



Full wwPDB NMR Structure Validation Report ⓘ

Dec 24, 2024 – 12:56 PM EST

PDB ID : 2K85
BMRB ID : 15938
Title : p190-A RhoGAP FF1 domain
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Deposited on : 2008-09-02

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.40

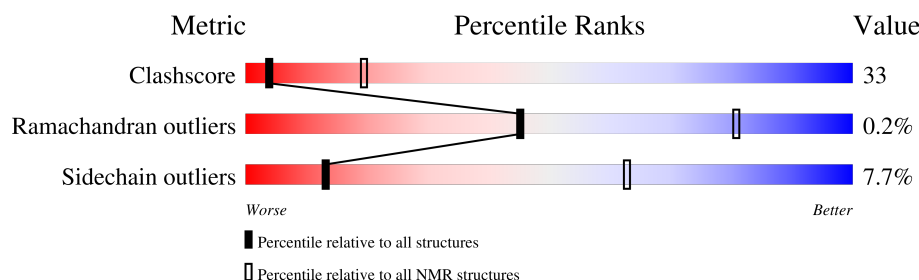
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 81%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	69	

2 Ensemble composition and analysis

This entry contains 15 models. Model 13 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:10-A:67 (58)	0.35	13

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1112 atoms, of which 557 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Glucocorticoid receptor DNA-binding factor 1.

Mol	Chain	Residues	Atoms						Trace
1	A	65	Total	C	H	N	O	S	0
			1112	353	557	101	100	1	

There are 4 discrepancies between the modelled and reference sequences:

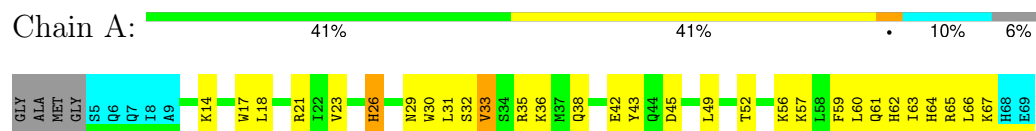
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q9NRY4
A	2	ALA	-	expression tag	UNP Q9NRY4
A	3	MET	-	expression tag	UNP Q9NRY4
A	4	GLY	-	expression tag	UNP Q9NRY4

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: Glucocorticoid receptor DNA-binding factor 1

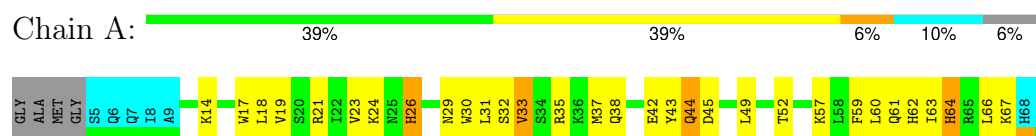


4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

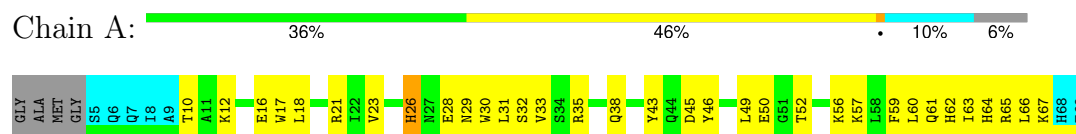
4.2.1 Score per residue for model 1

- Molecule 1: Glucocorticoid receptor DNA-binding factor 1



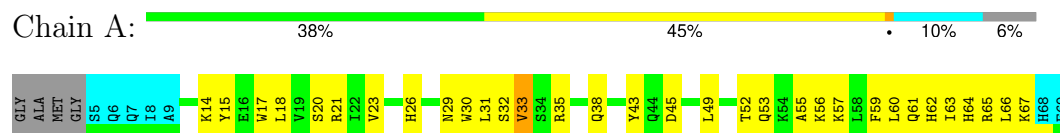
4.2.2 Score per residue for model 2

- Molecule 1: Glucocorticoid receptor DNA-binding factor 1



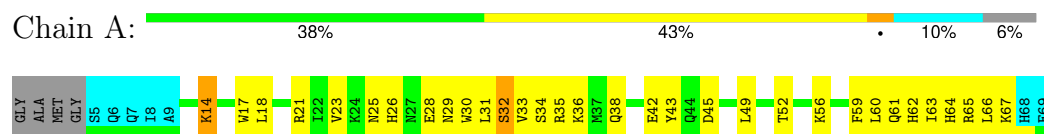
4.2.3 Score per residue for model 3

- Molecule 1: Glucocorticoid receptor DNA-binding factor 1



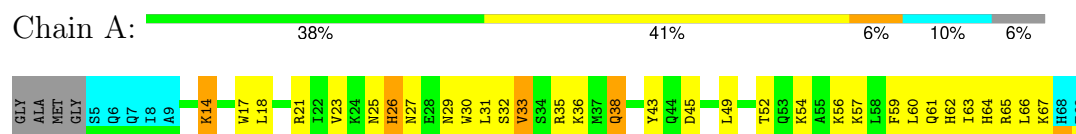
4.2.4 Score per residue for model 4

- Molecule 1: Glucocorticoid receptor DNA-binding factor 1



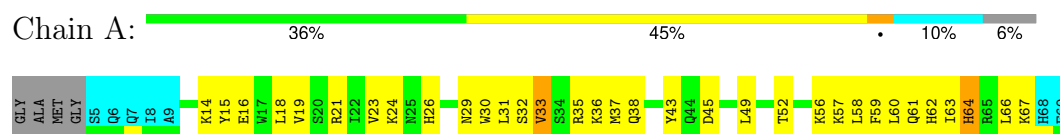
4.2.5 Score per residue for model 5

- Molecule 1: Glucocorticoid receptor DNA-binding factor 1



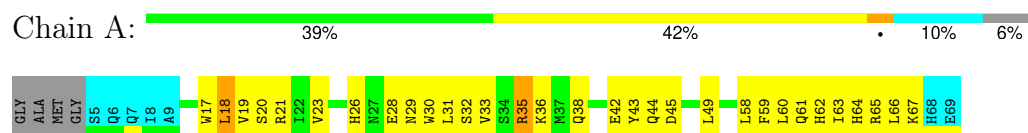
4.2.6 Score per residue for model 6

- Molecule 1: Glucocorticoid receptor DNA-binding factor 1



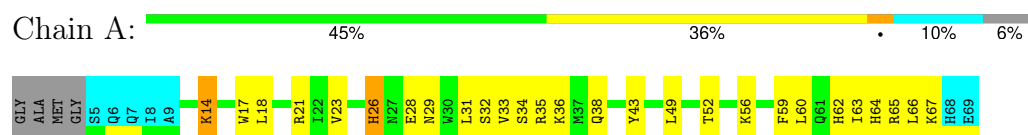
4.2.7 Score per residue for model 7

- Molecule 1: Glucocorticoid receptor DNA-binding factor 1



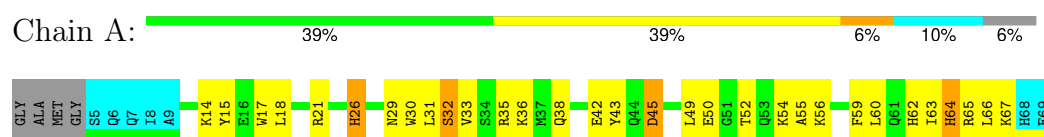
4.2.8 Score per residue for model 8

- Molecule 1: Glucocorticoid receptor DNA-binding factor 1



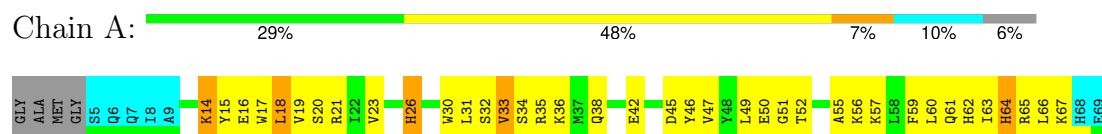
4.2.9 Score per residue for model 9

- Molecule 1: Glucocorticoid receptor DNA-binding factor 1



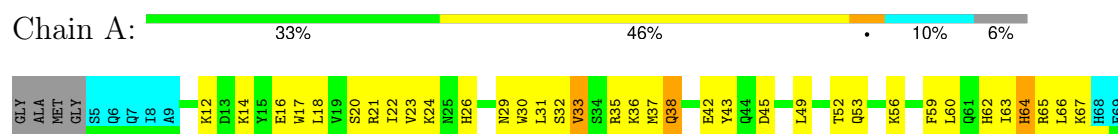
4.2.10 Score per residue for model 10

- Molecule 1: Glucocorticoid receptor DNA-binding factor 1



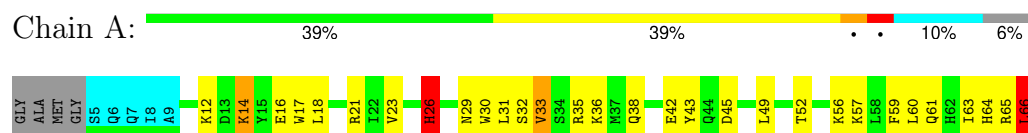
4.2.11 Score per residue for model 11

- Molecule 1: Glucocorticoid receptor DNA-binding factor 1



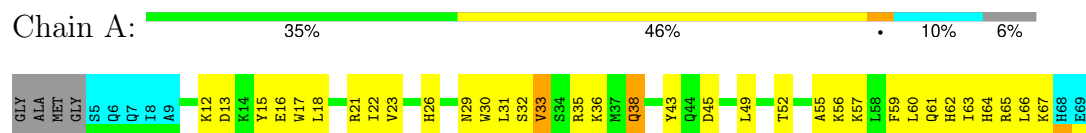
4.2.12 Score per residue for model 12

- Molecule 1: Glucocorticoid receptor DNA-binding factor 1



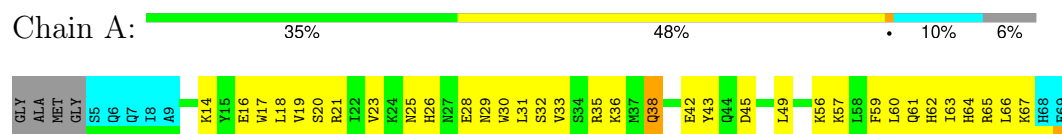
4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Glucocorticoid receptor DNA-binding factor 1



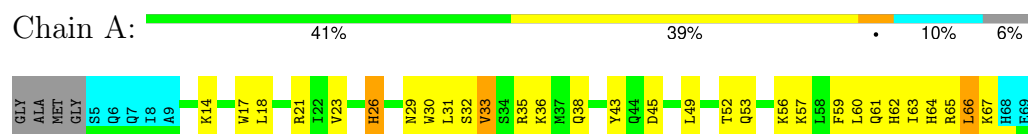
4.2.14 Score per residue for model 14

- Molecule 1: Glucocorticoid receptor DNA-binding factor 1



4.2.15 Score per residue for model 15

- Molecule 1: Glucocorticoid receptor DNA-binding factor 1



5 Refinement protocol and experimental data overview

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

Of the 80 calculated structures, 15 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
ARIA	structure solution	
ARIA	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	787
Number of shifts mapped to atoms	776
Number of unparsed shifts	0
Number of shifts with mapping errors	11
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

6 Model quality

6.1 Standard geometry

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

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	498	506	503	33±3
All	All	7470	7590	7545	495

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 33.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:HIS:HA	1:A:67:LYS:HE2	0.94	1.36	14	12
1:A:28:GLU:HB3	1:A:33:VAL:HG21	0.81	1.51	7	2
1:A:26:HIS:CE1	1:A:67:LYS:HG2	0.81	2.11	12	10
1:A:63:ILE:O	1:A:67:LYS:HG3	0.81	1.76	13	15
1:A:26:HIS:ND1	1:A:67:LYS:HG2	0.79	1.93	5	14
1:A:62:HIS:HA	1:A:65:ARG:HD3	0.77	1.56	8	4
1:A:23:VAL:HG22	1:A:33:VAL:HG11	0.77	1.56	11	8
1:A:26:HIS:HB3	1:A:66:LEU:HG	0.73	1.59	12	2
1:A:31:LEU:O	1:A:35:ARG:HG2	0.71	1.85	1	9
1:A:38:GLN:HA	1:A:43:TYR:CD1	0.68	2.24	15	9
1:A:32:SER:O	1:A:35:ARG:HB2	0.67	1.88	6	10
1:A:18:LEU:HD21	1:A:42:GLU:HG2	0.65	1.69	1	4
1:A:17:TRP:CE3	1:A:18:LEU:HD22	0.65	2.26	2	10
1:A:26:HIS:HB3	1:A:66:LEU:CG	0.64	2.22	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:TRP:NE1	1:A:56:LYS:HG2	0.64	2.08	9	1
1:A:64:HIS:HA	1:A:67:LYS:CE	0.63	2.23	3	6
1:A:35:ARG:O	1:A:38:GLN:HG2	0.63	1.93	9	6
1:A:17:TRP:CZ2	1:A:21:ARG:HD2	0.63	2.29	13	5
1:A:26:HIS:HB2	1:A:63:ILE:HG23	0.61	1.72	4	14
1:A:63:ILE:HA	1:A:66:LEU:HD12	0.60	1.73	14	10
1:A:38:GLN:HA	1:A:43:TYR:CD2	0.60	2.32	3	5
1:A:62:HIS:O	1:A:66:LEU:HG	0.60	1.96	1	12
1:A:45:ASP:O	1:A:49:LEU:HG	0.59	1.97	5	14
1:A:19:VAL:HA	1:A:37:MET:HE2	0.59	1.72	1	2
1:A:18:LEU:HD13	1:A:21:ARG:HD3	0.59	1.75	13	2
1:A:17:TRP:NE1	1:A:21:ARG:HB2	0.58	2.13	13	4
1:A:59:PHE:O	1:A:63:ILE:HG12	0.58	1.98	7	13
1:A:29:ASN:O	1:A:33:VAL:HG23	0.58	1.98	9	6
1:A:12:LYS:O	1:A:16:GLU:HG3	0.58	1.99	13	4
1:A:23:VAL:HA	1:A:28:GLU:HG2	0.57	1.77	2	2
1:A:61:GLN:O	1:A:65:ARG:HG2	0.57	2.00	2	4
1:A:56:LYS:O	1:A:59:PHE:HB3	0.57	1.99	11	6
1:A:42:GLU:HA	1:A:45:ASP:OD2	0.56	2.00	9	1
1:A:18:LEU:HG	1:A:42:GLU:HB2	0.56	1.77	11	6
1:A:64:HIS:O	1:A:67:LYS:HB2	0.55	2.02	9	6
1:A:32:SER:O	1:A:36:LYS:HG3	0.55	2.02	11	11
1:A:35:ARG:O	1:A:38:GLN:HG3	0.55	2.02	8	7
1:A:30:TRP:HA	1:A:33:VAL:CG2	0.54	2.31	15	6
1:A:26:HIS:HB3	1:A:66:LEU:CB	0.54	2.31	12	2
1:A:30:TRP:HB2	1:A:59:PHE:CD2	0.54	2.37	9	12
1:A:17:TRP:O	1:A:21:ARG:N	0.54	2.41	2	13
1:A:62:HIS:HA	1:A:65:ARG:HD2	0.54	1.78	5	1
1:A:29:ASN:O	1:A:33:VAL:HG22	0.53	2.03	11	8
1:A:23:VAL:HG12	1:A:66:LEU:HD21	0.53	1.80	15	2
1:A:20:SER:HA	1:A:62:HIS:CE1	0.53	2.39	11	2
1:A:62:HIS:HA	1:A:65:ARG:CD	0.52	2.33	5	1
1:A:28:GLU:HB3	1:A:33:VAL:CG2	0.52	2.30	7	2
1:A:63:ILE:O	1:A:66:LEU:HB2	0.52	2.05	13	6
1:A:14:LYS:O	1:A:18:LEU:HD23	0.52	2.05	3	11
1:A:57:LYS:O	1:A:61:GLN:HG2	0.51	2.05	1	4
1:A:60:LEU:O	1:A:63:ILE:HB	0.51	2.05	6	12
1:A:64:HIS:C	1:A:64:HIS:ND1	0.51	2.63	9	11
1:A:62:HIS:CE1	1:A:66:LEU:HD21	0.51	2.40	6	9
1:A:53:GLN:O	1:A:57:LYS:HG3	0.51	2.06	15	2
1:A:32:SER:HA	1:A:35:ARG:CG	0.51	2.35	3	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:VAL:O	1:A:23:VAL:HB	0.51	2.06	7	1
1:A:57:LYS:O	1:A:61:GLN:HG3	0.51	2.06	15	4
1:A:18:LEU:O	1:A:21:ARG:HG2	0.50	2.06	8	8
1:A:24:LYS:O	1:A:66:LEU:HD22	0.50	2.07	6	2
1:A:25:ASN:OD1	1:A:27:ASN:HB2	0.50	2.05	5	1
1:A:50:GLU:HB3	1:A:54:LYS:HD2	0.49	1.83	9	1
1:A:14:LYS:HB2	1:A:14:LYS:NZ	0.49	2.21	5	1
1:A:15:TYR:OH	1:A:55:ALA:HB1	0.49	2.08	9	4
1:A:17:TRP:CE2	1:A:21:ARG:HB2	0.49	2.43	15	3
1:A:54:LYS:HA	1:A:57:LYS:HB2	0.48	1.84	5	1
1:A:56:LYS:O	1:A:60:LEU:HD23	0.48	2.08	5	12
1:A:17:TRP:HA	1:A:20:SER:OG	0.48	2.09	10	2
1:A:16:GLU:HG2	1:A:58:LEU:HD11	0.48	1.86	6	1
1:A:32:SER:O	1:A:35:ARG:HB3	0.48	2.09	5	1
1:A:44:GLN:HA	1:A:44:GLN:HE21	0.47	1.68	1	1
1:A:14:LYS:HG2	1:A:42:GLU:HG2	0.47	1.86	10	1
1:A:59:PHE:CE1	1:A:63:ILE:HD11	0.47	2.44	5	3
1:A:32:SER:HA	1:A:35:ARG:HG2	0.47	1.86	3	1
1:A:23:VAL:HG22	1:A:28:GLU:HG3	0.46	1.86	7	1
1:A:46:TYR:CE1	1:A:50:GLU:HG3	0.46	2.45	2	2
1:A:64:HIS:HA	1:A:67:LYS:HE3	0.46	1.87	12	3
1:A:33:VAL:O	1:A:36:LYS:HB2	0.46	2.11	4	1
1:A:61:GLN:O	1:A:65:ARG:HG3	0.46	2.11	4	2
1:A:58:LEU:HA	1:A:61:GLN:HG2	0.46	1.88	7	1
1:A:31:LEU:HD22	1:A:31:LEU:N	0.45	2.27	6	13
1:A:18:LEU:HG	1:A:42:GLU:CB	0.45	2.41	10	2
1:A:32:SER:HA	1:A:35:ARG:HG3	0.45	1.89	10	1
1:A:18:LEU:HD21	1:A:42:GLU:CG	0.45	2.41	1	1
1:A:14:LYS:HG2	1:A:42:GLU:CG	0.45	2.41	10	1
1:A:31:LEU:H	1:A:31:LEU:HD22	0.44	1.73	11	1
1:A:64:HIS:ND1	1:A:64:HIS:C	0.44	2.69	7	3
1:A:23:VAL:HG12	1:A:66:LEU:CD1	0.44	2.43	4	3
1:A:63:ILE:HD13	1:A:66:LEU:HD12	0.44	1.88	8	1
1:A:23:VAL:HG21	1:A:59:PHE:CE1	0.44	2.47	1	3
1:A:61:GLN:O	1:A:64:HIS:HB3	0.44	2.12	4	6
1:A:32:SER:HA	1:A:35:ARG:HB2	0.43	1.88	5	1
1:A:16:GLU:O	1:A:19:VAL:HG12	0.43	2.12	10	1
1:A:13:ASP:O	1:A:16:GLU:HB2	0.43	2.12	13	1
1:A:20:SER:HB3	1:A:62:HIS:CE1	0.43	2.48	7	1
1:A:30:TRP:O	1:A:33:VAL:HG23	0.43	2.13	1	2
1:A:19:VAL:HG22	1:A:37:MET:HE1	0.43	1.89	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:VAL:O	1:A:51:GLY:HA2	0.43	2.13	10	1
1:A:38:GLN:HA	1:A:43:TYR:CE2	0.43	2.49	3	1
1:A:19:VAL:HG12	1:A:62:HIS:ND1	0.42	2.29	14	1
1:A:31:LEU:HD22	1:A:31:LEU:H	0.42	1.75	12	4
1:A:21:ARG:HG2	1:A:22:ILE:HG12	0.42	1.90	13	1
1:A:26:HIS:HB2	1:A:63:ILE:HD12	0.42	1.90	7	1
1:A:34:SER:HB3	1:A:43:TYR:OH	0.42	2.15	8	1
1:A:22:ILE:HG13	1:A:37:MET:HG3	0.42	1.91	11	1
1:A:15:TYR:O	1:A:18:LEU:HB2	0.42	2.15	6	2
1:A:33:VAL:O	1:A:37:MET:HG3	0.41	2.15	6	1
1:A:30:TRP:HA	1:A:33:VAL:HG23	0.41	1.92	13	4
1:A:18:LEU:CG	1:A:42:GLU:HB2	0.41	2.44	11	1
1:A:18:LEU:CD2	1:A:42:GLU:HB2	0.41	2.46	4	1
1:A:30:TRP:HB2	1:A:59:PHE:CE2	0.41	2.50	9	1
1:A:16:GLU:CG	1:A:58:LEU:HD11	0.41	2.45	6	1
1:A:26:HIS:HA	1:A:63:ILE:HD13	0.41	1.92	10	1
1:A:19:VAL:HA	1:A:37:MET:CE	0.41	2.44	1	1
1:A:26:HIS:HA	1:A:63:ILE:CD1	0.41	2.46	10	1
1:A:53:GLN:NE2	1:A:53:GLN:H	0.40	2.14	11	1
1:A:23:VAL:HG11	1:A:63:ILE:CD1	0.40	2.47	13	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	58/69 (84%)	50±2 (87±3%)	8±2 (13±3%)	0±0 (0±1%)	45	81
All	All	870/1035 (84%)	755 (87%)	113 (13%)	2 (0%)	45	81

All 2 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	26	HIS	1
1	A	66	LEU	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	54/61 (89%)	50±1 (92±2%)	4±1 (8±2%)	13	63
All	All	810/915 (89%)	748 (92%)	62 (8%)	13	63

All 18 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	52	THR	13
1	A	33	VAL	9
1	A	26	HIS	8
1	A	64	HIS	5
1	A	14	LYS	5
1	A	38	GLN	4
1	A	44	GLN	2
1	A	25	ASN	2
1	A	32	SER	2
1	A	34	SER	2
1	A	18	LEU	2
1	A	66	LEU	2
1	A	10	THR	1
1	A	35	ARG	1
1	A	49	LEU	1
1	A	45	ASP	1
1	A	24	LYS	1
1	A	16	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 81% 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	787
Number of shifts mapped to atoms	776
Number of unparsed shifts	0
Number of shifts with mapping errors	11
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

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

- No matching atom found in the structure. All 11 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	MET	H	8.439	0.100	1
1	A	3	MET	HA	4.006	0.100	1
1	A	3	MET	HB2	1.047	0.100	2
1	A	3	MET	HG2	1.256	0.100	2
1	A	3	MET	HG3	1.174	0.100	2
1	A	3	MET	CA	53.014	0.300	1
1	A	4	GLY	H	8.34	0.100	1
1	A	4	GLY	HA2	4.0605	0.100	2
1	A	4	GLY	HA3	3.795	0.100	2
1	A	4	GLY	CA	42.813	0.300	1
1	A	4	GLY	N	110.646	0.300	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	67	2.26 ± 0.24	Should be applied
$^{13}\text{C}_\beta$	62	2.75 ± 0.12	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	62	0.34 ± 0.40	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 704 atoms were assigned a chemical shift out of a possible 867. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	230/289 (80%)	116/116 (100%)	58/116 (50%)	56/57 (98%)
Sidechain	404/484 (83%)	273/311 (88%)	124/149 (83%)	7/24 (29%)
Aromatic	70/94 (74%)	41/45 (91%)	27/41 (66%)	2/8 (25%)
Overall	704/867 (81%)	430/472 (91%)	209/306 (68%)	65/89 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 776 atoms were assigned a chemical shift out of a possible 960. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	256/324 (79%)	130/130 (100%)	65/130 (50%)	61/64 (95%)
Sidechain	445/534 (83%)	300/343 (87%)	137/165 (83%)	8/26 (31%)
Aromatic	75/102 (74%)	44/49 (90%)	29/43 (67%)	2/10 (20%)
Overall	776/960 (81%)	474/522 (91%)	231/338 (68%)	71/100 (71%)

7.1.4 Statistically unusual chemical shifts ⓘ

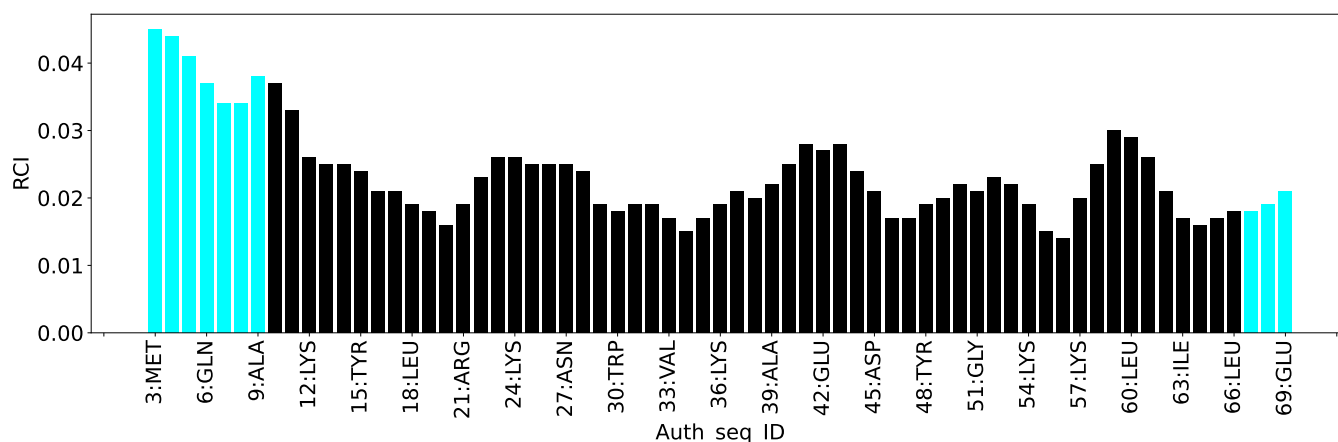
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	34	SER	HB3	1.55	2.49 – 5.20	-8.5
1	A	50	GLU	HB3	0.52	0.95 – 3.05	-7.0
1	A	56	LYS	HG3	-0.18	0.04 – 2.67	-5.8
1	A	34	SER	HB2	2.47	2.61 – 5.13	-5.6

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1497
Intra-residue ($ i-j =0$)	765
Sequential ($ i-j =1$)	315
Medium range ($ i-j >1$ and $ i-j <5$)	170
Long range ($ i-j \geq 5$)	177
Inter-chain	0
Hydrogen bond restraints	70
Disulfide bond restraints	0
Total dihedral-angle restraints	82
Number of unmapped restraints	10
Number of restraints per residue	22.9
Number of long range restraints per residue ¹	2.6

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)	58.7	0.2
0.2-0.5 (Medium)	83.8	0.5
>0.5 (Large)	22.1	2.51

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	0.5	1.77
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

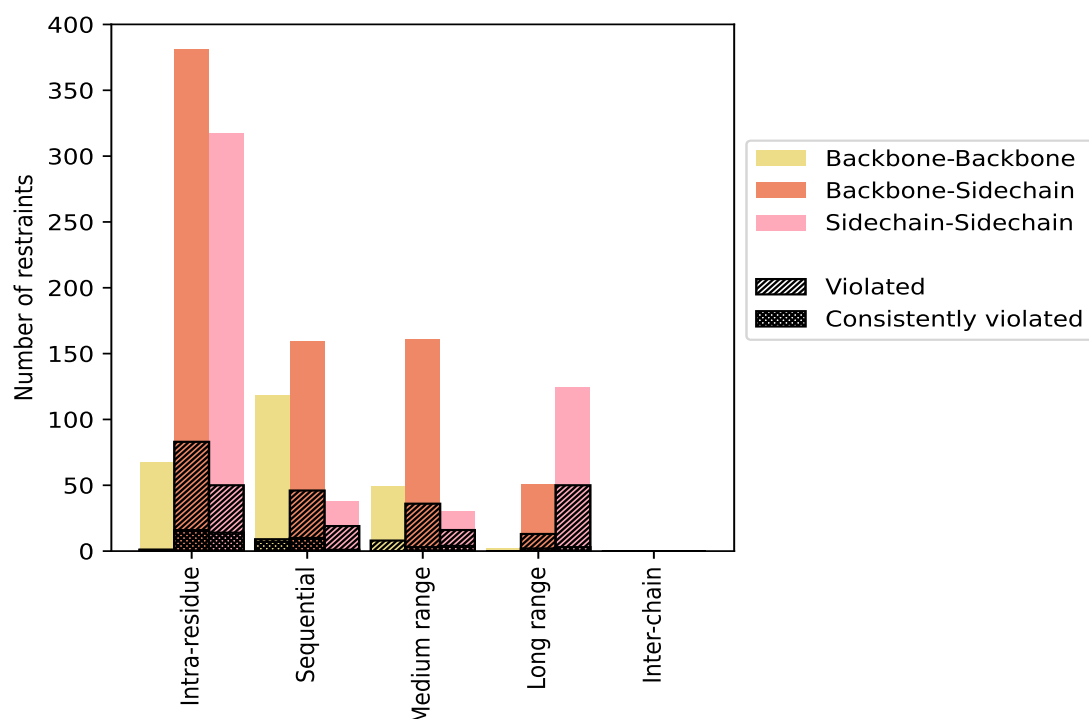
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	765	51.1	134	17.5	9.0	31	4.1	2.1
Backbone-Backbone	67	4.5	1	1.5	0.1	1	1.5	0.1
Backbone-Sidechain	381	25.5	83	21.8	5.5	16	4.2	1.1
Sidechain-Sidechain	317	21.2	50	15.8	3.3	14	4.4	0.9
Sequential ($i-j =1$)	315	21.0	74	23.5	4.9	18	5.7	1.2
Backbone-Backbone	118	7.9	9	7.6	0.6	7	5.9	0.5
Backbone-Sidechain	159	10.6	46	28.9	3.1	10	6.3	0.7
Sidechain-Sidechain	38	2.5	19	50.0	1.3	1	2.6	0.1
Medium range ($i-j >1$ & $i-j <5$)	170	11.4	55	32.4	3.7	7	4.1	0.5
Backbone-Backbone	49	3.3	8	16.3	0.5	0	0.0	0.0
Backbone-Sidechain	91	6.1	31	34.1	2.1	3	3.3	0.2
Sidechain-Sidechain	30	2.0	16	53.3	1.1	4	13.3	0.3
Long range ($i-j \geq 5$)	177	11.8	63	35.6	4.2	5	2.8	0.3
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	51	3.4	13	25.5	0.9	2	3.9	0.1
Sidechain-Sidechain	124	8.3	50	40.3	3.3	3	2.4	0.2
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	70	4.7	5	7.1	0.3	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1497	100.0	331	22.1	22.1	61	4.1	4.1
Backbone-Backbone	236	15.8	18	7.6	1.2	8	3.4	0.5
Backbone-Sidechain	752	50.2	178	23.7	11.9	31	4.1	2.1
Sidechain-Sidechain	509	34.0	135	26.5	9.0	22	4.3	1.5

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

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

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	74	43	25	23	0	165	0.3	1.39	0.19	0.27
2	71	47	22	26	0	166	0.29	1.29	0.17	0.26
3	79	48	29	23	0	179	0.31	1.37	0.21	0.25
4	71	47	25	24	0	167	0.33	1.87	0.25	0.26
5	65	43	32	23	0	163	0.29	1.96	0.22	0.22
6	68	46	28	21	0	163	0.31	1.42	0.2	0.27
7	66	48	25	28	0	167	0.29	2.35	0.24	0.22
8	67	48	26	26	0	167	0.33	1.75	0.24	0.25
9	69	42	25	25	0	161	0.32	2.33	0.27	0.26
10	70	42	25	23	0	160	0.29	1.35	0.19	0.24

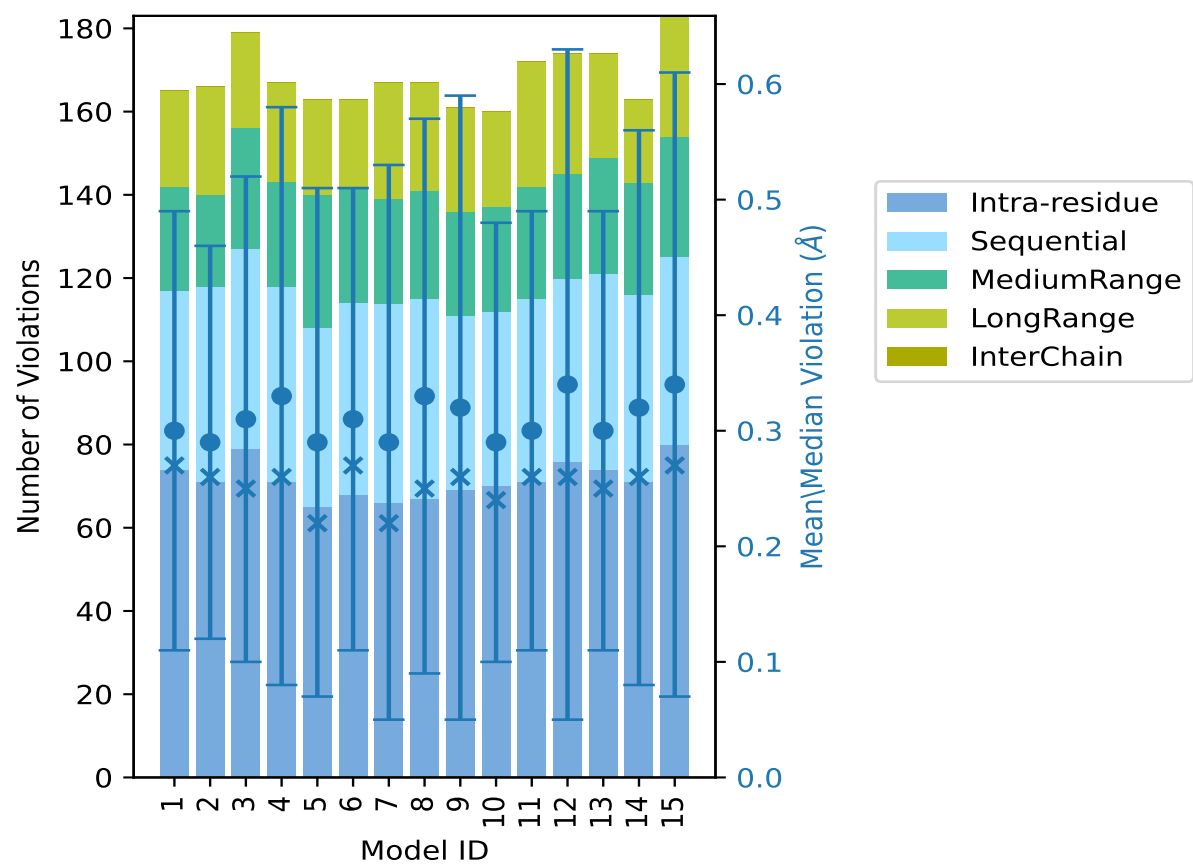
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	71	44	27	30	0	172	0.3	1.34	0.19	0.26
12	76	44	25	29	0	174	0.34	2.32	0.29	0.26
13	74	47	28	25	0	174	0.3	1.24	0.19	0.25
14	71	45	27	20	0	163	0.32	1.57	0.24	0.26
15	80	45	29	29	0	183	0.34	2.51	0.27	0.27

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

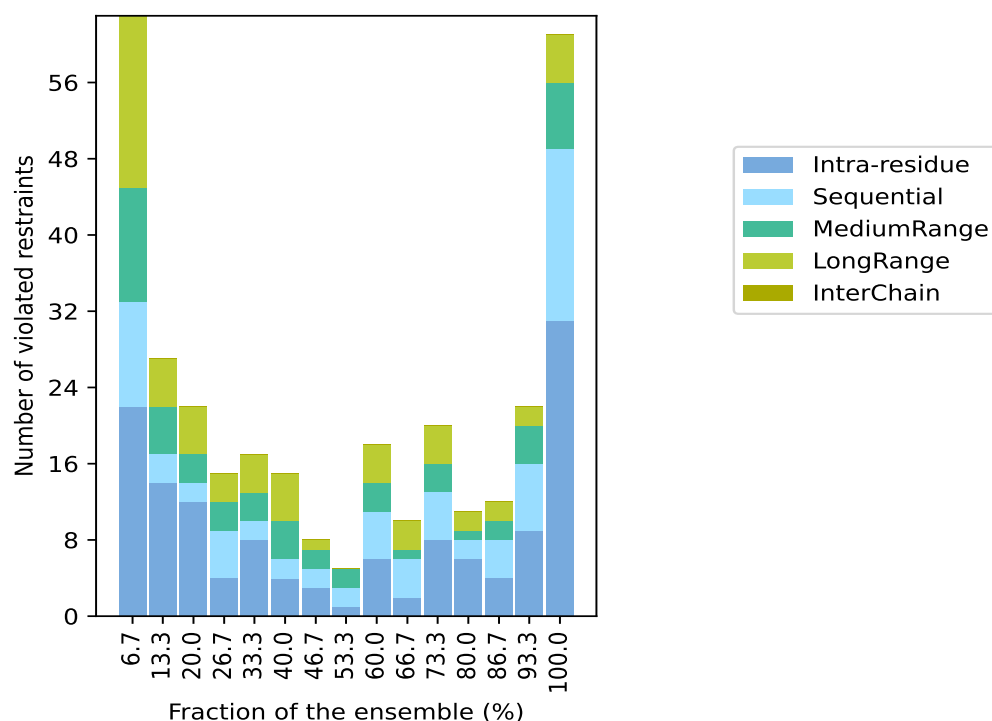
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1101(IR:631, SQ:241, MR:115, LR:114, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
22	11	12	18	0	63	1	6.7
14	3	5	5	0	27	2	13.3
12	2	3	5	0	22	3	20.0
4	5	3	3	0	15	4	26.7
8	2	3	4	0	17	5	33.3
4	2	4	5	0	15	6	40.0
3	2	2	1	0	8	7	46.7
1	2	2	0	0	5	8	53.3
6	5	3	4	0	18	9	60.0
2	4	1	3	0	10	10	66.7
8	5	3	4	0	20	11	73.3
6	2	1	2	0	11	12	80.0
4	4	2	2	0	12	13	86.7
9	7	4	2	0	22	14	93.3
31	18	7	5	0	61	15	100.0

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

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

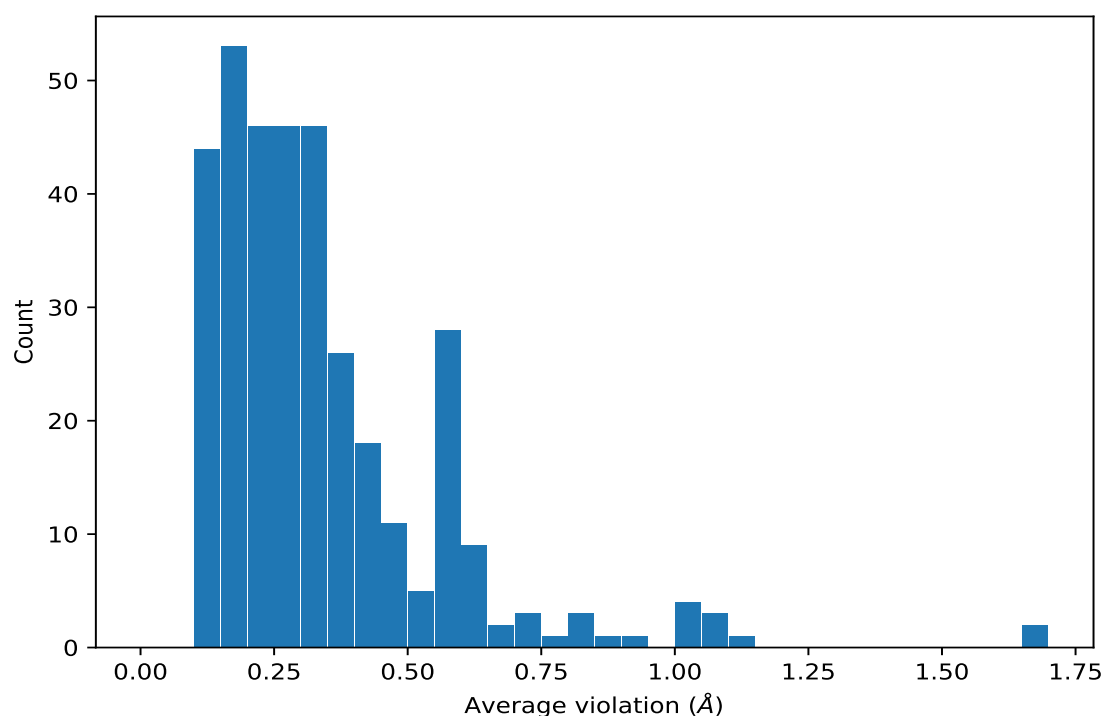
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,1341)	1:17:A:TRP:HE3	1:21:A:ARG:HB2	15	1.13	0.47	1.36
(1,13)	1:26:A:HIS:HD1	1:67:A:LYS:HD2	15	0.9	0.17	0.94
(1,1331)	1:23:A:VAL:H	1:33:A:VAL:HB	15	0.86	0.84	0.24
(1,1244)	1:26:A:HIS:HE1	1:67:A:LYS:HB2	15	0.73	0.43	0.93
(1,1275)	1:17:A:TRP:HD1	1:18:A:LEU:HA	15	0.6	0.12	0.56
(1,512)	1:8:A:ILE:H	1:8:A:ILE:HG21	15	0.59	0.03	0.6
(1,512)	1:8:A:ILE:H	1:8:A:ILE:HG22	15	0.59	0.03	0.6
(1,512)	1:8:A:ILE:H	1:8:A:ILE:HG23	15	0.59	0.03	0.6
(1,354)	1:59:A:PHE:H	1:58:A:LEU:HD22	15	0.57	0.03	0.57
(1,354)	1:59:A:PHE:H	1:58:A:LEU:HD23	15	0.57	0.03	0.57
(1,354)	1:59:A:PHE:H	1:58:A:LEU:HD21	15	0.57	0.03	0.57
(1,801)	1:23:A:VAL:H	1:22:A:ILE:HD11	15	0.56	0.14	0.63
(1,801)	1:23:A:VAL:H	1:22:A:ILE:HD13	15	0.56	0.14	0.63
(1,801)	1:23:A:VAL:H	1:22:A:ILE:HD12	15	0.56	0.14	0.63
(1,212)	1:17:A:TRP:HD1	1:17:A:TRP:HB3	15	0.55	0.01	0.54
(1,224)	1:48:A:TYR:H	1:48:A:TYR:HD2	15	0.48	0.06	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,645)	1:19:A:VAL:H	1:18:A:LEU:HD11	15	0.48	0.05	0.47
(1,645)	1:19:A:VAL:H	1:18:A:LEU:HD12	15	0.48	0.05	0.47
(1,645)	1:19:A:VAL:H	1:18:A:LEU:HD13	15	0.48	0.05	0.47
(1,241)	1:46:A:TYR:H	1:46:A:TYR:HD2	15	0.46	0.04	0.48
(1,241)	1:46:A:TYR:H	1:46:A:TYR:HD1	15	0.46	0.04	0.48
(1,1204)	1:18:A:LEU:HG	1:42:A:GLU:HA	15	0.44	0.23	0.34
(1,1069)	1:16:A:GLU:H	1:16:A:GLU:HB3	15	0.42	0.07	0.41
(1,1188)	1:59:A:PHE:HD2	1:60:A:LEU:HD11	15	0.41	0.07	0.41
(1,1188)	1:59:A:PHE:HD2	1:60:A:LEU:HD13	15	0.41	0.07	0.41
(1,1188)	1:59:A:PHE:HD2	1:60:A:LEU:HD12	15	0.41	0.07	0.41
(1,1053)	1:54:A:LYS:HD2	1:54:A:LYS:HA	15	0.41	0.1	0.35
(1,1066)	1:14:A:LYS:H	1:14:A:LYS:HG2	15	0.4	0.08	0.4
(1,402)	1:65:A:ARG:HB2	1:65:A:ARG:HA	15	0.38	0.02	0.37
(1,197)	1:30:A:TRP:HD1	1:30:A:TRP:HA	15	0.36	0.02	0.36
(1,1225)	1:47:A:VAL:HA	1:46:A:TYR:HA	15	0.35	0.01	0.35
(1,1425)	1:10:A:THR:H	1:13:A:ASP:HB2	15	0.34	0.22	0.21
(1,1364)	1:59:A:PHE:HE1	1:30:A:TRP:HE3	15	0.34	0.08	0.34
(1,1364)	1:59:A:PHE:HE2	1:30:A:TRP:HE3	15	0.34	0.08	0.34
(1,663)	1:64:A:HIS:HD1	1:64:A:HIS:HA	15	0.33	0.04	0.32
(1,1385)	1:67:A:LYS:HD2	1:64:A:HIS:HA	15	0.33	0.11	0.3
(1,1340)	1:17:A:TRP:HE3	1:21:A:ARG:HB3	15	0.33	0.04	0.32
(1,644)	1:18:A:LEU:HD12	1:18:A:LEU:HB2	15	0.32	0.05	0.34
(1,644)	1:18:A:LEU:HD13	1:18:A:LEU:HB2	15	0.32	0.05	0.34
(1,644)	1:18:A:LEU:HD11	1:18:A:LEU:HB2	15	0.32	0.05	0.34
(1,284)	1:21:A:ARG:HG2	1:21:A:ARG:HA	15	0.32	0.08	0.36
(1,658)	1:68:A:HIS:HD1	1:68:A:HIS:HA	15	0.32	0.01	0.32
(1,1015)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	15	0.31	0.04	0.31
(1,216)	1:17:A:TRP:HZ2	1:17:A:TRP:HH2	15	0.31	0.0	0.31
(1,425)	1:67:A:LYS:H	1:66:A:LEU:HG	15	0.3	0.06	0.29
(1,1056)	1:54:A:LYS:HG3	1:54:A:LYS:HB3	15	0.3	0.01	0.3
(1,449)	1:50:A:GLU:H	1:49:A:LEU:HD21	15	0.29	0.08	0.28
(1,449)	1:50:A:GLU:H	1:49:A:LEU:HD23	15	0.29	0.08	0.28
(1,449)	1:50:A:GLU:H	1:49:A:LEU:HD22	15	0.29	0.08	0.28
(1,718)	1:42:A:GLU:HA	1:41:A:PRO:HA	15	0.29	0.05	0.29
(1,308)	1:22:A:ILE:HG13	1:22:A:ILE:HA	15	0.28	0.04	0.3
(1,1389)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	15	0.27	0.08	0.3
(1,148)	1:22:A:ILE:H	1:21:A:ARG:HA	15	0.27	0.03	0.27
(1,1345)	1:64:A:HIS:HE1	1:68:A:HIS:HD1	15	0.27	0.05	0.25
(1,1232)	1:17:A:TRP:HE1	1:21:A:ARG:HG2	15	0.27	0.05	0.27
(1,471)	1:42:A:GLU:H	1:41:A:PRO:HB3	15	0.26	0.05	0.27
(1,1229)	1:58:A:LEU:HG	1:55:A:ALA:HA	15	0.26	0.03	0.27
(1,432)	1:68:A:HIS:H	1:68:A:HIS:HB2	15	0.25	0.02	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,220)	1:17:A:TRP:H	1:17:A:TRP:HE3	15	0.25	0.05	0.25
(1,820)	1:60:A:LEU:HG	1:60:A:LEU:HB2	15	0.24	0.01	0.24
(1,659)	1:68:A:HIS:HD1	1:68:A:HIS:HB2	15	0.22	0.05	0.24
(1,213)	1:17:A:TRP:HE1	1:17:A:TRP:HD1	15	0.21	0.0	0.21
(1,662)	1:64:A:HIS:H	1:64:A:HIS:HD1	15	0.21	0.05	0.21
(1,798)	1:28:A:GLU:H	1:27:A:ASN:HB3	15	0.2	0.05	0.22
(1,1357)	1:26:A:HIS:H	1:26:A:HIS:HD1	15	0.2	0.05	0.2
(1,365)	1:61:A:GLN:H	1:60:A:LEU:HG	15	0.2	0.02	0.2
(1,865)	1:21:A:ARG:HG3	1:21:A:ARG:HB3	15	0.19	0.0	0.19
(1,251)	1:46:A:TYR:HE1	1:46:A:TYR:HE2	15	0.18	0.0	0.18
(1,1274)	1:17:A:TRP:HE3	1:18:A:LEU:HA	15	0.17	0.03	0.18
(1,563)	1:32:A:SER:H	1:32:A:SER:HA	15	0.16	0.02	0.16
(1,217)	1:17:A:TRP:HH2	1:17:A:TRP:HZ3	15	0.16	0.0	0.16
(1,69)	1:10:A:THR:H	1:9:A:ALA:HA	15	0.16	0.01	0.16
(1,391)	1:64:A:HIS:H	1:63:A:ILE:HA	15	0.16	0.01	0.16
(1,32)	1:15:A:TYR:HE1	1:15:A:TYR:HB2	15	0.16	0.03	0.16
(1,68)	1:9:A:ALA:H	1:8:A:ILE:HA	15	0.16	0.02	0.15
(1,214)	1:17:A:TRP:HE1	1:17:A:TRP:HZ2	15	0.15	0.01	0.15
(1,163)	1:46:A:TYR:H	1:45:A:ASP:HA	15	0.14	0.01	0.14
(1,1413)	1:49:A:LEU:HD22	1:50:A:GLU:HG3	14	0.81	0.34	0.72
(1,1413)	1:49:A:LEU:HD21	1:50:A:GLU:HG3	14	0.81	0.34	0.72
(1,1413)	1:49:A:LEU:HD23	1:50:A:GLU:HG3	14	0.81	0.34	0.72
(1,1313)	1:33:A:VAL:HA	1:32:A:SER:HB3	14	0.67	0.36	0.68
(1,960)	1:56:A:LYS:H	1:56:A:LYS:HG2	14	0.44	0.08	0.42
(1,595)	1:54:A:LYS:HB2	1:54:A:LYS:HA	14	0.4	0.01	0.41
(1,1321)	1:64:A:HIS:HD1	1:65:A:ARG:HB3	14	0.39	0.16	0.38
(1,1000)	1:24:A:LYS:HG2	1:24:A:LYS:HD2	14	0.39	0.02	0.38
(1,320)	1:45:A:ASP:H	1:44:A:GLN:HG3	14	0.36	0.12	0.34
(1,12)	1:26:A:HIS:HD1	1:67:A:LYS:HB2	14	0.34	0.17	0.27
(1,1405)	1:7:A:GLN:HB2	1:7:A:GLN:HG3	14	0.34	0.0	0.34
(1,566)	1:32:A:SER:H	1:32:A:SER:HB3	14	0.34	0.04	0.32
(1,514)	1:8:A:ILE:HG12	1:8:A:ILE:HB	14	0.3	0.05	0.3
(1,1239)	1:65:A:ARG:HB3	1:62:A:HIS:HA	14	0.28	0.06	0.26
(1,837)	1:50:A:GLU:H	1:49:A:LEU:HG	14	0.27	0.01	0.27
(1,840)	1:32:A:SER:H	1:31:A:LEU:HG	14	0.26	0.04	0.26
(1,1337)	1:30:A:TRP:HD1	1:31:A:LEU:HG	14	0.25	0.04	0.24
(1,1101)	1:30:A:TRP:HD1	1:56:A:LYS:HD3	14	0.25	0.09	0.22
(1,1166)	1:36:A:LYS:HB3	1:33:A:VAL:HA	14	0.2	0.03	0.19
(1,617)	1:26:A:HIS:H	1:23:A:VAL:HA	14	0.2	0.07	0.18
(1,783)	1:64:A:HIS:H	1:61:A:GLN:HA	14	0.2	0.05	0.2
(1,536)	1:31:A:LEU:HG	1:31:A:LEU:HA	14	0.18	0.01	0.19
(1,533)	1:31:A:LEU:H	1:31:A:LEU:HG	14	0.17	0.02	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,834)	1:49:A:LEU:HD11	1:49:A:LEU:HB2	14	0.15	0.01	0.15
(1,834)	1:49:A:LEU:HD12	1:49:A:LEU:HB2	14	0.15	0.01	0.15
(1,834)	1:49:A:LEU:HD13	1:49:A:LEU:HB2	14	0.15	0.01	0.15
(1,1355)	1:62:A:HIS:HD1	1:63:A:ILE:HG12	13	0.59	0.23	0.6
(1,785)	1:64:A:HIS:HB2	1:61:A:GLN:HA	13	0.32	0.08	0.35
(1,1282)	1:21:A:ARG:HG3	1:18:A:LEU:HA	13	0.27	0.1	0.27
(1,551)	1:35:A:ARG:HB2	1:35:A:ARG:HA	13	0.21	0.02	0.22
(1,1078)	1:39:A:ALA:H	1:38:A:GLN:HB2	13	0.21	0.07	0.2
(1,1401)	1:7:A:GLN:HG2	1:7:A:GLN:HA	13	0.2	0.03	0.21
(1,1421)	1:23:A:VAL:H	1:62:A:HIS:HD1	13	0.18	0.05	0.19
(1,1047)	1:55:A:ALA:H	1:54:A:LYS:HG2	13	0.16	0.04	0.15
(1,681)	1:15:A:TYR:HE2	1:58:A:LEU:HB2	13	0.15	0.02	0.15
(1,1349)	1:22:A:ILE:H	1:23:A:VAL:HB	13	0.15	0.03	0.14
(1,227)	1:48:A:TYR:HD1	1:48:A:TYR:HA	13	0.14	0.02	0.13
(1,914)	1:41:A:PRO:HG3	1:41:A:PRO:HB2	13	0.12	0.01	0.12
(1,1372)	1:22:A:ILE:HD12	1:37:A:MET:HG3	12	0.6	0.3	0.6
(1,1372)	1:22:A:ILE:HD13	1:37:A:MET:HG3	12	0.6	0.3	0.6
(1,1372)	1:22:A:ILE:HD11	1:37:A:MET:HG3	12	0.6	0.3	0.6
(1,459)	1:52:A:THR:H	1:52:A:THR:HG21	12	0.55	0.11	0.52
(1,459)	1:52:A:THR:H	1:52:A:THR:HG22	12	0.55	0.11	0.52
(1,459)	1:52:A:THR:H	1:52:A:THR:HG23	12	0.55	0.11	0.52
(1,884)	1:65:A:ARG:H	1:65:A:ARG:HD2	12	0.44	0.24	0.4
(1,1376)	1:58:A:LEU:HD23	1:12:A:LYS:HE3	12	0.3	0.12	0.22
(1,1376)	1:58:A:LEU:HD21	1:12:A:LYS:HE3	12	0.3	0.12	0.22
(1,1376)	1:58:A:LEU:HD22	1:12:A:LYS:HE3	12	0.3	0.12	0.22
(1,935)	1:15:A:TYR:HD2	1:16:A:GLU:HB2	12	0.28	0.1	0.27
(1,866)	1:36:A:LYS:H	1:35:A:ARG:HG3	12	0.26	0.05	0.25
(1,1025)	1:36:A:LYS:HG3	1:36:A:LYS:HA	12	0.24	0.14	0.18
(1,218)	1:17:A:TRP:HE3	1:17:A:TRP:HB2	12	0.14	0.02	0.15
(1,795)	1:59:A:PHE:HE1	1:59:A:PHE:HB2	12	0.14	0.02	0.14
(1,1338)	1:64:A:HIS:H	1:62:A:HIS:HA	12	0.13	0.02	0.13
(1,905)	1:41:A:PRO:HG2	1:41:A:PRO:HA	12	0.12	0.02	0.12
(1,554)	1:35:A:ARG:HB2	1:35:A:ARG:HD2	11	0.64	0.03	0.65
(1,1154)	1:19:A:VAL:HG23	1:23:A:VAL:HG23	11	0.59	0.09	0.57
(1,1154)	1:19:A:VAL:HG21	1:23:A:VAL:HG23	11	0.59	0.09	0.57
(1,1154)	1:19:A:VAL:HG23	1:23:A:VAL:HG22	11	0.59	0.09	0.57
(1,1154)	1:19:A:VAL:HG22	1:23:A:VAL:HG23	11	0.59	0.09	0.57
(1,1154)	1:19:A:VAL:HG22	1:23:A:VAL:HG22	11	0.59	0.09	0.57
(1,1154)	1:19:A:VAL:HG21	1:23:A:VAL:HG21	11	0.59	0.09	0.57
(1,1154)	1:19:A:VAL:HG22	1:23:A:VAL:HG21	11	0.59	0.09	0.57
(1,1152)	1:19:A:VAL:HG23	1:23:A:VAL:HB	11	0.55	0.05	0.55
(1,1152)	1:19:A:VAL:HG21	1:23:A:VAL:HB	11	0.55	0.05	0.55

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1152)	1:19:A:VAL:HG22	1:23:A:VAL:HB	11	0.55	0.05	0.55
(1,1358)	1:23:A:VAL:H	1:19:A:VAL:HG23	11	0.49	0.05	0.48
(1,1358)	1:23:A:VAL:H	1:19:A:VAL:HG21	11	0.49	0.05	0.48
(1,1358)	1:23:A:VAL:H	1:19:A:VAL:HG22	11	0.49	0.05	0.48
(1,404)	1:65:A:ARG:HG2	1:65:A:ARG:HB2	11	0.41	0.04	0.4
(1,684)	1:62:A:HIS:HD1	1:23:A:VAL:HG11	11	0.37	0.15	0.39
(1,684)	1:62:A:HIS:HD1	1:23:A:VAL:HG13	11	0.37	0.15	0.39
(1,684)	1:62:A:HIS:HD1	1:23:A:VAL:HG12	11	0.37	0.15	0.39
(1,947)	1:62:A:HIS:H	1:61:A:GLN:HG3	11	0.34	0.16	0.3
(1,1127)	1:18:A:LEU:HG	1:43:A:TYR:HB3	11	0.27	0.15	0.21
(1,373)	1:61:A:GLN:HG3	1:61:A:GLN:HA	11	0.27	0.07	0.26
(1,886)	1:65:A:ARG:HD3	1:65:A:ARG:HA	11	0.25	0.08	0.27
(1,553)	1:35:A:ARG:HG3	1:35:A:ARG:HA	11	0.25	0.04	0.26
(1,873)	1:66:A:LEU:H	1:65:A:ARG:HG2	11	0.25	0.04	0.26
(1,489)	1:24:A:LYS:H	1:23:A:VAL:HG22	11	0.23	0.06	0.24
(1,489)	1:24:A:LYS:H	1:23:A:VAL:HG21	11	0.23	0.06	0.24
(1,489)	1:24:A:LYS:H	1:23:A:VAL:HG23	11	0.23	0.06	0.24
(1,1327)	1:64:A:HIS:HD1	1:69:A:GLU:HG2	11	0.23	0.15	0.17
(1,958)	1:53:A:GLN:HB2	1:53:A:GLN:HG2	11	0.21	0.03	0.21
(1,334)	1:57:A:LYS:H	1:56:A:LYS:HB2	11	0.21	0.08	0.19
(1,1095)	1:59:A:PHE:HD2	1:30:A:TRP:HA	11	0.18	0.05	0.18
(1,660)	1:68:A:HIS:HD1	1:68:A:HIS:HB3	11	0.16	0.04	0.16
(1,646)	1:19:A:VAL:H	1:18:A:LEU:HG	11	0.15	0.02	0.15
(1,26)	1:10:A:THR:HA	1:10:A:THR:HB	11	0.14	0.04	0.13
(1,565)	1:33:A:VAL:H	1:32:A:SER:HB3	10	0.43	0.12	0.42
(1,1382)	1:39:A:ALA:HB2	1:38:A:GLN:HG2	10	0.39	0.07	0.39
(1,1382)	1:39:A:ALA:HB3	1:38:A:GLN:HG2	10	0.39	0.07	0.39
(1,1382)	1:39:A:ALA:HB1	1:38:A:GLN:HG2	10	0.39	0.07	0.39
(1,1155)	1:19:A:VAL:HG21	1:62:A:HIS:HB3	10	0.38	0.16	0.38
(1,1155)	1:19:A:VAL:HG23	1:62:A:HIS:HB3	10	0.38	0.16	0.38
(1,1155)	1:19:A:VAL:HG22	1:62:A:HIS:HB3	10	0.38	0.16	0.38
(1,1004)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	10	0.37	0.17	0.35
(1,986)	1:58:A:LEU:HD11	1:12:A:LYS:HE3	10	0.34	0.08	0.34
(1,986)	1:58:A:LEU:HD13	1:12:A:LYS:HE3	10	0.34	0.08	0.34
(1,986)	1:58:A:LEU:HD12	1:12:A:LYS:HE3	10	0.34	0.08	0.34
(1,887)	1:65:A:ARG:HD2	1:65:A:ARG:HA	10	0.25	0.08	0.28
(1,867)	1:36:A:LYS:H	1:35:A:ARG:HD2	10	0.24	0.04	0.24
(1,762)	1:35:A:ARG:HD2	1:32:A:SER:HA	10	0.2	0.1	0.16
(1,1423)	1:26:A:HIS:HD1	1:66:A:LEU:HA	10	0.14	0.03	0.14
(1,703)	1:48:A:TYR:HD2	1:49:A:LEU:HB2	10	0.13	0.02	0.12
(1,1021)	1:57:A:LYS:HD2	1:57:A:LYS:HB2	9	0.58	0.12	0.61
(1,475)	1:33:A:VAL:HG22	1:33:A:VAL:HA	9	0.53	0.05	0.53

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,475)	1:33:A:VAL:HG23	1:33:A:VAL:HA	9	0.53	0.05	0.53
(1,475)	1:33:A:VAL:HG21	1:33:A:VAL:HA	9	0.53	0.05	0.53
(1,1007)	1:57:A:LYS:H	1:57:A:LYS:HE2	9	0.52	0.43	0.28
(1,1008)	1:57:A:LYS:H	1:57:A:LYS:HD2	9	0.51	0.42	0.38
(1,1175)	1:26:A:HIS:HE1	1:27:A:ASN:HD22	9	0.43	0.37	0.22
(1,1133)	1:30:A:TRP:HZ3	1:59:A:PHE:HB3	9	0.33	0.18	0.37
(1,1100)	1:30:A:TRP:HD1	1:56:A:LYS:HE2	9	0.33	0.11	0.36
(1,2)	1:66:A:LEU:HD23	1:25:A:ASN:HA	9	0.3	0.25	0.2
(1,2)	1:66:A:LEU:HD21	1:25:A:ASN:HA	9	0.3	0.25	0.2
(1,2)	1:66:A:LEU:HD22	1:25:A:ASN:HA	9	0.3	0.25	0.2
(1,757)	1:33:A:VAL:HB	1:30:A:TRP:HA	9	0.25	0.05	0.26
(1,705)	1:68:A:HIS:HD1	1:67:A:LYS:HG2	9	0.24	0.15	0.22
(1,467)	1:54:A:LYS:H	1:53:A:GLN:HG2	9	0.23	0.06	0.22
(1,926)	1:51:A:GLY:H	1:50:A:GLU:HG3	9	0.22	0.11	0.21
(1,422)	1:66:A:LEU:H	1:66:A:LEU:HD12	9	0.21	0.05	0.24
(1,422)	1:66:A:LEU:H	1:66:A:LEU:HD11	9	0.21	0.05	0.24
(1,422)	1:66:A:LEU:H	1:66:A:LEU:HD13	9	0.21	0.05	0.24
(1,481)	1:33:A:VAL:H	1:33:A:VAL:HB	9	0.21	0.03	0.22
(1,1117)	1:30:A:TRP:HE3	1:33:A:VAL:HB	9	0.18	0.05	0.2
(1,1426)	1:68:A:HIS:HD1	1:64:A:HIS:HB2	9	0.18	0.04	0.18
(1,1124)	1:15:A:TYR:HD2	1:55:A:ALA:HA	9	0.16	0.03	0.14
(1,434)	1:69:A:GLU:H	1:68:A:HIS:HB3	9	0.14	0.02	0.14
(1,1326)	1:64:A:HIS:HD1	1:67:A:LYS:HE2	8	0.64	0.21	0.72
(1,441)	1:69:A:GLU:H	1:69:A:GLU:HB3	8	0.31	0.16	0.26
(1,1187)	1:59:A:PHE:HE2	1:60:A:LEU:HD13	8	0.17	0.04	0.16
(1,1187)	1:59:A:PHE:HE2	1:60:A:LEU:HD12	8	0.17	0.04	0.16
(1,1187)	1:59:A:PHE:HE2	1:60:A:LEU:HD11	8	0.17	0.04	0.16
(1,651)	1:21:A:ARG:HB2	1:18:A:LEU:HA	8	0.14	0.03	0.13
(1,901)	1:40:A:SER:H	1:41:A:PRO:HD2	8	0.14	0.02	0.13
(1,653)	1:67:A:LYS:HB2	1:67:A:LYS:HE2	7	0.66	0.13	0.66
(1,1017)	1:57:A:LYS:HG3	1:57:A:LYS:HE2	7	0.34	0.22	0.21
(1,1226)	1:47:A:VAL:HG21	1:44:A:GLN:HA	7	0.27	0.12	0.24
(1,1226)	1:47:A:VAL:HG22	1:44:A:GLN:HA	7	0.27	0.12	0.24
(1,1226)	1:47:A:VAL:HG23	1:44:A:GLN:HA	7	0.27	0.12	0.24
(1,584)	1:13:A:ASP:H	1:12:A:LYS:HB2	7	0.21	0.06	0.23
(1,1315)	1:18:A:LEU:HG	1:42:A:GLU:HG3	7	0.15	0.05	0.12
(1,1296)	1:60:A:LEU:HG	1:57:A:LYS:HA	7	0.12	0.02	0.12
(3,10)	1:13:A:ASP:O	1:17:A:TRP:H	7	0.12	0.02	0.12
(1,242)	1:47:A:VAL:H	1:46:A:TYR:HB2	7	0.12	0.01	0.11
(1,1134)	1:30:A:TRP:HZ3	1:30:A:TRP:HA	7	0.12	0.01	0.11
(1,1269)	1:58:A:LEU:HD13	1:16:A:GLU:HG3	6	0.57	0.19	0.56
(1,1269)	1:58:A:LEU:HD12	1:16:A:GLU:HG3	6	0.57	0.19	0.56

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1269)	1:58:A:LEU:HD11	1:16:A:GLU:HG3	6	0.57	0.19	0.56
(1,1393)	1:26:A:HIS:HE1	1:67:A:LYS:HG3	6	0.41	0.11	0.44
(1,338)	1:57:A:LYS:H	1:57:A:LYS:HG2	6	0.38	0.14	0.36
(1,1219)	1:56:A:LYS:HB2	1:53:A:GLN:HA	6	0.32	0.16	0.31
(1,1286)	1:36:A:LYS:HG2	1:33:A:VAL:HA	6	0.29	0.08	0.3
(1,1419)	1:27:A:ASN:H	1:63:A:ILE:HD12	6	0.27	0.13	0.26
(1,1419)	1:27:A:ASN:H	1:63:A:ILE:HD13	6	0.27	0.13	0.26
(1,1081)	1:43:A:TYR:HE1	1:38:A:GLN:HB2	6	0.25	0.19	0.13
(1,1081)	1:43:A:TYR:HE2	1:38:A:GLN:HB2	6	0.25	0.19	0.13
(1,755)	1:22:A:ILE:HG12	1:19:A:VAL:HA	6	0.2	0.06	0.2
(1,1183)	1:69:A:GLU:H	1:68:A:HIS:H	6	0.18	0.07	0.16
(1,790)	1:67:A:LYS:HB2	1:64:A:HIS:HA	6	0.16	0.06	0.14
(1,558)	1:35:A:ARG:H	1:35:A:ARG:HD2	6	0.14	0.05	0.11
(1,24)	1:63:A:ILE:HD11	1:26:A:HIS:HB3	6	0.14	0.03	0.15
(1,24)	1:63:A:ILE:HD12	1:26:A:HIS:HB3	6	0.14	0.03	0.15
(1,24)	1:63:A:ILE:HD13	1:26:A:HIS:HB3	6	0.14	0.03	0.15
(1,1050)	1:54:A:LYS:HG3	1:54:A:LYS:HA	6	0.14	0.02	0.13
(1,1354)	1:62:A:HIS:HD1	1:63:A:ILE:HA	6	0.14	0.02	0.14
(1,666)	1:62:A:HIS:HD1	1:62:A:HIS:HA	6	0.12	0.01	0.13
(1,1242)	1:66:A:LEU:HD11	1:26:A:HIS:HB2	5	1.07	1.1	0.31
(1,1242)	1:66:A:LEU:HD12	1:26:A:HIS:HB2	5	1.07	1.1	0.31
(1,1242)	1:66:A:LEU:HD13	1:26:A:HIS:HB2	5	1.07	1.1	0.31
(1,741)	1:61:A:GLN:HE21	1:61:A:GLN:HG3	5	0.44	0.04	0.42
(1,1407)	1:8:A:ILE:HD13	1:5:A:SER:HA	5	0.4	0.15	0.5
(1,1407)	1:8:A:ILE:HD11	1:5:A:SER:HA	5	0.4	0.15	0.5
(1,1407)	1:8:A:ILE:HD12	1:5:A:SER:HA	5	0.4	0.15	0.5
(1,997)	1:24:A:LYS:HD2	1:24:A:LYS:HB2	5	0.38	0.12	0.4
(1,1415)	1:24:A:LYS:HG3	1:24:A:LYS:HA	5	0.34	0.07	0.32
(1,1406)	1:8:A:ILE:HD13	1:5:A:SER:HB2	5	0.32	0.23	0.23
(1,1406)	1:8:A:ILE:HD11	1:5:A:SER:HB2	5	0.32	0.23	0.23
(1,1406)	1:8:A:ILE:HD12	1:5:A:SER:HB2	5	0.32	0.23	0.23
(1,483)	1:34:A:SER:H	1:33:A:VAL:HG22	5	0.25	0.08	0.27
(1,483)	1:34:A:SER:H	1:33:A:VAL:HG21	5	0.25	0.08	0.27
(1,1001)	1:24:A:LYS:HD2	1:24:A:LYS:HB3	5	0.24	0.07	0.28
(1,627)	1:16:A:GLU:HG3	1:16:A:GLU:HA	5	0.22	0.07	0.23
(1,811)	1:66:A:LEU:H	1:66:A:LEU:HD22	5	0.21	0.05	0.21
(1,811)	1:66:A:LEU:H	1:66:A:LEU:HD23	5	0.21	0.05	0.21
(1,811)	1:66:A:LEU:H	1:66:A:LEU:HD21	5	0.21	0.05	0.21
(1,776)	1:61:A:GLN:HB3	1:58:A:LEU:HA	5	0.21	0.08	0.21
(1,487)	1:59:A:PHE:HD1	1:19:A:VAL:HG23	5	0.19	0.04	0.2
(1,487)	1:59:A:PHE:HD1	1:19:A:VAL:HG21	5	0.19	0.04	0.2
(1,487)	1:59:A:PHE:HD1	1:19:A:VAL:HG22	5	0.19	0.04	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1107)	1:43:A:TYR:HE1	1:34:A:SER:HB2	5	0.18	0.03	0.18
(1,1107)	1:43:A:TYR:HE2	1:34:A:SER:HB2	5	0.18	0.03	0.18
(1,312)	1:40:A:SER:H	1:40:A:SER:HB3	5	0.14	0.01	0.14
(1,629)	1:16:A:GLU:H	1:16:A:GLU:HG2	5	0.14	0.02	0.13
(3,20)	1:18:A:LEU:O	1:22:A:ILE:H	5	0.14	0.02	0.14
(1,1387)	1:68:A:HIS:HD1	1:67:A:LYS:HE2	5	0.13	0.03	0.11
(1,1098)	1:30:A:TRP:HD1	1:56:A:LYS:HG2	5	0.12	0.02	0.12
(1,1381)	1:49:A:LEU:HD23	1:7:A:GLN:HG2	4	0.38	0.21	0.34
(1,1381)	1:49:A:LEU:HD22	1:7:A:GLN:HG2	4	0.38	0.21	0.34
(1,268)	1:19:A:VAL:H	1:19:A:VAL:HG22	4	0.34	0.02	0.34
(1,268)	1:19:A:VAL:H	1:19:A:VAL:HG23	4	0.34	0.02	0.34
(1,403)	1:65:A:ARG:HG2	1:65:A:ARG:HA	4	0.32	0.14	0.32
(1,874)	1:65:A:ARG:HG3	1:65:A:ARG:HA	4	0.31	0.04	0.3
(1,1291)	1:57:A:LYS:HB2	1:54:A:LYS:HA	4	0.31	0.09	0.32
(1,20)	1:67:A:LYS:HG2	1:26:A:HIS:HB2	4	0.3	0.11	0.26
(1,1302)	1:63:A:ILE:HG12	1:60:A:LEU:HA	4	0.26	0.17	0.2
(1,858)	1:22:A:ILE:H	1:21:A:ARG:HG3	4	0.26	0.05	0.28
(1,1213)	1:30:A:TRP:HE3	1:37:A:MET:HE3	4	0.26	0.07	0.28
(1,1213)	1:30:A:TRP:HE3	1:37:A:MET:HE1	4	0.26	0.07	0.28
(1,269)	1:20:A:SER:H	1:19:A:VAL:HB	4	0.22	0.02	0.21
(1,1168)	1:68:A:HIS:HE1	1:67:A:LYS:HE2	4	0.2	0.05	0.22
(1,1417)	1:25:A:ASN:H	1:24:A:LYS:HG3	4	0.18	0.02	0.18
(1,777)	1:61:A:GLN:HG2	1:58:A:LEU:HA	4	0.15	0.04	0.14
(1,1276)	1:17:A:TRP:HZ3	1:18:A:LEU:HA	4	0.12	0.02	0.11
(1,614)	1:28:A:GLU:H	1:28:A:GLU:HB3	4	0.11	0.01	0.11
(1,1308)	1:33:A:VAL:HG13	1:28:A:GLU:HG2	3	1.0	0.34	1.21
(1,1308)	1:33:A:VAL:HG12	1:28:A:GLU:HG2	3	1.0	0.34	1.21
(1,1012)	1:57:A:LYS:HD2	1:57:A:LYS:HA	3	0.73	0.45	0.94
(1,1029)	1:36:A:LYS:HG2	1:36:A:LYS:HE2	3	0.64	0.05	0.64
(1,1037)	1:36:A:LYS:HD2	1:36:A:LYS:HB2	3	0.48	0.06	0.48
(1,1003)	1:24:A:LYS:HG2	1:24:A:LYS:HE2	3	0.39	0.06	0.35
(1,1016)	1:57:A:LYS:HG2	1:57:A:LYS:HE2	3	0.38	0.03	0.37
(1,1040)	1:37:A:MET:H	1:36:A:LYS:HG3	3	0.38	0.14	0.3
(1,885)	1:65:A:ARG:H	1:65:A:ARG:HD3	3	0.37	0.15	0.45
(1,721)	1:62:A:HIS:HE1	1:20:A:SER:HB3	3	0.37	0.19	0.49
(1,1180)	1:7:A:GLN:HE22	1:7:A:GLN:HG3	3	0.27	0.08	0.32
(1,7)	1:66:A:LEU:HD23	1:24:A:LYS:HA	3	0.26	0.05	0.24
(1,7)	1:66:A:LEU:HD22	1:24:A:LYS:HA	3	0.26	0.05	0.24
(1,954)	1:53:A:GLN:HG2	1:53:A:GLN:HA	3	0.22	0.04	0.25
(1,1149)	1:62:A:HIS:H	1:19:A:VAL:HG11	3	0.21	0.06	0.24
(1,872)	1:65:A:ARG:H	1:65:A:ARG:HG2	3	0.19	0.06	0.22
(1,1272)	1:16:A:GLU:HB3	1:13:A:ASP:HA	3	0.16	0.05	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,288)	1:21:A:ARG:H	1:21:A:ARG:HG2	3	0.15	0.05	0.12
(1,437)	1:69:A:GLU:HB2	1:69:A:GLU:HA	3	0.15	0.01	0.14
(1,1241)	1:63:A:ILE:HG22	1:26:A:HIS:HB3	3	0.14	0.02	0.14
(1,1241)	1:63:A:ILE:HG23	1:26:A:HIS:HB3	3	0.14	0.02	0.14
(1,1330)	1:17:A:TRP:HZ3	1:14:A:LYS:HG2	3	0.13	0.02	0.13
(1,1087)	1:56:A:LYS:H	1:53:A:GLN:HA	3	0.13	0.02	0.13
(1,1076)	1:38:A:GLN:H	1:38:A:GLN:HB2	3	0.11	0.0	0.11
(1,1323)	1:64:A:HIS:HD1	1:65:A:ARG:HG3	3	0.11	0.0	0.11
(1,10)	1:66:A:LEU:HD13	1:26:A:HIS:HA	2	1.65	0.04	1.65
(1,10)	1:66:A:LEU:HD11	1:26:A:HIS:HA	2	1.65	0.04	1.65
(1,414)	1:66:A:LEU:HD22	1:66:A:LEU:HA	2	1.04	0.22	1.04
(1,557)	1:35:A:ARG:HD2	1:35:A:ARG:HA	2	1.04	0.01	1.04
(1,417)	1:66:A:LEU:H	1:66:A:LEU:HG	2	0.77	0.04	0.77
(1,995)	1:24:A:LYS:HD2	1:24:A:LYS:HA	2	0.7	0.03	0.7
(1,1159)	1:62:A:HIS:HD1	1:66:A:LEU:HD13	2	0.61	0.03	0.61
(1,1159)	1:62:A:HIS:HD1	1:66:A:LEU:HD12	2	0.61	0.03	0.61
(1,421)	1:66:A:LEU:HD21	1:66:A:LEU:HB3	2	0.46	0.16	0.46
(1,870)	1:35:A:ARG:HG2	1:35:A:ARG:HB2	2	0.38	0.01	0.38
(1,5)	1:25:A:ASN:HB2	1:25:A:ASN:HA	2	0.32	0.09	0.32
(1,1304)	1:65:A:ARG:HB3	1:65:A:ARG:HD3	2	0.27	0.03	0.27
(1,1174)	1:44:A:GLN:HE21	1:43:A:TYR:HD2	2	0.24	0.12	0.24
(1,1174)	1:44:A:GLN:HE21	1:43:A:TYR:HD1	2	0.24	0.12	0.24
(1,763)	1:35:A:ARG:HG2	1:32:A:SER:HA	2	0.24	0.06	0.24
(1,488)	1:43:A:TYR:HD2	1:47:A:VAL:HG23	2	0.23	0.09	0.23
(1,488)	1:43:A:TYR:HD1	1:47:A:VAL:HG21	2	0.23	0.09	0.23
(1,466)	1:53:A:GLN:H	1:53:A:GLN:HB2	2	0.19	0.0	0.19
(1,1346)	1:43:A:TYR:HD1	1:37:A:MET:HG2	2	0.18	0.04	0.18
(1,1359)	1:23:A:VAL:H	1:19:A:VAL:HG11	2	0.18	0.01	0.18
(1,1359)	1:23:A:VAL:H	1:19:A:VAL:HG12	2	0.18	0.01	0.18
(1,562)	1:36:A:LYS:H	1:35:A:ARG:HG2	2	0.18	0.06	0.18
(1,1373)	1:22:A:ILE:HD13	1:37:A:MET:HG2	2	0.18	0.01	0.18
(1,1373)	1:22:A:ILE:HD11	1:37:A:MET:HG2	2	0.18	0.01	0.18
(1,984)	1:46:A:TYR:HE1	1:12:A:LYS:HG2	2	0.18	0.04	0.18
(1,946)	1:62:A:HIS:H	1:61:A:GLN:HG2	2	0.17	0.02	0.17
(1,494)	1:67:A:LYS:H	1:67:A:LYS:HG3	2	0.16	0.03	0.16
(1,369)	1:61:A:GLN:H	1:61:A:GLN:HB2	2	0.15	0.01	0.15
(1,18)	1:66:A:LEU:HB3	1:26:A:HIS:HB2	2	0.14	0.02	0.14
(1,237)	1:43:A:TYR:HD2	1:43:A:TYR:HA	2	0.13	0.02	0.13
(3,16)	1:16:A:GLU:O	1:20:A:SER:H	2	0.13	0.01	0.13
(3,17)	1:17:A:TRP:O	1:21:A:ARG:N	2	0.12	0.02	0.12
(1,1006)	1:57:A:LYS:H	1:57:A:LYS:HG3	2	0.12	0.01	0.12
(1,1284)	1:34:A:SER:HB3	1:31:A:LEU:HA	2	0.12	0.01	0.12

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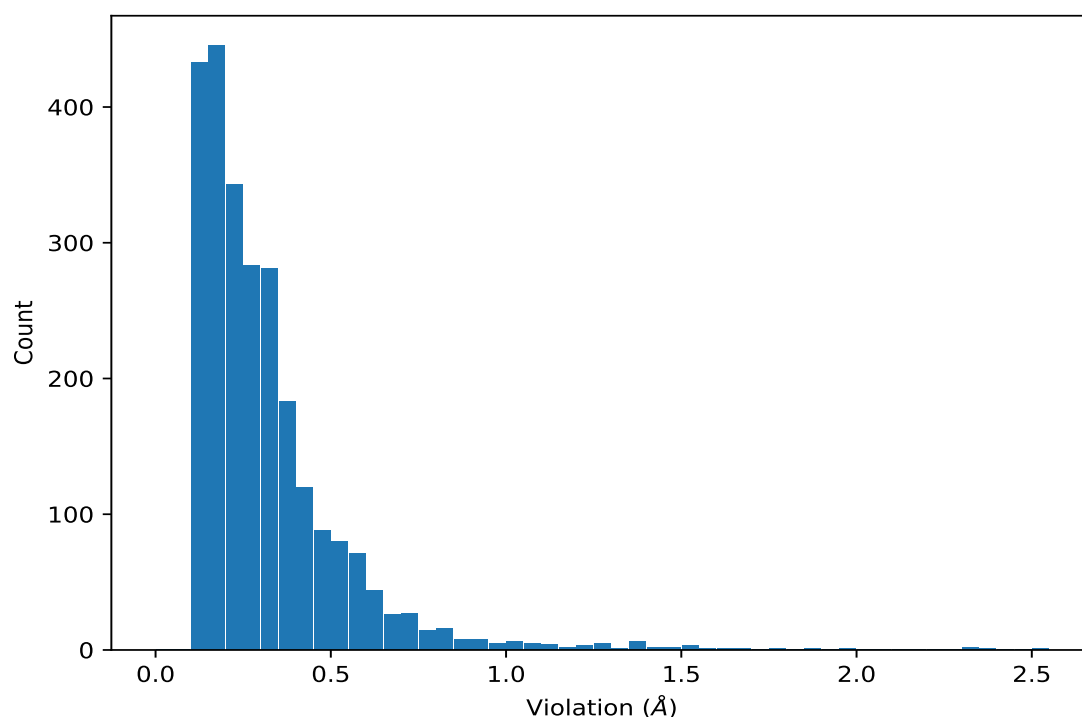
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,996)	1:24:A:LYS:HG2	1:24:A:LYS:HA	2	0.11	0.0	0.11

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)
(1,1242)	1:66:A:LEU:HD11	1:26:A:HIS:HB2	15	2.51
(1,1331)	1:23:A:VAL:H	1:33:A:VAL:HB	7	2.35
(1,1331)	1:23:A:VAL:H	1:33:A:VAL:HB	9	2.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1242)	1:66:A:LEU:HD12	1:26:A:HIS:HB2	12	2.32
(1,1413)	1:49:A:LEU:HD22	1:50:A:GLU:HG3	5	1.96
(1,1331)	1:23:A:VAL:H	1:33:A:VAL:HB	4	1.87
(1,1331)	1:23:A:VAL:H	1:33:A:VAL:HB	8	1.75
(1,10)	1:66:A:LEU:HD11	1:26:A:HIS:HA	15	1.69
(1,10)	1:66:A:LEU:HD13	1:26:A:HIS:HA	12	1.61
(1,1313)	1:33:A:VAL:HA	1:32:A:SER:HB3	14	1.57
(1,1341)	1:17:A:TRP:HE3	1:21:A:ARG:HB2	8	1.53
(1,1008)	1:57:A:LYS:H	1:57:A:LYS:HD2	12	1.53
(1,1341)	1:17:A:TRP:HE3	1:21:A:ARG:HB2	4	1.52
(1,1331)	1:23:A:VAL:H	1:33:A:VAL:HB	14	1.49
(1,1341)	1:17:A:TRP:HE3	1:21:A:ARG:HB2	5	1.46
(1,1341)	1:17:A:TRP:HE3	1:21:A:ARG:HB2	6	1.42
(1,1341)	1:17:A:TRP:HE3	1:21:A:ARG:HB2	9	1.41
(1,1341)	1:17:A:TRP:HE3	1:21:A:ARG:HB2	1	1.39
(1,1341)	1:17:A:TRP:HE3	1:21:A:ARG:HB2	3	1.37
(1,1007)	1:57:A:LYS:H	1:57:A:LYS:HE2	14	1.37
(1,1341)	1:17:A:TRP:HE3	1:21:A:ARG:HB2	12	1.36
(1,1341)	1:17:A:TRP:HE3	1:21:A:ARG:HB2	7	1.35
(1,1341)	1:17:A:TRP:HE3	1:21:A:ARG:HB2	10	1.35
(1,1341)	1:17:A:TRP:HE3	1:21:A:ARG:HB2	11	1.34
(1,1331)	1:23:A:VAL:H	1:33:A:VAL:HB	2	1.29
(1,530)	1:31:A:LEU:HD12	1:31:A:LEU:HA	4	1.29
(1,1308)	1:33:A:VAL:HG12	1:28:A:GLU:HG2	9	1.28
(1,414)	1:66:A:LEU:HD22	1:66:A:LEU:HA	15	1.26
(1,1244)	1:26:A:HIS:HE1	1:67:A:LYS:HB2	10	1.25
(1,1244)	1:26:A:HIS:HE1	1:67:A:LYS:HB2	13	1.24
(1,1244)	1:26:A:HIS:HE1	1:67:A:LYS:HB2	11	1.22
(1,1308)	1:33:A:VAL:HG13	1:28:A:GLU:HG2	8	1.21
(1,1244)	1:26:A:HIS:HE1	1:67:A:LYS:HB2	6	1.18
(1,1007)	1:57:A:LYS:H	1:57:A:LYS:HE2	13	1.17
(1,1012)	1:57:A:LYS:HD2	1:57:A:LYS:HA	3	1.14
(1,13)	1:26:A:HIS:HD1	1:67:A:LYS:HD2	3	1.13
(1,1244)	1:26:A:HIS:HE1	1:67:A:LYS:HB2	3	1.11
(1,13)	1:26:A:HIS:HD1	1:67:A:LYS:HD2	9	1.11
(1,1175)	1:26:A:HIS:HE1	1:27:A:ASN:HD22	8	1.08
(1,13)	1:26:A:HIS:HD1	1:67:A:LYS:HD2	14	1.08
(1,1372)	1:22:A:ILE:HD13	1:37:A:MET:HG3	4	1.07
(1,1244)	1:26:A:HIS:HE1	1:67:A:LYS:HB2	1	1.07
(1,1175)	1:26:A:HIS:HE1	1:27:A:ASN:HD22	14	1.06
(1,557)	1:35:A:ARG:HD2	1:35:A:ARG:HA	12	1.04
(1,557)	1:35:A:ARG:HD2	1:35:A:ARG:HA	10	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1372)	1:22:A:ILE:HD13	1:37:A:MET:HG3	8	1.01
(1,13)	1:26:A:HIS:HD1	1:67:A:LYS:HD2	1	1.01
(1,1204)	1:18:A:LEU:HG	1:42:A:GLU:HA	13	1.0
(1,13)	1:26:A:HIS:HD1	1:67:A:LYS:HD2	6	1.0
(1,13)	1:26:A:HIS:HD1	1:67:A:LYS:HD2	10	0.99
(1,1313)	1:33:A:VAL:HA	1:32:A:SER:HB3	4	0.97
(1,1244)	1:26:A:HIS:HE1	1:67:A:LYS:HB2	14	0.97
(1,13)	1:26:A:HIS:HD1	1:67:A:LYS:HD2	11	0.97
(1,1355)	1:62:A:HIS:HD1	1:63:A:ILE:HG12	12	0.95
(1,1012)	1:57:A:LYS:HD2	1:57:A:LYS:HA	15	0.94
(1,13)	1:26:A:HIS:HD1	1:67:A:LYS:HD2	12	0.94
(1,1413)	1:49:A:LEU:HD21	1:50:A:GLU:HG3	3	0.93
(1,1244)	1:26:A:HIS:HE1	1:67:A:LYS:HB2	9	0.93
(1,1313)	1:33:A:VAL:HA	1:32:A:SER:HB3	9	0.92
(1,2)	1:66:A:LEU:HD23	1:25:A:ASN:HA	12	0.92
(1,1413)	1:49:A:LEU:HD21	1:50:A:GLU:HG3	9	0.9
(1,1372)	1:22:A:ILE:HD11	1:37:A:MET:HG3	6	0.9
(1,1355)	1:62:A:HIS:HD1	1:63:A:ILE:HG12	4	0.88
(1,1321)	1:64:A:HIS:HD1	1:65:A:ARG:HB3	13	0.88
(1,13)	1:26:A:HIS:HD1	1:67:A:LYS:HD2	13	0.87
(1,1326)	1:64:A:HIS:HD1	1:67:A:LYS:HE2	8	0.86
(1,1313)	1:33:A:VAL:HA	1:32:A:SER:HB3	8	0.86
(1,1204)	1:18:A:LEU:HG	1:42:A:GLU:HA	8	0.86
(1,1425)	1:10:A:THR:H	1:13:A:ASP:HB2	15	0.85
(1,1355)	1:62:A:HIS:HD1	1:63:A:ILE:HG12	7	0.85
(1,13)	1:26:A:HIS:HD1	1:67:A:LYS:HD2	4	0.84
(1,1413)	1:49:A:LEU:HD22	1:50:A:GLU:HG3	14	0.83
(1,1372)	1:22:A:ILE:HD12	1:37:A:MET:HG3	3	0.83
(1,1313)	1:33:A:VAL:HA	1:32:A:SER:HB3	3	0.83
(1,1269)	1:58:A:LEU:HD11	1:16:A:GLU:HG3	11	0.83
(1,1046)	1:54:A:LYS:H	1:54:A:LYS:HG2	1	0.83
(1,414)	1:66:A:LEU:HD22	1:66:A:LEU:HA	12	0.83
(1,13)	1:26:A:HIS:HD1	1:67:A:LYS:HD2	2	0.83
(1,884)	1:65:A:ARG:H	1:65:A:ARG:HD2	1	0.82
(1,653)	1:67:A:LYS:HB2	1:67:A:LYS:HE2	15	0.82
(1,13)	1:26:A:HIS:HD1	1:67:A:LYS:HD2	15	0.82
(1,1413)	1:49:A:LEU:HD22	1:50:A:GLU:HG3	2	0.81
(1,884)	1:65:A:ARG:H	1:65:A:ARG:HD2	4	0.81
(1,417)	1:66:A:LEU:H	1:66:A:LEU:HG	15	0.81
(1,884)	1:65:A:ARG:H	1:65:A:ARG:HD2	14	0.8
(1,459)	1:52:A:THR:H	1:52:A:THR:HG23	7	0.8
(1,653)	1:67:A:LYS:HB2	1:67:A:LYS:HE2	7	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1326)	1:64:A:HIS:HD1	1:67:A:LYS:HE2	15	0.78
(1,801)	1:23:A:VAL:H	1:22:A:ILE:HD12	7	0.78
(1,1326)	1:64:A:HIS:HD1	1:67:A:LYS:HE2	2	0.77
(1,1275)	1:17:A:TRP:HD1	1:18:A:LEU:HA	10	0.77
(1,1275)	1:17:A:TRP:HD1	1:18:A:LEU:HA	11	0.77
(1,1413)	1:49:A:LEU:HD22	1:50:A:GLU:HG3	4	0.76
(1,1275)	1:17:A:TRP:HD1	1:18:A:LEU:HA	3	0.76
(1,516)	1:8:A:ILE:HD12	1:8:A:ILE:HB	4	0.76
(1,320)	1:45:A:ASP:H	1:44:A:GLN:HG3	12	0.76
(1,1355)	1:62:A:HIS:HD1	1:63:A:ILE:HG12	15	0.75
(1,1313)	1:33:A:VAL:HA	1:32:A:SER:HB3	5	0.75
(1,1154)	1:19:A:VAL:HG23	1:23:A:VAL:HG22	5	0.75
(1,653)	1:67:A:LYS:HB2	1:67:A:LYS:HE2	2	0.75
(1,1406)	1:8:A:ILE:HD11	1:5:A:SER:HB2	4	0.74
(1,1372)	1:22:A:ILE:HD11	1:37:A:MET:HG3	5	0.74
(1,1355)	1:62:A:HIS:HD1	1:63:A:ILE:HG12	6	0.74
(1,1313)	1:33:A:VAL:HA	1:32:A:SER:HB3	15	0.74
(1,1275)	1:17:A:TRP:HD1	1:18:A:LEU:HA	7	0.74
(1,1204)	1:18:A:LEU:HG	1:42:A:GLU:HA	5	0.74
(1,995)	1:24:A:LYS:HD2	1:24:A:LYS:HA	10	0.74
(1,977)	1:56:A:LYS:HD2	1:56:A:LYS:HB2	9	0.74
(1,1413)	1:49:A:LEU:HD21	1:50:A:GLU:HG3	15	0.73
(1,1326)	1:64:A:HIS:HD1	1:67:A:LYS:HE2	7	0.73
(1,1155)	1:19:A:VAL:HG23	1:62:A:HIS:HB3	15	0.73
(1,1021)	1:57:A:LYS:HD2	1:57:A:LYS:HB2	6	0.73
(1,417)	1:66:A:LEU:H	1:66:A:LEU:HG	12	0.73
(1,1372)	1:22:A:ILE:HD13	1:37:A:MET:HG3	15	0.72
(1,1326)	1:64:A:HIS:HD1	1:67:A:LYS:HE2	12	0.72
(1,1275)	1:17:A:TRP:HD1	1:18:A:LEU:HA	6	0.72
(1,1017)	1:57:A:LYS:HG3	1:57:A:LYS:HE2	3	0.72
(1,517)	1:8:A:ILE:HG22	1:8:A:ILE:HG12	4	0.72
(1,459)	1:52:A:THR:H	1:52:A:THR:HG21	14	0.72
(1,1425)	1:10:A:THR:H	1:13:A:ASP:HB2	13	0.71
(1,1381)	1:49:A:LEU:HD23	1:7:A:GLN:HG2	6	0.71
(1,1008)	1:57:A:LYS:H	1:57:A:LYS:HD2	8	0.71
(1,1413)	1:49:A:LEU:HD22	1:50:A:GLU:HG3	7	0.7
(1,1029)	1:36:A:LYS:HG2	1:36:A:LYS:HE2	4	0.7
(1,1021)	1:57:A:LYS:HD2	1:57:A:LYS:HB2	7	0.7
(1,1008)	1:57:A:LYS:H	1:57:A:LYS:HD2	6	0.7
(1,1004)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	8	0.7
(1,1413)	1:49:A:LEU:HD22	1:50:A:GLU:HG3	1	0.69
(1,1021)	1:57:A:LYS:HD2	1:57:A:LYS:HB2	15	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,801)	1:23:A:VAL:H	1:22:A:ILE:HD12	9	0.69
(1,554)	1:35:A:ARG:HB2	1:35:A:ARG:HD2	13	0.69
(1,1413)	1:49:A:LEU:HD23	1:50:A:GLU:HG3	13	0.68
(1,1269)	1:58:A:LEU:HD11	1:16:A:GLU:HG3	13	0.68
(1,1154)	1:19:A:VAL:HG23	1:23:A:VAL:HG23	3	0.68
(1,995)	1:24:A:LYS:HD2	1:24:A:LYS:HA	11	0.67
(1,801)	1:23:A:VAL:H	1:22:A:ILE:HD11	13	0.67
(1,554)	1:35:A:ARG:HB2	1:35:A:ARG:HD2	4	0.67
(1,12)	1:26:A:HIS:HD1	1:67:A:LYS:HB2	3	0.67
(1,1413)	1:49:A:LEU:HD21	1:50:A:GLU:HG3	12	0.66
(1,801)	1:23:A:VAL:H	1:22:A:ILE:HD11	1	0.66
(1,801)	1:23:A:VAL:H	1:22:A:ILE:HD11	11	0.66
(1,653)	1:67:A:LYS:HB2	1:67:A:LYS:HE2	8	0.66
(1,554)	1:35:A:ARG:HB2	1:35:A:ARG:HD2	1	0.66
(1,1275)	1:17:A:TRP:HD1	1:18:A:LEU:HA	12	0.65
(1,1154)	1:19:A:VAL:HG22	1:23:A:VAL:HG23	6	0.65
(1,1154)	1:19:A:VAL:HG23	1:23:A:VAL:HG23	13	0.65
(1,1021)	1:57:A:LYS:HD2	1:57:A:LYS:HB2	9	0.65
(1,947)	1:62:A:HIS:H	1:61:A:GLN:HG3	11	0.65
(1,801)	1:23:A:VAL:H	1:22:A:ILE:HD12	14	0.65
(1,554)	1:35:A:ARG:HB2	1:35:A:ARG:HD2	3	0.65
(1,554)	1:35:A:ARG:HB2	1:35:A:ARG:HD2	6	0.65
(1,554)	1:35:A:ARG:HB2	1:35:A:ARG:HD2	9	0.65
(1,13)	1:26:A:HIS:HD1	1:67:A:LYS:HD2	7	0.65
(1,1159)	1:62:A:HIS:HD1	1:66:A:LEU:HD13	12	0.64
(1,1029)	1:36:A:LYS:HG2	1:36:A:LYS:HE2	5	0.64
(1,801)	1:23:A:VAL:H	1:22:A:ILE:HD12	10	0.64
(1,554)	1:35:A:ARG:HB2	1:35:A:ARG:HD2	15	0.64
(1,1275)	1:17:A:TRP:HD1	1:18:A:LEU:HA	9	0.63
(1,947)	1:62:A:HIS:H	1:61:A:GLN:HG3	4	0.63
(1,801)	1:23:A:VAL:H	1:22:A:ILE:HD11	12	0.63
(1,565)	1:33:A:VAL:H	1:32:A:SER:HB3	4	0.63
(1,554)	1:35:A:ARG:HB2	1:35:A:ARG:HD2	2	0.63
(1,512)	1:8:A:ILE:H	1:8:A:ILE:HG23	12	0.63
(1,1413)	1:49:A:LEU:HD22	1:50:A:GLU:HG3	11	0.62
(1,1326)	1:64:A:HIS:HD1	1:67:A:LYS:HE2	3	0.62
(1,1313)	1:33:A:VAL:HA	1:32:A:SER:HB3	7	0.62
(1,1219)	1:56:A:LYS:HB2	1:53:A:GLN:HA	8	0.62
(1,1152)	1:19:A:VAL:HG23	1:23:A:VAL:HB	13	0.62
(1,1081)	1:43:A:TYR:HE2	1:38:A:GLN:HB2	8	0.62
(1,801)	1:23:A:VAL:H	1:22:A:ILE:HD13	2	0.62
(1,705)	1:68:A:HIS:HD1	1:67:A:LYS:HG2	12	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,512)	1:8:A:ILE:H	1:8:A:ILE:HG21	3	0.62
(1,512)	1:8:A:ILE:H	1:8:A:ILE:HG22	5	0.62
(1,421)	1:66:A:LEU:HD21	1:66:A:LEU:HB3	12	0.62
(1,354)	1:59:A:PHE:H	1:58:A:LEU:HD22	13	0.62
(1,1355)	1:62:A:HIS:HD1	1:63:A:ILE:HG12	5	0.61
(1,1154)	1:19:A:VAL:HG23	1:23:A:VAL:HG23	1	0.61
(1,1152)	1:19:A:VAL:HG23	1:23:A:VAL:HB	5	0.61
(1,1127)	1:18:A:LEU:HG	1:43:A:TYR:HB3	10	0.61
(1,1021)	1:57:A:LYS:HD2	1:57:A:LYS:HB2	8	0.61
(1,1007)	1:57:A:LYS:H	1:57:A:LYS:HE2	2	0.61
(1,684)	1:62:A:HIS:HD1	1:23:A:VAL:HG13	7	0.61
(1,554)	1:35:A:ARG:HB2	1:35:A:ARG:HD2	11	0.61
(1,554)	1:35:A:ARG:HB2	1:35:A:ARG:HD2	14	0.61
(1,459)	1:52:A:THR:H	1:52:A:THR:HG21	8	0.61
(1,354)	1:59:A:PHE:H	1:58:A:LEU:HD21	9	0.61
(1,224)	1:48:A:TYR:H	1:48:A:TYR:HD2	9	0.61
(1,1355)	1:62:A:HIS:HD1	1:63:A:ILE:HG12	9	0.6
(1,1175)	1:26:A:HIS:HE1	1:27:A:ASN:HD22	9	0.6
(1,1152)	1:19:A:VAL:HG21	1:23:A:VAL:HB	14	0.6
(1,512)	1:8:A:ILE:H	1:8:A:ILE:HG21	2	0.6
(1,512)	1:8:A:ILE:H	1:8:A:ILE:HG21	4	0.6
(1,512)	1:8:A:ILE:H	1:8:A:ILE:HG23	7	0.6
(1,512)	1:8:A:ILE:H	1:8:A:ILE:HG22	13	0.6
(1,512)	1:8:A:ILE:H	1:8:A:ILE:HG21	15	0.6
(1,354)	1:59:A:PHE:H	1:58:A:LEU:HD21	11	0.6
(1,13)	1:26:A:HIS:HD1	1:67:A:LYS:HD2	8	0.6
(1,1152)	1:19:A:VAL:HG22	1:23:A:VAL:HB	8	0.59
(1,653)	1:67:A:LYS:HB2	1:67:A:LYS:HE2	4	0.59
(1,512)	1:8:A:ILE:H	1:8:A:ILE:HG22	6	0.59
(1,512)	1:8:A:ILE:H	1:8:A:ILE:HG22	8	0.59
(1,512)	1:8:A:ILE:H	1:8:A:ILE:HG23	9	0.59
(1,475)	1:33:A:VAL:HG23	1:33:A:VAL:HA	15	0.59
(1,354)	1:59:A:PHE:H	1:58:A:LEU:HD21	4	0.59
(1,354)	1:59:A:PHE:H	1:58:A:LEU:HD23	14	0.59
(1,13)	1:26:A:HIS:HD1	1:67:A:LYS:HD2	5	0.59
(1,1358)	1:23:A:VAL:H	1:19:A:VAL:HG22	7	0.58
(1,1313)	1:33:A:VAL:HA	1:32:A:SER:HB3	1	0.58
(1,1159)	1:62:A:HIS:HD1	1:66:A:LEU:HD12	15	0.58
(1,1133)	1:30:A:TRP:HZ3	1:59:A:PHE:HB3	6	0.58
(1,1053)	1:54:A:LYS:HD2	1:54:A:LYS:HA	8	0.58
(1,1040)	1:37:A:MET:H	1:36:A:LYS:HG3	2	0.58
(1,1029)	1:36:A:LYS:HG2	1:36:A:LYS:HE2	2	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1021)	1:57:A:LYS:HD2	1:57:A:LYS:HB2	3	0.58
(1,1017)	1:57:A:LYS:HG3	1:57:A:LYS:HE2	12	0.58
(1,1004)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	14	0.58
(1,653)	1:67:A:LYS:HB2	1:67:A:LYS:HE2	12	0.58
(1,512)	1:8:A:ILE:H	1:8:A:ILE:HG21	11	0.58
(1,354)	1:59:A:PHE:H	1:58:A:LEU:HD21	6	0.58
(1,354)	1:59:A:PHE:H	1:58:A:LEU:HD22	12	0.58
(1,1385)	1:67:A:LYS:HD2	1:64:A:HIS:HA	8	0.57
(1,1327)	1:64:A:HIS:HD1	1:69:A:GLU:HG2	1	0.57
(1,1269)	1:58:A:LEU:HD12	1:16:A:GLU:HG3	15	0.57
(1,1154)	1:19:A:VAL:HG21	1:23:A:VAL:HG23	4	0.57
(1,1127)	1:18:A:LEU:HG	1:43:A:TYR:HB3	12	0.57
(1,1053)	1:54:A:LYS:HD2	1:54:A:LYS:HA	2	0.57
(1,645)	1:19:A:VAL:H	1:18:A:LEU:HD12	10	0.57
(1,645)	1:19:A:VAL:H	1:18:A:LEU:HD11	15	0.57
(1,475)	1:33:A:VAL:HG23	1:33:A:VAL:HA	6	0.57
(1,459)	1:52:A:THR:H	1:52:A:THR:HG21	1	0.57
(1,354)	1:59:A:PHE:H	1:58:A:LEU:HD23	2	0.57
(1,354)	1:59:A:PHE:H	1:58:A:LEU:HD23	10	0.57
(1,338)	1:57:A:LYS:H	1:57:A:LYS:HG2	14	0.57
(1,2)	1:66:A:LEU:HD23	1:25:A:ASN:HA	15	0.57
(1,1413)	1:49:A:LEU:HD23	1:50:A:GLU:HG3	6	0.56
(1,1275)	1:17:A:TRP:HD1	1:18:A:LEU:HA	1	0.56
(1,1269)	1:58:A:LEU:HD13	1:16:A:GLU:HG3	12	0.56
(1,1188)	1:59:A:PHE:HD2	1:60:A:LEU:HD12	5	0.56
(1,1154)	1:19:A:VAL:HG21	1:23:A:VAL:HG23	9	0.56
(1,1152)	1:19:A:VAL:HG22	1:23:A:VAL:HB	6	0.56
(1,1008)	1:57:A:LYS:H	1:57:A:LYS:HD2	7	0.56
(1,565)	1:33:A:VAL:H	1:32:A:SER:HB3	5	0.56
(1,565)	1:33:A:VAL:H	1:32:A:SER:HB3	9	0.56
(1,554)	1:35:A:ARG:HB2	1:35:A:ARG:HD2	8	0.56
(1,475)	1:33:A:VAL:HG23	1:33:A:VAL:HA	11	0.56
(1,354)	1:59:A:PHE:H	1:58:A:LEU:HD22	8	0.56
(1,224)	1:48:A:TYR:H	1:48:A:TYR:HD2	3	0.56
(1,212)	1:17:A:TRP:HD1	1:17:A:TRP:HB3	2	0.56
(1,212)	1:17:A:TRP:HD1	1:17:A:TRP:HB3	3	0.56
(1,212)	1:17:A:TRP:HD1	1:17:A:TRP:HB3	14	0.56
(1,1425)	1:10:A:THR:H	1:13:A:ASP:HB2	11	0.55
(1,1358)	1:23:A:VAL:H	1:19:A:VAL:HG21	9	0.55
(1,1355)	1:62:A:HIS:HD1	1:63:A:ILE:HG12	11	0.55
(1,1154)	1:19:A:VAL:HG22	1:23:A:VAL:HG22	8	0.55
(1,1152)	1:19:A:VAL:HG23	1:23:A:VAL:HB	1	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1152)	1:19:A:VAL:HG22	1:23:A:VAL:HB	7	0.55
(1,1037)	1:36:A:LYS:HD2	1:36:A:LYS:HB2	1	0.55
(1,645)	1:19:A:VAL:H	1:18:A:LEU:HD13	14	0.55
(1,512)	1:8:A:ILE:H	1:8:A:ILE:HG22	10	0.55
(1,475)	1:33:A:VAL:HG21	1:33:A:VAL:HA	12	0.55
(1,459)	1:52:A:THR:H	1:52:A:THR:HG21	4	0.55
(1,354)	1:59:A:PHE:H	1:58:A:LEU:HD22	1	0.55
(1,354)	1:59:A:PHE:H	1:58:A:LEU:HD23	7	0.55
(1,354)	1:59:A:PHE:H	1:58:A:LEU:HD21	15	0.55
(1,212)	1:17:A:TRP:HD1	1:17:A:TRP:HB3	10	0.55
(1,212)	1:17:A:TRP:HD1	1:17:A:TRP:HB3	12	0.55
(1,212)	1:17:A:TRP:HD1	1:17:A:TRP:HB3	15	0.55
(1,12)	1:26:A:HIS:HD1	1:67:A:LYS:HB2	10	0.55
(1,1407)	1:8:A:ILE:HD12	1:5:A:SER:HA	6	0.54
(1,1385)	1:67:A:LYS:HD2	1:64:A:HIS:HA	5	0.54
(1,1358)	1:23:A:VAL:H	1:19:A:VAL:HG23	1	0.54
(1,1269)	1:58:A:LEU:HD13	1:16:A:GLU:HG3	2	0.54
(1,1152)	1:19:A:VAL:HG21	1:23:A:VAL:HB	4	0.54
(1,960)	1:56:A:LYS:H	1:56:A:LYS:HG2	15	0.54
(1,441)	1:69:A:GLU:H	1:69:A:GLU:HB3	10	0.54
(1,354)	1:59:A:PHE:H	1:58:A:LEU:HD23	3	0.54
(1,212)	1:17:A:TRP:HD1	1:17:A:TRP:HB3	1	0.54
(1,212)	1:17:A:TRP:HD1	1:17:A:TRP:HB3	4	0.54
(1,212)	1:17:A:TRP:HD1	1:17:A:TRP:HB3	5	0.54
(1,212)	1:17:A:TRP:HD1	1:17:A:TRP:HB3	6	0.54
(1,212)	1:17:A:TRP:HD1	1:17:A:TRP:HB3	7	0.54
(1,212)	1:17:A:TRP:HD1	1:17:A:TRP:HB3	8	0.54
(1,212)	1:17:A:TRP:HD1	1:17:A:TRP:HB3	9	0.54
(1,212)	1:17:A:TRP:HD1	1:17:A:TRP:HB3	11	0.54
(1,212)	1:17:A:TRP:HD1	1:17:A:TRP:HB3	13	0.54
(1,1425)	1:10:A:THR:H	1:13:A:ASP:HB2	12	0.53
(1,1419)	1:27:A:ASN:H	1:63:A:ILE:HD13	14	0.53
(1,1393)	1:26:A:HIS:HE1	1:67:A:LYS:HG3	13	0.53
(1,1358)	1:23:A:VAL:H	1:19:A:VAL:HG21	14	0.53
(1,1302)	1:63:A:ILE:HG12	1:60:A:LEU:HA	10	0.53
(1,1066)	1:14:A:LYS:H	1:14:A:LYS:HG2	5	0.53
(1,1053)	1:54:A:LYS:HD2	1:54:A:LYS:HA	5	0.53
(1,1025)	1:36:A:LYS:HG3	1:36:A:LYS:HA	3	0.53
(1,997)	1:24:A:LYS:HD2	1:24:A:LYS:HB2	13	0.53
(1,960)	1:56:A:LYS:H	1:56:A:LYS:HG2	1	0.53
(1,935)	1:15:A:TYR:HD2	1:16:A:GLU:HB2	13	0.53
(1,645)	1:19:A:VAL:H	1:18:A:LEU:HD11	3	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,512)	1:8:A:ILE:H	1:8:A:ILE:HG21	1	0.53
(1,475)	1:33:A:VAL:HG23	1:33:A:VAL:HA	5	0.53
(1,459)	1:52:A:THR:H	1:52:A:THR:HG22	11	0.53
(1,449)	1:50:A:GLU:H	1:49:A:LEU:HD22	8	0.53
(1,224)	1:48:A:TYR:H	1:48:A:TYR:HD2	8	0.53
(1,224)	1:48:A:TYR:H	1:48:A:TYR:HD2	13	0.53
(1,224)	1:48:A:TYR:H	1:48:A:TYR:HD2	14	0.53
(1,12)	1:26:A:HIS:HD1	1:67:A:LYS:HB2	13	0.53
(1,1364)	1:59:A:PHE:HE1	1:30:A:TRP:HE3	11	0.52
(1,1308)	1:33:A:VAL:HG13	1:28:A:GLU:HG2	7	0.52
(1,1069)	1:16:A:GLU:H	1:16:A:GLU:HB3	11	0.52
(1,1069)	1:16:A:GLU:H	1:16:A:GLU:HB3	13	0.52
(1,1053)	1:54:A:LYS:HD2	1:54:A:LYS:HA	14	0.52
(1,1053)	1:54:A:LYS:HD2	1:54:A:LYS:HA	15	0.52
(1,1021)	1:57:A:LYS:HD2	1:57:A:LYS:HB2	12	0.52
(1,960)	1:56:A:LYS:H	1:56:A:LYS:HG2	3	0.52
(1,960)	1:56:A:LYS:H	1:56:A:LYS:HG2	12	0.52
(1,721)	1:62:A:HIS:HE1	1:20:A:SER:HB3	11	0.52
(1,512)	1:8:A:ILE:H	1:8:A:ILE:HG23	14	0.52
(1,475)	1:33:A:VAL:HG22	1:33:A:VAL:HA	1	0.52
(1,475)	1:33:A:VAL:HG23	1:33:A:VAL:HA	3	0.52
(1,441)	1:69:A:GLU:H	1:69:A:GLU:HB3	6	0.52
(1,354)	1:59:A:PHE:H	1:58:A:LEU:HD22	5	0.52
(1,338)	1:57:A:LYS:H	1:57:A:LYS:HG2	12	0.52
(1,12)	1:26:A:HIS:HD1	1:67:A:LYS:HB2	6	0.52
(1,1154)	1:19:A:VAL:HG21	1:23:A:VAL:HG21	14	0.51
(1,1133)	1:30:A:TRP:HZ3	1:59:A:PHE:HB3	13	0.51
(1,1066)	1:14:A:LYS:H	1:14:A:LYS:HG2	6	0.51
(1,1007)	1:57:A:LYS:H	1:57:A:LYS:HE2	11	0.51
(1,885)	1:65:A:ARG:H	1:65:A:ARG:HD3	14	0.51
(1,884)	1:65:A:ARG:H	1:65:A:ARG:HD2	6	0.51
(1,645)	1:19:A:VAL:H	1:18:A:LEU:HD12	2	0.51
(1,241)	1:46:A:TYR:H	1:46:A:TYR:HD1	11	0.51
(1,224)	1:48:A:TYR:H	1:48:A:TYR:HD2	10	0.51
(1,12)	1:26:A:HIS:HD1	1:67:A:LYS:HB2	11	0.51
(1,1407)	1:8:A:ILE:HD13	1:5:A:SER:HA	1	0.5
(1,1407)	1:8:A:ILE:HD13	1:5:A:SER:HA	9	0.5
(1,1384)	1:11:A:ALA:HB1	1:45:A:ASP:HB3	9	0.5
(1,1376)	1:58:A:LEU:HD23	1:12:A:LYS:HE3	8	0.5
(1,1275)	1:17:A:TRP:HD1	1:18:A:LEU:HA	4	0.5
(1,1275)	1:17:A:TRP:HD1	1:18:A:LEU:HA	15	0.5
(1,1155)	1:19:A:VAL:HG21	1:62:A:HIS:HB3	5	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1154)	1:19:A:VAL:HG22	1:23:A:VAL:HG21	15	0.5
(1,1152)	1:19:A:VAL:HG21	1:23:A:VAL:HB	9	0.5
(1,1069)	1:16:A:GLU:H	1:16:A:GLU:HB3	4	0.5
(1,960)	1:56:A:LYS:H	1:56:A:LYS:HG2	6	0.5
(1,684)	1:62:A:HIS:HD1	1:23:A:VAL:HG11	4	0.5
(1,645)	1:19:A:VAL:H	1:18:A:LEU:HD11	1	0.5
(1,475)	1:33:A:VAL:HG21	1:33:A:VAL:HA	13	0.5
(1,459)	1:52:A:THR:H	1:52:A:THR:HG22	2	0.5
(1,241)	1:46:A:TYR:H	1:46:A:TYR:HD2	1	0.5
(1,1382)	1:39:A:ALA:HB1	1:38:A:GLN:HG2	15	0.49
(1,1372)	1:22:A:ILE:HD13	1:37:A:MET:HG3	14	0.49
(1,1358)	1:23:A:VAL:H	1:19:A:VAL:HG23	13	0.49
(1,1321)	1:64:A:HIS:HD1	1:65:A:ARG:HB3	15	0.49
(1,1275)	1:17:A:TRP:HD1	1:18:A:LEU:HA	5	0.49
(1,1275)	1:17:A:TRP:HD1	1:18:A:LEU:HA	14	0.49
(1,1152)	1:19:A:VAL:HG23	1:23:A:VAL:HB	3	0.49
(1,1133)	1:30:A:TRP:HZ3	1:59:A:PHE:HB3	12	0.49
(1,1100)	1:30:A:TRP:HD1	1:56:A:LYS:HE2	14	0.49
(1,1069)	1:16:A:GLU:H	1:16:A:GLU:HB3	15	0.49
(1,741)	1:61:A:GLN:HE21	1:61:A:GLN:HG3	9	0.49
(1,721)	1:62:A:HIS:HE1	1:20:A:SER:HB3	12	0.49
(1,459)	1:52:A:THR:H	1:52:A:THR:HG22	13	0.49
(1,241)	1:46:A:TYR:H	1:46:A:TYR:HD1	4	0.49
(1,241)	1:46:A:TYR:H	1:46:A:TYR:HD1	7	0.49
(1,241)	1:46:A:TYR:H	1:46:A:TYR:HD2	15	0.49
(1,224)	1:48:A:TYR:H	1:48:A:TYR:HD2	4	0.49
(1,1413)	1:49:A:LEU:HD23	1:50:A:GLU:HG3	10	0.48
(1,1393)	1:26:A:HIS:HE1	1:67:A:LYS:HG3	3	0.48
(1,1393)	1:26:A:HIS:HE1	1:67:A:LYS:HG3	10	0.48
(1,1358)	1:23:A:VAL:H	1:19:A:VAL:HG23	3	0.48
(1,1327)	1:64:A:HIS:HD1	1:69:A:GLU:HG2	3	0.48
(1,1313)	1:33:A:VAL:HA	1:32:A:SER:HB3	12	0.48
(1,1188)	1:59:A:PHE:HD2	1:60:A:LEU:HD12	6	0.48
(1,1188)	1:59:A:PHE:HD2	1:60:A:LEU:HD12	8	0.48
(1,1152)	1:19:A:VAL:HG22	1:23:A:VAL:HB	15	0.48
(1,1133)	1:30:A:TRP:HZ3	1:59:A:PHE:HB3	11	0.48
(1,1066)	1:14:A:LYS:H	1:14:A:LYS:HG2	14	0.48
(1,1037)	1:36:A:LYS:HD2	1:36:A:LYS:HB2	3	0.48
(1,1004)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	2	0.48
(1,1003)	1:24:A:LYS:HG2	1:24:A:LYS:HE2	11	0.48
(1,986)	1:58:A:LEU:HD13	1:12:A:LYS:HE3	3	0.48
(1,960)	1:56:A:LYS:H	1:56:A:LYS:HG2	14	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,741)	1:61:A:GLN:HE21	1:61:A:GLN:HG3	3	0.48
(1,684)	1:62:A:HIS:HD1	1:23:A:VAL:HG12	6	0.48
(1,645)	1:19:A:VAL:H	1:18:A:LEU:HD11	13	0.48
(1,404)	1:65:A:ARG:HG2	1:65:A:ARG:HB2	6	0.48
(1,404)	1:65:A:ARG:HG2	1:65:A:ARG:HB2	14	0.48
(1,241)	1:46:A:TYR:H	1:46:A:TYR:HD2	9	0.48
(1,241)	1:46:A:TYR:H	1:46:A:TYR:HD1	10	0.48
(1,241)	1:46:A:TYR:H	1:46:A:TYR:HD2	12	0.48
(1,224)	1:48:A:TYR:H	1:48:A:TYR:HD2	5	0.48
(1,20)	1:67:A:LYS:HG2	1:26:A:HIS:HB2	14	0.48
(1,1376)	1:58:A:LEU:HD22	1:12:A:LYS:HE3	15	0.47
(1,1363)	1:33:A:VAL:HG23	1:28:A:GLU:HB3	15	0.47
(1,1358)	1:23:A:VAL:H	1:19:A:VAL:HG22	8	0.47
(1,1355)	1:62:A:HIS:HD1	1:63:A:ILE:HG12	8	0.47
(1,1355)	1:62:A:HIS:HD1	1:63:A:ILE:HG12	13	0.47
(1,1282)	1:21:A:ARG:HG3	1:18:A:LEU:HA	15	0.47
(1,1275)	1:17:A:TRP:HD1	1:18:A:LEU:HA	2	0.47
(1,1275)	1:17:A:TRP:HD1	1:18:A:LEU:HA	8	0.47
(1,1188)	1:59:A:PHE:HD2	1:60:A:LEU:HD11	11	0.47
(1,1066)	1:14:A:LYS:H	1:14:A:LYS:HG2	10	0.47
(1,926)	1:51:A:GLY:H	1:50:A:GLU:HG3	11	0.47
(1,645)	1:19:A:VAL:H	1:18:A:LEU:HD13	5	0.47
(1,459)	1:52:A:THR:H	1:52:A:THR:HG21	9	0.47
(1,459)	1:52:A:THR:H	1:52:A:THR:HG21	12	0.47
(1,1425)	1:10:A:THR:H	1:13:A:ASP:HB2	3	0.46
(1,1415)	1:24:A:LYS:HG3	1:24:A:LYS:HA	4	0.46
(1,1376)	1:58:A:LEU:HD22	1:12:A:LYS:HE3	9	0.46
(1,1358)	1:23:A:VAL:H	1:19:A:VAL:HG21	4	0.46
(1,1275)	1:17:A:TRP:HD1	1:18:A:LEU:HA	13	0.46
(1,1226)	1:47:A:VAL:HG22	1:44:A:GLN:HA	8	0.46
(1,1069)	1:16:A:GLU:H	1:16:A:GLU:HB3	10	0.46
(1,1017)	1:57:A:LYS:HG3	1:57:A:LYS:HE2	15	0.46
(1,1004)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	1	0.46
(1,997)	1:24:A:LYS:HD2	1:24:A:LYS:HB2	8	0.46
(1,645)	1:19:A:VAL:H	1:18:A:LEU:HD11	4	0.46
(1,645)	1:19:A:VAL:H	1:18:A:LEU:HD13	8	0.46
(1,565)	1:33:A:VAL:H	1:32:A:SER:HB3	8	0.46
(1,459)	1:52:A:THR:H	1:52:A:THR:HG23	3	0.46
(1,403)	1:65:A:ARG:HG2	1:65:A:ARG:HA	10	0.46
(1,241)	1:46:A:TYR:H	1:46:A:TYR:HD2	2	0.46
(1,224)	1:48:A:TYR:H	1:48:A:TYR:HD2	2	0.46
(1,1382)	1:39:A:ALA:HB3	1:38:A:GLN:HG2	14	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1364)	1:59:A:PHE:HE1	1:30:A:TRP:HE3	14	0.45
(1,1358)	1:23:A:VAL:H	1:19:A:VAL:HG22	15	0.45
(1,1313)	1:33:A:VAL:HA	1:32:A:SER:HB3	13	0.45
(1,1155)	1:19:A:VAL:HG21	1:62:A:HIS:HB3	3	0.45
(1,1103)	1:30:A:TRP:HD1	1:31:A:LEU:HD11	4	0.45
(1,1066)	1:14:A:LYS:H	1:14:A:LYS:HG2	12	0.45
(1,885)	1:65:A:ARG:H	1:65:A:ARG:HD3	6	0.45
(1,884)	1:65:A:ARG:H	1:65:A:ARG:HD2	11	0.45
(1,645)	1:19:A:VAL:H	1:18:A:LEU:HD12	12	0.45
(1,403)	1:65:A:ARG:HG2	1:65:A:ARG:HA	2	0.45
(1,338)	1:57:A:LYS:H	1:57:A:LYS:HG2	13	0.45
(1,241)	1:46:A:TYR:H	1:46:A:TYR:HD1	8	0.45
(1,224)	1:48:A:TYR:H	1:48:A:TYR:HD2	11	0.45
(1,1358)	1:23:A:VAL:H	1:19:A:VAL:HG23	5	0.44
(1,1204)	1:18:A:LEU:HG	1:42:A:GLU:HA	15	0.44
(1,1188)	1:59:A:PHE:HD2	1:60:A:LEU:HD12	15	0.44
(1,1155)	1:19:A:VAL:HG22	1:62:A:HIS:HB3	9	0.44
(1,1154)	1:19:A:VAL:HG22	1:23:A:VAL:HG23	7	0.44
(1,1101)	1:30:A:TRP:HD1	1:56:A:LYS:HD3	1	0.44
(1,1066)	1:14:A:LYS:H	1:14:A:LYS:HG2	1	0.44
(1,1066)	1:14:A:LYS:H	1:14:A:LYS:HG2	7	0.44
(1,1025)	1:36:A:LYS:HG3	1:36:A:LYS:HA	1	0.44
(1,1025)	1:36:A:LYS:HG3	1:36:A:LYS:HA	2	0.44
(1,653)	1:67:A:LYS:HB2	1:67:A:LYS:HE2	3	0.44
(1,645)	1:19:A:VAL:H	1:18:A:LEU:HD11	9	0.44
(1,645)	1:19:A:VAL:H	1:18:A:LEU:HD11	11	0.44
(1,441)	1:69:A:GLU:H	1:69:A:GLU:HB3	3	0.44
(1,224)	1:48:A:TYR:H	1:48:A:TYR:HD2	12	0.44
(1,1382)	1:39:A:ALA:HB3	1:38:A:GLN:HG2	13	0.43
(1,1372)	1:22:A:ILE:HD12	1:37:A:MET:HG3	2	0.43
(1,1358)	1:23:A:VAL:H	1:19:A:VAL:HG22	6	0.43
(1,1326)	1:64:A:HIS:HD1	1:67:A:LYS:HE2	4	0.43
(1,1291)	1:57:A:LYS:HB2	1:54:A:LYS:HA	12	0.43
(1,1101)	1:30:A:TRP:HD1	1:56:A:LYS:HD3	15	0.43
(1,1053)	1:54:A:LYS:HD2	1:54:A:LYS:HA	9	0.43
(1,1016)	1:57:A:LYS:HG2	1:57:A:LYS:HE2	3	0.43
(1,986)	1:58:A:LEU:HD13	1:12:A:LYS:HE3	15	0.43
(1,922)	1:50:A:GLU:H	1:50:A:GLU:HG2	5	0.43
(1,801)	1:23:A:VAL:H	1:22:A:ILE:HD11	3	0.43
(1,801)	1:23:A:VAL:H	1:22:A:ILE:HD12	4	0.43
(1,684)	1:62:A:HIS:HD1	1:23:A:VAL:HG13	8	0.43
(1,334)	1:57:A:LYS:H	1:56:A:LYS:HB2	8	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,241)	1:46:A:TYR:H	1:46:A:TYR:HD2	13	0.43
(1,241)	1:46:A:TYR:H	1:46:A:TYR:HD2	14	0.43
(1,224)	1:48:A:TYR:H	1:48:A:TYR:HD2	1	0.43
(1,1385)	1:67:A:LYS:HD2	1:64:A:HIS:HA	7	0.42
(1,1321)	1:64:A:HIS:HD1	1:65:A:ARG:HB3	4	0.42
(1,1188)	1:59:A:PHE:HD2	1:60:A:LEU:HD13	3	0.42
(1,1188)	1:59:A:PHE:HD2	1:60:A:LEU:HD13	4	0.42
(1,1069)	1:16:A:GLU:H	1:16:A:GLU:HB3	2	0.42
(1,1069)	1:16:A:GLU:H	1:16:A:GLU:HB3	14	0.42
(1,1021)	1:57:A:LYS:HD2	1:57:A:LYS:HB2	1	0.42
(1,1000)	1:24:A:LYS:HG2	1:24:A:LYS:HD2	1	0.42
(1,960)	1:56:A:LYS:H	1:56:A:LYS:HG2	5	0.42
(1,960)	1:56:A:LYS:H	1:56:A:LYS:HG2	7	0.42
(1,741)	1:61:A:GLN:HE21	1:61:A:GLN:HG3	10	0.42
(1,595)	1:54:A:LYS:HB2	1:54:A:LYS:HA	2	0.42
(1,595)	1:54:A:LYS:HB2	1:54:A:LYS:HA	5	0.42
(1,595)	1:54:A:LYS:HB2	1:54:A:LYS:HA	14	0.42
(1,566)	1:32:A:SER:H	1:32:A:SER:HB3	13	0.42
(1,565)	1:33:A:VAL:H	1:32:A:SER:HB3	3	0.42
(1,565)	1:33:A:VAL:H	1:32:A:SER:HB3	15	0.42
(1,241)	1:46:A:TYR:H	1:46:A:TYR:HD2	5	0.42
(1,224)	1:48:A:TYR:H	1:48:A:TYR:HD2	6	0.42
(1,19)	1:66:A:LEU:HD13	1:26:A:HIS:HB3	15	0.42
(1,5)	1:25:A:ASN:HB2	1:25:A:ASN:HA	15	0.42
(1,1393)	1:26:A:HIS:HE1	1:67:A:LYS:HG3	11	0.41
(1,1389)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	8	0.41
(1,1382)	1:39:A:ALA:HB3	1:38:A:GLN:HG2	3	0.41
(1,1381)	1:49:A:LEU:HD23	1:7:A:GLN:HG2	11	0.41
(1,1376)	1:58:A:LEU:HD21	1:12:A:LYS:HE3	3	0.41
(1,1321)	1:64:A:HIS:HD1	1:65:A:ARG:HB3	14	0.41
(1,1286)	1:36:A:LYS:HG2	1:33:A:VAL:HA	4	0.41
(1,1239)	1:65:A:ARG:HB3	1:62:A:HIS:HA	3	0.41
(1,1226)	1:47:A:VAL:HG21	1:44:A:GLN:HA	5	0.41
(1,1204)	1:18:A:LEU:HG	1:42:A:GLU:HA	4	0.41
(1,1188)	1:59:A:PHE:HD2	1:60:A:LEU:HD11	10	0.41
(1,1188)	1:59:A:PHE:HD2	1:60:A:LEU:HD11	12	0.41
(1,1069)	1:16:A:GLU:H	1:16:A:GLU:HB3	1	0.41
(1,1000)	1:24:A:LYS:HG2	1:24:A:LYS:HD2	13	0.41
(1,986)	1:58:A:LEU:HD13	1:12:A:LYS:HE3	8	0.41
(1,986)	1:58:A:LEU:HD13	1:12:A:LYS:HE3	9	0.41
(1,960)	1:56:A:LYS:H	1:56:A:LYS:HG2	10	0.41
(1,884)	1:65:A:ARG:H	1:65:A:ARG:HD2	8	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,741)	1:61:A:GLN:HE21	1:61:A:GLN:HG3	14	0.41
(1,741)	1:61:A:GLN:HE21	1:61:A:GLN:HG3	15	0.41
(1,663)	1:64:A:HIS:HD1	1:64:A:HIS:HA	10	0.41
(1,645)	1:19:A:VAL:H	1:18:A:LEU:HD12	7	0.41
(1,595)	1:54:A:LYS:HB2	1:54:A:LYS:HA	3	0.41
(1,595)	1:54:A:LYS:HB2	1:54:A:LYS:HA	4	0.41
(1,595)	1:54:A:LYS:HB2	1:54:A:LYS:HA	7	0.41
(1,595)	1:54:A:LYS:HB2	1:54:A:LYS:HA	11	0.41
(1,595)	1:54:A:LYS:HB2	1:54:A:LYS:HA	13	0.41
(1,595)	1:54:A:LYS:HB2	1:54:A:LYS:HA	15	0.41
(1,475)	1:33:A:VAL:HG22	1:33:A:VAL:HA	10	0.41
(1,404)	1:65:A:ARG:HG2	1:65:A:ARG:HB2	1	0.41
(1,404)	1:65:A:ARG:HG2	1:65:A:ARG:HB2	4	0.41
(1,404)	1:65:A:ARG:HG2	1:65:A:ARG:HB2	7	0.41
(1,320)	1:45:A:ASP:H	1:44:A:GLN:HG3	14	0.41
(1,224)	1:48:A:TYR:H	1:48:A:TYR:HD2	15	0.41
(1,1385)	1:67:A:LYS:HD2	1:64:A:HIS:HA	15	0.4
(1,1382)	1:39:A:ALA:HB1	1:38:A:GLN:HG2	8	0.4
(1,1340)	1:17:A:TRP:HE3	1:21:A:ARG:HB3	8	0.4
(1,1321)	1:64:A:HIS:HD1	1:65:A:ARG:HB3	1	0.4
(1,1321)	1:64:A:HIS:HD1	1:65:A:ARG:HB3	6	0.4
(1,1282)	1:21:A:ARG:HG3	1:18:A:LEU:HA	2	0.4
(1,1204)	1:18:A:LEU:HG	1:42:A:GLU:HA	2	0.4
(1,1188)	1:59:A:PHE:HD2	1:60:A:LEU:HD12	7	0.4
(1,1155)	1:19:A:VAL:HG23	1:62:A:HIS:HB3	8	0.4
(1,1069)	1:16:A:GLU:H	1:16:A:GLU:HB3	6	0.4
(1,1069)	1:16:A:GLU:H	1:16:A:GLU:HB3	12	0.4
(1,1066)	1:14:A:LYS:H	1:14:A:LYS:HG2	15	0.4
(1,1037)	1:36:A:LYS:HD2	1:36:A:LYS:HB2	2	0.4
(1,1000)	1:24:A:LYS:HG2	1:24:A:LYS:HD2	3	0.4
(1,1000)	1:24:A:LYS:HG2	1:24:A:LYS:HD2	8	0.4
(1,1000)	1:24:A:LYS:HG2	1:24:A:LYS:HD2	10	0.4
(1,997)	1:24:A:LYS:HD2	1:24:A:LYS:HB2	1	0.4
(1,960)	1:56:A:LYS:H	1:56:A:LYS:HG2	2	0.4
(1,884)	1:65:A:ARG:H	1:65:A:ARG:HD2	9	0.4
(1,801)	1:23:A:VAL:H	1:22:A:ILE:HD13	6	0.4
(1,785)	1:64:A:HIS:HB2	1:61:A:GLN:HA	1	0.4
(1,785)	1:64:A:HIS:HB2	1:61:A:GLN:HA	10	0.4
(1,785)	1:64:A:HIS:HB2	1:61:A:GLN:HA	11	0.4
(1,785)	1:64:A:HIS:HB2	1:61:A:GLN:HA	13	0.4
(1,684)	1:62:A:HIS:HD1	1:23:A:VAL:HG12	13	0.4
(1,663)	1:64:A:HIS:HD1	1:64:A:HIS:HA	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,645)	1:19:A:VAL:H	1:18:A:LEU:HD12	6	0.4
(1,595)	1:54:A:LYS:HB2	1:54:A:LYS:HA	10	0.4
(1,595)	1:54:A:LYS:HB2	1:54:A:LYS:HA	12	0.4
(1,404)	1:65:A:ARG:HG2	1:65:A:ARG:HB2	9	0.4
(1,402)	1:65:A:ARG:HB2	1:65:A:ARG:HA	3	0.4
(1,402)	1:65:A:ARG:HB2	1:65:A:ARG:HA	10	0.4
(1,402)	1:65:A:ARG:HB2	1:65:A:ARG:HA	12	0.4
(1,1406)	1:8:A:ILE:HD11	1:5:A:SER:HB2	12	0.39
(1,1385)	1:67:A:LYS:HD2	1:64:A:HIS:HA	12	0.39
(1,1377)	1:58:A:LEU:HD23	1:12:A:LYS:HE2	4	0.39
(1,1341)	1:17:A:TRP:HE3	1:21:A:ARG:HB2	2	0.39
(1,1340)	1:17:A:TRP:HE3	1:21:A:ARG:HB3	4	0.39
(1,1321)	1:64:A:HIS:HD1	1:65:A:ARG:HB3	5	0.39
(1,1282)	1:21:A:ARG:HG3	1:18:A:LEU:HA	14	0.39
(1,1188)	1:59:A:PHE:HD2	1:60:A:LEU:HD11	1	0.39
(1,1188)	1:59:A:PHE:HD2	1:60:A:LEU:HD12	14	0.39
(1,1100)	1:30:A:TRP:HD1	1:56:A:LYS:HE2	4	0.39
(1,1000)	1:24:A:LYS:HG2	1:24:A:LYS:HD2	9	0.39
(1,1000)	1:24:A:LYS:HG2	1:24:A:LYS:HD2	15	0.39
(1,935)	1:15:A:TYR:HD2	1:16:A:GLU:HB2	4	0.39
(1,870)	1:35:A:ARG:HG2	1:35:A:ARG:HB2	12	0.39
(1,801)	1:23:A:VAL:H	1:22:A:ILE:HD12	8	0.39
(1,762)	1:35:A:ARG:HD2	1:32:A:SER:HA	11	0.39
(1,684)	1:62:A:HIS:HD1	1:23:A:VAL:HG11	1	0.39
(1,663)	1:64:A:HIS:HD1	1:64:A:HIS:HA	12	0.39
(1,595)	1:54:A:LYS:HB2	1:54:A:LYS:HA	6	0.39
(1,595)	1:54:A:LYS:HB2	1:54:A:LYS:HA	9	0.39
(1,425)	1:67:A:LYS:H	1:66:A:LEU:HG	7	0.39
(1,425)	1:67:A:LYS:H	1:66:A:LEU:HG	8	0.39
(1,404)	1:65:A:ARG:HG2	1:65:A:ARG:HB2	8	0.39
(1,404)	1:65:A:ARG:HG2	1:65:A:ARG:HB2	11	0.39
(1,402)	1:65:A:ARG:HB2	1:65:A:ARG:HA	2	0.39
(1,402)	1:65:A:ARG:HB2	1:65:A:ARG:HA	14	0.39
(1,373)	1:61:A:GLN:HG3	1:61:A:GLN:HA	11	0.39
(1,284)	1:21:A:ARG:HG2	1:21:A:ARG:HA	4	0.39
(1,284)	1:21:A:ARG:HG2	1:21:A:ARG:HA	8	0.39
(1,241)	1:46:A:TYR:H	1:46:A:TYR:HD2	3	0.39
(1,241)	1:46:A:TYR:H	1:46:A:TYR:HD1	6	0.39
(1,224)	1:48:A:TYR:H	1:48:A:TYR:HD2	7	0.39
(1,197)	1:30:A:TRP:HD1	1:30:A:TRP:HA	6	0.39
(1,12)	1:26:A:HIS:HD1	1:67:A:LYS:HB2	1	0.39
(1,1382)	1:39:A:ALA:HB2	1:38:A:GLN:HG2	2	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1364)	1:59:A:PHE:HE1	1:30:A:TRP:HE3	2	0.38
(1,1364)	1:59:A:PHE:HE1	1:30:A:TRP:HE3	12	0.38
(1,1341)	1:17:A:TRP:HE3	1:21:A:ARG:HB2	13	0.38
(1,1321)	1:64:A:HIS:HD1	1:65:A:ARG:HB3	7	0.38
(1,1244)	1:26:A:HIS:HE1	1:67:A:LYS:HB2	12	0.38
(1,1225)	1:47:A:VAL:HA	1:46:A:TYR:HA	2	0.38
(1,1219)	1:56:A:LYS:HB2	1:53:A:GLN:HA	5	0.38
(1,1204)	1:18:A:LEU:HG	1:42:A:GLU:HA	3	0.38
(1,1100)	1:30:A:TRP:HD1	1:56:A:LYS:HE2	13	0.38
(1,1081)	1:43:A:TYR:HE1	1:38:A:GLN:HB2	10	0.38
(1,1053)	1:54:A:LYS:HD2	1:54:A:LYS:HA	6	0.38
(1,1008)	1:57:A:LYS:H	1:57:A:LYS:HD2	15	0.38
(1,1000)	1:24:A:LYS:HG2	1:24:A:LYS:HD2	5	0.38
(1,1000)	1:24:A:LYS:HG2	1:24:A:LYS:HD2	6	0.38
(1,1000)	1:24:A:LYS:HG2	1:24:A:LYS:HD2	12	0.38
(1,960)	1:56:A:LYS:H	1:56:A:LYS:HG2	11	0.38
(1,960)	1:56:A:LYS:H	1:56:A:LYS:HG2	13	0.38
(1,874)	1:65:A:ARG:HG3	1:65:A:ARG:HA	12	0.38
(1,801)	1:23:A:VAL:H	1:22:A:ILE:HD11	15	0.38
(1,718)	1:42:A:GLU:HA	1:41:A:PRO:HA	1	0.38
(1,644)	1:18:A:LEU:HD13	1:18:A:LEU:HB2	2	0.38
(1,644)	1:18:A:LEU:HD12	1:18:A:LEU:HB2	13	0.38
(1,617)	1:26:A:HIS:H	1:23:A:VAL:HA	14	0.38
(1,566)	1:32:A:SER:H	1:32:A:SER:HB3	12	0.38
(1,459)	1:52:A:THR:H	1:52:A:THR:HG22	6	0.38
(1,404)	1:65:A:ARG:HG2	1:65:A:ARG:HB2	13	0.38
(1,402)	1:65:A:ARG:HB2	1:65:A:ARG:HA	6	0.38
(1,284)	1:21:A:ARG:HG2	1:21:A:ARG:HA	5	0.38
(1,197)	1:30:A:TRP:HD1	1:30:A:TRP:HA	2	0.38
(1,197)	1:30:A:TRP:HD1	1:30:A:TRP:HA	13	0.38
(1,1415)	1:24:A:LYS:HG3	1:24:A:LYS:HA	10	0.37
(1,1382)	1:39:A:ALA:HB2	1:38:A:GLN:HG2	5	0.37
(1,1382)	1:39:A:ALA:HB3	1:38:A:GLN:HG2	6	0.37
(1,1364)	1:59:A:PHE:HE2	1:30:A:TRP:HE3	5	0.37
(1,1364)	1:59:A:PHE:HE1	1:30:A:TRP:HE3	13	0.37
(1,1345)	1:64:A:HIS:HE1	1:68:A:HIS:HD1	10	0.37
(1,1321)	1:64:A:HIS:HD1	1:65:A:ARG:HB3	9	0.37
(1,1239)	1:65:A:ARG:HB3	1:62:A:HIS:HA	7	0.37
(1,1225)	1:47:A:VAL:HA	1:46:A:TYR:HA	1	0.37
(1,1225)	1:47:A:VAL:HA	1:46:A:TYR:HA	3	0.37
(1,1225)	1:47:A:VAL:HA	1:46:A:TYR:HA	7	0.37
(1,1155)	1:19:A:VAL:HG22	1:62:A:HIS:HB3	14	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1133)	1:30:A:TRP:HZ3	1:59:A:PHE:HB3	2	0.37
(1,1100)	1:30:A:TRP:HD1	1:56:A:LYS:HE2	11	0.37
(1,1069)	1:16:A:GLU:H	1:16:A:GLU:HB3	8	0.37
(1,1066)	1:14:A:LYS:H	1:14:A:LYS:HG2	11	0.37
(1,1016)	1:57:A:LYS:HG2	1:57:A:LYS:HE2	12	0.37
(1,1000)	1:24:A:LYS:HG2	1:24:A:LYS:HD2	2	0.37
(1,1000)	1:24:A:LYS:HG2	1:24:A:LYS:HD2	14	0.37
(1,947)	1:62:A:HIS:H	1:61:A:GLN:HG3	8	0.37
(1,886)	1:65:A:ARG:HD3	1:65:A:ARG:HA	4	0.37
(1,870)	1:35:A:ARG:HG2	1:35:A:ARG:HB2	10	0.37
(1,801)	1:23:A:VAL:H	1:22:A:ILE:HD13	5	0.37
(1,785)	1:64:A:HIS:HB2	1:61:A:GLN:HA	6	0.37
(1,663)	1:64:A:HIS:HD1	1:64:A:HIS:HA	14	0.37
(1,644)	1:18:A:LEU:HD12	1:18:A:LEU:HB2	1	0.37
(1,595)	1:54:A:LYS:HB2	1:54:A:LYS:HA	8	0.37
(1,566)	1:32:A:SER:H	1:32:A:SER:HB3	5	0.37
(1,566)	1:32:A:SER:H	1:32:A:SER:HB3	7	0.37
(1,565)	1:33:A:VAL:H	1:32:A:SER:HB3	1	0.37
(1,425)	1:67:A:LYS:H	1:66:A:LEU:HG	4	0.37
(1,425)	1:67:A:LYS:H	1:66:A:LEU:HG	5	0.37
(1,404)	1:65:A:ARG:HG2	1:65:A:ARG:HB2	15	0.37
(1,402)	1:65:A:ARG:HB2	1:65:A:ARG:HA	5	0.37
(1,402)	1:65:A:ARG:HB2	1:65:A:ARG:HA	11	0.37
(1,402)	1:65:A:ARG:HB2	1:65:A:ARG:HA	15	0.37
(1,320)	1:45:A:ASP:H	1:44:A:GLN:HG3	2	0.37
(1,284)	1:21:A:ARG:HG2	1:21:A:ARG:HA	1	0.37
(1,284)	1:21:A:ARG:HG2	1:21:A:ARG:HA	3	0.37
(1,284)	1:21:A:ARG:HG2	1:21:A:ARG:HA	6	0.37
(1,284)	1:21:A:ARG:HG2	1:21:A:ARG:HA	7	0.37
(1,268)	1:19:A:VAL:H	1:19:A:VAL:HG23	2	0.37
(1,197)	1:30:A:TRP:HD1	1:30:A:TRP:HA	4	0.37
(1,1393)	1:26:A:HIS:HE1	1:67:A:LYS:HG3	6	0.36
(1,1372)	1:22:A:ILE:HD12	1:37:A:MET:HG3	1	0.36
(1,1364)	1:59:A:PHE:HE2	1:30:A:TRP:HE3	8	0.36
(1,1340)	1:17:A:TRP:HE3	1:21:A:ARG:HB3	2	0.36
(1,1340)	1:17:A:TRP:HE3	1:21:A:ARG:HB3	9	0.36
(1,1282)	1:21:A:ARG:HG3	1:18:A:LEU:HA	13	0.36
(1,1225)	1:47:A:VAL:HA	1:46:A:TYR:HA	4	0.36
(1,1225)	1:47:A:VAL:HA	1:46:A:TYR:HA	13	0.36
(1,1219)	1:56:A:LYS:HB2	1:53:A:GLN:HA	14	0.36
(1,1174)	1:44:A:GLN:HE21	1:43:A:TYR:HD2	8	0.36
(1,1100)	1:30:A:TRP:HD1	1:56:A:LYS:HE2	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1069)	1:16:A:GLU:H	1:16:A:GLU:HB3	7	0.36
(1,1069)	1:16:A:GLU:H	1:16:A:GLU:HB3	9	0.36
(1,1021)	1:57:A:LYS:HD2	1:57:A:LYS:HB2	4	0.36
(1,1004)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	10	0.36
(1,1000)	1:24:A:LYS:HG2	1:24:A:LYS:HD2	4	0.36
(1,947)	1:62:A:HIS:H	1:61:A:GLN:HG3	5	0.36
(1,935)	1:15:A:TYR:HD2	1:16:A:GLU:HB2	11	0.36
(1,842)	1:31:A:LEU:HB3	1:31:A:LEU:HG	4	0.36
(1,785)	1:64:A:HIS:HB2	1:61:A:GLN:HA	12	0.36
(1,644)	1:18:A:LEU:HD11	1:18:A:LEU:HB2	5	0.36
(1,644)	1:18:A:LEU:HD11	1:18:A:LEU:HB2	8	0.36
(1,644)	1:18:A:LEU:HD12	1:18:A:LEU:HB2	11	0.36
(1,565)	1:33:A:VAL:H	1:32:A:SER:HB3	7	0.36
(1,402)	1:65:A:ARG:HB2	1:65:A:ARG:HA	1	0.36
(1,402)	1:65:A:ARG:HB2	1:65:A:ARG:HA	4	0.36
(1,402)	1:65:A:ARG:HB2	1:65:A:ARG:HA	7	0.36
(1,402)	1:65:A:ARG:HB2	1:65:A:ARG:HA	8	0.36
(1,402)	1:65:A:ARG:HB2	1:65:A:ARG:HA	9	0.36
(1,402)	1:65:A:ARG:HB2	1:65:A:ARG:HA	13	0.36
(1,320)	1:45:A:ASP:H	1:44:A:GLN:HG3	6	0.36
(1,284)	1:21:A:ARG:HG2	1:21:A:ARG:HA	9	0.36
(1,284)	1:21:A:ARG:HG2	1:21:A:ARG:HA	12	0.36
(1,197)	1:30:A:TRP:HD1	1:30:A:TRP:HA	3	0.36
(1,197)	1:30:A:TRP:HD1	1:30:A:TRP:HA	8	0.36
(1,197)	1:30:A:TRP:HD1	1:30:A:TRP:HA	11	0.36
(1,197)	1:30:A:TRP:HD1	1:30:A:TRP:HA	12	0.36
(1,197)	1:30:A:TRP:HD1	1:30:A:TRP:HA	14	0.36
(1,1405)	1:7:A:GLN:HB2	1:7:A:GLN:HG3	2	0.35
(1,1389)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	6	0.35
(1,1389)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	9	0.35
(1,1340)	1:17:A:TRP:HE3	1:21:A:ARG:HB3	5	0.35
(1,1321)	1:64:A:HIS:HD1	1:65:A:ARG:HB3	8	0.35
(1,1291)	1:57:A:LYS:HB2	1:54:A:LYS:HA	9	0.35
(1,1232)	1:17:A:TRP:HE1	1:21:A:ARG:HG2	11	0.35
(1,1225)	1:47:A:VAL:HA	1:46:A:TYR:HA	5	0.35
(1,1225)	1:47:A:VAL:HA	1:46:A:TYR:HA	9	0.35
(1,1225)	1:47:A:VAL:HA	1:46:A:TYR:HA	10	0.35
(1,1225)	1:47:A:VAL:HA	1:46:A:TYR:HA	11	0.35
(1,1225)	1:47:A:VAL:HA	1:46:A:TYR:HA	14	0.35
(1,1188)	1:59:A:PHE:HD2	1:60:A:LEU:HD13	2	0.35
(1,1188)	1:59:A:PHE:HD2	1:60:A:LEU:HD13	13	0.35
(1,1155)	1:19:A:VAL:HG21	1:62:A:HIS:HB3	13	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1078)	1:39:A:ALA:H	1:38:A:GLN:HB2	2	0.35
(1,1066)	1:14:A:LYS:H	1:14:A:LYS:HG2	2	0.35
(1,1066)	1:14:A:LYS:H	1:14:A:LYS:HG2	3	0.35
(1,1053)	1:54:A:LYS:HD2	1:54:A:LYS:HA	7	0.35
(1,1016)	1:57:A:LYS:HG2	1:57:A:LYS:HE2	15	0.35
(1,1015)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	2	0.35
(1,1015)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	8	0.35
(1,1015)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	11	0.35
(1,1015)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	13	0.35
(1,1003)	1:24:A:LYS:HG2	1:24:A:LYS:HE2	2	0.35
(1,1000)	1:24:A:LYS:HG2	1:24:A:LYS:HD2	7	0.35
(1,986)	1:58:A:LEU:HD12	1:12:A:LYS:HE3	5	0.35
(1,947)	1:62:A:HIS:H	1:61:A:GLN:HG3	12	0.35
(1,933)	1:69:A:GLU:HB3	1:69:A:GLU:HG2	5	0.35
(1,785)	1:64:A:HIS:HB2	1:61:A:GLN:HA	8	0.35
(1,663)	1:64:A:HIS:HD1	1:64:A:HIS:HA	11	0.35
(1,566)	1:32:A:SER:H	1:32:A:SER:HB3	1	0.35
(1,566)	1:32:A:SER:H	1:32:A:SER:HB3	15	0.35
(1,320)	1:45:A:ASP:H	1:44:A:GLN:HG3	4	0.35
(1,320)	1:45:A:ASP:H	1:44:A:GLN:HG3	8	0.35
(1,284)	1:21:A:ARG:HG2	1:21:A:ARG:HA	10	0.35
(1,197)	1:30:A:TRP:HD1	1:30:A:TRP:HA	10	0.35
(1,1405)	1:7:A:GLN:HB2	1:7:A:GLN:HG3	3	0.34
(1,1405)	1:7:A:GLN:HB2	1:7:A:GLN:HG3	4	0.34
(1,1405)	1:7:A:GLN:HB2	1:7:A:GLN:HG3	5	0.34
(1,1405)	1:7:A:GLN:HB2	1:7:A:GLN:HG3	8	0.34
(1,1405)	1:7:A:GLN:HB2	1:7:A:GLN:HG3	9	0.34
(1,1405)	1:7:A:GLN:HB2	1:7:A:GLN:HG3	10	0.34
(1,1405)	1:7:A:GLN:HB2	1:7:A:GLN:HG3	11	0.34
(1,1405)	1:7:A:GLN:HB2	1:7:A:GLN:HG3	12	0.34
(1,1405)	1:7:A:GLN:HB2	1:7:A:GLN:HG3	13	0.34
(1,1405)	1:7:A:GLN:HB2	1:7:A:GLN:HG3	14	0.34
(1,1405)	1:7:A:GLN:HB2	1:7:A:GLN:HG3	15	0.34
(1,1385)	1:67:A:LYS:HD2	1:64:A:HIS:HA	2	0.34
(1,1382)	1:39:A:ALA:HB1	1:38:A:GLN:HG2	11	0.34
(1,1364)	1:59:A:PHE:HE1	1:30:A:TRP:HE3	15	0.34
(1,1355)	1:62:A:HIS:HD1	1:63:A:ILE:HG12	3	0.34
(1,1345)	1:64:A:HIS:HE1	1:68:A:HIS:HD1	9	0.34
(1,1341)	1:17:A:TRP:HE3	1:21:A:ARG:HB2	14	0.34
(1,1321)	1:64:A:HIS:HD1	1:65:A:ARG:HB3	11	0.34
(1,1244)	1:26:A:HIS:HE1	1:67:A:LYS:HB2	2	0.34
(1,1232)	1:17:A:TRP:HE1	1:21:A:ARG:HG2	14	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1225)	1:47:A:VAL:HA	1:46:A:TYR:HA	8	0.34
(1,1225)	1:47:A:VAL:HA	1:46:A:TYR:HA	12	0.34
(1,1225)	1:47:A:VAL:HA	1:46:A:TYR:HA	15	0.34
(1,1204)	1:18:A:LEU:HG	1:42:A:GLU:HA	1	0.34
(1,1204)	1:18:A:LEU:HG	1:42:A:GLU:HA	14	0.34
(1,1143)	1:47:A:VAL:HG11	1:52:A:THR:HG23	7	0.34
(1,1100)	1:30:A:TRP:HD1	1:56:A:LYS:HE2	15	0.34
(1,1069)	1:16:A:GLU:H	1:16:A:GLU:HB3	3	0.34
(1,1056)	1:54:A:LYS:HG3	1:54:A:LYS:HB3	1	0.34
(1,1015)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	7	0.34
(1,1004)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	4	0.34
(1,1003)	1:24:A:LYS:HG2	1:24:A:LYS:HE2	14	0.34
(1,866)	1:36:A:LYS:H	1:35:A:ARG:HG3	6	0.34
(1,718)	1:42:A:GLU:HA	1:41:A:PRO:HA	2	0.34
(1,718)	1:42:A:GLU:HA	1:41:A:PRO:HA	14	0.34
(1,684)	1:62:A:HIS:HD1	1:23:A:VAL:HG12	9	0.34
(1,663)	1:64:A:HIS:HD1	1:64:A:HIS:HA	8	0.34
(1,644)	1:18:A:LEU:HD13	1:18:A:LEU:HB2	6	0.34
(1,644)	1:18:A:LEU:HD12	1:18:A:LEU:HB2	15	0.34
(1,483)	1:34:A:SER:H	1:33:A:VAL:HG21	14	0.34
(1,467)	1:54:A:LYS:H	1:53:A:GLN:HG2	3	0.34
(1,449)	1:50:A:GLU:H	1:49:A:LEU:HD22	6	0.34
(1,425)	1:67:A:LYS:H	1:66:A:LEU:HG	3	0.34
(1,404)	1:65:A:ARG:HG2	1:65:A:ARG:HB2	5	0.34
(1,320)	1:45:A:ASP:H	1:44:A:GLN:HG3	1	0.34
(1,320)	1:45:A:ASP:H	1:44:A:GLN:HG3	15	0.34
(1,308)	1:22:A:ILE:HG13	1:22:A:ILE:HA	2	0.34
(1,308)	1:22:A:ILE:HG13	1:22:A:ILE:HA	13	0.34
(1,268)	1:19:A:VAL:H	1:19:A:VAL:HG22	10	0.34
(1,197)	1:30:A:TRP:HD1	1:30:A:TRP:HA	5	0.34
(1,197)	1:30:A:TRP:HD1	1:30:A:TRP:HA	7	0.34
(1,197)	1:30:A:TRP:HD1	1:30:A:TRP:HA	9	0.34
(1,104)	1:11:A:ALA:H	1:10:A:THR:HG23	2	0.34
(1,1425)	1:10:A:THR:H	1:13:A:ASP:HB2	1	0.33
(1,1405)	1:7:A:GLN:HB2	1:7:A:GLN:HG3	1	0.33
(1,1405)	1:7:A:GLN:HB2	1:7:A:GLN:HG3	7	0.33
(1,1385)	1:67:A:LYS:HD2	1:64:A:HIS:HA	4	0.33
(1,1364)	1:59:A:PHE:HE1	1:30:A:TRP:HE3	1	0.33
(1,1345)	1:64:A:HIS:HE1	1:68:A:HIS:HD1	3	0.33
(1,1341)	1:17:A:TRP:HE3	1:21:A:ARG:HB2	15	0.33
(1,1340)	1:17:A:TRP:HE3	1:21:A:ARG:HB3	12	0.33
(1,1340)	1:17:A:TRP:HE3	1:21:A:ARG:HB3	15	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1286)	1:36:A:LYS:HG2	1:33:A:VAL:HA	5	0.33
(1,1225)	1:47:A:VAL:HA	1:46:A:TYR:HA	6	0.33
(1,1213)	1:30:A:TRP:HE3	1:37:A:MET:HE3	10	0.33
(1,1183)	1:69:A:GLU:H	1:68:A:HIS:H	5	0.33
(1,1180)	1:7:A:GLN:HE22	1:7:A:GLN:HG3	7	0.33
(1,1101)	1:30:A:TRP:HD1	1:56:A:LYS:HD3	14	0.33
(1,1078)	1:39:A:ALA:H	1:38:A:GLN:HB2	11	0.33
(1,1053)	1:54:A:LYS:HD2	1:54:A:LYS:HA	10	0.33
(1,1053)	1:54:A:LYS:HD2	1:54:A:LYS:HA	11	0.33
(1,1015)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	4	0.33
(1,1015)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	6	0.33
(1,986)	1:58:A:LEU:HD12	1:12:A:LYS:HE3	11	0.33
(1,887)	1:65:A:ARG:HD2	1:65:A:ARG:HA	4	0.33
(1,887)	1:65:A:ARG:HD2	1:65:A:ARG:HA	8	0.33
(1,887)	1:65:A:ARG:HD2	1:65:A:ARG:HA	15	0.33
(1,886)	1:65:A:ARG:HD3	1:65:A:ARG:HA	1	0.33
(1,866)	1:36:A:LYS:H	1:35:A:ARG:HG3	11	0.33
(1,840)	1:32:A:SER:H	1:31:A:LEU:HG	6	0.33
(1,840)	1:32:A:SER:H	1:31:A:LEU:HG	11	0.33
(1,785)	1:64:A:HIS:HB2	1:61:A:GLN:HA	2	0.33
(1,755)	1:22:A:ILE:HG12	1:19:A:VAL:HA	7	0.33
(1,718)	1:42:A:GLU:HA	1:41:A:PRO:HA	12	0.33
(1,684)	1:62:A:HIS:HD1	1:23:A:VAL:HG11	3	0.33
(1,684)	1:62:A:HIS:HD1	1:23:A:VAL:HG13	10	0.33
(1,663)	1:64:A:HIS:HD1	1:64:A:HIS:HA	3	0.33
(1,658)	1:68:A:HIS:HD1	1:68:A:HIS:HA	5	0.33
(1,658)	1:68:A:HIS:HD1	1:68:A:HIS:HA	6	0.33
(1,658)	1:68:A:HIS:HD1	1:68:A:HIS:HA	8	0.33
(1,658)	1:68:A:HIS:HD1	1:68:A:HIS:HA	10	0.33
(1,658)	1:68:A:HIS:HD1	1:68:A:HIS:HA	12	0.33
(1,644)	1:18:A:LEU:HD12	1:18:A:LEU:HB2	4	0.33
(1,514)	1:8:A:ILE:HG12	1:8:A:ILE:HB	9	0.33
(1,514)	1:8:A:ILE:HG12	1:8:A:ILE:HB	10	0.33
(1,514)	1:8:A:ILE:HG12	1:8:A:ILE:HB	13	0.33
(1,514)	1:8:A:ILE:HG12	1:8:A:ILE:HB	14	0.33
(1,489)	1:24:A:LYS:H	1:23:A:VAL:HG22	9	0.33
(1,471)	1:42:A:GLU:H	1:41:A:PRO:HB3	2	0.33
(1,449)	1:50:A:GLU:H	1:49:A:LEU:HD21	1	0.33
(1,425)	1:67:A:LYS:H	1:66:A:LEU:HG	11	0.33
(1,373)	1:61:A:GLN:HG3	1:61:A:GLN:HA	4	0.33
(1,373)	1:61:A:GLN:HG3	1:61:A:GLN:HA	7	0.33
(1,308)	1:22:A:ILE:HG13	1:22:A:ILE:HA	1	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,308)	1:22:A:ILE:HG13	1:22:A:ILE:HA	14	0.33
(1,268)	1:19:A:VAL:H	1:19:A:VAL:HG22	11	0.33
(1,220)	1:17:A:TRP:H	1:17:A:TRP:HE3	15	0.33
(1,197)	1:30:A:TRP:HD1	1:30:A:TRP:HA	1	0.33
(1,197)	1:30:A:TRP:HD1	1:30:A:TRP:HA	15	0.33
(1,7)	1:66:A:LEU:HD23	1:24:A:LYS:HA	12	0.33
(1,1415)	1:24:A:LYS:HG3	1:24:A:LYS:HA	1	0.32
(1,1389)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	3	0.32
(1,1389)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	10	0.32
(1,1389)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	11	0.32
(1,1355)	1:62:A:HIS:HD1	1:63:A:ILE:HG12	2	0.32
(1,1345)	1:64:A:HIS:HE1	1:68:A:HIS:HD1	11	0.32
(1,1340)	1:17:A:TRP:HE3	1:21:A:ARG:HB3	1	0.32
(1,1286)	1:36:A:LYS:HG2	1:33:A:VAL:HA	14	0.32
(1,1239)	1:65:A:ARG:HB3	1:62:A:HIS:HA	5	0.32
(1,1226)	1:47:A:VAL:HG22	1:44:A:GLN:HA	6	0.32
(1,1204)	1:18:A:LEU:HG	1:42:A:GLU:HA	6	0.32
(1,1180)	1:7:A:GLN:HE22	1:7:A:GLN:HG3	1	0.32
(1,1066)	1:14:A:LYS:H	1:14:A:LYS:HG2	8	0.32
(1,1053)	1:54:A:LYS:HD2	1:54:A:LYS:HA	3	0.32
(1,1053)	1:54:A:LYS:HD2	1:54:A:LYS:HA	4	0.32
(1,986)	1:58:A:LEU:HD11	1:12:A:LYS:HE3	12	0.32
(1,886)	1:65:A:ARG:HD3	1:65:A:ARG:HA	5	0.32
(1,866)	1:36:A:LYS:H	1:35:A:ARG:HG3	4	0.32
(1,840)	1:32:A:SER:H	1:31:A:LEU:HG	5	0.32
(1,762)	1:35:A:ARG:HD2	1:32:A:SER:HA	13	0.32
(1,718)	1:42:A:GLU:HA	1:41:A:PRO:HA	7	0.32
(1,663)	1:64:A:HIS:HD1	1:64:A:HIS:HA	5	0.32
(1,663)	1:64:A:HIS:HD1	1:64:A:HIS:HA	6	0.32
(1,663)	1:64:A:HIS:HD1	1:64:A:HIS:HA	15	0.32
(1,658)	1:68:A:HIS:HD1	1:68:A:HIS:HA	1	0.32
(1,658)	1:68:A:HIS:HD1	1:68:A:HIS:HA	3	0.32
(1,658)	1:68:A:HIS:HD1	1:68:A:HIS:HA	4	0.32
(1,658)	1:68:A:HIS:HD1	1:68:A:HIS:HA	9	0.32
(1,658)	1:68:A:HIS:HD1	1:68:A:HIS:HA	11	0.32
(1,658)	1:68:A:HIS:HD1	1:68:A:HIS:HA	15	0.32
(1,644)	1:18:A:LEU:HD12	1:18:A:LEU:HB2	3	0.32
(1,566)	1:32:A:SER:H	1:32:A:SER:HB3	2	0.32
(1,566)	1:32:A:SER:H	1:32:A:SER:HB3	3	0.32
(1,566)	1:32:A:SER:H	1:32:A:SER:HB3	4	0.32
(1,566)	1:32:A:SER:H	1:32:A:SER:HB3	8	0.32
(1,514)	1:8:A:ILE:HG12	1:8:A:ILE:HB	8	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,488)	1:43:A:TYR:HD2	1:47:A:VAL:HG23	10	0.32
(1,483)	1:34:A:SER:H	1:33:A:VAL:HG22	2	0.32
(1,471)	1:42:A:GLU:H	1:41:A:PRO:HB3	12	0.32
(1,425)	1:67:A:LYS:H	1:66:A:LEU:HG	2	0.32
(1,320)	1:45:A:ASP:H	1:44:A:GLN:HG3	7	0.32
(1,148)	1:22:A:ILE:H	1:21:A:ARG:HA	13	0.32
(1,148)	1:22:A:ILE:H	1:21:A:ARG:HA	14	0.32
(1,1389)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	13	0.31
(1,1364)	1:59:A:PHE:HE1	1:30:A:TRP:HE3	6	0.31
(1,1364)	1:59:A:PHE:HE1	1:30:A:TRP:HE3	7	0.31
(1,1340)	1:17:A:TRP:HE3	1:21:A:ARG:HB3	6	0.31
(1,1340)	1:17:A:TRP:HE3	1:21:A:ARG:HB3	14	0.31
(1,1244)	1:26:A:HIS:HE1	1:67:A:LYS:HB2	4	0.31
(1,1242)	1:66:A:LEU:HD11	1:26:A:HIS:HB2	14	0.31
(1,1239)	1:65:A:ARG:HB3	1:62:A:HIS:HA	2	0.31
(1,1232)	1:17:A:TRP:HE1	1:21:A:ARG:HG2	2	0.31
(1,1232)	1:17:A:TRP:HE1	1:21:A:ARG:HG2	15	0.31
(1,1229)	1:58:A:LEU:HG	1:55:A:ALA:HA	6	0.31
(1,1213)	1:30:A:TRP:HE3	1:37:A:MET:HE1	9	0.31
(1,1066)	1:14:A:LYS:H	1:14:A:LYS:HG2	13	0.31
(1,1056)	1:54:A:LYS:HG3	1:54:A:LYS:HB3	9	0.31
(1,1053)	1:54:A:LYS:HD2	1:54:A:LYS:HA	12	0.31
(1,1053)	1:54:A:LYS:HD2	1:54:A:LYS:HA	13	0.31
(1,1015)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	3	0.31
(1,1015)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	9	0.31
(1,960)	1:56:A:LYS:H	1:56:A:LYS:HG2	8	0.31
(1,887)	1:65:A:ARG:HD2	1:65:A:ARG:HA	11	0.31
(1,886)	1:65:A:ARG:HD3	1:65:A:ARG:HA	11	0.31
(1,874)	1:65:A:ARG:HG3	1:65:A:ARG:HA	3	0.31
(1,866)	1:36:A:LYS:H	1:35:A:ARG:HG3	7	0.31
(1,858)	1:22:A:ILE:H	1:21:A:ARG:HG3	14	0.31
(1,785)	1:64:A:HIS:HB2	1:61:A:GLN:HA	15	0.31
(1,776)	1:61:A:GLN:HB3	1:58:A:LEU:HA	14	0.31
(1,718)	1:42:A:GLU:HA	1:41:A:PRO:HA	13	0.31
(1,705)	1:68:A:HIS:HD1	1:67:A:LYS:HG2	2	0.31
(1,658)	1:68:A:HIS:HD1	1:68:A:HIS:HA	2	0.31
(1,658)	1:68:A:HIS:HD1	1:68:A:HIS:HA	7	0.31
(1,644)	1:18:A:LEU:HD13	1:18:A:LEU:HB2	12	0.31
(1,627)	1:16:A:GLU:HG3	1:16:A:GLU:HA	15	0.31
(1,566)	1:32:A:SER:H	1:32:A:SER:HB3	9	0.31
(1,566)	1:32:A:SER:H	1:32:A:SER:HB3	10	0.31
(1,489)	1:24:A:LYS:H	1:23:A:VAL:HG22	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,471)	1:42:A:GLU:H	1:41:A:PRO:HB3	1	0.31
(1,471)	1:42:A:GLU:H	1:41:A:PRO:HB3	15	0.31
(1,441)	1:69:A:GLU:H	1:69:A:GLU:HB3	5	0.31
(1,421)	1:66:A:LEU:HD21	1:66:A:LEU:HB3	15	0.31
(1,320)	1:45:A:ASP:H	1:44:A:GLN:HG3	9	0.31
(1,320)	1:45:A:ASP:H	1:44:A:GLN:HG3	13	0.31
(1,308)	1:22:A:ILE:HG13	1:22:A:ILE:HA	7	0.31
(1,308)	1:22:A:ILE:HG13	1:22:A:ILE:HA	12	0.31
(1,284)	1:21:A:ARG:HG2	1:21:A:ARG:HA	11	0.31
(1,268)	1:19:A:VAL:H	1:19:A:VAL:HG23	12	0.31
(1,220)	1:17:A:TRP:H	1:17:A:TRP:HE3	2	0.31
(1,220)	1:17:A:TRP:H	1:17:A:TRP:HE3	13	0.31
(1,216)	1:17:A:TRP:HZ2	1:17:A:TRP:HH2	1	0.31
(1,216)	1:17:A:TRP:HZ2	1:17:A:TRP:HH2	2	0.31
(1,216)	1:17:A:TRP:HZ2	1:17:A:TRP:HH2	3	0.31
(1,216)	1:17:A:TRP:HZ2	1:17:A:TRP:HH2	4	0.31
(1,216)	1:17:A:TRP:HZ2	1:17:A:TRP:HH2	5	0.31
(1,216)	1:17:A:TRP:HZ2	1:17:A:TRP:HH2	6	0.31
(1,216)	1:17:A:TRP:HZ2	1:17:A:TRP:HH2	7	0.31
(1,216)	1:17:A:TRP:HZ2	1:17:A:TRP:HH2	8	0.31
(1,216)	1:17:A:TRP:HZ2	1:17:A:TRP:HH2	9	0.31
(1,216)	1:17:A:TRP:HZ2	1:17:A:TRP:HH2	10	0.31
(1,216)	1:17:A:TRP:HZ2	1:17:A:TRP:HH2	11	0.31
(1,216)	1:17:A:TRP:HZ2	1:17:A:TRP:HH2	12	0.31
(1,216)	1:17:A:TRP:HZ2	1:17:A:TRP:HH2	13	0.31
(1,216)	1:17:A:TRP:HZ2	1:17:A:TRP:HH2	14	0.31
(1,216)	1:17:A:TRP:HZ2	1:17:A:TRP:HH2	15	0.31
(1,148)	1:22:A:ILE:H	1:21:A:ARG:HA	2	0.31
(1,148)	1:22:A:ILE:H	1:21:A:ARG:HA	15	0.31
(1,1389)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	1	0.3
(1,1389)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	14	0.3
(1,1385)	1:67:A:LYS:HD2	1:64:A:HIS:HA	10	0.3
(1,1357)	1:26:A:HIS:H	1:26:A:HIS:HD1	8	0.3
(1,1345)	1:64:A:HIS:HE1	1:68:A:HIS:HD1	2	0.3
(1,1345)	1:64:A:HIS:HE1	1:68:A:HIS:HD1	6	0.3
(1,1340)	1:17:A:TRP:HE3	1:21:A:ARG:HB3	7	0.3
(1,1340)	1:17:A:TRP:HE3	1:21:A:ARG:HB3	11	0.3
(1,1337)	1:30:A:TRP:HD1	1:31:A:LEU:HG	6	0.3
(1,1337)	1:30:A:TRP:HD1	1:31:A:LEU:HG	13	0.3
(1,1327)	1:64:A:HIS:HD1	1:69:A:GLU:HG2	4	0.3
(1,1304)	1:65:A:ARG:HB3	1:65:A:ARG:HD3	3	0.3
(1,1291)	1:57:A:LYS:HB2	1:54:A:LYS:HA	13	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1232)	1:17:A:TRP:HE1	1:21:A:ARG:HG2	12	0.3
(1,1232)	1:17:A:TRP:HE1	1:21:A:ARG:HG2	13	0.3
(1,1229)	1:58:A:LEU:HG	1:55:A:ALA:HA	1	0.3
(1,1148)	1:15:A:TYR:HD2	1:46:A:TYR:HE2	4	0.3
(1,1100)	1:30:A:TRP:HD1	1:56:A:LYS:HE2	8	0.3
(1,1069)	1:16:A:GLU:H	1:16:A:GLU:HB3	5	0.3
(1,1066)	1:14:A:LYS:H	1:14:A:LYS:HG2	4	0.3
(1,1056)	1:54:A:LYS:HG3	1:54:A:LYS:HB3	2	0.3
(1,1056)	1:54:A:LYS:HG3	1:54:A:LYS:HB3	3	0.3
(1,1056)	1:54:A:LYS:HG3	1:54:A:LYS:HB3	4	0.3
(1,1056)	1:54:A:LYS:HG3	1:54:A:LYS:HB3	5	0.3
(1,1056)	1:54:A:LYS:HG3	1:54:A:LYS:HB3	6	0.3
(1,1056)	1:54:A:LYS:HG3	1:54:A:LYS:HB3	8	0.3
(1,1056)	1:54:A:LYS:HG3	1:54:A:LYS:HB3	10	0.3
(1,1056)	1:54:A:LYS:HG3	1:54:A:LYS:HB3	13	0.3
(1,1056)	1:54:A:LYS:HG3	1:54:A:LYS:HB3	14	0.3
(1,1056)	1:54:A:LYS:HG3	1:54:A:LYS:HB3	15	0.3
(1,1053)	1:54:A:LYS:HD2	1:54:A:LYS:HA	1	0.3
(1,1040)	1:37:A:MET:H	1:36:A:LYS:HG3	1	0.3
(1,1015)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	12	0.3
(1,1001)	1:24:A:LYS:HD2	1:24:A:LYS:HB3	3	0.3
(1,1001)	1:24:A:LYS:HD2	1:24:A:LYS:HB3	15	0.3
(1,947)	1:62:A:HIS:H	1:61:A:GLN:HG3	10	0.3
(1,926)	1:51:A:GLY:H	1:50:A:GLU:HG3	12	0.3
(1,887)	1:65:A:ARG:HD2	1:65:A:ARG:HA	9	0.3
(1,867)	1:36:A:LYS:H	1:35:A:ARG:HD2	14	0.3
(1,837)	1:50:A:GLU:H	1:49:A:LEU:HG	5	0.3
(1,837)	1:50:A:GLU:H	1:49:A:LEU:HG	7	0.3
(1,798)	1:28:A:GLU:H	1:27:A:ASN:HB3	9	0.3
(1,763)	1:35:A:ARG:HG2	1:32:A:SER:HA	7	0.3
(1,762)	1:35:A:ARG:HD2	1:32:A:SER:HA	6	0.3
(1,757)	1:33:A:VAL:HB	1:30:A:TRP:HA	6	0.3
(1,757)	1:33:A:VAL:HB	1:30:A:TRP:HA	11	0.3
(1,757)	1:33:A:VAL:HB	1:30:A:TRP:HA	15	0.3
(1,663)	1:64:A:HIS:HD1	1:64:A:HIS:HA	9	0.3
(1,663)	1:64:A:HIS:HD1	1:64:A:HIS:HA	13	0.3
(1,658)	1:68:A:HIS:HD1	1:68:A:HIS:HA	14	0.3
(1,644)	1:18:A:LEU:HD12	1:18:A:LEU:HB2	9	0.3
(1,553)	1:35:A:ARG:HG3	1:35:A:ARG:HA	13	0.3
(1,553)	1:35:A:ARG:HG3	1:35:A:ARG:HA	14	0.3
(1,514)	1:8:A:ILE:HG12	1:8:A:ILE:HB	2	0.3
(1,514)	1:8:A:ILE:HG12	1:8:A:ILE:HB	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,514)	1:8:A:ILE:HG12	1:8:A:ILE:HB	5	0.3
(1,514)	1:8:A:ILE:HG12	1:8:A:ILE:HB	7	0.3
(1,514)	1:8:A:ILE:HG12	1:8:A:ILE:HB	11	0.3
(1,514)	1:8:A:ILE:HG12	1:8:A:ILE:HB	12	0.3
(1,514)	1:8:A:ILE:HG12	1:8:A:ILE:HB	15	0.3
(1,449)	1:50:A:GLU:H	1:49:A:LEU:HD21	11	0.3
(1,308)	1:22:A:ILE:HG13	1:22:A:ILE:HA	9	0.3
(1,308)	1:22:A:ILE:HG13	1:22:A:ILE:HA	10	0.3
(1,220)	1:17:A:TRP:H	1:17:A:TRP:HE3	12	0.3
(1,1419)	1:27:A:ASN:H	1:63:A:ILE:HD12	1	0.29
(1,1419)	1:27:A:ASN:H	1:63:A:ILE:HD13	9	0.29
(1,1415)	1:24:A:LYS:HG3	1:24:A:LYS:HA	13	0.29
(1,1407)	1:8:A:ILE:HD12	1:5:A:SER:HA	13	0.29
(1,1389)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	12	0.29
(1,1372)	1:22:A:ILE:HD13	1:37:A:MET:HG3	7	0.29
(1,1364)	1:59:A:PHE:HE1	1:30:A:TRP:HE3	9	0.29
(1,1364)	1:59:A:PHE:HE1	1:30:A:TRP:HE3	10	0.29
(1,1340)	1:17:A:TRP:HE3	1:21:A:ARG:HB3	3	0.29
(1,1340)	1:17:A:TRP:HE3	1:21:A:ARG:HB3	13	0.29
(1,1337)	1:30:A:TRP:HD1	1:31:A:LEU:HG	12	0.29
(1,1282)	1:21:A:ARG:HG3	1:18:A:LEU:HA	11	0.29
(1,1232)	1:17:A:TRP:HE1	1:21:A:ARG:HG2	10	0.29
(1,1229)	1:58:A:LEU:HG	1:55:A:ALA:HA	14	0.29
(1,1204)	1:18:A:LEU:HG	1:42:A:GLU:HA	12	0.29
(1,1127)	1:18:A:LEU:HG	1:43:A:TYR:HB3	5	0.29
(1,1095)	1:59:A:PHE:HD2	1:30:A:TRP:HA	6	0.29
(1,1078)	1:39:A:ALA:H	1:38:A:GLN:HB2	1	0.29
(1,1066)	1:14:A:LYS:H	1:14:A:LYS:HG2	9	0.29
(1,1056)	1:54:A:LYS:HG3	1:54:A:LYS:HB3	7	0.29
(1,1056)	1:54:A:LYS:HG3	1:54:A:LYS:HB3	11	0.29
(1,960)	1:56:A:LYS:H	1:56:A:LYS:HG2	4	0.29
(1,947)	1:62:A:HIS:H	1:61:A:GLN:HG3	2	0.29
(1,874)	1:65:A:ARG:HG3	1:65:A:ARG:HA	2	0.29
(1,873)	1:66:A:LEU:H	1:65:A:ARG:HG2	7	0.29
(1,873)	1:66:A:LEU:H	1:65:A:ARG:HG2	8	0.29
(1,867)	1:36:A:LYS:H	1:35:A:ARG:HD2	9	0.29
(1,858)	1:22:A:ILE:H	1:21:A:ARG:HG3	15	0.29
(1,718)	1:42:A:GLU:HA	1:41:A:PRO:HA	9	0.29
(1,718)	1:42:A:GLU:HA	1:41:A:PRO:HA	15	0.29
(1,663)	1:64:A:HIS:HD1	1:64:A:HIS:HA	1	0.29
(1,663)	1:64:A:HIS:HD1	1:64:A:HIS:HA	7	0.29
(1,662)	1:64:A:HIS:H	1:64:A:HIS:HD1	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,658)	1:68:A:HIS:HD1	1:68:A:HIS:HA	13	0.29
(1,566)	1:32:A:SER:H	1:32:A:SER:HB3	6	0.29
(1,566)	1:32:A:SER:H	1:32:A:SER:HB3	11	0.29
(1,514)	1:8:A:ILE:HG12	1:8:A:ILE:HB	6	0.29
(1,489)	1:24:A:LYS:H	1:23:A:VAL:HG22	1	0.29
(1,471)	1:42:A:GLU:H	1:41:A:PRO:HB3	6	0.29
(1,471)	1:42:A:GLU:H	1:41:A:PRO:HB3	7	0.29
(1,467)	1:54:A:LYS:H	1:53:A:GLN:HG2	1	0.29
(1,449)	1:50:A:GLU:H	1:49:A:LEU:HD21	2	0.29
(1,449)	1:50:A:GLU:H	1:49:A:LEU:HD21	7	0.29
(1,449)	1:50:A:GLU:H	1:49:A:LEU:HD23	15	0.29
(1,432)	1:68:A:HIS:H	1:68:A:HIS:HB2	13	0.29
(1,425)	1:67:A:LYS:H	1:66:A:LEU:HG	6	0.29
(1,425)	1:67:A:LYS:H	1:66:A:LEU:HG	10	0.29
(1,320)	1:45:A:ASP:H	1:44:A:GLN:HG3	10	0.29
(1,148)	1:22:A:ILE:H	1:21:A:ARG:HA	1	0.29
(1,1425)	1:10:A:THR:H	1:13:A:ASP:HB2	6	0.28
(1,1372)	1:22:A:ILE:HD12	1:37:A:MET:HG3	12	0.28
(1,1345)	1:64:A:HIS:HE1	1:68:A:HIS:HD1	1	0.28
(1,1340)	1:17:A:TRP:HE3	1:21:A:ARG:HB3	10	0.28
(1,1337)	1:30:A:TRP:HD1	1:31:A:LEU:HG	15	0.28
(1,1282)	1:21:A:ARG:HG3	1:18:A:LEU:HA	9	0.28
(1,1244)	1:26:A:HIS:HE1	1:67:A:LYS:HB2	15	0.28
(1,1239)	1:65:A:ARG:HB3	1:62:A:HIS:HA	1	0.28
(1,1229)	1:58:A:LEU:HG	1:55:A:ALA:HA	12	0.28
(1,1117)	1:30:A:TRP:HE3	1:33:A:VAL:HB	15	0.28
(1,1101)	1:30:A:TRP:HD1	1:56:A:LYS:HD3	6	0.28
(1,1015)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	1	0.28
(1,1007)	1:57:A:LYS:H	1:57:A:LYS:HE2	5	0.28
(1,1001)	1:24:A:LYS:HD2	1:24:A:LYS:HB3	6	0.28
(1,935)	1:15:A:TYR:HD2	1:16:A:GLU:HB2	1	0.28
(1,886)	1:65:A:ARG:HD3	1:65:A:ARG:HA	8	0.28
(1,884)	1:65:A:ARG:H	1:65:A:ARG:HD2	15	0.28
(1,873)	1:66:A:LEU:H	1:65:A:ARG:HG2	5	0.28
(1,840)	1:32:A:SER:H	1:31:A:LEU:HG	12	0.28
(1,840)	1:32:A:SER:H	1:31:A:LEU:HG	13	0.28
(1,837)	1:50:A:GLU:H	1:49:A:LEU:HG	1	0.28
(1,837)	1:50:A:GLU:H	1:49:A:LEU:HG	2	0.28
(1,837)	1:50:A:GLU:H	1:49:A:LEU:HG	6	0.28
(1,785)	1:64:A:HIS:HB2	1:61:A:GLN:HA	14	0.28
(1,776)	1:61:A:GLN:HB3	1:58:A:LEU:HA	15	0.28
(1,659)	1:68:A:HIS:HD1	1:68:A:HIS:HB2	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,659)	1:68:A:HIS:HD1	1:68:A:HIS:HB2	9	0.28
(1,553)	1:35:A:ARG:HG3	1:35:A:ARG:HA	3	0.28
(1,471)	1:42:A:GLU:H	1:41:A:PRO:HB3	8	0.28
(1,449)	1:50:A:GLU:H	1:49:A:LEU:HD23	12	0.28
(1,425)	1:67:A:LYS:H	1:66:A:LEU:HG	13	0.28
(1,422)	1:66:A:LEU:H	1:66:A:LEU:HD13	13	0.28
(1,373)	1:61:A:GLN:HG3	1:61:A:GLN:HA	1	0.28
(1,338)	1:57:A:LYS:H	1:57:A:LYS:HG2	2	0.28
(1,334)	1:57:A:LYS:H	1:56:A:LYS:HB2	4	0.28
(1,320)	1:45:A:ASP:H	1:44:A:GLN:HG3	11	0.28
(1,220)	1:17:A:TRP:H	1:17:A:TRP:HE3	11	0.28
(1,220)	1:17:A:TRP:H	1:17:A:TRP:HE3	14	0.28
(1,148)	1:22:A:ILE:H	1:21:A:ARG:HA	7	0.28
(1,148)	1:22:A:ILE:H	1:21:A:ARG:HA	9	0.28
(1,20)	1:67:A:LYS:HG2	1:26:A:HIS:HB2	12	0.28
(1,1421)	1:23:A:VAL:H	1:62:A:HIS:HD1	12	0.27
(1,1385)	1:67:A:LYS:HD2	1:64:A:HIS:HA	1	0.27
(1,1385)	1:67:A:LYS:HD2	1:64:A:HIS:HA	11	0.27
(1,1337)	1:30:A:TRP:HD1	1:31:A:LEU:HG	3	0.27
(1,1337)	1:30:A:TRP:HD1	1:31:A:LEU:HG	11	0.27
(1,1302)	1:63:A:ILE:HG12	1:60:A:LEU:HA	1	0.27
(1,1286)	1:36:A:LYS:HG2	1:33:A:VAL:HA	15	0.27
(1,1282)	1:21:A:ARG:HG3	1:18:A:LEU:HA	7	0.27
(1,1239)	1:65:A:ARG:HB3	1:62:A:HIS:HA	10	0.27
(1,1239)	1:65:A:ARG:HB3	1:62:A:HIS:HA	14	0.27
(1,1236)	1:30:A:TRP:HE1	1:31:A:LEU:HD11	4	0.27
(1,1232)	1:17:A:TRP:HE1	1:21:A:ARG:HG2	3	0.27
(1,1232)	1:17:A:TRP:HE1	1:21:A:ARG:HG2	7	0.27
(1,1229)	1:58:A:LEU:HG	1:55:A:ALA:HA	2	0.27
(1,1229)	1:58:A:LEU:HG	1:55:A:ALA:HA	11	0.27
(1,1229)	1:58:A:LEU:HG	1:55:A:ALA:HA	13	0.27
(1,1229)	1:58:A:LEU:HG	1:55:A:ALA:HA	15	0.27
(1,1204)	1:18:A:LEU:HG	1:42:A:GLU:HA	7	0.27
(1,1204)	1:18:A:LEU:HG	1:42:A:GLU:HA	9	0.27
(1,1166)	1:36:A:LYS:HB3	1:33:A:VAL:HA	6	0.27
(1,1161)	1:62:A:HIS:HE1	1:66:A:LEU:HD22	15	0.27
(1,1149)	1:62:A:HIS:H	1:19:A:VAL:HG11	2	0.27
(1,1056)	1:54:A:LYS:HG3	1:54:A:LYS:HB3	12	0.27
(1,1015)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	10	0.27
(1,1015)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	15	0.27
(1,997)	1:24:A:LYS:HD2	1:24:A:LYS:HB2	4	0.27
(1,947)	1:62:A:HIS:H	1:61:A:GLN:HG3	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,938)	1:45:A:ASP:H	1:44:A:GLN:HB3	3	0.27
(1,935)	1:15:A:TYR:HD2	1:16:A:GLU:HB2	2	0.27
(1,935)	1:15:A:TYR:HD2	1:16:A:GLU:HB2	6	0.27
(1,935)	1:15:A:TYR:HD2	1:16:A:GLU:HB2	12	0.27
(1,886)	1:65:A:ARG:HD3	1:65:A:ARG:HA	9	0.27
(1,874)	1:65:A:ARG:HG3	1:65:A:ARG:HA	10	0.27
(1,873)	1:66:A:LEU:H	1:65:A:ARG:HG2	6	0.27
(1,873)	1:66:A:LEU:H	1:65:A:ARG:HG2	11	0.27
(1,867)	1:36:A:LYS:H	1:35:A:ARG:HD2	1	0.27
(1,866)	1:36:A:LYS:H	1:35:A:ARG:HG3	8	0.27
(1,840)	1:32:A:SER:H	1:31:A:LEU:HG	3	0.27
(1,840)	1:32:A:SER:H	1:31:A:LEU:HG	15	0.27
(1,837)	1:50:A:GLU:H	1:49:A:LEU:HG	3	0.27
(1,837)	1:50:A:GLU:H	1:49:A:LEU:HG	12	0.27
(1,837)	1:50:A:GLU:H	1:49:A:LEU:HG	13	0.27
(1,811)	1:66:A:LEU:H	1:66:A:LEU:HD23	11	0.27
(1,811)	1:66:A:LEU:H	1:66:A:LEU:HD22	14	0.27
(1,798)	1:28:A:GLU:H	1:27:A:ASN:HB3	8	0.27
(1,790)	1:67:A:LYS:HB2	1:64:A:HIS:HA	15	0.27
(1,785)	1:64:A:HIS:HB2	1:61:A:GLN:HA	9	0.27
(1,783)	1:64:A:HIS:H	1:61:A:GLN:HA	10	0.27
(1,718)	1:42:A:GLU:HA	1:41:A:PRO:HA	6	0.27
(1,662)	1:64:A:HIS:H	1:64:A:HIS:HD1	4	0.27
(1,662)	1:64:A:HIS:H	1:64:A:HIS:HD1	13	0.27
(1,659)	1:68:A:HIS:HD1	1:68:A:HIS:HB2	10	0.27
(1,627)	1:16:A:GLU:HG3	1:16:A:GLU:HA	4	0.27
(1,617)	1:26:A:HIS:H	1:23:A:VAL:HA	4	0.27
(1,617)	1:26:A:HIS:H	1:23:A:VAL:HA	11	0.27
(1,584)	1:13:A:ASP:H	1:12:A:LYS:HB2	6	0.27
(1,553)	1:35:A:ARG:HG3	1:35:A:ARG:HA	2	0.27
(1,489)	1:24:A:LYS:H	1:23:A:VAL:HG21	8	0.27
(1,489)	1:24:A:LYS:H	1:23:A:VAL:HG22	10	0.27
(1,483)	1:34:A:SER:H	1:33:A:VAL:HG21	4	0.27
(1,471)	1:42:A:GLU:H	1:41:A:PRO:HB3	10	0.27
(1,471)	1:42:A:GLU:H	1:41:A:PRO:HB3	11	0.27
(1,449)	1:50:A:GLU:H	1:49:A:LEU:HD21	4	0.27
(1,432)	1:68:A:HIS:H	1:68:A:HIS:HB2	1	0.27
(1,432)	1:68:A:HIS:H	1:68:A:HIS:HB2	6	0.27
(1,432)	1:68:A:HIS:H	1:68:A:HIS:HB2	9	0.27
(1,425)	1:67:A:LYS:H	1:66:A:LEU:HG	14	0.27
(1,373)	1:61:A:GLN:HG3	1:61:A:GLN:HA	2	0.27
(1,308)	1:22:A:ILE:HG13	1:22:A:ILE:HA	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,148)	1:22:A:ILE:H	1:21:A:ARG:HA	10	0.27
(1,12)	1:26:A:HIS:HD1	1:67:A:LYS:HB2	2	0.27
(1,12)	1:26:A:HIS:HD1	1:67:A:LYS:HB2	9	0.27
(1,1396)	1:44:A:GLN:HE21	1:43:A:TYR:HE2	11	0.26
(1,1381)	1:49:A:LEU:HD23	1:7:A:GLN:HG2	2	0.26
(1,1357)	1:26:A:HIS:H	1:26:A:HIS:HD1	5	0.26
(1,1331)	1:23:A:VAL:H	1:33:A:VAL:HB	13	0.26
(1,1321)	1:64:A:HIS:HD1	1:65:A:ARG:HB3	3	0.26
(1,1315)	1:18:A:LEU:HG	1:42:A:GLU:HG3	9	0.26
(1,1239)	1:65:A:ARG:HB3	1:62:A:HIS:HA	9	0.26
(1,1232)	1:17:A:TRP:HE1	1:21:A:ARG:HG2	9	0.26
(1,1229)	1:58:A:LEU:HG	1:55:A:ALA:HA	3	0.26
(1,1229)	1:58:A:LEU:HG	1:55:A:ALA:HA	5	0.26
(1,1219)	1:56:A:LYS:HB2	1:53:A:GLN:HA	4	0.26
(1,1204)	1:18:A:LEU:HG	1:42:A:GLU:HA	11	0.26
(1,1101)	1:30:A:TRP:HD1	1:56:A:LYS:HD3	3	0.26
(1,1040)	1:37:A:MET:H	1:36:A:LYS:HG3	3	0.26
(1,1015)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	14	0.26
(1,1004)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	13	0.26
(1,986)	1:58:A:LEU:HD13	1:12:A:LYS:HE3	10	0.26
(1,954)	1:53:A:GLN:HG2	1:53:A:GLN:HA	2	0.26
(1,873)	1:66:A:LEU:H	1:65:A:ARG:HG2	13	0.26
(1,867)	1:36:A:LYS:H	1:35:A:ARG:HD2	15	0.26
(1,858)	1:22:A:ILE:H	1:21:A:ARG:HG3	2	0.26
(1,840)	1:32:A:SER:H	1:31:A:LEU:HG	1	0.26
(1,837)	1:50:A:GLU:H	1:49:A:LEU:HG	4	0.26
(1,837)	1:50:A:GLU:H	1:49:A:LEU:HG	9	0.26
(1,837)	1:50:A:GLU:H	1:49:A:LEU:HG	10	0.26
(1,837)	1:50:A:GLU:H	1:49:A:LEU:HG	11	0.26
(1,837)	1:50:A:GLU:H	1:49:A:LEU:HG	15	0.26
(1,820)	1:60:A:LEU:HG	1:60:A:LEU:HB2	7	0.26
(1,820)	1:60:A:LEU:HG	1:60:A:LEU:HB2	8	0.26
(1,783)	1:64:A:HIS:H	1:61:A:GLN:HA	13	0.26
(1,757)	1:33:A:VAL:HB	1:30:A:TRP:HA	1	0.26
(1,757)	1:33:A:VAL:HB	1:30:A:TRP:HA	5	0.26
(1,757)	1:33:A:VAL:HB	1:30:A:TRP:HA	13	0.26
(1,718)	1:42:A:GLU:HA	1:41:A:PRO:HA	3	0.26
(1,718)	1:42:A:GLU:HA	1:41:A:PRO:HA	11	0.26
(1,705)	1:68:A:HIS:HD1	1:67:A:LYS:HG2	5	0.26
(1,663)	1:64:A:HIS:HD1	1:64:A:HIS:HA	4	0.26
(1,659)	1:68:A:HIS:HD1	1:68:A:HIS:HB2	11	0.26
(1,644)	1:18:A:LEU:HD13	1:18:A:LEU:HB2	7	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,644)	1:18:A:LEU:HD11	1:18:A:LEU:HB2	14	0.26
(1,617)	1:26:A:HIS:H	1:23:A:VAL:HA	6	0.26
(1,565)	1:33:A:VAL:H	1:32:A:SER:HB3	13	0.26
(1,565)	1:33:A:VAL:H	1:32:A:SER:HB3	14	0.26
(1,553)	1:35:A:ARG:HG3	1:35:A:ARG:HA	9	0.26
(1,553)	1:35:A:ARG:HG3	1:35:A:ARG:HA	15	0.26
(1,471)	1:42:A:GLU:H	1:41:A:PRO:HB3	3	0.26
(1,471)	1:42:A:GLU:H	1:41:A:PRO:HB3	9	0.26
(1,467)	1:54:A:LYS:H	1:53:A:GLN:HG2	13	0.26
(1,449)	1:50:A:GLU:H	1:49:A:LEU:HD21	14	0.26
(1,432)	1:68:A:HIS:H	1:68:A:HIS:HB2	3	0.26
(1,432)	1:68:A:HIS:H	1:68:A:HIS:HB2	5	0.26
(1,432)	1:68:A:HIS:H	1:68:A:HIS:HB2	14	0.26
(1,432)	1:68:A:HIS:H	1:68:A:HIS:HB2	15	0.26
(1,373)	1:61:A:GLN:HG3	1:61:A:GLN:HA	12	0.26
(1,308)	1:22:A:ILE:HG13	1:22:A:ILE:HA	15	0.26
(1,102)	1:39:A:ALA:H	1:38:A:GLN:H	10	0.26
(1,1426)	1:68:A:HIS:HD1	1:64:A:HIS:HB2	4	0.25
(1,1415)	1:24:A:LYS:HG3	1:24:A:LYS:HA	8	0.25
(1,1385)	1:67:A:LYS:HD2	1:64:A:HIS:HA	9	0.25
(1,1345)	1:64:A:HIS:HE1	1:68:A:HIS:HD1	4	0.25
(1,1345)	1:64:A:HIS:HE1	1:68:A:HIS:HD1	13	0.25
(1,1345)	1:64:A:HIS:HE1	1:68:A:HIS:HD1	14	0.25
(1,1337)	1:30:A:TRP:HD1	1:31:A:LEU:HG	10	0.25
(1,1286)	1:36:A:LYS:HG2	1:33:A:VAL:HA	2	0.25
(1,1282)	1:21:A:ARG:HG3	1:18:A:LEU:HA	12	0.25
(1,1244)	1:26:A:HIS:HE1	1:67:A:LYS:HB2	5	0.25
(1,1239)	1:65:A:ARG:HB3	1:62:A:HIS:HA	4	0.25
(1,1239)	1:65:A:ARG:HB3	1:62:A:HIS:HA	8	0.25
(1,1229)	1:58:A:LEU:HG	1:55:A:ALA:HA	8	0.25
(1,1229)	1:58:A:LEU:HG	1:55:A:ALA:HA	10	0.25
(1,1187)	1:59:A:PHE:HE2	1:60:A:LEU:HD12	7	0.25
(1,1175)	1:26:A:HIS:HE1	1:27:A:ASN:HD22	12	0.25
(1,1168)	1:68:A:HIS:HE1	1:67:A:LYS:HE2	15	0.25
(1,1166)	1:36:A:LYS:HB3	1:33:A:VAL:HA	14	0.25
(1,1095)	1:59:A:PHE:HD2	1:30:A:TRP:HA	12	0.25
(1,1015)	1:57:A:LYS:HD2	1:57:A:LYS:HE2	5	0.25
(1,958)	1:53:A:GLN:HB2	1:53:A:GLN:HG2	3	0.25
(1,958)	1:53:A:GLN:HB2	1:53:A:GLN:HG2	9	0.25
(1,954)	1:53:A:GLN:HG2	1:53:A:GLN:HA	9	0.25
(1,926)	1:51:A:GLY:H	1:50:A:GLU:HG3	3	0.25
(1,887)	1:65:A:ARG:HD2	1:65:A:ARG:HA	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,886)	1:65:A:ARG:HD3	1:65:A:ARG:HA	15	0.25
(1,884)	1:65:A:ARG:H	1:65:A:ARG:HD2	2	0.25
(1,884)	1:65:A:ARG:H	1:65:A:ARG:HD2	10	0.25
(1,867)	1:36:A:LYS:H	1:35:A:ARG:HD2	2	0.25
(1,866)	1:36:A:LYS:H	1:35:A:ARG:HG3	2	0.25
(1,866)	1:36:A:LYS:H	1:35:A:ARG:HG3	9	0.25
(1,840)	1:32:A:SER:H	1:31:A:LEU:HG	10	0.25
(1,837)	1:50:A:GLU:H	1:49:A:LEU:HG	14	0.25
(1,820)	1:60:A:LEU:HG	1:60:A:LEU:HB2	1	0.25
(1,820)	1:60:A:LEU:HG	1:60:A:LEU:HB2	9	0.25
(1,820)	1:60:A:LEU:HG	1:60:A:LEU:HB2	11	0.25
(1,820)	1:60:A:LEU:HG	1:60:A:LEU:HB2	13	0.25
(1,757)	1:33:A:VAL:HB	1:30:A:TRP:HA	3	0.25
(1,757)	1:33:A:VAL:HB	1:30:A:TRP:HA	12	0.25
(1,727)	1:25:A:ASN:H	1:25:A:ASN:HB3	14	0.25
(1,659)	1:68:A:HIS:HD1	1:68:A:HIS:HB2	1	0.25
(1,659)	1:68:A:HIS:HD1	1:68:A:HIS:HB2	3	0.25
(1,659)	1:68:A:HIS:HD1	1:68:A:HIS:HB2	14	0.25
(1,584)	1:13:A:ASP:H	1:12:A:LYS:HB2	10	0.25
(1,553)	1:35:A:ARG:HG3	1:35:A:ARG:HA	1	0.25
(1,467)	1:54:A:LYS:H	1:53:A:GLN:HG2	6	0.25
(1,449)	1:50:A:GLU:H	1:49:A:LEU:HD23	9	0.25
(1,449)	1:50:A:GLU:H	1:49:A:LEU:HD22	10	0.25
(1,449)	1:50:A:GLU:H	1:49:A:LEU:HD22	13	0.25
(1,432)	1:68:A:HIS:H	1:68:A:HIS:HB2	2	0.25
(1,432)	1:68:A:HIS:H	1:68:A:HIS:HB2	8	0.25
(1,425)	1:67:A:LYS:H	1:66:A:LEU:HG	9	0.25
(1,422)	1:66:A:LEU:H	1:66:A:LEU:HD12	1	0.25
(1,373)	1:61:A:GLN:HG3	1:61:A:GLN:HA	5	0.25
(1,373)	1:61:A:GLN:HG3	1:61:A:GLN:HA	8	0.25
(1,373)	1:61:A:GLN:HG3	1:61:A:GLN:HA	10	0.25
(1,338)	1:57:A:LYS:H	1:57:A:LYS:HG2	11	0.25
(1,308)	1:22:A:ILE:HG13	1:22:A:ILE:HA	8	0.25
(1,308)	1:22:A:ILE:HG13	1:22:A:ILE:HA	11	0.25
(1,220)	1:17:A:TRP:H	1:17:A:TRP:HE3	3	0.25
(1,220)	1:17:A:TRP:H	1:17:A:TRP:HE3	5	0.25
(1,148)	1:22:A:ILE:H	1:21:A:ARG:HA	3	0.25
(1,148)	1:22:A:ILE:H	1:21:A:ARG:HA	11	0.25
(1,148)	1:22:A:ILE:H	1:21:A:ARG:HA	12	0.25
(1,2)	1:66:A:LEU:HD22	1:25:A:ASN:HA	8	0.25
(1,1419)	1:27:A:ASN:H	1:63:A:ILE:HD13	8	0.24
(1,1401)	1:7:A:GLN:HG2	1:7:A:GLN:HA	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1357)	1:26:A:HIS:H	1:26:A:HIS:HD1	15	0.24
(1,1337)	1:30:A:TRP:HD1	1:31:A:LEU:HG	1	0.24
(1,1337)	1:30:A:TRP:HD1	1:31:A:LEU:HG	2	0.24
(1,1337)	1:30:A:TRP:HD1	1:31:A:LEU:HG	5	0.24
(1,1331)	1:23:A:VAL:H	1:33:A:VAL:HB	10	0.24
(1,1304)	1:65:A:ARG:HB3	1:65:A:ARG:HD3	12	0.24
(1,1239)	1:65:A:ARG:HB3	1:62:A:HIS:HA	6	0.24
(1,1239)	1:65:A:ARG:HB3	1:62:A:HIS:HA	13	0.24
(1,1232)	1:17:A:TRP:HE1	1:21:A:ARG:HG2	6	0.24
(1,1229)	1:58:A:LEU:HG	1:55:A:ALA:HA	4	0.24
(1,1226)	1:47:A:VAL:HG21	1:44:A:GLN:HA	10	0.24
(1,1213)	1:30:A:TRP:HE3	1:37:A:MET:HE1	13	0.24
(1,1204)	1:18:A:LEU:HG	1:42:A:GLU:HA	10	0.24
(1,1149)	1:62:A:HIS:H	1:19:A:VAL:HG11	11	0.24
(1,1101)	1:30:A:TRP:HD1	1:56:A:LYS:HD3	2	0.24
(1,1078)	1:39:A:ALA:H	1:38:A:GLN:HB2	12	0.24
(1,1047)	1:55:A:ALA:H	1:54:A:LYS:HG2	6	0.24
(1,1047)	1:55:A:ALA:H	1:54:A:LYS:HG2	8	0.24
(1,1007)	1:57:A:LYS:H	1:57:A:LYS:HE2	3	0.24
(1,986)	1:58:A:LEU:HD11	1:12:A:LYS:HE3	2	0.24
(1,958)	1:53:A:GLN:HB2	1:53:A:GLN:HG2	2	0.24
(1,887)	1:65:A:ARG:HD2	1:65:A:ARG:HA	7	0.24
(1,873)	1:66:A:LEU:H	1:65:A:ARG:HG2	14	0.24
(1,872)	1:65:A:ARG:H	1:65:A:ARG:HG2	13	0.24
(1,866)	1:36:A:LYS:H	1:35:A:ARG:HG3	15	0.24
(1,840)	1:32:A:SER:H	1:31:A:LEU:HG	2	0.24
(1,820)	1:60:A:LEU:HG	1:60:A:LEU:HB2	2	0.24
(1,820)	1:60:A:LEU:HG	1:60:A:LEU:HB2	4	0.24
(1,820)	1:60:A:LEU:HG	1:60:A:LEU:HB2	5	0.24
(1,820)	1:60:A:LEU:HG	1:60:A:LEU:HB2	6	0.24
(1,820)	1:60:A:LEU:HG	1:60:A:LEU:HB2	10	0.24
(1,820)	1:60:A:LEU:HG	1:60:A:LEU:HB2	12	0.24
(1,798)	1:28:A:GLU:H	1:27:A:ASN:HB3	3	0.24
(1,798)	1:28:A:GLU:H	1:27:A:ASN:HB3	7	0.24
(1,798)	1:28:A:GLU:H	1:27:A:ASN:HB3	13	0.24
(1,783)	1:64:A:HIS:H	1:61:A:GLN:HA	1	0.24
(1,783)	1:64:A:HIS:H	1:61:A:GLN:HA	2	0.24
(1,718)	1:42:A:GLU:HA	1:41:A:PRO:HA	4	0.24
(1,662)	1:64:A:HIS:H	1:64:A:HIS:HD1	14	0.24
(1,659)	1:68:A:HIS:HD1	1:68:A:HIS:HB2	13	0.24
(1,584)	1:13:A:ASP:H	1:12:A:LYS:HB2	7	0.24
(1,562)	1:36:A:LYS:H	1:35:A:ARG:HG2	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,553)	1:35:A:ARG:HG3	1:35:A:ARG:HA	8	0.24
(1,489)	1:24:A:LYS:H	1:23:A:VAL:HG22	3	0.24
(1,481)	1:33:A:VAL:H	1:33:A:VAL:HB	15	0.24
(1,432)	1:68:A:HIS:H	1:68:A:HIS:HB2	4	0.24
(1,432)	1:68:A:HIS:H	1:68:A:HIS:HB2	10	0.24
(1,432)	1:68:A:HIS:H	1:68:A:HIS:HB2	11	0.24
(1,422)	1:66:A:LEU:H	1:66:A:LEU:HD11	3	0.24
(1,422)	1:66:A:LEU:H	1:66:A:LEU:HD12	5	0.24
(1,422)	1:66:A:LEU:H	1:66:A:LEU:HD11	8	0.24
(1,320)	1:45:A:ASP:H	1:44:A:GLN:HG3	5	0.24
(1,308)	1:22:A:ILE:HG13	1:22:A:ILE:HA	3	0.24
(1,308)	1:22:A:ILE:HG13	1:22:A:ILE:HA	6	0.24
(1,269)	1:20:A:SER:H	1:19:A:VAL:HB	10	0.24
(1,148)	1:22:A:ILE:H	1:21:A:ARG:HA	8	0.24
(1,20)	1:67:A:LYS:HG2	1:26:A:HIS:HB2	9	0.24
(1,12)	1:26:A:HIS:HD1	1:67:A:LYS:HB2	5	0.24
(1,7)	1:66:A:LEU:HD23	1:24:A:LYS:HA	15	0.24
(1,1421)	1:23:A:VAL:H	1:62:A:HIS:HD1	7	0.23
(1,1406)	1:8:A:ILE:HD13	1:5:A:SER:HB2	3	0.23
(1,1401)	1:7:A:GLN:HG2	1:7:A:GLN:HA	13	0.23
(1,1385)	1:67:A:LYS:HD2	1:64:A:HIS:HA	6	0.23
(1,1376)	1:58:A:LEU:HD23	1:12:A:LYS:HE3	1	0.23
(1,1376)	1:58:A:LEU:HD21	1:12:A:LYS:HE3	2	0.23
(1,1364)	1:59:A:PHE:HE1	1:30:A:TRP:HE3	4	0.23
(1,1357)	1:26:A:HIS:H	1:26:A:HIS:HD1	2	0.23
(1,1357)	1:26:A:HIS:H	1:26:A:HIS:HD1	11	0.23
(1,1346)	1:43:A:TYR:HD1	1:37:A:MET:HG2	11	0.23
(1,1345)	1:64:A:HIS:HE1	1:68:A:HIS:HD1	15	0.23
(1,1337)	1:30:A:TRP:HD1	1:31:A:LEU:HG	9	0.23
(1,1331)	1:23:A:VAL:H	1:33:A:VAL:HB	12	0.23
(1,1321)	1:64:A:HIS:HD1	1:65:A:ARG:HB3	10	0.23
(1,1272)	1:16:A:GLU:HB3	1:13:A:ASP:HA	5	0.23
(1,1168)	1:68:A:HIS:HE1	1:67:A:LYS:HE2	12	0.23
(1,1155)	1:19:A:VAL:HG23	1:62:A:HIS:HB3	6	0.23
(1,1127)	1:18:A:LEU:HG	1:43:A:TYR:HB3	6	0.23
(1,1117)	1:30:A:TRP:HE3	1:33:A:VAL:HB	1	0.23
(1,1101)	1:30:A:TRP:HD1	1:56:A:LYS:HD3	7	0.23
(1,1001)	1:24:A:LYS:HD2	1:24:A:LYS:HB3	11	0.23
(1,958)	1:53:A:GLN:HB2	1:53:A:GLN:HG2	6	0.23
(1,958)	1:53:A:GLN:HB2	1:53:A:GLN:HG2	13	0.23
(1,886)	1:65:A:ARG:HD3	1:65:A:ARG:HA	13	0.23
(1,873)	1:66:A:LEU:H	1:65:A:ARG:HG2	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,840)	1:32:A:SER:H	1:31:A:LEU:HG	8	0.23
(1,840)	1:32:A:SER:H	1:31:A:LEU:HG	14	0.23
(1,820)	1:60:A:LEU:HG	1:60:A:LEU:HB2	3	0.23
(1,820)	1:60:A:LEU:HG	1:60:A:LEU:HB2	14	0.23
(1,820)	1:60:A:LEU:HG	1:60:A:LEU:HB2	15	0.23
(1,783)	1:64:A:HIS:H	1:61:A:GLN:HA	6	0.23
(1,783)	1:64:A:HIS:H	1:61:A:GLN:HA	8	0.23
(1,718)	1:42:A:GLU:HA	1:41:A:PRO:HA	10	0.23
(1,705)	1:68:A:HIS:HD1	1:67:A:LYS:HG2	7	0.23
(1,692)	1:46:A:TYR:HD1	1:11:A:ALA:HB2	7	0.23
(1,660)	1:68:A:HIS:HD1	1:68:A:HIS:HB3	12	0.23
(1,627)	1:16:A:GLU:HG3	1:16:A:GLU:HA	14	0.23
(1,617)	1:26:A:HIS:H	1:23:A:VAL:HA	13	0.23
(1,584)	1:13:A:ASP:H	1:12:A:LYS:HB2	3	0.23
(1,584)	1:13:A:ASP:H	1:12:A:LYS:HB2	14	0.23
(1,558)	1:35:A:ARG:H	1:35:A:ARG:HD2	6	0.23
(1,487)	1:59:A:PHE:HD1	1:19:A:VAL:HG23	3	0.23
(1,481)	1:33:A:VAL:H	1:33:A:VAL:HB	6	0.23
(1,481)	1:33:A:VAL:H	1:33:A:VAL:HB	11	0.23
(1,449)	1:50:A:GLU:H	1:49:A:LEU:HD23	3	0.23
(1,365)	1:61:A:GLN:H	1:60:A:LEU:HG	6	0.23
(1,288)	1:21:A:ARG:H	1:21:A:ARG:HG2	15	0.23
(1,148)	1:22:A:ILE:H	1:21:A:ARG:HA	4	0.23
(1,148)	1:22:A:ILE:H	1:21:A:ARG:HA	5	0.23
(1,148)	1:22:A:ILE:H	1:21:A:ARG:HA	6	0.23
(1,26)	1:10:A:THR:HA	1:10:A:THR:HB	2	0.23
(1,5)	1:25:A:ASN:HB2	1:25:A:ASN:HA	14	0.23
(1,1426)	1:68:A:HIS:HD1	1:64:A:HIS:HB2	13	0.22
(1,1421)	1:23:A:VAL:H	1:62:A:HIS:HD1	1	0.22
(1,1421)	1:23:A:VAL:H	1:62:A:HIS:HD1	13	0.22
(1,1421)	1:23:A:VAL:H	1:62:A:HIS:HD1	15	0.22
(1,1401)	1:7:A:GLN:HG2	1:7:A:GLN:HA	4	0.22
(1,1401)	1:7:A:GLN:HG2	1:7:A:GLN:HA	9	0.22
(1,1389)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	7	0.22
(1,1385)	1:67:A:LYS:HD2	1:64:A:HIS:HA	13	0.22
(1,1385)	1:67:A:LYS:HD2	1:64:A:HIS:HA	14	0.22
(1,1382)	1:39:A:ALA:HB2	1:38:A:GLN:HG2	10	0.22
(1,1376)	1:58:A:LEU:HD23	1:12:A:LYS:HE3	5	0.22
(1,1376)	1:58:A:LEU:HD22	1:12:A:LYS:HE3	6	0.22
(1,1376)	1:58:A:LEU:HD22	1:12:A:LYS:HE3	11	0.22
(1,1357)	1:26:A:HIS:H	1:26:A:HIS:HD1	1	0.22
(1,1349)	1:22:A:ILE:H	1:23:A:VAL:HB	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1345)	1:64:A:HIS:HE1	1:68:A:HIS:HD1	5	0.22
(1,1345)	1:64:A:HIS:HE1	1:68:A:HIS:HD1	12	0.22
(1,1331)	1:23:A:VAL:H	1:33:A:VAL:HB	1	0.22
(1,1313)	1:33:A:VAL:HA	1:32:A:SER:HB3	2	0.22
(1,1274)	1:17:A:TRP:HE3	1:18:A:LEU:HA	4	0.22
(1,1239)	1:65:A:ARG:HB3	1:62:A:HIS:HA	15	0.22
(1,1232)	1:17:A:TRP:HE1	1:21:A:ARG:HG2	1	0.22
(1,1188)	1:59:A:PHE:HD2	1:60:A:LEU:HD13	9	0.22
(1,1175)	1:26:A:HIS:HE1	1:27:A:ASN:HD22	5	0.22
(1,1166)	1:36:A:LYS:HB3	1:33:A:VAL:HA	8	0.22
(1,1166)	1:36:A:LYS:HB3	1:33:A:VAL:HA	11	0.22
(1,1155)	1:19:A:VAL:HG23	1:62:A:HIS:HB3	7	0.22
(1,1095)	1:59:A:PHE:HD2	1:30:A:TRP:HA	2	0.22
(1,1078)	1:39:A:ALA:H	1:38:A:GLN:HB2	6	0.22
(1,1025)	1:36:A:LYS:HG3	1:36:A:LYS:HA	13	0.22
(1,1008)	1:57:A:LYS:H	1:57:A:LYS:HD2	3	0.22
(1,1008)	1:57:A:LYS:H	1:57:A:LYS:HD2	9	0.22
(1,1007)	1:57:A:LYS:H	1:57:A:LYS:HE2	1	0.22
(1,1004)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	12	0.22
(1,997)	1:24:A:LYS:HD2	1:24:A:LYS:HB2	10	0.22
(1,986)	1:58:A:LEU:HD12	1:12:A:LYS:HE3	7	0.22
(1,984)	1:46:A:TYR:HE1	1:12:A:LYS:HG2	8	0.22
(1,935)	1:15:A:TYR:HD2	1:16:A:GLU:HB2	3	0.22
(1,935)	1:15:A:TYR:HD2	1:16:A:GLU:HB2	15	0.22
(1,926)	1:51:A:GLY:H	1:50:A:GLU:HG3	15	0.22
(1,873)	1:66:A:LEU:H	1:65:A:ARG:HG2	9	0.22
(1,872)	1:65:A:ARG:H	1:65:A:ARG:HG2	5	0.22
(1,867)	1:36:A:LYS:H	1:35:A:ARG:HD2	3	0.22
(1,867)	1:36:A:LYS:H	1:35:A:ARG:HD2	4	0.22
(1,867)	1:36:A:LYS:H	1:35:A:ARG:HD2	8	0.22
(1,866)	1:36:A:LYS:H	1:35:A:ARG:HG3	13	0.22
(1,798)	1:28:A:GLU:H	1:27:A:ASN:HB3	6	0.22
(1,798)	1:28:A:GLU:H	1:27:A:ASN:HB3	10	0.22
(1,798)	1:28:A:GLU:H	1:27:A:ASN:HB3	15	0.22
(1,785)	1:64:A:HIS:HB2	1:61:A:GLN:HA	5	0.22
(1,783)	1:64:A:HIS:H	1:61:A:GLN:HA	11	0.22
(1,755)	1:22:A:ILE:HG12	1:19:A:VAL:HA	1	0.22
(1,718)	1:42:A:GLU:HA	1:41:A:PRO:HA	8	0.22
(1,705)	1:68:A:HIS:HD1	1:67:A:LYS:HG2	8	0.22
(1,662)	1:64:A:HIS:H	1:64:A:HIS:HD1	5	0.22
(1,662)	1:64:A:HIS:H	1:64:A:HIS:HD1	15	0.22
(1,660)	1:68:A:HIS:HD1	1:68:A:HIS:HB3	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,660)	1:68:A:HIS:HD1	1:68:A:HIS:HB3	5	0.22
(1,551)	1:35:A:ARG:HB2	1:35:A:ARG:HA	1	0.22
(1,551)	1:35:A:ARG:HB2	1:35:A:ARG:HA	2	0.22
(1,551)	1:35:A:ARG:HB2	1:35:A:ARG:HA	3	0.22
(1,551)	1:35:A:ARG:HB2	1:35:A:ARG:HA	4	0.22
(1,551)	1:35:A:ARG:HB2	1:35:A:ARG:HA	6	0.22
(1,551)	1:35:A:ARG:HB2	1:35:A:ARG:HA	8	0.22
(1,551)	1:35:A:ARG:HB2	1:35:A:ARG:HA	9	0.22
(1,551)	1:35:A:ARG:HB2	1:35:A:ARG:HA	10	0.22
(1,551)	1:35:A:ARG:HB2	1:35:A:ARG:HA	11	0.22
(1,551)	1:35:A:ARG:HB2	1:35:A:ARG:HA	13	0.22
(1,551)	1:35:A:ARG:HB2	1:35:A:ARG:HA	14	0.22
(1,551)	1:35:A:ARG:HB2	1:35:A:ARG:HA	15	0.22
(1,489)	1:24:A:LYS:H	1:23:A:VAL:HG23	15	0.22
(1,481)	1:33:A:VAL:H	1:33:A:VAL:HB	5	0.22
(1,481)	1:33:A:VAL:H	1:33:A:VAL:HB	12	0.22
(1,467)	1:54:A:LYS:H	1:53:A:GLN:HG2	5	0.22
(1,441)	1:69:A:GLU:H	1:69:A:GLU:HB3	4	0.22
(1,432)	1:68:A:HIS:H	1:68:A:HIS:HB2	7	0.22
(1,422)	1:66:A:LEU:H	1:66:A:LEU:HD11	10	0.22
(1,365)	1:61:A:GLN:H	1:60:A:LEU:HG	2	0.22
(1,365)	1:61:A:GLN:H	1:60:A:LEU:HG	4	0.22
(1,365)	1:61:A:GLN:H	1:60:A:LEU:HG	8	0.22
(1,365)	1:61:A:GLN:H	1:60:A:LEU:HG	12	0.22
(1,334)	1:57:A:LYS:H	1:56:A:LYS:HB2	14	0.22
(1,269)	1:20:A:SER:H	1:19:A:VAL:HB	11	0.22
(1,220)	1:17:A:TRP:H	1:17:A:TRP:HE3	1	0.22
(1,220)	1:17:A:TRP:H	1:17:A:TRP:HE3	9	0.22
(1,213)	1:17:A:TRP:HE1	1:17:A:TRP:HD1	3	0.22
(1,213)	1:17:A:TRP:HE1	1:17:A:TRP:HD1	6	0.22
(1,7)	1:66:A:LEU:HD22	1:24:A:LYS:HA	13	0.22
(1,1426)	1:68:A:HIS:HD1	1:64:A:HIS:HB2	8	0.21
(1,1425)	1:10:A:THR:H	1:13:A:ASP:HB2	2	0.21
(1,1423)	1:26:A:HIS:HD1	1:66:A:LEU:HA	1	0.21
(1,1421)	1:23:A:VAL:H	1:62:A:HIS:HD1	3	0.21
(1,1401)	1:7:A:GLN:HG2	1:7:A:GLN:HA	3	0.21
(1,1401)	1:7:A:GLN:HG2	1:7:A:GLN:HA	8	0.21
(1,1401)	1:7:A:GLN:HG2	1:7:A:GLN:HA	11	0.21
(1,1393)	1:26:A:HIS:HE1	1:67:A:LYS:HG3	1	0.21
(1,1376)	1:58:A:LEU:HD21	1:12:A:LYS:HE3	10	0.21
(1,1376)	1:58:A:LEU:HD23	1:12:A:LYS:HE3	12	0.21
(1,1357)	1:26:A:HIS:H	1:26:A:HIS:HD1	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1345)	1:64:A:HIS:HE1	1:68:A:HIS:HD1	7	0.21
(1,1337)	1:30:A:TRP:HD1	1:31:A:LEU:HG	14	0.21
(1,1331)	1:23:A:VAL:H	1:33:A:VAL:HB	3	0.21
(1,1313)	1:33:A:VAL:HA	1:32:A:SER:HB3	6	0.21
(1,1282)	1:21:A:ARG:HG3	1:18:A:LEU:HA	10	0.21
(1,1274)	1:17:A:TRP:HE3	1:18:A:LEU:HA	7	0.21
(1,1274)	1:17:A:TRP:HE3	1:18:A:LEU:HA	9	0.21
(1,1274)	1:17:A:TRP:HE3	1:18:A:LEU:HA	10	0.21
(1,1269)	1:58:A:LEU:HD12	1:16:A:GLU:HG3	4	0.21
(1,1264)	1:45:A:ASP:HB2	1:42:A:GLU:HA	9	0.21
(1,1244)	1:26:A:HIS:HE1	1:67:A:LYS:HB2	7	0.21
(1,1229)	1:58:A:LEU:HG	1:55:A:ALA:HA	7	0.21
(1,1226)	1:47:A:VAL:HG21	1:44:A:GLN:HA	11	0.21
(1,1168)	1:68:A:HIS:HE1	1:67:A:LYS:HE2	2	0.21
(1,1157)	1:19:A:VAL:HG11	1:62:A:HIS:HB2	7	0.21
(1,1127)	1:18:A:LEU:HG	1:43:A:TYR:HB3	3	0.21
(1,1127)	1:18:A:LEU:HG	1:43:A:TYR:HB3	9	0.21
(1,1124)	1:15:A:TYR:HD2	1:55:A:ALA:HA	15	0.21
(1,1117)	1:30:A:TRP:HE3	1:33:A:VAL:HB	3	0.21
(1,1107)	1:43:A:TYR:HE1	1:34:A:SER:HB2	12	0.21
(1,1101)	1:30:A:TRP:HD1	1:56:A:LYS:HD3	10	0.21
(1,1101)	1:30:A:TRP:HD1	1:56:A:LYS:HD3	12	0.21
(1,1080)	1:43:A:TYR:HE1	1:38:A:GLN:HA	10	0.21
(1,1025)	1:36:A:LYS:HG3	1:36:A:LYS:HA	12	0.21
(1,1017)	1:57:A:LYS:HG3	1:57:A:LYS:HE2	6	0.21
(1,958)	1:53:A:GLN:HB2	1:53:A:GLN:HG2	1	0.21
(1,958)	1:53:A:GLN:HB2	1:53:A:GLN:HG2	5	0.21
(1,958)	1:53:A:GLN:HB2	1:53:A:GLN:HG2	8	0.21
(1,947)	1:62:A:HIS:H	1:61:A:GLN:HG3	15	0.21
(1,935)	1:15:A:TYR:HD2	1:16:A:GLU:HB2	9	0.21
(1,926)	1:51:A:GLY:H	1:50:A:GLU:HG3	1	0.21
(1,873)	1:66:A:LEU:H	1:65:A:ARG:HG2	1	0.21
(1,867)	1:36:A:LYS:H	1:35:A:ARG:HD2	10	0.21
(1,811)	1:66:A:LEU:H	1:66:A:LEU:HD23	4	0.21
(1,777)	1:61:A:GLN:HG2	1:58:A:LEU:HA	7	0.21
(1,776)	1:61:A:GLN:HB3	1:58:A:LEU:HA	11	0.21
(1,718)	1:42:A:GLU:HA	1:41:A:PRO:HA	5	0.21
(1,705)	1:68:A:HIS:HD1	1:67:A:LYS:HG2	15	0.21
(1,662)	1:64:A:HIS:H	1:64:A:HIS:HD1	8	0.21
(1,662)	1:64:A:HIS:H	1:64:A:HIS:HD1	9	0.21
(1,662)	1:64:A:HIS:H	1:64:A:HIS:HD1	11	0.21
(1,659)	1:68:A:HIS:HD1	1:68:A:HIS:HB2	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,659)	1:68:A:HIS:HD1	1:68:A:HIS:HB2	8	0.21
(1,563)	1:32:A:SER:H	1:32:A:SER:HA	5	0.21
(1,487)	1:59:A:PHE:HD1	1:19:A:VAL:HG23	5	0.21
(1,483)	1:34:A:SER:H	1:33:A:VAL:HG22	7	0.21
(1,471)	1:42:A:GLU:H	1:41:A:PRO:HB3	13	0.21
(1,471)	1:42:A:GLU:H	1:41:A:PRO:HB3	14	0.21
(1,425)	1:67:A:LYS:H	1:66:A:LEU:HG	1	0.21
(1,425)	1:67:A:LYS:H	1:66:A:LEU:HG	12	0.21
(1,425)	1:67:A:LYS:H	1:66:A:LEU:HG	15	0.21
(1,419)	1:66:A:LEU:HD11	1:66:A:LEU:HB2	12	0.21
(1,365)	1:61:A:GLN:H	1:60:A:LEU:HG	1	0.21
(1,365)	1:61:A:GLN:H	1:60:A:LEU:HG	15	0.21
(1,338)	1:57:A:LYS:H	1:57:A:LYS:HG2	4	0.21
(1,334)	1:57:A:LYS:H	1:56:A:LYS:HB2	5	0.21
(1,284)	1:21:A:ARG:HG2	1:21:A:ARG:HA	2	0.21
(1,220)	1:17:A:TRP:H	1:17:A:TRP:HE3	8	0.21
(1,213)	1:17:A:TRP:HE1	1:17:A:TRP:HD1	1	0.21
(1,213)	1:17:A:TRP:HE1	1:17:A:TRP:HD1	2	0.21
(1,213)	1:17:A:TRP:HE1	1:17:A:TRP:HD1	4	0.21
(1,213)	1:17:A:TRP:HE1	1:17:A:TRP:HD1	5	0.21
(1,213)	1:17:A:TRP:HE1	1:17:A:TRP:HD1	7	0.21
(1,213)	1:17:A:TRP:HE1	1:17:A:TRP:HD1	8	0.21
(1,213)	1:17:A:TRP:HE1	1:17:A:TRP:HD1	9	0.21
(1,213)	1:17:A:TRP:HE1	1:17:A:TRP:HD1	10	0.21
(1,213)	1:17:A:TRP:HE1	1:17:A:TRP:HD1	11	0.21
(1,213)	1:17:A:TRP:HE1	1:17:A:TRP:HD1	12	0.21
(1,213)	1:17:A:TRP:HE1	1:17:A:TRP:HD1	13	0.21
(1,213)	1:17:A:TRP:HE1	1:17:A:TRP:HD1	14	0.21
(1,213)	1:17:A:TRP:HE1	1:17:A:TRP:HD1	15	0.21
(1,12)	1:26:A:HIS:HD1	1:67:A:LYS:HB2	12	0.21
(1,12)	1:26:A:HIS:HD1	1:67:A:LYS:HB2	15	0.21
(1,2)	1:66:A:LEU:HD23	1:25:A:ASN:HA	5	0.21
(1,1426)	1:68:A:HIS:HD1	1:64:A:HIS:HB2	15	0.2
(1,1389)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	2	0.2
(1,1385)	1:67:A:LYS:HD2	1:64:A:HIS:HA	3	0.2
(1,1357)	1:26:A:HIS:H	1:26:A:HIS:HD1	6	0.2
(1,1357)	1:26:A:HIS:H	1:26:A:HIS:HD1	14	0.2
(1,1349)	1:22:A:ILE:H	1:23:A:VAL:HB	10	0.2
(1,1331)	1:23:A:VAL:H	1:33:A:VAL:HB	15	0.2
(1,1326)	1:64:A:HIS:HD1	1:67:A:LYS:HE2	5	0.2
(1,1239)	1:65:A:ARG:HB3	1:62:A:HIS:HA	12	0.2
(1,1232)	1:17:A:TRP:HE1	1:21:A:ARG:HG2	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1187)	1:59:A:PHE:HE2	1:60:A:LEU:HD11	11	0.2
(1,1166)	1:36:A:LYS:HB3	1:33:A:VAL:HA	1	0.2
(1,1166)	1:36:A:LYS:HB3	1:33:A:VAL:HA	2	0.2
(1,1133)	1:30:A:TRP:HZ3	1:59:A:PHE:HB3	9	0.2
(1,1124)	1:15:A:TYR:HD2	1:55:A:ALA:HA	14	0.2
(1,1117)	1:30:A:TRP:HE3	1:33:A:VAL:HB	5	0.2
(1,1117)	1:30:A:TRP:HE3	1:33:A:VAL:HB	12	0.2
(1,1107)	1:43:A:TYR:HE2	1:34:A:SER:HB2	7	0.2
(1,1100)	1:30:A:TRP:HD1	1:56:A:LYS:HE2	7	0.2
(1,1095)	1:59:A:PHE:HD2	1:30:A:TRP:HA	7	0.2
(1,1095)	1:59:A:PHE:HD2	1:30:A:TRP:HA	15	0.2
(1,1078)	1:39:A:ALA:H	1:38:A:GLN:HB2	7	0.2
(1,1078)	1:39:A:ALA:H	1:38:A:GLN:HB2	14	0.2
(1,958)	1:53:A:GLN:HB2	1:53:A:GLN:HG2	12	0.2
(1,947)	1:62:A:HIS:H	1:61:A:GLN:HG3	13	0.2
(1,935)	1:15:A:TYR:HD2	1:16:A:GLU:HB2	7	0.2
(1,866)	1:36:A:LYS:H	1:35:A:ARG:HG3	3	0.2
(1,829)	1:49:A:LEU:HG	1:49:A:LEU:HA	8	0.2
(1,798)	1:28:A:GLU:H	1:27:A:ASN:HB3	11	0.2
(1,790)	1:67:A:LYS:HB2	1:64:A:HIS:HA	7	0.2
(1,755)	1:22:A:ILE:HG12	1:19:A:VAL:HA	9	0.2
(1,662)	1:64:A:HIS:H	1:64:A:HIS:HD1	1	0.2
(1,662)	1:64:A:HIS:H	1:64:A:HIS:HD1	6	0.2
(1,659)	1:68:A:HIS:HD1	1:68:A:HIS:HB2	15	0.2
(1,617)	1:26:A:HIS:H	1:23:A:VAL:HA	8	0.2
(1,563)	1:32:A:SER:H	1:32:A:SER:HA	4	0.2
(1,558)	1:35:A:ARG:H	1:35:A:ARG:HD2	14	0.2
(1,553)	1:35:A:ARG:HG3	1:35:A:ARG:HA	4	0.2
(1,553)	1:35:A:ARG:HG3	1:35:A:ARG:HA	11	0.2
(1,536)	1:31:A:LEU:HG	1:31:A:LEU:HA	2	0.2
(1,536)	1:31:A:LEU:HG	1:31:A:LEU:HA	7	0.2
(1,533)	1:31:A:LEU:H	1:31:A:LEU:HG	7	0.2
(1,489)	1:24:A:LYS:H	1:23:A:VAL:HG22	13	0.2
(1,487)	1:59:A:PHE:HD1	1:19:A:VAL:HG22	15	0.2
(1,481)	1:33:A:VAL:H	1:33:A:VAL:HB	1	0.2
(1,481)	1:33:A:VAL:H	1:33:A:VAL:HB	13	0.2
(1,373)	1:61:A:GLN:HG3	1:61:A:GLN:HA	3	0.2
(1,365)	1:61:A:GLN:H	1:60:A:LEU:HG	3	0.2
(1,308)	1:22:A:ILE:HG13	1:22:A:ILE:HA	5	0.2
(1,284)	1:21:A:ARG:HG2	1:21:A:ARG:HA	14	0.2
(1,269)	1:20:A:SER:H	1:19:A:VAL:HB	2	0.2
(1,269)	1:20:A:SER:H	1:19:A:VAL:HB	12	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,220)	1:17:A:TRP:H	1:17:A:TRP:HE3	6	0.2
(1,220)	1:17:A:TRP:H	1:17:A:TRP:HE3	7	0.2
(1,68)	1:9:A:ALA:H	1:8:A:ILE:HA	15	0.2
(1,32)	1:15:A:TYR:HE1	1:15:A:TYR:HB2	3	0.2
(1,2)	1:66:A:LEU:HD23	1:25:A:ASN:HA	3	0.2
(1,1425)	1:10:A:THR:H	1:13:A:ASP:HB2	5	0.19
(1,1425)	1:10:A:THR:H	1:13:A:ASP:HB2	8	0.19
(1,1421)	1:23:A:VAL:H	1:62:A:HIS:HD1	4	0.19
(1,1419)	1:27:A:ASN:H	1:63:A:ILE:HD12	10	0.19
(1,1417)	1:25:A:ASN:H	1:24:A:LYS:HG3	4	0.19
(1,1417)	1:25:A:ASN:H	1:24:A:LYS:HG3	8	0.19
(1,1401)	1:7:A:GLN:HG2	1:7:A:GLN:HA	1	0.19
(1,1401)	1:7:A:GLN:HG2	1:7:A:GLN:HA	2	0.19
(1,1401)	1:7:A:GLN:HG2	1:7:A:GLN:HA	10	0.19
(1,1401)	1:7:A:GLN:HG2	1:7:A:GLN:HA	15	0.19
(1,1376)	1:58:A:LEU:HD21	1:12:A:LYS:HE3	7	0.19
(1,1373)	1:22:A:ILE:HD11	1:37:A:MET:HG2	9	0.19
(1,1364)	1:59:A:PHE:HE1	1:30:A:TRP:HE3	3	0.19
(1,1359)	1:23:A:VAL:H	1:19:A:VAL:HG12	11	0.19
(1,1357)	1:26:A:HIS:H	1:26:A:HIS:HD1	13	0.19
(1,1321)	1:64:A:HIS:HD1	1:65:A:ARG:HB3	2	0.19
(1,1315)	1:18:A:LEU:HG	1:42:A:GLU:HG3	11	0.19
(1,1274)	1:17:A:TRP:HE3	1:18:A:LEU:HA	5	0.19
(1,1274)	1:17:A:TRP:HE3	1:18:A:LEU:HA	6	0.19
(1,1219)	1:56:A:LYS:HB2	1:53:A:GLN:HA	6	0.19
(1,1215)	1:30:A:TRP:HE1	1:56:A:LYS:HB3	9	0.19
(1,1187)	1:59:A:PHE:HE2	1:60:A:LEU:HD13	4	0.19
(1,1175)	1:26:A:HIS:HE1	1:27:A:ASN:HD22	15	0.19
(1,1166)	1:36:A:LYS:HB3	1:33:A:VAL:HA	9	0.19
(1,1166)	1:36:A:LYS:HB3	1:33:A:VAL:HA	10	0.19
(1,1166)	1:36:A:LYS:HB3	1:33:A:VAL:HA	13	0.19
(1,1166)	1:36:A:LYS:HB3	1:33:A:VAL:HA	15	0.19
(1,1127)	1:18:A:LEU:HG	1:43:A:TYR:HB3	8	0.19
(1,1127)	1:18:A:LEU:HG	1:43:A:TYR:HB3	14	0.19
(1,1124)	1:15:A:TYR:HD2	1:55:A:ALA:HA	11	0.19
(1,1101)	1:30:A:TRP:HD1	1:56:A:LYS:HD3	4	0.19
(1,1078)	1:39:A:ALA:H	1:38:A:GLN:HB2	4	0.19
(1,1078)	1:39:A:ALA:H	1:38:A:GLN:HB2	9	0.19
(1,958)	1:53:A:GLN:HB2	1:53:A:GLN:HG2	4	0.19
(1,946)	1:62:A:HIS:H	1:61:A:GLN:HG2	15	0.19
(1,866)	1:36:A:LYS:H	1:35:A:ARG:HG3	1	0.19
(1,866)	1:36:A:LYS:H	1:35:A:ARG:HG3	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,865)	1:21:A:ARG:HG3	1:21:A:ARG:HB3	1	0.19
(1,865)	1:21:A:ARG:HG3	1:21:A:ARG:HB3	2	0.19
(1,865)	1:21:A:ARG:HG3	1:21:A:ARG:HB3	4	0.19
(1,865)	1:21:A:ARG:HG3	1:21:A:ARG:HB3	5	0.19
(1,865)	1:21:A:ARG:HG3	1:21:A:ARG:HB3	7	0.19
(1,865)	1:21:A:ARG:HG3	1:21:A:ARG:HB3	8	0.19
(1,865)	1:21:A:ARG:HG3	1:21:A:ARG:HB3	9	0.19
(1,865)	1:21:A:ARG:HG3	1:21:A:ARG:HB3	10	0.19
(1,865)	1:21:A:ARG:HG3	1:21:A:ARG:HB3	11	0.19
(1,865)	1:21:A:ARG:HG3	1:21:A:ARG:HB3	12	0.19
(1,865)	1:21:A:ARG:HG3	1:21:A:ARG:HB3	13	0.19
(1,840)	1:32:A:SER:H	1:31:A:LEU:HG	9	0.19
(1,783)	1:64:A:HIS:H	1:61:A:GLN:HA	12	0.19
(1,755)	1:22:A:ILE:HG12	1:19:A:VAL:HA	13	0.19
(1,662)	1:64:A:HIS:H	1:64:A:HIS:HD1	3	0.19
(1,660)	1:68:A:HIS:HD1	1:68:A:HIS:HB3	7	0.19
(1,644)	1:18:A:LEU:HD13	1:18:A:LEU:HB2	10	0.19
(1,617)	1:26:A:HIS:H	1:23:A:VAL:HA	2	0.19
(1,553)	1:35:A:ARG:HG3	1:35:A:ARG:HA	6	0.19
(1,536)	1:31:A:LEU:HG	1:31:A:LEU:HA	3	0.19
(1,536)	1:31:A:LEU:HG	1:31:A:LEU:HA	8	0.19
(1,536)	1:31:A:LEU:HG	1:31:A:LEU:HA	11	0.19
(1,536)	1:31:A:LEU:HG	1:31:A:LEU:HA	12	0.19
(1,536)	1:31:A:LEU:HG	1:31:A:LEU:HA	13	0.19
(1,536)	1:31:A:LEU:HG	1:31:A:LEU:HA	14	0.19
(1,533)	1:31:A:LEU:H	1:31:A:LEU:HG	1	0.19
(1,533)	1:31:A:LEU:H	1:31:A:LEU:HG	8	0.19
(1,494)	1:67:A:LYS:H	1:67:A:LYS:HG3	12	0.19
(1,489)	1:24:A:LYS:H	1:23:A:VAL:HG23	14	0.19
(1,481)	1:33:A:VAL:H	1:33:A:VAL:HB	3	0.19
(1,467)	1:54:A:LYS:H	1:53:A:GLN:HG2	4	0.19
(1,466)	1:53:A:GLN:H	1:53:A:GLN:HB2	2	0.19
(1,466)	1:53:A:GLN:H	1:53:A:GLN:HB2	9	0.19
(1,441)	1:69:A:GLU:H	1:69:A:GLU:HB3	8	0.19
(1,422)	1:66:A:LEU:H	1:66:A:LEU:HD11	7	0.19
(1,403)	1:65:A:ARG:HG2	1:65:A:ARG:HA	12	0.19
(1,365)	1:61:A:GLN:H	1:60:A:LEU:HG	7	0.19
(1,365)	1:61:A:GLN:H	1:60:A:LEU:HG	10	0.19
(1,365)	1:61:A:GLN:H	1:60:A:LEU:HG	13	0.19
(1,334)	1:57:A:LYS:H	1:56:A:LYS:HB2	3	0.19
(1,334)	1:57:A:LYS:H	1:56:A:LYS:HB2	6	0.19
(1,334)	1:57:A:LYS:H	1:56:A:LYS:HB2	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,284)	1:21:A:ARG:HG2	1:21:A:ARG:HA	13	0.19
(1,220)	1:17:A:TRP:H	1:17:A:TRP:HE3	10	0.19
(1,32)	1:15:A:TYR:HE1	1:15:A:TYR:HB2	5	0.19
(1,26)	1:10:A:THR:HA	1:10:A:THR:HB	6	0.19
(1,1426)	1:68:A:HIS:HD1	1:64:A:HIS:HB2	7	0.18
(1,1425)	1:10:A:THR:H	1:13:A:ASP:HB2	14	0.18
(1,1359)	1:23:A:VAL:H	1:19:A:VAL:HG11	10	0.18
(1,1331)	1:23:A:VAL:H	1:33:A:VAL:HB	5	0.18
(1,1331)	1:23:A:VAL:H	1:33:A:VAL:HB	6	0.18
(1,1282)	1:21:A:ARG:HG3	1:18:A:LEU:HA	6	0.18
(1,1274)	1:17:A:TRP:HE3	1:18:A:LEU:HA	1	0.18
(1,1274)	1:17:A:TRP:HE3	1:18:A:LEU:HA	3	0.18
(1,1274)	1:17:A:TRP:HE3	1:18:A:LEU:HA	8	0.18
(1,1232)	1:17:A:TRP:HE1	1:21:A:ARG:HG2	4	0.18
(1,1232)	1:17:A:TRP:HE1	1:21:A:ARG:HG2	8	0.18
(1,1229)	1:58:A:LEU:HG	1:55:A:ALA:HA	9	0.18
(1,1183)	1:69:A:GLU:H	1:68:A:HIS:H	3	0.18
(1,1166)	1:36:A:LYS:HB3	1:33:A:VAL:HA	3	0.18
(1,1166)	1:36:A:LYS:HB3	1:33:A:VAL:HA	5	0.18
(1,1166)	1:36:A:LYS:HB3	1:33:A:VAL:HA	7	0.18
(1,1127)	1:18:A:LEU:HG	1:43:A:TYR:HB3	11	0.18
(1,1124)	1:15:A:TYR:HD2	1:55:A:ALA:HA	13	0.18
(1,1107)	1:43:A:TYR:HE1	1:34:A:SER:HB2	11	0.18
(1,1104)	1:30:A:TRP:HD1	1:31:A:LEU:HD21	4	0.18
(1,1101)	1:30:A:TRP:HD1	1:56:A:LYS:HD3	5	0.18
(1,1095)	1:59:A:PHE:HD2	1:30:A:TRP:HA	3	0.18
(1,1050)	1:54:A:LYS:HG3	1:54:A:LYS:HA	15	0.18
(1,1047)	1:55:A:ALA:H	1:54:A:LYS:HG2	5	0.18
(1,1025)	1:36:A:LYS:HG3	1:36:A:LYS:HA	6	0.18
(1,1025)	1:36:A:LYS:HG3	1:36:A:LYS:HA	7	0.18
(1,886)	1:65:A:ARG:HD3	1:65:A:ARG:HA	6	0.18
(1,867)	1:36:A:LYS:H	1:35:A:ARG:HD2	6	0.18
(1,865)	1:21:A:ARG:HG3	1:21:A:ARG:HB3	3	0.18
(1,865)	1:21:A:ARG:HG3	1:21:A:ARG:HB3	6	0.18
(1,865)	1:21:A:ARG:HG3	1:21:A:ARG:HB3	14	0.18
(1,865)	1:21:A:ARG:HG3	1:21:A:ARG:HB3	15	0.18
(1,840)	1:32:A:SER:H	1:31:A:LEU:HG	7	0.18
(1,798)	1:28:A:GLU:H	1:27:A:ASN:HB3	12	0.18
(1,795)	1:59:A:PHE:HE1	1:59:A:PHE:HB2	6	0.18
(1,783)	1:64:A:HIS:H	1:61:A:GLN:HA	4	0.18
(1,762)	1:35:A:ARG:HD2	1:32:A:SER:HA	2	0.18
(1,681)	1:15:A:TYR:HE2	1:58:A:LEU:HB2	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,681)	1:15:A:TYR:HE2	1:58:A:LEU:HB2	9	0.18
(1,651)	1:21:A:ARG:HB2	1:18:A:LEU:HA	6	0.18
(1,651)	1:21:A:ARG:HB2	1:18:A:LEU:HA	7	0.18
(1,646)	1:19:A:VAL:H	1:18:A:LEU:HG	14	0.18
(1,646)	1:19:A:VAL:H	1:18:A:LEU:HG	15	0.18
(1,629)	1:16:A:GLU:H	1:16:A:GLU:HG2	5	0.18
(1,627)	1:16:A:GLU:HG3	1:16:A:GLU:HA	11	0.18
(1,563)	1:32:A:SER:H	1:32:A:SER:HA	6	0.18
(1,536)	1:31:A:LEU:HG	1:31:A:LEU:HA	1	0.18
(1,536)	1:31:A:LEU:HG	1:31:A:LEU:HA	5	0.18
(1,536)	1:31:A:LEU:HG	1:31:A:LEU:HA	6	0.18
(1,533)	1:31:A:LEU:H	1:31:A:LEU:HG	2	0.18
(1,533)	1:31:A:LEU:H	1:31:A:LEU:HG	9	0.18
(1,533)	1:31:A:LEU:H	1:31:A:LEU:HG	14	0.18
(1,486)	1:43:A:TYR:HE2	1:47:A:VAL:HG23	10	0.18
(1,471)	1:42:A:GLU:H	1:41:A:PRO:HB3	4	0.18
(1,432)	1:68:A:HIS:H	1:68:A:HIS:HB2	12	0.18
(1,365)	1:61:A:GLN:H	1:60:A:LEU:HG	14	0.18
(1,251)	1:46:A:TYR:HE1	1:46:A:TYR:HE2	3	0.18
(1,251)	1:46:A:TYR:HE1	1:46:A:TYR:HE2	4	0.18
(1,251)	1:46:A:TYR:HE1	1:46:A:TYR:HE2	5	0.18
(1,251)	1:46:A:TYR:HE1	1:46:A:TYR:HE2	6	0.18
(1,251)	1:46:A:TYR:HE1	1:46:A:TYR:HE2	7	0.18
(1,251)	1:46:A:TYR:HE1	1:46:A:TYR:HE2	9	0.18
(1,251)	1:46:A:TYR:HE1	1:46:A:TYR:HE2	12	0.18
(1,251)	1:46:A:TYR:HE1	1:46:A:TYR:HE2	14	0.18
(1,251)	1:46:A:TYR:HE1	1:46:A:TYR:HE2	15	0.18
(1,68)	1:9:A:ALA:H	1:8:A:ILE:HA	8	0.18
(1,68)	1:9:A:ALA:H	1:8:A:ILE:HA	9	0.18
(1,68)	1:9:A:ALA:H	1:8:A:ILE:HA	10	0.18
(1,32)	1:15:A:TYR:HE1	1:15:A:TYR:HB2	9	0.18
(1,32)	1:15:A:TYR:HE1	1:15:A:TYR:HB2	12	0.18
(1,20)	1:67:A:LYS:HG2	1:26:A:HIS:HB2	8	0.18
(1,1425)	1:10:A:THR:H	1:13:A:ASP:HB2	7	0.17
(1,1425)	1:10:A:THR:H	1:13:A:ASP:HB2	9	0.17
(1,1425)	1:10:A:THR:H	1:13:A:ASP:HB2	10	0.17
(1,1421)	1:23:A:VAL:H	1:62:A:HIS:HD1	9	0.17
(1,1421)	1:23:A:VAL:H	1:62:A:HIS:HD1	10	0.17
(1,1417)	1:25:A:ASN:H	1:24:A:LYS:HG3	13	0.17
(1,1401)	1:7:A:GLN:HG2	1:7:A:GLN:HA	12	0.17
(1,1389)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	5	0.17
(1,1387)	1:68:A:HIS:HD1	1:67:A:LYS:HE2	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1373)	1:22:A:ILE:HD13	1:37:A:MET:HG2	1	0.17
(1,1357)	1:26:A:HIS:H	1:26:A:HIS:HD1	10	0.17
(1,1349)	1:22:A:ILE:H	1:23:A:VAL:HB	13	0.17
(1,1345)	1:64:A:HIS:HE1	1:68:A:HIS:HD1	8	0.17
(1,1337)	1:30:A:TRP:HD1	1:31:A:LEU:HG	7	0.17
(1,1337)	1:30:A:TRP:HD1	1:31:A:LEU:HG	8	0.17
(1,1327)	1:64:A:HIS:HD1	1:69:A:GLU:HG2	7	0.17
(1,1327)	1:64:A:HIS:HD1	1:69:A:GLU:HG2	8	0.17
(1,1327)	1:64:A:HIS:HD1	1:69:A:GLU:HG2	12	0.17
(1,1327)	1:64:A:HIS:HD1	1:69:A:GLU:HG2	13	0.17
(1,1291)	1:57:A:LYS:HB2	1:54:A:LYS:HA	3	0.17
(1,1282)	1:21:A:ARG:HG3	1:18:A:LEU:HA	1	0.17
(1,1274)	1:17:A:TRP:HE3	1:18:A:LEU:HA	12	0.17
(1,1244)	1:26:A:HIS:HE1	1:67:A:LYS:HB2	8	0.17
(1,1187)	1:59:A:PHE:HE2	1:60:A:LEU:HD13	2	0.17
(1,1127)	1:18:A:LEU:HG	1:43:A:TYR:HB3	7	0.17
(1,1107)	1:43:A:TYR:HE1	1:34:A:SER:HB2	2	0.17
(1,1101)	1:30:A:TRP:HD1	1:56:A:LYS:HD3	8	0.17
(1,1095)	1:59:A:PHE:HD2	1:30:A:TRP:HA	14	0.17
(1,1047)	1:55:A:ALA:H	1:54:A:LYS:HG2	9	0.17
(1,1047)	1:55:A:ALA:H	1:54:A:LYS:HG2	11	0.17
(1,1025)	1:36:A:LYS:HG3	1:36:A:LYS:HA	10	0.17
(1,1025)	1:36:A:LYS:HG3	1:36:A:LYS:HA	11	0.17
(1,926)	1:51:A:GLY:H	1:50:A:GLU:HG3	8	0.17
(1,905)	1:41:A:PRO:HG2	1:41:A:PRO:HA	4	0.17
(1,901)	1:40:A:SER:H	1:41:A:PRO:HD2	4	0.17
(1,901)	1:40:A:SER:H	1:41:A:PRO:HD2	6	0.17
(1,887)	1:65:A:ARG:HD2	1:65:A:ARG:HA	6	0.17
(1,884)	1:65:A:ARG:H	1:65:A:ARG:HD2	12	0.17
(1,858)	1:22:A:ILE:H	1:21:A:ARG:HG3	13	0.17
(1,834)	1:49:A:LEU:HD12	1:49:A:LEU:HB2	3	0.17
(1,798)	1:28:A:GLU:H	1:27:A:ASN:HB3	5	0.17
(1,795)	1:59:A:PHE:HE1	1:59:A:PHE:HB2	11	0.17
(1,783)	1:64:A:HIS:H	1:61:A:GLN:HA	14	0.17
(1,763)	1:35:A:ARG:HG2	1:32:A:SER:HA	10	0.17
(1,762)	1:35:A:ARG:HD2	1:32:A:SER:HA	4	0.17
(1,703)	1:48:A:TYR:HD2	1:49:A:LEU:HB2	11	0.17
(1,681)	1:15:A:TYR:HE2	1:58:A:LEU:HB2	4	0.17
(1,681)	1:15:A:TYR:HE2	1:58:A:LEU:HB2	7	0.17
(1,660)	1:68:A:HIS:HD1	1:68:A:HIS:HB3	8	0.17
(1,659)	1:68:A:HIS:HD1	1:68:A:HIS:HB2	7	0.17
(1,617)	1:26:A:HIS:H	1:23:A:VAL:HA	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,617)	1:26:A:HIS:H	1:23:A:VAL:HA	10	0.17
(1,563)	1:32:A:SER:H	1:32:A:SER:HA	10	0.17
(1,563)	1:32:A:SER:H	1:32:A:SER:HA	11	0.17
(1,563)	1:32:A:SER:H	1:32:A:SER:HA	15	0.17
(1,536)	1:31:A:LEU:HG	1:31:A:LEU:HA	9	0.17
(1,536)	1:31:A:LEU:HG	1:31:A:LEU:HA	10	0.17
(1,536)	1:31:A:LEU:HG	1:31:A:LEU:HA	15	0.17
(1,533)	1:31:A:LEU:H	1:31:A:LEU:HG	5	0.17
(1,533)	1:31:A:LEU:H	1:31:A:LEU:HG	13	0.17
(1,533)	1:31:A:LEU:H	1:31:A:LEU:HG	15	0.17
(1,467)	1:54:A:LYS:H	1:53:A:GLN:HG2	11	0.17
(1,467)	1:54:A:LYS:H	1:53:A:GLN:HG2	12	0.17
(1,437)	1:69:A:GLU:HB2	1:69:A:GLU:HA	3	0.17
(1,434)	1:69:A:GLU:H	1:68:A:HIS:HB3	10	0.17
(1,434)	1:69:A:GLU:H	1:68:A:HIS:HB3	13	0.17
(1,403)	1:65:A:ARG:HG2	1:65:A:ARG:HA	3	0.17
(1,391)	1:64:A:HIS:H	1:63:A:ILE:HA	1	0.17
(1,391)	1:64:A:HIS:H	1:63:A:ILE:HA	4	0.17
(1,391)	1:64:A:HIS:H	1:63:A:ILE:HA	6	0.17
(1,391)	1:64:A:HIS:H	1:63:A:ILE:HA	8	0.17
(1,365)	1:61:A:GLN:H	1:60:A:LEU:HG	5	0.17
(1,365)	1:61:A:GLN:H	1:60:A:LEU:HG	11	0.17
(1,251)	1:46:A:TYR:HE1	1:46:A:TYR:HE2	1	0.17
(1,251)	1:46:A:TYR:HE1	1:46:A:TYR:HE2	2	0.17
(1,251)	1:46:A:TYR:HE1	1:46:A:TYR:HE2	8	0.17
(1,251)	1:46:A:TYR:HE1	1:46:A:TYR:HE2	10	0.17
(1,251)	1:46:A:TYR:HE1	1:46:A:TYR:HE2	11	0.17
(1,251)	1:46:A:TYR:HE1	1:46:A:TYR:HE2	13	0.17
(1,227)	1:48:A:TYR:HD1	1:48:A:TYR:HA	12	0.17
(1,220)	1:17:A:TRP:H	1:17:A:TRP:HE3	4	0.17
(1,218)	1:17:A:TRP:HE3	1:17:A:TRP:HB2	6	0.17
(1,218)	1:17:A:TRP:HE3	1:17:A:TRP:HB2	11	0.17
(1,217)	1:17:A:TRP:HH2	1:17:A:TRP:HZ3	1	0.17
(1,217)	1:17:A:TRP:HH2	1:17:A:TRP:HZ3	4	0.17
(1,217)	1:17:A:TRP:HH2	1:17:A:TRP:HZ3	6	0.17
(1,217)	1:17:A:TRP:HH2	1:17:A:TRP:HZ3	8	0.17
(1,217)	1:17:A:TRP:HH2	1:17:A:TRP:HZ3	14	0.17
(1,69)	1:10:A:THR:H	1:9:A:ALA:HA	1	0.17
(1,69)	1:10:A:THR:H	1:9:A:ALA:HA	6	0.17
(1,69)	1:10:A:THR:H	1:9:A:ALA:HA	7	0.17
(1,69)	1:10:A:THR:H	1:9:A:ALA:HA	10	0.17
(1,69)	1:10:A:THR:H	1:9:A:ALA:HA	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:10:A:THR:H	1:9:A:ALA:HA	12	0.17
(1,68)	1:9:A:ALA:H	1:8:A:ILE:HA	4	0.17
(1,32)	1:15:A:TYR:HE1	1:15:A:TYR:HB2	1	0.17
(1,32)	1:15:A:TYR:HE1	1:15:A:TYR:HB2	7	0.17
(1,24)	1:63:A:ILE:HD11	1:26:A:HIS:HB3	2	0.17
(1,24)	1:63:A:ILE:HD11	1:26:A:HIS:HB3	15	0.17
(1,2)	1:66:A:LEU:HD21	1:25:A:ASN:HA	9	0.17
(1,2)	1:66:A:LEU:HD21	1:25:A:ASN:HA	11	0.17
(3,20)	1:18:A:LEU:O	1:22:A:ILE:H	11	0.16
(1,1426)	1:68:A:HIS:HD1	1:64:A:HIS:HB2	3	0.16
(1,1425)	1:10:A:THR:H	1:13:A:ASP:HB2	4	0.16
(1,1406)	1:8:A:ILE:HD12	1:5:A:SER:HB2	14	0.16
(1,1357)	1:26:A:HIS:H	1:26:A:HIS:HD1	9	0.16
(1,1355)	1:62:A:HIS:HD1	1:63:A:ILE:HG12	1	0.16
(1,1354)	1:62:A:HIS:HD1	1:63:A:ILE:HA	13	0.16
(1,1351)	1:59:A:PHE:HZ	1:28:A:GLU:HB3	15	0.16
(1,1349)	1:22:A:ILE:H	1:23:A:VAL:HB	12	0.16
(1,1338)	1:64:A:HIS:H	1:62:A:HIS:HA	1	0.16
(1,1338)	1:64:A:HIS:H	1:62:A:HIS:HA	3	0.16
(1,1330)	1:17:A:TRP:HZ3	1:14:A:LYS:HG2	4	0.16
(1,1274)	1:17:A:TRP:HE3	1:18:A:LEU:HA	14	0.16
(1,1241)	1:63:A:ILE:HG22	1:26:A:HIS:HB3	2	0.16
(1,1187)	1:59:A:PHE:HE2	1:60:A:LEU:HD12	5	0.16
(1,1183)	1:69:A:GLU:H	1:68:A:HIS:H	8	0.16
(1,1183)	1:69:A:GLU:H	1:68:A:HIS:H	15	0.16
(1,1175)	1:26:A:HIS:HE1	1:27:A:ASN:HD22	7	0.16
(1,1166)	1:36:A:LYS:HB3	1:33:A:VAL:HA	12	0.16
(1,1155)	1:19:A:VAL:HG21	1:62:A:HIS:HB3	1	0.16
(1,1117)	1:30:A:TRP:HE3	1:33:A:VAL:HB	11	0.16
(1,1095)	1:59:A:PHE:HD2	1:30:A:TRP:HA	13	0.16
(1,1078)	1:39:A:ALA:H	1:38:A:GLN:HB2	3	0.16
(1,1050)	1:54:A:LYS:HG3	1:54:A:LYS:HA	2	0.16
(1,1047)	1:55:A:ALA:H	1:54:A:LYS:HG2	10	0.16
(1,1017)	1:57:A:LYS:HG3	1:57:A:LYS:HE2	4	0.16
(1,1004)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	5	0.16
(1,954)	1:53:A:GLN:HG2	1:53:A:GLN:HA	11	0.16
(1,885)	1:65:A:ARG:H	1:65:A:ARG:HD3	7	0.16
(1,873)	1:66:A:LEU:H	1:65:A:ARG:HG2	4	0.16
(1,834)	1:49:A:LEU:HD13	1:49:A:LEU:HB2	4	0.16
(1,834)	1:49:A:LEU:HD11	1:49:A:LEU:HB2	7	0.16
(1,834)	1:49:A:LEU:HD12	1:49:A:LEU:HB2	9	0.16
(1,834)	1:49:A:LEU:HD12	1:49:A:LEU:HB2	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,834)	1:49:A:LEU:HD11	1:49:A:LEU:HB2	13	0.16
(1,795)	1:59:A:PHE:HE1	1:59:A:PHE:HB2	12	0.16
(1,790)	1:67:A:LYS:HB2	1:64:A:HIS:HA	2	0.16
(1,703)	1:48:A:TYR:HD2	1:49:A:LEU:HB2	3	0.16
(1,681)	1:15:A:TYR:HE2	1:58:A:LEU:HB2	13	0.16
(1,681)	1:15:A:TYR:HE2	1:58:A:LEU:HB2	15	0.16
(1,660)	1:68:A:HIS:HD1	1:68:A:HIS:HB3	4	0.16
(1,646)	1:19:A:VAL:H	1:18:A:LEU:HG	1	0.16
(1,617)	1:26:A:HIS:H	1:23:A:VAL:HA	3	0.16
(1,563)	1:32:A:SER:H	1:32:A:SER:HA	3	0.16
(1,563)	1:32:A:SER:H	1:32:A:SER:HA	9	0.16
(1,563)	1:32:A:SER:H	1:32:A:SER:HA	13	0.16
(1,563)	1:32:A:SER:H	1:32:A:SER:HA	14	0.16
(1,533)	1:31:A:LEU:H	1:31:A:LEU:HG	3	0.16
(1,533)	1:31:A:LEU:H	1:31:A:LEU:HG	12	0.16
(1,487)	1:59:A:PHE:HD1	1:19:A:VAL:HG21	14	0.16
(1,471)	1:42:A:GLU:H	1:41:A:PRO:HB3	5	0.16
(1,441)	1:69:A:GLU:H	1:69:A:GLU:HB3	15	0.16
(1,391)	1:64:A:HIS:H	1:63:A:ILE:HA	3	0.16
(1,391)	1:64:A:HIS:H	1:63:A:ILE:HA	11	0.16
(1,391)	1:64:A:HIS:H	1:63:A:ILE:HA	13	0.16
(1,391)	1:64:A:HIS:H	1:63:A:ILE:HA	14	0.16
(1,369)	1:61:A:GLN:H	1:61:A:GLN:HB2	7	0.16
(1,365)	1:61:A:GLN:H	1:60:A:LEU:HG	9	0.16
(1,334)	1:57:A:LYS:H	1:56:A:LYS:HB2	13	0.16
(1,284)	1:21:A:ARG:HG2	1:21:A:ARG:HA	15	0.16
(1,227)	1:48:A:TYR:HD1	1:48:A:TYR:HA	5	0.16
(1,218)	1:17:A:TRP:HE3	1:17:A:TRP:HB2	10	0.16
(1,217)	1:17:A:TRP:HH2	1:17:A:TRP:HZ3	2	0.16
(1,217)	1:17:A:TRP:HH2	1:17:A:TRP:HZ3	3	0.16
(1,217)	1:17:A:TRP:HH2	1:17:A:TRP:HZ3	5	0.16
(1,217)	1:17:A:TRP:HH2	1:17:A:TRP:HZ3	7	0.16
(1,217)	1:17:A:TRP:HH2	1:17:A:TRP:HZ3	9	0.16
(1,217)	1:17:A:TRP:HH2	1:17:A:TRP:HZ3	10	0.16
(1,217)	1:17:A:TRP:HH2	1:17:A:TRP:HZ3	11	0.16
(1,217)	1:17:A:TRP:HH2	1:17:A:TRP:HZ3	12	0.16
(1,217)	1:17:A:TRP:HH2	1:17:A:TRP:HZ3	13	0.16
(1,217)	1:17:A:TRP:HH2	1:17:A:TRP:HZ3	15	0.16
(1,214)	1:17:A:TRP:HE1	1:17:A:TRP:HZ2	4	0.16
(1,214)	1:17:A:TRP:HE1	1:17:A:TRP:HZ2	8	0.16
(1,69)	1:10:A:THR:H	1:9:A:ALA:HA	2	0.16
(1,69)	1:10:A:THR:H	1:9:A:ALA:HA	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:10:A:THR:H	1:9:A:ALA:HA	5	0.16
(1,69)	1:10:A:THR:H	1:9:A:ALA:HA	14	0.16
(1,68)	1:9:A:ALA:H	1:8:A:ILE:HA	1	0.16
(1,68)	1:9:A:ALA:H	1:8:A:ILE:HA	6	0.16
(1,32)	1:15:A:TYR:HE1	1:15:A:TYR:HB2	2	0.16
(1,32)	1:15:A:TYR:HE1	1:15:A:TYR:HB2	6	0.16
(1,26)	1:10:A:THR:HA	1:10:A:THR:HB	1	0.16
(1,12)	1:26:A:HIS:HD1	1:67:A:LYS:HB2	4	0.16
(3,20)	1:18:A:LEU:O	1:22:A:ILE:H	10	0.15
(3,10)	1:13:A:ASP:O	1:17:A:TRP:H	3	0.15
(1,1423)	1:26:A:HIS:HD1	1:66:A:LEU:HA	4	0.15
(1,1423)	1:26:A:HIS:HD1	1:66:A:LEU:HA	6	0.15
(1,1423)	1:26:A:HIS:HD1	1:66:A:LEU:HA	11	0.15
(1,1421)	1:23:A:VAL:H	1:62:A:HIS:HD1	2	0.15
(1,1417)	1:25:A:ASN:H	1:24:A:LYS:HG3	1	0.15
(1,1407)	1:8:A:ILE:HD11	1:5:A:SER:HA	4	0.15
(1,1389)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	4	0.15
(1,1354)	1:62:A:HIS:HD1	1:63:A:ILE:HA	9	0.15
(1,1349)	1:22:A:ILE:H	1:23:A:VAL:HB	3	0.15
(1,1296)	1:60:A:LEU:HG	1:57:A:LYS:HA	2	0.15
(1,1296)	1:60:A:LEU:HG	1:57:A:LYS:HA	14	0.15
(1,1286)	1:36:A:LYS:HG2	1:33:A:VAL:HA	8	0.15
(1,1282)	1:21:A:ARG:HG3	1:18:A:LEU:HA	4	0.15
(1,1276)	1:17:A:TRP:HZ3	1:18:A:LEU:HA	4	0.15
(1,1187)	1:59:A:PHE:HE2	1:60:A:LEU:HD12	8	0.15
(1,1180)	1:7:A:GLN:HE22	1:7:A:GLN:HG3	6	0.15
(1,1134)	1:30:A:TRP:HZ3	1:30:A:TRP:HA	9	0.15
(1,1117)	1:30:A:TRP:HE3	1:33:A:VAL:HB	6	0.15
(1,1101)	1:30:A:TRP:HD1	1:56:A:LYS:HD3	13	0.15
(1,1098)	1:30:A:TRP:HD1	1:56:A:LYS:HG2	5	0.15
(1,1087)	1:56:A:LYS:H	1:53:A:GLN:HA	6	0.15
(1,1078)	1:39:A:ALA:H	1:38:A:GLN:HB2	5	0.15
(1,1047)	1:55:A:ALA:H	1:54:A:LYS:HG2	4	0.15
(1,1047)	1:55:A:ALA:H	1:54:A:LYS:HG2	14	0.15
(1,1017)	1:57:A:LYS:HG3	1:57:A:LYS:HE2	13	0.15
(1,1007)	1:57:A:LYS:H	1:57:A:LYS:HE2	4	0.15
(1,946)	1:62:A:HIS:H	1:61:A:GLN:HG2	13	0.15
(1,935)	1:15:A:TYR:HD2	1:16:A:GLU:HB2	5	0.15
(1,914)	1:41:A:PRO:HG3	1:41:A:PRO:HB2	4	0.15
(1,834)	1:49:A:LEU:HD11	1:49:A:LEU:HB2	2	0.15
(1,834)	1:49:A:LEU:HD11	1:49:A:LEU:HB2	5	0.15
(1,834)	1:49:A:LEU:HD13	1:49:A:LEU:HB2	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,834)	1:49:A:LEU:HD12	1:49:A:LEU:HB2	14	0.15
(1,811)	1:66:A:LEU:H	1:66:A:LEU:HD22	2	0.15
(1,811)	1:66:A:LEU:H	1:66:A:LEU:HD21	6	0.15
(1,795)	1:59:A:PHE:HE1	1:59:A:PHE:HB2	13	0.15
(1,762)	1:35:A:ARG:HD2	1:32:A:SER:HA	8	0.15
(1,755)	1:22:A:ILE:HG12	1:19:A:VAL:HA	14	0.15
(1,703)	1:48:A:TYR:HD2	1:49:A:LEU:HB2	10	0.15
(1,681)	1:15:A:TYR:HE2	1:58:A:LEU:HB2	6	0.15
(1,681)	1:15:A:TYR:HE2	1:58:A:LEU:HB2	11	0.15
(1,660)	1:68:A:HIS:HD1	1:68:A:HIS:HB3	15	0.15
(1,659)	1:68:A:HIS:HD1	1:68:A:HIS:HB2	2	0.15
(1,651)	1:21:A:ARG:HB2	1:18:A:LEU:HA	3	0.15
(1,646)	1:19:A:VAL:H	1:18:A:LEU:HG	6	0.15
(1,646)	1:19:A:VAL:H	1:18:A:LEU:HG	7	0.15
(1,646)	1:19:A:VAL:H	1:18:A:LEU:HG	9	0.15
(1,617)	1:26:A:HIS:H	1:23:A:VAL:HA	12	0.15
(1,604)	1:29:A:ASN:H	1:28:A:GLU:HG3	9	0.15
(1,602)	1:28:A:GLU:HG3	1:28:A:GLU:HA	15	0.15
(1,563)	1:32:A:SER:H	1:32:A:SER:HA	1	0.15
(1,563)	1:32:A:SER:H	1:32:A:SER:HA	7	0.15
(1,563)	1:32:A:SER:H	1:32:A:SER:HA	8	0.15
(1,533)	1:31:A:LEU:H	1:31:A:LEU:HG	6	0.15
(1,533)	1:31:A:LEU:H	1:31:A:LEU:HG	10	0.15
(1,533)	1:31:A:LEU:H	1:31:A:LEU:HG	11	0.15
(1,489)	1:24:A:LYS:H	1:23:A:VAL:HG22	6	0.15
(1,467)	1:54:A:LYS:H	1:53:A:GLN:HG2	8	0.15
(1,449)	1:50:A:GLU:H	1:49:A:LEU:HD22	5	0.15
(1,434)	1:69:A:GLU:H	1:68:A:HIS:HB3	7	0.15
(1,434)	1:69:A:GLU:H	1:68:A:HIS:HB3	11	0.15
(1,391)	1:64:A:HIS:H	1:63:A:ILE:HA	5	0.15
(1,391)	1:64:A:HIS:H	1:63:A:ILE:HA	7	0.15
(1,391)	1:64:A:HIS:H	1:63:A:ILE:HA	9	0.15
(1,391)	1:64:A:HIS:H	1:63:A:ILE:HA	10	0.15
(1,391)	1:64:A:HIS:H	1:63:A:ILE:HA	12	0.15
(1,391)	1:64:A:HIS:H	1:63:A:ILE:HA	15	0.15
(1,312)	1:40:A:SER:H	1:40:A:SER:HB3	8	0.15
(1,237)	1:43:A:TYR:HD2	1:43:A:TYR:HA	13	0.15
(1,227)	1:48:A:TYR:HD1	1:48:A:TYR:HA	4	0.15
(1,227)	1:48:A:TYR:HD1	1:48:A:TYR:HA	11	0.15
(1,227)	1:48:A:TYR:HD1	1:48:A:TYR:HA	15	0.15
(1,218)	1:17:A:TRP:HE3	1:17:A:TRP:HB2	3	0.15
(1,218)	1:17:A:TRP:HE3	1:17:A:TRP:HB2	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	1:17:A:TRP:HE3	1:17:A:TRP:HB2	9	0.15
(1,214)	1:17:A:TRP:HE1	1:17:A:TRP:HZ2	1	0.15
(1,214)	1:17:A:TRP:HE1	1:17:A:TRP:HZ2	2	0.15
(1,214)	1:17:A:TRP:HE1	1:17:A:TRP:HZ2	5	0.15
(1,214)	1:17:A:TRP:HE1	1:17:A:TRP:HZ2	9	0.15
(1,214)	1:17:A:TRP:HE1	1:17:A:TRP:HZ2	10	0.15
(1,214)	1:17:A:TRP:HE1	1:17:A:TRP:HZ2	11	0.15
(1,214)	1:17:A:TRP:HE1	1:17:A:TRP:HZ2	12	0.15
(1,214)	1:17:A:TRP:HE1	1:17:A:TRP:HZ2	14	0.15
(1,214)	1:17:A:TRP:HE1	1:17:A:TRP:HZ2	15	0.15
(1,163)	1:46:A:TYR:H	1:45:A:ASP:HA	1	0.15
(1,163)	1:46:A:TYR:H	1:45:A:ASP:HA	4	0.15
(1,163)	1:46:A:TYR:H	1:45:A:ASP:HA	6	0.15
(1,163)	1:46:A:TYR:H	1:45:A:ASP:HA	7	0.15
(1,163)	1:46:A:TYR:H	1:45:A:ASP:HA	10	0.15
(1,163)	1:46:A:TYR:H	1:45:A:ASP:HA	11	0.15
(1,163)	1:46:A:TYR:H	1:45:A:ASP:HA	14	0.15
(1,69)	1:10:A:THR:H	1:9:A:ALA:HA	3	0.15
(1,69)	1:10:A:THR:H	1:9:A:ALA:HA	8	0.15
(1,69)	1:10:A:THR:H	1:9:A:ALA:HA	9	0.15
(1,69)	1:10:A:THR:H	1:9:A:ALA:HA	13	0.15
(1,68)	1:9:A:ALA:H	1:8:A:ILE:HA	2	0.15
(1,68)	1:9:A:ALA:H	1:8:A:ILE:HA	5	0.15
(1,68)	1:9:A:ALA:H	1:8:A:ILE:HA	7	0.15
(1,68)	1:9:A:ALA:H	1:8:A:ILE:HA	11	0.15
(1,32)	1:15:A:TYR:HE1	1:15:A:TYR:HB2	8	0.15
(1,32)	1:15:A:TYR:HE1	1:15:A:TYR:HB2	11	0.15
(1,26)	1:10:A:THR:HA	1:10:A:THR:HB	15	0.15
(1,24)	1:63:A:ILE:HD12	1:26:A:HIS:HB3	3	0.15
(1,18)	1:66:A:LEU:HB3	1:26:A:HIS:HB2	14	0.15
(3,20)	1:18:A:LEU:O	1:22:A:ILE:H	3	0.14
(3,17)	1:17:A:TRP:O	1:21:A:ARG:N	2	0.14
(3,16)	1:16:A:GLU:O	1:20:A:SER:H	10	0.14
(3,10)	1:13:A:ASP:O	1:17:A:TRP:H	13	0.14
(1,1426)	1:68:A:HIS:HD1	1:64:A:HIS:HB2	14	0.14
(1,1423)	1:26:A:HIS:HD1	1:66:A:LEU:HA	2	0.14
(1,1423)	1:26:A:HIS:HD1	1:66:A:LEU:HA	13	0.14
(1,1387)	1:68:A:HIS:HD1	1:67:A:LYS:HE2	15	0.14
(1,1381)	1:49:A:LEU:HD22	1:7:A:GLN:HG2	15	0.14
(1,1357)	1:26:A:HIS:H	1:26:A:HIS:HD1	4	0.14
(1,1354)	1:62:A:HIS:HD1	1:63:A:ILE:HA	4	0.14
(1,1349)	1:22:A:ILE:H	1:23:A:VAL:HB	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1349)	1:22:A:ILE:H	1:23:A:VAL:HB	5	0.14
(1,1346)	1:43:A:TYR:HD1	1:37:A:MET:HG2	2	0.14
(1,1338)	1:64:A:HIS:H	1:62:A:HIS:HA	5	0.14
(1,1338)	1:64:A:HIS:H	1:62:A:HIS:HA	9	0.14
(1,1338)	1:64:A:HIS:H	1:62:A:HIS:HA	11	0.14
(1,1338)	1:64:A:HIS:H	1:62:A:HIS:HA	13	0.14
(1,1315)	1:18:A:LEU:HG	1:42:A:GLU:HG3	7	0.14
(1,1307)	1:33:A:VAL:HG11	1:28:A:GLU:HG3	4	0.14
(1,1303)	1:65:A:ARG:HB3	1:65:A:ARG:HD2	15	0.14
(1,1302)	1:63:A:ILE:HG12	1:60:A:LEU:HA	14	0.14
(1,1274)	1:17:A:TRP:HE3	1:18:A:LEU:HA	13	0.14
(1,1265)	1:14:A:LYS:HB2	1:11:A:ALA:HA	13	0.14
(1,1245)	1:26:A:HIS:HE1	1:67:A:LYS:HD2	10	0.14
(1,1241)	1:63:A:ILE:HG23	1:26:A:HIS:HB3	11	0.14
(1,1213)	1:30:A:TRP:HE3	1:37:A:MET:HE3	1	0.14
(1,1202)	1:18:A:LEU:HG	1:42:A:GLU:HB2	11	0.14
(1,1175)	1:26:A:HIS:HE1	1:27:A:ASN:HD22	4	0.14
(1,1127)	1:18:A:LEU:HG	1:43:A:TYR:HB3	4	0.14
(1,1124)	1:15:A:TYR:HD2	1:55:A:ALA:HA	8	0.14
(1,1124)	1:15:A:TYR:HD2	1:55:A:ALA:HA	10	0.14
(1,1108)	1:43:A:TYR:HE2	1:34:A:SER:HB3	9	0.14
(1,1098)	1:30:A:TRP:HD1	1:56:A:LYS:HG2	14	0.14
(1,1081)	1:43:A:TYR:HE1	1:38:A:GLN:HB2	13	0.14
(1,1078)	1:39:A:ALA:H	1:38:A:GLN:HB2	13	0.14
(1,1050)	1:54:A:LYS:HG3	1:54:A:LYS:HA	5	0.14
(1,1047)	1:55:A:ALA:H	1:54:A:LYS:HG2	12	0.14
(1,1047)	1:55:A:ALA:H	1:54:A:LYS:HG2	13	0.14
(1,1008)	1:57:A:LYS:H	1:57:A:LYS:HD2	13	0.14
(1,1007)	1:57:A:LYS:H	1:57:A:LYS:HE2	10	0.14
(1,1004)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	9	0.14
(1,914)	1:41:A:PRO:HG3	1:41:A:PRO:HB2	14	0.14
(1,905)	1:41:A:PRO:HG2	1:41:A:PRO:HA	14	0.14
(1,886)	1:65:A:ARG:HD3	1:65:A:ARG:HA	7	0.14
(1,834)	1:49:A:LEU:HD13	1:49:A:LEU:HB2	6	0.14
(1,834)	1:49:A:LEU:HD12	1:49:A:LEU:HB2	15	0.14
(1,798)	1:28:A:GLU:H	1:27:A:ASN:HB3	2	0.14
(1,798)	1:28:A:GLU:H	1:27:A:ASN:HB3	4	0.14
(1,798)	1:28:A:GLU:H	1:27:A:ASN:HB3	14	0.14
(1,795)	1:59:A:PHE:HE1	1:59:A:PHE:HB2	7	0.14
(1,795)	1:59:A:PHE:HE1	1:59:A:PHE:HB2	8	0.14
(1,783)	1:64:A:HIS:H	1:61:A:GLN:HA	5	0.14
(1,777)	1:61:A:GLN:HG2	1:58:A:LEU:HA	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,777)	1:61:A:GLN:HG2	1:58:A:LEU:HA	15	0.14
(1,755)	1:22:A:ILE:HG12	1:19:A:VAL:HA	11	0.14
(1,705)	1:68:A:HIS:HD1	1:67:A:LYS:HG2	10	0.14
(1,681)	1:15:A:TYR:HE2	1:58:A:LEU:HB2	5	0.14
(1,666)	1:62:A:HIS:HD1	1:62:A:HIS:HA	13	0.14
(1,662)	1:64:A:HIS:H	1:64:A:HIS:HD1	12	0.14
(1,659)	1:68:A:HIS:HD1	1:68:A:HIS:HB2	5	0.14
(1,646)	1:19:A:VAL:H	1:18:A:LEU:HG	5	0.14
(1,646)	1:19:A:VAL:H	1:18:A:LEU:HG	13	0.14
(1,633)	1:16:A:GLU:H	1:16:A:GLU:HG3	14	0.14
(1,629)	1:16:A:GLU:H	1:16:A:GLU:HG2	9	0.14
(1,617)	1:26:A:HIS:H	1:23:A:VAL:HA	1	0.14
(1,563)	1:32:A:SER:H	1:32:A:SER:HA	12	0.14
(1,551)	1:35:A:ARG:HB2	1:35:A:ARG:HA	12	0.14
(1,488)	1:43:A:TYR:HD1	1:47:A:VAL:HG21	4	0.14
(1,437)	1:69:A:GLU:HB2	1:69:A:GLU:HA	6	0.14
(1,437)	1:69:A:GLU:HB2	1:69:A:GLU:HA	10	0.14
(1,434)	1:69:A:GLU:H	1:68:A:HIS:HB3	9	0.14
(1,434)	1:69:A:GLU:H	1:68:A:HIS:HB3	12	0.14
(1,420)	1:66:A:LEU:HD13	1:66:A:LEU:HB3	15	0.14
(1,391)	1:64:A:HIS:H	1:63:A:ILE:HA	2	0.14
(1,369)	1:61:A:GLN:H	1:61:A:GLN:HB2	3	0.14
(1,334)	1:57:A:LYS:H	1:56:A:LYS:HB2	7	0.14
(1,334)	1:57:A:LYS:H	1:56:A:LYS:HB2	10	0.14
(1,312)	1:40:A:SER:H	1:40:A:SER:HB3	6	0.14
(1,312)	1:40:A:SER:H	1:40:A:SER:HB3	10	0.14
(1,242)	1:47:A:VAL:H	1:46:A:TYR:HB2	13	0.14
(1,227)	1:48:A:TYR:HD1	1:48:A:TYR:HA	2	0.14
(1,218)	1:17:A:TRP:HE3	1:17:A:TRP:HB2	1	0.14
(1,214)	1:17:A:TRP:HE1	1:17:A:TRP:HZ2	3	0.14
(1,214)	1:17:A:TRP:HE1	1:17:A:TRP:HZ2	6	0.14
(1,214)	1:17:A:TRP:HE1	1:17:A:TRP:HZ2	7	0.14
(1,214)	1:17:A:TRP:HE1	1:17:A:TRP:HZ2	13	0.14
(1,163)	1:46:A:TYR:H	1:45:A:ASP:HA	2	0.14
(1,163)	1:46:A:TYR:H	1:45:A:ASP:HA	5	0.14
(1,163)	1:46:A:TYR:H	1:45:A:ASP:HA	8	0.14
(1,163)	1:46:A:TYR:H	1:45:A:ASP:HA	9	0.14
(1,163)	1:46:A:TYR:H	1:45:A:ASP:HA	12	0.14
(1,163)	1:46:A:TYR:H	1:45:A:ASP:HA	13	0.14
(1,163)	1:46:A:TYR:H	1:45:A:ASP:HA	15	0.14
(1,68)	1:9:A:ALA:H	1:8:A:ILE:HA	3	0.14
(1,68)	1:9:A:ALA:H	1:8:A:ILE:HA	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:15:A:TYR:HE1	1:15:A:TYR:HB2	4	0.14
(1,26)	1:10:A:THR:HA	1:10:A:THR:HB	8	0.14
(1,24)	1:63:A:ILE:HD11	1:26:A:HIS:HB3	11	0.14
(1,12)	1:26:A:HIS:HD1	1:67:A:LYS:HB2	7	0.14
(1,12)	1:26:A:HIS:HD1	1:67:A:LYS:HB2	8	0.14
(1,2)	1:66:A:LEU:HD21	1:25:A:ASN:HA	7	0.14
(1,1426)	1:68:A:HIS:HD1	1:64:A:HIS:HB2	2	0.13
(1,1423)	1:26:A:HIS:HD1	1:66:A:LEU:HA	3	0.13
(1,1423)	1:26:A:HIS:HD1	1:66:A:LEU:HA	5	0.13
(1,1372)	1:22:A:ILE:HD12	1:37:A:MET:HG3	11	0.13
(1,1357)	1:26:A:HIS:H	1:26:A:HIS:HD1	7	0.13
(1,1354)	1:62:A:HIS:HD1	1:63:A:ILE:HA	7	0.13
(1,1349)	1:22:A:ILE:H	1:23:A:VAL:HB	2	0.13
(1,1331)	1:23:A:VAL:H	1:33:A:VAL:HB	11	0.13
(1,1330)	1:17:A:TRP:HZ3	1:14:A:LYS:HG2	8	0.13
(1,1327)	1:64:A:HIS:HD1	1:69:A:GLU:HG2	11	0.13
(1,1327)	1:64:A:HIS:HD1	1:69:A:GLU:HG2	15	0.13
(1,1313)	1:33:A:VAL:HA	1:32:A:SER:HB3	11	0.13
(1,1284)	1:34:A:SER:HB3	1:31:A:LEU:HA	1	0.13
(1,1274)	1:17:A:TRP:HE3	1:18:A:LEU:HA	11	0.13
(1,1274)	1:17:A:TRP:HE3	1:18:A:LEU:HA	15	0.13
(1,1226)	1:47:A:VAL:HG23	1:44:A:GLN:HA	12	0.13
(1,1219)	1:56:A:LYS:HB2	1:53:A:GLN:HA	11	0.13
(1,1187)	1:59:A:PHE:HE2	1:60:A:LEU:HD11	12	0.13
(1,1183)	1:69:A:GLU:H	1:68:A:HIS:H	6	0.13
(1,1175)	1:26:A:HIS:HE1	1:27:A:ASN:HD22	11	0.13
(1,1174)	1:44:A:GLN:HE21	1:43:A:TYR:HD1	14	0.13
(1,1149)	1:62:A:HIS:H	1:19:A:VAL:HG11	5	0.13
(1,1107)	1:43:A:TYR:HE1	1:34:A:SER:HB2	8	0.13
(1,1095)	1:59:A:PHE:HD2	1:30:A:TRP:HA	9	0.13
(1,1087)	1:56:A:LYS:H	1:53:A:GLN:HA	8	0.13
(1,1025)	1:36:A:LYS:HG3	1:36:A:LYS:HA	14	0.13
(1,1006)	1:57:A:LYS:H	1:57:A:LYS:HG3	3	0.13
(1,984)	1:46:A:TYR:HE1	1:12:A:LYS:HG2	5	0.13
(1,958)	1:53:A:GLN:HB2	1:53:A:GLN:HG2	7	0.13
(1,926)	1:51:A:GLY:H	1:50:A:GLU:HG3	14	0.13
(1,914)	1:41:A:PRO:HG3	1:41:A:PRO:HB2	3	0.13
(1,905)	1:41:A:PRO:HG2	1:41:A:PRO:HA	3	0.13
(1,905)	1:41:A:PRO:HG2	1:41:A:PRO:HA	6	0.13
(1,901)	1:40:A:SER:H	1:41:A:PRO:HD2	3	0.13
(1,901)	1:40:A:SER:H	1:41:A:PRO:HD2	10	0.13
(1,901)	1:40:A:SER:H	1:41:A:PRO:HD2	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,901)	1:40:A:SER:H	1:41:A:PRO:HD2	14	0.13
(1,890)	1:66:A:LEU:H	1:65:A:ARG:HB3	12	0.13
(1,887)	1:65:A:ARG:HD2	1:65:A:ARG:HA	3	0.13
(1,884)	1:65:A:ARG:H	1:65:A:ARG:HD2	7	0.13
(1,834)	1:49:A:LEU:HD11	1:49:A:LEU:HB2	1	0.13
(1,834)	1:49:A:LEU:HD12	1:49:A:LEU:HB2	11	0.13
(1,827)	1:50:A:GLU:H	1:49:A:LEU:HB3	8	0.13
(1,798)	1:28:A:GLU:H	1:27:A:ASN:HB3	1	0.13
(1,795)	1:59:A:PHE:HE1	1:59:A:PHE:HB2	2	0.13
(1,795)	1:59:A:PHE:HE1	1:59:A:PHE:HB2	9	0.13
(1,783)	1:64:A:HIS:H	1:61:A:GLN:HA	9	0.13
(1,783)	1:64:A:HIS:H	1:61:A:GLN:HA	15	0.13
(1,776)	1:61:A:GLN:HB3	1:58:A:LEU:HA	1	0.13
(1,703)	1:48:A:TYR:HD2	1:49:A:LEU:HB2	9	0.13
(1,703)	1:48:A:TYR:HD2	1:49:A:LEU:HB2	13	0.13
(1,681)	1:15:A:TYR:HE2	1:58:A:LEU:HB2	8	0.13
(1,681)	1:15:A:TYR:HE2	1:58:A:LEU:HB2	12	0.13
(1,666)	1:62:A:HIS:HD1	1:62:A:HIS:HA	2	0.13
(1,666)	1:62:A:HIS:HD1	1:62:A:HIS:HA	3	0.13
(1,666)	1:62:A:HIS:HD1	1:62:A:HIS:HA	10	0.13
(1,662)	1:64:A:HIS:H	1:64:A:HIS:HD1	2	0.13
(1,651)	1:21:A:ARG:HB2	1:18:A:LEU:HA	4	0.13
(1,651)	1:21:A:ARG:HB2	1:18:A:LEU:HA	10	0.13
(1,651)	1:21:A:ARG:HB2	1:18:A:LEU:HA	11	0.13
(1,646)	1:19:A:VAL:H	1:18:A:LEU:HG	2	0.13
(1,646)	1:19:A:VAL:H	1:18:A:LEU:HG	3	0.13
(1,629)	1:16:A:GLU:H	1:16:A:GLU:HG2	7	0.13
(1,614)	1:28:A:GLU:H	1:28:A:GLU:HB3	9	0.13
(1,563)	1:32:A:SER:H	1:32:A:SER:HA	2	0.13
(1,552)	1:35:A:ARG:HG2	1:35:A:ARG:HA	5	0.13
(1,494)	1:67:A:LYS:H	1:67:A:LYS:HG3	15	0.13
(1,487)	1:59:A:PHE:HD1	1:19:A:VAL:HG23	13	0.13
(1,481)	1:33:A:VAL:H	1:33:A:VAL:HB	10	0.13
(1,434)	1:69:A:GLU:H	1:68:A:HIS:HB3	1	0.13
(1,422)	1:66:A:LEU:H	1:66:A:LEU:HD12	4	0.13
(1,422)	1:66:A:LEU:H	1:66:A:LEU:HD12	9	0.13
(1,373)	1:61:A:GLN:HG3	1:61:A:GLN:HA	9	0.13
(1,312)	1:40:A:SER:H	1:40:A:SER:HB3	11	0.13
(1,242)	1:47:A:VAL:H	1:46:A:TYR:HB2	15	0.13
(1,227)	1:48:A:TYR:HD1	1:48:A:TYR:HA	1	0.13
(1,227)	1:48:A:TYR:HD1	1:48:A:TYR:HA	3	0.13
(1,227)	1:48:A:TYR:HD1	1:48:A:TYR:HA	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:48:A:TYR:HD1	1:48:A:TYR:HA	7	0.13
(1,218)	1:17:A:TRP:HE3	1:17:A:TRP:HB2	4	0.13
(1,218)	1:17:A:TRP:HE3	1:17:A:TRP:HB2	5	0.13
(1,218)	1:17:A:TRP:HE3	1:17:A:TRP:HB2	8	0.13
(1,163)	1:46:A:TYR:H	1:45:A:ASP:HA	3	0.13
(1,32)	1:15:A:TYR:HE1	1:15:A:TYR:HB2	10	0.13
(1,26)	1:10:A:THR:HA	1:10:A:THR:HB	7	0.13
(1,26)	1:10:A:THR:HA	1:10:A:THR:HB	13	0.13
(3,20)	1:18:A:LEU:O	1:22:A:ILE:H	6	0.12
(3,16)	1:16:A:GLU:O	1:20:A:SER:H	11	0.12
(3,10)	1:13:A:ASP:O	1:17:A:TRP:H	2	0.12
(3,10)	1:13:A:ASP:O	1:17:A:TRP:H	12	0.12
(1,1426)	1:68:A:HIS:HD1	1:64:A:HIS:HB2	5	0.12
(1,1423)	1:26:A:HIS:HD1	1:66:A:LEU:HA	10	0.12
(1,1421)	1:23:A:VAL:H	1:62:A:HIS:HD1	5	0.12
(1,1421)	1:23:A:VAL:H	1:62:A:HIS:HD1	6	0.12
(1,1398)	1:6:A:GLN:H	1:6:A:GLN:HB2	15	0.12
(1,1357)	1:26:A:HIS:H	1:26:A:HIS:HD1	3	0.12
(1,1354)	1:62:A:HIS:HD1	1:63:A:ILE:HA	6	0.12
(1,1349)	1:22:A:ILE:H	1:23:A:VAL:HB	8	0.12
(1,1349)	1:22:A:ILE:H	1:23:A:VAL:HB	9	0.12
(1,1349)	1:22:A:ILE:H	1:23:A:VAL:HB	14	0.12
(1,1339)	1:44:A:GLN:HE22	1:44:A:GLN:HG2	14	0.12
(1,1338)	1:64:A:HIS:H	1:62:A:HIS:HA	10	0.12
(1,1327)	1:64:A:HIS:HD1	1:69:A:GLU:HG2	2	0.12
(1,1323)	1:64:A:HIS:HD1	1:65:A:ARG:HG3	2	0.12
(1,1315)	1:18:A:LEU:HG	1:42:A:GLU:HG3	1	0.12
(1,1315)	1:18:A:LEU:HG	1:42:A:GLU:HG3	6	0.12
(1,1311)	1:66:A:LEU:HD13	1:24:A:LYS:HA	7	0.12
(1,1296)	1:60:A:LEU:HG	1:57:A:LYS:HA	5	0.12
(1,1296)	1:60:A:LEU:HG	1:57:A:LYS:HA	12	0.12
(1,1282)	1:21:A:ARG:HG3	1:18:A:LEU:HA	5	0.12
(1,1272)	1:16:A:GLU:HB3	1:13:A:ASP:HA	3	0.12
(1,1272)	1:16:A:GLU:HB3	1:13:A:ASP:HA	12	0.12
(1,1262)	1:7:A:GLN:HA	1:10:A:THR:HB	6	0.12
(1,1241)	1:63:A:ILE:HG22	1:26:A:HIS:HB3	6	0.12
(1,1226)	1:47:A:VAL:HG23	1:44:A:GLN:HA	9	0.12
(1,1187)	1:59:A:PHE:HE2	1:60:A:LEU:HD12	6	0.12
(1,1134)	1:30:A:TRP:HZ3	1:30:A:TRP:HA	12	0.12
(1,1133)	1:30:A:TRP:HZ3	1:59:A:PHE:HB3	4	0.12
(1,1133)	1:30:A:TRP:HZ3	1:59:A:PHE:HB3	5	0.12
(1,1133)	1:30:A:TRP:HZ3	1:59:A:PHE:HB3	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1124)	1:15:A:TYR:HD2	1:55:A:ALA:HA	2	0.12
(1,1124)	1:15:A:TYR:HD2	1:55:A:ALA:HA	4	0.12
(1,1124)	1:15:A:TYR:HD2	1:55:A:ALA:HA	12	0.12
(1,1117)	1:30:A:TRP:HE3	1:33:A:VAL:HB	10	0.12
(1,1098)	1:30:A:TRP:HD1	1:56:A:LYS:HG2	8	0.12
(1,1095)	1:59:A:PHE:HD2	1:30:A:TRP:HA	1	0.12
(1,1081)	1:43:A:TYR:HE2	1:38:A:GLN:HB2	12	0.12
(1,1078)	1:39:A:ALA:H	1:38:A:GLN:HB2	15	0.12
(1,1076)	1:38:A:GLN:H	1:38:A:GLN:HB2	10	0.12
(1,1050)	1:54:A:LYS:HG3	1:54:A:LYS:HA	11	0.12
(1,1050)	1:54:A:LYS:HG3	1:54:A:LYS:HA	14	0.12
(1,1047)	1:55:A:ALA:H	1:54:A:LYS:HG2	7	0.12
(1,1025)	1:36:A:LYS:HG3	1:36:A:LYS:HA	8	0.12
(1,1017)	1:57:A:LYS:HG3	1:57:A:LYS:HE2	1	0.12
(1,926)	1:51:A:GLY:H	1:50:A:GLU:HG3	10	0.12
(1,926)	1:51:A:GLY:H	1:50:A:GLU:HG3	13	0.12
(1,914)	1:41:A:PRO:HG3	1:41:A:PRO:HB2	5	0.12
(1,914)	1:41:A:PRO:HG3	1:41:A:PRO:HB2	6	0.12
(1,914)	1:41:A:PRO:HG3	1:41:A:PRO:HB2	7	0.12
(1,914)	1:41:A:PRO:HG3	1:41:A:PRO:HB2	13	0.12
(1,905)	1:41:A:PRO:HG2	1:41:A:PRO:HA	7	0.12
(1,905)	1:41:A:PRO:HG2	1:41:A:PRO:HA	11	0.12
(1,905)	1:41:A:PRO:HG2	1:41:A:PRO:HA	13	0.12
(1,901)	1:40:A:SER:H	1:41:A:PRO:HD2	8	0.12
(1,887)	1:65:A:ARG:HD2	1:65:A:ARG:HA	13	0.12
(1,795)	1:59:A:PHE:HE1	1:59:A:PHE:HB2	3	0.12
(1,795)	1:59:A:PHE:HE1	1:59:A:PHE:HB2	15	0.12
(1,762)	1:35:A:ARG:HD2	1:32:A:SER:HA	1	0.12
(1,762)	1:35:A:ARG:HD2	1:32:A:SER:HA	5	0.12
(1,762)	1:35:A:ARG:HD2	1:32:A:SER:HA	15	0.12
(1,703)	1:48:A:TYR:HD2	1:49:A:LEU:HB2	14	0.12
(1,681)	1:15:A:TYR:HE2	1:58:A:LEU:HB2	1	0.12
(1,681)	1:15:A:TYR:HE2	1:58:A:LEU:HB2	10	0.12
(1,666)	1:62:A:HIS:HD1	1:62:A:HIS:HA	1	0.12
(1,662)	1:64:A:HIS:H	1:64:A:HIS:HD1	10	0.12
(1,660)	1:68:A:HIS:HD1	1:68:A:HIS:HB3	3	0.12
(1,652)	1:19:A:VAL:HB	1:16:A:GLU:HA	11	0.12
(1,651)	1:21:A:ARG:HB2	1:18:A:LEU:HA	9	0.12
(1,646)	1:19:A:VAL:H	1:18:A:LEU:HG	4	0.12
(1,629)	1:16:A:GLU:H	1:16:A:GLU:HG2	3	0.12
(1,584)	1:13:A:ASP:H	1:12:A:LYS:HB2	1	0.12
(1,562)	1:36:A:LYS:H	1:35:A:ARG:HG2	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,483)	1:34:A:SER:H	1:33:A:VAL:HG21	8	0.12
(1,434)	1:69:A:GLU:H	1:68:A:HIS:HB3	2	0.12
(1,334)	1:57:A:LYS:H	1:56:A:LYS:HB2	2	0.12
(1,312)	1:40:A:SER:H	1:40:A:SER:HB3	7	0.12
(1,288)	1:21:A:ARG:H	1:21:A:ARG:HG2	14	0.12
(1,242)	1:47:A:VAL:H	1:46:A:TYR:HB2	3	0.12
(1,227)	1:48:A:TYR:HD1	1:48:A:TYR:HA	13	0.12
(1,227)	1:48:A:TYR:HD1	1:48:A:TYR:HA	14	0.12
(1,218)	1:17:A:TRP:HE3	1:17:A:TRP:HB2	12	0.12
(1,218)	1:17:A:TRP:HE3	1:17:A:TRP:HB2	13	0.12
(1,69)	1:10:A:THR:H	1:9:A:ALA:HA	15	0.12
(1,68)	1:9:A:ALA:H	1:8:A:ILE:HA	12	0.12
(1,32)	1:15:A:TYR:HE1	1:15:A:TYR:HB2	13	0.12
(1,32)	1:15:A:TYR:HE1	1:15:A:TYR:HB2	14	0.12
(1,32)	1:15:A:TYR:HE1	1:15:A:TYR:HB2	15	0.12
(1,18)	1:66:A:LEU:HB3	1:26:A:HIS:HB2	2	0.12
(3,20)	1:18:A:LEU:O	1:22:A:ILE:H	8	0.11
(3,10)	1:13:A:ASP:O	1:17:A:TRP:H	5	0.11
(3,10)	1:13:A:ASP:O	1:17:A:TRP:H	15	0.11
(1,1423)	1:26:A:HIS:HD1	1:66:A:LEU:HA	7	0.11
(1,1421)	1:23:A:VAL:H	1:62:A:HIS:HD1	8	0.11
(1,1419)	1:27:A:ASN:H	1:63:A:ILE:HD13	3	0.11
(1,1401)	1:7:A:GLN:HG2	1:7:A:GLN:HA	14	0.11
(1,1389)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	15	0.11
(1,1387)	1:68:A:HIS:HD1	1:67:A:LYS:HE2	7	0.11
(1,1387)	1:68:A:HIS:HD1	1:67:A:LYS:HE2	8	0.11
(1,1354)	1:62:A:HIS:HD1	1:63:A:ILE:HA	8	0.11
(1,1349)	1:22:A:ILE:H	1:23:A:VAL:HB	6	0.11
(1,1349)	1:22:A:ILE:H	1:23:A:VAL:HB	7	0.11
(1,1338)	1:64:A:HIS:H	1:62:A:HIS:HA	2	0.11
(1,1338)	1:64:A:HIS:H	1:62:A:HIS:HA	6	0.11
(1,1338)	1:64:A:HIS:H	1:62:A:HIS:HA	7	0.11
(1,1338)	1:64:A:HIS:H	1:62:A:HIS:HA	14	0.11
(1,1330)	1:17:A:TRP:HZ3	1:14:A:LYS:HG2	9	0.11
(1,1323)	1:64:A:HIS:HD1	1:65:A:ARG:HG3	3	0.11
(1,1323)	1:64:A:HIS:HD1	1:65:A:ARG:HG3	10	0.11
(1,1302)	1:63:A:ILE:HG12	1:60:A:LEU:HA	13	0.11
(1,1296)	1:60:A:LEU:HG	1:57:A:LYS:HA	3	0.11
(1,1296)	1:60:A:LEU:HG	1:57:A:LYS:HA	6	0.11
(1,1296)	1:60:A:LEU:HG	1:57:A:LYS:HA	7	0.11
(1,1284)	1:34:A:SER:HB3	1:31:A:LEU:HA	7	0.11
(1,1276)	1:17:A:TRP:HZ3	1:18:A:LEU:HA	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1276)	1:17:A:TRP:HZ3	1:18:A:LEU:HA	14	0.11
(1,1259)	1:9:A:ALA:H	1:6:A:GLN:HA	15	0.11
(1,1242)	1:66:A:LEU:HD13	1:26:A:HIS:HB2	13	0.11
(1,1183)	1:69:A:GLU:H	1:68:A:HIS:H	4	0.11
(1,1168)	1:68:A:HIS:HE1	1:67:A:LYS:HE2	3	0.11
(1,1137)	1:36:A:LYS:H	1:34:A:SER:HA	7	0.11
(1,1134)	1:30:A:TRP:HZ3	1:30:A:TRP:HA	1	0.11
(1,1134)	1:30:A:TRP:HZ3	1:30:A:TRP:HA	7	0.11
(1,1134)	1:30:A:TRP:HZ3	1:30:A:TRP:HA	10	0.11
(1,1134)	1:30:A:TRP:HZ3	1:30:A:TRP:HA	13	0.11
(1,1117)	1:30:A:TRP:HE3	1:33:A:VAL:HB	13	0.11
(1,1101)	1:30:A:TRP:HD1	1:56:A:LYS:HD3	11	0.11
(1,1081)	1:43:A:TYR:HE1	1:38:A:GLN:HB2	5	0.11
(1,1076)	1:38:A:GLN:H	1:38:A:GLN:HB2	1	0.11
(1,1076)	1:38:A:GLN:H	1:38:A:GLN:HB2	8	0.11
(1,1050)	1:54:A:LYS:HG3	1:54:A:LYS:HA	4	0.11
(1,1047)	1:55:A:ALA:H	1:54:A:LYS:HG2	2	0.11
(1,1047)	1:55:A:ALA:H	1:54:A:LYS:HG2	3	0.11
(1,1025)	1:36:A:LYS:HG3	1:36:A:LYS:HA	9	0.11
(1,1012)	1:57:A:LYS:HD2	1:57:A:LYS:HA	12	0.11
(1,1006)	1:57:A:LYS:H	1:57:A:LYS:HG3	15	0.11
(1,1001)	1:24:A:LYS:HD2	1:24:A:LYS:HB3	7	0.11
(1,996)	1:24:A:LYS:HG2	1:24:A:LYS:HA	15	0.11
(1,914)	1:41:A:PRO:HG3	1:41:A:PRO:HB2	9	0.11
(1,914)	1:41:A:PRO:HG3	1:41:A:PRO:HB2	10	0.11
(1,914)	1:41:A:PRO:HG3	1:41:A:PRO:HB2	11	0.11
(1,914)	1:41:A:PRO:HG3	1:41:A:PRO:HB2	12	0.11
(1,905)	1:41:A:PRO:HG2	1:41:A:PRO:HA	5	0.11
(1,905)	1:41:A:PRO:HG2	1:41:A:PRO:HA	9	0.11
(1,905)	1:41:A:PRO:HG2	1:41:A:PRO:HA	10	0.11
(1,905)	1:41:A:PRO:HG2	1:41:A:PRO:HA	12	0.11
(1,901)	1:40:A:SER:H	1:41:A:PRO:HD2	7	0.11
(1,886)	1:65:A:ARG:HD3	1:65:A:ARG:HA	14	0.11
(1,795)	1:59:A:PHE:HE1	1:59:A:PHE:HB2	5	0.11
(1,791)	1:67:A:LYS:HG2	1:64:A:HIS:HA	12	0.11
(1,790)	1:67:A:LYS:HB2	1:64:A:HIS:HA	4	0.11
(1,790)	1:67:A:LYS:HB2	1:64:A:HIS:HA	5	0.11
(1,783)	1:64:A:HIS:H	1:61:A:GLN:HA	3	0.11
(1,777)	1:61:A:GLN:HG2	1:58:A:LEU:HA	9	0.11
(1,776)	1:61:A:GLN:HB3	1:58:A:LEU:HA	5	0.11
(1,762)	1:35:A:ARG:HD2	1:32:A:SER:HA	9	0.11
(1,757)	1:33:A:VAL:HB	1:30:A:TRP:HA	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,720)	1:15:A:TYR:HD1	1:18:A:LEU:HG	14	0.11
(1,705)	1:68:A:HIS:HD1	1:67:A:LYS:HG2	11	0.11
(1,703)	1:48:A:TYR:HD2	1:49:A:LEU:HB2	5	0.11
(1,703)	1:48:A:TYR:HD2	1:49:A:LEU:HB2	12	0.11
(1,684)	1:62:A:HIS:HD1	1:23:A:VAL:HG13	5	0.11
(1,660)	1:68:A:HIS:HD1	1:68:A:HIS:HB3	1	0.11
(1,660)	1:68:A:HIS:HD1	1:68:A:HIS:HB3	13	0.11
(1,660)	1:68:A:HIS:HD1	1:68:A:HIS:HB3	14	0.11
(1,659)	1:68:A:HIS:HD1	1:68:A:HIS:HB2	12	0.11
(1,629)	1:16:A:GLU:H	1:16:A:GLU:HG2	8	0.11
(1,627)	1:16:A:GLU:HG3	1:16:A:GLU:HA	13	0.11
(1,617)	1:26:A:HIS:H	1:23:A:VAL:HA	15	0.11
(1,614)	1:28:A:GLU:H	1:28:A:GLU:HB3	15	0.11
(1,584)	1:13:A:ASP:H	1:12:A:LYS:HB2	9	0.11
(1,558)	1:35:A:ARG:H	1:35:A:ARG:HD2	1	0.11
(1,558)	1:35:A:ARG:H	1:35:A:ARG:HD2	10	0.11
(1,558)	1:35:A:ARG:H	1:35:A:ARG:HD2	11	0.11
(1,514)	1:8:A:ILE:HG12	1:8:A:ILE:HB	1	0.11
(1,489)	1:24:A:LYS:H	1:23:A:VAL:HG22	4	0.11
(1,455)	1:50:A:GLU:H	1:50:A:GLU:HG3	5	0.11
(1,441)	1:69:A:GLU:H	1:69:A:GLU:HB3	9	0.11
(1,434)	1:69:A:GLU:H	1:68:A:HIS:HB3	6	0.11
(1,288)	1:21:A:ARG:H	1:21:A:ARG:HG2	13	0.11
(1,242)	1:47:A:VAL:H	1:46:A:TYR:HB2	5	0.11
(1,242)	1:47:A:VAL:H	1:46:A:TYR:HB2	11	0.11
(1,242)	1:47:A:VAL:H	1:46:A:TYR:HB2	12	0.11
(1,237)	1:43:A:TYR:HD2	1:43:A:TYR:HA	1	0.11
(1,227)	1:48:A:TYR:HD1	1:48:A:TYR:HA	9	0.11
(1,26)	1:10:A:THR:HA	1:10:A:THR:HB	3	0.11
(1,24)	1:63:A:ILE:HD13	1:26:A:HIS:HB3	13	0.11
(1,2)	1:66:A:LEU:HD21	1:25:A:ASN:HA	4	0.11
(3,33)	1:40:A:SER:O	1:44:A:GLN:N	3	0.1
(3,17)	1:17:A:TRP:O	1:21:A:ARG:N	13	0.1
(3,10)	1:13:A:ASP:O	1:17:A:TRP:H	11	0.1
(1,1406)	1:8:A:ILE:HD13	1:5:A:SER:HB2	5	0.1
(1,1387)	1:68:A:HIS:HD1	1:67:A:LYS:HE2	12	0.1
(1,1338)	1:64:A:HIS:H	1:62:A:HIS:HA	8	0.1
(1,1327)	1:64:A:HIS:HD1	1:69:A:GLU:HG2	14	0.1
(1,1315)	1:18:A:LEU:HG	1:42:A:GLU:HG3	12	0.1
(1,1315)	1:18:A:LEU:HG	1:42:A:GLU:HG3	14	0.1
(1,1276)	1:17:A:TRP:HZ3	1:18:A:LEU:HA	7	0.1
(1,1274)	1:17:A:TRP:HE3	1:18:A:LEU:HA	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1242)	1:66:A:LEU:HD11	1:26:A:HIS:HB2	10	0.1
(1,1214)	1:30:A:TRP:HZ3	1:37:A:MET:HE3	1	0.1
(1,1134)	1:30:A:TRP:HZ3	1:30:A:TRP:HA	3	0.1
(1,1100)	1:30:A:TRP:HD1	1:56:A:LYS:HE2	12	0.1
(1,1098)	1:30:A:TRP:HD1	1:56:A:LYS:HG2	1	0.1
(1,1098)	1:30:A:TRP:HD1	1:56:A:LYS:HG2	7	0.1
(1,1095)	1:59:A:PHE:HD2	1:30:A:TRP:HA	4	0.1
(1,1087)	1:56:A:LYS:H	1:53:A:GLN:HA	14	0.1
(1,1081)	1:43:A:TYR:HE1	1:38:A:GLN:HB2	15	0.1
(1,1049)	1:54:A:LYS:HG2	1:54:A:LYS:HB2	1	0.1
(1,1008)	1:57:A:LYS:H	1:57:A:LYS:HD2	14	0.1
(1,996)	1:24:A:LYS:HG2	1:24:A:LYS:HA	11	0.1
(1,947)	1:62:A:HIS:H	1:61:A:GLN:HG3	6	0.1
(1,914)	1:41:A:PRO:HG3	1:41:A:PRO:HB2	1	0.1
(1,914)	1:41:A:PRO:HG3	1:41:A:PRO:HB2	2	0.1
(1,905)	1:41:A:PRO:HG2	1:41:A:PRO:HA	2	0.1
(1,872)	1:65:A:ARG:H	1:65:A:ARG:HG2	15	0.1
(1,795)	1:59:A:PHE:HE1	1:59:A:PHE:HB2	14	0.1
(1,790)	1:67:A:LYS:HB2	1:64:A:HIS:HA	12	0.1
(1,785)	1:64:A:HIS:HB2	1:61:A:GLN:HA	3	0.1
(1,781)	1:64:A:HIS:H	1:60:A:LEU:HA	5	0.1
(1,753)	1:22:A:ILE:H	1:19:A:VAL:HA	11	0.1
(1,721)	1:62:A:HIS:HE1	1:20:A:SER:HB3	2	0.1
(1,705)	1:68:A:HIS:HD1	1:67:A:LYS:HG2	3	0.1
(1,703)	1:48:A:TYR:HD2	1:49:A:LEU:HB2	1	0.1
(1,703)	1:48:A:TYR:HD2	1:49:A:LEU:HB2	7	0.1
(1,684)	1:62:A:HIS:HD1	1:23:A:VAL:HG13	11	0.1
(1,666)	1:62:A:HIS:HD1	1:62:A:HIS:HA	14	0.1
(1,651)	1:21:A:ARG:HB2	1:18:A:LEU:HA	8	0.1
(1,617)	1:26:A:HIS:H	1:23:A:VAL:HA	7	0.1
(1,614)	1:28:A:GLU:H	1:28:A:GLU:HB3	12	0.1
(1,614)	1:28:A:GLU:H	1:28:A:GLU:HB3	13	0.1
(1,612)	1:28:A:GLU:H	1:28:A:GLU:HG3	9	0.1
(1,558)	1:35:A:ARG:H	1:35:A:ARG:HD2	2	0.1
(1,513)	1:8:A:ILE:H	1:8:A:ILE:HD12	15	0.1
(1,275)	1:21:A:ARG:H	1:20:A:SER:HB3	10	0.1
(1,242)	1:47:A:VAL:H	1:46:A:TYR:HB2	6	0.1
(1,68)	1:9:A:ALA:H	1:8:A:ILE:HA	14	0.1
(1,26)	1:10:A:THR:HA	1:10:A:THR:HB	10	0.1
(1,26)	1:10:A:THR:HA	1:10:A:THR:HB	11	0.1
(1,26)	1:10:A:THR:HA	1:10:A:THR:HB	14	0.1
(1,24)	1:63:A:ILE:HD11	1:26:A:HIS:HB3	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:63:A:ILE:HG22	1:26:A:HIS:HB2	4	0.1

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

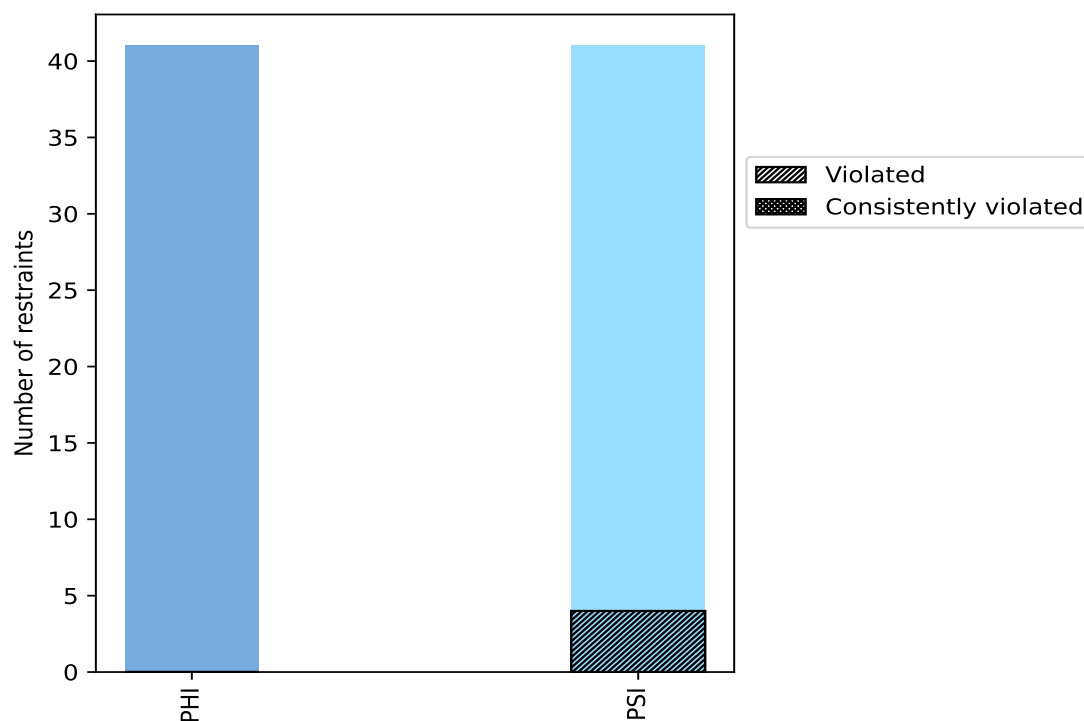
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	41	50.0	0	0.0	0.0	0	0.0	0.0
PSI	41	50.0	4	9.8	4.9	0	0.0	0.0
Total	82	100.0	4	4.9	4.9	0	0.0	0.0

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

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



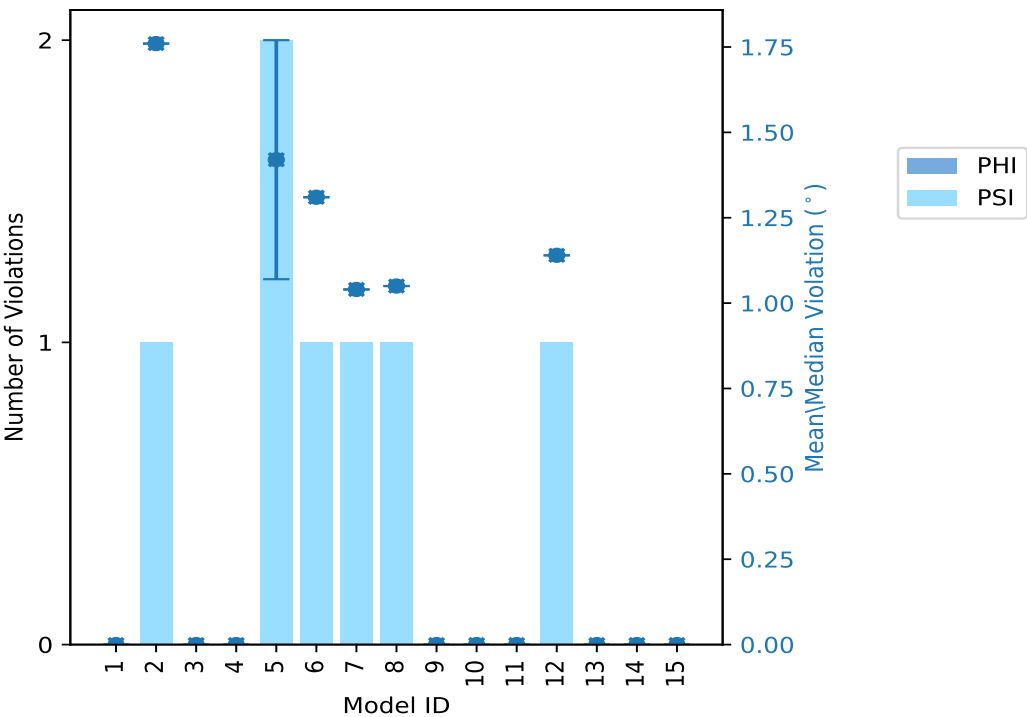
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	0	0	0.0	0.0	0.0	0.0
2	0	1	1	1.76	1.76	0.0	1.76
3	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0.0	0.0	0.0	0.0
5	0	2	2	1.42	1.77	0.35	1.42
6	0	1	1	1.31	1.31	0.0	1.31
7	0	1	1	1.04	1.04	0.0	1.04
8	0	1	1	1.05	1.05	0.0	1.05
9	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0.0	0.0	0.0	0.0
11	0	0	0	0.0	0.0	0.0	0.0
12	0	1	1	1.14	1.14	0.0	1.14
13	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0.0	0.0	0.0	0.0

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

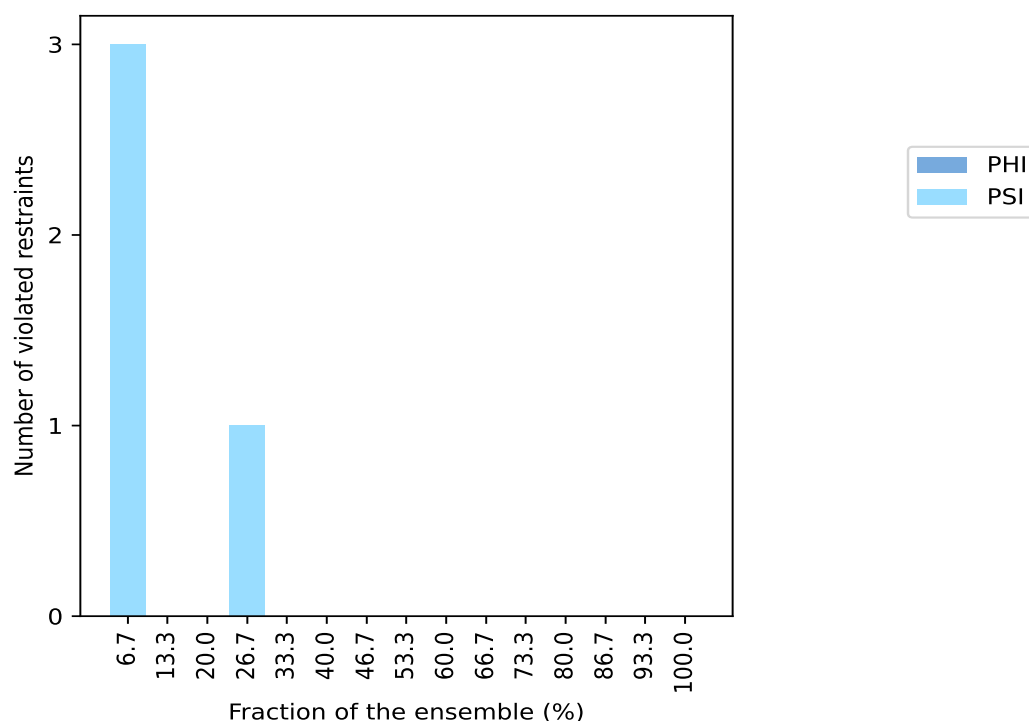
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	3	3	1	6.7
0	0	0	2	13.3
0	0	0	3	20.0
0	1	1	4	26.7
0	0	0	5	33.3
0	0	0	6	40.0
0	0	0	7	46.7
0	0	0	8	53.3
0	0	0	9	60.0
0	0	0	10	66.7
0	0	0	11	73.3
0	0	0	12	80.0
0	0	0	13	86.7
0	0	0	14	93.3
0	0	0	15	100.0

¹ Number of models with violations

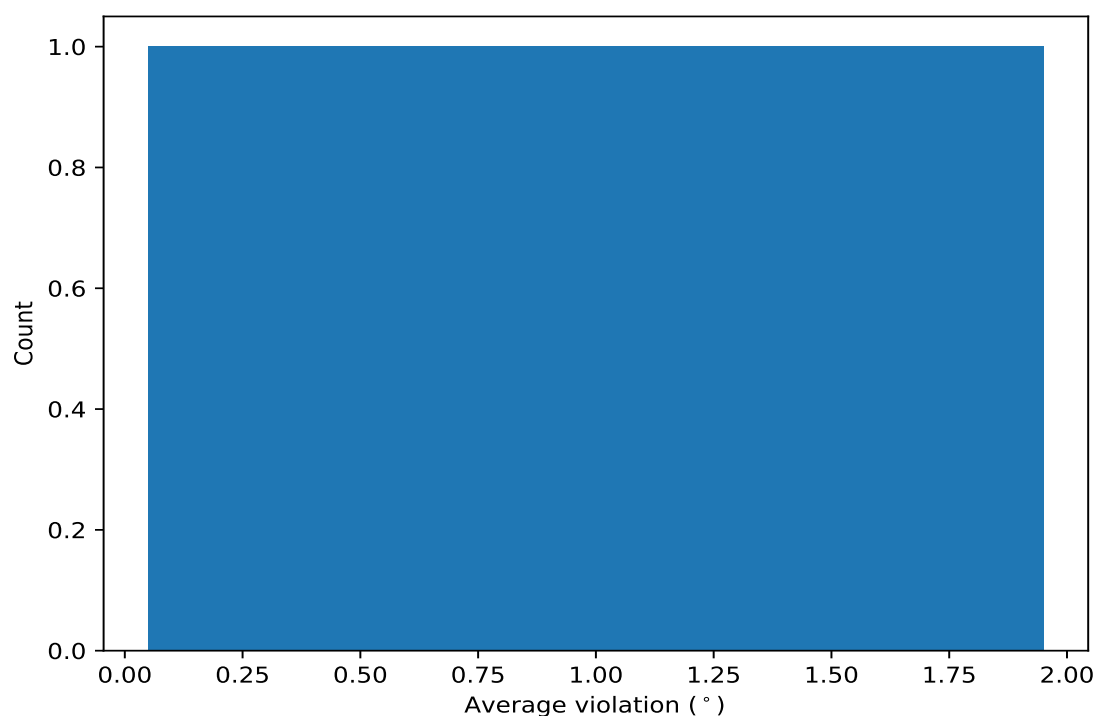
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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



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

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

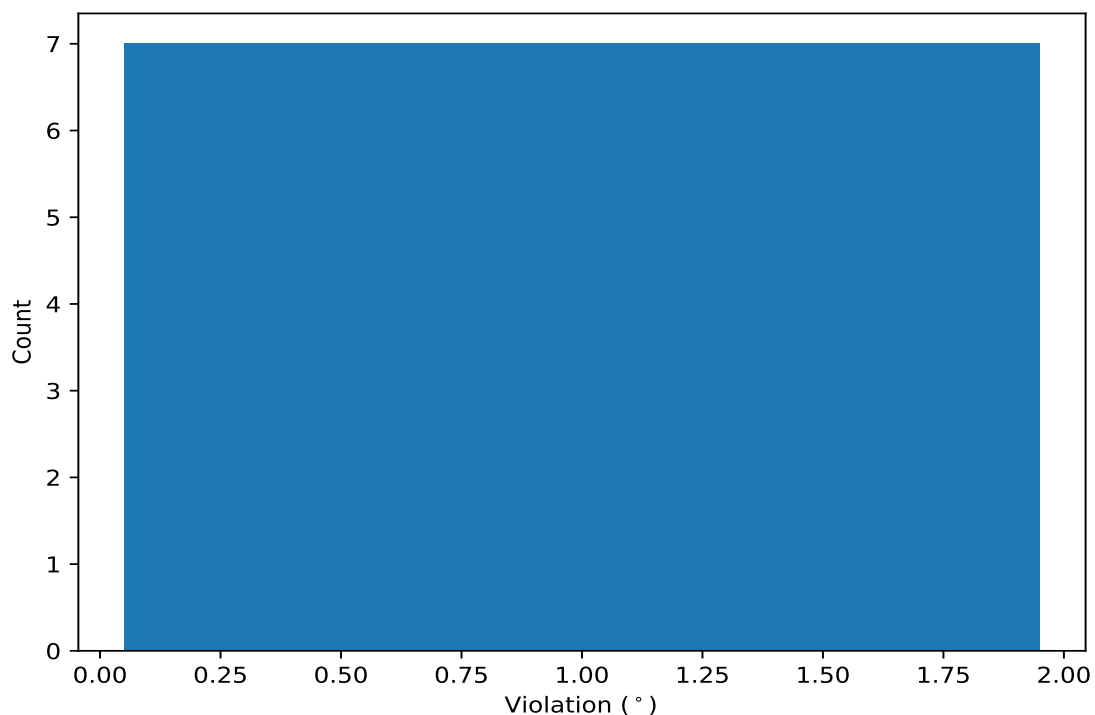
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,24)	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	1:22:A:ILE:N	4	1.32	0.28	1.23

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,24)	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	1:22:A:ILE:N	5	1.77
(1,22)	1:20:A:SER:N	1:20:A:SER:CA	1:20:A:SER:C	1:21:A:ARG:N	2	1.76
(1,24)	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	1:22:A:ILE:N	6	1.31
(1,24)	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	1:22:A:ILE:N	12	1.14
(1,52)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:GLN:N	5	1.07
(1,24)	1:21:A:ARG:N	1:21:A:ARG:CA	1:21:A:ARG:C	1:22:A:ILE:N	8	1.05
(1,48)	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	1:48:A:TYR:N	7	1.04