,150)	1:33:A:LYS:HG2	1:33:A:LYS:HA	10	0.38	0.26	0.31
(1,304)	1:11:A:ARG:H	1:10:A:SER:HB2	10	0.38	0.07	0.4
(1,442)	1:38:A:ARG:H	1:38:A:ARG:HB2	10	0.38	0.13	0.45
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD21	10	0.38	0.17	0.3
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD22	10	0.38	0.17	0.3
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD23	10	0.38	0.17	0.3
(1,527)	1:58:A:VAL:H	1:57:A:CYS:H	10	0.38	0.1	0.36
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB1	10	0.38	0.03	0.38
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB2	10	0.38	0.03	0.38
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB3	10	0.38	0.03	0.38
(1,266)	1:3:A:GLN:H	1:4:A:ASP:H	10	0.35	0.14	0.3
(1,438)	1:38:A:ARG:H	1:36:A:ARG:HB2	10	0.34	0.15	0.34
(1,441)	1:38:A:ARG:H	1:38:A:ARG:HA	10	0.33	0.04	0.34
(1,246)	1:56:A:THR:HG21	1:56:A:THR:HB	10	0.33	0.0	0.33
(1,246)	1:56:A:THR:HG22	1:56:A:THR:HB	10	0.33	0.0	0.33
(1,246)	1:56:A:THR:HG23	1:56:A:THR:HB	10	0.33	0.0	0.33
(1,80)	1:22:A:ASN:HD21	1:22:A:ASN:HD22	10	0.33	0.0	0.33
(1,151)	1:34:A:THR:HA	1:23:A:TYR:HA	10	0.33	0.07	0.32
(1,330)	1:15:A:LYS:H	1:15:A:LYS:HB2	10	0.33	0.04	0.34
(1,64)	1:19:A:SER:HA	1:19:A:SER:HB3	10	0.32	0.02	0.32
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD21	10	0.32	0.09	0.3
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD22	10	0.32	0.09	0.3
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD23	10	0.32	0.09	0.3
(1,389)	1:27:A:LYS:H	1:27:A:LYS:HB2	10	0.32	0.17	0.31
(1,308)	1:12:A:ASN:H	1:11:A:ARG:HA	10	0.31	0.07	0.32
(1,214)	1:50:A:LEU:HD21	1:54:A:GLU:HB2	10	0.31	0.03	0.3
(1,214)	1:50:A:LEU:HD22	1:54:A:GLU:HB2	10	0.31	0.03	0.3
(1,214)	1:50:A:LEU:HD23	1:54:A:GLU:HB2	10	0.31	0.03	0.3
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG21	10	0.3	0.01	0.3
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG22	10	0.3	0.01	0.3
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG23	10	0.3	0.01	0.3
(1,248)	1:57:A:CYS:HA	1:7:A:CYS:HA	10	0.3	0.08	0.31
(1,363)	1:21:A:THR:H	1:21:A:THR:HA	10	0.3	0.08	0.24
(1,198)	1:47:A:PHE:HB3	1:47:A:PHE:HB2	10	0.3	0.0	0.3
(1,230)	1:53:A:CYS:HB3	1:53:A:CYS:HB2	10	0.3	0.0	0.3
(1,262)	1:61:A:GLU:HG2	1:61:A:GLU:HG3	10	0.3	0.0	0.3
(1,186)	1:38:A:ARG:HD3	1:38:A:ARG:HG3	10	0.3	0.06	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,222)	1:51:A:GLU:HG3	1:51:A:GLU:HG2	10	0.3	0.0	0.3
(1,237)	1:54:A:GLU:HB2	1:54:A:GLU:HB3	10	0.3	0.0	0.3
(1,289)	1:8:A:GLN:HE21	1:8:A:GLN:HE22	10	0.3	0.0	0.3
(1,316)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	10	0.3	0.0	0.3
(1,130)	1:30:A:SER:HB3	1:30:A:SER:HB2	10	0.3	0.0	0.3
(1,267)	1:3:A:GLN:HE21	1:3:A:GLN:HE22	10	0.3	0.0	0.3
(1,181)	1:37:A:TYR:HB3	1:37:A:TYR:HB2	10	0.3	0.0	0.3
(1,140)	1:32:A:CYS:HB3	1:32:A:CYS:HB2	10	0.29	0.0	0.29
(1,134)	1:32:A:CYS:HA	1:25:A:TYR:HB3	10	0.28	0.26	0.2
(1,495)	1:52:A:ASP:H	1:52:A:ASP:HB3	10	0.28	0.09	0.3
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG11	10	0.28	0.07	0.29
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG12	10	0.28	0.07	0.29
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG13	10	0.28	0.07	0.29
(1,327)	1:14:A:GLY:H	1:14:A:GLY:HA3	10	0.28	0.07	0.26
(1,243)	1:55:A:ALA:HB1	1:55:A:ALA:H	10	0.28	0.01	0.28
(1,243)	1:55:A:ALA:HB2	1:55:A:ALA:H	10	0.28	0.01	0.28
(1,243)	1:55:A:ALA:HB3	1:55:A:ALA:H	10	0.28	0.01	0.28
(1,55)	1:15:A:LYS:HA	1:15:A:LYS:HB3	10	0.27	0.04	0.29
(1,314)	1:12:A:ASN:HD21	1:12:A:ASN:HB3	10	0.27	0.03	0.28
(1,169)	1:35:A:PHE:HE1	1:37:A:TYR:HA	10	0.27	0.06	0.24
(1,245)	1:56:A:THR:HG21	1:53:A:CYS:HA	10	0.26	0.06	0.26
(1,245)	1:56:A:THR:HG22	1:53:A:CYS:HA	10	0.26	0.06	0.26
(1,245)	1:56:A:THR:HG23	1:53:A:CYS:HA	10	0.26	0.06	0.26
(1,9)	1:4:A:ASP:HB2	1:4:A:ASP:HB3	10	0.26	0.0	0.26
(1,125)	1:27:A:LYS:HB3	1:27:A:LYS:HG3	10	0.25	0.02	0.26
(1,29)	1:10:A:SER:HB3	1:10:A:SER:HB2	10	0.25	0.0	0.25
(1,440)	1:38:A:ARG:H	1:37:A:TYR:HB3	10	0.25	0.1	0.18
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG21	10	0.24	0.04	0.24
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG22	10	0.24	0.04	0.24
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG23	10	0.24	0.04	0.24
(1,511)	1:55:A:ALA:H	1:54:A:GLU:HG3	10	0.24	0.06	0.24
(1,21)	1:8:A:GLN:HA	1:8:A:GLN:HB3	10	0.22	0.03	0.22
(1,102)	1:24:A:TYR:HD1	1:24:A:TYR:HA	10	0.21	0.05	0.21
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG21	10	0.21	0.02	0.2
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG22	10	0.21	0.02	0.2
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG23	10	0.21	0.02	0.2
(1,238)	1:54:A:GLU:HB2	1:55:A:ALA:H	10	0.21	0.04	0.22
(1,406)	1:30:A:SER:H	1:30:A:SER:HB2	10	0.19	0.05	0.19
(2,29)	1:59:A:THR:H	1:55:A:ALA:O	10	0.18	0.02	0.18
(1,141)	1:32:A:CYS:HB3	1:50:A:LEU:HB3	10	0.17	0.05	0.16
(1,65)	1:19:A:SER:HA	1:19:A:SER:HB2	10	0.16	0.03	0.16
(1,540)	1:61:A:GLU:H	1:61:A:GLU:HA	10	0.16	0.04	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,501)	1:53:A:CYS:H	1:52:A:ASP:HB2	10	0.16	0.03	0.15
(1,136)	1:32:A:CYS:HA	1:32:A:CYS:HB3	10	0.15	0.02	0.15
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG21	10	0.15	0.01	0.15
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG22	10	0.15	0.01	0.15
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG23	10	0.15	0.01	0.15
(1,255)	1:58:A:VAL:HG11	1:58:A:VAL:HB	10	0.14	0.0	0.14
(1,255)	1:58:A:VAL:HG12	1:58:A:VAL:HB	10	0.14	0.0	0.14
(1,255)	1:58:A:VAL:HG13	1:58:A:VAL:HB	10	0.14	0.0	0.14
(1,144)	1:33:A:LYS:HA	1:33:A:LYS:HD2	9	0.67	0.32	0.75
(1,350)	1:18:A:GLY:H	1:19:A:SER:H	9	0.63	0.26	0.66
(1,456)	1:43:A:ASN:H	1:43:A:ASN:HB3	9	0.56	0.29	0.66
(1,340)	1:17:A:SER:H	1:16:A:GLY:HA3	9	0.53	0.17	0.45
(1,351)	1:19:A:SER:H	1:18:A:GLY:HA3	9	0.48	0.28	0.4
(1,443)	1:38:A:ARG:H	1:39:A:GLY:H	9	0.44	0.07	0.43
(1,292)	1:9:A:LEU:H	1:8:A:GLN:H	9	0.41	0.19	0.44
(1,454)	1:43:A:ASN:H	1:12:A:ASN:HB3	9	0.41	0.26	0.28
(1,249)	1:57:A:CYS:HA	1:7:A:CYS:HB2	9	0.41	0.13	0.42
(1,543)	1:61:A:GLU:H	1:61:A:GLU:HG2	9	0.39	0.17	0.38
(1,465)	1:48:A:LYS:H	1:49:A:THR:H	9	0.39	0.13	0.38
(1,23)	1:9:A:LEU:HA	1:5:A:TYR:HB3	9	0.39	0.24	0.44
(1,446)	1:40:A:SER:H	1:40:A:SER:HB3	9	0.38	0.2	0.33
(1,459)	1:47:A:PHE:H	1:46:A:ARG:HG2	9	0.36	0.11	0.41
(1,269)	1:4:A:ASP:H	1:3:A:GLN:HB3	9	0.35	0.29	0.21
(1,449)	1:41:A:GLY:H	1:40:A:SER:HA	9	0.35	0.21	0.35
(1,281)	1:7:A:CYS:H	1:6:A:ARG:HG3	9	0.35	0.16	0.28
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD11	9	0.34	0.15	0.34
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD12	9	0.34	0.15	0.34
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD13	9	0.34	0.15	0.34
(1,475)	1:50:A:LEU:H	1:49:A:THR:HB	9	0.33	0.15	0.32
(1,354)	1:19:A:SER:H	1:19:A:SER:HB3	9	0.31	0.16	0.27
(1,458)	1:47:A:PHE:H	1:46:A:ARG:HG3	9	0.3	0.03	0.31
(1,322)	1:13:A:TYR:H	1:13:A:TYR:HB2	9	0.3	0.2	0.19
(1,402)	1:30:A:SER:H	1:27:A:LYS:HA	9	0.29	0.12	0.24
(1,208)	1:48:A:LYS:HD3	1:48:A:LYS:HA	9	0.28	0.1	0.28
(1,353)	1:19:A:SER:H	1:19:A:SER:HA	9	0.28	0.06	0.29
(1,234)	1:54:A:GLU:HA	1:58:A:VAL:HB	9	0.27	0.14	0.21
(1,542)	1:61:A:GLU:H	1:61:A:GLU:HG3	9	0.26	0.15	0.21
(1,49)	1:12:A:ASN:HA	1:12:A:ASN:HB2	9	0.25	0.05	0.26
(1,462)	1:48:A:LYS:H	1:48:A:LYS:HB2	9	0.25	0.11	0.2
(1,164)	1:35:A:PHE:HD1	1:34:A:THR:HA	9	0.24	0.1	0.24
(1,165)	1:35:A:PHE:HD1	1:34:A:THR:HB	9	0.24	0.05	0.25
(1,172)	1:36:A:ARG:HA	1:21:A:THR:HA	9	0.24	0.1	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,88)	1:23:A:TYR:HE1	1:49:A:THR:HA	9	0.24	0.11	0.21
(1,394)	1:28:A:ALA:H	1:29:A:THR:H	9	0.22	0.06	0.22
(1,321)	1:13:A:TYR:H	1:13:A:TYR:HB3	9	0.22	0.07	0.24
(1,541)	1:61:A:GLU:H	1:61:A:GLU:HB2	9	0.22	0.23	0.16
(1,426)	1:35:A:PHE:H	1:34:A:THR:HB	9	0.22	0.06	0.22
(1,259)	1:61:A:GLU:HA	1:61:A:GLU:HG2	9	0.2	0.06	0.21
(1,148)	1:33:A:LYS:HE3	1:33:A:LYS:HD2	9	0.2	0.03	0.2
(1,506)	1:54:A:GLU:H	1:53:A:CYS:HB3	9	0.19	0.08	0.19
(1,146)	1:33:A:LYS:HA	1:33:A:LYS:HG3	9	0.19	0.05	0.19
(1,481)	1:51:A:GLU:H	1:50:A:LEU:H	9	0.18	0.06	0.19
(1,513)	1:55:A:ALA:H	1:56:A:THR:H	9	0.18	0.03	0.18
(1,503)	1:53:A:CYS:H	1:53:A:CYS:HB2	9	0.18	0.03	0.18
(2,31)	1:60:A:ALA:H	1:56:A:THR:O	9	0.15	0.03	0.15
(1,528)	1:58:A:VAL:H	1:58:A:VAL:HA	9	0.15	0.02	0.15
(1,419)	1:34:A:THR:H	1:33:A:LYS:HB3	8	0.7	0.32	0.68
(1,182)	1:37:A:TYR:HB2	1:20:A:PHE:HB3	8	0.49	0.39	0.3
(1,310)	1:12:A:ASN:H	1:11:A:ARG:HG3	8	0.48	0.2	0.43
(1,325)	1:14:A:GLY:H	1:13:A:TYR:HB3	8	0.44	0.33	0.33
(1,299)	1:10:A:SER:H	1:9:A:LEU:HB3	8	0.43	0.14	0.36
(1,264)	1:3:A:GLN:H	1:3:A:GLN:HB2	8	0.41	0.27	0.38
(1,347)	1:18:A:GLY:H	1:17:A:SER:HB2	8	0.39	0.22	0.27
(1,313)	1:12:A:ASN:H	1:12:A:ASN:HB2	8	0.39	0.32	0.24
(1,453)	1:42:A:GLY:H	1:41:A:GLY:HA2	8	0.39	0.22	0.38
(1,94)	1:24:A:TYR:HB3	1:11:A:ARG:HB3	8	0.37	0.11	0.37
(1,344)	1:17:A:SER:H	1:18:A:GLY:H	8	0.36	0.13	0.32
(1,396)	1:28:A:ALA:H	1:30:A:SER:H	8	0.34	0.12	0.37
(1,227)	1:53:A:CYS:HB3	1:32:A:CYS:HB2	8	0.33	0.1	0.31
(1,312)	1:12:A:ASN:H	1:12:A:ASN:HB3	8	0.33	0.11	0.36
(1,307)	1:11:A:ARG:H	1:11:A:ARG:HG2	8	0.32	0.1	0.34
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD11	8	0.32	0.08	0.34
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD12	8	0.32	0.08	0.34
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD13	8	0.32	0.08	0.34
(1,261)	1:61:A:GLU:HG2	1:59:A:THR:HA	8	0.28	0.13	0.28
(1,271)	1:4:A:ASP:H	1:4:A:ASP:HB3	8	0.24	0.15	0.19
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG21	8	0.24	0.09	0.2
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG22	8	0.24	0.09	0.2
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG23	8	0.24	0.09	0.2
(1,272)	1:4:A:ASP:H	1:4:A:ASP:HB2	8	0.23	0.08	0.21
(1,171)	1:35:A:PHE:HE1	1:37:A:TYR:HB2	8	0.23	0.09	0.2
(1,444)	1:39:A:GLY:H	1:40:A:SER:H	8	0.22	0.05	0.24
(1,194)	1:47:A:PHE:HA	1:46:A:ARG:HG2	8	0.22	0.1	0.16
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD21	8	0.22	0.05	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD22	8	0.22	0.05	0.24
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD23	8	0.22	0.05	0.24
(1,6)	1:3:A:GLN:HB3	1:3:A:GLN:HA	8	0.22	0.14	0.15
(1,490)	1:52:A:ASP:H	1:49:A:THR:HB	8	0.2	0.06	0.2
(1,526)	1:58:A:VAL:H	1:54:A:GLU:HA	8	0.2	0.07	0.2
(1,273)	1:5:A:TYR:H	1:4:A:ASP:HB2	8	0.2	0.04	0.22
(1,445)	1:40:A:SER:H	1:40:A:SER:HA	8	0.2	0.13	0.16
(1,287)	1:8:A:GLN:H	1:7:A:CYS:HA	8	0.19	0.11	0.12
(1,401)	1:29:A:THR:H	1:29:A:THR:HG21	8	0.18	0.05	0.17
(1,401)	1:29:A:THR:H	1:29:A:THR:HG22	8	0.18	0.05	0.17
(1,401)	1:29:A:THR:H	1:29:A:THR:HG23	8	0.18	0.05	0.17
(1,496)	1:52:A:ASP:H	1:52:A:ASP:HB2	8	0.17	0.05	0.17
(1,348)	1:18:A:GLY:H	1:18:A:GLY:HA3	8	0.16	0.04	0.16
(1,224)	1:52:A:ASP:HA	1:52:A:ASP:HB2	8	0.16	0.03	0.16
(1,539)	1:61:A:GLU:H	1:60:A:ALA:HA	8	0.15	0.03	0.14
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG21	8	0.14	0.05	0.12
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG22	8	0.14	0.05	0.12
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG23	8	0.14	0.05	0.12
(1,505)	1:54:A:GLU:H	1:53:A:CYS:H	8	0.13	0.03	0.12
(1,346)	1:18:A:GLY:H	1:17:A:SER:HA	8	0.12	0.01	0.12
(1,447)	1:40:A:SER:H	1:40:A:SER:HB2	7	0.48	0.19	0.55
(1,183)	1:37:A:TYR:HB2	1:22:A:ASN:HB2	7	0.46	0.32	0.35
(1,463)	1:48:A:LYS:H	1:48:A:LYS:HD3	7	0.43	0.23	0.32
(1,455)	1:43:A:ASN:H	1:12:A:ASN:HB2	7	0.36	0.16	0.41
(1,464)	1:48:A:LYS:H	1:48:A:LYS:HD2	7	0.34	0.11	0.39
(1,358)	1:20:A:PHE:H	1:20:A:PHE:HB3	7	0.33	0.11	0.34
(1,326)	1:14:A:GLY:H	1:13:A:TYR:HB2	7	0.29	0.07	0.27
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG21	7	0.29	0.1	0.33
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG22	7	0.29	0.1	0.33
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG23	7	0.29	0.1	0.33
(1,492)	1:52:A:ASP:H	1:51:A:GLU:HG3	7	0.28	0.08	0.3
(1,199)	1:47:A:PHE:HB3	1:53:A:CYS:HA	7	0.27	0.13	0.28
(1,328)	1:14:A:GLY:H	1:14:A:GLY:HA2	7	0.27	0.16	0.18
(1,73)	1:20:A:PHE:HA	1:20:A:PHE:HB2	7	0.27	0.1	0.32
(1,434)	1:36:A:ARG:H	1:36:A:ARG:HG2	7	0.27	0.08	0.24
(1,343)	1:17:A:SER:H	1:17:A:SER:HB3	7	0.26	0.11	0.19
(1,297)	1:9:A:LEU:H	1:9:A:LEU:HG	7	0.25	0.18	0.15
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD11	7	0.24	0.04	0.24
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD12	7	0.24	0.04	0.24
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD13	7	0.24	0.04	0.24
(1,302)	1:10:A:SER:H	1:10:A:SER:HB3	7	0.24	0.09	0.21
(1,332)	1:15:A:LYS:H	1:15:A:LYS:HG2	7	0.23	0.04	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,306)	1:11:A:ARG:H	1:11:A:ARG:HB3	7	0.22	0.1	0.18
(1,418)	1:34:A:THR:H	1:33:A:LYS:HA	7	0.21	0.12	0.14
(1,333)	1:15:A:LYS:H	1:16:A:GLY:H	7	0.2	0.06	0.23
(1,420)	1:34:A:THR:H	1:33:A:LYS:HD3	7	0.2	0.06	0.18
(1,355)	1:20:A:PHE:H	1:19:A:SER:HA	7	0.19	0.15	0.12
(1,478)	1:50:A:LEU:H	1:50:A:LEU:HB2	7	0.19	0.03	0.18
(1,282)	1:7:A:CYS:H	1:6:A:ARG:HG2	7	0.17	0.09	0.15
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG21	7	0.17	0.04	0.16
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG22	7	0.17	0.04	0.16
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG23	7	0.17	0.04	0.16
(1,188)	1:40:A:SER:HA	1:41:A:GLY:HA2	7	0.17	0.05	0.16
(1,335)	1:16:A:GLY:H	1:15:A:LYS:HB3	7	0.17	0.05	0.14
(1,518)	1:56:A:THR:H	1:56:A:THR:HG21	7	0.16	0.03	0.17
(1,518)	1:56:A:THR:H	1:56:A:THR:HG22	7	0.16	0.03	0.17
(1,518)	1:56:A:THR:H	1:56:A:THR:HG23	7	0.16	0.03	0.17
(1,480)	1:51:A:GLU:H	1:49:A:THR:HB	7	0.16	0.07	0.13
(1,483)	1:51:A:GLU:H	1:50:A:LEU:HB3	7	0.16	0.03	0.17
(1,225)	1:53:A:CYS:H	1:53:A:CYS:HB3	7	0.15	0.03	0.14
(1,433)	1:36:A:ARG:H	1:36:A:ARG:HB2	7	0.15	0.03	0.14
(1,430)	1:36:A:ARG:H	1:35:A:PHE:HA	7	0.14	0.03	0.15
(1,126)	1:27:A:LYS:HB2	1:27:A:LYS:HA	7	0.14	0.02	0.14
(1,461)	1:48:A:LYS:H	1:48:A:LYS:HA	7	0.14	0.02	0.14
(1,42)	1:11:A:ARG:HD2	1:11:A:ARG:HB2	6	0.72	0.36	0.82
(1,362)	1:21:A:THR:H	1:20:A:PHE:HB2	6	0.38	0.26	0.3
(1,303)	1:11:A:ARG:H	1:10:A:SER:HA	6	0.36	0.34	0.2
(1,311)	1:12:A:ASN:H	1:11:A:ARG:HG2	6	0.28	0.22	0.22
(1,469)	1:49:A:THR:H	1:48:A:LYS:HB2	6	0.25	0.1	0.22
(1,424)	1:35:A:PHE:H	1:22:A:ASN:H	6	0.24	0.07	0.22
(1,451)	1:41:A:GLY:H	1:41:A:GLY:HA2	6	0.23	0.08	0.21
(1,384)	1:26:A:ASP:H	1:26:A:ASP:HB2	6	0.22	0.09	0.2
(1,380)	1:25:A:TYR:H	1:25:A:TYR:HB3	6	0.21	0.12	0.16
(1,187)	1:40:A:SER:HA	1:41:A:GLY:HA3	6	0.2	0.05	0.22
(1,474)	1:50:A:LEU:H	1:49:A:THR:HA	6	0.2	0.05	0.2
(1,383)	1:26:A:ASP:H	1:26:A:ASP:HB3	6	0.19	0.05	0.18
(1,285)	1:7:A:CYS:H	1:7:A:CYS:HB2	6	0.19	0.07	0.18
(1,487)	1:51:A:GLU:H	1:51:A:GLU:HG3	6	0.18	0.07	0.16
(1,388)	1:27:A:LYS:H	1:27:A:LYS:HB3	6	0.17	0.04	0.18
(1,185)	1:37:A:TYR:HB2	1:46:A:ARG:HG3	6	0.17	0.05	0.15
(1,291)	1:9:A:LEU:H	1:5:A:TYR:HB3	6	0.16	0.06	0.13
(1,391)	1:28:A:ALA:H	1:27:A:LYS:HA	6	0.16	0.04	0.16
(1,24)	1:9:A:LEU:HA	1:9:A:LEU:HG	6	0.14	0.03	0.14
(1,298)	1:10:A:SER:H	1:9:A:LEU:HA	5	0.47	0.15	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,34)	1:11:A:ARG:HB3	1:11:A:ARG:HG2	5	0.41	0.11	0.43
(1,168)	1:35:A:PHE:HD1	1:37:A:TYR:HB2	5	0.27	0.07	0.32
(1,417)	1:33:A:LYS:H	1:33:A:LYS:HB3	5	0.24	0.15	0.18
(1,295)	1:9:A:LEU:H	1:9:A:LEU:HA	5	0.24	0.15	0.12
(1,410)	1:32:A:CYS:H	1:31:A:SER:HA	5	0.22	0.08	0.2
(1,498)	1:53:A:CYS:H	1:47:A:PHE:HB3	5	0.2	0.08	0.16
(1,290)	1:9:A:LEU:H	1:5:A:TYR:HA	5	0.18	0.12	0.13
(1,423)	1:35:A:PHE:H	1:21:A:THR:HG21	5	0.18	0.06	0.17
(1,423)	1:35:A:PHE:H	1:21:A:THR:HG22	5	0.18	0.06	0.17
(1,423)	1:35:A:PHE:H	1:21:A:THR:HG23	5	0.18	0.06	0.17
(1,177)	1:36:A:ARG:HG2	1:35:A:PHE:HA	5	0.17	0.07	0.12
(1,278)	1:6:A:ARG:H	1:6:A:ARG:HG2	5	0.17	0.07	0.14
(1,277)	1:6:A:ARG:H	1:6:A:ARG:HG3	5	0.16	0.01	0.16
(1,450)	1:41:A:GLY:H	1:41:A:GLY:HA3	5	0.16	0.02	0.16
(1,192)	1:46:A:ARG:HA	1:46:A:ARG:HG3	5	0.15	0.02	0.15
(1,439)	1:38:A:ARG:H	1:37:A:TYR:HA	5	0.15	0.06	0.11
(1,497)	1:52:A:ASP:H	1:53:A:CYS:H	5	0.14	0.02	0.14
(1,425)	1:35:A:PHE:H	1:34:A:THR:HA	5	0.14	0.01	0.14
(1,270)	1:4:A:ASP:H	1:4:A:ASP:HA	5	0.13	0.02	0.13
(1,203)	1:48:A:LYS:HA	1:22:A:ASN:HA	5	0.12	0.02	0.11
(1,138)	1:32:A:CYS:HA	1:50:A:LEU:HB2	5	0.11	0.02	0.1
(1,147)	1:33:A:LYS:HE3	1:33:A:LYS:HD3	4	0.44	0.08	0.44
(1,360)	1:21:A:THR:H	1:20:A:PHE:HA	4	0.4	0.03	0.4
(1,190)	1:40:A:SER:HB2	1:40:A:SER:HA	4	0.34	0.22	0.34
(1,5)	1:3:A:GLN:HA	1:3:A:GLN:HB2	4	0.31	0.14	0.3
(1,381)	1:25:A:TYR:H	1:25:A:TYR:HB2	4	0.29	0.27	0.14
(1,45)	1:11:A:ARG:HG3	1:11:A:ARG:HB3	4	0.27	0.08	0.29
(1,504)	1:54:A:GLU:H	1:50:A:LEU:HD21	4	0.24	0.06	0.24
(1,504)	1:54:A:GLU:H	1:50:A:LEU:HD22	4	0.24	0.06	0.24
(1,504)	1:54:A:GLU:H	1:50:A:LEU:HD23	4	0.24	0.06	0.24
(1,260)	1:61:A:GLU:HG3	1:61:A:GLU:HA	4	0.22	0.15	0.16
(1,263)	1:3:A:GLN:H	1:3:A:GLN:HA	4	0.21	0.19	0.11
(1,488)	1:51:A:GLU:H	1:51:A:GLU:HG2	4	0.21	0.04	0.22
(1,376)	1:24:A:TYR:H	1:34:A:THR:HA	4	0.21	0.02	0.2
(1,338)	1:16:A:GLY:H	1:16:A:GLY:HA2	4	0.19	0.04	0.19
(1,468)	1:49:A:THR:H	1:48:A:LYS:HB3	4	0.18	0.01	0.18
(1,369)	1:23:A:TYR:H	1:22:A:ASN:HB3	4	0.18	0.04	0.17
(1,413)	1:32:A:CYS:H	1:32:A:CYS:HB2	4	0.17	0.04	0.18
(1,466)	1:49:A:THR:H	1:47:A:PHE:HB3	4	0.16	0.06	0.16
(1,436)	1:37:A:TYR:H	1:36:A:ARG:HB2	4	0.14	0.04	0.14
(1,61)	1:17:A:SER:HA	1:17:A:SER:HB2	4	0.14	0.01	0.15
(1,500)	1:53:A:CYS:H	1:52:A:ASP:HB3	4	0.14	0.03	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,375)	1:24:A:TYR:H	1:33:A:LYS:H	4	0.13	0.02	0.14
(1,385)	1:26:A:ASP:H	1:32:A:CYS:HA	4	0.13	0.02	0.13
(1,408)	1:31:A:SER:H	1:30:A:SER:HA	4	0.13	0.03	0.13
(1,536)	1:60:A:ALA:H	1:59:A:THR:HB	4	0.13	0.03	0.12
(1,367)	1:22:A:ASN:H	1:22:A:ASN:HB2	4	0.13	0.02	0.12
(1,320)	1:13:A:TYR:H	1:13:A:TYR:HA	4	0.12	0.02	0.12
(1,531)	1:59:A:THR:H	1:58:A:VAL:HB	4	0.12	0.01	0.12
(1,431)	1:36:A:ARG:H	1:36:A:ARG:HA	4	0.12	0.01	0.12
(1,170)	1:35:A:PHE:HE1	1:37:A:TYR:HA	4	0.11	0.02	0.11
(1,189)	1:40:A:SER:HB3	1:40:A:SER:HA	3	0.53	0.06	0.52
(1,493)	1:52:A:ASP:H	1:51:A:GLU:HG2	3	0.26	0.09	0.31
(1,210)	1:49:A:THR:HB	1:51:A:GLU:HG2	3	0.2	0.12	0.12
(1,205)	1:48:A:LYS:HB3	1:48:A:LYS:HA	3	0.2	0.04	0.22
(1,499)	1:53:A:CYS:H	1:50:A:LEU:HA	3	0.19	0.06	0.17
(1,525)	1:57:A:CYS:H	1:57:A:CYS:HB2	3	0.19	0.02	0.17
(1,30)	1:11:A:ARG:HA	1:10:A:SER:HA	3	0.18	0.06	0.15
(1,429)	1:35:A:PHE:H	1:35:A:PHE:HD1	3	0.18	0.08	0.14
(1,284)	1:7:A:CYS:H	1:7:A:CYS:HB3	3	0.18	0.01	0.17
(1,524)	1:57:A:CYS:H	1:57:A:CYS:HB3	3	0.18	0.02	0.17
(1,135)	1:32:A:CYS:HA	1:25:A:TYR:HB2	3	0.17	0.1	0.1
(1,471)	1:49:A:THR:H	1:49:A:THR:HG21	3	0.16	0.03	0.18
(1,471)	1:49:A:THR:H	1:49:A:THR:HG22	3	0.16	0.03	0.18
(1,471)	1:49:A:THR:H	1:49:A:THR:HG23	3	0.16	0.03	0.18
(1,371)	1:23:A:TYR:H	1:23:A:TYR:HD1	3	0.16	0.02	0.16
(1,93)	1:24:A:TYR:HA	1:47:A:PHE:HB3	3	0.15	0.02	0.15
(1,336)	1:16:A:GLY:H	1:15:A:LYS:HG2	3	0.14	0.04	0.11
(1,364)	1:22:A:ASN:H	1:21:A:THR:HA	3	0.13	0.0	0.13
(1,486)	1:51:A:GLU:H	1:51:A:GLU:HB3	3	0.13	0.0	0.13
(1,242)	1:55:A:ALA:HB1	1:52:A:ASP:HA	3	0.13	0.0	0.13
(1,242)	1:55:A:ALA:HB2	1:52:A:ASP:HA	3	0.13	0.0	0.13
(1,242)	1:55:A:ALA:HB3	1:52:A:ASP:HA	3	0.13	0.0	0.13
(1,279)	1:6:A:ARG:H	1:7:A:CYS:H	3	0.12	0.01	0.13
(1,160)	1:35:A:PHE:HA	1:36:A:ARG:HA	3	0.12	0.01	0.12
(1,398)	1:29:A:THR:H	1:28:A:ALA:HA	3	0.12	0.01	0.12
(1,256)	1:59:A:THR:HA	1:58:A:VAL:HG11	3	0.11	0.01	0.11
(1,256)	1:59:A:THR:HA	1:58:A:VAL:HG12	3	0.11	0.01	0.11
(1,256)	1:59:A:THR:HA	1:58:A:VAL:HG13	3	0.11	0.01	0.11
(1,158)	1:35:A:PHE:HA	1:34:A:THR:HB	3	0.11	0.0	0.11
(1,473)	1:49:A:THR:H	1:52:A:ASP:HB2	2	0.16	0.06	0.16
(1,16)	1:7:A:CYS:HA	1:6:A:ARG:HA	2	0.14	0.03	0.14
(1,131)	1:30:A:SER:HB2	1:29:A:THR:HA	2	0.14	0.0	0.14
(1,293)	1:9:A:LEU:H	1:8:A:GLN:HA	2	0.14	0.03	0.14

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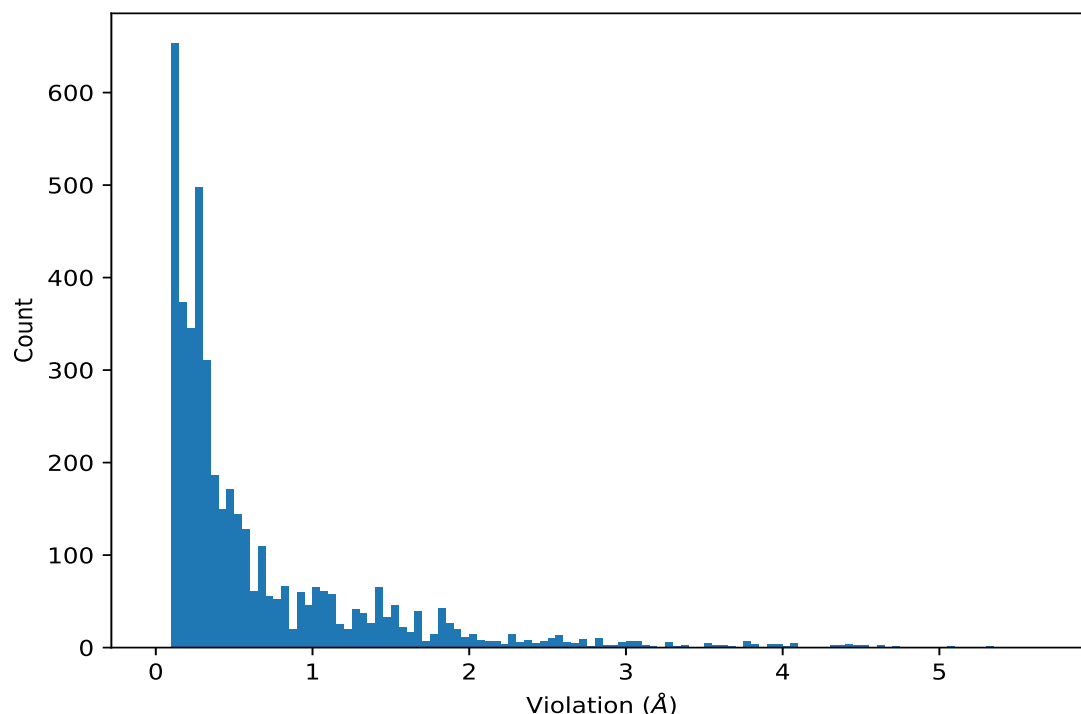
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,397)	1:29:A:THR:H	1:27:A:LYS:HA	2	0.12	0.01	0.12
(1,395)	1:28:A:ALA:H	1:29:A:THR:HG21	2	0.12	0.01	0.12
(1,395)	1:28:A:ALA:H	1:29:A:THR:HG22	2	0.12	0.01	0.12
(1,395)	1:28:A:ALA:H	1:29:A:THR:HG23	2	0.12	0.01	0.12
(1,28)	1:10:A:SER:HB3	1:10:A:SER:HA	2	0.12	0.0	0.12
(1,155)	1:34:A:THR:HB	1:21:A:THR:HA	2	0.12	0.0	0.12
(1,422)	1:35:A:PHE:H	1:21:A:THR:HA	2	0.12	0.0	0.12
(1,7)	1:4:A:ASP:HA	1:4:A:ASP:HB2	2	0.11	0.01	0.11
(1,32)	1:11:A:ARG:HA	1:11:A:ARG:HB2	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,109)	1:24:A:TYR:HE1	1:11:A:ARG:HG3	6	5.66
(1,109)	1:24:A:TYR:HE1	1:11:A:ARG:HG3	8	5.35
(1,109)	1:24:A:TYR:HE1	1:11:A:ARG:HG3	1	5.33
(1,109)	1:24:A:TYR:HE1	1:11:A:ARG:HG3	3	5.29
(1,109)	1:24:A:TYR:HE1	1:11:A:ARG:HG3	4	5.13
(1,98)	1:24:A:TYR:HD1	1:11:A:ARG:HD3	7	5.08
(1,98)	1:24:A:TYR:HD1	1:11:A:ARG:HD3	9	5.07
(1,109)	1:24:A:TYR:HE1	1:11:A:ARG:HG3	2	4.96
(1,112)	1:24:A:TYR:HE1	1:26:A:ASP:HA	8	4.76
(1,112)	1:24:A:TYR:HE1	1:26:A:ASP:HA	9	4.72
(1,98)	1:24:A:TYR:HD1	1:11:A:ARG:HD3	10	4.72
(1,98)	1:24:A:TYR:HD1	1:11:A:ARG:HD3	5	4.64
(1,107)	1:24:A:TYR:HE1	1:11:A:ARG:HD3	7	4.62
(1,100)	1:24:A:TYR:HD1	1:11:A:ARG:HG3	6	4.62
(1,110)	1:24:A:TYR:HE1	1:11:A:ARG:HG2	8	4.54
(1,110)	1:24:A:TYR:HE1	1:11:A:ARG:HG2	1	4.51
(1,107)	1:24:A:TYR:HE1	1:11:A:ARG:HD3	9	4.51
(1,112)	1:24:A:TYR:HE1	1:26:A:ASP:HA	7	4.46
(1,110)	1:24:A:TYR:HE1	1:11:A:ARG:HG2	4	4.46
(1,112)	1:24:A:TYR:HE1	1:26:A:ASP:HA	5	4.45
(1,112)	1:24:A:TYR:HE1	1:26:A:ASP:HA	4	4.44
(1,98)	1:24:A:TYR:HD1	1:11:A:ARG:HD3	2	4.44
(1,98)	1:24:A:TYR:HD1	1:11:A:ARG:HD3	8	4.44
(1,112)	1:24:A:TYR:HE1	1:26:A:ASP:HA	10	4.4
(1,100)	1:24:A:TYR:HD1	1:11:A:ARG:HG3	1	4.39
(1,110)	1:24:A:TYR:HE1	1:11:A:ARG:HG2	6	4.36
(1,98)	1:24:A:TYR:HD1	1:11:A:ARG:HD3	1	4.36
(1,98)	1:24:A:TYR:HD1	1:11:A:ARG:HD3	4	4.35
(1,110)	1:24:A:TYR:HE1	1:11:A:ARG:HG2	2	4.34
(1,100)	1:24:A:TYR:HD1	1:11:A:ARG:HG3	3	4.33
(1,110)	1:24:A:TYR:HE1	1:11:A:ARG:HG2	3	4.29
(1,100)	1:24:A:TYR:HD1	1:11:A:ARG:HG3	8	4.22
(1,107)	1:24:A:TYR:HE1	1:11:A:ARG:HD3	10	4.18
(1,110)	1:24:A:TYR:HE1	1:11:A:ARG:HG2	5	4.09
(1,107)	1:24:A:TYR:HE1	1:11:A:ARG:HD3	5	4.09
(1,100)	1:24:A:TYR:HD1	1:11:A:ARG:HG3	2	4.09
(1,112)	1:24:A:TYR:HE1	1:26:A:ASP:HA	2	4.07
(1,101)	1:24:A:TYR:HD1	1:11:A:ARG:HG2	8	4.07
(1,100)	1:24:A:TYR:HD1	1:11:A:ARG:HG3	4	4.04
(1,109)	1:24:A:TYR:HE1	1:11:A:ARG:HG3	5	4.0
(1,112)	1:24:A:TYR:HE1	1:26:A:ASP:HA	6	3.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,110)	1:24:A:TYR:HE1	1:11:A:ARG:HG2	10	3.95
(1,104)	1:24:A:TYR:HD1	1:25:A:TYR:HA	3	3.95
(1,101)	1:24:A:TYR:HD1	1:11:A:ARG:HG2	4	3.95
(1,110)	1:24:A:TYR:HE1	1:11:A:ARG:HG2	7	3.94
(1,112)	1:24:A:TYR:HE1	1:26:A:ASP:HA	1	3.93
(1,98)	1:24:A:TYR:HD1	1:11:A:ARG:HD3	3	3.93
(1,104)	1:24:A:TYR:HD1	1:25:A:TYR:HA	6	3.92
(1,112)	1:24:A:TYR:HE1	1:26:A:ASP:HA	3	3.86
(1,104)	1:24:A:TYR:HD1	1:25:A:TYR:HA	8	3.83
(1,101)	1:24:A:TYR:HD1	1:11:A:ARG:HG2	1	3.83
(1,109)	1:24:A:TYR:HE1	1:11:A:ARG:HG3	7	3.82
(1,104)	1:24:A:TYR:HD1	1:25:A:TYR:HA	4	3.81
(1,101)	1:24:A:TYR:HD1	1:11:A:ARG:HG2	2	3.8
(1,98)	1:24:A:TYR:HD1	1:11:A:ARG:HD3	6	3.78
(1,104)	1:24:A:TYR:HD1	1:25:A:TYR:HA	7	3.77
(1,104)	1:24:A:TYR:HD1	1:25:A:TYR:HA	9	3.77
(1,109)	1:24:A:TYR:HE1	1:11:A:ARG:HG3	10	3.76
(1,104)	1:24:A:TYR:HD1	1:25:A:TYR:HA	5	3.76
(1,104)	1:24:A:TYR:HD1	1:25:A:TYR:HA	1	3.75
(1,110)	1:24:A:TYR:HE1	1:11:A:ARG:HG2	9	3.71
(1,104)	1:24:A:TYR:HD1	1:25:A:TYR:HA	2	3.69
(1,104)	1:24:A:TYR:HD1	1:25:A:TYR:HA	10	3.66
(1,107)	1:24:A:TYR:HE1	1:11:A:ARG:HD3	1	3.65
(1,101)	1:24:A:TYR:HD1	1:11:A:ARG:HG2	5	3.65
(1,99)	1:24:A:TYR:HD1	1:11:A:ARG:HD2	5	3.64
(1,107)	1:24:A:TYR:HE1	1:11:A:ARG:HD3	2	3.58
(1,101)	1:24:A:TYR:HD1	1:11:A:ARG:HG2	6	3.58
(1,101)	1:24:A:TYR:HD1	1:11:A:ARG:HG2	3	3.57
(1,109)	1:24:A:TYR:HE1	1:11:A:ARG:HG3	9	3.55
(1,108)	1:24:A:TYR:HE1	1:11:A:ARG:HD2	7	3.54
(1,101)	1:24:A:TYR:HD1	1:11:A:ARG:HG2	7	3.53
(1,101)	1:24:A:TYR:HD1	1:11:A:ARG:HG2	10	3.53
(1,108)	1:24:A:TYR:HE1	1:11:A:ARG:HD2	5	3.51
(1,99)	1:24:A:TYR:HD1	1:11:A:ARG:HD2	1	3.38
(1,99)	1:24:A:TYR:HD1	1:11:A:ARG:HD2	10	3.38
(1,108)	1:24:A:TYR:HE1	1:11:A:ARG:HD2	9	3.37
(1,101)	1:24:A:TYR:HD1	1:11:A:ARG:HG2	9	3.33
(1,108)	1:24:A:TYR:HE1	1:11:A:ARG:HD2	10	3.31
(1,107)	1:24:A:TYR:HE1	1:11:A:ARG:HD3	8	3.3
(1,99)	1:24:A:TYR:HD1	1:11:A:ARG:HD2	7	3.3
(1,107)	1:24:A:TYR:HE1	1:11:A:ARG:HD3	4	3.29
(1,100)	1:24:A:TYR:HD1	1:11:A:ARG:HG3	5	3.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,107)	1:24:A:TYR:HE1	1:11:A:ARG:HD3	3	3.26
(1,99)	1:24:A:TYR:HD1	1:11:A:ARG:HD2	6	3.25
(1,106)	1:24:A:TYR:HE1	1:11:A:ARG:HB2	6	3.21
(1,108)	1:24:A:TYR:HE1	1:11:A:ARG:HD2	1	3.17
(1,99)	1:24:A:TYR:HD1	1:11:A:ARG:HD2	3	3.17
(1,100)	1:24:A:TYR:HD1	1:11:A:ARG:HG3	7	3.12
(1,99)	1:24:A:TYR:HD1	1:11:A:ARG:HD2	9	3.11
(1,107)	1:24:A:TYR:HE1	1:11:A:ARG:HD3	6	3.1
(1,59)	1:16:A:GLY:HA2	1:15:A:LYS:HA	4	3.09
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD11	7	3.09
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD12	7	3.09
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD13	7	3.09
(1,59)	1:16:A:GLY:HA2	1:15:A:LYS:HA	9	3.07
(1,96)	1:24:A:TYR:HD1	1:11:A:ARG:HA	10	3.06
(1,59)	1:16:A:GLY:HA2	1:15:A:LYS:HA	1	3.06
(1,108)	1:24:A:TYR:HE1	1:11:A:ARG:HD2	6	3.05
(1,120)	1:26:A:ASP:HB2	1:32:A:CYS:HA	7	3.04
(1,120)	1:26:A:ASP:HB2	1:32:A:CYS:HA	8	3.03
(1,99)	1:24:A:TYR:HD1	1:11:A:ARG:HD2	2	3.03
(1,120)	1:26:A:ASP:HB2	1:32:A:CYS:HA	4	3.01
(1,59)	1:16:A:GLY:HA2	1:15:A:LYS:HA	7	3.01
(1,100)	1:24:A:TYR:HD1	1:11:A:ARG:HG3	10	3.0
(1,59)	1:16:A:GLY:HA2	1:15:A:LYS:HA	3	2.98
(1,96)	1:24:A:TYR:HD1	1:11:A:ARG:HA	8	2.97
(1,96)	1:24:A:TYR:HD1	1:11:A:ARG:HA	4	2.96
(1,59)	1:16:A:GLY:HA2	1:15:A:LYS:HA	10	2.96
(1,108)	1:24:A:TYR:HE1	1:11:A:ARG:HD2	3	2.95
(1,59)	1:16:A:GLY:HA2	1:15:A:LYS:HA	6	2.95
(1,59)	1:16:A:GLY:HA2	1:15:A:LYS:HA	2	2.93
(1,120)	1:26:A:ASP:HB2	1:32:A:CYS:HA	9	2.91
(1,106)	1:24:A:TYR:HE1	1:11:A:ARG:HB2	10	2.91
(1,59)	1:16:A:GLY:HA2	1:15:A:LYS:HA	5	2.9
(1,106)	1:24:A:TYR:HE1	1:11:A:ARG:HB2	8	2.88
(1,100)	1:24:A:TYR:HD1	1:11:A:ARG:HG3	9	2.88
(1,63)	1:18:A:GLY:HA3	1:18:A:GLY:HA2	2	2.82
(1,63)	1:18:A:GLY:HA3	1:18:A:GLY:HA2	1	2.81
(1,63)	1:18:A:GLY:HA3	1:18:A:GLY:HA2	3	2.81
(1,63)	1:18:A:GLY:HA3	1:18:A:GLY:HA2	4	2.81
(1,63)	1:18:A:GLY:HA3	1:18:A:GLY:HA2	5	2.81
(1,63)	1:18:A:GLY:HA3	1:18:A:GLY:HA2	6	2.81
(1,63)	1:18:A:GLY:HA3	1:18:A:GLY:HA2	7	2.81
(1,63)	1:18:A:GLY:HA3	1:18:A:GLY:HA2	8	2.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:18:A:GLY:HA3	1:18:A:GLY:HA2	9	2.81
(1,63)	1:18:A:GLY:HA3	1:18:A:GLY:HA2	10	2.81
(1,120)	1:26:A:ASP:HB2	1:32:A:CYS:HA	1	2.8
(1,99)	1:24:A:TYR:HD1	1:11:A:ARG:HD2	4	2.75
(1,108)	1:24:A:TYR:HE1	1:11:A:ARG:HD2	2	2.74
(1,99)	1:24:A:TYR:HD1	1:11:A:ARG:HD2	8	2.74
(1,120)	1:26:A:ASP:HB2	1:32:A:CYS:HA	3	2.73
(1,120)	1:26:A:ASP:HB2	1:32:A:CYS:HA	5	2.73
(1,120)	1:26:A:ASP:HB2	1:32:A:CYS:HA	6	2.7
(1,106)	1:24:A:TYR:HE1	1:11:A:ARG:HB2	4	2.7
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD11	5	2.7
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD12	5	2.7
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD13	5	2.7
(1,120)	1:26:A:ASP:HB2	1:32:A:CYS:HA	2	2.69
(1,96)	1:24:A:TYR:HD1	1:11:A:ARG:HA	7	2.69
(1,59)	1:16:A:GLY:HA2	1:15:A:LYS:HA	8	2.68
(1,70)	1:19:A:SER:HB3	1:36:A:ARG:HD3	8	2.67
(1,52)	1:13:A:TYR:HA	1:14:A:GLY:HA2	3	2.67
(1,60)	1:17:A:SER:HA	1:17:A:SER:HB3	7	2.65
(1,52)	1:13:A:TYR:HA	1:14:A:GLY:HA2	9	2.65
(1,70)	1:19:A:SER:HB3	1:36:A:ARG:HD3	7	2.64
(1,106)	1:24:A:TYR:HE1	1:11:A:ARG:HB2	7	2.63
(1,60)	1:17:A:SER:HA	1:17:A:SER:HB3	5	2.63
(1,60)	1:17:A:SER:HA	1:17:A:SER:HB3	3	2.62
(1,60)	1:17:A:SER:HA	1:17:A:SER:HB3	6	2.59
(1,60)	1:17:A:SER:HA	1:17:A:SER:HB3	9	2.59
(1,96)	1:24:A:TYR:HD1	1:11:A:ARG:HA	9	2.58
(1,60)	1:17:A:SER:HA	1:17:A:SER:HB3	1	2.58
(1,60)	1:17:A:SER:HA	1:17:A:SER:HB3	4	2.58
(1,60)	1:17:A:SER:HA	1:17:A:SER:HB3	8	2.58
(1,121)	1:27:A:LYS:HA	1:27:A:LYS:HB3	3	2.57
(1,121)	1:27:A:LYS:HA	1:27:A:LYS:HB3	5	2.57
(1,121)	1:27:A:LYS:HA	1:27:A:LYS:HB3	1	2.56
(1,121)	1:27:A:LYS:HA	1:27:A:LYS:HB3	2	2.56
(1,121)	1:27:A:LYS:HA	1:27:A:LYS:HB3	6	2.56
(1,121)	1:27:A:LYS:HA	1:27:A:LYS:HB3	8	2.56
(1,121)	1:27:A:LYS:HA	1:27:A:LYS:HB3	9	2.56
(1,60)	1:17:A:SER:HA	1:17:A:SER:HB3	10	2.56
(1,121)	1:27:A:LYS:HA	1:27:A:LYS:HB3	7	2.55
(1,96)	1:24:A:TYR:HD1	1:11:A:ARG:HA	5	2.55
(1,121)	1:27:A:LYS:HA	1:27:A:LYS:HB3	4	2.54
(1,108)	1:24:A:TYR:HE1	1:11:A:ARG:HD2	8	2.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:24:A:TYR:HD1	1:11:A:ARG:HB2	6	2.53
(1,70)	1:19:A:SER:HB3	1:36:A:ARG:HD3	4	2.53
(1,60)	1:17:A:SER:HA	1:17:A:SER:HB3	2	2.53
(1,52)	1:13:A:TYR:HA	1:14:A:GLY:HA2	1	2.53
(1,89)	1:24:A:TYR:HA	1:11:A:ARG:HA	9	2.52
(1,108)	1:24:A:TYR:HE1	1:11:A:ARG:HD2	4	2.5
(1,120)	1:26:A:ASP:HB2	1:32:A:CYS:HA	10	2.48
(1,106)	1:24:A:TYR:HE1	1:11:A:ARG:HB2	1	2.48
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD11	2	2.46
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD12	2	2.46
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD13	2	2.46
(1,92)	1:24:A:TYR:HA	1:25:A:TYR:HB3	3	2.45
(1,89)	1:24:A:TYR:HA	1:11:A:ARG:HA	10	2.45
(1,68)	1:19:A:SER:HA	1:36:A:ARG:HD3	9	2.44
(1,92)	1:24:A:TYR:HA	1:25:A:TYR:HB3	9	2.43
(1,70)	1:19:A:SER:HB3	1:36:A:ARG:HD3	10	2.42
(1,106)	1:24:A:TYR:HE1	1:11:A:ARG:HB2	5	2.41
(1,89)	1:24:A:TYR:HA	1:11:A:ARG:HA	3	2.41
(1,92)	1:24:A:TYR:HA	1:25:A:TYR:HB3	2	2.4
(1,89)	1:24:A:TYR:HA	1:11:A:ARG:HA	7	2.4
(1,92)	1:24:A:TYR:HA	1:25:A:TYR:HB3	10	2.39
(1,106)	1:24:A:TYR:HE1	1:11:A:ARG:HB2	3	2.36
(1,92)	1:24:A:TYR:HA	1:25:A:TYR:HB3	4	2.36
(1,92)	1:24:A:TYR:HA	1:25:A:TYR:HB3	5	2.36
(1,89)	1:24:A:TYR:HA	1:11:A:ARG:HA	2	2.36
(1,89)	1:24:A:TYR:HA	1:11:A:ARG:HA	5	2.36
(1,68)	1:19:A:SER:HA	1:36:A:ARG:HD3	5	2.34
(1,92)	1:24:A:TYR:HA	1:25:A:TYR:HB3	1	2.33
(1,89)	1:24:A:TYR:HA	1:11:A:ARG:HA	1	2.33
(1,52)	1:13:A:TYR:HA	1:14:A:GLY:HA2	5	2.33
(1,92)	1:24:A:TYR:HA	1:25:A:TYR:HB3	8	2.32
(1,92)	1:24:A:TYR:HA	1:25:A:TYR:HB3	6	2.31
(1,70)	1:19:A:SER:HB3	1:36:A:ARG:HD3	5	2.3
(1,52)	1:13:A:TYR:HA	1:14:A:GLY:HA2	4	2.3
(1,52)	1:13:A:TYR:HA	1:14:A:GLY:HA2	7	2.3
(1,89)	1:24:A:TYR:HA	1:11:A:ARG:HA	6	2.29
(1,121)	1:27:A:LYS:HA	1:27:A:LYS:HB3	10	2.28
(1,106)	1:24:A:TYR:HE1	1:11:A:ARG:HB2	9	2.28
(1,106)	1:24:A:TYR:HE1	1:11:A:ARG:HB2	2	2.27
(1,68)	1:19:A:SER:HA	1:36:A:ARG:HD3	7	2.27
(1,68)	1:19:A:SER:HA	1:36:A:ARG:HD3	10	2.27
(1,62)	1:17:A:SER:HA	1:18:A:GLY:HA2	8	2.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:13:A:TYR:HA	1:14:A:GLY:HA2	2	2.27
(1,113)	1:24:A:TYR:HE1	1:26:A:ASP:HB2	10	2.26
(1,92)	1:24:A:TYR:HA	1:25:A:TYR:HB3	7	2.26
(1,68)	1:19:A:SER:HA	1:36:A:ARG:HD3	1	2.25
(1,52)	1:13:A:TYR:HA	1:14:A:GLY:HA2	6	2.25
(1,70)	1:19:A:SER:HB3	1:36:A:ARG:HD3	3	2.23
(1,68)	1:19:A:SER:HA	1:36:A:ARG:HD3	2	2.21
(1,68)	1:19:A:SER:HA	1:36:A:ARG:HD3	8	2.21
(1,20)	1:7:A:CYS:HB2	1:3:A:GLN:HG3	8	2.2
(1,96)	1:24:A:TYR:HD1	1:11:A:ARG:HA	1	2.19
(1,68)	1:19:A:SER:HA	1:36:A:ARG:HD3	3	2.19
(1,20)	1:7:A:CYS:HB2	1:3:A:GLN:HG3	10	2.19
(1,70)	1:19:A:SER:HB3	1:36:A:ARG:HD3	6	2.18
(1,62)	1:17:A:SER:HA	1:18:A:GLY:HA2	4	2.18
(1,62)	1:17:A:SER:HA	1:18:A:GLY:HA2	7	2.17
(1,62)	1:17:A:SER:HA	1:18:A:GLY:HA2	2	2.16
(1,68)	1:19:A:SER:HA	1:36:A:ARG:HD3	6	2.12
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD11	3	2.12
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD12	3	2.12
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD13	3	2.12
(1,77)	1:22:A:ASN:HA	1:22:A:ASN:HB3	4	2.1
(1,77)	1:22:A:ASN:HA	1:22:A:ASN:HB3	5	2.1
(1,77)	1:22:A:ASN:HA	1:22:A:ASN:HB3	6	2.1
(1,96)	1:24:A:TYR:HD1	1:11:A:ARG:HA	2	2.09
(1,77)	1:22:A:ASN:HA	1:22:A:ASN:HB3	7	2.09
(1,62)	1:17:A:SER:HA	1:18:A:GLY:HA2	5	2.09
(1,52)	1:13:A:TYR:HA	1:14:A:GLY:HA2	8	2.09
(1,62)	1:17:A:SER:HA	1:18:A:GLY:HA2	6	2.08
(1,62)	1:17:A:SER:HA	1:18:A:GLY:HA2	1	2.07
(1,96)	1:24:A:TYR:HD1	1:11:A:ARG:HA	6	2.06
(1,62)	1:17:A:SER:HA	1:18:A:GLY:HA2	9	2.06
(1,339)	1:16:A:GLY:H	1:38:A:ARG:HG3	8	2.05
(1,77)	1:22:A:ASN:HA	1:22:A:ASN:HB3	10	2.05
(1,62)	1:17:A:SER:HA	1:18:A:GLY:HA2	3	2.05
(1,77)	1:22:A:ASN:HA	1:22:A:ASN:HB3	3	2.04
(1,123)	1:27:A:LYS:HA	1:27:A:LYS:HE3	6	2.03
(1,62)	1:17:A:SER:HA	1:18:A:GLY:HA2	10	2.03
(1,20)	1:7:A:CYS:HB2	1:3:A:GLN:HG3	5	2.02
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG11	7	2.01
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG12	7	2.01
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG13	7	2.01
(1,113)	1:24:A:TYR:HE1	1:26:A:ASP:HB2	8	2.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,70)	1:19:A:SER:HB3	1:36:A:ARG:HD3	1	2.01
(1,95)	1:24:A:TYR:HB3	1:11:A:ARG:HB2	6	2.0
(1,77)	1:22:A:ASN:HA	1:22:A:ASN:HB3	1	2.0
(1,52)	1:13:A:TYR:HA	1:14:A:GLY:HA2	10	2.0
(1,96)	1:24:A:TYR:HD1	1:11:A:ARG:HA	3	1.99
(1,89)	1:24:A:TYR:HA	1:11:A:ARG:HA	8	1.99
(1,77)	1:22:A:ASN:HA	1:22:A:ASN:HB3	2	1.99
(1,128)	1:27:A:LYS:HE3	1:27:A:LYS:HG3	1	1.98
(1,128)	1:27:A:LYS:HE3	1:27:A:LYS:HG3	3	1.98
(1,20)	1:7:A:CYS:HB2	1:3:A:GLN:HG3	3	1.98
(1,128)	1:27:A:LYS:HE3	1:27:A:LYS:HG3	2	1.97
(1,128)	1:27:A:LYS:HE3	1:27:A:LYS:HG3	4	1.97
(1,128)	1:27:A:LYS:HE3	1:27:A:LYS:HG3	6	1.97
(1,128)	1:27:A:LYS:HE3	1:27:A:LYS:HG3	7	1.97
(1,128)	1:27:A:LYS:HE3	1:27:A:LYS:HG3	8	1.97
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG11	7	1.95
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG12	7	1.95
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG13	7	1.95
(1,91)	1:24:A:TYR:HA	1:24:A:TYR:HB3	1	1.95
(1,91)	1:24:A:TYR:HA	1:24:A:TYR:HB3	2	1.94
(1,128)	1:27:A:LYS:HE3	1:27:A:LYS:HG3	5	1.93
(1,123)	1:27:A:LYS:HA	1:27:A:LYS:HE3	4	1.93
(1,91)	1:24:A:TYR:HA	1:24:A:TYR:HB3	3	1.93
(1,91)	1:24:A:TYR:HA	1:24:A:TYR:HB3	6	1.93
(1,91)	1:24:A:TYR:HA	1:24:A:TYR:HB3	8	1.93
(1,91)	1:24:A:TYR:HA	1:24:A:TYR:HB3	9	1.93
(1,53)	1:13:A:TYR:HB3	1:13:A:TYR:HA	5	1.93
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG11	8	1.92
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG12	8	1.92
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG13	8	1.92
(1,113)	1:24:A:TYR:HE1	1:26:A:ASP:HB2	4	1.92
(1,91)	1:24:A:TYR:HA	1:24:A:TYR:HB3	5	1.92
(1,68)	1:19:A:SER:HA	1:36:A:ARG:HD3	4	1.92
(1,53)	1:13:A:TYR:HB3	1:13:A:TYR:HA	9	1.92
(1,53)	1:13:A:TYR:HB3	1:13:A:TYR:HA	10	1.91
(1,123)	1:27:A:LYS:HA	1:27:A:LYS:HE3	1	1.9
(1,123)	1:27:A:LYS:HA	1:27:A:LYS:HE3	7	1.9
(1,105)	1:24:A:TYR:HE1	1:11:A:ARG:HB3	8	1.89
(1,91)	1:24:A:TYR:HA	1:24:A:TYR:HB3	10	1.89
(1,89)	1:24:A:TYR:HA	1:11:A:ARG:HA	4	1.89
(1,77)	1:22:A:ASN:HA	1:22:A:ASN:HB3	8	1.89
(1,77)	1:22:A:ASN:HA	1:22:A:ASN:HB3	9	1.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG11	8	1.88
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG12	8	1.88
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG13	8	1.88
(1,152)	1:34:A:THR:HA	1:33:A:LYS:HE3	5	1.88
(1,91)	1:24:A:TYR:HA	1:24:A:TYR:HB3	7	1.88
(1,152)	1:34:A:THR:HA	1:33:A:LYS:HE3	4	1.87
(1,105)	1:24:A:TYR:HE1	1:11:A:ARG:HB3	4	1.87
(1,97)	1:24:A:TYR:HD1	1:11:A:ARG:HB2	8	1.87
(1,91)	1:24:A:TYR:HA	1:24:A:TYR:HB3	4	1.87
(1,128)	1:27:A:LYS:HE3	1:27:A:LYS:HG3	9	1.86
(1,265)	1:3:A:GLN:H	1:3:A:GLN:HG3	8	1.85
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG11	10	1.85
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG12	10	1.85
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG13	10	1.85
(1,97)	1:24:A:TYR:HD1	1:11:A:ARG:HB2	1	1.85
(1,53)	1:13:A:TYR:HB3	1:13:A:TYR:HA	7	1.85
(1,25)	1:9:A:LEU:HD11	1:9:A:LEU:HA	5	1.85
(1,25)	1:9:A:LEU:HD12	1:9:A:LEU:HA	5	1.85
(1,25)	1:9:A:LEU:HD13	1:9:A:LEU:HA	5	1.85
(1,25)	1:9:A:LEU:HD11	1:9:A:LEU:HA	8	1.84
(1,25)	1:9:A:LEU:HD12	1:9:A:LEU:HA	8	1.84
(1,25)	1:9:A:LEU:HD13	1:9:A:LEU:HA	8	1.84
(1,53)	1:13:A:TYR:HB3	1:13:A:TYR:HA	3	1.83
(1,25)	1:9:A:LEU:HD11	1:9:A:LEU:HA	2	1.83
(1,25)	1:9:A:LEU:HD12	1:9:A:LEU:HA	2	1.83
(1,25)	1:9:A:LEU:HD13	1:9:A:LEU:HA	2	1.83
(1,25)	1:9:A:LEU:HD11	1:9:A:LEU:HA	3	1.83
(1,25)	1:9:A:LEU:HD12	1:9:A:LEU:HA	3	1.83
(1,25)	1:9:A:LEU:HD13	1:9:A:LEU:HA	3	1.83
(1,25)	1:9:A:LEU:HD11	1:9:A:LEU:HA	7	1.83
(1,25)	1:9:A:LEU:HD12	1:9:A:LEU:HA	7	1.83
(1,25)	1:9:A:LEU:HD13	1:9:A:LEU:HA	7	1.83
(1,22)	1:8:A:GLN:HA	1:27:A:LYS:HE3	5	1.83
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG11	9	1.82
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG12	9	1.82
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG13	9	1.82
(1,113)	1:24:A:TYR:HE1	1:26:A:ASP:HB2	9	1.82
(1,97)	1:24:A:TYR:HD1	1:11:A:ARG:HB2	10	1.82
(1,53)	1:13:A:TYR:HB3	1:13:A:TYR:HA	1	1.82
(1,25)	1:9:A:LEU:HD11	1:9:A:LEU:HA	4	1.82
(1,25)	1:9:A:LEU:HD12	1:9:A:LEU:HA	4	1.82
(1,25)	1:9:A:LEU:HD13	1:9:A:LEU:HA	4	1.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:9:A:LEU:HD11	1:9:A:LEU:HA	6	1.82
(1,25)	1:9:A:LEU:HD12	1:9:A:LEU:HA	6	1.82
(1,25)	1:9:A:LEU:HD13	1:9:A:LEU:HA	6	1.82
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG11	3	1.81
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG12	3	1.81
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG13	3	1.81
(1,70)	1:19:A:SER:HB3	1:36:A:ARG:HD3	9	1.81
(1,53)	1:13:A:TYR:HB3	1:13:A:TYR:HA	2	1.81
(1,53)	1:13:A:TYR:HB3	1:13:A:TYR:HA	6	1.81
(1,53)	1:13:A:TYR:HB3	1:13:A:TYR:HA	8	1.81
(1,37)	1:11:A:ARG:HD3	1:11:A:ARG:HA	2	1.81
(1,25)	1:9:A:LEU:HD11	1:9:A:LEU:HA	9	1.81
(1,25)	1:9:A:LEU:HD12	1:9:A:LEU:HA	9	1.81
(1,25)	1:9:A:LEU:HD13	1:9:A:LEU:HA	9	1.81
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG11	10	1.8
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG12	10	1.8
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG13	10	1.8
(1,145)	1:33:A:LYS:HA	1:33:A:LYS:HE3	3	1.8
(1,123)	1:27:A:LYS:HA	1:27:A:LYS:HE3	9	1.8
(1,53)	1:13:A:TYR:HB3	1:13:A:TYR:HA	4	1.8
(1,152)	1:34:A:THR:HA	1:33:A:LYS:HE3	2	1.78
(1,97)	1:24:A:TYR:HD1	1:11:A:ARG:HB2	3	1.78
(1,25)	1:9:A:LEU:HD11	1:9:A:LEU:HA	10	1.78
(1,25)	1:9:A:LEU:HD12	1:9:A:LEU:HA	10	1.78
(1,25)	1:9:A:LEU:HD13	1:9:A:LEU:HA	10	1.78
(1,339)	1:16:A:GLY:H	1:38:A:ARG:HG3	10	1.77
(1,37)	1:11:A:ARG:HD3	1:11:A:ARG:HA	8	1.77
(1,25)	1:9:A:LEU:HD11	1:9:A:LEU:HA	1	1.77
(1,25)	1:9:A:LEU:HD12	1:9:A:LEU:HA	1	1.77
(1,25)	1:9:A:LEU:HD13	1:9:A:LEU:HA	1	1.77
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG11	4	1.76
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG12	4	1.76
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG13	4	1.76
(1,123)	1:27:A:LYS:HA	1:27:A:LYS:HE3	2	1.76
(1,22)	1:8:A:GLN:HA	1:27:A:LYS:HE3	4	1.76
(1,286)	1:7:A:CYS:H	1:8:A:GLN:HG3	6	1.74
(1,247)	1:57:A:CYS:HA	1:3:A:GLN:HG3	3	1.74
(1,105)	1:24:A:TYR:HE1	1:11:A:ARG:HB3	5	1.74
(1,76)	1:22:A:ASN:HA	1:21:A:THR:HB	1	1.73
(1,67)	1:19:A:SER:HA	1:36:A:ARG:HB3	10	1.73
(1,76)	1:22:A:ASN:HA	1:21:A:THR:HB	3	1.72
(1,37)	1:11:A:ARG:HD3	1:11:A:ARG:HA	3	1.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG11	5	1.7
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG12	5	1.7
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG13	5	1.7
(1,97)	1:24:A:TYR:HD1	1:11:A:ARG:HB2	4	1.7
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG21	3	1.7
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG22	3	1.7
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG23	3	1.7
(1,37)	1:11:A:ARG:HD3	1:11:A:ARG:HA	4	1.7
(1,247)	1:57:A:CYS:HA	1:3:A:GLN:HG3	1	1.69
(1,145)	1:33:A:LYS:HA	1:33:A:LYS:HE3	2	1.69
(1,37)	1:11:A:ARG:HD3	1:11:A:ARG:HA	1	1.69
(1,111)	1:24:A:TYR:HE1	1:24:A:TYR:HD1	1	1.68
(1,111)	1:24:A:TYR:HE1	1:24:A:TYR:HD1	2	1.68
(1,111)	1:24:A:TYR:HE1	1:24:A:TYR:HD1	3	1.68
(1,111)	1:24:A:TYR:HE1	1:24:A:TYR:HD1	5	1.68
(1,111)	1:24:A:TYR:HE1	1:24:A:TYR:HD1	6	1.68
(1,111)	1:24:A:TYR:HE1	1:24:A:TYR:HD1	7	1.68
(1,111)	1:24:A:TYR:HE1	1:24:A:TYR:HD1	8	1.68
(1,111)	1:24:A:TYR:HE1	1:24:A:TYR:HD1	9	1.68
(1,111)	1:24:A:TYR:HE1	1:24:A:TYR:HD1	10	1.68
(1,97)	1:24:A:TYR:HD1	1:11:A:ARG:HB2	7	1.68
(1,76)	1:22:A:ASN:HA	1:21:A:THR:HB	2	1.68
(1,39)	1:11:A:ARG:HD3	1:11:A:ARG:HD2	1	1.68
(1,39)	1:11:A:ARG:HD3	1:11:A:ARG:HD2	2	1.68
(1,39)	1:11:A:ARG:HD3	1:11:A:ARG:HD2	3	1.68
(1,39)	1:11:A:ARG:HD3	1:11:A:ARG:HD2	4	1.68
(1,39)	1:11:A:ARG:HD3	1:11:A:ARG:HD2	5	1.68
(1,39)	1:11:A:ARG:HD3	1:11:A:ARG:HD2	6	1.68
(1,39)	1:11:A:ARG:HD3	1:11:A:ARG:HD2	7	1.68
(1,39)	1:11:A:ARG:HD3	1:11:A:ARG:HD2	8	1.68
(1,39)	1:11:A:ARG:HD3	1:11:A:ARG:HD2	9	1.68
(1,39)	1:11:A:ARG:HD3	1:11:A:ARG:HD2	10	1.68
(1,37)	1:11:A:ARG:HD3	1:11:A:ARG:HA	6	1.68
(1,111)	1:24:A:TYR:HE1	1:24:A:TYR:HD1	4	1.67
(1,67)	1:19:A:SER:HA	1:36:A:ARG:HB3	4	1.67
(1,123)	1:27:A:LYS:HA	1:27:A:LYS:HE3	8	1.66
(1,113)	1:24:A:TYR:HE1	1:26:A:ASP:HB2	2	1.66
(1,67)	1:19:A:SER:HA	1:36:A:ARG:HB3	2	1.66
(1,20)	1:7:A:CYS:HB2	1:3:A:GLN:HG3	6	1.66
(1,247)	1:57:A:CYS:HA	1:3:A:GLN:HG3	5	1.65
(1,184)	1:37:A:TYR:HB2	1:46:A:ARG:HB3	1	1.65
(1,247)	1:57:A:CYS:HA	1:3:A:GLN:HG3	8	1.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:22:A:ASN:HA	1:21:A:THR:HB	5	1.64
(1,76)	1:22:A:ASN:HA	1:21:A:THR:HB	6	1.64
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG11	6	1.63
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG12	6	1.63
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG13	6	1.63
(1,76)	1:22:A:ASN:HA	1:21:A:THR:HB	8	1.63
(1,76)	1:22:A:ASN:HA	1:21:A:THR:HB	9	1.63
(1,184)	1:37:A:TYR:HB2	1:46:A:ARG:HB3	5	1.62
(1,76)	1:22:A:ASN:HA	1:21:A:THR:HB	7	1.62
(1,286)	1:7:A:CYS:H	1:8:A:GLN:HG3	1	1.61
(1,184)	1:37:A:TYR:HB2	1:46:A:ARG:HB3	2	1.61
(1,76)	1:22:A:ASN:HA	1:21:A:THR:HB	10	1.61
(1,184)	1:37:A:TYR:HB2	1:46:A:ARG:HB3	7	1.6
(1,70)	1:19:A:SER:HB3	1:36:A:ARG:HD3	2	1.6
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG11	3	1.59
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG12	3	1.59
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG13	3	1.59
(1,22)	1:8:A:GLN:HA	1:27:A:LYS:HE3	1	1.59
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG11	1	1.58
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG12	1	1.58
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG13	1	1.58
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG11	9	1.58
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG12	9	1.58
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG13	9	1.58
(1,113)	1:24:A:TYR:HE1	1:26:A:ASP:HB2	5	1.58
(1,113)	1:24:A:TYR:HE1	1:26:A:ASP:HB2	7	1.58
(1,105)	1:24:A:TYR:HE1	1:11:A:ARG:HB3	2	1.58
(1,184)	1:37:A:TYR:HB2	1:46:A:ARG:HB3	3	1.57
(1,184)	1:37:A:TYR:HB2	1:46:A:ARG:HB3	10	1.57
(1,123)	1:27:A:LYS:HA	1:27:A:LYS:HE3	5	1.57
(1,97)	1:24:A:TYR:HD1	1:11:A:ARG:HB2	2	1.57
(1,184)	1:37:A:TYR:HB2	1:46:A:ARG:HB3	4	1.56
(1,58)	1:16:A:GLY:HA3	1:16:A:GLY:HA2	4	1.55
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD11	1	1.55
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD12	1	1.55
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD13	1	1.55
(1,390)	1:27:A:LYS:H	1:27:A:LYS:HE3	6	1.54
(1,390)	1:27:A:LYS:H	1:27:A:LYS:HE3	7	1.54
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD11	8	1.54
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD12	8	1.54
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD13	8	1.54
(1,254)	1:58:A:VAL:HG11	1:54:A:GLU:HB3	8	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,254)	1:58:A:VAL:HG12	1:54:A:GLU:HB3	8	1.54
(1,254)	1:58:A:VAL:HG13	1:54:A:GLU:HB3	8	1.54
(1,113)	1:24:A:TYR:HE1	1:26:A:ASP:HB2	6	1.54
(1,95)	1:24:A:TYR:HB3	1:11:A:ARG:HB2	3	1.54
(1,58)	1:16:A:GLY:HA3	1:16:A:GLY:HA2	1	1.54
(1,58)	1:16:A:GLY:HA3	1:16:A:GLY:HA2	2	1.54
(1,58)	1:16:A:GLY:HA3	1:16:A:GLY:HA2	3	1.54
(1,58)	1:16:A:GLY:HA3	1:16:A:GLY:HA2	9	1.54
(1,197)	1:47:A:PHE:HB3	1:23:A:TYR:HB3	6	1.53
(1,184)	1:37:A:TYR:HB2	1:46:A:ARG:HB3	9	1.53
(1,76)	1:22:A:ASN:HA	1:21:A:THR:HB	4	1.53
(1,58)	1:16:A:GLY:HA3	1:16:A:GLY:HA2	5	1.53
(1,58)	1:16:A:GLY:HA3	1:16:A:GLY:HA2	6	1.53
(1,58)	1:16:A:GLY:HA3	1:16:A:GLY:HA2	7	1.53
(1,58)	1:16:A:GLY:HA3	1:16:A:GLY:HA2	8	1.53
(1,58)	1:16:A:GLY:HA3	1:16:A:GLY:HA2	10	1.53
(1,294)	1:9:A:LEU:H	1:8:A:GLN:HG3	10	1.52
(1,286)	1:7:A:CYS:H	1:8:A:GLN:HG3	2	1.52
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG11	6	1.52
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG12	6	1.52
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG13	6	1.52
(1,113)	1:24:A:TYR:HE1	1:26:A:ASP:HB2	1	1.52
(1,105)	1:24:A:TYR:HE1	1:11:A:ARG:HB3	9	1.52
(1,254)	1:58:A:VAL:HG11	1:54:A:GLU:HB3	10	1.51
(1,254)	1:58:A:VAL:HG12	1:54:A:GLU:HB3	10	1.51
(1,254)	1:58:A:VAL:HG13	1:54:A:GLU:HB3	10	1.51
(1,247)	1:57:A:CYS:HA	1:3:A:GLN:HG3	4	1.51
(1,247)	1:57:A:CYS:HA	1:3:A:GLN:HG3	10	1.51
(1,123)	1:27:A:LYS:HA	1:27:A:LYS:HE3	3	1.51
(1,103)	1:24:A:TYR:HD1	1:24:A:TYR:HB3	4	1.51
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG21	9	1.51
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG22	9	1.51
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG23	9	1.51
(1,390)	1:27:A:LYS:H	1:27:A:LYS:HE3	2	1.5
(1,390)	1:27:A:LYS:H	1:27:A:LYS:HE3	5	1.5
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG11	2	1.5
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG12	2	1.5
(1,235)	1:54:A:GLU:HA	1:58:A:VAL:HG13	2	1.5
(1,103)	1:24:A:TYR:HD1	1:24:A:TYR:HB3	3	1.5
(1,103)	1:24:A:TYR:HD1	1:24:A:TYR:HB3	7	1.5
(1,339)	1:16:A:GLY:H	1:38:A:ARG:HG3	2	1.49
(1,294)	1:9:A:LEU:H	1:8:A:GLN:HG3	9	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,103)	1:24:A:TYR:HD1	1:24:A:TYR:HB3	6	1.49
(1,97)	1:24:A:TYR:HD1	1:11:A:ARG:HB2	5	1.49
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG21	8	1.49
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG22	8	1.49
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG23	8	1.49
(1,419)	1:34:A:THR:H	1:33:A:LYS:HB3	3	1.48
(1,390)	1:27:A:LYS:H	1:27:A:LYS:HE3	3	1.48
(1,390)	1:27:A:LYS:H	1:27:A:LYS:HE3	8	1.48
(1,286)	1:7:A:CYS:H	1:8:A:GLN:HG3	8	1.48
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG21	4	1.48
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG22	4	1.48
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG23	4	1.48
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG21	7	1.48
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG22	7	1.48
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG23	7	1.48
(1,139)	1:32:A:CYS:HB3	1:23:A:TYR:HB3	10	1.47
(1,103)	1:24:A:TYR:HD1	1:24:A:TYR:HB3	5	1.47
(1,103)	1:24:A:TYR:HD1	1:24:A:TYR:HB3	8	1.47
(1,103)	1:24:A:TYR:HD1	1:24:A:TYR:HB3	9	1.47
(1,103)	1:24:A:TYR:HD1	1:24:A:TYR:HB3	10	1.47
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD11	9	1.47
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD12	9	1.47
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD13	9	1.47
(1,390)	1:27:A:LYS:H	1:27:A:LYS:HE3	1	1.46
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG21	9	1.46
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG22	9	1.46
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG23	9	1.46
(1,184)	1:37:A:TYR:HB2	1:46:A:ARG:HB3	6	1.46
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG21	5	1.46
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG22	5	1.46
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG23	5	1.46
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG11	1	1.45
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG12	1	1.45
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG13	1	1.45
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG11	2	1.45
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG12	2	1.45
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG13	2	1.45
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG21	10	1.45
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG22	10	1.45
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG23	10	1.45
(1,390)	1:27:A:LYS:H	1:27:A:LYS:HE3	4	1.44
(1,339)	1:16:A:GLY:H	1:38:A:ARG:HG3	6	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,254)	1:58:A:VAL:HG11	1:54:A:GLU:HB3	7	1.44
(1,254)	1:58:A:VAL:HG12	1:54:A:GLU:HB3	7	1.44
(1,254)	1:58:A:VAL:HG13	1:54:A:GLU:HB3	7	1.44
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG21	4	1.44
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG22	4	1.44
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG23	4	1.44
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG21	6	1.44
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG22	6	1.44
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG23	6	1.44
(1,103)	1:24:A:TYR:HD1	1:24:A:TYR:HB3	1	1.44
(1,95)	1:24:A:TYR:HB3	1:11:A:ARG:HB2	1	1.44
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG11	5	1.43
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG12	5	1.43
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG13	5	1.43
(1,254)	1:58:A:VAL:HG11	1:54:A:GLU:HB3	3	1.43
(1,254)	1:58:A:VAL:HG12	1:54:A:GLU:HB3	3	1.43
(1,254)	1:58:A:VAL:HG13	1:54:A:GLU:HB3	3	1.43
(1,254)	1:58:A:VAL:HG11	1:54:A:GLU:HB3	4	1.43
(1,254)	1:58:A:VAL:HG12	1:54:A:GLU:HB3	4	1.43
(1,254)	1:58:A:VAL:HG13	1:54:A:GLU:HB3	4	1.43
(1,139)	1:32:A:CYS:HB3	1:23:A:TYR:HB3	7	1.43
(1,139)	1:32:A:CYS:HB3	1:23:A:TYR:HB3	8	1.43
(1,105)	1:24:A:TYR:HE1	1:11:A:ARG:HB3	1	1.43
(1,103)	1:24:A:TYR:HD1	1:24:A:TYR:HB3	2	1.43
(1,69)	1:19:A:SER:HB3	1:19:A:SER:HB2	1	1.43
(1,69)	1:19:A:SER:HB3	1:19:A:SER:HB2	2	1.43
(1,69)	1:19:A:SER:HB3	1:19:A:SER:HB2	3	1.43
(1,69)	1:19:A:SER:HB3	1:19:A:SER:HB2	4	1.43
(1,69)	1:19:A:SER:HB3	1:19:A:SER:HB2	5	1.43
(1,69)	1:19:A:SER:HB3	1:19:A:SER:HB2	6	1.43
(1,69)	1:19:A:SER:HB3	1:19:A:SER:HB2	7	1.43
(1,69)	1:19:A:SER:HB3	1:19:A:SER:HB2	8	1.43
(1,69)	1:19:A:SER:HB3	1:19:A:SER:HB2	9	1.43
(1,69)	1:19:A:SER:HB3	1:19:A:SER:HB2	10	1.43
(1,67)	1:19:A:SER:HA	1:36:A:ARG:HB3	8	1.43
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG11	4	1.42
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG12	4	1.42
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG13	4	1.42
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG11	6	1.42
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG12	6	1.42
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG13	6	1.42
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG11	7	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG12	7	1.42
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG13	7	1.42
(1,247)	1:57:A:CYS:HA	1:3:A:GLN:HG3	2	1.42
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG11	4	1.42
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG12	4	1.42
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG13	4	1.42
(1,67)	1:19:A:SER:HA	1:36:A:ARG:HB3	5	1.42
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG11	3	1.41
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG12	3	1.41
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG13	3	1.41
(1,356)	1:20:A:PHE:H	1:19:A:SER:HB2	2	1.41
(1,105)	1:24:A:TYR:HE1	1:11:A:ARG:HB3	10	1.41
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG11	8	1.4
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG12	8	1.4
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG13	8	1.4
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG11	9	1.4
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG12	9	1.4
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG13	9	1.4
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG11	10	1.4
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG12	10	1.4
(1,530)	1:58:A:VAL:H	1:58:A:VAL:HG13	10	1.4
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG21	7	1.4
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG22	7	1.4
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG23	7	1.4
(1,254)	1:58:A:VAL:HG11	1:54:A:GLU:HB3	9	1.39
(1,254)	1:58:A:VAL:HG12	1:54:A:GLU:HB3	9	1.39
(1,254)	1:58:A:VAL:HG13	1:54:A:GLU:HB3	9	1.39
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG11	5	1.39
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG12	5	1.39
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG13	5	1.39
(1,339)	1:16:A:GLY:H	1:38:A:ARG:HG3	4	1.37
(1,128)	1:27:A:LYS:HE3	1:27:A:LYS:HG3	10	1.37
(1,67)	1:19:A:SER:HA	1:36:A:ARG:HB3	3	1.37
(1,20)	1:7:A:CYS:HB2	1:3:A:GLN:HG3	4	1.37
(1,286)	1:7:A:CYS:H	1:8:A:GLN:HG3	10	1.35
(1,163)	1:35:A:PHE:HD1	1:34:A:THR:HA	3	1.35
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG21	6	1.35
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG22	6	1.35
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG23	6	1.35
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG11	2	1.34
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG12	2	1.34
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG13	2	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:19:A:SER:HA	1:36:A:ARG:HA	10	1.34
(1,20)	1:7:A:CYS:HB2	1:3:A:GLN:HG3	9	1.34
(1,241)	1:55:A:ALA:HA	1:54:A:GLU:HG3	9	1.33
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG21	8	1.33
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG22	8	1.33
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG23	8	1.33
(1,127)	1:27:A:LYS:HE3	1:27:A:LYS:HB3	10	1.33
(1,105)	1:24:A:TYR:HE1	1:11:A:ARG:HB3	7	1.33
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG21	2	1.33
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG22	2	1.33
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG23	2	1.33
(1,67)	1:19:A:SER:HA	1:36:A:ARG:HB3	1	1.33
(1,265)	1:3:A:GLN:H	1:3:A:GLN:HG3	2	1.32
(1,163)	1:35:A:PHE:HD1	1:34:A:THR:HA	7	1.32
(1,294)	1:9:A:LEU:H	1:8:A:GLN:HG3	5	1.31
(1,254)	1:58:A:VAL:HG11	1:54:A:GLU:HB3	5	1.31
(1,254)	1:58:A:VAL:HG12	1:54:A:GLU:HB3	5	1.31
(1,254)	1:58:A:VAL:HG13	1:54:A:GLU:HB3	5	1.31
(1,241)	1:55:A:ALA:HA	1:54:A:GLU:HG3	3	1.31
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG21	10	1.31
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG22	10	1.31
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG23	10	1.31
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD21	6	1.31
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD22	6	1.31
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD23	6	1.31
(1,86)	1:23:A:TYR:HD1	1:48:A:LYS:HA	5	1.31
(1,241)	1:55:A:ALA:HA	1:54:A:GLU:HG3	4	1.3
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG21	1	1.3
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG22	1	1.3
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG23	1	1.3
(1,97)	1:24:A:TYR:HD1	1:11:A:ARG:HB2	9	1.3
(1,86)	1:23:A:TYR:HD1	1:48:A:LYS:HA	9	1.3
(1,66)	1:19:A:SER:HA	1:36:A:ARG:HA	7	1.3
(1,20)	1:7:A:CYS:HB2	1:3:A:GLN:HG3	1	1.3
(1,254)	1:58:A:VAL:HG11	1:54:A:GLU:HB3	2	1.29
(1,254)	1:58:A:VAL:HG12	1:54:A:GLU:HB3	2	1.29
(1,254)	1:58:A:VAL:HG13	1:54:A:GLU:HB3	2	1.29
(1,254)	1:58:A:VAL:HG11	1:54:A:GLU:HB3	6	1.29
(1,254)	1:58:A:VAL:HG12	1:54:A:GLU:HB3	6	1.29
(1,254)	1:58:A:VAL:HG13	1:54:A:GLU:HB3	6	1.29
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG21	2	1.29
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG22	2	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG23	2	1.29
(1,197)	1:47:A:PHE:HB3	1:23:A:TYR:HB3	1	1.29
(1,197)	1:47:A:PHE:HB3	1:23:A:TYR:HB3	2	1.29
(1,86)	1:23:A:TYR:HD1	1:48:A:LYS:HA	6	1.29
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG21	1	1.29
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG22	1	1.29
(1,83)	1:23:A:TYR:HA	1:34:A:THR:HG23	1	1.29
(1,37)	1:11:A:ARG:HD3	1:11:A:ARG:HA	5	1.29
(1,37)	1:11:A:ARG:HD3	1:11:A:ARG:HA	9	1.29
(1,294)	1:9:A:LEU:H	1:8:A:GLN:HG3	2	1.28
(1,294)	1:9:A:LEU:H	1:8:A:GLN:HG3	4	1.28
(1,184)	1:37:A:TYR:HB2	1:46:A:ARG:HB3	8	1.28
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD21	1	1.28
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD22	1	1.28
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD23	1	1.28
(1,86)	1:23:A:TYR:HD1	1:48:A:LYS:HA	7	1.28
(1,390)	1:27:A:LYS:H	1:27:A:LYS:HE3	9	1.27
(1,294)	1:9:A:LEU:H	1:8:A:GLN:HG3	3	1.27
(1,139)	1:32:A:CYS:HB3	1:23:A:TYR:HB3	9	1.27
(1,79)	1:22:A:ASN:HB2	1:22:A:ASN:HB3	1	1.27
(1,79)	1:22:A:ASN:HB2	1:22:A:ASN:HB3	2	1.27
(1,79)	1:22:A:ASN:HB2	1:22:A:ASN:HB3	3	1.27
(1,79)	1:22:A:ASN:HB2	1:22:A:ASN:HB3	4	1.27
(1,79)	1:22:A:ASN:HB2	1:22:A:ASN:HB3	5	1.27
(1,79)	1:22:A:ASN:HB2	1:22:A:ASN:HB3	6	1.27
(1,79)	1:22:A:ASN:HB2	1:22:A:ASN:HB3	7	1.27
(1,79)	1:22:A:ASN:HB2	1:22:A:ASN:HB3	8	1.27
(1,79)	1:22:A:ASN:HB2	1:22:A:ASN:HB3	9	1.27
(1,79)	1:22:A:ASN:HB2	1:22:A:ASN:HB3	10	1.27
(1,241)	1:55:A:ALA:HA	1:54:A:GLU:HG3	7	1.26
(1,241)	1:55:A:ALA:HA	1:54:A:GLU:HG3	10	1.26
(1,86)	1:23:A:TYR:HD1	1:48:A:LYS:HA	1	1.26
(1,241)	1:55:A:ALA:HA	1:54:A:GLU:HG3	5	1.25
(1,241)	1:55:A:ALA:HA	1:54:A:GLU:HG3	8	1.25
(1,197)	1:47:A:PHE:HB3	1:23:A:TYR:HB3	4	1.24
(1,66)	1:19:A:SER:HA	1:36:A:ARG:HA	8	1.24
(1,325)	1:14:A:GLY:H	1:13:A:TYR:HB3	5	1.23
(1,241)	1:55:A:ALA:HA	1:54:A:GLU:HG3	1	1.23
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD21	2	1.23
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD22	2	1.23
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD23	2	1.23
(1,254)	1:58:A:VAL:HG11	1:54:A:GLU:HB3	1	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,254)	1:58:A:VAL:HG12	1:54:A:GLU:HB3	1	1.22
(1,254)	1:58:A:VAL:HG13	1:54:A:GLU:HB3	1	1.22
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG21	5	1.22
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG22	5	1.22
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG23	5	1.22
(1,22)	1:8:A:GLN:HA	1:27:A:LYS:HE3	9	1.22
(1,241)	1:55:A:ALA:HA	1:54:A:GLU:HG3	2	1.21
(1,163)	1:35:A:PHE:HD1	1:34:A:THR:HA	1	1.21
(1,144)	1:33:A:LYS:HA	1:33:A:LYS:HD2	6	1.21
(1,139)	1:32:A:CYS:HB3	1:23:A:TYR:HB3	3	1.21
(1,113)	1:24:A:TYR:HE1	1:26:A:ASP:HB2	3	1.21
(1,66)	1:19:A:SER:HA	1:36:A:ARG:HA	9	1.21
(1,163)	1:35:A:PHE:HD1	1:34:A:THR:HA	2	1.2
(1,197)	1:47:A:PHE:HB3	1:23:A:TYR:HB3	5	1.19
(1,183)	1:37:A:TYR:HB2	1:22:A:ASN:HB2	6	1.19
(1,87)	1:23:A:TYR:HD1	1:49:A:THR:HA	5	1.19
(1,54)	1:14:A:GLY:HA3	1:14:A:GLY:HA2	3	1.19
(1,54)	1:14:A:GLY:HA3	1:14:A:GLY:HA2	9	1.19
(1,42)	1:11:A:ARG:HD2	1:11:A:ARG:HB2	10	1.19
(1,241)	1:55:A:ALA:HA	1:54:A:GLU:HG3	6	1.18
(1,163)	1:35:A:PHE:HD1	1:34:A:THR:HA	9	1.18
(1,105)	1:24:A:TYR:HE1	1:11:A:ARG:HB3	3	1.18
(1,54)	1:14:A:GLY:HA3	1:14:A:GLY:HA2	1	1.18
(1,54)	1:14:A:GLY:HA3	1:14:A:GLY:HA2	7	1.18
(1,286)	1:7:A:CYS:H	1:8:A:GLN:HG3	9	1.17
(1,149)	1:33:A:LYS:HE3	1:33:A:LYS:HG3	3	1.17
(1,139)	1:32:A:CYS:HB3	1:23:A:TYR:HB3	5	1.17
(1,67)	1:19:A:SER:HA	1:36:A:ARG:HB3	6	1.17
(1,67)	1:19:A:SER:HA	1:36:A:ARG:HB3	7	1.17
(1,54)	1:14:A:GLY:HA3	1:14:A:GLY:HA2	2	1.17
(1,54)	1:14:A:GLY:HA3	1:14:A:GLY:HA2	4	1.17
(1,54)	1:14:A:GLY:HA3	1:14:A:GLY:HA2	5	1.17
(1,54)	1:14:A:GLY:HA3	1:14:A:GLY:HA2	6	1.17
(1,54)	1:14:A:GLY:HA3	1:14:A:GLY:HA2	8	1.17
(1,54)	1:14:A:GLY:HA3	1:14:A:GLY:HA2	10	1.17
(1,139)	1:32:A:CYS:HB3	1:23:A:TYR:HB3	6	1.16
(1,95)	1:24:A:TYR:HB3	1:11:A:ARG:HB2	2	1.16
(1,393)	1:28:A:ALA:H	1:28:A:ALA:HB3	3	1.15
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD11	9	1.15
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD12	9	1.15
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD13	9	1.15
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD11	10	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD12	10	1.15
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD13	10	1.15
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG21	3	1.15
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG22	3	1.15
(1,223)	1:51:A:GLU:HG2	1:49:A:THR:HG23	3	1.15
(1,22)	1:8:A:GLN:HA	1:27:A:LYS:HE3	8	1.15
(1,309)	1:12:A:ASN:H	1:11:A:ARG:HB2	1	1.14
(1,309)	1:12:A:ASN:H	1:11:A:ARG:HB2	4	1.14
(1,247)	1:57:A:CYS:HA	1:3:A:GLN:HG3	7	1.14
(1,150)	1:33:A:LYS:HG2	1:33:A:LYS:HA	3	1.14
(1,22)	1:8:A:GLN:HA	1:27:A:LYS:HE3	10	1.14
(1,393)	1:28:A:ALA:H	1:28:A:ALA:HB3	1	1.13
(1,393)	1:28:A:ALA:H	1:28:A:ALA:HB3	6	1.13
(1,393)	1:28:A:ALA:H	1:28:A:ALA:HB3	9	1.13
(1,309)	1:12:A:ASN:H	1:11:A:ARG:HB2	8	1.13
(1,145)	1:33:A:LYS:HA	1:33:A:LYS:HE3	10	1.13
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD21	8	1.13
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD22	8	1.13
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD23	8	1.13
(1,66)	1:19:A:SER:HA	1:36:A:ARG:HA	4	1.13
(1,38)	1:11:A:ARG:HD3	1:11:A:ARG:HB2	3	1.13
(1,509)	1:54:A:GLU:H	1:54:A:GLU:HG3	2	1.12
(1,393)	1:28:A:ALA:H	1:28:A:ALA:HB3	2	1.12
(1,393)	1:28:A:ALA:H	1:28:A:ALA:HB3	4	1.12
(1,393)	1:28:A:ALA:H	1:28:A:ALA:HB3	5	1.12
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD11	1	1.12
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD12	1	1.12
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD13	1	1.12
(1,215)	1:50:A:LEU:HD21	1:54:A:GLU:HG3	7	1.12
(1,215)	1:50:A:LEU:HD22	1:54:A:GLU:HG3	7	1.12
(1,215)	1:50:A:LEU:HD23	1:54:A:GLU:HG3	7	1.12
(1,163)	1:35:A:PHE:HD1	1:34:A:THR:HA	6	1.12
(1,152)	1:34:A:THR:HA	1:33:A:LYS:HE3	3	1.12
(1,145)	1:33:A:LYS:HA	1:33:A:LYS:HE3	9	1.12
(1,66)	1:19:A:SER:HA	1:36:A:ARG:HA	5	1.12
(1,393)	1:28:A:ALA:H	1:28:A:ALA:HB3	7	1.11
(1,393)	1:28:A:ALA:H	1:28:A:ALA:HB3	8	1.11
(1,303)	1:11:A:ARG:H	1:10:A:SER:HA	6	1.11
(1,215)	1:50:A:LEU:HD21	1:54:A:GLU:HG3	8	1.11
(1,215)	1:50:A:LEU:HD22	1:54:A:GLU:HG3	8	1.11
(1,215)	1:50:A:LEU:HD23	1:54:A:GLU:HG3	8	1.11
(1,163)	1:35:A:PHE:HD1	1:34:A:THR:HA	10	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,145)	1:33:A:LYS:HA	1:33:A:LYS:HE3	1	1.11
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD21	4	1.11
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD22	4	1.11
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD23	4	1.11
(1,95)	1:24:A:TYR:HB3	1:11:A:ARG:HB2	8	1.11
(1,38)	1:11:A:ARG:HD3	1:11:A:ARG:HB2	4	1.11
(1,378)	1:25:A:TYR:H	1:24:A:TYR:HB3	5	1.1
(1,269)	1:4:A:ASP:H	1:3:A:GLN:HB3	2	1.1
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG11	1	1.1
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG12	1	1.1
(1,133)	1:31:A:SER:HB3	1:58:A:VAL:HG13	1	1.1
(1,509)	1:54:A:GLU:H	1:54:A:GLU:HG3	1	1.09
(1,509)	1:54:A:GLU:H	1:54:A:GLU:HG3	6	1.09
(1,456)	1:43:A:ASN:H	1:43:A:ASN:HB3	3	1.09
(1,393)	1:28:A:ALA:H	1:28:A:ALA:HB3	10	1.09
(1,378)	1:25:A:TYR:H	1:24:A:TYR:HB3	4	1.09
(1,339)	1:16:A:GLY:H	1:38:A:ARG:HG3	7	1.09
(1,215)	1:50:A:LEU:HD21	1:54:A:GLU:HG3	10	1.09
(1,215)	1:50:A:LEU:HD22	1:54:A:GLU:HG3	10	1.09
(1,215)	1:50:A:LEU:HD23	1:54:A:GLU:HG3	10	1.09
(1,149)	1:33:A:LYS:HE3	1:33:A:LYS:HG3	5	1.09
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD21	9	1.09
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD22	9	1.09
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD23	9	1.09
(1,86)	1:23:A:TYR:HD1	1:48:A:LYS:HA	3	1.09
(1,509)	1:54:A:GLU:H	1:54:A:GLU:HG3	8	1.08
(1,378)	1:25:A:TYR:H	1:24:A:TYR:HB3	3	1.08
(1,378)	1:25:A:TYR:H	1:24:A:TYR:HB3	9	1.08
(1,139)	1:32:A:CYS:HB3	1:23:A:TYR:HB3	4	1.08
(1,95)	1:24:A:TYR:HB3	1:11:A:ARG:HB2	7	1.08
(1,38)	1:11:A:ARG:HD3	1:11:A:ARG:HB2	2	1.08
(1,38)	1:11:A:ARG:HD3	1:11:A:ARG:HB2	8	1.08
(1,11)	1:5:A:TYR:HB3	1:8:A:GLN:HG3	6	1.08
(1,509)	1:54:A:GLU:H	1:54:A:GLU:HG3	4	1.07
(1,509)	1:54:A:GLU:H	1:54:A:GLU:HG3	5	1.07
(1,509)	1:54:A:GLU:H	1:54:A:GLU:HG3	10	1.07
(1,163)	1:35:A:PHE:HD1	1:34:A:THR:HA	5	1.07
(1,163)	1:35:A:PHE:HD1	1:34:A:THR:HA	8	1.07
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD21	3	1.07
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD22	3	1.07
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD23	3	1.07
(1,534)	1:59:A:THR:H	1:59:A:THR:HG21	4	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,534)	1:59:A:THR:H	1:59:A:THR:HG22	4	1.06
(1,534)	1:59:A:THR:H	1:59:A:THR:HG23	4	1.06
(1,454)	1:43:A:ASN:H	1:12:A:ASN:HB3	4	1.06
(1,390)	1:27:A:LYS:H	1:27:A:LYS:HE3	10	1.06
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD11	3	1.06
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD12	3	1.06
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD13	3	1.06
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD11	4	1.06
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD12	4	1.06
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD13	4	1.06
(1,215)	1:50:A:LEU:HD21	1:54:A:GLU:HG3	3	1.06
(1,215)	1:50:A:LEU:HD22	1:54:A:GLU:HG3	3	1.06
(1,215)	1:50:A:LEU:HD23	1:54:A:GLU:HG3	3	1.06
(1,149)	1:33:A:LYS:HE3	1:33:A:LYS:HG3	4	1.06
(1,134)	1:32:A:CYS:HA	1:25:A:TYR:HB3	10	1.06
(1,509)	1:54:A:GLU:H	1:54:A:GLU:HG3	3	1.05
(1,378)	1:25:A:TYR:H	1:24:A:TYR:HB3	8	1.05
(1,339)	1:16:A:GLY:H	1:38:A:ARG:HG3	9	1.05
(1,215)	1:50:A:LEU:HD21	1:54:A:GLU:HG3	1	1.05
(1,215)	1:50:A:LEU:HD22	1:54:A:GLU:HG3	1	1.05
(1,215)	1:50:A:LEU:HD23	1:54:A:GLU:HG3	1	1.05
(1,215)	1:50:A:LEU:HD21	1:54:A:GLU:HG3	6	1.05
(1,215)	1:50:A:LEU:HD22	1:54:A:GLU:HG3	6	1.05
(1,215)	1:50:A:LEU:HD23	1:54:A:GLU:HG3	6	1.05
(1,145)	1:33:A:LYS:HA	1:33:A:LYS:HE3	7	1.05
(1,139)	1:32:A:CYS:HB3	1:23:A:TYR:HB3	2	1.05
(1,87)	1:23:A:TYR:HD1	1:49:A:THR:HA	6	1.05
(1,66)	1:19:A:SER:HA	1:36:A:ARG:HA	3	1.05
(1,38)	1:11:A:ARG:HD3	1:11:A:ARG:HB2	1	1.05
(1,37)	1:11:A:ARG:HD3	1:11:A:ARG:HA	7	1.05
(1,534)	1:59:A:THR:H	1:59:A:THR:HG21	2	1.04
(1,534)	1:59:A:THR:H	1:59:A:THR:HG22	2	1.04
(1,534)	1:59:A:THR:H	1:59:A:THR:HG23	2	1.04
(1,534)	1:59:A:THR:H	1:59:A:THR:HG21	3	1.04
(1,534)	1:59:A:THR:H	1:59:A:THR:HG22	3	1.04
(1,534)	1:59:A:THR:H	1:59:A:THR:HG23	3	1.04
(1,534)	1:59:A:THR:H	1:59:A:THR:HG21	7	1.04
(1,534)	1:59:A:THR:H	1:59:A:THR:HG22	7	1.04
(1,534)	1:59:A:THR:H	1:59:A:THR:HG23	7	1.04
(1,378)	1:25:A:TYR:H	1:24:A:TYR:HB3	7	1.04
(1,313)	1:12:A:ASN:H	1:12:A:ASN:HB2	4	1.04
(1,309)	1:12:A:ASN:H	1:11:A:ARG:HB2	3	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD11	7	1.04
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD12	7	1.04
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD13	7	1.04
(1,286)	1:7:A:CYS:H	1:8:A:GLN:HG3	4	1.04
(1,286)	1:7:A:CYS:H	1:8:A:GLN:HG3	7	1.04
(1,149)	1:33:A:LYS:HE3	1:33:A:LYS:HG3	2	1.04
(1,534)	1:59:A:THR:H	1:59:A:THR:HG21	6	1.03
(1,534)	1:59:A:THR:H	1:59:A:THR:HG22	6	1.03
(1,534)	1:59:A:THR:H	1:59:A:THR:HG23	6	1.03
(1,534)	1:59:A:THR:H	1:59:A:THR:HG21	8	1.03
(1,534)	1:59:A:THR:H	1:59:A:THR:HG22	8	1.03
(1,534)	1:59:A:THR:H	1:59:A:THR:HG23	8	1.03
(1,534)	1:59:A:THR:H	1:59:A:THR:HG21	10	1.03
(1,534)	1:59:A:THR:H	1:59:A:THR:HG22	10	1.03
(1,534)	1:59:A:THR:H	1:59:A:THR:HG23	10	1.03
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD11	2	1.03
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD12	2	1.03
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD13	2	1.03
(1,197)	1:47:A:PHE:HB3	1:23:A:TYR:HB3	3	1.03
(1,163)	1:35:A:PHE:HD1	1:34:A:THR:HA	4	1.03
(1,11)	1:5:A:TYR:HB3	1:8:A:GLN:HG3	4	1.03
(1,11)	1:5:A:TYR:HB3	1:8:A:GLN:HG3	5	1.03
(1,534)	1:59:A:THR:H	1:59:A:THR:HG21	5	1.02
(1,534)	1:59:A:THR:H	1:59:A:THR:HG22	5	1.02
(1,534)	1:59:A:THR:H	1:59:A:THR:HG23	5	1.02
(1,378)	1:25:A:TYR:H	1:24:A:TYR:HB3	6	1.02
(1,339)	1:16:A:GLY:H	1:38:A:ARG:HG3	5	1.02
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD11	5	1.02
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD12	5	1.02
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD13	5	1.02
(1,264)	1:3:A:GLN:H	1:3:A:GLN:HB2	2	1.02
(1,182)	1:37:A:TYR:HB2	1:20:A:PHE:HB3	3	1.02
(1,152)	1:34:A:THR:HA	1:33:A:LYS:HE3	8	1.02
(1,95)	1:24:A:TYR:HB3	1:11:A:ARG:HB2	4	1.02
(1,48)	1:12:A:ASN:HA	1:12:A:ASN:HB3	6	1.02
(1,48)	1:12:A:ASN:HA	1:12:A:ASN:HB3	7	1.02
(1,11)	1:5:A:TYR:HB3	1:8:A:GLN:HG3	3	1.02
(1,509)	1:54:A:GLU:H	1:54:A:GLU:HG3	7	1.01
(1,197)	1:47:A:PHE:HB3	1:23:A:TYR:HB3	8	1.01
(1,66)	1:19:A:SER:HA	1:36:A:ARG:HA	1	1.01
(1,48)	1:12:A:ASN:HA	1:12:A:ASN:HB3	1	1.01
(1,48)	1:12:A:ASN:HA	1:12:A:ASN:HB3	3	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:12:A:ASN:HA	1:12:A:ASN:HB3	5	1.01
(1,48)	1:12:A:ASN:HA	1:12:A:ASN:HB3	9	1.01
(1,265)	1:3:A:GLN:H	1:3:A:GLN:HG3	7	1.0
(1,197)	1:47:A:PHE:HB3	1:23:A:TYR:HB3	9	1.0
(1,139)	1:32:A:CYS:HB3	1:23:A:TYR:HB3	1	1.0
(1,86)	1:23:A:TYR:HD1	1:48:A:LYS:HA	4	1.0
(1,86)	1:23:A:TYR:HD1	1:48:A:LYS:HA	10	1.0
(1,72)	1:20:A:PHE:HA	1:20:A:PHE:HB3	4	1.0
(1,72)	1:20:A:PHE:HA	1:20:A:PHE:HB3	10	1.0
(1,48)	1:12:A:ASN:HA	1:12:A:ASN:HB3	2	1.0
(1,42)	1:11:A:ARG:HD2	1:11:A:ARG:HB2	7	1.0
(1,378)	1:25:A:TYR:H	1:24:A:TYR:HB3	10	0.99
(1,294)	1:9:A:LEU:H	1:8:A:GLN:HG3	7	0.99
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD21	10	0.99
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD22	10	0.99
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD23	10	0.99
(1,40)	1:11:A:ARG:HD3	1:11:A:ARG:HG3	7	0.99
(1,509)	1:54:A:GLU:H	1:54:A:GLU:HG3	9	0.98
(1,318)	1:13:A:TYR:H	1:12:A:ASN:HB3	3	0.98
(1,318)	1:13:A:TYR:H	1:12:A:ASN:HB3	6	0.98
(1,215)	1:50:A:LEU:HD21	1:54:A:GLU:HG3	2	0.98
(1,215)	1:50:A:LEU:HD22	1:54:A:GLU:HG3	2	0.98
(1,215)	1:50:A:LEU:HD23	1:54:A:GLU:HG3	2	0.98
(1,182)	1:37:A:TYR:HB2	1:20:A:PHE:HB3	9	0.98
(1,145)	1:33:A:LYS:HA	1:33:A:LYS:HE3	8	0.98
(1,87)	1:23:A:TYR:HD1	1:49:A:THR:HA	1	0.98
(1,72)	1:20:A:PHE:HA	1:20:A:PHE:HB3	2	0.98
(1,40)	1:11:A:ARG:HD3	1:11:A:ARG:HG3	3	0.98
(1,40)	1:11:A:ARG:HD3	1:11:A:ARG:HG3	9	0.98
(1,215)	1:50:A:LEU:HD21	1:54:A:GLU:HG3	9	0.97
(1,215)	1:50:A:LEU:HD22	1:54:A:GLU:HG3	9	0.97
(1,215)	1:50:A:LEU:HD23	1:54:A:GLU:HG3	9	0.97
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD21	7	0.97
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD22	7	0.97
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD23	7	0.97
(1,95)	1:24:A:TYR:HB3	1:11:A:ARG:HB2	10	0.97
(1,72)	1:20:A:PHE:HA	1:20:A:PHE:HB3	3	0.97
(1,72)	1:20:A:PHE:HA	1:20:A:PHE:HB3	9	0.97
(1,48)	1:12:A:ASN:HA	1:12:A:ASN:HB3	4	0.97
(1,40)	1:11:A:ARG:HD3	1:11:A:ARG:HG3	1	0.97
(1,40)	1:11:A:ARG:HD3	1:11:A:ARG:HG3	4	0.97
(1,40)	1:11:A:ARG:HD3	1:11:A:ARG:HG3	6	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:11:A:ARG:HD3	1:11:A:ARG:HG3	8	0.97
(1,331)	1:15:A:LYS:H	1:15:A:LYS:HG3	8	0.96
(1,323)	1:13:A:TYR:H	1:14:A:GLY:H	4	0.96
(1,323)	1:13:A:TYR:H	1:14:A:GLY:H	5	0.96
(1,318)	1:13:A:TYR:H	1:12:A:ASN:HB3	7	0.96
(1,265)	1:3:A:GLN:H	1:3:A:GLN:HG3	10	0.96
(1,215)	1:50:A:LEU:HD21	1:54:A:GLU:HG3	4	0.96
(1,215)	1:50:A:LEU:HD22	1:54:A:GLU:HG3	4	0.96
(1,215)	1:50:A:LEU:HD23	1:54:A:GLU:HG3	4	0.96
(1,197)	1:47:A:PHE:HB3	1:23:A:TYR:HB3	10	0.96
(1,176)	1:36:A:ARG:HD3	1:36:A:ARG:HA	4	0.96
(1,87)	1:23:A:TYR:HD1	1:49:A:THR:HA	7	0.96
(1,86)	1:23:A:TYR:HD1	1:48:A:LYS:HA	8	0.96
(1,40)	1:11:A:ARG:HD3	1:11:A:ARG:HG3	2	0.96
(1,36)	1:11:A:ARG:HB2	1:11:A:ARG:HG2	3	0.96
(1,351)	1:19:A:SER:H	1:18:A:GLY:HA3	10	0.95
(1,350)	1:18:A:GLY:H	1:19:A:SER:H	1	0.95
(1,309)	1:12:A:ASN:H	1:11:A:ARG:HB2	2	0.95
(1,152)	1:34:A:THR:HA	1:33:A:LYS:HE3	6	0.95
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD21	5	0.95
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD22	5	0.95
(1,142)	1:32:A:CYS:HB2	1:50:A:LEU:HD23	5	0.95
(1,40)	1:11:A:ARG:HD3	1:11:A:ARG:HG3	10	0.95
(1,38)	1:11:A:ARG:HD3	1:11:A:ARG:HB2	5	0.95
(1,36)	1:11:A:ARG:HB2	1:11:A:ARG:HG2	2	0.95
(1,36)	1:11:A:ARG:HB2	1:11:A:ARG:HG2	4	0.95
(1,36)	1:11:A:ARG:HB2	1:11:A:ARG:HG2	8	0.95
(1,20)	1:7:A:CYS:HB2	1:3:A:GLN:HG3	7	0.95
(1,472)	1:49:A:THR:H	1:52:A:ASP:HB3	5	0.94
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD11	7	0.94
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD12	7	0.94
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD13	7	0.94
(1,182)	1:37:A:TYR:HB2	1:20:A:PHE:HB3	2	0.94
(1,87)	1:23:A:TYR:HD1	1:49:A:THR:HA	3	0.94
(1,40)	1:11:A:ARG:HD3	1:11:A:ARG:HG3	5	0.94
(1,36)	1:11:A:ARG:HB2	1:11:A:ARG:HG2	1	0.94
(1,350)	1:18:A:GLY:H	1:19:A:SER:H	3	0.93
(1,286)	1:7:A:CYS:H	1:8:A:GLN:HG3	5	0.93
(1,35)	1:11:A:ARG:HB2	1:11:A:ARG:HB3	9	0.93
(1,448)	1:41:A:GLY:H	1:40:A:SER:H	7	0.92
(1,378)	1:25:A:TYR:H	1:24:A:TYR:HB3	1	0.92
(1,215)	1:50:A:LEU:HD21	1:54:A:GLU:HG3	5	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:50:A:LEU:HD22	1:54:A:GLU:HG3	5	0.92
(1,215)	1:50:A:LEU:HD23	1:54:A:GLU:HG3	5	0.92
(1,67)	1:19:A:SER:HA	1:36:A:ARG:HB3	9	0.92
(1,66)	1:19:A:SER:HA	1:36:A:ARG:HA	2	0.92
(1,35)	1:11:A:ARG:HB2	1:11:A:ARG:HB3	1	0.92
(1,35)	1:11:A:ARG:HB2	1:11:A:ARG:HB3	2	0.92
(1,35)	1:11:A:ARG:HB2	1:11:A:ARG:HB3	3	0.92
(1,35)	1:11:A:ARG:HB2	1:11:A:ARG:HB3	4	0.92
(1,35)	1:11:A:ARG:HB2	1:11:A:ARG:HB3	5	0.92
(1,35)	1:11:A:ARG:HB2	1:11:A:ARG:HB3	6	0.92
(1,35)	1:11:A:ARG:HB2	1:11:A:ARG:HB3	7	0.92
(1,35)	1:11:A:ARG:HB2	1:11:A:ARG:HB3	8	0.92
(1,35)	1:11:A:ARG:HB2	1:11:A:ARG:HB3	10	0.92
(1,534)	1:59:A:THR:H	1:59:A:THR:HG21	9	0.91
(1,534)	1:59:A:THR:H	1:59:A:THR:HG22	9	0.91
(1,534)	1:59:A:THR:H	1:59:A:THR:HG23	9	0.91
(1,378)	1:25:A:TYR:H	1:24:A:TYR:HB3	2	0.91
(1,345)	1:17:A:SER:H	1:38:A:ARG:HA	5	0.91
(1,318)	1:13:A:TYR:H	1:12:A:ASN:HB3	10	0.91
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD11	5	0.91
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD12	5	0.91
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD13	5	0.91
(1,176)	1:36:A:ARG:HD3	1:36:A:ARG:HA	2	0.91
(1,42)	1:11:A:ARG:HD2	1:11:A:ARG:HB2	5	0.91
(1,23)	1:9:A:LEU:HA	1:5:A:TYR:HB3	6	0.91
(1,463)	1:48:A:LYS:H	1:48:A:LYS:HD3	10	0.9
(1,341)	1:17:A:SER:H	1:16:A:GLY:HA2	4	0.9
(1,197)	1:47:A:PHE:HB3	1:23:A:TYR:HB3	7	0.9
(1,144)	1:33:A:LYS:HA	1:33:A:LYS:HD2	1	0.9
(1,95)	1:24:A:TYR:HB3	1:11:A:ARG:HB2	5	0.9
(1,82)	1:23:A:TYR:HA	1:34:A:THR:HB	6	0.9
(1,72)	1:20:A:PHE:HA	1:20:A:PHE:HB3	8	0.9
(1,36)	1:11:A:ARG:HB2	1:11:A:ARG:HG2	6	0.9
(1,144)	1:33:A:LYS:HA	1:33:A:LYS:HD2	8	0.89
(1,86)	1:23:A:TYR:HD1	1:48:A:LYS:HA	2	0.89
(1,72)	1:20:A:PHE:HA	1:20:A:PHE:HB3	7	0.89
(1,361)	1:21:A:THR:H	1:20:A:PHE:HB3	7	0.88
(1,82)	1:23:A:TYR:HA	1:34:A:THR:HB	1	0.88
(1,82)	1:23:A:TYR:HA	1:34:A:THR:HB	5	0.88
(1,145)	1:33:A:LYS:HA	1:33:A:LYS:HE3	6	0.87
(1,124)	1:27:A:LYS:HA	1:27:A:LYS:HG3	3	0.87
(1,87)	1:23:A:TYR:HD1	1:49:A:THR:HA	9	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,82)	1:23:A:TYR:HA	1:34:A:THR:HB	2	0.87
(1,82)	1:23:A:TYR:HA	1:34:A:THR:HB	9	0.87
(1,351)	1:19:A:SER:H	1:18:A:GLY:HA3	6	0.86
(1,318)	1:13:A:TYR:H	1:12:A:ASN:HB3	2	0.86
(1,176)	1:36:A:ARG:HD3	1:36:A:ARG:HA	3	0.86
(1,114)	1:25:A:TYR:HA	1:32:A:CYS:HA	10	0.86
(1,105)	1:24:A:TYR:HE1	1:11:A:ARG:HB3	6	0.86
(1,87)	1:23:A:TYR:HD1	1:49:A:THR:HA	8	0.86
(1,85)	1:23:A:TYR:HD1	1:23:A:TYR:HB3	3	0.86
(1,85)	1:23:A:TYR:HD1	1:23:A:TYR:HB3	7	0.86
(1,82)	1:23:A:TYR:HA	1:34:A:THR:HB	8	0.86
(1,541)	1:61:A:GLU:H	1:61:A:GLU:HB2	5	0.85
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD11	6	0.85
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD12	6	0.85
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD13	6	0.85
(1,265)	1:3:A:GLN:H	1:3:A:GLN:HG3	1	0.85
(1,196)	1:47:A:PHE:HA	1:48:A:LYS:HD3	5	0.85
(1,124)	1:27:A:LYS:HA	1:27:A:LYS:HG3	8	0.85
(1,85)	1:23:A:TYR:HD1	1:23:A:TYR:HB3	1	0.85
(1,85)	1:23:A:TYR:HD1	1:23:A:TYR:HB3	2	0.85
(1,85)	1:23:A:TYR:HD1	1:23:A:TYR:HB3	4	0.85
(1,85)	1:23:A:TYR:HD1	1:23:A:TYR:HB3	5	0.85
(1,85)	1:23:A:TYR:HD1	1:23:A:TYR:HB3	8	0.85
(1,85)	1:23:A:TYR:HD1	1:23:A:TYR:HB3	10	0.85
(1,37)	1:11:A:ARG:HD3	1:11:A:ARG:HA	10	0.85
(1,11)	1:5:A:TYR:HB3	1:8:A:GLN:HG3	9	0.85
(1,449)	1:41:A:GLY:H	1:40:A:SER:HA	4	0.84
(1,152)	1:34:A:THR:HA	1:33:A:LYS:HE3	7	0.84
(1,350)	1:18:A:GLY:H	1:19:A:SER:H	5	0.83
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD11	3	0.83
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD12	3	0.83
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD13	3	0.83
(1,124)	1:27:A:LYS:HA	1:27:A:LYS:HG3	2	0.83
(1,124)	1:27:A:LYS:HA	1:27:A:LYS:HG3	5	0.83
(1,85)	1:23:A:TYR:HD1	1:23:A:TYR:HB3	6	0.83
(1,85)	1:23:A:TYR:HD1	1:23:A:TYR:HB3	9	0.83
(1,82)	1:23:A:TYR:HA	1:34:A:THR:HB	10	0.83
(1,50)	1:12:A:ASN:HB3	1:12:A:ASN:HB2	1	0.83
(1,50)	1:12:A:ASN:HB3	1:12:A:ASN:HB2	5	0.83
(1,50)	1:12:A:ASN:HB3	1:12:A:ASN:HB2	8	0.83
(1,50)	1:12:A:ASN:HB3	1:12:A:ASN:HB2	10	0.83
(1,340)	1:17:A:SER:H	1:16:A:GLY:HA3	10	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:13:A:TYR:H	1:12:A:ASN:HB3	1	0.82
(1,286)	1:7:A:CYS:H	1:8:A:GLN:HG3	3	0.82
(1,265)	1:3:A:GLN:H	1:3:A:GLN:HG3	3	0.82
(1,196)	1:47:A:PHE:HA	1:48:A:LYS:HD3	4	0.82
(1,114)	1:25:A:TYR:HA	1:32:A:CYS:HA	6	0.82
(1,82)	1:23:A:TYR:HA	1:34:A:THR:HB	7	0.82
(1,50)	1:12:A:ASN:HB3	1:12:A:ASN:HB2	2	0.82
(1,50)	1:12:A:ASN:HB3	1:12:A:ASN:HB2	3	0.82
(1,50)	1:12:A:ASN:HB3	1:12:A:ASN:HB2	4	0.82
(1,50)	1:12:A:ASN:HB3	1:12:A:ASN:HB2	7	0.82
(1,50)	1:12:A:ASN:HB3	1:12:A:ASN:HB2	9	0.82
(1,26)	1:9:A:LEU:HD11	1:45:A:ASN:HB2	5	0.82
(1,26)	1:9:A:LEU:HD12	1:45:A:ASN:HB2	5	0.82
(1,26)	1:9:A:LEU:HD13	1:45:A:ASN:HB2	5	0.82
(1,11)	1:5:A:TYR:HB3	1:8:A:GLN:HG3	7	0.82
(1,313)	1:12:A:ASN:H	1:12:A:ASN:HB2	8	0.81
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD11	9	0.81
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD12	9	0.81
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD13	9	0.81
(1,124)	1:27:A:LYS:HA	1:27:A:LYS:HG3	1	0.81
(1,82)	1:23:A:TYR:HA	1:34:A:THR:HB	4	0.81
(1,71)	1:19:A:SER:HB2	1:36:A:ARG:HD3	4	0.81
(1,66)	1:19:A:SER:HA	1:36:A:ARG:HA	6	0.81
(1,50)	1:12:A:ASN:HB3	1:12:A:ASN:HB2	6	0.81
(1,543)	1:61:A:GLU:H	1:61:A:GLU:HG2	5	0.8
(1,361)	1:21:A:THR:H	1:20:A:PHE:HB3	5	0.8
(1,361)	1:21:A:THR:H	1:20:A:PHE:HB3	8	0.8
(1,310)	1:12:A:ASN:H	1:11:A:ARG:HG3	2	0.8
(1,124)	1:27:A:LYS:HA	1:27:A:LYS:HG3	4	0.8
(1,114)	1:25:A:TYR:HA	1:32:A:CYS:HA	4	0.8
(1,114)	1:25:A:TYR:HA	1:32:A:CYS:HA	7	0.8
(1,84)	1:23:A:TYR:HD1	1:22:A:ASN:HA	2	0.8
(1,84)	1:23:A:TYR:HD1	1:22:A:ASN:HA	6	0.8
(1,84)	1:23:A:TYR:HD1	1:22:A:ASN:HA	9	0.8
(1,38)	1:11:A:ARG:HD3	1:11:A:ARG:HB2	6	0.8
(1,356)	1:20:A:PHE:H	1:19:A:SER:HB2	10	0.79
(1,323)	1:13:A:TYR:H	1:14:A:GLY:H	10	0.79
(1,176)	1:36:A:ARG:HD3	1:36:A:ARG:HA	1	0.79
(1,176)	1:36:A:ARG:HD3	1:36:A:ARG:HA	6	0.79
(1,152)	1:34:A:THR:HA	1:33:A:LYS:HE3	1	0.79
(1,124)	1:27:A:LYS:HA	1:27:A:LYS:HG3	7	0.79
(1,90)	1:24:A:TYR:HA	1:23:A:TYR:HA	8	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,82)	1:23:A:TYR:HA	1:34:A:THR:HB	3	0.79
(1,36)	1:11:A:ARG:HB2	1:11:A:ARG:HG2	5	0.79
(1,447)	1:40:A:SER:H	1:40:A:SER:HB2	1	0.78
(1,389)	1:27:A:LYS:H	1:27:A:LYS:HB2	10	0.78
(1,361)	1:21:A:THR:H	1:20:A:PHE:HB3	6	0.78
(1,345)	1:17:A:SER:H	1:38:A:ARG:HA	1	0.78
(1,124)	1:27:A:LYS:HA	1:27:A:LYS:HG3	9	0.78
(1,452)	1:42:A:GLY:H	1:41:A:GLY:HA3	1	0.77
(1,352)	1:19:A:SER:H	1:18:A:GLY:HA2	7	0.77
(1,347)	1:18:A:GLY:H	1:17:A:SER:HB2	4	0.77
(1,213)	1:50:A:LEU:HD11	1:51:A:GLU:HG2	5	0.77
(1,213)	1:50:A:LEU:HD12	1:51:A:GLU:HG2	5	0.77
(1,213)	1:50:A:LEU:HD13	1:51:A:GLU:HG2	5	0.77
(1,176)	1:36:A:ARG:HD3	1:36:A:ARG:HA	9	0.77
(1,144)	1:33:A:LYS:HA	1:33:A:LYS:HD2	7	0.77
(1,90)	1:24:A:TYR:HA	1:23:A:TYR:HA	3	0.77
(1,90)	1:24:A:TYR:HA	1:23:A:TYR:HA	4	0.77
(1,90)	1:24:A:TYR:HA	1:23:A:TYR:HA	7	0.77
(1,90)	1:24:A:TYR:HA	1:23:A:TYR:HA	9	0.77
(1,90)	1:24:A:TYR:HA	1:23:A:TYR:HA	10	0.77
(1,84)	1:23:A:TYR:HD1	1:22:A:ASN:HA	3	0.77
(1,472)	1:49:A:THR:H	1:52:A:ASP:HB3	3	0.76
(1,411)	1:32:A:CYS:H	1:31:A:SER:HB3	7	0.76
(1,381)	1:25:A:TYR:H	1:25:A:TYR:HB2	10	0.76
(1,361)	1:21:A:THR:H	1:20:A:PHE:HB3	1	0.76
(1,352)	1:19:A:SER:H	1:18:A:GLY:HA2	8	0.76
(1,340)	1:17:A:SER:H	1:16:A:GLY:HA3	6	0.76
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD11	1	0.76
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD12	1	0.76
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD13	1	0.76
(1,152)	1:34:A:THR:HA	1:33:A:LYS:HE3	10	0.76
(1,114)	1:25:A:TYR:HA	1:32:A:CYS:HA	8	0.76
(1,90)	1:24:A:TYR:HA	1:23:A:TYR:HA	1	0.76
(1,362)	1:21:A:THR:H	1:20:A:PHE:HB2	1	0.75
(1,351)	1:19:A:SER:H	1:18:A:GLY:HA3	4	0.75
(1,311)	1:12:A:ASN:H	1:11:A:ARG:HG2	2	0.75
(1,299)	1:10:A:SER:H	1:9:A:LEU:HB3	6	0.75
(1,144)	1:33:A:LYS:HA	1:33:A:LYS:HD2	10	0.75
(1,124)	1:27:A:LYS:HA	1:27:A:LYS:HG3	6	0.75
(1,114)	1:25:A:TYR:HA	1:32:A:CYS:HA	3	0.75
(1,90)	1:24:A:TYR:HA	1:23:A:TYR:HA	2	0.75
(1,90)	1:24:A:TYR:HA	1:23:A:TYR:HA	5	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,90)	1:24:A:TYR:HA	1:23:A:TYR:HA	6	0.75
(1,87)	1:23:A:TYR:HD1	1:49:A:THR:HA	4	0.75
(1,18)	1:7:A:CYS:HA	1:57:A:CYS:HB2	1	0.75
(1,452)	1:42:A:GLY:H	1:41:A:GLY:HA3	6	0.74
(1,323)	1:13:A:TYR:H	1:14:A:GLY:H	2	0.74
(1,114)	1:25:A:TYR:HA	1:32:A:CYS:HA	2	0.74
(1,114)	1:25:A:TYR:HA	1:32:A:CYS:HA	5	0.74
(1,114)	1:25:A:TYR:HA	1:32:A:CYS:HA	9	0.74
(1,51)	1:13:A:TYR:HA	1:13:A:TYR:HB2	5	0.74
(1,51)	1:13:A:TYR:HA	1:13:A:TYR:HB2	10	0.74
(1,11)	1:5:A:TYR:HB3	1:8:A:GLN:HG3	10	0.74
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG21	1	0.73
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG22	1	0.73
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG23	1	0.73
(1,446)	1:40:A:SER:H	1:40:A:SER:HB3	8	0.73
(1,294)	1:9:A:LEU:H	1:8:A:GLN:HG3	1	0.73
(1,292)	1:9:A:LEU:H	1:8:A:GLN:H	8	0.73
(1,265)	1:3:A:GLN:H	1:3:A:GLN:HG3	9	0.73
(1,176)	1:36:A:ARG:HD3	1:36:A:ARG:HA	10	0.73
(1,122)	1:27:A:LYS:HA	1:27:A:LYS:HB2	10	0.73
(1,42)	1:11:A:ARG:HD2	1:11:A:ARG:HB2	9	0.73
(1,36)	1:11:A:ARG:HB2	1:11:A:ARG:HG2	9	0.73
(1,456)	1:43:A:ASN:H	1:43:A:ASN:HB3	6	0.72
(1,119)	1:26:A:ASP:HB2	1:26:A:ASP:HB3	1	0.72
(1,119)	1:26:A:ASP:HB2	1:26:A:ASP:HB3	2	0.72
(1,119)	1:26:A:ASP:HB2	1:26:A:ASP:HB3	3	0.72
(1,119)	1:26:A:ASP:HB2	1:26:A:ASP:HB3	4	0.72
(1,119)	1:26:A:ASP:HB2	1:26:A:ASP:HB3	5	0.72
(1,119)	1:26:A:ASP:HB2	1:26:A:ASP:HB3	6	0.72
(1,119)	1:26:A:ASP:HB2	1:26:A:ASP:HB3	7	0.72
(1,119)	1:26:A:ASP:HB2	1:26:A:ASP:HB3	8	0.72
(1,119)	1:26:A:ASP:HB2	1:26:A:ASP:HB3	9	0.72
(1,119)	1:26:A:ASP:HB2	1:26:A:ASP:HB3	10	0.72
(1,95)	1:24:A:TYR:HB3	1:11:A:ARG:HB2	9	0.72
(1,75)	1:21:A:THR:HB	1:21:A:THR:HA	8	0.72
(1,56)	1:15:A:LYS:HA	1:15:A:LYS:HB2	1	0.72
(1,51)	1:13:A:TYR:HA	1:13:A:TYR:HB2	9	0.72
(1,26)	1:9:A:LEU:HD11	1:45:A:ASN:HB2	7	0.72
(1,26)	1:9:A:LEU:HD12	1:45:A:ASN:HB2	7	0.72
(1,26)	1:9:A:LEU:HD13	1:45:A:ASN:HB2	7	0.72
(1,347)	1:18:A:GLY:H	1:17:A:SER:HB2	6	0.71
(1,340)	1:17:A:SER:H	1:16:A:GLY:HA3	4	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:13:A:TYR:H	1:12:A:ASN:HB3	5	0.71
(1,310)	1:12:A:ASN:H	1:11:A:ARG:HG3	7	0.71
(1,309)	1:12:A:ASN:H	1:11:A:ARG:HB2	9	0.71
(1,211)	1:49:A:THR:HG21	1:49:A:THR:HA	5	0.71
(1,211)	1:49:A:THR:HG22	1:49:A:THR:HA	5	0.71
(1,211)	1:49:A:THR:HG23	1:49:A:THR:HA	5	0.71
(1,211)	1:49:A:THR:HG21	1:49:A:THR:HA	7	0.71
(1,211)	1:49:A:THR:HG22	1:49:A:THR:HA	7	0.71
(1,211)	1:49:A:THR:HG23	1:49:A:THR:HA	7	0.71
(1,176)	1:36:A:ARG:HD3	1:36:A:ARG:HA	5	0.71
(1,176)	1:36:A:ARG:HD3	1:36:A:ARG:HA	8	0.71
(1,114)	1:25:A:TYR:HA	1:32:A:CYS:HA	1	0.71
(1,75)	1:21:A:THR:HB	1:21:A:THR:HA	3	0.71
(1,75)	1:21:A:THR:HB	1:21:A:THR:HA	10	0.71
(1,71)	1:19:A:SER:HB2	1:36:A:ARG:HD3	3	0.71
(1,56)	1:15:A:LYS:HA	1:15:A:LYS:HB2	7	0.71
(1,38)	1:11:A:ARG:HD3	1:11:A:ARG:HB2	10	0.71
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG21	5	0.7
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG22	5	0.7
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG23	5	0.7
(1,456)	1:43:A:ASN:H	1:43:A:ASN:HB3	5	0.7
(1,350)	1:18:A:GLY:H	1:19:A:SER:H	7	0.7
(1,211)	1:49:A:THR:HG21	1:49:A:THR:HA	10	0.7
(1,211)	1:49:A:THR:HG22	1:49:A:THR:HA	10	0.7
(1,211)	1:49:A:THR:HG23	1:49:A:THR:HA	10	0.7
(1,75)	1:21:A:THR:HB	1:21:A:THR:HA	1	0.7
(1,75)	1:21:A:THR:HB	1:21:A:THR:HA	2	0.7
(1,75)	1:21:A:THR:HB	1:21:A:THR:HA	7	0.7
(1,75)	1:21:A:THR:HB	1:21:A:THR:HA	9	0.7
(1,71)	1:19:A:SER:HB2	1:36:A:ARG:HD3	7	0.7
(1,56)	1:15:A:LYS:HA	1:15:A:LYS:HB2	2	0.7
(1,56)	1:15:A:LYS:HA	1:15:A:LYS:HB2	3	0.7
(1,56)	1:15:A:LYS:HA	1:15:A:LYS:HB2	5	0.7
(1,56)	1:15:A:LYS:HA	1:15:A:LYS:HB2	9	0.7
(1,18)	1:7:A:CYS:HA	1:57:A:CYS:HB2	3	0.7
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG21	7	0.69
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG22	7	0.69
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG23	7	0.69
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD21	10	0.69
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD22	10	0.69
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD23	10	0.69
(1,144)	1:33:A:LYS:HA	1:33:A:LYS:HD2	9	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:21:A:THR:HB	1:21:A:THR:HA	4	0.69
(1,75)	1:21:A:THR:HB	1:21:A:THR:HA	5	0.69
(1,75)	1:21:A:THR:HB	1:21:A:THR:HA	6	0.69
(1,71)	1:19:A:SER:HB2	1:36:A:ARG:HD3	5	0.69
(1,456)	1:43:A:ASN:H	1:43:A:ASN:HB3	1	0.68
(1,419)	1:34:A:THR:H	1:33:A:LYS:HB3	4	0.68
(1,419)	1:34:A:THR:H	1:33:A:LYS:HB3	9	0.68
(1,419)	1:34:A:THR:H	1:33:A:LYS:HB3	10	0.68
(1,362)	1:21:A:THR:H	1:20:A:PHE:HB2	5	0.68
(1,322)	1:13:A:TYR:H	1:13:A:TYR:HB2	5	0.68
(1,211)	1:49:A:THR:HG21	1:49:A:THR:HA	9	0.68
(1,211)	1:49:A:THR:HG22	1:49:A:THR:HA	9	0.68
(1,211)	1:49:A:THR:HG23	1:49:A:THR:HA	9	0.68
(1,152)	1:34:A:THR:HA	1:33:A:LYS:HE3	9	0.68
(1,56)	1:15:A:LYS:HA	1:15:A:LYS:HB2	6	0.68
(1,46)	1:11:A:ARG:HG3	1:11:A:ARG:HB2	5	0.68
(1,46)	1:11:A:ARG:HG3	1:11:A:ARG:HB2	9	0.68
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD11	7	0.68
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD12	7	0.68
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD13	7	0.68
(1,453)	1:42:A:GLY:H	1:41:A:GLY:HA2	7	0.67
(1,419)	1:34:A:THR:H	1:33:A:LYS:HB3	5	0.67
(1,411)	1:32:A:CYS:H	1:31:A:SER:HB3	6	0.67
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD11	2	0.67
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD12	2	0.67
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD13	2	0.67
(1,211)	1:49:A:THR:HG21	1:49:A:THR:HA	1	0.67
(1,211)	1:49:A:THR:HG22	1:49:A:THR:HA	1	0.67
(1,211)	1:49:A:THR:HG23	1:49:A:THR:HA	1	0.67
(1,176)	1:36:A:ARG:HD3	1:36:A:ARG:HA	7	0.67
(1,118)	1:26:A:ASP:HA	1:26:A:ASP:HB2	7	0.67
(1,41)	1:11:A:ARG:HD3	1:11:A:ARG:HG2	8	0.67
(1,18)	1:7:A:CYS:HA	1:57:A:CYS:HB2	2	0.67
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG21	9	0.66
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG22	9	0.66
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG23	9	0.66
(1,456)	1:43:A:ASN:H	1:43:A:ASN:HB3	10	0.66
(1,350)	1:18:A:GLY:H	1:19:A:SER:H	8	0.66
(1,265)	1:3:A:GLN:H	1:3:A:GLN:HG3	6	0.66
(1,211)	1:49:A:THR:HG21	1:49:A:THR:HA	3	0.66
(1,211)	1:49:A:THR:HG22	1:49:A:THR:HA	3	0.66
(1,211)	1:49:A:THR:HG23	1:49:A:THR:HA	3	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,211)	1:49:A:THR:HG21	1:49:A:THR:HA	4	0.66
(1,211)	1:49:A:THR:HG22	1:49:A:THR:HA	4	0.66
(1,211)	1:49:A:THR:HG23	1:49:A:THR:HA	4	0.66
(1,116)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	7	0.66
(1,116)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	10	0.66
(1,84)	1:23:A:TYR:HD1	1:22:A:ASN:HA	1	0.66
(1,72)	1:20:A:PHE:HA	1:20:A:PHE:HB3	6	0.66
(1,43)	1:11:A:ARG:HD2	1:11:A:ARG:HG3	5	0.66
(1,4)	1:1:A:PRO:HD2	1:1:A:PRO:HG3	1	0.66
(1,4)	1:1:A:PRO:HD2	1:1:A:PRO:HG3	4	0.66
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG21	3	0.65
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG22	3	0.65
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG23	3	0.65
(1,323)	1:13:A:TYR:H	1:14:A:GLY:H	7	0.65
(1,322)	1:13:A:TYR:H	1:13:A:TYR:HB2	10	0.65
(1,310)	1:12:A:ASN:H	1:11:A:ARG:HG3	10	0.65
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD11	10	0.65
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD12	10	0.65
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD13	10	0.65
(1,211)	1:49:A:THR:HG21	1:49:A:THR:HA	2	0.65
(1,211)	1:49:A:THR:HG22	1:49:A:THR:HA	2	0.65
(1,211)	1:49:A:THR:HG23	1:49:A:THR:HA	2	0.65
(1,191)	1:46:A:ARG:HA	1:46:A:ARG:HB3	1	0.65
(1,191)	1:46:A:ARG:HA	1:46:A:ARG:HB3	2	0.65
(1,191)	1:46:A:ARG:HA	1:46:A:ARG:HB3	3	0.65
(1,191)	1:46:A:ARG:HA	1:46:A:ARG:HB3	4	0.65
(1,191)	1:46:A:ARG:HA	1:46:A:ARG:HB3	6	0.65
(1,191)	1:46:A:ARG:HA	1:46:A:ARG:HB3	7	0.65
(1,191)	1:46:A:ARG:HA	1:46:A:ARG:HB3	8	0.65
(1,124)	1:27:A:LYS:HA	1:27:A:LYS:HG3	10	0.65
(1,116)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	1	0.65
(1,116)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	2	0.65
(1,116)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	3	0.65
(1,116)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	4	0.65
(1,116)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	5	0.65
(1,116)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	6	0.65
(1,116)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	8	0.65
(1,116)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	9	0.65
(1,71)	1:19:A:SER:HB2	1:36:A:ARG:HD3	8	0.65
(1,51)	1:13:A:TYR:HA	1:13:A:TYR:HB2	7	0.65
(1,46)	1:11:A:ARG:HG3	1:11:A:ARG:HB2	7	0.65
(1,41)	1:11:A:ARG:HD3	1:11:A:ARG:HG2	2	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:8:A:GLN:HA	1:27:A:LYS:HE3	2	0.65
(1,341)	1:17:A:SER:H	1:16:A:GLY:HA2	10	0.64
(1,325)	1:14:A:GLY:H	1:13:A:TYR:HB3	10	0.64
(1,323)	1:13:A:TYR:H	1:14:A:GLY:H	6	0.64
(1,319)	1:13:A:TYR:H	1:12:A:ASN:HB2	5	0.64
(1,309)	1:12:A:ASN:H	1:11:A:ARG:HB2	6	0.64
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD11	4	0.64
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD12	4	0.64
(1,300)	1:10:A:SER:H	1:9:A:LEU:HD13	4	0.64
(1,247)	1:57:A:CYS:HA	1:3:A:GLN:HG3	6	0.64
(1,211)	1:49:A:THR:HG21	1:49:A:THR:HA	6	0.64
(1,211)	1:49:A:THR:HG22	1:49:A:THR:HA	6	0.64
(1,211)	1:49:A:THR:HG23	1:49:A:THR:HA	6	0.64
(1,196)	1:47:A:PHE:HA	1:48:A:LYS:HD3	7	0.64
(1,191)	1:46:A:ARG:HA	1:46:A:ARG:HB3	9	0.64
(1,191)	1:46:A:ARG:HA	1:46:A:ARG:HB3	10	0.64
(1,41)	1:11:A:ARG:HD3	1:11:A:ARG:HG2	4	0.64
(1,41)	1:11:A:ARG:HD3	1:11:A:ARG:HG2	9	0.64
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG21	2	0.63
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG22	2	0.63
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG23	2	0.63
(1,463)	1:48:A:LYS:H	1:48:A:LYS:HD3	8	0.63
(1,453)	1:42:A:GLY:H	1:41:A:GLY:HA2	4	0.63
(1,419)	1:34:A:THR:H	1:33:A:LYS:HB3	7	0.63
(1,298)	1:10:A:SER:H	1:9:A:LEU:HA	6	0.63
(1,149)	1:33:A:LYS:HE3	1:33:A:LYS:HG3	8	0.63
(1,46)	1:11:A:ARG:HG3	1:11:A:ARG:HB2	10	0.63
(1,43)	1:11:A:ARG:HD2	1:11:A:ARG:HG3	10	0.63
(1,41)	1:11:A:ARG:HD3	1:11:A:ARG:HG2	1	0.63
(1,41)	1:11:A:ARG:HD3	1:11:A:ARG:HG2	6	0.63
(1,455)	1:43:A:ASN:H	1:12:A:ASN:HB2	5	0.62
(1,352)	1:19:A:SER:H	1:18:A:GLY:HA2	9	0.62
(1,350)	1:18:A:GLY:H	1:19:A:SER:H	10	0.62
(1,240)	1:54:A:GLU:HG3	1:54:A:GLU:HB3	1	0.62
(1,240)	1:54:A:GLU:HG3	1:54:A:GLU:HB3	2	0.62
(1,240)	1:54:A:GLU:HG3	1:54:A:GLU:HB3	5	0.62
(1,240)	1:54:A:GLU:HG3	1:54:A:GLU:HB3	6	0.62
(1,240)	1:54:A:GLU:HG3	1:54:A:GLU:HB3	7	0.62
(1,240)	1:54:A:GLU:HG3	1:54:A:GLU:HB3	10	0.62
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD21	7	0.62
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD22	7	0.62
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD23	7	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,211)	1:49:A:THR:HG21	1:49:A:THR:HA	8	0.62
(1,211)	1:49:A:THR:HG22	1:49:A:THR:HA	8	0.62
(1,211)	1:49:A:THR:HG23	1:49:A:THR:HA	8	0.62
(1,191)	1:46:A:ARG:HA	1:46:A:ARG:HB3	5	0.62
(1,46)	1:11:A:ARG:HG3	1:11:A:ARG:HB2	6	0.62
(1,36)	1:11:A:ARG:HB2	1:11:A:ARG:HG2	7	0.62
(1,542)	1:61:A:GLU:H	1:61:A:GLU:HG3	5	0.61
(1,452)	1:42:A:GLY:H	1:41:A:GLY:HA3	7	0.61
(1,447)	1:40:A:SER:H	1:40:A:SER:HB2	9	0.61
(1,446)	1:40:A:SER:H	1:40:A:SER:HB3	1	0.61
(1,344)	1:17:A:SER:H	1:18:A:GLY:H	5	0.61
(1,240)	1:54:A:GLU:HG3	1:54:A:GLU:HB3	3	0.61
(1,240)	1:54:A:GLU:HG3	1:54:A:GLU:HB3	4	0.61
(1,240)	1:54:A:GLU:HG3	1:54:A:GLU:HB3	8	0.61
(1,240)	1:54:A:GLU:HG3	1:54:A:GLU:HB3	9	0.61
(1,189)	1:40:A:SER:HB3	1:40:A:SER:HA	6	0.61
(1,118)	1:26:A:ASP:HA	1:26:A:ASP:HB2	2	0.61
(1,41)	1:11:A:ARG:HD3	1:11:A:ARG:HG2	3	0.61
(1,36)	1:11:A:ARG:HB2	1:11:A:ARG:HG2	10	0.61
(1,22)	1:8:A:GLN:HA	1:27:A:LYS:HE3	6	0.61
(1,472)	1:49:A:THR:H	1:52:A:ASP:HB3	7	0.6
(1,456)	1:43:A:ASN:H	1:43:A:ASN:HB3	2	0.6
(1,453)	1:42:A:GLY:H	1:41:A:GLY:HA2	10	0.6
(1,448)	1:41:A:GLY:H	1:40:A:SER:H	8	0.6
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB1	7	0.6
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB2	7	0.6
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB3	7	0.6
(1,352)	1:19:A:SER:H	1:18:A:GLY:HA2	4	0.6
(1,339)	1:16:A:GLY:H	1:38:A:ARG:HG3	3	0.6
(1,331)	1:15:A:LYS:H	1:15:A:LYS:HG3	10	0.6
(1,319)	1:13:A:TYR:H	1:12:A:ASN:HB2	8	0.6
(1,281)	1:7:A:CYS:H	1:6:A:ARG:HG3	7	0.6
(1,271)	1:4:A:ASP:H	1:4:A:ASP:HB3	8	0.6
(1,118)	1:26:A:ASP:HA	1:26:A:ASP:HB2	6	0.6
(1,118)	1:26:A:ASP:HA	1:26:A:ASP:HB2	9	0.6
(1,404)	1:30:A:SER:H	1:29:A:THR:HG21	6	0.59
(1,404)	1:30:A:SER:H	1:29:A:THR:HG22	6	0.59
(1,404)	1:30:A:SER:H	1:29:A:THR:HG23	6	0.59
(1,350)	1:18:A:GLY:H	1:19:A:SER:H	9	0.59
(1,319)	1:13:A:TYR:H	1:12:A:ASN:HB2	9	0.59
(1,309)	1:12:A:ASN:H	1:11:A:ARG:HB2	7	0.59
(1,301)	1:10:A:SER:H	1:10:A:SER:HA	6	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,122)	1:27:A:LYS:HA	1:27:A:LYS:HB2	5	0.59
(1,118)	1:26:A:ASP:HA	1:26:A:ASP:HB2	4	0.59
(1,118)	1:26:A:ASP:HA	1:26:A:ASP:HB2	8	0.59
(1,94)	1:24:A:TYR:HB3	1:11:A:ARG:HB3	8	0.59
(1,51)	1:13:A:TYR:HA	1:13:A:TYR:HB2	3	0.59
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG21	10	0.58
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG22	10	0.58
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG23	10	0.58
(1,475)	1:50:A:LEU:H	1:49:A:THR:HB	7	0.58
(1,438)	1:38:A:ARG:H	1:36:A:ARG:HB2	2	0.58
(1,359)	1:20:A:PHE:H	1:20:A:PHE:HB2	1	0.58
(1,359)	1:20:A:PHE:H	1:20:A:PHE:HB2	6	0.58
(1,281)	1:7:A:CYS:H	1:6:A:ARG:HG3	8	0.58
(1,261)	1:61:A:GLU:HG2	1:59:A:THR:HA	1	0.58
(1,149)	1:33:A:LYS:HE3	1:33:A:LYS:HG3	6	0.58
(1,72)	1:20:A:PHE:HA	1:20:A:PHE:HB3	1	0.58
(1,72)	1:20:A:PHE:HA	1:20:A:PHE:HB3	5	0.58
(1,41)	1:11:A:ARG:HD3	1:11:A:ARG:HG2	7	0.58
(1,472)	1:49:A:THR:H	1:52:A:ASP:HB3	9	0.57
(1,447)	1:40:A:SER:H	1:40:A:SER:HB2	8	0.57
(1,411)	1:32:A:CYS:H	1:31:A:SER:HB3	2	0.57
(1,411)	1:32:A:CYS:H	1:31:A:SER:HB3	4	0.57
(1,404)	1:30:A:SER:H	1:29:A:THR:HG21	4	0.57
(1,404)	1:30:A:SER:H	1:29:A:THR:HG22	4	0.57
(1,404)	1:30:A:SER:H	1:29:A:THR:HG23	4	0.57
(1,309)	1:12:A:ASN:H	1:11:A:ARG:HB2	10	0.57
(1,249)	1:57:A:CYS:HA	1:7:A:CYS:HB2	2	0.57
(1,149)	1:33:A:LYS:HE3	1:33:A:LYS:HG3	7	0.57
(1,127)	1:27:A:LYS:HE3	1:27:A:LYS:HB3	6	0.57
(1,122)	1:27:A:LYS:HA	1:27:A:LYS:HB2	3	0.57
(1,11)	1:5:A:TYR:HB3	1:8:A:GLN:HG3	2	0.57
(1,472)	1:49:A:THR:H	1:52:A:ASP:HB3	8	0.56
(1,454)	1:43:A:ASN:H	1:12:A:ASN:HB3	10	0.56
(1,411)	1:32:A:CYS:H	1:31:A:SER:HB3	8	0.56
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB1	2	0.56
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB2	2	0.56
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB3	2	0.56
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB1	9	0.56
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB2	9	0.56
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB3	9	0.56
(1,266)	1:3:A:GLN:H	1:4:A:ASP:H	1	0.56
(1,213)	1:50:A:LEU:HD11	1:51:A:GLU:HG2	1	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,213)	1:50:A:LEU:HD12	1:51:A:GLU:HG2	1	0.56
(1,213)	1:50:A:LEU:HD13	1:51:A:GLU:HG2	1	0.56
(1,190)	1:40:A:SER:HB2	1:40:A:SER:HA	1	0.56
(1,149)	1:33:A:LYS:HE3	1:33:A:LYS:HG3	10	0.56
(1,127)	1:27:A:LYS:HE3	1:27:A:LYS:HB3	5	0.56
(1,118)	1:26:A:ASP:HA	1:26:A:ASP:HB2	1	0.56
(1,117)	1:26:A:ASP:HA	1:26:A:ASP:HB3	1	0.56
(1,117)	1:26:A:ASP:HA	1:26:A:ASP:HB3	2	0.56
(1,117)	1:26:A:ASP:HA	1:26:A:ASP:HB3	3	0.56
(1,117)	1:26:A:ASP:HA	1:26:A:ASP:HB3	4	0.56
(1,117)	1:26:A:ASP:HA	1:26:A:ASP:HB3	5	0.56
(1,117)	1:26:A:ASP:HA	1:26:A:ASP:HB3	6	0.56
(1,117)	1:26:A:ASP:HA	1:26:A:ASP:HB3	8	0.56
(1,117)	1:26:A:ASP:HA	1:26:A:ASP:HB3	9	0.56
(1,117)	1:26:A:ASP:HA	1:26:A:ASP:HB3	10	0.56
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG21	6	0.56
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG22	6	0.56
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG23	6	0.56
(1,57)	1:15:A:LYS:HA	1:15:A:LYS:HG2	10	0.56
(1,51)	1:13:A:TYR:HA	1:13:A:TYR:HB2	2	0.56
(1,51)	1:13:A:TYR:HA	1:13:A:TYR:HB2	6	0.56
(1,44)	1:11:A:ARG:HD2	1:11:A:ARG:HG2	3	0.56
(1,44)	1:11:A:ARG:HD2	1:11:A:ARG:HG2	7	0.56
(1,44)	1:11:A:ARG:HD2	1:11:A:ARG:HG2	9	0.56
(1,26)	1:9:A:LEU:HD11	1:45:A:ASN:HB2	1	0.56
(1,26)	1:9:A:LEU:HD12	1:45:A:ASN:HB2	1	0.56
(1,26)	1:9:A:LEU:HD13	1:45:A:ASN:HB2	1	0.56
(1,22)	1:8:A:GLN:HA	1:27:A:LYS:HE3	3	0.56
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD11	8	0.56
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD12	8	0.56
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD13	8	0.56
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG21	4	0.55
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG22	4	0.55
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG23	4	0.55
(1,447)	1:40:A:SER:H	1:40:A:SER:HB2	5	0.55
(1,446)	1:40:A:SER:H	1:40:A:SER:HB3	3	0.55
(1,443)	1:38:A:ARG:H	1:39:A:GLY:H	7	0.55
(1,442)	1:38:A:ARG:H	1:38:A:ARG:HB2	4	0.55
(1,404)	1:30:A:SER:H	1:29:A:THR:HG21	7	0.55
(1,404)	1:30:A:SER:H	1:29:A:THR:HG22	7	0.55
(1,404)	1:30:A:SER:H	1:29:A:THR:HG23	7	0.55
(1,404)	1:30:A:SER:H	1:29:A:THR:HG21	8	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,404)	1:30:A:SER:H	1:29:A:THR:HG22	8	0.55
(1,404)	1:30:A:SER:H	1:29:A:THR:HG23	8	0.55
(1,359)	1:20:A:PHE:H	1:20:A:PHE:HB2	5	0.55
(1,355)	1:20:A:PHE:H	1:19:A:SER:HA	2	0.55
(1,352)	1:19:A:SER:H	1:18:A:GLY:HA2	6	0.55
(1,297)	1:9:A:LEU:H	1:9:A:LEU:HG	8	0.55
(1,292)	1:9:A:LEU:H	1:8:A:GLN:H	4	0.55
(1,213)	1:50:A:LEU:HD11	1:51:A:GLU:HG2	3	0.55
(1,213)	1:50:A:LEU:HD12	1:51:A:GLU:HG2	3	0.55
(1,213)	1:50:A:LEU:HD13	1:51:A:GLU:HG2	3	0.55
(1,190)	1:40:A:SER:HB2	1:40:A:SER:HA	8	0.55
(1,149)	1:33:A:LYS:HE3	1:33:A:LYS:HG3	1	0.55
(1,149)	1:33:A:LYS:HE3	1:33:A:LYS:HG3	9	0.55
(1,87)	1:23:A:TYR:HD1	1:49:A:THR:HA	10	0.55
(1,71)	1:19:A:SER:HB2	1:36:A:ARG:HD3	10	0.55
(1,51)	1:13:A:TYR:HA	1:13:A:TYR:HB2	1	0.55
(1,51)	1:13:A:TYR:HA	1:13:A:TYR:HB2	4	0.55
(1,44)	1:11:A:ARG:HD2	1:11:A:ARG:HG2	1	0.55
(1,44)	1:11:A:ARG:HD2	1:11:A:ARG:HG2	6	0.55
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD11	4	0.55
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD12	4	0.55
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD13	4	0.55
(1,352)	1:19:A:SER:H	1:18:A:GLY:HA2	3	0.54
(1,352)	1:19:A:SER:H	1:18:A:GLY:HA2	5	0.54
(1,298)	1:10:A:SER:H	1:9:A:LEU:HA	2	0.54
(1,298)	1:10:A:SER:H	1:9:A:LEU:HA	4	0.54
(1,294)	1:9:A:LEU:H	1:8:A:GLN:HG3	8	0.54
(1,263)	1:3:A:GLN:H	1:3:A:GLN:HA	8	0.54
(1,249)	1:57:A:CYS:HA	1:7:A:CYS:HB2	8	0.54
(1,122)	1:27:A:LYS:HA	1:27:A:LYS:HB2	8	0.54
(1,118)	1:26:A:ASP:HA	1:26:A:ASP:HB2	3	0.54
(1,118)	1:26:A:ASP:HA	1:26:A:ASP:HB2	5	0.54
(1,117)	1:26:A:ASP:HA	1:26:A:ASP:HB3	7	0.54
(1,84)	1:23:A:TYR:HD1	1:22:A:ASN:HA	8	0.54
(1,78)	1:22:A:ASN:HA	1:22:A:ASN:HB2	3	0.54
(1,78)	1:22:A:ASN:HA	1:22:A:ASN:HB2	4	0.54
(1,78)	1:22:A:ASN:HA	1:22:A:ASN:HB2	5	0.54
(1,78)	1:22:A:ASN:HA	1:22:A:ASN:HB2	6	0.54
(1,78)	1:22:A:ASN:HA	1:22:A:ASN:HB2	7	0.54
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG21	1	0.54
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG22	1	0.54
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG23	1	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG21	2	0.54
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG22	2	0.54
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG23	2	0.54
(1,57)	1:15:A:LYS:HA	1:15:A:LYS:HG2	8	0.54
(1,44)	1:11:A:ARG:HD2	1:11:A:ARG:HG2	2	0.54
(1,44)	1:11:A:ARG:HD2	1:11:A:ARG:HG2	4	0.54
(1,44)	1:11:A:ARG:HD2	1:11:A:ARG:HG2	8	0.54
(1,38)	1:11:A:ARG:HD3	1:11:A:ARG:HB2	7	0.54
(1,38)	1:11:A:ARG:HD3	1:11:A:ARG:HB2	9	0.54
(1,8)	1:4:A:ASP:HB3	1:4:A:ASP:HA	8	0.54
(1,3)	1:1:A:PRO:HD3	1:1:A:PRO:HG3	9	0.54
(1,465)	1:48:A:LYS:H	1:49:A:THR:H	8	0.53
(1,452)	1:42:A:GLY:H	1:41:A:GLY:HA3	3	0.53
(1,452)	1:42:A:GLY:H	1:41:A:GLY:HA3	8	0.53
(1,445)	1:40:A:SER:H	1:40:A:SER:HA	3	0.53
(1,438)	1:38:A:ARG:H	1:36:A:ARG:HB2	10	0.53
(1,417)	1:33:A:LYS:H	1:33:A:LYS:HB3	3	0.53
(1,411)	1:32:A:CYS:H	1:31:A:SER:HB3	5	0.53
(1,359)	1:20:A:PHE:H	1:20:A:PHE:HB2	2	0.53
(1,319)	1:13:A:TYR:H	1:12:A:ASN:HB2	4	0.53
(1,292)	1:9:A:LEU:H	1:8:A:GLN:H	10	0.53
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD21	8	0.53
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD22	8	0.53
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD23	8	0.53
(1,147)	1:33:A:LYS:HE3	1:33:A:LYS:HD3	2	0.53
(1,78)	1:22:A:ASN:HA	1:22:A:ASN:HB2	10	0.53
(1,57)	1:15:A:LYS:HA	1:15:A:LYS:HG2	4	0.53
(1,47)	1:11:A:ARG:HG3	1:11:A:ARG:HG2	1	0.53
(1,47)	1:11:A:ARG:HG3	1:11:A:ARG:HG2	5	0.53
(1,3)	1:1:A:PRO:HD3	1:1:A:PRO:HG3	1	0.53
(1,527)	1:58:A:VAL:H	1:57:A:CYS:H	2	0.52
(1,465)	1:48:A:LYS:H	1:49:A:THR:H	3	0.52
(1,465)	1:48:A:LYS:H	1:49:A:THR:H	4	0.52
(1,411)	1:32:A:CYS:H	1:31:A:SER:HB3	1	0.52
(1,354)	1:19:A:SER:H	1:19:A:SER:HB3	6	0.52
(1,344)	1:17:A:SER:H	1:18:A:GLY:H	1	0.52
(1,309)	1:12:A:ASN:H	1:11:A:ARG:HB2	5	0.52
(1,264)	1:3:A:GLN:H	1:3:A:GLN:HB2	9	0.52
(1,249)	1:57:A:CYS:HA	1:7:A:CYS:HB2	1	0.52
(1,189)	1:40:A:SER:HB3	1:40:A:SER:HA	8	0.52
(1,84)	1:23:A:TYR:HD1	1:22:A:ASN:HA	10	0.52
(1,78)	1:22:A:ASN:HA	1:22:A:ASN:HB2	1	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,78)	1:22:A:ASN:HA	1:22:A:ASN:HB2	2	0.52
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG21	3	0.52
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG22	3	0.52
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG23	3	0.52
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG21	8	0.52
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG22	8	0.52
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG23	8	0.52
(1,71)	1:19:A:SER:HB2	1:36:A:ARG:HD3	2	0.52
(1,47)	1:11:A:ARG:HG3	1:11:A:ARG:HG2	2	0.52
(1,47)	1:11:A:ARG:HG3	1:11:A:ARG:HG2	3	0.52
(1,47)	1:11:A:ARG:HG3	1:11:A:ARG:HG2	4	0.52
(1,47)	1:11:A:ARG:HG3	1:11:A:ARG:HG2	6	0.52
(1,47)	1:11:A:ARG:HG3	1:11:A:ARG:HG2	7	0.52
(1,47)	1:11:A:ARG:HG3	1:11:A:ARG:HG2	8	0.52
(1,47)	1:11:A:ARG:HG3	1:11:A:ARG:HG2	9	0.52
(1,47)	1:11:A:ARG:HG3	1:11:A:ARG:HG2	10	0.52
(1,46)	1:11:A:ARG:HG3	1:11:A:ARG:HB2	1	0.52
(1,44)	1:11:A:ARG:HD2	1:11:A:ARG:HG2	10	0.52
(1,3)	1:1:A:PRO:HD3	1:1:A:PRO:HG3	3	0.52
(1,3)	1:1:A:PRO:HD3	1:1:A:PRO:HG3	4	0.52
(1,3)	1:1:A:PRO:HD3	1:1:A:PRO:HG3	5	0.52
(1,3)	1:1:A:PRO:HD3	1:1:A:PRO:HG3	6	0.52
(1,3)	1:1:A:PRO:HD3	1:1:A:PRO:HG3	7	0.52
(1,3)	1:1:A:PRO:HD3	1:1:A:PRO:HG3	8	0.52
(1,3)	1:1:A:PRO:HD3	1:1:A:PRO:HG3	10	0.52
(1,527)	1:58:A:VAL:H	1:57:A:CYS:H	6	0.51
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG21	6	0.51
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG22	6	0.51
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG23	6	0.51
(1,465)	1:48:A:LYS:H	1:49:A:THR:H	2	0.51
(1,411)	1:32:A:CYS:H	1:31:A:SER:HB3	3	0.51
(1,411)	1:32:A:CYS:H	1:31:A:SER:HB3	9	0.51
(1,354)	1:19:A:SER:H	1:19:A:SER:HB3	4	0.51
(1,328)	1:14:A:GLY:H	1:14:A:GLY:HA2	3	0.51
(1,310)	1:12:A:ASN:H	1:11:A:ARG:HG3	9	0.51
(1,299)	1:10:A:SER:H	1:9:A:LEU:HB3	8	0.51
(1,292)	1:9:A:LEU:H	1:8:A:GLN:H	7	0.51
(1,266)	1:3:A:GLN:H	1:4:A:ASP:H	9	0.51
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG11	9	0.51
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG12	9	0.51
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG13	9	0.51
(1,213)	1:50:A:LEU:HD11	1:51:A:GLU:HG2	9	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,213)	1:50:A:LEU:HD12	1:51:A:GLU:HG2	9	0.51
(1,213)	1:50:A:LEU:HD13	1:51:A:GLU:HG2	9	0.51
(1,204)	1:48:A:LYS:HA	1:48:A:LYS:HD2	10	0.51
(1,196)	1:47:A:PHE:HA	1:48:A:LYS:HD3	3	0.51
(1,183)	1:37:A:TYR:HB2	1:22:A:ASN:HB2	9	0.51
(1,127)	1:27:A:LYS:HE3	1:27:A:LYS:HB3	3	0.51
(1,81)	1:23:A:TYR:HA	1:23:A:TYR:HB3	7	0.51
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG21	4	0.51
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG22	4	0.51
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG23	4	0.51
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG21	5	0.51
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG22	5	0.51
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG23	5	0.51
(1,71)	1:19:A:SER:HB2	1:36:A:ARG:HD3	1	0.51
(1,44)	1:11:A:ARG:HD2	1:11:A:ARG:HG2	5	0.51
(1,34)	1:11:A:ARG:HB3	1:11:A:ARG:HG2	10	0.51
(1,23)	1:9:A:LEU:HA	1:5:A:TYR:HB3	4	0.51
(1,22)	1:8:A:GLN:HA	1:27:A:LYS:HE3	7	0.51
(1,3)	1:1:A:PRO:HD3	1:1:A:PRO:HG3	2	0.51
(1,475)	1:50:A:LEU:H	1:49:A:THR:HB	5	0.5
(1,472)	1:49:A:THR:H	1:52:A:ASP:HB3	4	0.5
(1,443)	1:38:A:ARG:H	1:39:A:GLY:H	3	0.5
(1,396)	1:28:A:ALA:H	1:30:A:SER:H	2	0.5
(1,358)	1:20:A:PHE:H	1:20:A:PHE:HB3	9	0.5
(1,341)	1:17:A:SER:H	1:16:A:GLY:HA2	7	0.5
(1,297)	1:9:A:LEU:H	1:9:A:LEU:HG	6	0.5
(1,265)	1:3:A:GLN:H	1:3:A:GLN:HG3	4	0.5
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG11	8	0.5
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG12	8	0.5
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG13	8	0.5
(1,204)	1:48:A:LYS:HA	1:48:A:LYS:HD2	5	0.5
(1,196)	1:47:A:PHE:HA	1:48:A:LYS:HD3	10	0.5
(1,147)	1:33:A:LYS:HE3	1:33:A:LYS:HD3	3	0.5
(1,118)	1:26:A:ASP:HA	1:26:A:ASP:HB2	10	0.5
(1,84)	1:23:A:TYR:HD1	1:22:A:ASN:HA	5	0.5
(1,81)	1:23:A:TYR:HA	1:23:A:TYR:HB3	9	0.5
(1,46)	1:11:A:ARG:HG3	1:11:A:ARG:HB2	2	0.5
(1,34)	1:11:A:ARG:HB3	1:11:A:ARG:HG2	7	0.5
(1,23)	1:9:A:LEU:HA	1:5:A:TYR:HB3	1	0.5
(1,6)	1:3:A:GLN:HB3	1:3:A:GLN:HA	8	0.5
(1,455)	1:43:A:ASN:H	1:12:A:ASN:HB2	4	0.49
(1,453)	1:42:A:GLY:H	1:41:A:GLY:HA2	3	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:42:A:GLY:H	1:41:A:GLY:HA3	2	0.49
(1,442)	1:38:A:ARG:H	1:38:A:ARG:HB2	1	0.49
(1,442)	1:38:A:ARG:H	1:38:A:ARG:HB2	5	0.49
(1,402)	1:30:A:SER:H	1:27:A:LYS:HA	7	0.49
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB1	1	0.49
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB2	1	0.49
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB3	1	0.49
(1,266)	1:3:A:GLN:H	1:4:A:ASP:H	4	0.49
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG11	4	0.49
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG12	4	0.49
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG13	4	0.49
(1,249)	1:57:A:CYS:HA	1:7:A:CYS:HB2	3	0.49
(1,244)	1:55:A:ALA:HB1	1:56:A:THR:HB	4	0.49
(1,244)	1:55:A:ALA:HB2	1:56:A:THR:HB	4	0.49
(1,244)	1:55:A:ALA:HB3	1:56:A:THR:HB	4	0.49
(1,244)	1:55:A:ALA:HB1	1:56:A:THR:HB	6	0.49
(1,244)	1:55:A:ALA:HB2	1:56:A:THR:HB	6	0.49
(1,244)	1:55:A:ALA:HB3	1:56:A:THR:HB	6	0.49
(1,227)	1:53:A:CYS:HB3	1:32:A:CYS:HB2	10	0.49
(1,127)	1:27:A:LYS:HE3	1:27:A:LYS:HB3	1	0.49
(1,127)	1:27:A:LYS:HE3	1:27:A:LYS:HB3	4	0.49
(1,127)	1:27:A:LYS:HE3	1:27:A:LYS:HB3	8	0.49
(1,122)	1:27:A:LYS:HA	1:27:A:LYS:HB2	6	0.49
(1,81)	1:23:A:TYR:HA	1:23:A:TYR:HB3	3	0.49
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG21	7	0.49
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG22	7	0.49
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG23	7	0.49
(1,46)	1:11:A:ARG:HG3	1:11:A:ARG:HB2	3	0.49
(1,46)	1:11:A:ARG:HG3	1:11:A:ARG:HB2	4	0.49
(1,46)	1:11:A:ARG:HG3	1:11:A:ARG:HB2	8	0.49
(1,5)	1:3:A:GLN:HA	1:3:A:GLN:HB2	1	0.49
(1,1)	1:1:A:PRO:HB3	1:1:A:PRO:HD2	9	0.49
(1,527)	1:58:A:VAL:H	1:57:A:CYS:H	4	0.48
(1,464)	1:48:A:LYS:H	1:48:A:LYS:HD2	10	0.48
(1,448)	1:41:A:GLY:H	1:40:A:SER:H	1	0.48
(1,443)	1:38:A:ARG:H	1:39:A:GLY:H	4	0.48
(1,359)	1:20:A:PHE:H	1:20:A:PHE:HB2	9	0.48
(1,354)	1:19:A:SER:H	1:19:A:SER:HB3	10	0.48
(1,352)	1:19:A:SER:H	1:18:A:GLY:HA2	1	0.48
(1,347)	1:18:A:GLY:H	1:17:A:SER:HB2	10	0.48
(1,331)	1:15:A:LYS:H	1:15:A:LYS:HG3	9	0.48
(1,328)	1:14:A:GLY:H	1:14:A:GLY:HA2	9	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,319)	1:13:A:TYR:H	1:12:A:ASN:HB2	1	0.48
(1,319)	1:13:A:TYR:H	1:12:A:ASN:HB2	2	0.48
(1,319)	1:13:A:TYR:H	1:12:A:ASN:HB2	10	0.48
(1,298)	1:10:A:SER:H	1:9:A:LEU:HA	8	0.48
(1,281)	1:7:A:CYS:H	1:6:A:ARG:HG3	5	0.48
(1,266)	1:3:A:GLN:H	1:4:A:ASP:H	5	0.48
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG11	6	0.48
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG12	6	0.48
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG13	6	0.48
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG11	10	0.48
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG12	10	0.48
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG13	10	0.48
(1,88)	1:23:A:TYR:HE1	1:49:A:THR:HA	5	0.48
(1,81)	1:23:A:TYR:HA	1:23:A:TYR:HB3	8	0.48
(1,81)	1:23:A:TYR:HA	1:23:A:TYR:HB3	10	0.48
(1,56)	1:15:A:LYS:HA	1:15:A:LYS:HB2	8	0.48
(1,51)	1:13:A:TYR:HA	1:13:A:TYR:HB2	8	0.48
(1,48)	1:12:A:ASN:HA	1:12:A:ASN:HB3	8	0.48
(1,26)	1:9:A:LEU:HD11	1:45:A:ASN:HB2	4	0.48
(1,26)	1:9:A:LEU:HD12	1:45:A:ASN:HB2	4	0.48
(1,26)	1:9:A:LEU:HD13	1:45:A:ASN:HB2	4	0.48
(1,26)	1:9:A:LEU:HD11	1:45:A:ASN:HB2	6	0.48
(1,26)	1:9:A:LEU:HD12	1:45:A:ASN:HB2	6	0.48
(1,26)	1:9:A:LEU:HD13	1:45:A:ASN:HB2	6	0.48
(1,543)	1:61:A:GLU:H	1:61:A:GLU:HG2	8	0.47
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG21	8	0.47
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG22	8	0.47
(1,522)	1:57:A:CYS:H	1:56:A:THR:HG23	8	0.47
(1,475)	1:50:A:LEU:H	1:49:A:THR:HB	3	0.47
(1,472)	1:49:A:THR:H	1:52:A:ASP:HB3	1	0.47
(1,464)	1:48:A:LYS:H	1:48:A:LYS:HD2	6	0.47
(1,442)	1:38:A:ARG:H	1:38:A:ARG:HB2	2	0.47
(1,442)	1:38:A:ARG:H	1:38:A:ARG:HB2	10	0.47
(1,402)	1:30:A:SER:H	1:27:A:LYS:HA	9	0.47
(1,380)	1:25:A:TYR:H	1:25:A:TYR:HB3	10	0.47
(1,343)	1:17:A:SER:H	1:17:A:SER:HB3	9	0.47
(1,318)	1:13:A:TYR:H	1:12:A:ASN:HB3	8	0.47
(1,304)	1:11:A:ARG:H	1:10:A:SER:HB2	6	0.47
(1,260)	1:61:A:GLU:HG3	1:61:A:GLU:HA	5	0.47
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG11	3	0.47
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG12	3	0.47
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG13	3	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,234)	1:54:A:GLU:HA	1:58:A:VAL:HB	6	0.47
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD21	10	0.47
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD22	10	0.47
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD23	10	0.47
(1,208)	1:48:A:LYS:HD3	1:48:A:LYS:HA	6	0.47
(1,196)	1:47:A:PHE:HA	1:48:A:LYS:HD3	9	0.47
(1,189)	1:40:A:SER:HB3	1:40:A:SER:HA	1	0.47
(1,172)	1:36:A:ARG:HA	1:21:A:THR:HA	5	0.47
(1,151)	1:34:A:THR:HA	1:23:A:TYR:HA	6	0.47
(1,143)	1:33:A:LYS:HA	1:33:A:LYS:HB3	7	0.47
(1,143)	1:33:A:LYS:HA	1:33:A:LYS:HB3	8	0.47
(1,143)	1:33:A:LYS:HA	1:33:A:LYS:HB3	10	0.47
(1,122)	1:27:A:LYS:HA	1:27:A:LYS:HB2	1	0.47
(1,122)	1:27:A:LYS:HA	1:27:A:LYS:HB2	2	0.47
(1,81)	1:23:A:TYR:HA	1:23:A:TYR:HB3	5	0.47
(1,78)	1:22:A:ASN:HA	1:22:A:ASN:HB2	8	0.47
(1,78)	1:22:A:ASN:HA	1:22:A:ASN:HB2	9	0.47
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG21	9	0.47
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG22	9	0.47
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG23	9	0.47
(1,57)	1:15:A:LYS:HA	1:15:A:LYS:HG2	2	0.47
(1,57)	1:15:A:LYS:HA	1:15:A:LYS:HG2	6	0.47
(1,43)	1:11:A:ARG:HD2	1:11:A:ARG:HG3	1	0.47
(1,43)	1:11:A:ARG:HD2	1:11:A:ARG:HG3	7	0.47
(1,495)	1:52:A:ASP:H	1:52:A:ASP:HB3	5	0.46
(1,454)	1:43:A:ASN:H	1:12:A:ASN:HB3	6	0.46
(1,359)	1:20:A:PHE:H	1:20:A:PHE:HB2	10	0.46
(1,340)	1:17:A:SER:H	1:16:A:GLY:HA3	3	0.46
(1,331)	1:15:A:LYS:H	1:15:A:LYS:HG3	3	0.46
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG11	7	0.46
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG12	7	0.46
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG13	7	0.46
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD21	7	0.46
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD22	7	0.46
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD23	7	0.46
(1,227)	1:53:A:CYS:HB3	1:32:A:CYS:HB2	3	0.46
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG21	5	0.46
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG22	5	0.46
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG23	5	0.46
(1,183)	1:37:A:TYR:HB2	1:22:A:ASN:HB2	8	0.46
(1,171)	1:35:A:PHE:HE1	1:37:A:TYR:HB2	2	0.46
(1,143)	1:33:A:LYS:HA	1:33:A:LYS:HB3	1	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,143)	1:33:A:LYS:HA	1:33:A:LYS:HB3	2	0.46
(1,143)	1:33:A:LYS:HA	1:33:A:LYS:HB3	4	0.46
(1,143)	1:33:A:LYS:HA	1:33:A:LYS:HB3	6	0.46
(1,143)	1:33:A:LYS:HA	1:33:A:LYS:HB3	9	0.46
(1,122)	1:27:A:LYS:HA	1:27:A:LYS:HB2	4	0.46
(1,122)	1:27:A:LYS:HA	1:27:A:LYS:HB2	9	0.46
(1,94)	1:24:A:TYR:HB3	1:11:A:ARG:HB3	3	0.46
(1,81)	1:23:A:TYR:HA	1:23:A:TYR:HB3	1	0.46
(1,81)	1:23:A:TYR:HA	1:23:A:TYR:HB3	2	0.46
(1,43)	1:11:A:ARG:HD2	1:11:A:ARG:HG3	3	0.46
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD11	5	0.46
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD12	5	0.46
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD13	5	0.46
(1,459)	1:47:A:PHE:H	1:46:A:ARG:HG2	5	0.45
(1,452)	1:42:A:GLY:H	1:41:A:GLY:HA3	5	0.45
(1,443)	1:38:A:ARG:H	1:39:A:GLY:H	1	0.45
(1,404)	1:30:A:SER:H	1:29:A:THR:HG21	5	0.45
(1,404)	1:30:A:SER:H	1:29:A:THR:HG22	5	0.45
(1,404)	1:30:A:SER:H	1:29:A:THR:HG23	5	0.45
(1,341)	1:17:A:SER:H	1:16:A:GLY:HA2	6	0.45
(1,340)	1:17:A:SER:H	1:16:A:GLY:HA3	2	0.45
(1,340)	1:17:A:SER:H	1:16:A:GLY:HA3	8	0.45
(1,331)	1:15:A:LYS:H	1:15:A:LYS:HG3	2	0.45
(1,331)	1:15:A:LYS:H	1:15:A:LYS:HG3	4	0.45
(1,312)	1:12:A:ASN:H	1:12:A:ASN:HB3	10	0.45
(1,306)	1:11:A:ARG:H	1:11:A:ARG:HB3	1	0.45
(1,299)	1:10:A:SER:H	1:9:A:LEU:HB3	10	0.45
(1,244)	1:55:A:ALA:HB1	1:56:A:THR:HB	8	0.45
(1,244)	1:55:A:ALA:HB2	1:56:A:THR:HB	8	0.45
(1,244)	1:55:A:ALA:HB3	1:56:A:THR:HB	8	0.45
(1,234)	1:54:A:GLU:HA	1:58:A:VAL:HB	1	0.45
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD21	6	0.45
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD22	6	0.45
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD23	6	0.45
(1,199)	1:47:A:PHE:HB3	1:53:A:CYS:HA	3	0.45
(1,143)	1:33:A:LYS:HA	1:33:A:LYS:HB3	5	0.45
(1,87)	1:23:A:TYR:HD1	1:49:A:THR:HA	2	0.45
(1,81)	1:23:A:TYR:HA	1:23:A:TYR:HB3	6	0.45
(1,43)	1:11:A:ARG:HD2	1:11:A:ARG:HG3	2	0.45
(1,43)	1:11:A:ARG:HD2	1:11:A:ARG:HG3	4	0.45
(1,43)	1:11:A:ARG:HD2	1:11:A:ARG:HG3	6	0.45
(1,23)	1:9:A:LEU:HA	1:5:A:TYR:HB3	7	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:7:A:CYS:HA	1:57:A:CYS:HB2	8	0.45
(1,462)	1:48:A:LYS:H	1:48:A:LYS:HB2	5	0.44
(1,459)	1:47:A:PHE:H	1:46:A:ARG:HG2	7	0.44
(1,459)	1:47:A:PHE:H	1:46:A:ARG:HG2	9	0.44
(1,438)	1:38:A:ARG:H	1:36:A:ARG:HB2	7	0.44
(1,404)	1:30:A:SER:H	1:29:A:THR:HG21	1	0.44
(1,404)	1:30:A:SER:H	1:29:A:THR:HG22	1	0.44
(1,404)	1:30:A:SER:H	1:29:A:THR:HG23	1	0.44
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB1	6	0.44
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB2	6	0.44
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB3	6	0.44
(1,396)	1:28:A:ALA:H	1:30:A:SER:H	9	0.44
(1,362)	1:21:A:THR:H	1:20:A:PHE:HB2	6	0.44
(1,304)	1:11:A:ARG:H	1:10:A:SER:HB2	3	0.44
(1,295)	1:9:A:LEU:H	1:9:A:LEU:HA	6	0.44
(1,292)	1:9:A:LEU:H	1:8:A:GLN:H	1	0.44
(1,269)	1:4:A:ASP:H	1:3:A:GLN:HB3	4	0.44
(1,248)	1:57:A:CYS:HA	1:7:A:CYS:HA	2	0.44
(1,234)	1:54:A:GLU:HA	1:58:A:VAL:HB	2	0.44
(1,127)	1:27:A:LYS:HE3	1:27:A:LYS:HB3	9	0.44
(1,122)	1:27:A:LYS:HA	1:27:A:LYS:HB2	7	0.44
(1,84)	1:23:A:TYR:HD1	1:22:A:ASN:HA	7	0.44
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG21	10	0.44
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG22	10	0.44
(1,74)	1:21:A:THR:HA	1:21:A:THR:HG23	10	0.44
(1,57)	1:15:A:LYS:HA	1:15:A:LYS:HG2	3	0.44
(1,23)	1:9:A:LEU:HA	1:5:A:TYR:HB3	8	0.44
(1,1)	1:1:A:PRO:HB3	1:1:A:PRO:HD2	5	0.44
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB1	4	0.43
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB2	4	0.43
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB3	4	0.43
(1,462)	1:48:A:LYS:H	1:48:A:LYS:HB2	7	0.43
(1,459)	1:47:A:PHE:H	1:46:A:ARG:HG2	6	0.43
(1,443)	1:38:A:ARG:H	1:39:A:GLY:H	6	0.43
(1,443)	1:38:A:ARG:H	1:39:A:GLY:H	8	0.43
(1,442)	1:38:A:ARG:H	1:38:A:ARG:HB2	9	0.43
(1,440)	1:38:A:ARG:H	1:37:A:TYR:HB3	10	0.43
(1,396)	1:28:A:ALA:H	1:30:A:SER:H	7	0.43
(1,360)	1:21:A:THR:H	1:20:A:PHE:HA	10	0.43
(1,358)	1:20:A:PHE:H	1:20:A:PHE:HB3	3	0.43
(1,352)	1:19:A:SER:H	1:18:A:GLY:HA2	10	0.43
(1,351)	1:19:A:SER:H	1:18:A:GLY:HA3	2	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,307)	1:11:A:ARG:H	1:11:A:ARG:HG2	4	0.43
(1,307)	1:11:A:ARG:H	1:11:A:ARG:HG2	8	0.43
(1,304)	1:11:A:ARG:H	1:10:A:SER:HB2	4	0.43
(1,264)	1:3:A:GLN:H	1:3:A:GLN:HB2	4	0.43
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG11	2	0.43
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG12	2	0.43
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG13	2	0.43
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG11	5	0.43
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG12	5	0.43
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG13	5	0.43
(1,213)	1:50:A:LEU:HD11	1:51:A:GLU:HG2	4	0.43
(1,213)	1:50:A:LEU:HD12	1:51:A:GLU:HG2	4	0.43
(1,213)	1:50:A:LEU:HD13	1:51:A:GLU:HG2	4	0.43
(1,204)	1:48:A:LYS:HA	1:48:A:LYS:HD2	6	0.43
(1,204)	1:48:A:LYS:HA	1:48:A:LYS:HD2	7	0.43
(1,196)	1:47:A:PHE:HA	1:48:A:LYS:HD3	6	0.43
(1,182)	1:37:A:TYR:HB2	1:20:A:PHE:HB3	10	0.43
(1,127)	1:27:A:LYS:HE3	1:27:A:LYS:HB3	7	0.43
(1,57)	1:15:A:LYS:HA	1:15:A:LYS:HG2	9	0.43
(1,56)	1:15:A:LYS:HA	1:15:A:LYS:HB2	4	0.43
(1,34)	1:11:A:ARG:HB3	1:11:A:ARG:HG2	9	0.43
(1,1)	1:1:A:PRO:HB3	1:1:A:PRO:HD2	6	0.43
(1,1)	1:1:A:PRO:HB3	1:1:A:PRO:HD2	8	0.43
(1,527)	1:58:A:VAL:H	1:57:A:CYS:H	9	0.42
(1,449)	1:41:A:GLY:H	1:40:A:SER:HA	3	0.42
(1,443)	1:38:A:ARG:H	1:39:A:GLY:H	10	0.42
(1,438)	1:38:A:ARG:H	1:36:A:ARG:HB2	6	0.42
(1,419)	1:34:A:THR:H	1:33:A:LYS:HB3	8	0.42
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB1	4	0.42
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB2	4	0.42
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB3	4	0.42
(1,354)	1:19:A:SER:H	1:19:A:SER:HB3	8	0.42
(1,341)	1:17:A:SER:H	1:16:A:GLY:HA2	1	0.42
(1,312)	1:12:A:ASN:H	1:12:A:ASN:HB3	3	0.42
(1,312)	1:12:A:ASN:H	1:12:A:ASN:HB3	8	0.42
(1,290)	1:9:A:LEU:H	1:5:A:TYR:HA	10	0.42
(1,249)	1:57:A:CYS:HA	1:7:A:CYS:HB2	10	0.42
(1,244)	1:55:A:ALA:HB1	1:56:A:THR:HB	5	0.42
(1,244)	1:55:A:ALA:HB2	1:56:A:THR:HB	5	0.42
(1,244)	1:55:A:ALA:HB3	1:56:A:THR:HB	5	0.42
(1,204)	1:48:A:LYS:HA	1:48:A:LYS:HD2	3	0.42
(1,199)	1:47:A:PHE:HB3	1:53:A:CYS:HA	9	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,151)	1:34:A:THR:HA	1:23:A:TYR:HA	1	0.42
(1,94)	1:24:A:TYR:HB3	1:11:A:ARG:HB3	4	0.42
(1,81)	1:23:A:TYR:HA	1:23:A:TYR:HB3	4	0.42
(1,6)	1:3:A:GLN:HB3	1:3:A:GLN:HA	2	0.42
(1,5)	1:3:A:GLN:HA	1:3:A:GLN:HB2	4	0.42
(1,1)	1:1:A:PRO:HB3	1:1:A:PRO:HD2	3	0.42
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB1	9	0.41
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB2	9	0.41
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB3	9	0.41
(1,459)	1:47:A:PHE:H	1:46:A:ARG:HG2	8	0.41
(1,455)	1:43:A:ASN:H	1:12:A:ASN:HB2	3	0.41
(1,455)	1:43:A:ASN:H	1:12:A:ASN:HB2	9	0.41
(1,449)	1:41:A:GLY:H	1:40:A:SER:HA	10	0.41
(1,448)	1:41:A:GLY:H	1:40:A:SER:H	3	0.41
(1,446)	1:40:A:SER:H	1:40:A:SER:HB3	9	0.41
(1,434)	1:36:A:ARG:H	1:36:A:ARG:HG2	7	0.41
(1,418)	1:34:A:THR:H	1:33:A:LYS:HA	6	0.41
(1,363)	1:21:A:THR:H	1:21:A:THR:HA	4	0.41
(1,363)	1:21:A:THR:H	1:21:A:THR:HA	7	0.41
(1,360)	1:21:A:THR:H	1:20:A:PHE:HA	8	0.41
(1,340)	1:17:A:SER:H	1:16:A:GLY:HA3	7	0.41
(1,331)	1:15:A:LYS:H	1:15:A:LYS:HG3	6	0.41
(1,326)	1:14:A:GLY:H	1:13:A:TYR:HB2	5	0.41
(1,312)	1:12:A:ASN:H	1:12:A:ASN:HB3	1	0.41
(1,304)	1:11:A:ARG:H	1:10:A:SER:HB2	2	0.41
(1,304)	1:11:A:ARG:H	1:10:A:SER:HB2	8	0.41
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD11	6	0.41
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD12	6	0.41
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD13	6	0.41
(1,295)	1:9:A:LEU:H	1:9:A:LEU:HA	8	0.41
(1,204)	1:48:A:LYS:HA	1:48:A:LYS:HD2	9	0.41
(1,164)	1:35:A:PHE:HD1	1:34:A:THR:HA	3	0.41
(1,127)	1:27:A:LYS:HE3	1:27:A:LYS:HB3	2	0.41
(1,71)	1:19:A:SER:HB2	1:36:A:ARG:HD3	6	0.41
(1,56)	1:15:A:LYS:HA	1:15:A:LYS:HB2	10	0.41
(1,43)	1:11:A:ARG:HD2	1:11:A:ARG:HG3	8	0.41
(1,11)	1:5:A:TYR:HB3	1:8:A:GLN:HG3	8	0.41
(1,1)	1:1:A:PRO:HB3	1:1:A:PRO:HD2	10	0.41
(1,492)	1:52:A:ASP:H	1:51:A:GLU:HG3	9	0.4
(1,459)	1:47:A:PHE:H	1:46:A:ARG:HG2	3	0.4
(1,443)	1:38:A:ARG:H	1:39:A:GLY:H	5	0.4
(1,438)	1:38:A:ARG:H	1:36:A:ARG:HB2	8	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:21:A:THR:H	1:21:A:THR:HA	8	0.4
(1,360)	1:21:A:THR:H	1:20:A:PHE:HA	4	0.4
(1,351)	1:19:A:SER:H	1:18:A:GLY:HA3	9	0.4
(1,344)	1:17:A:SER:H	1:18:A:GLY:H	4	0.4
(1,341)	1:17:A:SER:H	1:16:A:GLY:HA2	9	0.4
(1,340)	1:17:A:SER:H	1:16:A:GLY:HA3	9	0.4
(1,308)	1:12:A:ASN:H	1:11:A:ARG:HA	5	0.4
(1,307)	1:11:A:ARG:H	1:11:A:ARG:HG2	2	0.4
(1,269)	1:4:A:ASP:H	1:3:A:GLN:HB3	1	0.4
(1,269)	1:4:A:ASP:H	1:3:A:GLN:HB3	8	0.4
(1,244)	1:55:A:ALA:HB1	1:56:A:THR:HB	2	0.4
(1,244)	1:55:A:ALA:HB2	1:56:A:THR:HB	2	0.4
(1,244)	1:55:A:ALA:HB3	1:56:A:THR:HB	2	0.4
(1,196)	1:47:A:PHE:HA	1:48:A:LYS:HD3	1	0.4
(1,194)	1:47:A:PHE:HA	1:46:A:ARG:HG2	8	0.4
(1,186)	1:38:A:ARG:HD3	1:38:A:ARG:HG3	9	0.4
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG21	9	0.4
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG22	9	0.4
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG23	9	0.4
(1,94)	1:24:A:TYR:HB3	1:11:A:ARG:HB3	6	0.4
(1,43)	1:11:A:ARG:HD2	1:11:A:ARG:HG3	9	0.4
(1,41)	1:11:A:ARG:HD3	1:11:A:ARG:HG2	10	0.4
(1,26)	1:9:A:LEU:HD11	1:45:A:ASN:HB2	2	0.4
(1,26)	1:9:A:LEU:HD12	1:45:A:ASN:HB2	2	0.4
(1,26)	1:9:A:LEU:HD13	1:45:A:ASN:HB2	2	0.4
(1,543)	1:61:A:GLU:H	1:61:A:GLU:HG2	10	0.39
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB1	8	0.39
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB2	8	0.39
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB3	8	0.39
(1,469)	1:49:A:THR:H	1:48:A:LYS:HB2	7	0.39
(1,464)	1:48:A:LYS:H	1:48:A:LYS:HD2	5	0.39
(1,464)	1:48:A:LYS:H	1:48:A:LYS:HD2	7	0.39
(1,463)	1:48:A:LYS:H	1:48:A:LYS:HD3	6	0.39
(1,452)	1:42:A:GLY:H	1:41:A:GLY:HA3	4	0.39
(1,451)	1:41:A:GLY:H	1:41:A:GLY:HA2	8	0.39
(1,404)	1:30:A:SER:H	1:29:A:THR:HG21	2	0.39
(1,404)	1:30:A:SER:H	1:29:A:THR:HG22	2	0.39
(1,404)	1:30:A:SER:H	1:29:A:THR:HG23	2	0.39
(1,396)	1:28:A:ALA:H	1:30:A:SER:H	6	0.39
(1,363)	1:21:A:THR:H	1:21:A:THR:HA	10	0.39
(1,343)	1:17:A:SER:H	1:17:A:SER:HB3	7	0.39
(1,304)	1:11:A:ARG:H	1:10:A:SER:HB2	9	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,287)	1:8:A:GLN:H	1:7:A:CYS:HA	6	0.39
(1,264)	1:3:A:GLN:H	1:3:A:GLN:HB2	1	0.39
(1,227)	1:53:A:CYS:HB3	1:32:A:CYS:HB2	7	0.39
(1,115)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	1	0.39
(1,115)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	2	0.39
(1,115)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	3	0.39
(1,115)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	4	0.39
(1,115)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	5	0.39
(1,115)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	6	0.39
(1,115)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	8	0.39
(1,115)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	9	0.39
(1,543)	1:61:A:GLU:H	1:61:A:GLU:HG2	1	0.38
(1,543)	1:61:A:GLU:H	1:61:A:GLU:HG2	3	0.38
(1,543)	1:61:A:GLU:H	1:61:A:GLU:HG2	9	0.38
(1,542)	1:61:A:GLU:H	1:61:A:GLU:HG3	4	0.38
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB1	3	0.38
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB2	3	0.38
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB3	3	0.38
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB1	7	0.38
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB2	7	0.38
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB3	7	0.38
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB1	10	0.38
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB2	10	0.38
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB3	10	0.38
(1,527)	1:58:A:VAL:H	1:57:A:CYS:H	3	0.38
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD11	2	0.38
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD12	2	0.38
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD13	2	0.38
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD11	4	0.38
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD12	4	0.38
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD13	4	0.38
(1,465)	1:48:A:LYS:H	1:49:A:THR:H	9	0.38
(1,441)	1:38:A:ARG:H	1:38:A:ARG:HA	5	0.38
(1,404)	1:30:A:SER:H	1:29:A:THR:HG21	9	0.38
(1,404)	1:30:A:SER:H	1:29:A:THR:HG22	9	0.38
(1,404)	1:30:A:SER:H	1:29:A:THR:HG23	9	0.38
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB1	8	0.38
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB2	8	0.38
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB3	8	0.38
(1,361)	1:21:A:THR:H	1:20:A:PHE:HB3	2	0.38
(1,341)	1:17:A:SER:H	1:16:A:GLY:HA2	8	0.38
(1,331)	1:15:A:LYS:H	1:15:A:LYS:HG3	5	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,330)	1:15:A:LYS:H	1:15:A:LYS:HB2	9	0.38
(1,319)	1:13:A:TYR:H	1:12:A:ASN:HB2	6	0.38
(1,318)	1:13:A:TYR:H	1:12:A:ASN:HB3	4	0.38
(1,308)	1:12:A:ASN:H	1:11:A:ARG:HA	7	0.38
(1,308)	1:12:A:ASN:H	1:11:A:ARG:HA	9	0.38
(1,292)	1:9:A:LEU:H	1:8:A:GLN:H	9	0.38
(1,272)	1:4:A:ASP:H	1:4:A:ASP:HB2	2	0.38
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD21	8	0.38
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD22	8	0.38
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD23	8	0.38
(1,214)	1:50:A:LEU:HD21	1:54:A:GLU:HB2	5	0.38
(1,214)	1:50:A:LEU:HD22	1:54:A:GLU:HB2	5	0.38
(1,214)	1:50:A:LEU:HD23	1:54:A:GLU:HB2	5	0.38
(1,164)	1:35:A:PHE:HD1	1:34:A:THR:HA	7	0.38
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG21	4	0.38
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG22	4	0.38
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG23	4	0.38
(1,150)	1:33:A:LYS:HG2	1:33:A:LYS:HA	6	0.38
(1,115)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	7	0.38
(1,115)	1:25:A:TYR:HE1	1:25:A:TYR:HD1	10	0.38
(1,84)	1:23:A:TYR:HD1	1:22:A:ASN:HA	4	0.38
(1,57)	1:15:A:LYS:HA	1:15:A:LYS:HG2	5	0.38
(1,18)	1:7:A:CYS:HA	1:57:A:CYS:HB2	9	0.38
(1,4)	1:1:A:PRO:HD2	1:1:A:PRO:HG3	9	0.38
(1,472)	1:49:A:THR:H	1:52:A:ASP:HB3	2	0.37
(1,452)	1:42:A:GLY:H	1:41:A:GLY:HA3	9	0.37
(1,449)	1:41:A:GLY:H	1:40:A:SER:HA	7	0.37
(1,448)	1:41:A:GLY:H	1:40:A:SER:H	2	0.37
(1,448)	1:41:A:GLY:H	1:40:A:SER:H	9	0.37
(1,448)	1:41:A:GLY:H	1:40:A:SER:H	10	0.37
(1,447)	1:40:A:SER:H	1:40:A:SER:HB2	6	0.37
(1,441)	1:38:A:ARG:H	1:38:A:ARG:HA	1	0.37
(1,441)	1:38:A:ARG:H	1:38:A:ARG:HA	10	0.37
(1,418)	1:34:A:THR:H	1:33:A:LYS:HA	2	0.37
(1,384)	1:26:A:ASP:H	1:26:A:ASP:HB2	7	0.37
(1,341)	1:17:A:SER:H	1:16:A:GLY:HA2	2	0.37
(1,331)	1:15:A:LYS:H	1:15:A:LYS:HG3	7	0.37
(1,327)	1:14:A:GLY:H	1:14:A:GLY:HA3	5	0.37
(1,327)	1:14:A:GLY:H	1:14:A:GLY:HA3	6	0.37
(1,319)	1:13:A:TYR:H	1:12:A:ASN:HB2	3	0.37
(1,307)	1:11:A:ARG:H	1:11:A:ARG:HG2	3	0.37
(1,304)	1:11:A:ARG:H	1:10:A:SER:HB2	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,304)	1:11:A:ARG:H	1:10:A:SER:HB2	5	0.37
(1,302)	1:10:A:SER:H	1:10:A:SER:HB3	2	0.37
(1,302)	1:10:A:SER:H	1:10:A:SER:HB3	4	0.37
(1,299)	1:10:A:SER:H	1:9:A:LEU:HB3	3	0.37
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD11	8	0.37
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD12	8	0.37
(1,296)	1:9:A:LEU:H	1:9:A:LEU:HD13	8	0.37
(1,287)	1:8:A:GLN:H	1:7:A:CYS:HA	10	0.37
(1,282)	1:7:A:CYS:H	1:6:A:ARG:HG2	1	0.37
(1,264)	1:3:A:GLN:H	1:3:A:GLN:HB2	7	0.37
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG11	1	0.37
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG12	1	0.37
(1,253)	1:58:A:VAL:HA	1:58:A:VAL:HG13	1	0.37
(1,248)	1:57:A:CYS:HA	1:7:A:CYS:HA	6	0.37
(1,210)	1:49:A:THR:HB	1:51:A:GLU:HG2	3	0.37
(1,186)	1:38:A:ARG:HD3	1:38:A:ARG:HG3	4	0.37
(1,169)	1:35:A:PHE:HE1	1:37:A:TYR:HA	4	0.37
(1,169)	1:35:A:PHE:HE1	1:37:A:TYR:HA	6	0.37
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG21	7	0.37
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG22	7	0.37
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG23	7	0.37
(1,151)	1:34:A:THR:HA	1:23:A:TYR:HA	7	0.37
(1,147)	1:33:A:LYS:HE3	1:33:A:LYS:HD3	5	0.37
(1,73)	1:20:A:PHE:HA	1:20:A:PHE:HB2	4	0.37
(1,48)	1:12:A:ASN:HA	1:12:A:ASN:HB3	10	0.37
(1,42)	1:11:A:ARG:HD2	1:11:A:ARG:HB2	6	0.37
(1,34)	1:11:A:ARG:HB3	1:11:A:ARG:HG2	5	0.37
(1,20)	1:7:A:CYS:HB2	1:3:A:GLN:HG3	2	0.37
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB1	2	0.36
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB2	2	0.36
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB3	2	0.36
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB1	5	0.36
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB2	5	0.36
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB3	5	0.36
(1,506)	1:54:A:GLU:H	1:53:A:CYS:HB3	10	0.36
(1,492)	1:52:A:ASP:H	1:51:A:GLU:HG3	4	0.36
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD11	3	0.36
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD12	3	0.36
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD13	3	0.36
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD11	9	0.36
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD12	9	0.36
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD13	9	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,475)	1:50:A:LEU:H	1:49:A:THR:HB	1	0.36
(1,469)	1:49:A:THR:H	1:48:A:LYS:HB2	5	0.36
(1,459)	1:47:A:PHE:H	1:46:A:ARG:HG2	1	0.36
(1,456)	1:43:A:ASN:H	1:43:A:ASN:HB3	9	0.36
(1,448)	1:41:A:GLY:H	1:40:A:SER:H	5	0.36
(1,441)	1:38:A:ARG:H	1:38:A:ARG:HA	3	0.36
(1,440)	1:38:A:ARG:H	1:37:A:TYR:HB3	2	0.36
(1,440)	1:38:A:ARG:H	1:37:A:TYR:HB3	7	0.36
(1,434)	1:36:A:ARG:H	1:36:A:ARG:HG2	6	0.36
(1,419)	1:34:A:THR:H	1:33:A:LYS:HB3	1	0.36
(1,402)	1:30:A:SER:H	1:27:A:LYS:HA	2	0.36
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB1	10	0.36
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB2	10	0.36
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB3	10	0.36
(1,360)	1:21:A:THR:H	1:20:A:PHE:HA	7	0.36
(1,352)	1:19:A:SER:H	1:18:A:GLY:HA2	2	0.36
(1,345)	1:17:A:SER:H	1:38:A:ARG:HA	2	0.36
(1,341)	1:17:A:SER:H	1:16:A:GLY:HA2	3	0.36
(1,330)	1:15:A:LYS:H	1:15:A:LYS:HB2	7	0.36
(1,327)	1:14:A:GLY:H	1:14:A:GLY:HA3	8	0.36
(1,325)	1:14:A:GLY:H	1:13:A:TYR:HB3	1	0.36
(1,319)	1:13:A:TYR:H	1:12:A:ASN:HB2	7	0.36
(1,308)	1:12:A:ASN:H	1:11:A:ARG:HA	2	0.36
(1,304)	1:11:A:ARG:H	1:10:A:SER:HB2	7	0.36
(1,248)	1:57:A:CYS:HA	1:7:A:CYS:HA	9	0.36
(1,245)	1:56:A:THR:HG21	1:53:A:CYS:HA	1	0.36
(1,245)	1:56:A:THR:HG22	1:53:A:CYS:HA	1	0.36
(1,245)	1:56:A:THR:HG23	1:53:A:CYS:HA	1	0.36
(1,244)	1:55:A:ALA:HB1	1:56:A:THR:HB	10	0.36
(1,244)	1:55:A:ALA:HB2	1:56:A:THR:HB	10	0.36
(1,244)	1:55:A:ALA:HB3	1:56:A:THR:HB	10	0.36
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD21	6	0.36
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD22	6	0.36
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD23	6	0.36
(1,213)	1:50:A:LEU:HD11	1:51:A:GLU:HG2	2	0.36
(1,213)	1:50:A:LEU:HD12	1:51:A:GLU:HG2	2	0.36
(1,213)	1:50:A:LEU:HD13	1:51:A:GLU:HG2	2	0.36
(1,204)	1:48:A:LYS:HA	1:48:A:LYS:HD2	4	0.36
(1,186)	1:38:A:ARG:HD3	1:38:A:ARG:HG3	1	0.36
(1,172)	1:36:A:ARG:HA	1:21:A:THR:HA	1	0.36
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD11	8	0.36
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD12	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD13	8	0.36
(1,1)	1:1:A:PRO:HB3	1:1:A:PRO:HD2	2	0.36
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB1	6	0.35
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB2	6	0.35
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB3	6	0.35
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG11	1	0.35
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG12	1	0.35
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG13	1	0.35
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG11	7	0.35
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG12	7	0.35
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG13	7	0.35
(1,465)	1:48:A:LYS:H	1:49:A:THR:H	5	0.35
(1,458)	1:47:A:PHE:H	1:46:A:ARG:HG3	4	0.35
(1,454)	1:43:A:ASN:H	1:12:A:ASN:HB3	1	0.35
(1,449)	1:41:A:GLY:H	1:40:A:SER:HA	2	0.35
(1,441)	1:38:A:ARG:H	1:38:A:ARG:HA	9	0.35
(1,424)	1:35:A:PHE:H	1:22:A:ASN:H	7	0.35
(1,396)	1:28:A:ALA:H	1:30:A:SER:H	1	0.35
(1,389)	1:27:A:LYS:H	1:27:A:LYS:HB2	7	0.35
(1,358)	1:20:A:PHE:H	1:20:A:PHE:HB3	4	0.35
(1,353)	1:19:A:SER:H	1:19:A:SER:HA	5	0.35
(1,330)	1:15:A:LYS:H	1:15:A:LYS:HB2	4	0.35
(1,330)	1:15:A:LYS:H	1:15:A:LYS:HB2	5	0.35
(1,330)	1:15:A:LYS:H	1:15:A:LYS:HB2	10	0.35
(1,326)	1:14:A:GLY:H	1:13:A:TYR:HB2	4	0.35
(1,310)	1:12:A:ASN:H	1:11:A:ARG:HG3	5	0.35
(1,299)	1:10:A:SER:H	1:9:A:LEU:HB3	1	0.35
(1,299)	1:10:A:SER:H	1:9:A:LEU:HB3	5	0.35
(1,248)	1:57:A:CYS:HA	1:7:A:CYS:HA	4	0.35
(1,213)	1:50:A:LEU:HD11	1:51:A:GLU:HG2	7	0.35
(1,213)	1:50:A:LEU:HD12	1:51:A:GLU:HG2	7	0.35
(1,213)	1:50:A:LEU:HD13	1:51:A:GLU:HG2	7	0.35
(1,208)	1:48:A:LYS:HD3	1:48:A:LYS:HA	3	0.35
(1,204)	1:48:A:LYS:HA	1:48:A:LYS:HD2	2	0.35
(1,194)	1:47:A:PHE:HA	1:46:A:ARG:HG2	6	0.35
(1,183)	1:37:A:TYR:HB2	1:22:A:ASN:HB2	1	0.35
(1,168)	1:35:A:PHE:HD1	1:37:A:TYR:HB2	4	0.35
(1,151)	1:34:A:THR:HA	1:23:A:TYR:HA	2	0.35
(1,150)	1:33:A:LYS:HG2	1:33:A:LYS:HA	8	0.35
(1,147)	1:33:A:LYS:HE3	1:33:A:LYS:HD3	4	0.35
(1,64)	1:19:A:SER:HA	1:19:A:SER:HB3	6	0.35
(1,45)	1:11:A:ARG:HG3	1:11:A:ARG:HB3	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:11:A:ARG:HD3	1:11:A:ARG:HG2	5	0.35
(1,18)	1:7:A:CYS:HA	1:57:A:CYS:HB2	4	0.35
(1,4)	1:1:A:PRO:HD2	1:1:A:PRO:HG3	5	0.35
(1,1)	1:1:A:PRO:HB3	1:1:A:PRO:HD2	7	0.35
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG11	2	0.34
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG12	2	0.34
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG13	2	0.34
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG11	6	0.34
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG12	6	0.34
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG13	6	0.34
(1,495)	1:52:A:ASP:H	1:52:A:ASP:HB3	7	0.34
(1,458)	1:47:A:PHE:H	1:46:A:ARG:HG3	7	0.34
(1,440)	1:38:A:ARG:H	1:37:A:TYR:HB3	4	0.34
(1,404)	1:30:A:SER:H	1:29:A:THR:HG21	3	0.34
(1,404)	1:30:A:SER:H	1:29:A:THR:HG22	3	0.34
(1,404)	1:30:A:SER:H	1:29:A:THR:HG23	3	0.34
(1,359)	1:20:A:PHE:H	1:20:A:PHE:HB2	8	0.34
(1,358)	1:20:A:PHE:H	1:20:A:PHE:HB3	5	0.34
(1,353)	1:19:A:SER:H	1:19:A:SER:HA	1	0.34
(1,344)	1:17:A:SER:H	1:18:A:GLY:H	6	0.34
(1,341)	1:17:A:SER:H	1:16:A:GLY:HA2	5	0.34
(1,331)	1:15:A:LYS:H	1:15:A:LYS:HG3	1	0.34
(1,330)	1:15:A:LYS:H	1:15:A:LYS:HB2	1	0.34
(1,323)	1:13:A:TYR:H	1:14:A:GLY:H	3	0.34
(1,308)	1:12:A:ASN:H	1:11:A:ARG:HA	8	0.34
(1,299)	1:10:A:SER:H	1:9:A:LEU:HB3	9	0.34
(1,272)	1:4:A:ASP:H	1:4:A:ASP:HB2	8	0.34
(1,249)	1:57:A:CYS:HA	1:7:A:CYS:HB2	9	0.34
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD21	1	0.34
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD22	1	0.34
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD23	1	0.34
(1,214)	1:50:A:LEU:HD21	1:54:A:GLU:HB2	2	0.34
(1,214)	1:50:A:LEU:HD22	1:54:A:GLU:HB2	2	0.34
(1,214)	1:50:A:LEU:HD23	1:54:A:GLU:HB2	2	0.34
(1,213)	1:50:A:LEU:HD11	1:51:A:GLU:HG2	6	0.34
(1,213)	1:50:A:LEU:HD12	1:51:A:GLU:HG2	6	0.34
(1,213)	1:50:A:LEU:HD13	1:51:A:GLU:HG2	6	0.34
(1,213)	1:50:A:LEU:HD11	1:51:A:GLU:HG2	10	0.34
(1,213)	1:50:A:LEU:HD12	1:51:A:GLU:HG2	10	0.34
(1,213)	1:50:A:LEU:HD13	1:51:A:GLU:HG2	10	0.34
(1,208)	1:48:A:LYS:HD3	1:48:A:LYS:HA	9	0.34
(1,199)	1:47:A:PHE:HB3	1:53:A:CYS:HA	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,150)	1:33:A:LYS:HG2	1:33:A:LYS:HA	2	0.34
(1,144)	1:33:A:LYS:HA	1:33:A:LYS:HD2	5	0.34
(1,94)	1:24:A:TYR:HB3	1:11:A:ARG:HB3	7	0.34
(1,73)	1:20:A:PHE:HA	1:20:A:PHE:HB2	2	0.34
(1,64)	1:19:A:SER:HA	1:19:A:SER:HB3	1	0.34
(1,64)	1:19:A:SER:HA	1:19:A:SER:HB3	2	0.34
(1,64)	1:19:A:SER:HA	1:19:A:SER:HB3	5	0.34
(1,45)	1:11:A:ARG:HG3	1:11:A:ARG:HB3	7	0.34
(1,18)	1:7:A:CYS:HA	1:57:A:CYS:HB2	5	0.34
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD11	4	0.34
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD12	4	0.34
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD13	4	0.34
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD11	6	0.34
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD12	6	0.34
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD13	6	0.34
(1,4)	1:1:A:PRO:HD2	1:1:A:PRO:HG3	3	0.34
(1,4)	1:1:A:PRO:HD2	1:1:A:PRO:HG3	6	0.34
(1,4)	1:1:A:PRO:HD2	1:1:A:PRO:HG3	8	0.34
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG11	5	0.33
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG12	5	0.33
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG13	5	0.33
(1,527)	1:58:A:VAL:H	1:57:A:CYS:H	1	0.33
(1,527)	1:58:A:VAL:H	1:57:A:CYS:H	8	0.33
(1,511)	1:55:A:ALA:H	1:54:A:GLU:HG3	7	0.33
(1,504)	1:54:A:GLU:H	1:50:A:LEU:HD21	10	0.33
(1,504)	1:54:A:GLU:H	1:50:A:LEU:HD22	10	0.33
(1,504)	1:54:A:GLU:H	1:50:A:LEU:HD23	10	0.33
(1,498)	1:53:A:CYS:H	1:47:A:PHE:HB3	9	0.33
(1,493)	1:52:A:ASP:H	1:51:A:GLU:HG2	1	0.33
(1,458)	1:47:A:PHE:H	1:46:A:ARG:HG3	1	0.33
(1,446)	1:40:A:SER:H	1:40:A:SER:HB3	5	0.33
(1,441)	1:38:A:ARG:H	1:38:A:ARG:HA	2	0.33
(1,410)	1:32:A:CYS:H	1:31:A:SER:HA	10	0.33
(1,404)	1:30:A:SER:H	1:29:A:THR:HG21	10	0.33
(1,404)	1:30:A:SER:H	1:29:A:THR:HG22	10	0.33
(1,404)	1:30:A:SER:H	1:29:A:THR:HG23	10	0.33
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB1	5	0.33
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB2	5	0.33
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB3	5	0.33
(1,358)	1:20:A:PHE:H	1:20:A:PHE:HB3	1	0.33
(1,353)	1:19:A:SER:H	1:19:A:SER:HA	3	0.33
(1,340)	1:17:A:SER:H	1:16:A:GLY:HA3	1	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,325)	1:14:A:GLY:H	1:13:A:TYR:HB3	4	0.33
(1,325)	1:14:A:GLY:H	1:13:A:TYR:HB3	7	0.33
(1,313)	1:12:A:ASN:H	1:12:A:ASN:HB2	10	0.33
(1,265)	1:3:A:GLN:H	1:3:A:GLN:HG3	5	0.33
(1,261)	1:61:A:GLU:HG2	1:59:A:THR:HA	5	0.33
(1,246)	1:56:A:THR:HG21	1:56:A:THR:HB	1	0.33
(1,246)	1:56:A:THR:HG22	1:56:A:THR:HB	1	0.33
(1,246)	1:56:A:THR:HG23	1:56:A:THR:HB	1	0.33
(1,246)	1:56:A:THR:HG21	1:56:A:THR:HB	2	0.33
(1,246)	1:56:A:THR:HG22	1:56:A:THR:HB	2	0.33
(1,246)	1:56:A:THR:HG23	1:56:A:THR:HB	2	0.33
(1,246)	1:56:A:THR:HG21	1:56:A:THR:HB	3	0.33
(1,246)	1:56:A:THR:HG22	1:56:A:THR:HB	3	0.33
(1,246)	1:56:A:THR:HG23	1:56:A:THR:HB	3	0.33
(1,246)	1:56:A:THR:HG21	1:56:A:THR:HB	4	0.33
(1,246)	1:56:A:THR:HG22	1:56:A:THR:HB	4	0.33
(1,246)	1:56:A:THR:HG23	1:56:A:THR:HB	4	0.33
(1,246)	1:56:A:THR:HG21	1:56:A:THR:HB	5	0.33
(1,246)	1:56:A:THR:HG22	1:56:A:THR:HB	5	0.33
(1,246)	1:56:A:THR:HG23	1:56:A:THR:HB	5	0.33
(1,246)	1:56:A:THR:HG21	1:56:A:THR:HB	5	0.33
(1,246)	1:56:A:THR:HG23	1:56:A:THR:HB	5	0.33
(1,246)	1:56:A:THR:HG21	1:56:A:THR:HB	6	0.33
(1,246)	1:56:A:THR:HG22	1:56:A:THR:HB	6	0.33
(1,246)	1:56:A:THR:HG23	1:56:A:THR:HB	6	0.33
(1,246)	1:56:A:THR:HG21	1:56:A:THR:HB	7	0.33
(1,246)	1:56:A:THR:HG22	1:56:A:THR:HB	7	0.33
(1,246)	1:56:A:THR:HG23	1:56:A:THR:HB	7	0.33
(1,246)	1:56:A:THR:HG21	1:56:A:THR:HB	8	0.33
(1,246)	1:56:A:THR:HG22	1:56:A:THR:HB	8	0.33
(1,246)	1:56:A:THR:HG23	1:56:A:THR:HB	8	0.33
(1,246)	1:56:A:THR:HG21	1:56:A:THR:HB	9	0.33
(1,246)	1:56:A:THR:HG22	1:56:A:THR:HB	9	0.33
(1,246)	1:56:A:THR:HG23	1:56:A:THR:HB	9	0.33
(1,246)	1:56:A:THR:HG21	1:56:A:THR:HB	10	0.33
(1,246)	1:56:A:THR:HG22	1:56:A:THR:HB	10	0.33
(1,246)	1:56:A:THR:HG23	1:56:A:THR:HB	10	0.33
(1,245)	1:56:A:THR:HG21	1:53:A:CYS:HA	6	0.33
(1,245)	1:56:A:THR:HG22	1:53:A:CYS:HA	6	0.33
(1,245)	1:56:A:THR:HG23	1:53:A:CYS:HA	6	0.33
(1,227)	1:53:A:CYS:HB3	1:32:A:CYS:HB2	4	0.33
(1,214)	1:50:A:LEU:HD21	1:54:A:GLU:HB2	4	0.33
(1,214)	1:50:A:LEU:HD22	1:54:A:GLU:HB2	4	0.33
(1,214)	1:50:A:LEU:HD23	1:54:A:GLU:HB2	4	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,186)	1:38:A:ARG:HD3	1:38:A:ARG:HG3	5	0.33
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG21	8	0.33
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG22	8	0.33
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG23	8	0.33
(1,151)	1:34:A:THR:HA	1:23:A:TYR:HA	10	0.33
(1,80)	1:22:A:ASN:HD21	1:22:A:ASN:HD22	1	0.33
(1,80)	1:22:A:ASN:HD21	1:22:A:ASN:HD22	2	0.33
(1,80)	1:22:A:ASN:HD21	1:22:A:ASN:HD22	3	0.33
(1,80)	1:22:A:ASN:HD21	1:22:A:ASN:HD22	4	0.33
(1,80)	1:22:A:ASN:HD21	1:22:A:ASN:HD22	5	0.33
(1,80)	1:22:A:ASN:HD21	1:22:A:ASN:HD22	6	0.33
(1,80)	1:22:A:ASN:HD21	1:22:A:ASN:HD22	7	0.33
(1,80)	1:22:A:ASN:HD21	1:22:A:ASN:HD22	9	0.33
(1,80)	1:22:A:ASN:HD21	1:22:A:ASN:HD22	10	0.33
(1,71)	1:19:A:SER:HB2	1:36:A:ARG:HD3	9	0.33
(1,64)	1:19:A:SER:HA	1:19:A:SER:HB3	10	0.33
(1,55)	1:15:A:LYS:HA	1:15:A:LYS:HB3	1	0.33
(1,4)	1:1:A:PRO:HD2	1:1:A:PRO:HG3	2	0.33
(1,4)	1:1:A:PRO:HD2	1:1:A:PRO:HG3	7	0.33
(1,4)	1:1:A:PRO:HD2	1:1:A:PRO:HG3	10	0.33
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB1	1	0.32
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB2	1	0.32
(1,538)	1:60:A:ALA:H	1:60:A:ALA:HB3	1	0.32
(1,527)	1:58:A:VAL:H	1:57:A:CYS:H	5	0.32
(1,495)	1:52:A:ASP:H	1:52:A:ASP:HB3	2	0.32
(1,495)	1:52:A:ASP:H	1:52:A:ASP:HB3	8	0.32
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD11	1	0.32
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD12	1	0.32
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD13	1	0.32
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD11	5	0.32
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD12	5	0.32
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD13	5	0.32
(1,475)	1:50:A:LEU:H	1:49:A:THR:HB	9	0.32
(1,463)	1:48:A:LYS:H	1:48:A:LYS:HD3	4	0.32
(1,463)	1:48:A:LYS:H	1:48:A:LYS:HD3	9	0.32
(1,406)	1:30:A:SER:H	1:30:A:SER:HB2	10	0.32
(1,402)	1:30:A:SER:H	1:27:A:LYS:HA	1	0.32
(1,396)	1:28:A:ALA:H	1:30:A:SER:H	4	0.32
(1,389)	1:27:A:LYS:H	1:27:A:LYS:HB2	4	0.32
(1,389)	1:27:A:LYS:H	1:27:A:LYS:HB2	9	0.32
(1,356)	1:20:A:PHE:H	1:19:A:SER:HB2	6	0.32
(1,356)	1:20:A:PHE:H	1:19:A:SER:HB2	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,353)	1:19:A:SER:H	1:19:A:SER:HA	2	0.32
(1,345)	1:17:A:SER:H	1:38:A:ARG:HA	4	0.32
(1,330)	1:15:A:LYS:H	1:15:A:LYS:HB2	2	0.32
(1,330)	1:15:A:LYS:H	1:15:A:LYS:HB2	3	0.32
(1,328)	1:14:A:GLY:H	1:14:A:GLY:HA2	1	0.32
(1,307)	1:11:A:ARG:H	1:11:A:ARG:HG2	6	0.32
(1,294)	1:9:A:LEU:H	1:8:A:GLN:HG3	6	0.32
(1,281)	1:7:A:CYS:H	1:6:A:ARG:HG3	9	0.32
(1,249)	1:57:A:CYS:HA	1:7:A:CYS:HB2	6	0.32
(1,249)	1:57:A:CYS:HA	1:7:A:CYS:HB2	7	0.32
(1,245)	1:56:A:THR:HG21	1:53:A:CYS:HA	5	0.32
(1,245)	1:56:A:THR:HG22	1:53:A:CYS:HA	5	0.32
(1,245)	1:56:A:THR:HG23	1:53:A:CYS:HA	5	0.32
(1,244)	1:55:A:ALA:HB1	1:56:A:THR:HB	1	0.32
(1,244)	1:55:A:ALA:HB2	1:56:A:THR:HB	1	0.32
(1,244)	1:55:A:ALA:HB3	1:56:A:THR:HB	1	0.32
(1,244)	1:55:A:ALA:HB1	1:56:A:THR:HB	3	0.32
(1,244)	1:55:A:ALA:HB2	1:56:A:THR:HB	3	0.32
(1,244)	1:55:A:ALA:HB3	1:56:A:THR:HB	3	0.32
(1,244)	1:55:A:ALA:HB1	1:56:A:THR:HB	9	0.32
(1,244)	1:55:A:ALA:HB2	1:56:A:THR:HB	9	0.32
(1,244)	1:55:A:ALA:HB3	1:56:A:THR:HB	9	0.32
(1,214)	1:50:A:LEU:HD21	1:54:A:GLU:HB2	9	0.32
(1,214)	1:50:A:LEU:HD22	1:54:A:GLU:HB2	9	0.32
(1,214)	1:50:A:LEU:HD23	1:54:A:GLU:HB2	9	0.32
(1,208)	1:48:A:LYS:HD3	1:48:A:LYS:HA	2	0.32
(1,186)	1:38:A:ARG:HD3	1:38:A:ARG:HG3	6	0.32
(1,168)	1:35:A:PHE:HD1	1:37:A:TYR:HB2	6	0.32
(1,168)	1:35:A:PHE:HD1	1:37:A:TYR:HB2	8	0.32
(1,165)	1:35:A:PHE:HD1	1:34:A:THR:HB	9	0.32
(1,145)	1:33:A:LYS:HA	1:33:A:LYS:HE3	4	0.32
(1,102)	1:24:A:TYR:HD1	1:24:A:TYR:HA	4	0.32
(1,88)	1:23:A:TYR:HE1	1:49:A:THR:HA	4	0.32
(1,80)	1:22:A:ASN:HD21	1:22:A:ASN:HD22	8	0.32
(1,73)	1:20:A:PHE:HA	1:20:A:PHE:HB2	3	0.32
(1,73)	1:20:A:PHE:HA	1:20:A:PHE:HB2	10	0.32
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD11	10	0.32
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD12	10	0.32
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD13	10	0.32
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD11	10	0.32
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD12	10	0.32
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD13	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:1:A:PRO:HB3	1:1:A:PRO:HD2	1	0.32
(1,527)	1:58:A:VAL:H	1:57:A:CYS:H	10	0.31
(1,493)	1:52:A:ASP:H	1:51:A:GLU:HG2	2	0.31
(1,480)	1:51:A:GLU:H	1:49:A:THR:HB	7	0.31
(1,462)	1:48:A:LYS:H	1:48:A:LYS:HB2	8	0.31
(1,458)	1:47:A:PHE:H	1:46:A:ARG:HG3	5	0.31
(1,458)	1:47:A:PHE:H	1:46:A:ARG:HG3	6	0.31
(1,449)	1:41:A:GLY:H	1:40:A:SER:HA	8	0.31
(1,441)	1:38:A:ARG:H	1:38:A:ARG:HA	6	0.31
(1,441)	1:38:A:ARG:H	1:38:A:ARG:HA	8	0.31
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG21	1	0.31
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG22	1	0.31
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG23	1	0.31
(1,424)	1:35:A:PHE:H	1:22:A:ASN:H	10	0.31
(1,389)	1:27:A:LYS:H	1:27:A:LYS:HB2	1	0.31
(1,389)	1:27:A:LYS:H	1:27:A:LYS:HB2	2	0.31
(1,384)	1:26:A:ASP:H	1:26:A:ASP:HB2	1	0.31
(1,359)	1:20:A:PHE:H	1:20:A:PHE:HB2	7	0.31
(1,345)	1:17:A:SER:H	1:38:A:ARG:HA	3	0.31
(1,344)	1:17:A:SER:H	1:18:A:GLY:H	3	0.31
(1,326)	1:14:A:GLY:H	1:13:A:TYR:HB2	2	0.31
(1,321)	1:13:A:TYR:H	1:13:A:TYR:HB3	7	0.31
(1,312)	1:12:A:ASN:H	1:12:A:ASN:HB3	2	0.31
(1,299)	1:10:A:SER:H	1:9:A:LEU:HB3	7	0.31
(1,248)	1:57:A:CYS:HA	1:7:A:CYS:HA	1	0.31
(1,248)	1:57:A:CYS:HA	1:7:A:CYS:HA	8	0.31
(1,245)	1:56:A:THR:HG21	1:53:A:CYS:HA	2	0.31
(1,245)	1:56:A:THR:HG22	1:53:A:CYS:HA	2	0.31
(1,245)	1:56:A:THR:HG23	1:53:A:CYS:HA	2	0.31
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD21	1	0.31
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD22	1	0.31
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD23	1	0.31
(1,214)	1:50:A:LEU:HD21	1:54:A:GLU:HB2	7	0.31
(1,214)	1:50:A:LEU:HD22	1:54:A:GLU:HB2	7	0.31
(1,214)	1:50:A:LEU:HD23	1:54:A:GLU:HB2	7	0.31
(1,198)	1:47:A:PHE:HB3	1:47:A:PHE:HB2	10	0.31
(1,196)	1:47:A:PHE:HA	1:48:A:LYS:HD3	2	0.31
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG21	1	0.31
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG22	1	0.31
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG23	1	0.31
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG21	2	0.31
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG22	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG23	2	0.31
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG21	4	0.31
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG22	4	0.31
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG23	4	0.31
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG21	5	0.31
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG22	5	0.31
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG23	5	0.31
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG21	9	0.31
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG22	9	0.31
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG23	9	0.31
(1,150)	1:33:A:LYS:HG2	1:33:A:LYS:HA	1	0.31
(1,150)	1:33:A:LYS:HG2	1:33:A:LYS:HA	7	0.31
(1,144)	1:33:A:LYS:HA	1:33:A:LYS:HD2	4	0.31
(1,141)	1:32:A:CYS:HB3	1:50:A:LEU:HB3	8	0.31
(1,135)	1:32:A:CYS:HA	1:25:A:TYR:HB2	10	0.31
(1,64)	1:19:A:SER:HA	1:19:A:SER:HB3	3	0.31
(1,64)	1:19:A:SER:HA	1:19:A:SER:HB3	7	0.31
(1,64)	1:19:A:SER:HA	1:19:A:SER:HB3	8	0.31
(1,49)	1:12:A:ASN:HA	1:12:A:ASN:HB2	5	0.31
(1,542)	1:61:A:GLU:H	1:61:A:GLU:HG3	3	0.3
(1,511)	1:55:A:ALA:H	1:54:A:GLU:HG3	8	0.3
(1,495)	1:52:A:ASP:H	1:52:A:ASP:HB3	9	0.3
(1,492)	1:52:A:ASP:H	1:51:A:GLU:HG3	1	0.3
(1,492)	1:52:A:ASP:H	1:51:A:GLU:HG3	10	0.3
(1,452)	1:42:A:GLY:H	1:41:A:GLY:HA3	10	0.3
(1,443)	1:38:A:ARG:H	1:39:A:GLY:H	9	0.3
(1,441)	1:38:A:ARG:H	1:38:A:ARG:HA	7	0.3
(1,410)	1:32:A:CYS:H	1:31:A:SER:HA	1	0.3
(1,394)	1:28:A:ALA:H	1:29:A:THR:H	2	0.3
(1,356)	1:20:A:PHE:H	1:19:A:SER:HB2	1	0.3
(1,356)	1:20:A:PHE:H	1:19:A:SER:HB2	8	0.3
(1,327)	1:14:A:GLY:H	1:14:A:GLY:HA3	10	0.3
(1,323)	1:13:A:TYR:H	1:14:A:GLY:H	9	0.3
(1,316)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	1	0.3
(1,316)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	2	0.3
(1,316)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	4	0.3
(1,316)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	5	0.3
(1,316)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	6	0.3
(1,316)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	7	0.3
(1,316)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	8	0.3
(1,316)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	9	0.3
(1,316)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	1:12:A:ASN:HD21	1:12:A:ASN:HB3	5	0.3
(1,289)	1:8:A:GLN:HE21	1:8:A:GLN:HE22	2	0.3
(1,289)	1:8:A:GLN:HE21	1:8:A:GLN:HE22	3	0.3
(1,289)	1:8:A:GLN:HE21	1:8:A:GLN:HE22	4	0.3
(1,289)	1:8:A:GLN:HE21	1:8:A:GLN:HE22	5	0.3
(1,289)	1:8:A:GLN:HE21	1:8:A:GLN:HE22	6	0.3
(1,289)	1:8:A:GLN:HE21	1:8:A:GLN:HE22	7	0.3
(1,289)	1:8:A:GLN:HE21	1:8:A:GLN:HE22	8	0.3
(1,289)	1:8:A:GLN:HE21	1:8:A:GLN:HE22	9	0.3
(1,289)	1:8:A:GLN:HE21	1:8:A:GLN:HE22	10	0.3
(1,278)	1:6:A:ARG:H	1:6:A:ARG:HG2	7	0.3
(1,267)	1:3:A:GLN:HE21	1:3:A:GLN:HE22	4	0.3
(1,267)	1:3:A:GLN:HE21	1:3:A:GLN:HE22	5	0.3
(1,267)	1:3:A:GLN:HE21	1:3:A:GLN:HE22	6	0.3
(1,267)	1:3:A:GLN:HE21	1:3:A:GLN:HE22	7	0.3
(1,267)	1:3:A:GLN:HE21	1:3:A:GLN:HE22	8	0.3
(1,267)	1:3:A:GLN:HE21	1:3:A:GLN:HE22	9	0.3
(1,267)	1:3:A:GLN:HE21	1:3:A:GLN:HE22	10	0.3
(1,266)	1:3:A:GLN:H	1:4:A:ASP:H	6	0.3
(1,266)	1:3:A:GLN:H	1:4:A:ASP:H	8	0.3
(1,262)	1:61:A:GLU:HG2	1:61:A:GLU:HG3	1	0.3
(1,262)	1:61:A:GLU:HG2	1:61:A:GLU:HG3	2	0.3
(1,262)	1:61:A:GLU:HG2	1:61:A:GLU:HG3	3	0.3
(1,262)	1:61:A:GLU:HG2	1:61:A:GLU:HG3	4	0.3
(1,262)	1:61:A:GLU:HG2	1:61:A:GLU:HG3	5	0.3
(1,262)	1:61:A:GLU:HG2	1:61:A:GLU:HG3	6	0.3
(1,262)	1:61:A:GLU:HG2	1:61:A:GLU:HG3	7	0.3
(1,262)	1:61:A:GLU:HG2	1:61:A:GLU:HG3	8	0.3
(1,262)	1:61:A:GLU:HG2	1:61:A:GLU:HG3	9	0.3
(1,262)	1:61:A:GLU:HG2	1:61:A:GLU:HG3	10	0.3
(1,261)	1:61:A:GLU:HG2	1:59:A:THR:HA	7	0.3
(1,237)	1:54:A:GLU:HB2	1:54:A:GLU:HB3	1	0.3
(1,237)	1:54:A:GLU:HB2	1:54:A:GLU:HB3	2	0.3
(1,237)	1:54:A:GLU:HB2	1:54:A:GLU:HB3	3	0.3
(1,237)	1:54:A:GLU:HB2	1:54:A:GLU:HB3	4	0.3
(1,237)	1:54:A:GLU:HB2	1:54:A:GLU:HB3	6	0.3
(1,237)	1:54:A:GLU:HB2	1:54:A:GLU:HB3	7	0.3
(1,237)	1:54:A:GLU:HB2	1:54:A:GLU:HB3	8	0.3
(1,237)	1:54:A:GLU:HB2	1:54:A:GLU:HB3	9	0.3
(1,237)	1:54:A:GLU:HB2	1:54:A:GLU:HB3	10	0.3
(1,230)	1:53:A:CYS:HB3	1:53:A:CYS:HB2	1	0.3
(1,230)	1:53:A:CYS:HB3	1:53:A:CYS:HB2	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:53:A:CYS:HB3	1:53:A:CYS:HB2	3	0.3
(1,230)	1:53:A:CYS:HB3	1:53:A:CYS:HB2	4	0.3
(1,230)	1:53:A:CYS:HB3	1:53:A:CYS:HB2	5	0.3
(1,230)	1:53:A:CYS:HB3	1:53:A:CYS:HB2	6	0.3
(1,230)	1:53:A:CYS:HB3	1:53:A:CYS:HB2	7	0.3
(1,230)	1:53:A:CYS:HB3	1:53:A:CYS:HB2	8	0.3
(1,230)	1:53:A:CYS:HB3	1:53:A:CYS:HB2	9	0.3
(1,230)	1:53:A:CYS:HB3	1:53:A:CYS:HB2	10	0.3
(1,222)	1:51:A:GLU:HG3	1:51:A:GLU:HG2	1	0.3
(1,222)	1:51:A:GLU:HG3	1:51:A:GLU:HG2	2	0.3
(1,222)	1:51:A:GLU:HG3	1:51:A:GLU:HG2	4	0.3
(1,222)	1:51:A:GLU:HG3	1:51:A:GLU:HG2	5	0.3
(1,222)	1:51:A:GLU:HG3	1:51:A:GLU:HG2	6	0.3
(1,222)	1:51:A:GLU:HG3	1:51:A:GLU:HG2	7	0.3
(1,222)	1:51:A:GLU:HG3	1:51:A:GLU:HG2	8	0.3
(1,222)	1:51:A:GLU:HG3	1:51:A:GLU:HG2	9	0.3
(1,222)	1:51:A:GLU:HG3	1:51:A:GLU:HG2	10	0.3
(1,214)	1:50:A:LEU:HD21	1:54:A:GLU:HB2	1	0.3
(1,214)	1:50:A:LEU:HD22	1:54:A:GLU:HB2	1	0.3
(1,214)	1:50:A:LEU:HD23	1:54:A:GLU:HB2	1	0.3
(1,214)	1:50:A:LEU:HD21	1:54:A:GLU:HB2	10	0.3
(1,214)	1:50:A:LEU:HD22	1:54:A:GLU:HB2	10	0.3
(1,214)	1:50:A:LEU:HD23	1:54:A:GLU:HB2	10	0.3
(1,198)	1:47:A:PHE:HB3	1:47:A:PHE:HB2	1	0.3
(1,198)	1:47:A:PHE:HB3	1:47:A:PHE:HB2	2	0.3
(1,198)	1:47:A:PHE:HB3	1:47:A:PHE:HB2	3	0.3
(1,198)	1:47:A:PHE:HB3	1:47:A:PHE:HB2	4	0.3
(1,198)	1:47:A:PHE:HB3	1:47:A:PHE:HB2	5	0.3
(1,198)	1:47:A:PHE:HB3	1:47:A:PHE:HB2	6	0.3
(1,198)	1:47:A:PHE:HB3	1:47:A:PHE:HB2	7	0.3
(1,198)	1:47:A:PHE:HB3	1:47:A:PHE:HB2	8	0.3
(1,198)	1:47:A:PHE:HB3	1:47:A:PHE:HB2	9	0.3
(1,181)	1:37:A:TYR:HB3	1:37:A:TYR:HB2	1	0.3
(1,181)	1:37:A:TYR:HB3	1:37:A:TYR:HB2	2	0.3
(1,181)	1:37:A:TYR:HB3	1:37:A:TYR:HB2	3	0.3
(1,181)	1:37:A:TYR:HB3	1:37:A:TYR:HB2	5	0.3
(1,181)	1:37:A:TYR:HB3	1:37:A:TYR:HB2	9	0.3
(1,181)	1:37:A:TYR:HB3	1:37:A:TYR:HB2	10	0.3
(1,169)	1:35:A:PHE:HE1	1:37:A:TYR:HA	3	0.3
(1,165)	1:35:A:PHE:HD1	1:34:A:THR:HB	10	0.3
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG21	3	0.3
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG22	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG23	3	0.3
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG21	6	0.3
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG22	6	0.3
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG23	6	0.3
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG21	7	0.3
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG22	7	0.3
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG23	7	0.3
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG21	8	0.3
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG22	8	0.3
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG23	8	0.3
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG21	10	0.3
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG22	10	0.3
(1,157)	1:34:A:THR:HB	1:34:A:THR:HG23	10	0.3
(1,151)	1:34:A:THR:HA	1:23:A:TYR:HA	9	0.3
(1,140)	1:32:A:CYS:HB3	1:32:A:CYS:HB2	1	0.3
(1,140)	1:32:A:CYS:HB3	1:32:A:CYS:HB2	4	0.3
(1,140)	1:32:A:CYS:HB3	1:32:A:CYS:HB2	6	0.3
(1,130)	1:30:A:SER:HB3	1:30:A:SER:HB2	1	0.3
(1,130)	1:30:A:SER:HB3	1:30:A:SER:HB2	3	0.3
(1,130)	1:30:A:SER:HB3	1:30:A:SER:HB2	4	0.3
(1,130)	1:30:A:SER:HB3	1:30:A:SER:HB2	5	0.3
(1,130)	1:30:A:SER:HB3	1:30:A:SER:HB2	6	0.3
(1,130)	1:30:A:SER:HB3	1:30:A:SER:HB2	9	0.3
(1,130)	1:30:A:SER:HB3	1:30:A:SER:HB2	10	0.3
(1,88)	1:23:A:TYR:HE1	1:49:A:THR:HA	6	0.3
(1,73)	1:20:A:PHE:HA	1:20:A:PHE:HB2	9	0.3
(1,64)	1:19:A:SER:HA	1:19:A:SER:HB3	4	0.3
(1,55)	1:15:A:LYS:HA	1:15:A:LYS:HB3	3	0.3
(1,55)	1:15:A:LYS:HA	1:15:A:LYS:HB3	7	0.3
(1,55)	1:15:A:LYS:HA	1:15:A:LYS:HB3	9	0.3
(1,18)	1:7:A:CYS:HA	1:57:A:CYS:HB2	6	0.3
(1,1)	1:1:A:PRO:HB3	1:1:A:PRO:HD2	4	0.3
(1,495)	1:52:A:ASP:H	1:52:A:ASP:HB3	3	0.29
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD11	9	0.29
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD12	9	0.29
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD13	9	0.29
(1,464)	1:48:A:LYS:H	1:48:A:LYS:HD2	9	0.29
(1,444)	1:39:A:GLY:H	1:40:A:SER:H	8	0.29
(1,429)	1:35:A:PHE:H	1:35:A:PHE:HD1	3	0.29
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG21	6	0.29
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG22	6	0.29
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG23	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG21	7	0.29
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG22	7	0.29
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG23	7	0.29
(1,426)	1:35:A:PHE:H	1:34:A:THR:HB	8	0.29
(1,426)	1:35:A:PHE:H	1:34:A:THR:HB	9	0.29
(1,356)	1:20:A:PHE:H	1:19:A:SER:HB2	3	0.29
(1,356)	1:20:A:PHE:H	1:19:A:SER:HB2	5	0.29
(1,356)	1:20:A:PHE:H	1:19:A:SER:HB2	9	0.29
(1,353)	1:19:A:SER:H	1:19:A:SER:HA	10	0.29
(1,345)	1:17:A:SER:H	1:38:A:ARG:HA	7	0.29
(1,345)	1:17:A:SER:H	1:38:A:ARG:HA	8	0.29
(1,333)	1:15:A:LYS:H	1:16:A:GLY:H	9	0.29
(1,322)	1:13:A:TYR:H	1:13:A:TYR:HB2	8	0.29
(1,316)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	3	0.29
(1,314)	1:12:A:ASN:HD21	1:12:A:ASN:HB3	2	0.29
(1,310)	1:12:A:ASN:H	1:11:A:ARG:HG3	8	0.29
(1,308)	1:12:A:ASN:H	1:11:A:ARG:HA	3	0.29
(1,292)	1:9:A:LEU:H	1:8:A:GLN:H	6	0.29
(1,289)	1:8:A:GLN:HE21	1:8:A:GLN:HE22	1	0.29
(1,285)	1:7:A:CYS:H	1:7:A:CYS:HB2	8	0.29
(1,271)	1:4:A:ASP:H	1:4:A:ASP:HB3	4	0.29
(1,267)	1:3:A:GLN:HE21	1:3:A:GLN:HE22	1	0.29
(1,267)	1:3:A:GLN:HE21	1:3:A:GLN:HE22	2	0.29
(1,267)	1:3:A:GLN:HE21	1:3:A:GLN:HE22	3	0.29
(1,259)	1:61:A:GLU:HA	1:61:A:GLU:HG2	3	0.29
(1,244)	1:55:A:ALA:HB1	1:56:A:THR:HB	7	0.29
(1,244)	1:55:A:ALA:HB2	1:56:A:THR:HB	7	0.29
(1,244)	1:55:A:ALA:HB3	1:56:A:THR:HB	7	0.29
(1,243)	1:55:A:ALA:HB1	1:55:A:ALA:H	2	0.29
(1,243)	1:55:A:ALA:HB2	1:55:A:ALA:H	2	0.29
(1,243)	1:55:A:ALA:HB3	1:55:A:ALA:H	2	0.29
(1,243)	1:55:A:ALA:HB1	1:55:A:ALA:H	10	0.29
(1,243)	1:55:A:ALA:HB2	1:55:A:ALA:H	10	0.29
(1,243)	1:55:A:ALA:HB3	1:55:A:ALA:H	10	0.29
(1,237)	1:54:A:GLU:HB2	1:54:A:GLU:HB3	5	0.29
(1,222)	1:51:A:GLU:HG3	1:51:A:GLU:HG2	3	0.29
(1,214)	1:50:A:LEU:HD21	1:54:A:GLU:HB2	6	0.29
(1,214)	1:50:A:LEU:HD22	1:54:A:GLU:HB2	6	0.29
(1,214)	1:50:A:LEU:HD23	1:54:A:GLU:HB2	6	0.29
(1,181)	1:37:A:TYR:HB3	1:37:A:TYR:HB2	4	0.29
(1,181)	1:37:A:TYR:HB3	1:37:A:TYR:HB2	6	0.29
(1,181)	1:37:A:TYR:HB3	1:37:A:TYR:HB2	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,181)	1:37:A:TYR:HB3	1:37:A:TYR:HB2	8	0.29
(1,177)	1:36:A:ARG:HG2	1:35:A:PHE:HA	10	0.29
(1,151)	1:34:A:THR:HA	1:23:A:TYR:HA	8	0.29
(1,150)	1:33:A:LYS:HG2	1:33:A:LYS:HA	10	0.29
(1,140)	1:32:A:CYS:HB3	1:32:A:CYS:HB2	2	0.29
(1,140)	1:32:A:CYS:HB3	1:32:A:CYS:HB2	3	0.29
(1,140)	1:32:A:CYS:HB3	1:32:A:CYS:HB2	5	0.29
(1,140)	1:32:A:CYS:HB3	1:32:A:CYS:HB2	7	0.29
(1,140)	1:32:A:CYS:HB3	1:32:A:CYS:HB2	8	0.29
(1,140)	1:32:A:CYS:HB3	1:32:A:CYS:HB2	9	0.29
(1,140)	1:32:A:CYS:HB3	1:32:A:CYS:HB2	10	0.29
(1,130)	1:30:A:SER:HB3	1:30:A:SER:HB2	2	0.29
(1,130)	1:30:A:SER:HB3	1:30:A:SER:HB2	7	0.29
(1,130)	1:30:A:SER:HB3	1:30:A:SER:HB2	8	0.29
(1,64)	1:19:A:SER:HA	1:19:A:SER:HB3	9	0.29
(1,57)	1:15:A:LYS:HA	1:15:A:LYS:HG2	7	0.29
(1,55)	1:15:A:LYS:HA	1:15:A:LYS:HB3	5	0.29
(1,49)	1:12:A:ASN:HA	1:12:A:ASN:HB2	2	0.29
(1,49)	1:12:A:ASN:HA	1:12:A:ASN:HB2	8	0.29
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD11	3	0.29
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD12	3	0.29
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD13	3	0.29
(1,543)	1:61:A:GLU:H	1:61:A:GLU:HG2	4	0.28
(1,543)	1:61:A:GLU:H	1:61:A:GLU:HG2	7	0.28
(1,511)	1:55:A:ALA:H	1:54:A:GLU:HG3	5	0.28
(1,496)	1:52:A:ASP:H	1:52:A:ASP:HB2	5	0.28
(1,490)	1:52:A:ASP:H	1:49:A:THR:HB	6	0.28
(1,487)	1:51:A:GLU:H	1:51:A:GLU:HG3	5	0.28
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD11	6	0.28
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD12	6	0.28
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD13	6	0.28
(1,463)	1:48:A:LYS:H	1:48:A:LYS:HD3	1	0.28
(1,458)	1:47:A:PHE:H	1:46:A:ARG:HG3	3	0.28
(1,458)	1:47:A:PHE:H	1:46:A:ARG:HG3	10	0.28
(1,454)	1:43:A:ASN:H	1:12:A:ASN:HB3	5	0.28
(1,442)	1:38:A:ARG:H	1:38:A:ARG:HB2	8	0.28
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG21	5	0.28
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG22	5	0.28
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG23	5	0.28
(1,389)	1:27:A:LYS:H	1:27:A:LYS:HB2	6	0.28
(1,383)	1:26:A:ASP:H	1:26:A:ASP:HB3	2	0.28
(1,353)	1:19:A:SER:H	1:19:A:SER:HA	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,351)	1:19:A:SER:H	1:18:A:GLY:HA3	7	0.28
(1,347)	1:18:A:GLY:H	1:17:A:SER:HB2	7	0.28
(1,344)	1:17:A:SER:H	1:18:A:GLY:H	8	0.28
(1,344)	1:17:A:SER:H	1:18:A:GLY:H	10	0.28
(1,343)	1:17:A:SER:H	1:17:A:SER:HB3	3	0.28
(1,332)	1:15:A:LYS:H	1:15:A:LYS:HG2	5	0.28
(1,332)	1:15:A:LYS:H	1:15:A:LYS:HG2	6	0.28
(1,325)	1:14:A:GLY:H	1:13:A:TYR:HB3	2	0.28
(1,314)	1:12:A:ASN:HD21	1:12:A:ASN:HB3	1	0.28
(1,314)	1:12:A:ASN:HD21	1:12:A:ASN:HB3	6	0.28
(1,314)	1:12:A:ASN:HD21	1:12:A:ASN:HB3	8	0.28
(1,314)	1:12:A:ASN:HD21	1:12:A:ASN:HB3	9	0.28
(1,312)	1:12:A:ASN:H	1:12:A:ASN:HB3	5	0.28
(1,310)	1:12:A:ASN:H	1:11:A:ARG:HG3	6	0.28
(1,308)	1:12:A:ASN:H	1:11:A:ARG:HA	4	0.28
(1,281)	1:7:A:CYS:H	1:6:A:ARG:HG3	2	0.28
(1,264)	1:3:A:GLN:H	1:3:A:GLN:HB2	10	0.28
(1,261)	1:61:A:GLU:HG2	1:59:A:THR:HA	2	0.28
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG21	1	0.28
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG22	1	0.28
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG23	1	0.28
(1,245)	1:56:A:THR:HG21	1:53:A:CYS:HA	10	0.28
(1,245)	1:56:A:THR:HG22	1:53:A:CYS:HA	10	0.28
(1,245)	1:56:A:THR:HG23	1:53:A:CYS:HA	10	0.28
(1,243)	1:55:A:ALA:HB1	1:55:A:ALA:H	1	0.28
(1,243)	1:55:A:ALA:HB2	1:55:A:ALA:H	1	0.28
(1,243)	1:55:A:ALA:HB3	1:55:A:ALA:H	1	0.28
(1,243)	1:55:A:ALA:HB1	1:55:A:ALA:H	5	0.28
(1,243)	1:55:A:ALA:HB2	1:55:A:ALA:H	5	0.28
(1,243)	1:55:A:ALA:HB3	1:55:A:ALA:H	5	0.28
(1,243)	1:55:A:ALA:HB1	1:55:A:ALA:H	6	0.28
(1,243)	1:55:A:ALA:HB2	1:55:A:ALA:H	6	0.28
(1,243)	1:55:A:ALA:HB3	1:55:A:ALA:H	6	0.28
(1,238)	1:54:A:GLU:HB2	1:55:A:ALA:H	7	0.28
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD21	2	0.28
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD22	2	0.28
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD23	2	0.28
(1,227)	1:53:A:CYS:HB3	1:32:A:CYS:HB2	5	0.28
(1,227)	1:53:A:CYS:HB3	1:32:A:CYS:HB2	9	0.28
(1,208)	1:48:A:LYS:HD3	1:48:A:LYS:HA	8	0.28
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG21	7	0.28
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG22	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG23	7	0.28
(1,199)	1:47:A:PHE:HB3	1:53:A:CYS:HA	6	0.28
(1,194)	1:47:A:PHE:HA	1:46:A:ARG:HG2	9	0.28
(1,169)	1:35:A:PHE:HE1	1:37:A:TYR:HA	8	0.28
(1,151)	1:34:A:THR:HA	1:23:A:TYR:HA	4	0.28
(1,146)	1:33:A:LYS:HA	1:33:A:LYS:HG3	3	0.28
(1,125)	1:27:A:LYS:HB3	1:27:A:LYS:HG3	6	0.28
(1,55)	1:15:A:LYS:HA	1:15:A:LYS:HB3	2	0.28
(1,49)	1:12:A:ASN:HA	1:12:A:ASN:HB2	1	0.28
(1,540)	1:61:A:GLU:H	1:61:A:GLU:HA	5	0.27
(1,526)	1:58:A:VAL:H	1:54:A:GLU:HA	2	0.27
(1,526)	1:58:A:VAL:H	1:54:A:GLU:HA	9	0.27
(1,511)	1:55:A:ALA:H	1:54:A:GLU:HG3	2	0.27
(1,499)	1:53:A:CYS:H	1:50:A:LEU:HA	6	0.27
(1,481)	1:51:A:GLU:H	1:50:A:LEU:H	6	0.27
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD11	4	0.27
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD12	4	0.27
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD13	4	0.27
(1,475)	1:50:A:LEU:H	1:49:A:THR:HB	6	0.27
(1,458)	1:47:A:PHE:H	1:46:A:ARG:HG3	2	0.27
(1,444)	1:39:A:GLY:H	1:40:A:SER:H	7	0.27
(1,439)	1:38:A:ARG:H	1:37:A:TYR:HA	7	0.27
(1,438)	1:38:A:ARG:H	1:36:A:ARG:HB2	3	0.27
(1,420)	1:34:A:THR:H	1:33:A:LYS:HD3	6	0.27
(1,420)	1:34:A:THR:H	1:33:A:LYS:HD3	8	0.27
(1,394)	1:28:A:ALA:H	1:29:A:THR:H	6	0.27
(1,394)	1:28:A:ALA:H	1:29:A:THR:H	9	0.27
(1,358)	1:20:A:PHE:H	1:20:A:PHE:HB3	6	0.27
(1,354)	1:19:A:SER:H	1:19:A:SER:HB3	9	0.27
(1,351)	1:19:A:SER:H	1:18:A:GLY:HA3	8	0.27
(1,327)	1:14:A:GLY:H	1:14:A:GLY:HA3	1	0.27
(1,326)	1:14:A:GLY:H	1:13:A:TYR:HB2	6	0.27
(1,322)	1:13:A:TYR:H	1:13:A:TYR:HB2	9	0.27
(1,321)	1:13:A:TYR:H	1:13:A:TYR:HB3	9	0.27
(1,311)	1:12:A:ASN:H	1:11:A:ARG:HG2	9	0.27
(1,281)	1:7:A:CYS:H	1:6:A:ARG:HG3	3	0.27
(1,281)	1:7:A:CYS:H	1:6:A:ARG:HG3	4	0.27
(1,261)	1:61:A:GLU:HG2	1:59:A:THR:HA	6	0.27
(1,243)	1:55:A:ALA:HB1	1:55:A:ALA:H	4	0.27
(1,243)	1:55:A:ALA:HB2	1:55:A:ALA:H	4	0.27
(1,243)	1:55:A:ALA:HB3	1:55:A:ALA:H	4	0.27
(1,243)	1:55:A:ALA:HB1	1:55:A:ALA:H	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,243)	1:55:A:ALA:HB2	1:55:A:ALA:H	7	0.27
(1,243)	1:55:A:ALA:HB3	1:55:A:ALA:H	7	0.27
(1,243)	1:55:A:ALA:HB1	1:55:A:ALA:H	8	0.27
(1,243)	1:55:A:ALA:HB2	1:55:A:ALA:H	8	0.27
(1,243)	1:55:A:ALA:HB3	1:55:A:ALA:H	8	0.27
(1,227)	1:53:A:CYS:HB3	1:32:A:CYS:HB2	2	0.27
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD21	5	0.27
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD22	5	0.27
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD23	5	0.27
(1,214)	1:50:A:LEU:HD21	1:54:A:GLU:HB2	3	0.27
(1,214)	1:50:A:LEU:HD22	1:54:A:GLU:HB2	3	0.27
(1,214)	1:50:A:LEU:HD23	1:54:A:GLU:HB2	3	0.27
(1,213)	1:50:A:LEU:HD11	1:51:A:GLU:HG2	8	0.27
(1,213)	1:50:A:LEU:HD12	1:51:A:GLU:HG2	8	0.27
(1,213)	1:50:A:LEU:HD13	1:51:A:GLU:HG2	8	0.27
(1,204)	1:48:A:LYS:HA	1:48:A:LYS:HD2	1	0.27
(1,188)	1:40:A:SER:HA	1:41:A:GLY:HA2	8	0.27
(1,187)	1:40:A:SER:HA	1:41:A:GLY:HA3	8	0.27
(1,185)	1:37:A:TYR:HB2	1:46:A:ARG:HG3	8	0.27
(1,183)	1:37:A:TYR:HB2	1:22:A:ASN:HB2	10	0.27
(1,164)	1:35:A:PHE:HD1	1:34:A:THR:HA	1	0.27
(1,150)	1:33:A:LYS:HG2	1:33:A:LYS:HA	9	0.27
(1,145)	1:33:A:LYS:HA	1:33:A:LYS:HE3	5	0.27
(1,125)	1:27:A:LYS:HB3	1:27:A:LYS:HG3	1	0.27
(1,125)	1:27:A:LYS:HB3	1:27:A:LYS:HG3	4	0.27
(1,125)	1:27:A:LYS:HB3	1:27:A:LYS:HG3	7	0.27
(1,125)	1:27:A:LYS:HB3	1:27:A:LYS:HG3	9	0.27
(1,102)	1:24:A:TYR:HD1	1:24:A:TYR:HA	7	0.27
(1,30)	1:11:A:ARG:HA	1:10:A:SER:HA	8	0.27
(1,9)	1:4:A:ASP:HB2	1:4:A:ASP:HB3	2	0.27
(1,9)	1:4:A:ASP:HB2	1:4:A:ASP:HB3	3	0.27
(1,542)	1:61:A:GLU:H	1:61:A:GLU:HG3	9	0.26
(1,526)	1:58:A:VAL:H	1:54:A:GLU:HA	4	0.26
(1,506)	1:54:A:GLU:H	1:53:A:CYS:HB3	8	0.26
(1,495)	1:52:A:ASP:H	1:52:A:ASP:HB3	4	0.26
(1,490)	1:52:A:ASP:H	1:49:A:THR:HB	9	0.26
(1,488)	1:51:A:GLU:H	1:51:A:GLU:HG2	1	0.26
(1,487)	1:51:A:GLU:H	1:51:A:GLU:HG3	10	0.26
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD11	6	0.26
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD12	6	0.26
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD13	6	0.26
(1,465)	1:48:A:LYS:H	1:49:A:THR:H	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,465)	1:48:A:LYS:H	1:49:A:THR:H	7	0.26
(1,454)	1:43:A:ASN:H	1:12:A:ASN:HB3	8	0.26
(1,453)	1:42:A:GLY:H	1:41:A:GLY:HA2	8	0.26
(1,446)	1:40:A:SER:H	1:40:A:SER:HB3	6	0.26
(1,441)	1:38:A:ARG:H	1:38:A:ARG:HA	4	0.26
(1,426)	1:35:A:PHE:H	1:34:A:THR:HB	3	0.26
(1,424)	1:35:A:PHE:H	1:22:A:ASN:H	4	0.26
(1,347)	1:18:A:GLY:H	1:17:A:SER:HB2	1	0.26
(1,347)	1:18:A:GLY:H	1:17:A:SER:HB2	9	0.26
(1,333)	1:15:A:LYS:H	1:16:A:GLY:H	7	0.26
(1,332)	1:15:A:LYS:H	1:15:A:LYS:HG2	1	0.26
(1,327)	1:14:A:GLY:H	1:14:A:GLY:HA3	7	0.26
(1,326)	1:14:A:GLY:H	1:13:A:TYR:HB2	8	0.26
(1,326)	1:14:A:GLY:H	1:13:A:TYR:HB2	9	0.26
(1,314)	1:12:A:ASN:HD21	1:12:A:ASN:HB3	3	0.26
(1,314)	1:12:A:ASN:HD21	1:12:A:ASN:HB3	4	0.26
(1,314)	1:12:A:ASN:HD21	1:12:A:ASN:HB3	7	0.26
(1,313)	1:12:A:ASN:H	1:12:A:ASN:HB2	7	0.26
(1,310)	1:12:A:ASN:H	1:11:A:ARG:HG3	3	0.26
(1,308)	1:12:A:ASN:H	1:11:A:ARG:HA	1	0.26
(1,308)	1:12:A:ASN:H	1:11:A:ARG:HA	10	0.26
(1,307)	1:11:A:ARG:H	1:11:A:ARG:HG2	10	0.26
(1,306)	1:11:A:ARG:H	1:11:A:ARG:HB3	3	0.26
(1,271)	1:4:A:ASP:H	1:4:A:ASP:HB3	10	0.26
(1,243)	1:55:A:ALA:HB1	1:55:A:ALA:H	3	0.26
(1,243)	1:55:A:ALA:HB2	1:55:A:ALA:H	3	0.26
(1,243)	1:55:A:ALA:HB3	1:55:A:ALA:H	3	0.26
(1,243)	1:55:A:ALA:HB1	1:55:A:ALA:H	9	0.26
(1,243)	1:55:A:ALA:HB2	1:55:A:ALA:H	9	0.26
(1,243)	1:55:A:ALA:HB3	1:55:A:ALA:H	9	0.26
(1,234)	1:54:A:GLU:HA	1:58:A:VAL:HB	5	0.26
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD21	5	0.26
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD22	5	0.26
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD23	5	0.26
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD21	2	0.26
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD22	2	0.26
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD23	2	0.26
(1,208)	1:48:A:LYS:HD3	1:48:A:LYS:HA	1	0.26
(1,204)	1:48:A:LYS:HA	1:48:A:LYS:HD2	8	0.26
(1,186)	1:38:A:ARG:HD3	1:38:A:ARG:HG3	3	0.26
(1,186)	1:38:A:ARG:HD3	1:38:A:ARG:HG3	8	0.26
(1,186)	1:38:A:ARG:HD3	1:38:A:ARG:HG3	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,164)	1:35:A:PHE:HD1	1:34:A:THR:HA	2	0.26
(1,143)	1:33:A:LYS:HA	1:33:A:LYS:HB3	3	0.26
(1,125)	1:27:A:LYS:HB3	1:27:A:LYS:HG3	2	0.26
(1,94)	1:24:A:TYR:HB3	1:11:A:ARG:HB3	1	0.26
(1,94)	1:24:A:TYR:HB3	1:11:A:ARG:HB3	9	0.26
(1,49)	1:12:A:ASN:HA	1:12:A:ASN:HB2	7	0.26
(1,21)	1:8:A:GLN:HA	1:8:A:GLN:HB3	3	0.26
(1,9)	1:4:A:ASP:HB2	1:4:A:ASP:HB3	1	0.26
(1,9)	1:4:A:ASP:HB2	1:4:A:ASP:HB3	4	0.26
(1,9)	1:4:A:ASP:HB2	1:4:A:ASP:HB3	5	0.26
(1,9)	1:4:A:ASP:HB2	1:4:A:ASP:HB3	6	0.26
(1,9)	1:4:A:ASP:HB2	1:4:A:ASP:HB3	7	0.26
(1,9)	1:4:A:ASP:HB2	1:4:A:ASP:HB3	8	0.26
(1,9)	1:4:A:ASP:HB2	1:4:A:ASP:HB3	9	0.26
(1,9)	1:4:A:ASP:HB2	1:4:A:ASP:HB3	10	0.26
(2,29)	1:59:A:THR:H	1:55:A:ALA:O	1	0.25
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG11	3	0.25
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG12	3	0.25
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG13	3	0.25
(1,504)	1:54:A:GLU:H	1:50:A:LEU:HD21	8	0.25
(1,504)	1:54:A:GLU:H	1:50:A:LEU:HD22	8	0.25
(1,504)	1:54:A:GLU:H	1:50:A:LEU:HD23	8	0.25
(1,490)	1:52:A:ASP:H	1:49:A:THR:HB	10	0.25
(1,488)	1:51:A:GLU:H	1:51:A:GLU:HG2	5	0.25
(1,475)	1:50:A:LEU:H	1:49:A:THR:HB	4	0.25
(1,474)	1:50:A:LEU:H	1:49:A:THR:HA	5	0.25
(1,474)	1:50:A:LEU:H	1:49:A:THR:HA	7	0.25
(1,472)	1:49:A:THR:H	1:52:A:ASP:HB3	6	0.25
(1,466)	1:49:A:THR:H	1:47:A:PHE:HB3	1	0.25
(1,454)	1:43:A:ASN:H	1:12:A:ASN:HB3	3	0.25
(1,454)	1:43:A:ASN:H	1:12:A:ASN:HB3	7	0.25
(1,444)	1:39:A:GLY:H	1:40:A:SER:H	5	0.25
(1,444)	1:39:A:GLY:H	1:40:A:SER:H	9	0.25
(1,442)	1:38:A:ARG:H	1:38:A:ARG:HB2	3	0.25
(1,442)	1:38:A:ARG:H	1:38:A:ARG:HB2	7	0.25
(1,438)	1:38:A:ARG:H	1:36:A:ARG:HB2	4	0.25
(1,434)	1:36:A:ARG:H	1:36:A:ARG:HG2	5	0.25
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG21	9	0.25
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG22	9	0.25
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG23	9	0.25
(1,423)	1:35:A:PHE:H	1:21:A:THR:HG21	7	0.25
(1,423)	1:35:A:PHE:H	1:21:A:THR:HG22	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,423)	1:35:A:PHE:H	1:21:A:THR:HG23	7	0.25
(1,420)	1:34:A:THR:H	1:33:A:LYS:HD3	1	0.25
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB1	3	0.25
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB2	3	0.25
(1,399)	1:29:A:THR:H	1:28:A:ALA:HB3	3	0.25
(1,394)	1:28:A:ALA:H	1:29:A:THR:H	1	0.25
(1,363)	1:21:A:THR:H	1:21:A:THR:HA	6	0.25
(1,354)	1:19:A:SER:H	1:19:A:SER:HB3	7	0.25
(1,347)	1:18:A:GLY:H	1:17:A:SER:HB2	3	0.25
(1,345)	1:17:A:SER:H	1:38:A:ARG:HA	9	0.25
(1,335)	1:16:A:GLY:H	1:15:A:LYS:HB3	1	0.25
(1,330)	1:15:A:LYS:H	1:15:A:LYS:HB2	6	0.25
(1,327)	1:14:A:GLY:H	1:14:A:GLY:HA3	2	0.25
(1,327)	1:14:A:GLY:H	1:14:A:GLY:HA3	4	0.25
(1,321)	1:13:A:TYR:H	1:13:A:TYR:HB3	3	0.25
(1,311)	1:12:A:ASN:H	1:11:A:ARG:HG2	5	0.25
(1,303)	1:11:A:ARG:H	1:10:A:SER:HA	3	0.25
(1,302)	1:10:A:SER:H	1:10:A:SER:HB3	7	0.25
(1,285)	1:7:A:CYS:H	1:7:A:CYS:HB2	1	0.25
(1,266)	1:3:A:GLN:H	1:4:A:ASP:H	3	0.25
(1,259)	1:61:A:GLU:HA	1:61:A:GLU:HG2	1	0.25
(1,259)	1:61:A:GLU:HA	1:61:A:GLU:HG2	4	0.25
(1,248)	1:57:A:CYS:HA	1:7:A:CYS:HA	3	0.25
(1,238)	1:54:A:GLU:HB2	1:55:A:ALA:H	9	0.25
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD21	9	0.25
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD22	9	0.25
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD23	9	0.25
(1,214)	1:50:A:LEU:HD21	1:54:A:GLU:HB2	8	0.25
(1,214)	1:50:A:LEU:HD22	1:54:A:GLU:HB2	8	0.25
(1,214)	1:50:A:LEU:HD23	1:54:A:GLU:HB2	8	0.25
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG21	8	0.25
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG22	8	0.25
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG23	8	0.25
(1,172)	1:36:A:ARG:HA	1:21:A:THR:HA	9	0.25
(1,169)	1:35:A:PHE:HE1	1:37:A:TYR:HA	5	0.25
(1,165)	1:35:A:PHE:HD1	1:34:A:THR:HB	1	0.25
(1,165)	1:35:A:PHE:HD1	1:34:A:THR:HB	7	0.25
(1,165)	1:35:A:PHE:HD1	1:34:A:THR:HB	8	0.25
(1,151)	1:34:A:THR:HA	1:23:A:TYR:HA	5	0.25
(1,150)	1:33:A:LYS:HG2	1:33:A:LYS:HA	4	0.25
(1,94)	1:24:A:TYR:HB3	1:11:A:ARG:HB3	10	0.25
(1,55)	1:15:A:LYS:HA	1:15:A:LYS:HB3	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:10:A:SER:HB3	1:10:A:SER:HB2	1	0.25
(1,29)	1:10:A:SER:HB3	1:10:A:SER:HB2	2	0.25
(1,29)	1:10:A:SER:HB3	1:10:A:SER:HB2	3	0.25
(1,29)	1:10:A:SER:HB3	1:10:A:SER:HB2	4	0.25
(1,29)	1:10:A:SER:HB3	1:10:A:SER:HB2	5	0.25
(1,29)	1:10:A:SER:HB3	1:10:A:SER:HB2	6	0.25
(1,29)	1:10:A:SER:HB3	1:10:A:SER:HB2	7	0.25
(1,29)	1:10:A:SER:HB3	1:10:A:SER:HB2	8	0.25
(1,29)	1:10:A:SER:HB3	1:10:A:SER:HB2	9	0.25
(1,29)	1:10:A:SER:HB3	1:10:A:SER:HB2	10	0.25
(1,21)	1:8:A:GLN:HA	1:8:A:GLN:HB3	1	0.25
(1,21)	1:8:A:GLN:HA	1:8:A:GLN:HB3	4	0.25
(1,21)	1:8:A:GLN:HA	1:8:A:GLN:HB3	5	0.25
(1,526)	1:58:A:VAL:H	1:54:A:GLU:HA	3	0.24
(1,511)	1:55:A:ALA:H	1:54:A:GLU:HG3	3	0.24
(1,503)	1:53:A:CYS:H	1:53:A:CYS:HB2	6	0.24
(1,498)	1:53:A:CYS:H	1:47:A:PHE:HB3	6	0.24
(1,492)	1:52:A:ASP:H	1:51:A:GLU:HG3	5	0.24
(1,481)	1:51:A:GLU:H	1:50:A:LEU:H	1	0.24
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD11	2	0.24
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD12	2	0.24
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD13	2	0.24
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD11	5	0.24
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD12	5	0.24
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD13	5	0.24
(1,474)	1:50:A:LEU:H	1:49:A:THR:HA	3	0.24
(1,458)	1:47:A:PHE:H	1:46:A:ARG:HG3	8	0.24
(1,455)	1:43:A:ASN:H	1:12:A:ASN:HB2	2	0.24
(1,451)	1:41:A:GLY:H	1:41:A:GLY:HA2	3	0.24
(1,438)	1:38:A:ARG:H	1:36:A:ARG:HB2	1	0.24
(1,434)	1:36:A:ARG:H	1:36:A:ARG:HG2	2	0.24
(1,423)	1:35:A:PHE:H	1:21:A:THR:HG21	4	0.24
(1,423)	1:35:A:PHE:H	1:21:A:THR:HG22	4	0.24
(1,423)	1:35:A:PHE:H	1:21:A:THR:HG23	4	0.24
(1,402)	1:30:A:SER:H	1:27:A:LYS:HA	8	0.24
(1,401)	1:29:A:THR:H	1:29:A:THR:HG21	7	0.24
(1,401)	1:29:A:THR:H	1:29:A:THR:HG22	7	0.24
(1,401)	1:29:A:THR:H	1:29:A:THR:HG23	7	0.24
(1,389)	1:27:A:LYS:H	1:27:A:LYS:HB2	8	0.24
(1,376)	1:24:A:TYR:H	1:34:A:THR:HA	5	0.24
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG21	3	0.24
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG22	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG23	3	0.24
(1,363)	1:21:A:THR:H	1:21:A:THR:HA	1	0.24
(1,363)	1:21:A:THR:H	1:21:A:THR:HA	9	0.24
(1,353)	1:19:A:SER:H	1:19:A:SER:HA	6	0.24
(1,345)	1:17:A:SER:H	1:38:A:ARG:HA	10	0.24
(1,338)	1:16:A:GLY:H	1:16:A:GLY:HA2	9	0.24
(1,335)	1:16:A:GLY:H	1:15:A:LYS:HB3	8	0.24
(1,330)	1:15:A:LYS:H	1:15:A:LYS:HB2	8	0.24
(1,321)	1:13:A:TYR:H	1:13:A:TYR:HB3	1	0.24
(1,321)	1:13:A:TYR:H	1:13:A:TYR:HB3	6	0.24
(1,321)	1:13:A:TYR:H	1:13:A:TYR:HB3	8	0.24
(1,312)	1:12:A:ASN:H	1:12:A:ASN:HB3	4	0.24
(1,291)	1:9:A:LEU:H	1:5:A:TYR:HB3	7	0.24
(1,291)	1:9:A:LEU:H	1:5:A:TYR:HB3	8	0.24
(1,273)	1:5:A:TYR:H	1:4:A:ASP:HB2	1	0.24
(1,273)	1:5:A:TYR:H	1:4:A:ASP:HB2	4	0.24
(1,272)	1:4:A:ASP:H	1:4:A:ASP:HB2	3	0.24
(1,266)	1:3:A:GLN:H	1:4:A:ASP:H	2	0.24
(1,259)	1:61:A:GLU:HA	1:61:A:GLU:HG2	9	0.24
(1,248)	1:57:A:CYS:HA	1:7:A:CYS:HA	10	0.24
(1,245)	1:56:A:THR:HG21	1:53:A:CYS:HA	7	0.24
(1,245)	1:56:A:THR:HG22	1:53:A:CYS:HA	7	0.24
(1,245)	1:56:A:THR:HG23	1:53:A:CYS:HA	7	0.24
(1,238)	1:54:A:GLU:HB2	1:55:A:ALA:H	3	0.24
(1,238)	1:54:A:GLU:HB2	1:55:A:ALA:H	8	0.24
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD21	4	0.24
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD22	4	0.24
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD23	4	0.24
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD21	3	0.24
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD22	3	0.24
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD23	3	0.24
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD21	4	0.24
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD22	4	0.24
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD23	4	0.24
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD21	1	0.24
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD22	1	0.24
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD23	1	0.24
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD21	4	0.24
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD22	4	0.24
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD23	4	0.24
(1,208)	1:48:A:LYS:HD3	1:48:A:LYS:HA	4	0.24
(1,187)	1:40:A:SER:HA	1:41:A:GLY:HA3	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,186)	1:38:A:ARG:HD3	1:38:A:ARG:HG3	2	0.24
(1,169)	1:35:A:PHE:HE1	1:37:A:TYR:HA	10	0.24
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG21	4	0.24
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG22	4	0.24
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG23	4	0.24
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG21	6	0.24
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG22	6	0.24
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG23	6	0.24
(1,165)	1:35:A:PHE:HD1	1:34:A:THR:HB	2	0.24
(1,164)	1:35:A:PHE:HD1	1:34:A:THR:HA	9	0.24
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG21	10	0.24
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG22	10	0.24
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG23	10	0.24
(1,148)	1:33:A:LYS:HE3	1:33:A:LYS:HD2	4	0.24
(1,125)	1:27:A:LYS:HB3	1:27:A:LYS:HG3	5	0.24
(1,125)	1:27:A:LYS:HB3	1:27:A:LYS:HG3	8	0.24
(1,49)	1:12:A:ASN:HA	1:12:A:ASN:HB2	3	0.24
(1,49)	1:12:A:ASN:HA	1:12:A:ASN:HB2	6	0.24
(1,49)	1:12:A:ASN:HA	1:12:A:ASN:HB2	10	0.24
(1,23)	1:9:A:LEU:HA	1:5:A:TYR:HB3	5	0.24
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG11	4	0.23
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG12	4	0.23
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG13	4	0.23
(1,513)	1:55:A:ALA:H	1:56:A:THR:H	7	0.23
(1,511)	1:55:A:ALA:H	1:54:A:GLU:HG3	4	0.23
(1,511)	1:55:A:ALA:H	1:54:A:GLU:HG3	9	0.23
(1,506)	1:54:A:GLU:H	1:53:A:CYS:HB3	7	0.23
(1,504)	1:54:A:GLU:H	1:50:A:LEU:HD21	7	0.23
(1,504)	1:54:A:GLU:H	1:50:A:LEU:HD22	7	0.23
(1,504)	1:54:A:GLU:H	1:50:A:LEU:HD23	7	0.23
(1,501)	1:53:A:CYS:H	1:52:A:ASP:HB2	5	0.23
(1,495)	1:52:A:ASP:H	1:52:A:ASP:HB3	1	0.23
(1,490)	1:52:A:ASP:H	1:49:A:THR:HB	4	0.23
(1,481)	1:51:A:GLU:H	1:50:A:LEU:H	9	0.23
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD11	1	0.23
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD12	1	0.23
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD13	1	0.23
(1,473)	1:49:A:THR:H	1:52:A:ASP:HB2	5	0.23
(1,469)	1:49:A:THR:H	1:48:A:LYS:HB2	8	0.23
(1,451)	1:41:A:GLY:H	1:41:A:GLY:HA2	7	0.23
(1,447)	1:40:A:SER:H	1:40:A:SER:HB2	4	0.23
(1,444)	1:39:A:GLY:H	1:40:A:SER:H	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,426)	1:35:A:PHE:H	1:34:A:THR:HB	2	0.23
(1,401)	1:29:A:THR:H	1:29:A:THR:HG21	9	0.23
(1,401)	1:29:A:THR:H	1:29:A:THR:HG22	9	0.23
(1,401)	1:29:A:THR:H	1:29:A:THR:HG23	9	0.23
(1,383)	1:26:A:ASP:H	1:26:A:ASP:HB3	6	0.23
(1,369)	1:23:A:TYR:H	1:22:A:ASN:HB3	2	0.23
(1,363)	1:21:A:THR:H	1:21:A:THR:HA	2	0.23
(1,363)	1:21:A:THR:H	1:21:A:THR:HA	5	0.23
(1,333)	1:15:A:LYS:H	1:16:A:GLY:H	4	0.23
(1,333)	1:15:A:LYS:H	1:16:A:GLY:H	8	0.23
(1,306)	1:11:A:ARG:H	1:11:A:ARG:HB3	4	0.23
(1,245)	1:56:A:THR:HG21	1:53:A:CYS:HA	3	0.23
(1,245)	1:56:A:THR:HG22	1:53:A:CYS:HA	3	0.23
(1,245)	1:56:A:THR:HG23	1:53:A:CYS:HA	3	0.23
(1,236)	1:54:A:GLU:HB3	1:58:A:VAL:HB	1	0.23
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD21	3	0.23
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD22	3	0.23
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD23	3	0.23
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD21	9	0.23
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD22	9	0.23
(1,231)	1:54:A:GLU:HA	1:50:A:LEU:HD23	9	0.23
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD21	9	0.23
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD22	9	0.23
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD23	9	0.23
(1,224)	1:52:A:ASP:HA	1:52:A:ASP:HB2	5	0.23
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD21	2	0.23
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD22	2	0.23
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD23	2	0.23
(1,205)	1:48:A:LYS:HB3	1:48:A:LYS:HA	5	0.23
(1,187)	1:40:A:SER:HA	1:41:A:GLY:HA3	3	0.23
(1,177)	1:36:A:ARG:HG2	1:35:A:PHE:HA	4	0.23
(1,171)	1:35:A:PHE:HE1	1:37:A:TYR:HB2	6	0.23
(1,169)	1:35:A:PHE:HE1	1:37:A:TYR:HA	2	0.23
(1,169)	1:35:A:PHE:HE1	1:37:A:TYR:HA	7	0.23
(1,168)	1:35:A:PHE:HD1	1:37:A:TYR:HB2	3	0.23
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG21	8	0.23
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG22	8	0.23
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG23	8	0.23
(1,148)	1:33:A:LYS:HE3	1:33:A:LYS:HD2	5	0.23
(1,148)	1:33:A:LYS:HE3	1:33:A:LYS:HD2	8	0.23
(1,146)	1:33:A:LYS:HA	1:33:A:LYS:HG3	5	0.23
(1,134)	1:32:A:CYS:HA	1:25:A:TYR:HB3	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,134)	1:32:A:CYS:HA	1:25:A:TYR:HB3	2	0.23
(1,134)	1:32:A:CYS:HA	1:25:A:TYR:HB3	9	0.23
(1,102)	1:24:A:TYR:HD1	1:24:A:TYR:HA	3	0.23
(1,88)	1:23:A:TYR:HE1	1:49:A:THR:HA	7	0.23
(1,45)	1:11:A:ARG:HG3	1:11:A:ARG:HB3	9	0.23
(1,21)	1:8:A:GLN:HA	1:8:A:GLN:HB3	7	0.23
(2,31)	1:60:A:ALA:H	1:56:A:THR:O	1	0.22
(1,525)	1:57:A:CYS:H	1:57:A:CYS:HB2	1	0.22
(1,506)	1:54:A:GLU:H	1:53:A:CYS:HB3	6	0.22
(1,478)	1:50:A:LEU:H	1:50:A:LEU:HB2	4	0.22
(1,478)	1:50:A:LEU:H	1:50:A:LEU:HB2	9	0.22
(1,462)	1:48:A:LYS:H	1:48:A:LYS:HB2	2	0.22
(1,447)	1:40:A:SER:H	1:40:A:SER:HB2	2	0.22
(1,446)	1:40:A:SER:H	1:40:A:SER:HB3	4	0.22
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG21	10	0.22
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG22	10	0.22
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG23	10	0.22
(1,426)	1:35:A:PHE:H	1:34:A:THR:HB	6	0.22
(1,413)	1:32:A:CYS:H	1:32:A:CYS:HB2	10	0.22
(1,406)	1:30:A:SER:H	1:30:A:SER:HB2	8	0.22
(1,401)	1:29:A:THR:H	1:29:A:THR:HG21	8	0.22
(1,401)	1:29:A:THR:H	1:29:A:THR:HG22	8	0.22
(1,401)	1:29:A:THR:H	1:29:A:THR:HG23	8	0.22
(1,394)	1:28:A:ALA:H	1:29:A:THR:H	3	0.22
(1,394)	1:28:A:ALA:H	1:29:A:THR:H	7	0.22
(1,391)	1:28:A:ALA:H	1:27:A:LYS:HA	2	0.22
(1,388)	1:27:A:LYS:H	1:27:A:LYS:HB3	6	0.22
(1,380)	1:25:A:TYR:H	1:25:A:TYR:HB3	7	0.22
(1,376)	1:24:A:TYR:H	1:34:A:THR:HA	6	0.22
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG21	2	0.22
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG22	2	0.22
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG23	2	0.22
(1,356)	1:20:A:PHE:H	1:19:A:SER:HB2	4	0.22
(1,350)	1:18:A:GLY:H	1:19:A:SER:H	6	0.22
(1,332)	1:15:A:LYS:H	1:15:A:LYS:HG2	2	0.22
(1,325)	1:14:A:GLY:H	1:13:A:TYR:HB3	6	0.22
(1,303)	1:11:A:ARG:H	1:10:A:SER:HA	2	0.22
(1,273)	1:5:A:TYR:H	1:4:A:ASP:HB2	2	0.22
(1,273)	1:5:A:TYR:H	1:4:A:ASP:HB2	3	0.22
(1,272)	1:4:A:ASP:H	1:4:A:ASP:HB2	1	0.22
(1,266)	1:3:A:GLN:H	1:4:A:ASP:H	7	0.22
(1,248)	1:57:A:CYS:HA	1:7:A:CYS:HA	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,245)	1:56:A:THR:HG21	1:53:A:CYS:HA	9	0.22
(1,245)	1:56:A:THR:HG22	1:53:A:CYS:HA	9	0.22
(1,245)	1:56:A:THR:HG23	1:53:A:CYS:HA	9	0.22
(1,238)	1:54:A:GLU:HB2	1:55:A:ALA:H	4	0.22
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD21	5	0.22
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD22	5	0.22
(1,228)	1:53:A:CYS:HB3	1:50:A:LEU:HD23	5	0.22
(1,225)	1:53:A:CYS:H	1:53:A:CYS:HB3	6	0.22
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD21	6	0.22
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD22	6	0.22
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD23	6	0.22
(1,205)	1:48:A:LYS:HB3	1:48:A:LYS:HA	7	0.22
(1,185)	1:37:A:TYR:HB2	1:46:A:ARG:HG3	3	0.22
(1,183)	1:37:A:TYR:HB2	1:22:A:ASN:HB2	3	0.22
(1,169)	1:35:A:PHE:HE1	1:37:A:TYR:HA	1	0.22
(1,165)	1:35:A:PHE:HD1	1:34:A:THR:HB	5	0.22
(1,146)	1:33:A:LYS:HA	1:33:A:LYS:HG3	6	0.22
(1,125)	1:27:A:LYS:HB3	1:27:A:LYS:HG3	3	0.22
(1,125)	1:27:A:LYS:HB3	1:27:A:LYS:HG3	10	0.22
(1,102)	1:24:A:TYR:HD1	1:24:A:TYR:HA	6	0.22
(1,55)	1:15:A:LYS:HA	1:15:A:LYS:HB3	4	0.22
(1,55)	1:15:A:LYS:HA	1:15:A:LYS:HB3	10	0.22
(1,34)	1:11:A:ARG:HB3	1:11:A:ARG:HG2	6	0.22
(1,21)	1:8:A:GLN:HA	1:8:A:GLN:HB3	9	0.22
(1,542)	1:61:A:GLU:H	1:61:A:GLU:HG3	1	0.21
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG11	10	0.21
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG12	10	0.21
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG13	10	0.21
(1,518)	1:56:A:THR:H	1:56:A:THR:HG21	3	0.21
(1,518)	1:56:A:THR:H	1:56:A:THR:HG22	3	0.21
(1,518)	1:56:A:THR:H	1:56:A:THR:HG23	3	0.21
(1,513)	1:55:A:ALA:H	1:56:A:THR:H	9	0.21
(1,492)	1:52:A:ASP:H	1:51:A:GLU:HG3	2	0.21
(1,481)	1:51:A:GLU:H	1:50:A:LEU:H	4	0.21
(1,469)	1:49:A:THR:H	1:48:A:LYS:HB2	10	0.21
(1,436)	1:37:A:TYR:H	1:36:A:ARG:HB2	4	0.21
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG21	3	0.21
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG22	3	0.21
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG23	3	0.21
(1,418)	1:34:A:THR:H	1:33:A:LYS:HA	1	0.21
(1,406)	1:30:A:SER:H	1:30:A:SER:HB2	7	0.21
(1,363)	1:21:A:THR:H	1:21:A:THR:HA	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,361)	1:21:A:THR:H	1:20:A:PHE:HB3	3	0.21
(1,353)	1:19:A:SER:H	1:19:A:SER:HA	7	0.21
(1,348)	1:18:A:GLY:H	1:18:A:GLY:HA3	5	0.21
(1,338)	1:16:A:GLY:H	1:16:A:GLY:HA2	8	0.21
(1,332)	1:15:A:LYS:H	1:15:A:LYS:HG2	3	0.21
(1,313)	1:12:A:ASN:H	1:12:A:ASN:HB2	2	0.21
(1,307)	1:11:A:ARG:H	1:11:A:ARG:HG2	1	0.21
(1,302)	1:10:A:SER:H	1:10:A:SER:HB3	5	0.21
(1,273)	1:5:A:TYR:H	1:4:A:ASP:HB2	9	0.21
(1,269)	1:4:A:ASP:H	1:3:A:GLN:HB3	6	0.21
(1,261)	1:61:A:GLU:HG2	1:59:A:THR:HA	10	0.21
(1,259)	1:61:A:GLU:HA	1:61:A:GLU:HG2	6	0.21
(1,238)	1:54:A:GLU:HB2	1:55:A:ALA:H	5	0.21
(1,234)	1:54:A:GLU:HA	1:58:A:VAL:HB	4	0.21
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD21	3	0.21
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD22	3	0.21
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD23	3	0.21
(1,187)	1:40:A:SER:HA	1:41:A:GLY:HA3	6	0.21
(1,171)	1:35:A:PHE:HE1	1:37:A:TYR:HB2	1	0.21
(1,171)	1:35:A:PHE:HE1	1:37:A:TYR:HB2	10	0.21
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG21	5	0.21
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG22	5	0.21
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG23	5	0.21
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG21	9	0.21
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG22	9	0.21
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG23	9	0.21
(1,151)	1:34:A:THR:HA	1:23:A:TYR:HA	3	0.21
(1,150)	1:33:A:LYS:HG2	1:33:A:LYS:HA	5	0.21
(1,148)	1:33:A:LYS:HE3	1:33:A:LYS:HD2	7	0.21
(1,146)	1:33:A:LYS:HA	1:33:A:LYS:HG3	1	0.21
(1,136)	1:32:A:CYS:HA	1:32:A:CYS:HB3	7	0.21
(1,134)	1:32:A:CYS:HA	1:25:A:TYR:HB3	3	0.21
(1,102)	1:24:A:TYR:HD1	1:24:A:TYR:HA	5	0.21
(1,102)	1:24:A:TYR:HD1	1:24:A:TYR:HA	8	0.21
(1,102)	1:24:A:TYR:HD1	1:24:A:TYR:HA	10	0.21
(1,88)	1:23:A:TYR:HE1	1:49:A:THR:HA	1	0.21
(1,65)	1:19:A:SER:HA	1:19:A:SER:HB2	9	0.21
(1,57)	1:15:A:LYS:HA	1:15:A:LYS:HG2	1	0.21
(1,21)	1:8:A:GLN:HA	1:8:A:GLN:HB3	10	0.21
(2,29)	1:59:A:THR:H	1:55:A:ALA:O	5	0.2
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG11	9	0.2
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG12	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG13	9	0.2
(1,524)	1:57:A:CYS:H	1:57:A:CYS:HB3	7	0.2
(1,513)	1:55:A:ALA:H	1:56:A:THR:H	5	0.2
(1,511)	1:55:A:ALA:H	1:54:A:GLU:HG3	6	0.2
(1,505)	1:54:A:GLU:H	1:53:A:CYS:H	8	0.2
(1,496)	1:52:A:ASP:H	1:52:A:ASP:HB2	7	0.2
(1,487)	1:51:A:GLU:H	1:51:A:GLU:HG3	9	0.2
(1,480)	1:51:A:GLU:H	1:49:A:THR:HB	9	0.2
(1,478)	1:50:A:LEU:H	1:50:A:LEU:HB2	6	0.2
(1,472)	1:49:A:THR:H	1:52:A:ASP:HB3	10	0.2
(1,464)	1:48:A:LYS:H	1:48:A:LYS:HD2	2	0.2
(1,463)	1:48:A:LYS:H	1:48:A:LYS:HD3	2	0.2
(1,462)	1:48:A:LYS:H	1:48:A:LYS:HB2	4	0.2
(1,454)	1:43:A:ASN:H	1:12:A:ASN:HB3	9	0.2
(1,444)	1:39:A:GLY:H	1:40:A:SER:H	1	0.2
(1,444)	1:39:A:GLY:H	1:40:A:SER:H	6	0.2
(1,434)	1:36:A:ARG:H	1:36:A:ARG:HG2	3	0.2
(1,434)	1:36:A:ARG:H	1:36:A:ARG:HG2	8	0.2
(1,434)	1:36:A:ARG:H	1:36:A:ARG:HG2	9	0.2
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG21	2	0.2
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG22	2	0.2
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG23	2	0.2
(1,417)	1:33:A:LYS:H	1:33:A:LYS:HB3	8	0.2
(1,410)	1:32:A:CYS:H	1:31:A:SER:HA	7	0.2
(1,406)	1:30:A:SER:H	1:30:A:SER:HB2	9	0.2
(1,402)	1:30:A:SER:H	1:27:A:LYS:HA	5	0.2
(1,402)	1:30:A:SER:H	1:27:A:LYS:HA	6	0.2
(1,401)	1:29:A:THR:H	1:29:A:THR:HG21	1	0.2
(1,401)	1:29:A:THR:H	1:29:A:THR:HG22	1	0.2
(1,401)	1:29:A:THR:H	1:29:A:THR:HG23	1	0.2
(1,394)	1:28:A:ALA:H	1:29:A:THR:H	4	0.2
(1,388)	1:27:A:LYS:H	1:27:A:LYS:HB3	4	0.2
(1,384)	1:26:A:ASP:H	1:26:A:ASP:HB2	10	0.2
(1,359)	1:20:A:PHE:H	1:20:A:PHE:HB2	4	0.2
(1,351)	1:19:A:SER:H	1:18:A:GLY:HA3	5	0.2
(1,348)	1:18:A:GLY:H	1:18:A:GLY:HA3	8	0.2
(1,345)	1:17:A:SER:H	1:38:A:ARG:HA	6	0.2
(1,336)	1:16:A:GLY:H	1:15:A:LYS:HG2	1	0.2
(1,335)	1:16:A:GLY:H	1:15:A:LYS:HB3	6	0.2
(1,332)	1:15:A:LYS:H	1:15:A:LYS:HG2	7	0.2
(1,323)	1:13:A:TYR:H	1:14:A:GLY:H	8	0.2
(1,321)	1:13:A:TYR:H	1:13:A:TYR:HB3	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,282)	1:7:A:CYS:H	1:6:A:ARG:HG2	3	0.2
(1,272)	1:4:A:ASP:H	1:4:A:ASP:HB2	9	0.2
(1,271)	1:4:A:ASP:H	1:4:A:ASP:HB3	7	0.2
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG21	3	0.2
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG22	3	0.2
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG23	3	0.2
(1,183)	1:37:A:TYR:HB2	1:22:A:ASN:HB2	7	0.2
(1,172)	1:36:A:ARG:HA	1:21:A:THR:HA	4	0.2
(1,172)	1:36:A:ARG:HA	1:21:A:THR:HA	6	0.2
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG21	2	0.2
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG22	2	0.2
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG23	2	0.2
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG21	3	0.2
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG22	3	0.2
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG23	3	0.2
(1,165)	1:35:A:PHE:HD1	1:34:A:THR:HB	6	0.2
(1,148)	1:33:A:LYS:HE3	1:33:A:LYS:HD2	9	0.2
(1,148)	1:33:A:LYS:HE3	1:33:A:LYS:HD2	10	0.2
(1,102)	1:24:A:TYR:HD1	1:24:A:TYR:HA	9	0.2
(1,55)	1:15:A:LYS:HA	1:15:A:LYS:HB3	8	0.2
(1,21)	1:8:A:GLN:HA	1:8:A:GLN:HB3	2	0.2
(1,18)	1:7:A:CYS:HA	1:57:A:CYS:HB2	7	0.2
(2,31)	1:60:A:ALA:H	1:56:A:THR:O	5	0.19
(2,29)	1:59:A:THR:H	1:55:A:ALA:O	10	0.19
(1,539)	1:61:A:GLU:H	1:60:A:ALA:HA	7	0.19
(1,518)	1:56:A:THR:H	1:56:A:THR:HG21	9	0.19
(1,518)	1:56:A:THR:H	1:56:A:THR:HG22	9	0.19
(1,518)	1:56:A:THR:H	1:56:A:THR:HG23	9	0.19
(1,513)	1:55:A:ALA:H	1:56:A:THR:H	8	0.19
(1,506)	1:54:A:GLU:H	1:53:A:CYS:HB3	1	0.19
(1,503)	1:53:A:CYS:H	1:53:A:CYS:HB2	1	0.19
(1,503)	1:53:A:CYS:H	1:53:A:CYS:HB2	7	0.19
(1,503)	1:53:A:CYS:H	1:53:A:CYS:HB2	10	0.19
(1,501)	1:53:A:CYS:H	1:52:A:ASP:HB2	7	0.19
(1,500)	1:53:A:CYS:H	1:52:A:ASP:HB3	2	0.19
(1,496)	1:52:A:ASP:H	1:52:A:ASP:HB2	3	0.19
(1,483)	1:51:A:GLU:H	1:50:A:LEU:HB3	2	0.19
(1,483)	1:51:A:GLU:H	1:50:A:LEU:HB3	9	0.19
(1,481)	1:51:A:GLU:H	1:50:A:LEU:H	3	0.19
(1,471)	1:49:A:THR:H	1:49:A:THR:HG21	6	0.19
(1,471)	1:49:A:THR:H	1:49:A:THR:HG22	6	0.19
(1,471)	1:49:A:THR:H	1:49:A:THR:HG23	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,468)	1:49:A:THR:H	1:48:A:LYS:HB3	5	0.19
(1,459)	1:47:A:PHE:H	1:46:A:ARG:HG2	10	0.19
(1,455)	1:43:A:ASN:H	1:12:A:ASN:HB2	7	0.19
(1,451)	1:41:A:GLY:H	1:41:A:GLY:HA2	6	0.19
(1,449)	1:41:A:GLY:H	1:40:A:SER:HA	1	0.19
(1,433)	1:36:A:ARG:H	1:36:A:ARG:HB2	6	0.19
(1,433)	1:36:A:ARG:H	1:36:A:ARG:HB2	7	0.19
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG21	4	0.19
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG22	4	0.19
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG23	4	0.19
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG21	8	0.19
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG22	8	0.19
(1,427)	1:35:A:PHE:H	1:34:A:THR:HG23	8	0.19
(1,426)	1:35:A:PHE:H	1:34:A:THR:HB	4	0.19
(1,426)	1:35:A:PHE:H	1:34:A:THR:HB	10	0.19
(1,413)	1:32:A:CYS:H	1:32:A:CYS:HB2	7	0.19
(1,410)	1:32:A:CYS:H	1:31:A:SER:HA	2	0.19
(1,406)	1:30:A:SER:H	1:30:A:SER:HB2	2	0.19
(1,406)	1:30:A:SER:H	1:30:A:SER:HB2	5	0.19
(1,402)	1:30:A:SER:H	1:27:A:LYS:HA	10	0.19
(1,384)	1:26:A:ASP:H	1:26:A:ASP:HB2	3	0.19
(1,383)	1:26:A:ASP:H	1:26:A:ASP:HB3	1	0.19
(1,376)	1:24:A:TYR:H	1:34:A:THR:HA	1	0.19
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG21	8	0.19
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG22	8	0.19
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG23	8	0.19
(1,350)	1:18:A:GLY:H	1:19:A:SER:H	2	0.19
(1,348)	1:18:A:GLY:H	1:18:A:GLY:HA3	10	0.19
(1,343)	1:17:A:SER:H	1:17:A:SER:HB3	2	0.19
(1,332)	1:15:A:LYS:H	1:15:A:LYS:HG2	9	0.19
(1,327)	1:14:A:GLY:H	1:14:A:GLY:HA3	9	0.19
(1,326)	1:14:A:GLY:H	1:13:A:TYR:HB2	7	0.19
(1,322)	1:13:A:TYR:H	1:13:A:TYR:HB2	6	0.19
(1,314)	1:12:A:ASN:HD21	1:12:A:ASN:HB3	10	0.19
(1,311)	1:12:A:ASN:H	1:11:A:ARG:HG2	6	0.19
(1,304)	1:11:A:ARG:H	1:10:A:SER:HB2	10	0.19
(1,303)	1:11:A:ARG:H	1:10:A:SER:HA	7	0.19
(1,303)	1:11:A:ARG:H	1:10:A:SER:HA	9	0.19
(1,302)	1:10:A:SER:H	1:10:A:SER:HB3	8	0.19
(1,284)	1:7:A:CYS:H	1:7:A:CYS:HB3	7	0.19
(1,272)	1:4:A:ASP:H	1:4:A:ASP:HB2	7	0.19
(1,260)	1:61:A:GLU:HG3	1:61:A:GLU:HA	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,238)	1:54:A:GLU:HB2	1:55:A:ALA:H	2	0.19
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG21	1	0.19
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG22	1	0.19
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG23	1	0.19
(1,188)	1:40:A:SER:HA	1:41:A:GLY:HA2	3	0.19
(1,188)	1:40:A:SER:HA	1:41:A:GLY:HA2	4	0.19
(1,186)	1:38:A:ARG:HD3	1:38:A:ARG:HG3	7	0.19
(1,171)	1:35:A:PHE:HE1	1:37:A:TYR:HB2	4	0.19
(1,169)	1:35:A:PHE:HE1	1:37:A:TYR:HA	9	0.19
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG21	1	0.19
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG22	1	0.19
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG23	1	0.19
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG21	7	0.19
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG22	7	0.19
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG23	7	0.19
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG21	10	0.19
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG22	10	0.19
(1,166)	1:35:A:PHE:HD1	1:34:A:THR:HG23	10	0.19
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG21	2	0.19
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG22	2	0.19
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG23	2	0.19
(1,148)	1:33:A:LYS:HE3	1:33:A:LYS:HD2	1	0.19
(1,146)	1:33:A:LYS:HA	1:33:A:LYS:HG3	4	0.19
(1,134)	1:32:A:CYS:HA	1:25:A:TYR:HB3	5	0.19
(1,134)	1:32:A:CYS:HA	1:25:A:TYR:HB3	8	0.19
(1,65)	1:19:A:SER:HA	1:19:A:SER:HB2	4	0.19
(1,65)	1:19:A:SER:HA	1:19:A:SER:HB2	7	0.19
(1,26)	1:9:A:LEU:HD11	1:45:A:ASN:HB2	3	0.19
(1,26)	1:9:A:LEU:HD12	1:45:A:ASN:HB2	3	0.19
(1,26)	1:9:A:LEU:HD13	1:45:A:ASN:HB2	3	0.19
(1,26)	1:9:A:LEU:HD11	1:45:A:ASN:HB2	9	0.19
(1,26)	1:9:A:LEU:HD12	1:45:A:ASN:HB2	9	0.19
(1,26)	1:9:A:LEU:HD13	1:45:A:ASN:HB2	9	0.19
(1,21)	1:8:A:GLN:HA	1:8:A:GLN:HB3	6	0.19
(2,29)	1:59:A:THR:H	1:55:A:ALA:O	2	0.18
(2,29)	1:59:A:THR:H	1:55:A:ALA:O	3	0.18
(2,29)	1:59:A:THR:H	1:55:A:ALA:O	6	0.18
(2,29)	1:59:A:THR:H	1:55:A:ALA:O	9	0.18
(1,539)	1:61:A:GLU:H	1:60:A:ALA:HA	9	0.18
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG11	8	0.18
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG12	8	0.18
(1,532)	1:59:A:THR:H	1:58:A:VAL:HG13	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,527)	1:58:A:VAL:H	1:57:A:CYS:H	7	0.18
(1,513)	1:55:A:ALA:H	1:56:A:THR:H	3	0.18
(1,503)	1:53:A:CYS:H	1:53:A:CYS:HB2	9	0.18
(1,496)	1:52:A:ASP:H	1:52:A:ASP:HB2	8	0.18
(1,490)	1:52:A:ASP:H	1:49:A:THR:HB	1	0.18
(1,488)	1:51:A:GLU:H	1:51:A:GLU:HG2	7	0.18
(1,483)	1:51:A:GLU:H	1:50:A:LEU:HB3	4	0.18
(1,478)	1:50:A:LEU:H	1:50:A:LEU:HB2	1	0.18
(1,478)	1:50:A:LEU:H	1:50:A:LEU:HB2	5	0.18
(1,471)	1:49:A:THR:H	1:49:A:THR:HG21	2	0.18
(1,471)	1:49:A:THR:H	1:49:A:THR:HG22	2	0.18
(1,471)	1:49:A:THR:H	1:49:A:THR:HG23	2	0.18
(1,468)	1:49:A:THR:H	1:48:A:LYS:HB3	2	0.18
(1,468)	1:49:A:THR:H	1:48:A:LYS:HB3	8	0.18
(1,462)	1:48:A:LYS:H	1:48:A:LYS:HB2	1	0.18
(1,462)	1:48:A:LYS:H	1:48:A:LYS:HB2	9	0.18
(1,461)	1:48:A:LYS:H	1:48:A:LYS:HA	2	0.18
(1,450)	1:41:A:GLY:H	1:41:A:GLY:HA3	3	0.18
(1,446)	1:40:A:SER:H	1:40:A:SER:HB3	7	0.18
(1,440)	1:38:A:ARG:H	1:37:A:TYR:HB3	3	0.18
(1,430)	1:36:A:ARG:H	1:35:A:PHE:HA	6	0.18
(1,424)	1:35:A:PHE:H	1:22:A:ASN:H	6	0.18
(1,420)	1:34:A:THR:H	1:33:A:LYS:HD3	7	0.18
(1,417)	1:33:A:LYS:H	1:33:A:LYS:HB3	2	0.18
(1,417)	1:33:A:LYS:H	1:33:A:LYS:HB3	7	0.18
(1,411)	1:32:A:CYS:H	1:31:A:SER:HB3	10	0.18
(1,406)	1:30:A:SER:H	1:30:A:SER:HB2	3	0.18
(1,396)	1:28:A:ALA:H	1:30:A:SER:H	5	0.18
(1,391)	1:28:A:ALA:H	1:27:A:LYS:HA	4	0.18
(1,388)	1:27:A:LYS:H	1:27:A:LYS:HB3	1	0.18
(1,388)	1:27:A:LYS:H	1:27:A:LYS:HB3	9	0.18
(1,383)	1:26:A:ASP:H	1:26:A:ASP:HB3	8	0.18
(1,381)	1:25:A:TYR:H	1:25:A:TYR:HB2	3	0.18
(1,380)	1:25:A:TYR:H	1:25:A:TYR:HB3	6	0.18
(1,376)	1:24:A:TYR:H	1:34:A:THR:HA	2	0.18
(1,371)	1:23:A:TYR:H	1:23:A:TYR:HD1	9	0.18
(1,361)	1:21:A:THR:H	1:20:A:PHE:HB3	4	0.18
(1,361)	1:21:A:THR:H	1:20:A:PHE:HB3	10	0.18
(1,355)	1:20:A:PHE:H	1:19:A:SER:HA	10	0.18
(1,348)	1:18:A:GLY:H	1:18:A:GLY:HA3	7	0.18
(1,344)	1:17:A:SER:H	1:18:A:GLY:H	9	0.18
(1,343)	1:17:A:SER:H	1:17:A:SER:HB3	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,343)	1:17:A:SER:H	1:17:A:SER:HB3	10	0.18
(1,328)	1:14:A:GLY:H	1:14:A:GLY:HA2	10	0.18
(1,322)	1:13:A:TYR:H	1:13:A:TYR:HB2	1	0.18
(1,308)	1:12:A:ASN:H	1:11:A:ARG:HA	6	0.18
(1,306)	1:11:A:ARG:H	1:11:A:ARG:HB3	6	0.18
(1,303)	1:11:A:ARG:H	1:10:A:SER:HA	5	0.18
(1,298)	1:10:A:SER:H	1:9:A:LEU:HA	7	0.18
(1,287)	1:8:A:GLN:H	1:7:A:CYS:HA	8	0.18
(1,285)	1:7:A:CYS:H	1:7:A:CYS:HB2	7	0.18
(1,285)	1:7:A:CYS:H	1:7:A:CYS:HB2	10	0.18
(1,282)	1:7:A:CYS:H	1:6:A:ARG:HG2	4	0.18
(1,281)	1:7:A:CYS:H	1:6:A:ARG:HG3	1	0.18
(1,278)	1:6:A:ARG:H	1:6:A:ARG:HG2	5	0.18
(1,277)	1:6:A:ARG:H	1:6:A:ARG:HG3	8	0.18
(1,273)	1:5:A:TYR:H	1:4:A:ASP:HB2	10	0.18
(1,271)	1:4:A:ASP:H	1:4:A:ASP:HB3	3	0.18
(1,269)	1:4:A:ASP:H	1:3:A:GLN:HB3	3	0.18
(1,268)	1:4:A:ASP:H	1:3:A:GLN:HA	8	0.18
(1,259)	1:61:A:GLU:HA	1:61:A:GLU:HG2	2	0.18
(1,248)	1:57:A:CYS:HA	1:7:A:CYS:HA	7	0.18
(1,245)	1:56:A:THR:HG21	1:53:A:CYS:HA	4	0.18
(1,245)	1:56:A:THR:HG22	1:53:A:CYS:HA	4	0.18
(1,245)	1:56:A:THR:HG23	1:53:A:CYS:HA	4	0.18
(1,224)	1:52:A:ASP:HA	1:52:A:ASP:HB2	7	0.18
(1,219)	1:51:A:GLU:HA	1:54:A:GLU:HB3	7	0.18
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG21	2	0.18
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG22	2	0.18
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG23	2	0.18
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG21	6	0.18
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG22	6	0.18
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG23	6	0.18
(1,192)	1:46:A:ARG:HA	1:46:A:ARG:HG3	6	0.18
(1,172)	1:36:A:ARG:HA	1:21:A:THR:HA	3	0.18
(1,172)	1:36:A:ARG:HA	1:21:A:THR:HA	7	0.18
(1,164)	1:35:A:PHE:HD1	1:34:A:THR:HA	6	0.18
(1,148)	1:33:A:LYS:HE3	1:33:A:LYS:HD2	6	0.18
(1,141)	1:32:A:CYS:HB3	1:50:A:LEU:HB3	7	0.18
(1,93)	1:24:A:TYR:HA	1:47:A:PHE:HB3	4	0.18
(1,88)	1:23:A:TYR:HE1	1:49:A:THR:HA	2	0.18
(1,24)	1:9:A:LEU:HA	1:9:A:LEU:HG	1	0.18
(1,24)	1:9:A:LEU:HA	1:9:A:LEU:HG	6	0.18
(1,16)	1:7:A:CYS:HA	1:6:A:ARG:HA	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:3:A:GLN:HB3	1:3:A:GLN:HA	1	0.18
(2,31)	1:60:A:ALA:H	1:56:A:THR:O	2	0.17
(2,29)	1:59:A:THR:H	1:55:A:ALA:O	7	0.17
(1,542)	1:61:A:GLU:H	1:61:A:GLU:HG3	7	0.17
(1,541)	1:61:A:GLU:H	1:61:A:GLU:HB2	4	0.17
(1,541)	1:61:A:GLU:H	1:61:A:GLU:HB2	8	0.17
(1,539)	1:61:A:GLU:H	1:60:A:ALA:HA	4	0.17
(1,536)	1:60:A:ALA:H	1:59:A:THR:HB	5	0.17
(1,528)	1:58:A:VAL:H	1:58:A:VAL:HA	2	0.17
(1,528)	1:58:A:VAL:H	1:58:A:VAL:HA	3	0.17
(1,528)	1:58:A:VAL:H	1:58:A:VAL:HA	6	0.17
(1,526)	1:58:A:VAL:H	1:54:A:GLU:HA	6	0.17
(1,525)	1:57:A:CYS:H	1:57:A:CYS:HB2	3	0.17
(1,525)	1:57:A:CYS:H	1:57:A:CYS:HB2	7	0.17
(1,524)	1:57:A:CYS:H	1:57:A:CYS:HB3	1	0.17
(1,518)	1:56:A:THR:H	1:56:A:THR:HG21	2	0.17
(1,518)	1:56:A:THR:H	1:56:A:THR:HG22	2	0.17
(1,518)	1:56:A:THR:H	1:56:A:THR:HG23	2	0.17
(1,518)	1:56:A:THR:H	1:56:A:THR:HG21	10	0.17
(1,518)	1:56:A:THR:H	1:56:A:THR:HG22	10	0.17
(1,518)	1:56:A:THR:H	1:56:A:THR:HG23	10	0.17
(1,513)	1:55:A:ALA:H	1:56:A:THR:H	2	0.17
(1,505)	1:54:A:GLU:H	1:53:A:CYS:H	10	0.17
(1,503)	1:53:A:CYS:H	1:53:A:CYS:HB2	5	0.17
(1,501)	1:53:A:CYS:H	1:52:A:ASP:HB2	3	0.17
(1,501)	1:53:A:CYS:H	1:52:A:ASP:HB2	9	0.17
(1,499)	1:53:A:CYS:H	1:50:A:LEU:HA	7	0.17
(1,497)	1:52:A:ASP:H	1:53:A:CYS:H	2	0.17
(1,492)	1:52:A:ASP:H	1:51:A:GLU:HG3	8	0.17
(1,490)	1:52:A:ASP:H	1:49:A:THR:HB	2	0.17
(1,483)	1:51:A:GLU:H	1:50:A:LEU:HB3	6	0.17
(1,481)	1:51:A:GLU:H	1:50:A:LEU:H	5	0.17
(1,469)	1:49:A:THR:H	1:48:A:LYS:HB2	6	0.17
(1,466)	1:49:A:THR:H	1:47:A:PHE:HB3	8	0.17
(1,464)	1:48:A:LYS:H	1:48:A:LYS:HD2	1	0.17
(1,462)	1:48:A:LYS:H	1:48:A:LYS:HB2	3	0.17
(1,453)	1:42:A:GLY:H	1:41:A:GLY:HA2	5	0.17
(1,451)	1:41:A:GLY:H	1:41:A:GLY:HA2	4	0.17
(1,450)	1:41:A:GLY:H	1:41:A:GLY:HA3	7	0.17
(1,440)	1:38:A:ARG:H	1:37:A:TYR:HB3	1	0.17
(1,440)	1:38:A:ARG:H	1:37:A:TYR:HB3	6	0.17
(1,440)	1:38:A:ARG:H	1:37:A:TYR:HB3	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:38:A:ARG:H	1:36:A:ARG:HB2	5	0.17
(1,430)	1:36:A:ARG:H	1:35:A:PHE:HA	7	0.17
(1,423)	1:35:A:PHE:H	1:21:A:THR:HG21	8	0.17
(1,423)	1:35:A:PHE:H	1:21:A:THR:HG22	8	0.17
(1,423)	1:35:A:PHE:H	1:21:A:THR:HG23	8	0.17
(1,420)	1:34:A:THR:H	1:33:A:LYS:HD3	10	0.17
(1,391)	1:28:A:ALA:H	1:27:A:LYS:HA	9	0.17
(1,369)	1:23:A:TYR:H	1:22:A:ASN:HB3	1	0.17
(1,369)	1:23:A:TYR:H	1:22:A:ASN:HB3	6	0.17
(1,362)	1:21:A:THR:H	1:20:A:PHE:HB2	10	0.17
(1,353)	1:19:A:SER:H	1:19:A:SER:HA	9	0.17
(1,338)	1:16:A:GLY:H	1:16:A:GLY:HA2	4	0.17
(1,306)	1:11:A:ARG:H	1:11:A:ARG:HB3	5	0.17
(1,293)	1:9:A:LEU:H	1:8:A:GLN:HA	8	0.17
(1,284)	1:7:A:CYS:H	1:7:A:CYS:HB3	6	0.17
(1,284)	1:7:A:CYS:H	1:7:A:CYS:HB3	10	0.17
(1,277)	1:6:A:ARG:H	1:6:A:ARG:HG3	3	0.17
(1,269)	1:4:A:ASP:H	1:3:A:GLN:HB3	5	0.17
(1,266)	1:3:A:GLN:H	1:4:A:ASP:H	10	0.17
(1,258)	1:59:A:THR:HB	1:59:A:THR:HA	1	0.17
(1,247)	1:57:A:CYS:HA	1:3:A:GLN:HG3	9	0.17
(1,238)	1:54:A:GLU:HB2	1:55:A:ALA:H	10	0.17
(1,234)	1:54:A:GLU:HA	1:58:A:VAL:HB	9	0.17
(1,234)	1:54:A:GLU:HA	1:58:A:VAL:HB	10	0.17
(1,225)	1:53:A:CYS:H	1:53:A:CYS:HB3	1	0.17
(1,208)	1:48:A:LYS:HD3	1:48:A:LYS:HA	7	0.17
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG21	4	0.17
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG22	4	0.17
(1,207)	1:48:A:LYS:HB2	1:49:A:THR:HG23	4	0.17
(1,203)	1:48:A:LYS:HA	1:22:A:ASN:HA	5	0.17
(1,194)	1:47:A:PHE:HA	1:46:A:ARG:HG2	1	0.17
(1,192)	1:46:A:ARG:HA	1:46:A:ARG:HG3	7	0.17
(1,182)	1:37:A:TYR:HB2	1:20:A:PHE:HB3	4	0.17
(1,172)	1:36:A:ARG:HA	1:21:A:THR:HA	8	0.17
(1,171)	1:35:A:PHE:HE1	1:37:A:TYR:HB2	7	0.17
(1,171)	1:35:A:PHE:HE1	1:37:A:TYR:HB2	8	0.17
(1,171)	1:35:A:PHE:HE1	1:37:A:TYR:HB2	9	0.17
(1,164)	1:35:A:PHE:HD1	1:34:A:THR:HA	10	0.17
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG21	7	0.17
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG22	7	0.17
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG23	7	0.17
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG21	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG22	10	0.17
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG23	10	0.17
(1,141)	1:32:A:CYS:HB3	1:50:A:LEU:HB3	6	0.17
(1,141)	1:32:A:CYS:HB3	1:50:A:LEU:HB3	9	0.17
(1,134)	1:32:A:CYS:HA	1:25:A:TYR:HB3	7	0.17
(1,126)	1:27:A:LYS:HB2	1:27:A:LYS:HA	7	0.17
(1,123)	1:27:A:LYS:HA	1:27:A:LYS:HE3	10	0.17
(1,65)	1:19:A:SER:HA	1:19:A:SER:HB2	8	0.17
(1,45)	1:11:A:ARG:HG3	1:11:A:ARG:HB3	5	0.17
(1,5)	1:3:A:GLN:HA	1:3:A:GLN:HB2	7	0.17
(1,5)	1:3:A:GLN:HA	1:3:A:GLN:HB2	9	0.17
(2,31)	1:60:A:ALA:H	1:56:A:THR:O	4	0.16
(2,29)	1:59:A:THR:H	1:55:A:ALA:O	4	0.16
(2,29)	1:59:A:THR:H	1:55:A:ALA:O	8	0.16
(1,541)	1:61:A:GLU:H	1:61:A:GLU:HB2	7	0.16
(1,541)	1:61:A:GLU:H	1:61:A:GLU:HB2	10	0.16
(1,534)	1:59:A:THR:H	1:59:A:THR:HG21	1	0.16
(1,534)	1:59:A:THR:H	1:59:A:THR:HG22	1	0.16
(1,534)	1:59:A:THR:H	1:59:A:THR:HG23	1	0.16
(1,528)	1:58:A:VAL:H	1:58:A:VAL:HA	1	0.16
(1,524)	1:57:A:CYS:H	1:57:A:CYS:HB3	9	0.16
(1,520)	1:57:A:CYS:H	1:56:A:THR:H	8	0.16
(1,513)	1:55:A:ALA:H	1:56:A:THR:H	4	0.16
(1,511)	1:55:A:ALA:H	1:54:A:GLU:HG3	10	0.16
(1,503)	1:53:A:CYS:H	1:53:A:CYS:HB2	2	0.16
(1,498)	1:53:A:CYS:H	1:47:A:PHE:HB3	5	0.16
(1,497)	1:52:A:ASP:H	1:53:A:CYS:H	9	0.16
(1,496)	1:52:A:ASP:H	1:52:A:ASP:HB2	9	0.16
(1,495)	1:52:A:ASP:H	1:52:A:ASP:HB3	6	0.16
(1,488)	1:51:A:GLU:H	1:51:A:GLU:HG2	10	0.16
(1,478)	1:50:A:LEU:H	1:50:A:LEU:HB2	3	0.16
(1,468)	1:49:A:THR:H	1:48:A:LYS:HB3	7	0.16
(1,461)	1:48:A:LYS:H	1:48:A:LYS:HA	3	0.16
(1,461)	1:48:A:LYS:H	1:48:A:LYS:HA	8	0.16
(1,453)	1:42:A:GLY:H	1:41:A:GLY:HA2	2	0.16
(1,450)	1:41:A:GLY:H	1:41:A:GLY:HA3	1	0.16
(1,448)	1:41:A:GLY:H	1:40:A:SER:H	4	0.16
(1,445)	1:40:A:SER:H	1:40:A:SER:HA	5	0.16
(1,445)	1:40:A:SER:H	1:40:A:SER:HA	6	0.16
(1,445)	1:40:A:SER:H	1:40:A:SER:HA	7	0.16
(1,445)	1:40:A:SER:H	1:40:A:SER:HA	8	0.16
(1,440)	1:38:A:ARG:H	1:37:A:TYR:HB3	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,436)	1:37:A:TYR:H	1:36:A:ARG:HB2	6	0.16
(1,426)	1:35:A:PHE:H	1:34:A:THR:HB	1	0.16
(1,425)	1:35:A:PHE:H	1:34:A:THR:HA	9	0.16
(1,424)	1:35:A:PHE:H	1:22:A:ASN:H	5	0.16
(1,424)	1:35:A:PHE:H	1:22:A:ASN:H	9	0.16
(1,413)	1:32:A:CYS:H	1:32:A:CYS:HB2	8	0.16
(1,408)	1:31:A:SER:H	1:30:A:SER:HA	4	0.16
(1,408)	1:31:A:SER:H	1:30:A:SER:HA	7	0.16
(1,406)	1:30:A:SER:H	1:30:A:SER:HB2	1	0.16
(1,402)	1:30:A:SER:H	1:27:A:LYS:HA	4	0.16
(1,394)	1:28:A:ALA:H	1:29:A:THR:H	5	0.16
(1,389)	1:27:A:LYS:H	1:27:A:LYS:HB2	3	0.16
(1,388)	1:27:A:LYS:H	1:27:A:LYS:HB3	7	0.16
(1,371)	1:23:A:TYR:H	1:23:A:TYR:HD1	7	0.16
(1,367)	1:22:A:ASN:H	1:22:A:ASN:HB2	7	0.16
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG21	10	0.16
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG22	10	0.16
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG23	10	0.16
(1,361)	1:21:A:THR:H	1:20:A:PHE:HB3	9	0.16
(1,343)	1:17:A:SER:H	1:17:A:SER:HB3	6	0.16
(1,322)	1:13:A:TYR:H	1:13:A:TYR:HB2	2	0.16
(1,313)	1:12:A:ASN:H	1:12:A:ASN:HB2	3	0.16
(1,313)	1:12:A:ASN:H	1:12:A:ASN:HB2	6	0.16
(1,307)	1:11:A:ARG:H	1:11:A:ARG:HG2	7	0.16
(1,290)	1:9:A:LEU:H	1:5:A:TYR:HA	7	0.16
(1,277)	1:6:A:ARG:H	1:6:A:ARG:HG3	4	0.16
(1,272)	1:4:A:ASP:H	1:4:A:ASP:HB2	10	0.16
(1,271)	1:4:A:ASP:H	1:4:A:ASP:HB3	2	0.16
(1,270)	1:4:A:ASP:H	1:4:A:ASP:HA	7	0.16
(1,269)	1:4:A:ASP:H	1:3:A:GLN:HB3	9	0.16
(1,259)	1:61:A:GLU:HA	1:61:A:GLU:HG2	7	0.16
(1,245)	1:56:A:THR:HG21	1:53:A:CYS:HA	8	0.16
(1,245)	1:56:A:THR:HG22	1:53:A:CYS:HA	8	0.16
(1,245)	1:56:A:THR:HG23	1:53:A:CYS:HA	8	0.16
(1,224)	1:52:A:ASP:HA	1:52:A:ASP:HB2	3	0.16
(1,224)	1:52:A:ASP:HA	1:52:A:ASP:HB2	8	0.16
(1,224)	1:52:A:ASP:HA	1:52:A:ASP:HB2	9	0.16
(1,220)	1:51:A:GLU:HB3	1:51:A:GLU:HG2	1	0.16
(1,199)	1:47:A:PHE:HB3	1:53:A:CYS:HA	10	0.16
(1,194)	1:47:A:PHE:HA	1:46:A:ARG:HG2	7	0.16
(1,194)	1:47:A:PHE:HA	1:46:A:ARG:HG2	10	0.16
(1,188)	1:40:A:SER:HA	1:41:A:GLY:HA2	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG21	6	0.16
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG22	6	0.16
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG23	6	0.16
(1,146)	1:33:A:LYS:HA	1:33:A:LYS:HG3	9	0.16
(1,144)	1:33:A:LYS:HA	1:33:A:LYS:HD2	3	0.16
(1,141)	1:32:A:CYS:HB3	1:50:A:LEU:HB3	1	0.16
(1,141)	1:32:A:CYS:HB3	1:50:A:LEU:HB3	2	0.16
(1,141)	1:32:A:CYS:HB3	1:50:A:LEU:HB3	4	0.16
(1,136)	1:32:A:CYS:HA	1:32:A:CYS:HB3	1	0.16
(1,136)	1:32:A:CYS:HA	1:32:A:CYS:HB3	3	0.16
(1,136)	1:32:A:CYS:HA	1:32:A:CYS:HB3	8	0.16
(1,134)	1:32:A:CYS:HA	1:25:A:TYR:HB3	4	0.16
(1,134)	1:32:A:CYS:HA	1:25:A:TYR:HB3	6	0.16
(1,65)	1:19:A:SER:HA	1:19:A:SER:HB2	3	0.16
(1,65)	1:19:A:SER:HA	1:19:A:SER:HB2	10	0.16
(1,23)	1:9:A:LEU:HA	1:5:A:TYR:HB3	9	0.16
(1,18)	1:7:A:CYS:HA	1:57:A:CYS:HB2	10	0.16
(2,31)	1:60:A:ALA:H	1:56:A:THR:O	6	0.15
(1,543)	1:61:A:GLU:H	1:61:A:GLU:HG2	2	0.15
(1,542)	1:61:A:GLU:H	1:61:A:GLU:HG3	2	0.15
(1,542)	1:61:A:GLU:H	1:61:A:GLU:HG3	10	0.15
(1,540)	1:61:A:GLU:H	1:61:A:GLU:HA	1	0.15
(1,540)	1:61:A:GLU:H	1:61:A:GLU:HA	3	0.15
(1,540)	1:61:A:GLU:H	1:61:A:GLU:HA	4	0.15
(1,540)	1:61:A:GLU:H	1:61:A:GLU:HA	7	0.15
(1,540)	1:61:A:GLU:H	1:61:A:GLU:HA	8	0.15
(1,540)	1:61:A:GLU:H	1:61:A:GLU:HA	9	0.15
(1,540)	1:61:A:GLU:H	1:61:A:GLU:HA	10	0.15
(1,539)	1:61:A:GLU:H	1:60:A:ALA:HA	6	0.15
(1,528)	1:58:A:VAL:H	1:58:A:VAL:HA	4	0.15
(1,528)	1:58:A:VAL:H	1:58:A:VAL:HA	9	0.15
(1,513)	1:55:A:ALA:H	1:56:A:THR:H	10	0.15
(1,511)	1:55:A:ALA:H	1:54:A:GLU:HG3	1	0.15
(1,506)	1:54:A:GLU:H	1:53:A:CYS:HB3	9	0.15
(1,504)	1:54:A:GLU:H	1:50:A:LEU:HD21	6	0.15
(1,504)	1:54:A:GLU:H	1:50:A:LEU:HD22	6	0.15
(1,504)	1:54:A:GLU:H	1:50:A:LEU:HD23	6	0.15
(1,503)	1:53:A:CYS:H	1:53:A:CYS:HB2	4	0.15
(1,501)	1:53:A:CYS:H	1:52:A:ASP:HB2	8	0.15
(1,495)	1:52:A:ASP:H	1:52:A:ASP:HB3	10	0.15
(1,490)	1:52:A:ASP:H	1:49:A:THR:HB	8	0.15
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD11	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD12	3	0.15
(1,479)	1:50:A:LEU:H	1:50:A:LEU:HD13	3	0.15
(1,474)	1:50:A:LEU:H	1:49:A:THR:HA	1	0.15
(1,474)	1:50:A:LEU:H	1:49:A:THR:HA	9	0.15
(1,465)	1:48:A:LYS:H	1:49:A:THR:H	10	0.15
(1,459)	1:47:A:PHE:H	1:46:A:ARG:HG2	2	0.15
(1,455)	1:43:A:ASN:H	1:12:A:ASN:HB2	10	0.15
(1,451)	1:41:A:GLY:H	1:41:A:GLY:HA2	1	0.15
(1,450)	1:41:A:GLY:H	1:41:A:GLY:HA3	9	0.15
(1,445)	1:40:A:SER:H	1:40:A:SER:HA	1	0.15
(1,442)	1:38:A:ARG:H	1:38:A:ARG:HB2	6	0.15
(1,440)	1:38:A:ARG:H	1:37:A:TYR:HB3	5	0.15
(1,430)	1:36:A:ARG:H	1:35:A:PHE:HA	2	0.15
(1,430)	1:36:A:ARG:H	1:35:A:PHE:HA	9	0.15
(1,420)	1:34:A:THR:H	1:33:A:LYS:HD3	9	0.15
(1,407)	1:30:A:SER:H	1:31:A:SER:H	6	0.15
(1,385)	1:26:A:ASP:H	1:32:A:CYS:HA	6	0.15
(1,383)	1:26:A:ASP:H	1:26:A:ASP:HB3	4	0.15
(1,375)	1:24:A:TYR:H	1:33:A:LYS:H	3	0.15
(1,372)	1:23:A:TYR:HD1	1:23:A:TYR:HA	6	0.15
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG21	1	0.15
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG22	1	0.15
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG23	1	0.15
(1,357)	1:20:A:PHE:H	1:20:A:PHE:HA	2	0.15
(1,348)	1:18:A:GLY:H	1:18:A:GLY:HA3	1	0.15
(1,346)	1:18:A:GLY:H	1:17:A:SER:HA	2	0.15
(1,337)	1:16:A:GLY:H	1:16:A:GLY:HA3	8	0.15
(1,333)	1:15:A:LYS:H	1:16:A:GLY:H	5	0.15
(1,328)	1:14:A:GLY:H	1:14:A:GLY:HA2	7	0.15
(1,327)	1:14:A:GLY:H	1:14:A:GLY:HA3	3	0.15
(1,324)	1:14:A:GLY:H	1:13:A:TYR:HA	5	0.15
(1,322)	1:13:A:TYR:H	1:13:A:TYR:HB2	3	0.15
(1,320)	1:13:A:TYR:H	1:13:A:TYR:HA	8	0.15
(1,313)	1:12:A:ASN:H	1:12:A:ASN:HB2	5	0.15
(1,297)	1:9:A:LEU:H	1:9:A:LEU:HG	2	0.15
(1,297)	1:9:A:LEU:H	1:9:A:LEU:HG	5	0.15
(1,297)	1:9:A:LEU:H	1:9:A:LEU:HG	7	0.15
(1,292)	1:9:A:LEU:H	1:8:A:GLN:H	3	0.15
(1,282)	1:7:A:CYS:H	1:6:A:ARG:HG2	8	0.15
(1,277)	1:6:A:ARG:H	1:6:A:ARG:HG3	1	0.15
(1,271)	1:4:A:ASP:H	1:4:A:ASP:HB3	1	0.15
(1,255)	1:58:A:VAL:HG11	1:58:A:VAL:HB	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,255)	1:58:A:VAL:HG12	1:58:A:VAL:HB	4	0.15
(1,255)	1:58:A:VAL:HG13	1:58:A:VAL:HB	4	0.15
(1,255)	1:58:A:VAL:HG11	1:58:A:VAL:HB	9	0.15
(1,255)	1:58:A:VAL:HG12	1:58:A:VAL:HB	9	0.15
(1,255)	1:58:A:VAL:HG13	1:58:A:VAL:HB	9	0.15
(1,238)	1:54:A:GLU:HB2	1:55:A:ALA:H	1	0.15
(1,227)	1:53:A:CYS:HB3	1:32:A:CYS:HB2	1	0.15
(1,225)	1:53:A:CYS:H	1:53:A:CYS:HB3	10	0.15
(1,221)	1:51:A:GLU:HB2	1:51:A:GLU:HG3	1	0.15
(1,205)	1:48:A:LYS:HB3	1:48:A:LYS:HA	8	0.15
(1,194)	1:47:A:PHE:HA	1:46:A:ARG:HG2	5	0.15
(1,192)	1:46:A:ARG:HA	1:46:A:ARG:HG3	9	0.15
(1,185)	1:37:A:TYR:HB2	1:46:A:ARG:HG3	9	0.15
(1,168)	1:35:A:PHE:HD1	1:37:A:TYR:HB2	2	0.15
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG21	1	0.15
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG22	1	0.15
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG23	1	0.15
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG21	2	0.15
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG22	2	0.15
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG23	2	0.15
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG21	5	0.15
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG22	5	0.15
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG23	5	0.15
(1,136)	1:32:A:CYS:HA	1:32:A:CYS:HB3	2	0.15
(1,136)	1:32:A:CYS:HA	1:32:A:CYS:HB3	4	0.15
(1,126)	1:27:A:LYS:HB2	1:27:A:LYS:HA	4	0.15
(1,126)	1:27:A:LYS:HB2	1:27:A:LYS:HA	9	0.15
(1,93)	1:24:A:TYR:HA	1:47:A:PHE:HB3	10	0.15
(1,88)	1:23:A:TYR:HE1	1:49:A:THR:HA	3	0.15
(1,65)	1:19:A:SER:HA	1:19:A:SER:HB2	2	0.15
(1,61)	1:17:A:SER:HA	1:17:A:SER:HB2	3	0.15
(1,61)	1:17:A:SER:HA	1:17:A:SER:HB2	7	0.15
(1,42)	1:11:A:ARG:HD2	1:11:A:ARG:HB2	1	0.15
(1,30)	1:11:A:ARG:HA	1:10:A:SER:HA	6	0.15
(1,23)	1:9:A:LEU:HA	1:5:A:TYR:HB3	3	0.15
(1,21)	1:8:A:GLN:HA	1:8:A:GLN:HB3	8	0.15
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD11	6	0.15
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD12	6	0.15
(1,12)	1:5:A:TYR:HB3	1:9:A:LEU:HD13	6	0.15
(1,6)	1:3:A:GLN:HB3	1:3:A:GLN:HA	3	0.15
(2,33)	1:61:A:GLU:H	1:57:A:CYS:O	1	0.14
(1,540)	1:61:A:GLU:H	1:61:A:GLU:HA	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,540)	1:61:A:GLU:H	1:61:A:GLU:HA	6	0.14
(1,531)	1:59:A:THR:H	1:58:A:VAL:HB	1	0.14
(1,526)	1:58:A:VAL:H	1:54:A:GLU:HA	5	0.14
(1,518)	1:56:A:THR:H	1:56:A:THR:HG21	1	0.14
(1,518)	1:56:A:THR:H	1:56:A:THR:HG22	1	0.14
(1,518)	1:56:A:THR:H	1:56:A:THR:HG23	1	0.14
(1,518)	1:56:A:THR:H	1:56:A:THR:HG21	7	0.14
(1,518)	1:56:A:THR:H	1:56:A:THR:HG22	7	0.14
(1,518)	1:56:A:THR:H	1:56:A:THR:HG23	7	0.14
(1,501)	1:53:A:CYS:H	1:52:A:ASP:HB2	1	0.14
(1,501)	1:53:A:CYS:H	1:52:A:ASP:HB2	4	0.14
(1,499)	1:53:A:CYS:H	1:50:A:LEU:HA	1	0.14
(1,497)	1:52:A:ASP:H	1:53:A:CYS:H	5	0.14
(1,486)	1:51:A:GLU:H	1:51:A:GLU:HB3	5	0.14
(1,483)	1:51:A:GLU:H	1:50:A:LEU:HB3	1	0.14
(1,480)	1:51:A:GLU:H	1:49:A:THR:HB	6	0.14
(1,478)	1:50:A:LEU:H	1:50:A:LEU:HB2	2	0.14
(1,474)	1:50:A:LEU:H	1:49:A:THR:HA	4	0.14
(1,466)	1:49:A:THR:H	1:47:A:PHE:HB3	3	0.14
(1,461)	1:48:A:LYS:H	1:48:A:LYS:HA	4	0.14
(1,457)	1:47:A:PHE:H	1:35:A:PHE:HE1	7	0.14
(1,456)	1:43:A:ASN:H	1:43:A:ASN:HB3	4	0.14
(1,445)	1:40:A:SER:H	1:40:A:SER:HA	9	0.14
(1,439)	1:38:A:ARG:H	1:37:A:TYR:HA	3	0.14
(1,433)	1:36:A:ARG:H	1:36:A:ARG:HB2	2	0.14
(1,433)	1:36:A:ARG:H	1:36:A:ARG:HB2	5	0.14
(1,433)	1:36:A:ARG:H	1:36:A:ARG:HB2	8	0.14
(1,429)	1:35:A:PHE:H	1:35:A:PHE:HD1	6	0.14
(1,425)	1:35:A:PHE:H	1:34:A:THR:HA	2	0.14
(1,425)	1:35:A:PHE:H	1:34:A:THR:HA	3	0.14
(1,418)	1:34:A:THR:H	1:33:A:LYS:HA	5	0.14
(1,401)	1:29:A:THR:H	1:29:A:THR:HG21	6	0.14
(1,401)	1:29:A:THR:H	1:29:A:THR:HG22	6	0.14
(1,401)	1:29:A:THR:H	1:29:A:THR:HG23	6	0.14
(1,391)	1:28:A:ALA:H	1:27:A:LYS:HA	1	0.14
(1,391)	1:28:A:ALA:H	1:27:A:LYS:HA	7	0.14
(1,389)	1:27:A:LYS:H	1:27:A:LYS:HB2	5	0.14
(1,385)	1:26:A:ASP:H	1:32:A:CYS:HA	2	0.14
(1,380)	1:25:A:TYR:H	1:25:A:TYR:HB3	1	0.14
(1,377)	1:25:A:TYR:H	1:24:A:TYR:HA	2	0.14
(1,375)	1:24:A:TYR:H	1:33:A:LYS:H	5	0.14
(1,375)	1:24:A:TYR:H	1:33:A:LYS:H	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,364)	1:22:A:ASN:H	1:21:A:THR:HA	3	0.14
(1,362)	1:21:A:THR:H	1:20:A:PHE:HB2	4	0.14
(1,359)	1:20:A:PHE:H	1:20:A:PHE:HB2	3	0.14
(1,351)	1:19:A:SER:H	1:18:A:GLY:HA3	3	0.14
(1,348)	1:18:A:GLY:H	1:18:A:GLY:HA3	3	0.14
(1,347)	1:18:A:GLY:H	1:17:A:SER:HB2	5	0.14
(1,339)	1:16:A:GLY:H	1:38:A:ARG:HG3	1	0.14
(1,338)	1:16:A:GLY:H	1:16:A:GLY:HA2	1	0.14
(1,335)	1:16:A:GLY:H	1:15:A:LYS:HB3	9	0.14
(1,333)	1:15:A:LYS:H	1:16:A:GLY:H	6	0.14
(1,318)	1:13:A:TYR:H	1:12:A:ASN:HB3	9	0.14
(1,302)	1:10:A:SER:H	1:10:A:SER:HB3	10	0.14
(1,291)	1:9:A:LEU:H	1:5:A:TYR:HB3	10	0.14
(1,281)	1:7:A:CYS:H	1:6:A:ARG:HG3	6	0.14
(1,278)	1:6:A:ARG:H	1:6:A:ARG:HG2	2	0.14
(1,278)	1:6:A:ARG:H	1:6:A:ARG:HG2	8	0.14
(1,277)	1:6:A:ARG:H	1:6:A:ARG:HG3	9	0.14
(1,273)	1:5:A:TYR:H	1:4:A:ASP:HB2	5	0.14
(1,272)	1:4:A:ASP:H	1:4:A:ASP:HB2	4	0.14
(1,270)	1:4:A:ASP:H	1:4:A:ASP:HA	4	0.14
(1,264)	1:3:A:GLN:H	1:3:A:GLN:HB2	6	0.14
(1,261)	1:61:A:GLU:HG2	1:59:A:THR:HA	9	0.14
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG21	8	0.14
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG22	8	0.14
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG23	8	0.14
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG21	10	0.14
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG22	10	0.14
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG23	10	0.14
(1,255)	1:58:A:VAL:HG11	1:58:A:VAL:HB	1	0.14
(1,255)	1:58:A:VAL:HG12	1:58:A:VAL:HB	1	0.14
(1,255)	1:58:A:VAL:HG13	1:58:A:VAL:HB	1	0.14
(1,255)	1:58:A:VAL:HG11	1:58:A:VAL:HB	2	0.14
(1,255)	1:58:A:VAL:HG12	1:58:A:VAL:HB	2	0.14
(1,255)	1:58:A:VAL:HG13	1:58:A:VAL:HB	2	0.14
(1,255)	1:58:A:VAL:HG11	1:58:A:VAL:HB	3	0.14
(1,255)	1:58:A:VAL:HG12	1:58:A:VAL:HB	3	0.14
(1,255)	1:58:A:VAL:HG13	1:58:A:VAL:HB	3	0.14
(1,255)	1:58:A:VAL:HG11	1:58:A:VAL:HB	5	0.14
(1,255)	1:58:A:VAL:HG12	1:58:A:VAL:HB	5	0.14
(1,255)	1:58:A:VAL:HG13	1:58:A:VAL:HB	5	0.14
(1,255)	1:58:A:VAL:HG11	1:58:A:VAL:HB	6	0.14
(1,255)	1:58:A:VAL:HG12	1:58:A:VAL:HB	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,255)	1:58:A:VAL:HG13	1:58:A:VAL:HB	6	0.14
(1,255)	1:58:A:VAL:HG11	1:58:A:VAL:HB	7	0.14
(1,255)	1:58:A:VAL:HG12	1:58:A:VAL:HB	7	0.14
(1,255)	1:58:A:VAL:HG13	1:58:A:VAL:HB	7	0.14
(1,255)	1:58:A:VAL:HG11	1:58:A:VAL:HB	8	0.14
(1,255)	1:58:A:VAL:HG12	1:58:A:VAL:HB	8	0.14
(1,255)	1:58:A:VAL:HG13	1:58:A:VAL:HB	8	0.14
(1,255)	1:58:A:VAL:HG11	1:58:A:VAL:HB	10	0.14
(1,255)	1:58:A:VAL:HG12	1:58:A:VAL:HB	10	0.14
(1,255)	1:58:A:VAL:HG13	1:58:A:VAL:HB	10	0.14
(1,249)	1:57:A:CYS:HA	1:7:A:CYS:HB2	4	0.14
(1,238)	1:54:A:GLU:HB2	1:55:A:ALA:H	6	0.14
(1,234)	1:54:A:GLU:HA	1:58:A:VAL:HB	3	0.14
(1,225)	1:53:A:CYS:H	1:53:A:CYS:HB3	5	0.14
(1,224)	1:52:A:ASP:HA	1:52:A:ASP:HB2	2	0.14
(1,192)	1:46:A:ARG:HA	1:46:A:ARG:HG3	10	0.14
(1,188)	1:40:A:SER:HA	1:41:A:GLY:HA2	1	0.14
(1,188)	1:40:A:SER:HA	1:41:A:GLY:HA2	2	0.14
(1,187)	1:40:A:SER:HA	1:41:A:GLY:HA3	1	0.14
(1,185)	1:37:A:TYR:HB2	1:46:A:ARG:HG3	6	0.14
(1,182)	1:37:A:TYR:HB2	1:20:A:PHE:HB3	6	0.14
(1,170)	1:35:A:PHE:HE1	1:37:A:TYR:HA	9	0.14
(1,165)	1:35:A:PHE:HD1	1:34:A:THR:HB	4	0.14
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG21	4	0.14
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG22	4	0.14
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG23	4	0.14
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG21	8	0.14
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG22	8	0.14
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG23	8	0.14
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG21	9	0.14
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG22	9	0.14
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG23	9	0.14
(1,141)	1:32:A:CYS:HB3	1:50:A:LEU:HB3	3	0.14
(1,141)	1:32:A:CYS:HB3	1:50:A:LEU:HB3	5	0.14
(1,138)	1:32:A:CYS:HA	1:50:A:LEU:HB2	10	0.14
(1,136)	1:32:A:CYS:HA	1:32:A:CYS:HB3	6	0.14
(1,131)	1:30:A:SER:HB2	1:29:A:THR:HA	6	0.14
(1,131)	1:30:A:SER:HB2	1:29:A:THR:HA	10	0.14
(1,126)	1:27:A:LYS:HB2	1:27:A:LYS:HA	1	0.14
(1,126)	1:27:A:LYS:HB2	1:27:A:LYS:HA	2	0.14
(1,65)	1:19:A:SER:HA	1:19:A:SER:HB2	5	0.14
(1,61)	1:17:A:SER:HA	1:17:A:SER:HB2	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:9:A:LEU:HD11	1:45:A:ASN:HB2	8	0.14
(1,26)	1:9:A:LEU:HD12	1:45:A:ASN:HB2	8	0.14
(1,26)	1:9:A:LEU:HD13	1:45:A:ASN:HB2	8	0.14
(1,24)	1:9:A:LEU:HA	1:9:A:LEU:HG	4	0.14
(1,24)	1:9:A:LEU:HA	1:9:A:LEU:HG	9	0.14
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD11	1	0.14
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD12	1	0.14
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD13	1	0.14
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD11	9	0.14
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD12	9	0.14
(1,14)	1:6:A:ARG:HA	1:9:A:LEU:HD13	9	0.14
(1,11)	1:5:A:TYR:HB3	1:8:A:GLN:HG3	1	0.14
(1,6)	1:3:A:GLN:HB3	1:3:A:GLN:HA	10	0.14
(2,31)	1:60:A:ALA:H	1:56:A:THR:O	8	0.13
(2,31)	1:60:A:ALA:H	1:56:A:THR:O	10	0.13
(1,539)	1:61:A:GLU:H	1:60:A:ALA:HA	1	0.13
(1,539)	1:61:A:GLU:H	1:60:A:ALA:HA	2	0.13
(1,539)	1:61:A:GLU:H	1:60:A:ALA:HA	3	0.13
(1,536)	1:60:A:ALA:H	1:59:A:THR:HB	8	0.13
(1,528)	1:58:A:VAL:H	1:58:A:VAL:HA	8	0.13
(1,528)	1:58:A:VAL:H	1:58:A:VAL:HA	10	0.13
(1,518)	1:56:A:THR:H	1:56:A:THR:HG21	5	0.13
(1,518)	1:56:A:THR:H	1:56:A:THR:HG22	5	0.13
(1,518)	1:56:A:THR:H	1:56:A:THR:HG23	5	0.13
(1,513)	1:55:A:ALA:H	1:56:A:THR:H	6	0.13
(1,505)	1:54:A:GLU:H	1:53:A:CYS:H	7	0.13
(1,501)	1:53:A:CYS:H	1:52:A:ASP:HB2	6	0.13
(1,500)	1:53:A:CYS:H	1:52:A:ASP:HB3	8	0.13
(1,498)	1:53:A:CYS:H	1:47:A:PHE:HB3	1	0.13
(1,497)	1:52:A:ASP:H	1:53:A:CYS:H	10	0.13
(1,496)	1:52:A:ASP:H	1:52:A:ASP:HB2	4	0.13
(1,493)	1:52:A:ASP:H	1:51:A:GLU:HG2	6	0.13
(1,487)	1:51:A:GLU:H	1:51:A:GLU:HG3	4	0.13
(1,487)	1:51:A:GLU:H	1:51:A:GLU:HG3	7	0.13
(1,486)	1:51:A:GLU:H	1:51:A:GLU:HB3	7	0.13
(1,486)	1:51:A:GLU:H	1:51:A:GLU:HB3	10	0.13
(1,483)	1:51:A:GLU:H	1:50:A:LEU:HB3	5	0.13
(1,481)	1:51:A:GLU:H	1:50:A:LEU:H	7	0.13
(1,480)	1:51:A:GLU:H	1:49:A:THR:HB	4	0.13
(1,461)	1:48:A:LYS:H	1:48:A:LYS:HA	5	0.13
(1,453)	1:42:A:GLY:H	1:41:A:GLY:HA2	6	0.13
(1,431)	1:36:A:ARG:H	1:36:A:ARG:HA	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,430)	1:36:A:ARG:H	1:35:A:PHE:HA	4	0.13
(1,425)	1:35:A:PHE:H	1:34:A:THR:HA	6	0.13
(1,418)	1:34:A:THR:H	1:33:A:LYS:HA	8	0.13
(1,406)	1:30:A:SER:H	1:30:A:SER:HB2	6	0.13
(1,401)	1:29:A:THR:H	1:29:A:THR:HG21	2	0.13
(1,401)	1:29:A:THR:H	1:29:A:THR:HG22	2	0.13
(1,401)	1:29:A:THR:H	1:29:A:THR:HG23	2	0.13
(1,401)	1:29:A:THR:H	1:29:A:THR:HG21	5	0.13
(1,401)	1:29:A:THR:H	1:29:A:THR:HG22	5	0.13
(1,401)	1:29:A:THR:H	1:29:A:THR:HG23	5	0.13
(1,398)	1:29:A:THR:H	1:28:A:ALA:HA	7	0.13
(1,397)	1:29:A:THR:H	1:27:A:LYS:HA	7	0.13
(1,395)	1:28:A:ALA:H	1:29:A:THR:HG21	1	0.13
(1,395)	1:28:A:ALA:H	1:29:A:THR:HG22	1	0.13
(1,395)	1:28:A:ALA:H	1:29:A:THR:HG23	1	0.13
(1,371)	1:23:A:TYR:H	1:23:A:TYR:HD1	2	0.13
(1,369)	1:23:A:TYR:H	1:22:A:ASN:HB3	9	0.13
(1,364)	1:22:A:ASN:H	1:21:A:THR:HA	1	0.13
(1,364)	1:22:A:ASN:H	1:21:A:THR:HA	2	0.13
(1,362)	1:21:A:THR:H	1:20:A:PHE:HB2	3	0.13
(1,355)	1:20:A:PHE:H	1:19:A:SER:HA	7	0.13
(1,354)	1:19:A:SER:H	1:19:A:SER:HB3	5	0.13
(1,346)	1:18:A:GLY:H	1:17:A:SER:HA	5	0.13
(1,346)	1:18:A:GLY:H	1:17:A:SER:HA	10	0.13
(1,328)	1:14:A:GLY:H	1:14:A:GLY:HA2	4	0.13
(1,323)	1:13:A:TYR:H	1:14:A:GLY:H	1	0.13
(1,311)	1:12:A:ASN:H	1:11:A:ARG:HG2	8	0.13
(1,306)	1:11:A:ARG:H	1:11:A:ARG:HB3	10	0.13
(1,302)	1:10:A:SER:H	1:10:A:SER:HB3	1	0.13
(1,290)	1:9:A:LEU:H	1:5:A:TYR:HA	2	0.13
(1,279)	1:6:A:ARG:H	1:7:A:CYS:H	5	0.13
(1,279)	1:6:A:ARG:H	1:7:A:CYS:H	7	0.13
(1,270)	1:4:A:ASP:H	1:4:A:ASP:HA	8	0.13
(1,269)	1:4:A:ASP:H	1:3:A:GLN:HB3	7	0.13
(1,260)	1:61:A:GLU:HG3	1:61:A:GLU:HA	1	0.13
(1,259)	1:61:A:GLU:HA	1:61:A:GLU:HG2	10	0.13
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG21	3	0.13
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG22	3	0.13
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG23	3	0.13
(1,256)	1:59:A:THR:HA	1:58:A:VAL:HG11	7	0.13
(1,256)	1:59:A:THR:HA	1:58:A:VAL:HG12	7	0.13
(1,256)	1:59:A:THR:HA	1:58:A:VAL:HG13	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:55:A:ALA:HB1	1:52:A:ASP:HA	3	0.13
(1,242)	1:55:A:ALA:HB2	1:52:A:ASP:HA	3	0.13
(1,242)	1:55:A:ALA:HB3	1:52:A:ASP:HA	3	0.13
(1,242)	1:55:A:ALA:HB1	1:52:A:ASP:HA	7	0.13
(1,242)	1:55:A:ALA:HB2	1:52:A:ASP:HA	7	0.13
(1,242)	1:55:A:ALA:HB3	1:52:A:ASP:HA	7	0.13
(1,225)	1:53:A:CYS:H	1:53:A:CYS:HB3	9	0.13
(1,224)	1:52:A:ASP:HA	1:52:A:ASP:HB2	4	0.13
(1,190)	1:40:A:SER:HB2	1:40:A:SER:HA	6	0.13
(1,185)	1:37:A:TYR:HB2	1:46:A:ARG:HG3	4	0.13
(1,182)	1:37:A:TYR:HB2	1:20:A:PHE:HB3	7	0.13
(1,164)	1:35:A:PHE:HD1	1:34:A:THR:HA	5	0.13
(1,164)	1:35:A:PHE:HD1	1:34:A:THR:HA	8	0.13
(1,160)	1:35:A:PHE:HA	1:36:A:ARG:HA	2	0.13
(1,146)	1:33:A:LYS:HA	1:33:A:LYS:HG3	7	0.13
(1,146)	1:33:A:LYS:HA	1:33:A:LYS:HG3	8	0.13
(1,146)	1:33:A:LYS:HA	1:33:A:LYS:HG3	10	0.13
(1,141)	1:32:A:CYS:HB3	1:50:A:LEU:HB3	10	0.13
(1,136)	1:32:A:CYS:HA	1:32:A:CYS:HB3	5	0.13
(1,136)	1:32:A:CYS:HA	1:32:A:CYS:HB3	9	0.13
(1,136)	1:32:A:CYS:HA	1:32:A:CYS:HB3	10	0.13
(1,102)	1:24:A:TYR:HD1	1:24:A:TYR:HA	1	0.13
(1,102)	1:24:A:TYR:HD1	1:24:A:TYR:HA	2	0.13
(1,93)	1:24:A:TYR:HA	1:47:A:PHE:HB3	7	0.13
(1,88)	1:23:A:TYR:HE1	1:49:A:THR:HA	8	0.13
(1,65)	1:19:A:SER:HA	1:19:A:SER:HB2	6	0.13
(1,6)	1:3:A:GLN:HB3	1:3:A:GLN:HA	6	0.13
(2,31)	1:60:A:ALA:H	1:56:A:THR:O	7	0.12
(1,541)	1:61:A:GLU:H	1:61:A:GLU:HB2	9	0.12
(1,536)	1:60:A:ALA:H	1:59:A:THR:HB	1	0.12
(1,531)	1:59:A:THR:H	1:58:A:VAL:HB	6	0.12
(1,531)	1:59:A:THR:H	1:58:A:VAL:HB	7	0.12
(1,519)	1:57:A:CYS:H	1:54:A:GLU:HA	2	0.12
(1,506)	1:54:A:GLU:H	1:53:A:CYS:HB3	2	0.12
(1,506)	1:54:A:GLU:H	1:53:A:CYS:HB3	3	0.12
(1,505)	1:54:A:GLU:H	1:53:A:CYS:H	3	0.12
(1,503)	1:53:A:CYS:H	1:53:A:CYS:HB2	8	0.12
(1,501)	1:53:A:CYS:H	1:52:A:ASP:HB2	2	0.12
(1,500)	1:53:A:CYS:H	1:52:A:ASP:HB3	9	0.12
(1,498)	1:53:A:CYS:H	1:47:A:PHE:HB3	3	0.12
(1,497)	1:52:A:ASP:H	1:53:A:CYS:H	7	0.12
(1,496)	1:52:A:ASP:H	1:52:A:ASP:HB2	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD11	8	0.12
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD12	8	0.12
(1,484)	1:51:A:GLU:H	1:50:A:LEU:HD13	8	0.12
(1,480)	1:51:A:GLU:H	1:49:A:THR:HB	1	0.12
(1,480)	1:51:A:GLU:H	1:49:A:THR:HB	8	0.12
(1,480)	1:51:A:GLU:H	1:49:A:THR:HB	10	0.12
(1,475)	1:50:A:LEU:H	1:49:A:THR:HB	10	0.12
(1,471)	1:49:A:THR:H	1:49:A:THR:HG21	8	0.12
(1,471)	1:49:A:THR:H	1:49:A:THR:HG22	8	0.12
(1,471)	1:49:A:THR:H	1:49:A:THR:HG23	8	0.12
(1,456)	1:43:A:ASN:H	1:43:A:ASN:HB3	7	0.12
(1,450)	1:41:A:GLY:H	1:41:A:GLY:HA3	8	0.12
(1,449)	1:41:A:GLY:H	1:40:A:SER:HA	6	0.12
(1,448)	1:41:A:GLY:H	1:40:A:SER:H	6	0.12
(1,433)	1:36:A:ARG:H	1:36:A:ARG:HB2	3	0.12
(1,431)	1:36:A:ARG:H	1:36:A:ARG:HA	4	0.12
(1,431)	1:36:A:ARG:H	1:36:A:ARG:HA	7	0.12
(1,430)	1:36:A:ARG:H	1:35:A:PHE:HA	8	0.12
(1,425)	1:35:A:PHE:H	1:34:A:THR:HA	1	0.12
(1,423)	1:35:A:PHE:H	1:21:A:THR:HG21	10	0.12
(1,423)	1:35:A:PHE:H	1:21:A:THR:HG22	10	0.12
(1,423)	1:35:A:PHE:H	1:21:A:THR:HG23	10	0.12
(1,422)	1:35:A:PHE:H	1:21:A:THR:HA	7	0.12
(1,418)	1:34:A:THR:H	1:33:A:LYS:HA	3	0.12
(1,418)	1:34:A:THR:H	1:33:A:LYS:HA	4	0.12
(1,413)	1:32:A:CYS:H	1:32:A:CYS:HB2	4	0.12
(1,406)	1:30:A:SER:H	1:30:A:SER:HB2	4	0.12
(1,401)	1:29:A:THR:H	1:29:A:THR:HG21	4	0.12
(1,401)	1:29:A:THR:H	1:29:A:THR:HG22	4	0.12
(1,401)	1:29:A:THR:H	1:29:A:THR:HG23	4	0.12
(1,398)	1:29:A:THR:H	1:28:A:ALA:HA	9	0.12
(1,397)	1:29:A:THR:H	1:27:A:LYS:HA	6	0.12
(1,396)	1:28:A:ALA:H	1:30:A:SER:H	10	0.12
(1,385)	1:26:A:ASP:H	1:32:A:CYS:HA	7	0.12
(1,384)	1:26:A:ASP:H	1:26:A:ASP:HB2	9	0.12
(1,383)	1:26:A:ASP:H	1:26:A:ASP:HB3	9	0.12
(1,380)	1:25:A:TYR:H	1:25:A:TYR:HB3	2	0.12
(1,368)	1:23:A:TYR:H	1:22:A:ASN:HA	2	0.12
(1,367)	1:22:A:ASN:H	1:22:A:ASN:HB2	4	0.12
(1,367)	1:22:A:ASN:H	1:22:A:ASN:HB2	10	0.12
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG21	4	0.12
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG22	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG23	4	0.12
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG21	5	0.12
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG22	5	0.12
(1,365)	1:22:A:ASN:H	1:21:A:THR:HG23	5	0.12
(1,355)	1:20:A:PHE:H	1:19:A:SER:HA	8	0.12
(1,346)	1:18:A:GLY:H	1:17:A:SER:HA	1	0.12
(1,346)	1:18:A:GLY:H	1:17:A:SER:HA	8	0.12
(1,335)	1:16:A:GLY:H	1:15:A:LYS:HB3	2	0.12
(1,335)	1:16:A:GLY:H	1:15:A:LYS:HB3	3	0.12
(1,335)	1:16:A:GLY:H	1:15:A:LYS:HB3	10	0.12
(1,333)	1:15:A:LYS:H	1:16:A:GLY:H	3	0.12
(1,320)	1:13:A:TYR:H	1:13:A:TYR:HA	3	0.12
(1,320)	1:13:A:TYR:H	1:13:A:TYR:HA	6	0.12
(1,312)	1:12:A:ASN:H	1:12:A:ASN:HB3	6	0.12
(1,306)	1:11:A:ARG:H	1:11:A:ARG:HB3	8	0.12
(1,297)	1:9:A:LEU:H	1:9:A:LEU:HG	3	0.12
(1,295)	1:9:A:LEU:H	1:9:A:LEU:HA	1	0.12
(1,295)	1:9:A:LEU:H	1:9:A:LEU:HA	7	0.12
(1,291)	1:9:A:LEU:H	1:5:A:TYR:HB3	9	0.12
(1,287)	1:8:A:GLN:H	1:7:A:CYS:HA	9	0.12
(1,261)	1:61:A:GLU:HG2	1:59:A:THR:HA	8	0.12
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG21	4	0.12
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG22	4	0.12
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG23	4	0.12
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG21	9	0.12
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG22	9	0.12
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG23	9	0.12
(1,251)	1:57:A:CYS:HA	1:57:A:CYS:HB2	1	0.12
(1,242)	1:55:A:ALA:HB1	1:52:A:ASP:HA	9	0.12
(1,242)	1:55:A:ALA:HB2	1:52:A:ASP:HA	9	0.12
(1,242)	1:55:A:ALA:HB3	1:52:A:ASP:HA	9	0.12
(1,225)	1:53:A:CYS:H	1:53:A:CYS:HB3	2	0.12
(1,225)	1:53:A:CYS:H	1:53:A:CYS:HB3	7	0.12
(1,210)	1:49:A:THR:HB	1:51:A:GLU:HG2	5	0.12
(1,210)	1:49:A:THR:HB	1:51:A:GLU:HG2	7	0.12
(1,208)	1:48:A:LYS:HD3	1:48:A:LYS:HA	5	0.12
(1,203)	1:48:A:LYS:HA	1:22:A:ASN:HA	4	0.12
(1,199)	1:47:A:PHE:HB3	1:53:A:CYS:HA	1	0.12
(1,199)	1:47:A:PHE:HB3	1:53:A:CYS:HA	4	0.12
(1,187)	1:40:A:SER:HA	1:41:A:GLY:HA3	7	0.12
(1,185)	1:37:A:TYR:HB2	1:46:A:ARG:HG3	10	0.12
(1,182)	1:37:A:TYR:HB2	1:20:A:PHE:HB3	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,177)	1:36:A:ARG:HG2	1:35:A:PHE:HA	2	0.12
(1,177)	1:36:A:ARG:HG2	1:35:A:PHE:HA	8	0.12
(1,174)	1:36:A:ARG:HA	1:36:A:ARG:HG2	7	0.12
(1,172)	1:36:A:ARG:HA	1:21:A:THR:HA	10	0.12
(1,160)	1:35:A:PHE:HA	1:36:A:ARG:HA	10	0.12
(1,155)	1:34:A:THR:HB	1:21:A:THR:HA	3	0.12
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG21	3	0.12
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG22	3	0.12
(1,154)	1:34:A:THR:HA	1:34:A:THR:HG23	3	0.12
(1,148)	1:33:A:LYS:HE3	1:33:A:LYS:HD2	3	0.12
(1,126)	1:27:A:LYS:HB2	1:27:A:LYS:HA	6	0.12
(1,126)	1:27:A:LYS:HB2	1:27:A:LYS:HA	10	0.12
(1,88)	1:23:A:TYR:HE1	1:49:A:THR:HA	10	0.12
(1,73)	1:20:A:PHE:HA	1:20:A:PHE:HB2	8	0.12
(1,65)	1:19:A:SER:HA	1:19:A:SER:HB2	1	0.12
(1,61)	1:17:A:SER:HA	1:17:A:SER:HB2	9	0.12
(1,49)	1:12:A:ASN:HA	1:12:A:ASN:HB2	9	0.12
(1,30)	1:11:A:ARG:HA	1:10:A:SER:HA	4	0.12
(1,28)	1:10:A:SER:HB3	1:10:A:SER:HA	8	0.12
(1,24)	1:9:A:LEU:HA	1:9:A:LEU:HG	3	0.12
(1,7)	1:4:A:ASP:HA	1:4:A:ASP:HB2	4	0.12
(1,6)	1:3:A:GLN:HB3	1:3:A:GLN:HA	5	0.12
(2,31)	1:60:A:ALA:H	1:56:A:THR:O	3	0.11
(2,23)	1:56:A:THR:H	1:52:A:ASP:O	7	0.11
(1,541)	1:61:A:GLU:H	1:61:A:GLU:HB2	2	0.11
(1,541)	1:61:A:GLU:H	1:61:A:GLU:HB2	6	0.11
(1,539)	1:61:A:GLU:H	1:60:A:ALA:HA	10	0.11
(1,526)	1:58:A:VAL:H	1:54:A:GLU:HA	7	0.11
(1,526)	1:58:A:VAL:H	1:54:A:GLU:HA	8	0.11
(1,505)	1:54:A:GLU:H	1:53:A:CYS:H	2	0.11
(1,505)	1:54:A:GLU:H	1:53:A:CYS:H	5	0.11
(1,501)	1:53:A:CYS:H	1:52:A:ASP:HB2	10	0.11
(1,500)	1:53:A:CYS:H	1:52:A:ASP:HB3	4	0.11
(1,490)	1:52:A:ASP:H	1:49:A:THR:HB	3	0.11
(1,481)	1:51:A:GLU:H	1:50:A:LEU:H	10	0.11
(1,475)	1:50:A:LEU:H	1:49:A:THR:HB	8	0.11
(1,469)	1:49:A:THR:H	1:48:A:LYS:HB2	9	0.11
(1,462)	1:48:A:LYS:H	1:48:A:LYS:HB2	6	0.11
(1,461)	1:48:A:LYS:H	1:48:A:LYS:HA	7	0.11
(1,461)	1:48:A:LYS:H	1:48:A:LYS:HA	9	0.11
(1,449)	1:41:A:GLY:H	1:40:A:SER:HA	5	0.11
(1,444)	1:39:A:GLY:H	1:40:A:SER:H	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:38:A:ARG:H	1:37:A:TYR:HA	1	0.11
(1,439)	1:38:A:ARG:H	1:37:A:TYR:HA	5	0.11
(1,439)	1:38:A:ARG:H	1:37:A:TYR:HA	6	0.11
(1,438)	1:38:A:ARG:H	1:36:A:ARG:HB2	9	0.11
(1,436)	1:37:A:TYR:H	1:36:A:ARG:HB2	5	0.11
(1,433)	1:36:A:ARG:H	1:36:A:ARG:HB2	9	0.11
(1,429)	1:35:A:PHE:H	1:35:A:PHE:HD1	4	0.11
(1,426)	1:35:A:PHE:H	1:34:A:THR:HB	7	0.11
(1,422)	1:35:A:PHE:H	1:21:A:THR:HA	8	0.11
(1,417)	1:33:A:LYS:H	1:33:A:LYS:HB3	4	0.11
(1,395)	1:28:A:ALA:H	1:29:A:THR:HG21	9	0.11
(1,395)	1:28:A:ALA:H	1:29:A:THR:HG22	9	0.11
(1,395)	1:28:A:ALA:H	1:29:A:THR:HG23	9	0.11
(1,385)	1:26:A:ASP:H	1:32:A:CYS:HA	5	0.11
(1,384)	1:26:A:ASP:H	1:26:A:ASP:HB2	5	0.11
(1,381)	1:25:A:TYR:H	1:25:A:TYR:HB2	2	0.11
(1,380)	1:25:A:TYR:H	1:25:A:TYR:HB3	8	0.11
(1,367)	1:22:A:ASN:H	1:22:A:ASN:HB2	9	0.11
(1,358)	1:20:A:PHE:H	1:20:A:PHE:HB3	2	0.11
(1,355)	1:20:A:PHE:H	1:19:A:SER:HA	1	0.11
(1,355)	1:20:A:PHE:H	1:19:A:SER:HA	5	0.11
(1,354)	1:19:A:SER:H	1:19:A:SER:HB3	1	0.11
(1,354)	1:19:A:SER:H	1:19:A:SER:HB3	3	0.11
(1,348)	1:18:A:GLY:H	1:18:A:GLY:HA3	2	0.11
(1,346)	1:18:A:GLY:H	1:17:A:SER:HA	3	0.11
(1,346)	1:18:A:GLY:H	1:17:A:SER:HA	7	0.11
(1,336)	1:16:A:GLY:H	1:15:A:LYS:HG2	7	0.11
(1,336)	1:16:A:GLY:H	1:15:A:LYS:HG2	10	0.11
(1,329)	1:15:A:LYS:H	1:15:A:LYS:HA	1	0.11
(1,328)	1:14:A:GLY:H	1:14:A:GLY:HA2	8	0.11
(1,322)	1:13:A:TYR:H	1:13:A:TYR:HB2	4	0.11
(1,315)	1:12:A:ASN:HD21	1:12:A:ASN:HB2	10	0.11
(1,305)	1:11:A:ARG:H	1:11:A:ARG:HA	1	0.11
(1,297)	1:9:A:LEU:H	1:9:A:LEU:HG	4	0.11
(1,293)	1:9:A:LEU:H	1:8:A:GLN:HA	1	0.11
(1,292)	1:9:A:LEU:H	1:8:A:GLN:H	2	0.11
(1,291)	1:9:A:LEU:H	1:5:A:TYR:HB3	2	0.11
(1,291)	1:9:A:LEU:H	1:5:A:TYR:HB3	4	0.11
(1,290)	1:9:A:LEU:H	1:5:A:TYR:HA	5	0.11
(1,287)	1:8:A:GLN:H	1:7:A:CYS:HA	1	0.11
(1,287)	1:8:A:GLN:H	1:7:A:CYS:HA	2	0.11
(1,287)	1:8:A:GLN:H	1:7:A:CYS:HA	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,285)	1:7:A:CYS:H	1:7:A:CYS:HB2	3	0.11
(1,285)	1:7:A:CYS:H	1:7:A:CYS:HB2	5	0.11
(1,282)	1:7:A:CYS:H	1:6:A:ARG:HG2	6	0.11
(1,282)	1:7:A:CYS:H	1:6:A:ARG:HG2	7	0.11
(1,279)	1:6:A:ARG:H	1:7:A:CYS:H	6	0.11
(1,278)	1:6:A:ARG:H	1:6:A:ARG:HG2	1	0.11
(1,273)	1:5:A:TYR:H	1:4:A:ASP:HB2	8	0.11
(1,271)	1:4:A:ASP:H	1:4:A:ASP:HB3	9	0.11
(1,270)	1:4:A:ASP:H	1:4:A:ASP:HA	1	0.11
(1,270)	1:4:A:ASP:H	1:4:A:ASP:HA	6	0.11
(1,264)	1:3:A:GLN:H	1:3:A:GLN:HB2	3	0.11
(1,263)	1:3:A:GLN:H	1:3:A:GLN:HA	10	0.11
(1,259)	1:61:A:GLU:HA	1:61:A:GLU:HG2	8	0.11
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG21	7	0.11
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG22	7	0.11
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG23	7	0.11
(1,256)	1:59:A:THR:HA	1:58:A:VAL:HG11	8	0.11
(1,256)	1:59:A:THR:HA	1:58:A:VAL:HG12	8	0.11
(1,256)	1:59:A:THR:HA	1:58:A:VAL:HG13	8	0.11
(1,234)	1:54:A:GLU:HA	1:58:A:VAL:HB	8	0.11
(1,224)	1:52:A:ASP:HA	1:52:A:ASP:HB2	1	0.11
(1,203)	1:48:A:LYS:HA	1:22:A:ASN:HA	1	0.11
(1,203)	1:48:A:LYS:HA	1:22:A:ASN:HA	3	0.11
(1,203)	1:48:A:LYS:HA	1:22:A:ASN:HA	7	0.11
(1,196)	1:47:A:PHE:HA	1:48:A:LYS:HD3	8	0.11
(1,195)	1:47:A:PHE:HA	1:47:A:PHE:HB3	10	0.11
(1,194)	1:47:A:PHE:HA	1:46:A:ARG:HG2	2	0.11
(1,192)	1:46:A:ARG:HA	1:46:A:ARG:HG3	1	0.11
(1,190)	1:40:A:SER:HB2	1:40:A:SER:HA	10	0.11
(1,177)	1:36:A:ARG:HG2	1:35:A:PHE:HA	9	0.11
(1,170)	1:35:A:PHE:HE1	1:37:A:TYR:HA	1	0.11
(1,160)	1:35:A:PHE:HA	1:36:A:ARG:HA	9	0.11
(1,158)	1:35:A:PHE:HA	1:34:A:THR:HB	2	0.11
(1,158)	1:35:A:PHE:HA	1:34:A:THR:HB	8	0.11
(1,155)	1:34:A:THR:HB	1:21:A:THR:HA	9	0.11
(1,138)	1:32:A:CYS:HA	1:50:A:LEU:HB2	7	0.11
(1,32)	1:11:A:ARG:HA	1:11:A:ARG:HB2	5	0.11
(1,31)	1:11:A:ARG:HA	1:11:A:ARG:HB3	5	0.11
(1,28)	1:10:A:SER:HB3	1:10:A:SER:HA	4	0.11
(1,26)	1:9:A:LEU:HD11	1:45:A:ASN:HB2	10	0.11
(1,26)	1:9:A:LEU:HD12	1:45:A:ASN:HB2	10	0.11
(1,26)	1:9:A:LEU:HD13	1:45:A:ASN:HB2	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:9:A:LEU:HA	1:9:A:LEU:HG	8	0.11
(1,23)	1:9:A:LEU:HA	1:5:A:TYR:HB3	10	0.11
(1,17)	1:7:A:CYS:HA	1:7:A:CYS:HB2	1	0.11
(1,16)	1:7:A:CYS:HA	1:6:A:ARG:HA	8	0.11
(1,15)	1:6:A:ARG:HG3	1:6:A:ARG:HA	7	0.11
(1,6)	1:3:A:GLN:HB3	1:3:A:GLN:HA	7	0.11
(1,542)	1:61:A:GLU:H	1:61:A:GLU:HG3	6	0.1
(1,541)	1:61:A:GLU:H	1:61:A:GLU:HB2	1	0.1
(1,536)	1:60:A:ALA:H	1:59:A:THR:HB	3	0.1
(1,531)	1:59:A:THR:H	1:58:A:VAL:HB	9	0.1
(1,528)	1:58:A:VAL:H	1:58:A:VAL:HA	7	0.1
(1,517)	1:56:A:THR:H	1:56:A:THR:HB	3	0.1
(1,506)	1:54:A:GLU:H	1:53:A:CYS:HB3	4	0.1
(1,505)	1:54:A:GLU:H	1:53:A:CYS:H	4	0.1
(1,505)	1:54:A:GLU:H	1:53:A:CYS:H	9	0.1
(1,496)	1:52:A:ASP:H	1:52:A:ASP:HB2	1	0.1
(1,487)	1:51:A:GLU:H	1:51:A:GLU:HG3	1	0.1
(1,483)	1:51:A:GLU:H	1:50:A:LEU:HB3	3	0.1
(1,481)	1:51:A:GLU:H	1:50:A:LEU:H	8	0.1
(1,473)	1:49:A:THR:H	1:52:A:ASP:HB2	7	0.1
(1,466)	1:49:A:THR:H	1:47:A:PHE:HB3	5	0.1
(1,446)	1:40:A:SER:H	1:40:A:SER:HB3	2	0.1
(1,445)	1:40:A:SER:H	1:40:A:SER:HA	10	0.1
(1,436)	1:37:A:TYR:H	1:36:A:ARG:HB2	1	0.1
(1,431)	1:36:A:ARG:H	1:36:A:ARG:HA	8	0.1
(1,430)	1:36:A:ARG:H	1:35:A:PHE:HA	3	0.1
(1,423)	1:35:A:PHE:H	1:21:A:THR:HG21	9	0.1
(1,423)	1:35:A:PHE:H	1:21:A:THR:HG22	9	0.1
(1,423)	1:35:A:PHE:H	1:21:A:THR:HG23	9	0.1
(1,420)	1:34:A:THR:H	1:33:A:LYS:HD3	2	0.1
(1,410)	1:32:A:CYS:H	1:31:A:SER:HA	9	0.1
(1,408)	1:31:A:SER:H	1:30:A:SER:HA	3	0.1
(1,408)	1:31:A:SER:H	1:30:A:SER:HA	6	0.1
(1,398)	1:29:A:THR:H	1:28:A:ALA:HA	2	0.1
(1,394)	1:28:A:ALA:H	1:29:A:THR:H	8	0.1
(1,391)	1:28:A:ALA:H	1:27:A:LYS:HA	6	0.1
(1,388)	1:27:A:LYS:H	1:27:A:LYS:HB3	2	0.1
(1,381)	1:25:A:TYR:H	1:25:A:TYR:HB2	7	0.1
(1,375)	1:24:A:TYR:H	1:33:A:LYS:H	10	0.1
(1,355)	1:20:A:PHE:H	1:19:A:SER:HA	9	0.1
(1,348)	1:18:A:GLY:H	1:18:A:GLY:HA3	6	0.1
(1,346)	1:18:A:GLY:H	1:17:A:SER:HA	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,325)	1:14:A:GLY:H	1:13:A:TYR:HB3	9	0.1
(1,321)	1:13:A:TYR:H	1:13:A:TYR:HB3	5	0.1
(1,321)	1:13:A:TYR:H	1:13:A:TYR:HB3	10	0.1
(1,320)	1:13:A:TYR:H	1:13:A:TYR:HA	1	0.1
(1,311)	1:12:A:ASN:H	1:11:A:ARG:HG2	4	0.1
(1,295)	1:9:A:LEU:H	1:9:A:LEU:HA	3	0.1
(1,290)	1:9:A:LEU:H	1:5:A:TYR:HA	6	0.1
(1,287)	1:8:A:GLN:H	1:7:A:CYS:HA	5	0.1
(1,282)	1:7:A:CYS:H	1:6:A:ARG:HG2	10	0.1
(1,280)	1:7:A:CYS:H	1:6:A:ARG:HA	8	0.1
(1,263)	1:3:A:GLN:H	1:3:A:GLN:HA	3	0.1
(1,263)	1:3:A:GLN:H	1:3:A:GLN:HA	5	0.1
(1,260)	1:61:A:GLU:HG3	1:61:A:GLU:HA	3	0.1
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG21	5	0.1
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG22	5	0.1
(1,257)	1:59:A:THR:HA	1:59:A:THR:HG23	5	0.1
(1,256)	1:59:A:THR:HA	1:58:A:VAL:HG11	3	0.1
(1,256)	1:59:A:THR:HA	1:58:A:VAL:HG12	3	0.1
(1,256)	1:59:A:THR:HA	1:58:A:VAL:HG13	3	0.1
(1,226)	1:53:A:CYS:HA	1:53:A:CYS:HB2	6	0.1
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD21	7	0.1
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD22	7	0.1
(1,216)	1:51:A:GLU:HA	1:50:A:LEU:HD23	7	0.1
(1,201)	1:47:A:PHE:HD1	1:47:A:PHE:HB3	6	0.1
(1,188)	1:40:A:SER:HA	1:41:A:GLY:HA2	10	0.1
(1,180)	1:37:A:TYR:HA	1:37:A:TYR:HB2	7	0.1
(1,170)	1:35:A:PHE:HE1	1:37:A:TYR:HA	2	0.1
(1,170)	1:35:A:PHE:HE1	1:37:A:TYR:HA	7	0.1
(1,158)	1:35:A:PHE:HA	1:34:A:THR:HB	1	0.1
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG21	3	0.1
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG22	3	0.1
(1,156)	1:34:A:THR:HB	1:21:A:THR:HG23	3	0.1
(1,138)	1:32:A:CYS:HA	1:50:A:LEU:HB2	3	0.1
(1,138)	1:32:A:CYS:HA	1:50:A:LEU:HB2	8	0.1
(1,138)	1:32:A:CYS:HA	1:50:A:LEU:HB2	9	0.1
(1,135)	1:32:A:CYS:HA	1:25:A:TYR:HB2	5	0.1
(1,135)	1:32:A:CYS:HA	1:25:A:TYR:HB2	7	0.1
(1,73)	1:20:A:PHE:HA	1:20:A:PHE:HB2	7	0.1
(1,32)	1:11:A:ARG:HA	1:11:A:ARG:HB2	6	0.1
(1,7)	1:4:A:ASP:HA	1:4:A:ASP:HB2	1	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found