



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 10:29 AM UTC

PDB ID : 2N3H / pdb_00002n3h
BMRB ID : 25138
Title : Solution structure of DRB4 dsRBD2 (viz. DRB4(81-151))
Authors : Deshmukh, M.; Chiliveri, S.
Deposited on : 2015-05-29

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

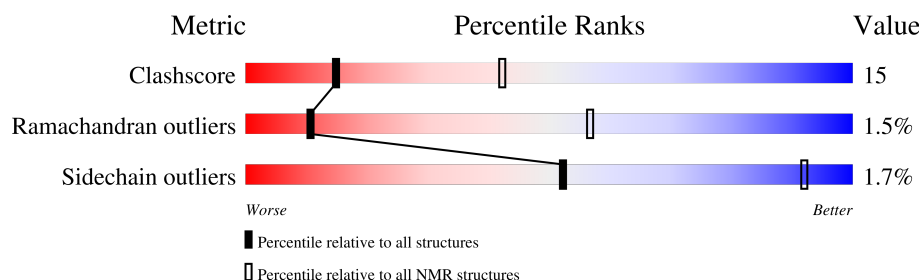
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 86%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	153	

2 Ensemble composition and analysis

This entry contains 20 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:82-A:149 (68)	0.47	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 4 clusters and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1069 atoms, of which 538 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Double-stranded RNA-binding protein 4.

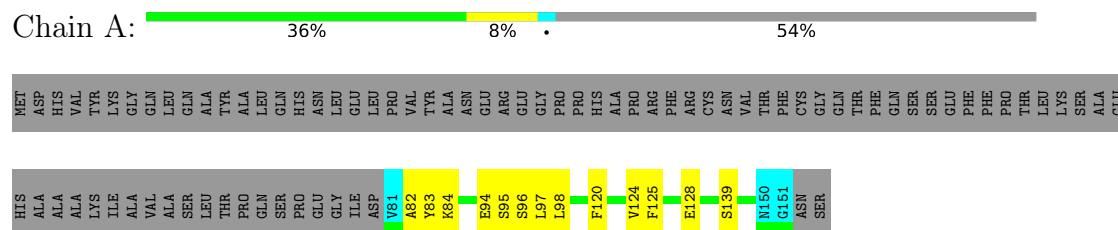
Mol	Chain	Residues	Atoms						Trace
1	A	71	Total	C	H	N	O	S	0
			1069	341	538	85	103	2	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Double-stranded RNA-binding protein 4

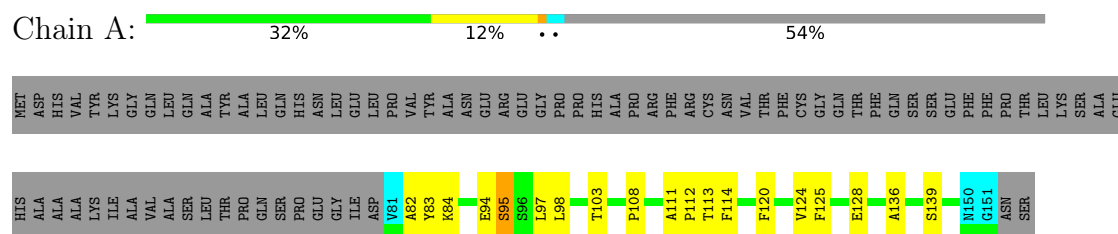


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

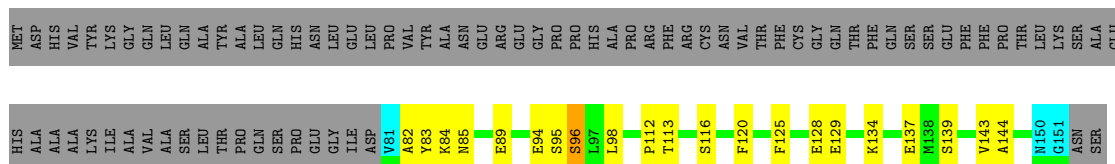
- Molecule 1: Double-stranded RNA-binding protein 4



4.2.2 Score per residue for model 2

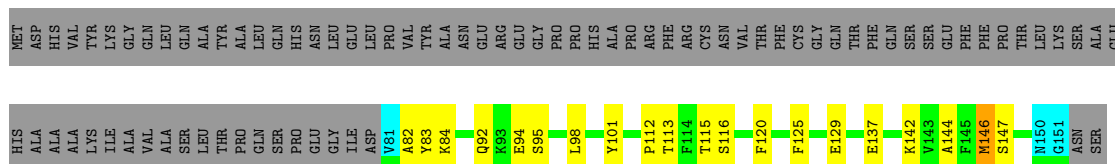
- Molecule 1: Double-stranded RNA-binding protein 4





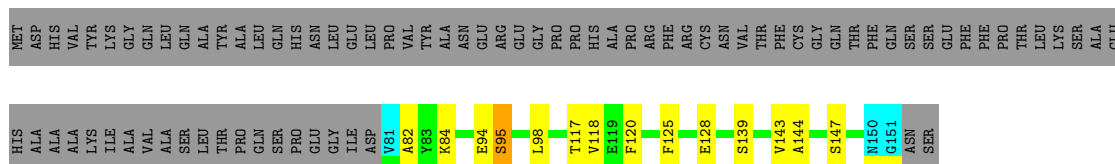
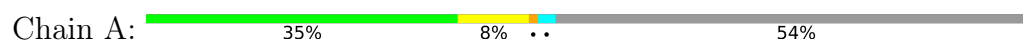
4.2.3 Score per residue for model 3

- Molecule 1: Double-stranded RNA-binding protein 4



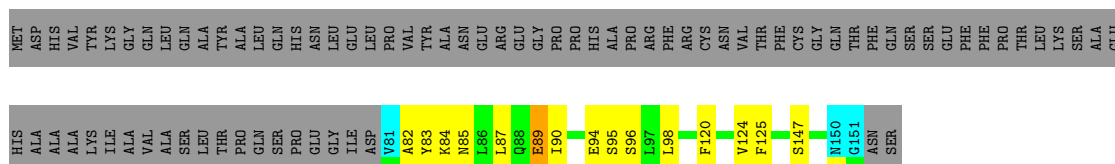
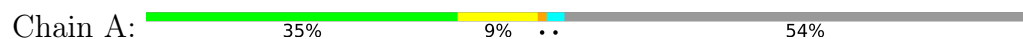
4.2.4 Score per residue for model 4

- Molecule 1: Double-stranded RNA-binding protein 4



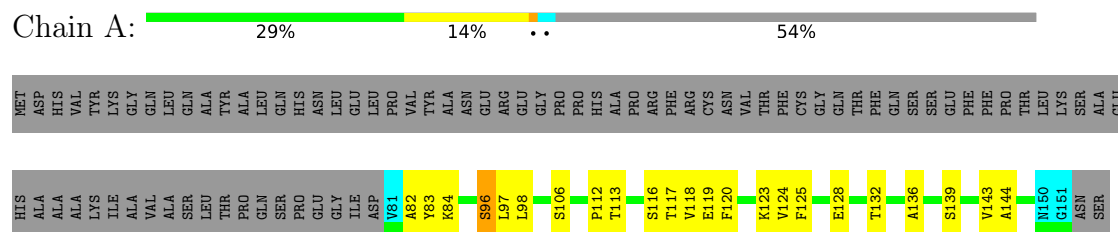
4.2.5 Score per residue for model 5

- Molecule 1: Double-stranded RNA-binding protein 4



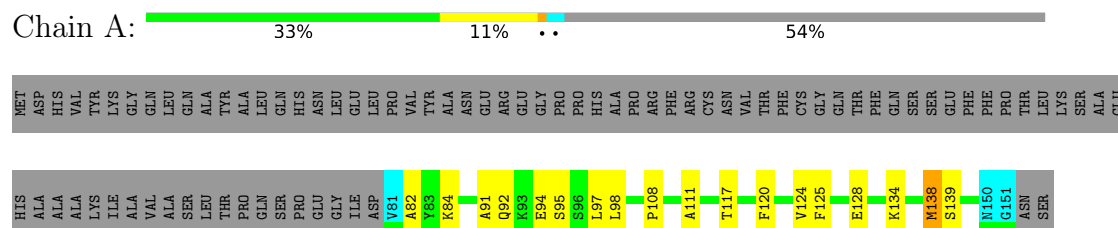
4.2.6 Score per residue for model 6

- Molecule 1: Double-stranded RNA-binding protein 4



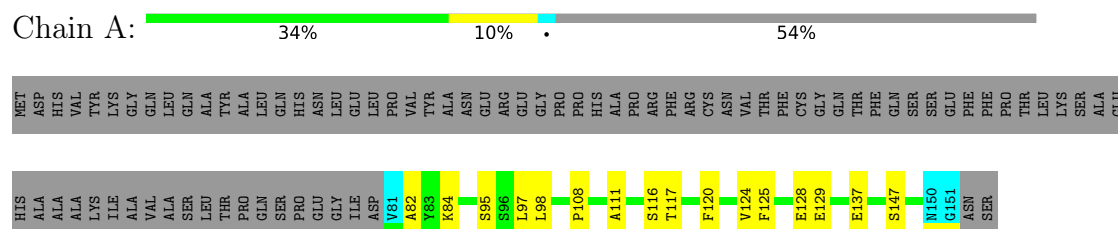
4.2.7 Score per residue for model 7

- Molecule 1: Double-stranded RNA-binding protein 4



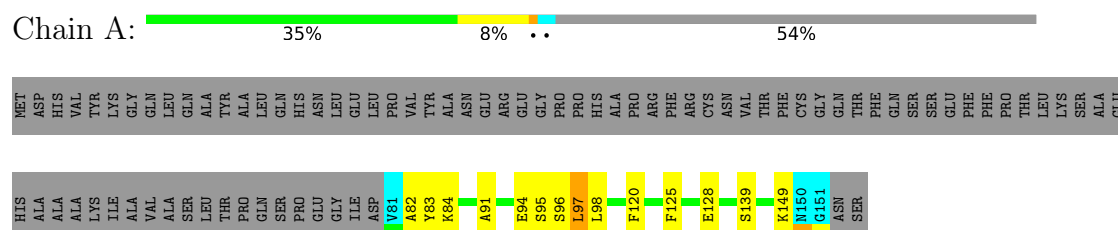
4.2.8 Score per residue for model 8

- Molecule 1: Double-stranded RNA-binding protein 4



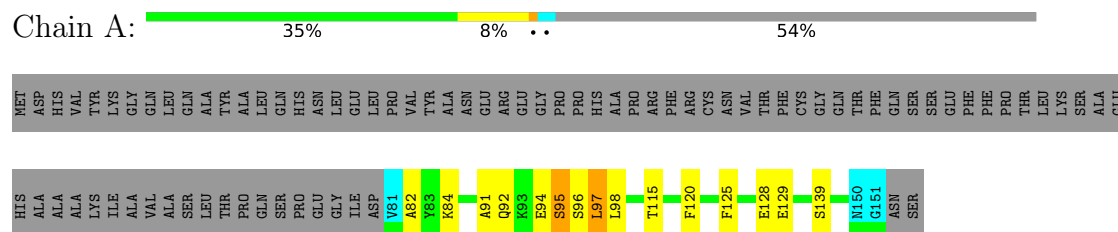
4.2.9 Score per residue for model 9

- Molecule 1: Double-stranded RNA-binding protein 4



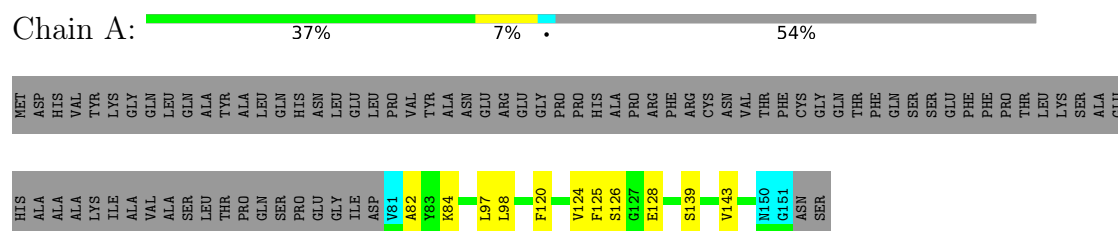
4.2.14 Score per residue for model 14

- Molecule 1: Double-stranded RNA-binding protein 4



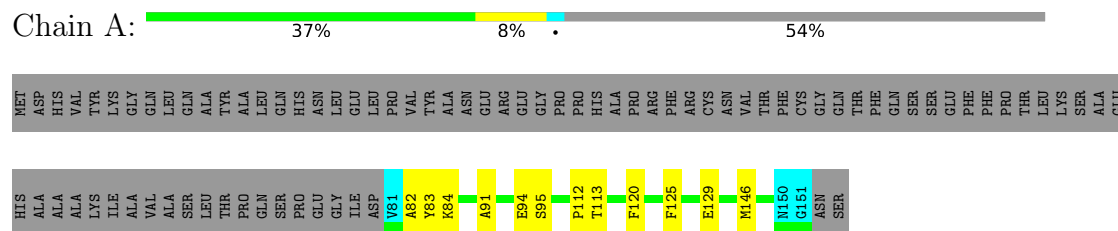
4.2.15 Score per residue for model 15

- Molecule 1: Double-stranded RNA-binding protein 4



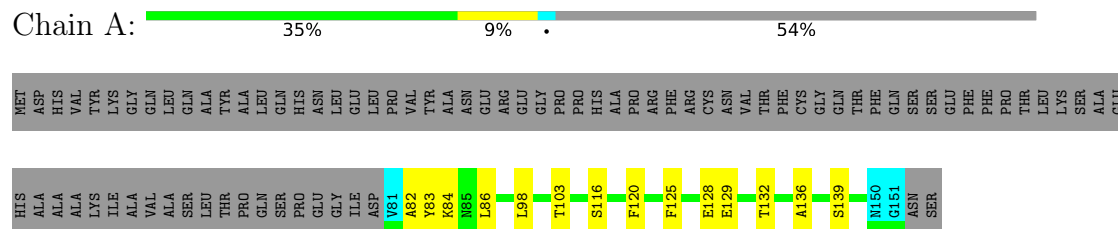
4.2.16 Score per residue for model 16

- Molecule 1: Double-stranded RNA-binding protein 4



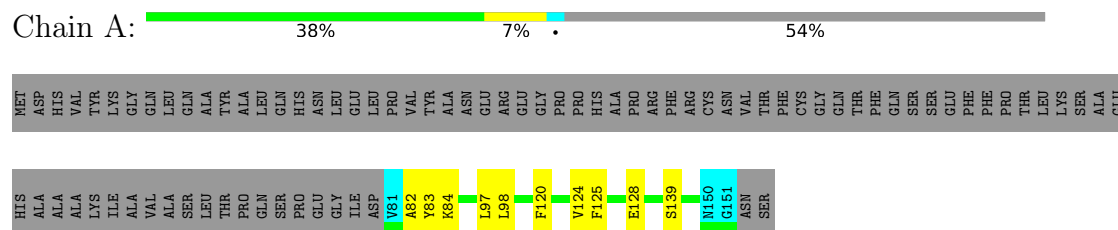
4.2.17 Score per residue for model 17

- Molecule 1: Double-stranded RNA-binding protein 4



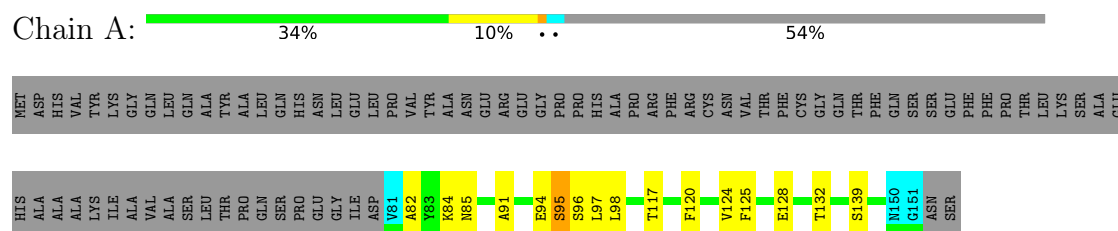
4.2.18 Score per residue for model 18

- Molecule 1: Double-stranded RNA-binding protein 4



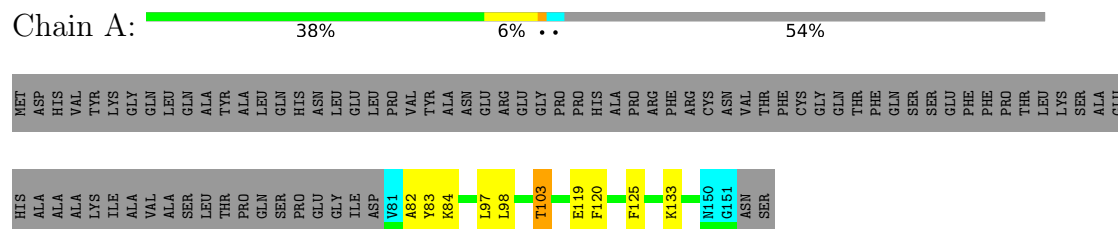
4.2.19 Score per residue for model 19

- Molecule 1: Double-stranded RNA-binding protein 4



4.2.20 Score per residue for model 20

- Molecule 1: Double-stranded RNA-binding protein 4



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
Sparky	structure solution	
Sparky	structure solution	
Sparky	structure solution	
Sparky	structure solution	
X-PLOR NIH	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	1658
Number of shifts mapped to atoms	788
Number of unparsed shifts	0
Number of shifts with mapping errors	870
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	512	521	521	16±3
All	All	10240	10420	10420	311

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:PHE:CZ	1:A:125:PHE:CE1	0.64	2.86	11	20
1:A:120:PHE:CE1	1:A:125:PHE:CD1	0.58	2.91	15	1
1:A:146:MET:N	1:A:146:MET:SD	0.58	2.76	3	1
1:A:138:MET:N	1:A:138:MET:SD	0.57	2.77	7	1
1:A:120:PHE:CE2	1:A:125:PHE:CD1	0.56	2.94	5	18
1:A:98:LEU:HD12	1:A:98:LEU:N	0.55	2.15	17	18
1:A:96:SER:OG	1:A:97:LEU:N	0.54	2.40	13	2
1:A:97:LEU:HD12	1:A:97:LEU:N	0.54	2.17	15	6
1:A:129:GLU:N	1:A:129:GLU:CD	0.54	2.66	16	2
1:A:129:GLU:N	1:A:129:GLU:OE1	0.54	2.41	2	1
1:A:82:ALA:C	1:A:84:LYS:N	0.54	2.66	5	20
1:A:129:GLU:CD	1:A:129:GLU:H	0.53	2.10	17	3
1:A:124:VAL:C	1:A:125:PHE:CD1	0.53	2.87	15	2
1:A:89:GLU:N	1:A:89:GLU:OE1	0.52	2.41	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:ALA:O	1:A:95:SER:N	0.52	2.43	9	5
1:A:128:GLU:H	1:A:139:SER:CB	0.51	2.18	6	3
1:A:142:LYS:O	1:A:146:MET:SD	0.51	2.68	3	1
1:A:146:MET:SD	1:A:146:MET:C	0.50	2.95	16	1
1:A:145:PHE:C	1:A:145:PHE:CD1	0.50	2.90	13	2
1:A:134:LYS:O	1:A:138:MET:SD	0.50	2.70	7	1
1:A:108:PRO:HG2	1:A:111:ALA:HB3	0.49	1.84	12	4
1:A:82:ALA:O	1:A:84:LYS:N	0.49	2.45	1	20
1:A:143:VAL:HG13	1:A:144:ALA:N	0.49	2.23	6	3
1:A:125:PHE:CD1	1:A:125:PHE:N	0.48	2.82	7	12
1:A:124:VAL:HG22	1:A:125:PHE:N	0.48	2.23	15	2
1:A:136:ALA:O	1:A:139:SER:OG	0.48	2.26	6	2
1:A:124:VAL:O	1:A:125:PHE:CD1	0.48	2.67	5	2
1:A:97:LEU:N	1:A:97:LEU:CD1	0.48	2.76	15	6
1:A:124:VAL:O	1:A:124:VAL:HG13	0.47	2.09	1	8
1:A:120:PHE:CE2	1:A:125:PHE:CE1	0.47	3.02	10	12
1:A:84:LYS:NZ	1:A:101:TYR:CE2	0.47	2.83	3	1
1:A:98:LEU:HD12	1:A:98:LEU:H	0.47	1.70	10	3
1:A:94:GLU:O	1:A:95:SER:CB	0.47	2.62	1	5
1:A:112:PRO:O	1:A:113:THR:HG23	0.47	2.10	11	7
1:A:106:SER:O	1:A:113:THR:O	0.46	2.33	6	1
1:A:98:LEU:H	1:A:98:LEU:CD1	0.46	2.22	10	4
1:A:94:GLU:C	1:A:96:SER:N	0.46	2.74	2	1
1:A:128:GLU:CG	1:A:129:GLU:N	0.46	2.78	10	3
1:A:129:GLU:CD	1:A:129:GLU:C	0.46	2.84	10	1
1:A:129:GLU:OE2	1:A:129:GLU:N	0.46	2.44	17	1
1:A:94:GLU:O	1:A:95:SER:C	0.46	2.59	9	5
1:A:82:ALA:C	1:A:84:LYS:H	0.45	2.20	13	20
1:A:117:THR:HG22	1:A:118:VAL:N	0.45	2.25	4	2
1:A:98:LEU:N	1:A:98:LEU:CD1	0.45	2.79	17	15
1:A:116:SER:OG	1:A:136:ALA:C	0.45	2.60	13	2
1:A:119:GLU:CD	1:A:119:GLU:C	0.44	2.85	20	1
1:A:96:SER:O	1:A:97:LEU:CB	0.44	2.65	9	3
1:A:117:THR:CG2	1:A:124:VAL:CG2	0.44	2.96	8	6
1:A:115:THR:OG1	1:A:129:GLU:CD	0.44	2.60	3	1
1:A:116:SER:OG	1:A:137:GLU:CD	0.44	2.61	3	3
1:A:128:GLU:CD	1:A:139:SER:OG	0.44	2.61	2	8
1:A:92:GLN:HE21	1:A:98:LEU:HD11	0.44	1.73	3	1
1:A:115:THR:OG1	1:A:129:GLU:OE1	0.44	2.36	14	2
1:A:85:ASN:O	1:A:89:GLU:CD	0.44	2.60	5	1
1:A:115:THR:OG1	1:A:129:GLU:OE2	0.44	2.36	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:SER:O	1:A:96:SER:O	0.44	2.36	2	1
1:A:92:GLN:CD	1:A:92:GLN:C	0.43	2.86	7	2
1:A:115:THR:HG1	1:A:129:GLU:CD	0.43	2.20	3	1
1:A:119:GLU:OE2	1:A:123:LYS:N	0.43	2.51	6	1
1:A:134:LYS:N	1:A:134:LYS:CD	0.42	2.82	11	2
1:A:128:GLU:O	1:A:128:GLU:CG	0.42	2.66	9	3
1:A:98:LEU:CD1	1:A:98:LEU:H	0.42	2.28	4	5
1:A:117:THR:CG2	1:A:118:VAL:N	0.42	2.82	4	1
1:A:103:THR:OG1	1:A:133:LYS:NZ	0.42	2.53	20	1
1:A:85:ASN:OD1	1:A:89:GLU:OE2	0.42	2.38	2	1
1:A:144:ALA:O	1:A:147:SER:OG	0.41	2.36	3	1
1:A:85:ASN:O	1:A:89:GLU:OE2	0.41	2.37	5	1
1:A:116:SER:OG	1:A:136:ALA:O	0.41	2.38	17	1
1:A:120:PHE:CD1	1:A:120:PHE:C	0.41	2.99	18	1
1:A:85:ASN:OD1	1:A:85:ASN:C	0.41	2.63	19	1
1:A:97:LEU:HD13	1:A:97:LEU:C	0.41	2.41	14	1
1:A:87:LEU:HD23	1:A:90:ILE:HD11	0.41	1.93	5	1
1:A:94:GLU:C	1:A:96:SER:H	0.41	2.23	2	1
1:A:128:GLU:OE2	1:A:139:SER:OG	0.41	2.37	19	1
1:A:126:SER:O	1:A:143:VAL:HG21	0.41	2.16	15	1
1:A:97:LEU:C	1:A:97:LEU:CD1	0.40	2.94	14	1
1:A:124:VAL:CG2	1:A:125:PHE:N	0.40	2.83	15	1
1:A:124:VAL:HG13	1:A:124:VAL:O	0.40	2.16	10	1
1:A:112:PRO:O	1:A:113:THR:CG2	0.40	2.69	11	2

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	68/153 (44%)	63±1 (93±2%)	4±2 (6±2%)	1±1 (2±1%)	11	57
All	All	1360/3060 (44%)	1259 (93%)	80 (6%)	21 (2%)	11	57

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

Mol	Chain	Res	Type	Models (Total)
1	A	83	TYR	14
1	A	96	SER	5
1	A	95	SER	2

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	54/124 (44%)	53±1 (98±2%)	1±1 (2±2%)	52	92
All	All	1080/2480 (44%)	1062 (98%)	18 (2%)	52	92

All 9 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	95	SER	4
1	A	103	THR	3
1	A	132	THR	3
1	A	97	LEU	2
1	A	86	LEU	2
1	A	114	PHE	1
1	A	146	MET	1
1	A	89	GLU	1
1	A	138	MET	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 86% 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	1658
Number of shifts mapped to atoms	788
Number of unparsed shifts	0
Number of shifts with mapping errors	870
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- No matching atom found in the structure. All 870 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	HIS	HA	3.68	0.02	1
1	A	3	HIS	HB2	2.58	0.02	2
1	A	3	HIS	HB3	2.2	0.02	2
1	A	3	HIS	C	175.9	0.3	1
1	A	3	HIS	CA	54.1	0.3	1
1	A	3	HIS	CB	28.2	0.3	1
1	A	4	VAL	H	6.86	0.02	1
1	A	4	VAL	HA	4.37	0.02	1
1	A	4	VAL	HB	1.99	0.02	1
1	A	4	VAL	HG11	0.48	0.02	1
1	A	4	VAL	HG12	0.48	0.02	1
1	A	4	VAL	HG13	0.48	0.02	1
1	A	4	VAL	HG21	-0.17	0.02	1
1	A	4	VAL	HG22	-0.17	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	VAL	HG23	-0.17	0.02	1
1	A	4	VAL	C	177.1	0.3	1
1	A	4	VAL	CA	60.4	0.3	1
1	A	4	VAL	CB	32.7	0.3	1
1	A	4	VAL	CG1	20.7	0.3	1
1	A	4	VAL	CG2	16.6	0.3	1
1	A	4	VAL	N	111.8	0.3	1
1	A	5	TYR	H	8.26	0.02	1
1	A	5	TYR	HA	4.19	0.02	1
1	A	5	TYR	HB2	3.09	0.02	2
1	A	5	TYR	HB3	2.75	0.02	2
1	A	5	TYR	HD1	6.94	0.02	3
1	A	5	TYR	HD2	7.01	0.02	3
1	A	5	TYR	C	177.9	0.3	1
1	A	5	TYR	CA	62.3	0.3	1
1	A	5	TYR	CB	39.6	0.3	1
1	A	5	TYR	N	123.6	0.3	1
1	A	6	LYS	H	8.48	0.02	1
1	A	6	LYS	C	180.5	0.3	1
1	A	6	LYS	CA	60.6	0.3	1
1	A	6	LYS	CB	31.6	0.3	1
1	A	6	LYS	N	121.2	0.3	1
1	A	7	GLY	H	8.7	0.02	1
1	A	7	GLY	HA2	3.71	0.02	2
1	A	7	GLY	HA3	3.78	0.02	2
1	A	7	GLY	C	176.5	0.3	1
1	A	7	GLY	CA	46.5	0.3	1
1	A	7	GLY	N	108.8	0.3	1
1	A	8	GLN	H	7.29	0.02	1
1	A	8	GLN	HA	4.03	0.02	1
1	A	8	GLN	HB2	2.08	0.02	2
1	A	8	GLN	HB3	2.19	0.02	2
1	A	8	GLN	HE21	6.94	0.02	1
1	A	8	GLN	HE22	6.45	0.02	1
1	A	8	GLN	HG2	2.48	0.02	1
1	A	8	GLN	HG3	2.48	0.02	1
1	A	8	GLN	C	178.9	0.3	1
1	A	8	GLN	CA	58.8	0.3	1
1	A	8	GLN	CB	28.5	0.3	1
1	A	8	GLN	CG	33.7	0.3	1
1	A	8	GLN	N	122.9	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	8	GLN	NE2	109.6	0.3	1
1	A	9	LEU	H	7.73	0.02	1
1	A	9	LEU	HA	3.8	0.02	1
1	A	9	LEU	HB2	1.22	0.02	2
1	A	9	LEU	HB3	1.45	0.02	2
1	A	9	LEU	HD11	0.18	0.02	1
1	A	9	LEU	HD12	0.18	0.02	1
1	A	9	LEU	HD13	0.18	0.02	1
1	A	9	LEU	HD21	0.37	0.02	1
1	A	9	LEU	HD22	0.37	0.02	1
1	A	9	LEU	HD23	0.37	0.02	1
1	A	9	LEU	HG	0.99	0.02	1
1	A	9	LEU	C	177.4	0.3	1
1	A	9	LEU	CA	57.1	0.3	1
1	A	9	LEU	CB	41.0	0.3	1
1	A	9	LEU	CD1	23.0	0.3	1
1	A	9	LEU	CD2	24.8	0.3	1
1	A	9	LEU	CG	26.1	0.3	1
1	A	9	LEU	N	121.7	0.3	1
1	A	10	GLN	H	7.75	0.02	1
1	A	10	GLN	HA	3.63	0.02	1
1	A	10	GLN	HB2	2.05	0.02	1
1	A	10	GLN	HB3	2.05	0.02	1
1	A	10	GLN	HE21	7.11	0.02	1
1	A	10	GLN	HE22	6.64	0.02	1
1	A	10	GLN	HG2	1.44	0.02	1
1	A	10	GLN	HG3	1.44	0.02	1
1	A	10	GLN	C	176.9	0.3	1
1	A	10	GLN	CA	59.5	0.3	1
1	A	10	GLN	CB	28.3	0.3	1
1	A	10	GLN	CG	33.4	0.3	1
1	A	10	GLN	N	119.0	0.3	1
1	A	10	GLN	NE2	111.7	0.3	1
1	A	11	ALA	H	8.09	0.02	1
1	A	11	ALA	HA	3.84	0.02	1
1	A	11	ALA	HB1	1.4	0.02	1
1	A	11	ALA	HB2	1.4	0.02	1
1	A	11	ALA	HB3	1.4	0.02	1
1	A	11	ALA	C	180.0	0.3	1
1	A	11	ALA	CA	55.0	0.3	1
1	A	11	ALA	CB	17.6	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	11	ALA	N	120.6	0.3	1
1	A	12	TYR	H	7.75	0.02	1
1	A	12	TYR	HA	4.13	0.02	1
1	A	12	TYR	HB2	3.14	0.02	2
1	A	12	TYR	HB3	3.08	0.02	2
1	A	12	TYR	HD1	7.04	0.02	1
1	A	12	TYR	HD2	7.04	0.02	1
1	A	12	TYR	HE1	7.04	0.02	1
1	A	12	TYR	HE2	7.04	0.02	1
1	A	12	TYR	C	177.7	0.3	1
1	A	12	TYR	CA	61.9	0.3	1
1	A	12	TYR	CB	38.3	0.3	1
1	A	12	TYR	N	120.8	0.3	1
1	A	13	ALA	H	8.26	0.02	1
1	A	13	ALA	HA	4.1	0.02	1
1	A	13	ALA	HB1	1.67	0.02	1
1	A	13	ALA	HB2	1.67	0.02	1
1	A	13	ALA	HB3	1.67	0.02	1
1	A	13	ALA	C	179.5	0.3	1
1	A	13	ALA	CA	55.8	0.3	1
1	A	13	ALA	CB	18.0	0.3	1
1	A	13	ALA	N	122.2	0.3	1
1	A	14	LEU	H	8.25	0.02	1
1	A	14	LEU	HA	4.09	0.02	1
1	A	14	LEU	HB2	1.46	0.02	1
1	A	14	LEU	HB3	1.46	0.02	1
1	A	14	LEU	HD11	0.84	0.02	1
1	A	14	LEU	HD12	0.84	0.02	1
1	A	14	LEU	HD13	0.84	0.02	1
1	A	14	LEU	HD21	0.84	0.02	1
1	A	14	LEU	HD22	0.84	0.02	1
1	A	14	LEU	HD23	0.84	0.02	1
1	A	14	LEU	HG	1.77	0.02	1
1	A	14	LEU	C	180.6	0.3	1
1	A	14	LEU	CA	57.3	0.3	1
1	A	14	LEU	CB	41.5	0.3	1
1	A	14	LEU	CD1	22.8	0.3	1
1	A	14	LEU	CD2	25.1	0.3	1
1	A	14	LEU	CG	26.6	0.3	1
1	A	14	LEU	N	117.6	0.3	1
1	A	15	GLN	H	8.11	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	15	GLN	HA	3.79	0.02	1
1	A	15	GLN	HB2	1.59	0.02	2
1	A	15	GLN	HB3	1.69	0.02	2
1	A	15	GLN	HG2	1.92	0.02	1
1	A	15	GLN	HG3	1.92	0.02	1
1	A	15	GLN	C	176.7	0.3	1
1	A	15	GLN	CA	58.0	0.3	1
1	A	15	GLN	CB	28.1	0.3	1
1	A	15	GLN	CG	32.9	0.3	1
1	A	15	GLN	N	120.0	0.3	1
1	A	16	HIS	H	7.25	0.02	1
1	A	16	HIS	HA	4.46	0.02	1
1	A	16	HIS	HB2	3.19	0.02	2
1	A	16	HIS	HB3	2.32	0.02	2
1	A	16	HIS	C	173.1	0.3	1
1	A	16	HIS	CA	55.9	0.3	1
1	A	16	HIS	CB	29.5	0.3	1
1	A	16	HIS	N	114.2	0.3	1
1	A	17	ASN	H	7.63	0.02	1
1	A	17	ASN	HA	4.33	0.02	1
1	A	17	ASN	HB2	2.65	0.02	2
1	A	17	ASN	HB3	3.0	0.02	2
1	A	17	ASN	C	173.8	0.3	1
1	A	17	ASN	CA	54.3	0.3	1
1	A	17	ASN	CB	36.6	0.3	1
1	A	17	ASN	N	118.2	0.3	1
1	A	18	LEU	H	8.53	0.02	1
1	A	18	LEU	HA	4.55	0.02	1
1	A	18	LEU	HB2	1.57	0.02	1
1	A	18	LEU	HB3	1.57	0.02	1
1	A	18	LEU	HD11	0.84	0.02	1
1	A	18	LEU	HD12	0.84	0.02	1
1	A	18	LEU	HD13	0.84	0.02	1
1	A	18	LEU	HD21	0.75	0.02	1
1	A	18	LEU	HD22	0.75	0.02	1
1	A	18	LEU	HD23	0.75	0.02	1
1	A	18	LEU	HG	1.47	0.02	1
1	A	18	LEU	C	176.4	0.3	1
1	A	18	LEU	CA	52.8	0.3	1
1	A	18	LEU	CB	44.2	0.3	1
1	A	18	LEU	CD1	22.0	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	18	LEU	CD2	22.2	0.3	1
1	A	18	LEU	CG	26.5	0.3	1
1	A	18	LEU	N	119.5	0.3	1
1	A	19	GLU	H	8.07	0.02	1
1	A	19	GLU	HA	4.01	0.02	1
1	A	19	GLU	HB2	1.95	0.02	2
1	A	19	GLU	HB3	1.86	0.02	2
1	A	19	GLU	HG2	2.3	0.02	1
1	A	19	GLU	HG3	2.3	0.02	1
1	A	19	GLU	C	176.6	0.3	1
1	A	19	GLU	CA	56.7	0.3	1
1	A	19	GLU	CB	29.3	0.3	1
1	A	19	GLU	CG	36.5	0.3	1
1	A	19	GLU	N	120.6	0.3	1
1	A	20	LEU	H	8.18	0.02	1
1	A	20	LEU	HA	4.37	0.02	1
1	A	20	LEU	HB2	1.67	0.02	1
1	A	20	LEU	HB3	1.67	0.02	1
1	A	20	LEU	HD11	0.92	0.02	1
1	A	20	LEU	HD12	0.92	0.02	1
1	A	20	LEU	HD13	0.92	0.02	1
1	A	20	LEU	HD21	0.92	0.02	1
1	A	20	LEU	HD22	0.92	0.02	1
1	A	20	LEU	HD23	0.92	0.02	1
1	A	20	LEU	C	175.5	0.3	1
1	A	20	LEU	CA	54.0	0.3	1
1	A	20	LEU	CB	39.4	0.3	1
1	A	20	LEU	N	122.5	0.3	1
1	A	21	PRO	HA	4.63	0.02	1
1	A	21	PRO	HB2	1.89	0.02	1
1	A	21	PRO	HB3	1.89	0.02	1
1	A	21	PRO	HD2	3.56	0.02	2
1	A	21	PRO	HD3	3.59	0.02	2
1	A	21	PRO	HG2	1.85	0.02	1
1	A	21	PRO	HG3	1.85	0.02	1
1	A	21	PRO	C	175.0	0.3	1
1	A	21	PRO	CA	62.4	0.3	1
1	A	21	PRO	CB	32.7	0.3	1
1	A	21	PRO	CD	49.8	0.3	1
1	A	21	PRO	CG	27.2	0.3	1
1	A	22	VAL	H	7.97	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	22	VAL	HA	4.3	0.02	1
1	A	22	VAL	HB	1.74	0.02	1
1	A	22	VAL	HG11	0.84	0.02	1
1	A	22	VAL	HG12	0.84	0.02	1
1	A	22	VAL	HG13	0.84	0.02	1
1	A	22	VAL	HG21	0.92	0.02	1
1	A	22	VAL	HG22	0.92	0.02	1
1	A	22	VAL	HG23	0.92	0.02	1
1	A	22	VAL	C	175.5	0.3	1
1	A	22	VAL	CA	61.3	0.3	1
1	A	22	VAL	CB	34.5	0.3	1
1	A	22	VAL	CG1	20.8	0.3	1
1	A	22	VAL	CG2	20.8	0.3	1
1	A	22	VAL	N	121.0	0.3	1
1	A	23	TYR	H	9.24	0.02	1
1	A	23	TYR	HA	4.82	0.02	1
1	A	23	TYR	HB2	2.77	0.02	1
1	A	23	TYR	HB3	2.77	0.02	1
1	A	23	TYR	HD1	6.88	0.02	1
1	A	23	TYR	HD2	6.88	0.02	1
1	A	23	TYR	HE1	6.88	0.02	1
1	A	23	TYR	HE2	6.88	0.02	1
1	A	23	TYR	C	174.7	0.3	1
1	A	23	TYR	CA	58.1	0.3	1
1	A	23	TYR	CB	40.0	0.3	1
1	A	23	TYR	N	131.0	0.3	1
1	A	24	ALA	H	8.7	0.02	1
1	A	24	ALA	HA	4.73	0.02	1
1	A	24	ALA	HB1	1.35	0.02	1
1	A	24	ALA	HB2	1.35	0.02	1
1	A	24	ALA	HB3	1.35	0.02	1
1	A	24	ALA	C	175.6	0.3	1
1	A	24	ALA	CA	51.2	0.3	1
1	A	24	ALA	CB	21.4	0.3	1
1	A	24	ALA	N	127.2	0.3	1
1	A	25	ASN	H	8.78	0.02	1
1	A	25	ASN	HA	5.68	0.02	1
1	A	25	ASN	HB2	2.62	0.02	2
1	A	25	ASN	HB3	2.44	0.02	2
1	A	25	ASN	HD21	7.66	0.02	1
1	A	25	ASN	HD22	6.81	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	25	ASN	C	173.5	0.3	1
1	A	25	ASN	CA	52.2	0.3	1
1	A	25	ASN	CB	44.6	0.3	1
1	A	25	ASN	N	117.0	0.3	1
1	A	25	ASN	ND2	116.4	0.3	1
1	A	26	GLU	H	8.88	0.02	1
1	A	26	GLU	HA	4.59	0.02	1
1	A	26	GLU	HB2	1.91	0.02	1
1	A	26	GLU	HB3	1.91	0.02	1
1	A	26	GLU	HG2	2.18	0.02	1
1	A	26	GLU	HG3	2.18	0.02	1
1	A	26	GLU	C	173.8	0.3	1
1	A	26	GLU	CA	54.7	0.3	1
1	A	26	GLU	CB	33.5	0.3	1
1	A	26	GLU	CG	36.2	0.3	1
1	A	26	GLU	N	121.3	0.3	1
1	A	27	ARG	H	8.48	0.02	1
1	A	27	ARG	HA	5.28	0.02	1
1	A	27	ARG	HB2	1.51	0.02	1
1	A	27	ARG	HB3	1.51	0.02	1
1	A	27	ARG	HD2	2.96	0.02	2
1	A	27	ARG	HD3	2.91	0.02	2
1	A	27	ARG	HG2	1.15	0.02	2
1	A	27	ARG	HG3	0.99	0.02	2
1	A	27	ARG	C	175.3	0.3	1
1	A	27	ARG	CA	53.9	0.3	1
1	A	27	ARG	CB	33.0	0.3	1
1	A	27	ARG	CD	43.4	0.3	1
1	A	27	ARG	CG	26.2	0.3	1
1	A	27	ARG	N	123.4	0.3	1
1	A	28	GLU	H	8.74	0.02	1
1	A	28	GLU	HA	4.53	0.02	1
1	A	28	GLU	HB2	1.36	0.02	1
1	A	28	GLU	HB3	1.36	0.02	1
1	A	28	GLU	HG2	1.71	0.02	2
1	A	28	GLU	HG3	1.83	0.02	2
1	A	28	GLU	C	174.8	0.3	1
1	A	28	GLU	CA	54.3	0.3	1
1	A	28	GLU	CB	33.1	0.3	1
1	A	28	GLU	CG	35.5	0.3	1
1	A	28	GLU	N	125.4	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	29	GLY	H	8.14	0.02	1
1	A	29	GLY	HA2	4.26	0.02	2
1	A	29	GLY	HA3	3.61	0.02	2
1	A	29	GLY	C	171.0	0.3	1
1	A	29	GLY	CA	43.6	0.3	1
1	A	29	GLY	N	107.9	0.3	1
1	A	31	PRO	HA	3.97	0.02	1
1	A	31	PRO	HB2	2.25	0.02	2
1	A	31	PRO	HB3	2.08	0.02	2
1	A	31	PRO	HD2	3.72	0.02	2
1	A	31	PRO	HD3	3.68	0.02	2
1	A	31	PRO	HG2	1.95	0.02	2
1	A	31	PRO	HG3	1.88	0.02	2
1	A	31	PRO	C	177.2	0.3	1
1	A	31	PRO	CA	65.1	0.3	1
1	A	31	PRO	CB	31.5	0.3	1
1	A	31	PRO	CG	27.5	0.3	1
1	A	32	HIS	H	7.35	0.02	1
1	A	32	HIS	HA	4.52	0.02	1
1	A	32	HIS	HB2	3.24	0.02	2
1	A	32	HIS	HB3	2.87	0.02	2
1	A	32	HIS	C	175.1	0.3	1
1	A	32	HIS	CA	55.7	0.3	1
1	A	32	HIS	CB	30.0	0.3	1
1	A	32	HIS	N	110.4	0.3	1
1	A	33	ALA	H	7.24	0.02	1
1	A	33	ALA	HA	4.53	0.02	1
1	A	33	ALA	HB1	0.87	0.02	1
1	A	33	ALA	HB2	0.87	0.02	1
1	A	33	ALA	HB3	0.87	0.02	1
1	A	33	ALA	C	175.1	0.3	1
1	A	33	ALA	CA	50.5	0.3	1
1	A	33	ALA	CB	18.3	0.3	1
1	A	33	ALA	N	125.9	0.3	1
1	A	34	PRO	HA	4.31	0.02	1
1	A	34	PRO	HB2	1.71	0.02	1
1	A	34	PRO	HB3	1.71	0.02	1
1	A	34	PRO	HD2	3.38	0.02	2
1	A	34	PRO	HD3	3.29	0.02	2
1	A	34	PRO	HG2	1.2	0.02	1
1	A	34	PRO	HG3	1.2	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	34	PRO	C	175.7	0.3	1
1	A	34	PRO	CA	62.6	0.3	1
1	A	34	PRO	CB	32.2	0.3	1
1	A	34	PRO	CD	49.3	0.3	1
1	A	34	PRO	CG	26.6	0.3	1
1	A	35	ARG	H	8.14	0.02	1
1	A	35	ARG	HA	4.74	0.02	1
1	A	35	ARG	HB2	1.33	0.02	1
1	A	35	ARG	HB3	1.33	0.02	1
1	A	35	ARG	HD2	2.62	0.02	2
1	A	35	ARG	HD3	2.85	0.02	2
1	A	35	ARG	HG2	1.24	0.02	1
1	A	35	ARG	HG3	1.24	0.02	1
1	A	35	ARG	C	174.6	0.3	1
1	A	35	ARG	CA	54.1	0.3	1
1	A	35	ARG	CB	33.1	0.3	1
1	A	35	ARG	CD	43.2	0.3	1
1	A	35	ARG	CG	26.7	0.3	1
1	A	35	ARG	N	117.1	0.3	1
1	A	36	PHE	H	9.42	0.02	1
1	A	36	PHE	HA	5.7	0.02	1
1	A	36	PHE	HB2	2.7	0.02	1
1	A	36	PHE	HB3	2.7	0.02	1
1	A	36	PHE	HD1	6.91	0.02	1
1	A	36	PHE	HD2	6.91	0.02	1
1	A	36	PHE	HE1	6.91	0.02	1
1	A	36	PHE	HE2	6.91	0.02	1
1	A	36	PHE	C	174.7	0.3	1
1	A	36	PHE	CA	57.2	0.3	1
1	A	36	PHE	CB	43.9	0.3	1
1	A	36	PHE	N	119.0	0.3	1
1	A	37	ARG	H	8.78	0.02	1
1	A	37	ARG	HA	4.97	0.02	1
1	A	37	ARG	HD2	2.93	0.02	2
1	A	37	ARG	HD3	2.88	0.02	2
1	A	37	ARG	HG2	0.92	0.02	2
1	A	37	ARG	HG3	0.96	0.02	2
1	A	37	ARG	C	176.0	0.3	1
1	A	37	ARG	CA	55.1	0.3	1
1	A	37	ARG	CB	34.0	0.3	1
1	A	37	ARG	CD	43.9	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	37	ARG	CG	25.9	0.3	1
1	A	37	ARG	N	122.9	0.3	1
1	A	38	CYS	H	9.34	0.02	1
1	A	38	CYS	HA	5.59	0.02	1
1	A	38	CYS	HB2	2.95	0.02	2
1	A	38	CYS	HB3	2.59	0.02	2
1	A	38	CYS	C	172.8	0.3	1
1	A	38	CYS	CA	58.2	0.3	1
1	A	38	CYS	CB	31.5	0.3	1
1	A	38	CYS	N	126.0	0.3	1
1	A	39	ASN	H	8.56	0.02	1
1	A	39	ASN	HA	5.32	0.02	1
1	A	39	ASN	HB2	2.47	0.02	1
1	A	39	ASN	HB3	2.47	0.02	1
1	A	39	ASN	HD21	7.3	0.02	1
1	A	39	ASN	HD22	6.69	0.02	1
1	A	39	ASN	C	172.8	0.3	1
1	A	39	ASN	CA	50.9	0.3	1
1	A	39	ASN	CB	42.4	0.3	1
1	A	39	ASN	N	118.7	0.3	1
1	A	39	ASN	ND2	115.7	0.3	1
1	A	40	VAL	H	8.8	0.02	1
1	A	40	VAL	HA	4.91	0.02	1
1	A	40	VAL	HB	1.48	0.02	1
1	A	40	VAL	HG11	0.66	0.02	1
1	A	40	VAL	HG12	0.66	0.02	1
1	A	40	VAL	HG13	0.66	0.02	1
1	A	40	VAL	HG21	-0.09	0.02	1
1	A	40	VAL	HG22	-0.09	0.02	1
1	A	40	VAL	HG23	-0.09	0.02	1
1	A	40	VAL	C	172.6	0.3	1
1	A	40	VAL	CA	58.1	0.3	1
1	A	40	VAL	CB	34.9	0.3	1
1	A	40	VAL	CG1	20.8	0.3	1
1	A	40	VAL	CG2	22.5	0.3	1
1	A	40	VAL	N	119.1	0.3	1
1	A	41	THR	H	8.86	0.02	1
1	A	41	THR	HA	5.36	0.02	1
1	A	41	THR	HB	3.76	0.02	1
1	A	41	THR	HG21	0.89	0.02	1
1	A	41	THR	HG22	0.89	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	41	THR	HG23	0.89	0.02	1
1	A	41	THR	C	174.2	0.3	1
1	A	41	THR	CA	61.4	0.3	1
1	A	41	THR	CB	69.5	0.3	1
1	A	41	THR	CG2	20.0	0.3	1
1	A	41	THR	N	126.8	0.3	1
1	A	42	PHE	H	9.4	0.02	1
1	A	42	PHE	HA	4.9	0.02	1
1	A	42	PHE	HB2	2.97	0.02	2
1	A	42	PHE	HB3	2.62	0.02	2
1	A	42	PHE	HD1	7.1	0.02	1
1	A	42	PHE	HD2	7.1	0.02	1
1	A	42	PHE	HE1	7.1	0.02	1
1	A	42	PHE	HE2	7.1	0.02	1
1	A	42	PHE	C	173.5	0.3	1
1	A	42	PHE	CA	56.5	0.3	1
1	A	42	PHE	CB	42.1	0.3	1
1	A	42	PHE	N	129.0	0.3	1
1	A	43	CYS	H	9.26	0.02	1
1	A	43	CYS	HA	3.59	0.02	1
1	A	43	CYS	HB2	2.79	0.02	2
1	A	43	CYS	HB3	2.29	0.02	2
1	A	43	CYS	C	174.8	0.3	1
1	A	43	CYS	CA	60.6	0.3	1
1	A	43	CYS	CB	25.2	0.3	1
1	A	43	CYS	N	126.0	0.3	1
1	A	44	GLY	H	8.66	0.02	1
1	A	44	GLY	HA2	3.88	0.02	2
1	A	44	GLY	HA3	3.42	0.02	2
1	A	44	GLY	C	173.1	0.3	1
1	A	44	GLY	CA	45.2	0.3	1
1	A	44	GLY	N	104.8	0.3	1
1	A	45	GLN	H	7.53	0.02	1
1	A	45	GLN	HA	4.36	0.02	1
1	A	45	GLN	HB2	1.41	0.02	1
1	A	45	GLN	HB3	1.41	0.02	1
1	A	45	GLN	HG2	1.75	0.02	2
1	A	45	GLN	HG3	1.85	0.02	2
1	A	45	GLN	C	173.0	0.3	1
1	A	45	GLN	CA	53.7	0.3	1
1	A	45	GLN	CB	32.2	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	45	GLN	CG	33.5	0.3	1
1	A	45	GLN	N	120.7	0.3	1
1	A	46	THR	H	8.29	0.02	1
1	A	46	THR	HA	4.77	0.02	1
1	A	46	THR	HB	3.55	0.02	1
1	A	46	THR	HG21	0.85	0.02	1
1	A	46	THR	HG22	0.85	0.02	1
1	A	46	THR	HG23	0.85	0.02	1
1	A	46	THR	C	173.2	0.3	1
1	A	46	THR	CA	61.9	0.3	1
1	A	46	THR	CB	69.7	0.3	1
1	A	46	THR	CG2	21.6	0.3	1
1	A	46	THR	N	119.0	0.3	1
1	A	47	PHE	H	9.38	0.02	1
1	A	47	PHE	HA	4.54	0.02	1
1	A	47	PHE	HB2	2.9	0.02	2
1	A	47	PHE	HB3	2.66	0.02	2
1	A	47	PHE	HD1	7.13	0.02	1
1	A	47	PHE	HD2	7.13	0.02	1
1	A	47	PHE	HE1	7.13	0.02	1
1	A	47	PHE	HE2	7.13	0.02	1
1	A	47	PHE	C	173.9	0.3	1
1	A	47	PHE	CA	56.6	0.3	1
1	A	47	PHE	CB	38.8	0.3	1
1	A	47	PHE	N	128.8	0.3	1
1	A	48	GLN	H	8.92	0.02	1
1	A	48	GLN	HA	4.44	0.02	1
1	A	48	GLN	HB2	2.11	0.02	2
1	A	48	GLN	HB3	1.83	0.02	2
1	A	48	GLN	HE21	7.79	0.02	1
1	A	48	GLN	HE22	7.25	0.02	1
1	A	48	GLN	C	174.9	0.3	1
1	A	48	GLN	CA	54.2	0.3	1
1	A	48	GLN	CB	32.0	0.3	1
1	A	48	GLN	N	124.8	0.3	1
1	A	48	GLN	NE2	116.9	0.3	1
1	A	49	SER	H	7.95	0.02	1
1	A	49	SER	C	175.2	0.3	1
1	A	49	SER	CA	57.5	0.3	1
1	A	49	SER	CB	63.3	0.3	1
1	A	49	SER	N	120.3	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	50	SER	HA	4.41	0.02	1
1	A	50	SER	HB2	3.94	0.02	2
1	A	50	SER	HB3	3.84	0.02	2
1	A	50	SER	C	174.3	0.3	1
1	A	50	SER	CA	59.1	0.3	1
1	A	50	SER	CB	63.7	0.3	1
1	A	51	GLU	H	7.71	0.02	1
1	A	51	GLU	HA	4.3	0.02	1
1	A	51	GLU	HB2	1.65	0.02	1
1	A	51	GLU	HB3	1.65	0.02	1
1	A	51	GLU	HG2	2.02	0.02	1
1	A	51	GLU	HG3	2.02	0.02	1
1	A	51	GLU	C	173.4	0.3	1
1	A	51	GLU	CA	55.4	0.3	1
1	A	51	GLU	CB	32.6	0.3	1
1	A	51	GLU	CG	36.6	0.3	1
1	A	51	GLU	N	123.3	0.3	1
1	A	52	PHE	H	8.1	0.02	1
1	A	52	PHE	HA	5.03	0.02	1
1	A	52	PHE	HB2	2.66	0.02	2
1	A	52	PHE	HB3	2.55	0.02	2
1	A	52	PHE	HD1	6.88	0.02	1
1	A	52	PHE	HD2	6.88	0.02	1
1	A	52	PHE	HE1	6.88	0.02	1
1	A	52	PHE	HE2	6.88	0.02	1
1	A	52	PHE	C	176.4	0.3	1
1	A	52	PHE	CA	56.7	0.3	1
1	A	52	PHE	CB	41.7	0.3	1
1	A	52	PHE	N	117.9	0.3	1
1	A	53	PHE	H	9.7	0.02	1
1	A	53	PHE	HA	4.86	0.02	1
1	A	53	PHE	HB2	3.3	0.02	1
1	A	53	PHE	HB3	3.3	0.02	1
1	A	53	PHE	HD1	7.29	0.02	1
1	A	53	PHE	HD2	7.29	0.02	1
1	A	53	PHE	HE1	7.29	0.02	1
1	A	53	PHE	HE2	7.29	0.02	1
1	A	53	PHE	C	175.2	0.3	1
1	A	53	PHE	CA	56.2	0.3	1
1	A	53	PHE	CB	43.0	0.3	1
1	A	53	PHE	N	119.3	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	54	PRO	HA	4.89	0.02	1
1	A	54	PRO	HB2	2.41	0.02	1
1	A	54	PRO	HB3	2.41	0.02	1
1	A	54	PRO	HD2	3.68	0.02	1
1	A	54	PRO	HD3	3.68	0.02	1
1	A	54	PRO	HG2	2.21	0.02	1
1	A	54	PRO	HG3	2.21	0.02	1
1	A	54	PRO	C	175.9	0.3	1
1	A	54	PRO	CA	63.9	0.3	1
1	A	54	PRO	CB	32.4	0.3	1
1	A	54	PRO	CG	27.1	0.3	1
1	A	55	THR	H	7.03	0.02	1
1	A	55	THR	HA	4.61	0.02	1
1	A	55	THR	HB	4.28	0.02	1
1	A	55	THR	HG21	1.21	0.02	1
1	A	55	THR	HG22	1.21	0.02	1
1	A	55	THR	HG23	1.21	0.02	1
1	A	55	THR	C	173.0	0.3	1
1	A	55	THR	CA	58.3	0.3	1
1	A	55	THR	CB	72.0	0.3	1
1	A	55	THR	CG2	21.6	0.3	1
1	A	55	THR	N	104.8	0.3	1
1	A	56	LEU	H	8.12	0.02	1
1	A	56	LEU	HA	3.31	0.02	1
1	A	56	LEU	HB2	1.05	0.02	2
1	A	56	LEU	HB3	0.07	0.02	2
1	A	56	LEU	HD11	0.53	0.02	1
1	A	56	LEU	HD12	0.53	0.02	1
1	A	56	LEU	HD13	0.53	0.02	1
1	A	56	LEU	HD21	0.47	0.02	1
1	A	56	LEU	HD22	0.47	0.02	1
1	A	56	LEU	HD23	0.47	0.02	1
1	A	56	LEU	HG	0.87	0.02	1
1	A	56	LEU	C	177.8	0.3	1
1	A	56	LEU	CA	56.9	0.3	1
1	A	56	LEU	CB	40.0	0.3	1
1	A	56	LEU	CD1	22.8	0.3	1
1	A	56	LEU	CD2	24.9	0.3	1
1	A	56	LEU	CG	26.3	0.3	1
1	A	56	LEU	N	126.7	0.3	1
1	A	57	LYS	H	8.05	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	57	LYS	HA	3.76	0.02	1
1	A	57	LYS	HB2	1.62	0.02	1
1	A	57	LYS	HB3	1.62	0.02	1
1	A	57	LYS	HD2	1.41	0.02	1
1	A	57	LYS	HD3	1.41	0.02	1
1	A	57	LYS	HE2	2.75	0.02	1
1	A	57	LYS	HE3	2.75	0.02	1
1	A	57	LYS	HG2	0.84	0.02	1
1	A	57	LYS	HG3	0.84	0.02	1
1	A	57	LYS	C	178.8	0.3	1
1	A	57	LYS	CA	59.3	0.3	1
1	A	57	LYS	CB	32.1	0.3	1
1	A	57	LYS	CD	28.8	0.3	1
1	A	57	LYS	CE	43.9	0.3	1
1	A	57	LYS	CG	24.6	0.3	1
1	A	57	LYS	N	118.4	0.3	1
1	A	58	SER	H	7.58	0.02	1
1	A	58	SER	HA	3.94	0.02	1
1	A	58	SER	HB2	3.64	0.02	1
1	A	58	SER	HB3	3.64	0.02	1
1	A	58	SER	C	174.9	0.3	1
1	A	58	SER	CA	62.3	0.3	1
1	A	58	SER	N	114.3	0.3	1
1	A	59	ALA	H	7.27	0.02	1
1	A	59	ALA	HA	3.82	0.02	1
1	A	59	ALA	HB1	1.63	0.02	1
1	A	59	ALA	HB2	1.63	0.02	1
1	A	59	ALA	HB3	1.63	0.02	1
1	A	59	ALA	C	180.0	0.3	1
1	A	59	ALA	CA	55.1	0.3	1
1	A	59	ALA	CB	19.2	0.3	1
1	A	59	ALA	N	125.4	0.3	1
1	A	60	GLU	H	8.57	0.02	1
1	A	60	GLU	HA	3.92	0.02	1
1	A	60	GLU	HB2	1.93	0.02	1
1	A	60	GLU	HB3	1.93	0.02	1
1	A	60	GLU	HG2	2.41	0.02	1
1	A	60	GLU	HG3	2.41	0.02	1
1	A	60	GLU	C	179.4	0.3	1
1	A	60	GLU	CA	59.6	0.3	1
1	A	60	GLU	CB	30.1	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	60	GLU	CG	37.4	0.3	1
1	A	60	GLU	N	120.6	0.3	1
1	A	61	HIS	H	7.93	0.02	1
1	A	61	HIS	HA	4.0	0.02	1
1	A	61	HIS	HB2	3.22	0.02	2
1	A	61	HIS	HB3	2.95	0.02	2
1	A	61	HIS	C	177.1	0.3	1
1	A	61	HIS	CA	61.3	0.3	1
1	A	61	HIS	CB	31.3	0.3	1
1	A	61	HIS	N	118.2	0.3	1
1	A	62	ALA	H	7.9	0.02	1
1	A	62	ALA	HA	3.87	0.02	1
1	A	62	ALA	HB1	1.25	0.02	1
1	A	62	ALA	HB2	1.25	0.02	1
1	A	62	ALA	HB3	1.25	0.02	1
1	A	62	ALA	C	180.5	0.3	1
1	A	62	ALA	CA	54.9	0.3	1
1	A	62	ALA	CB	19.9	0.3	1
1	A	62	ALA	N	122.3	0.3	1
1	A	63	ALA	H	7.56	0.02	1
1	A	63	ALA	HA	3.97	0.02	1
1	A	63	ALA	HB1	1.36	0.02	1
1	A	63	ALA	HB2	1.36	0.02	1
1	A	63	ALA	HB3	1.36	0.02	1
1	A	63	ALA	C	178.4	0.3	1
1	A	63	ALA	CA	55.0	0.3	1
1	A	63	ALA	CB	17.2	0.3	1
1	A	63	ALA	N	121.5	0.3	1
1	A	64	ALA	H	8.42	0.02	1
1	A	64	ALA	HA	3.69	0.02	1
1	A	64	ALA	HB1	1.42	0.02	1
1	A	64	ALA	HB2	1.42	0.02	1
1	A	64	ALA	HB3	1.42	0.02	1
1	A	64	ALA	C	178.2	0.3	1
1	A	64	ALA	CA	55.0	0.3	1
1	A	64	ALA	CB	17.3	0.3	1
1	A	64	ALA	N	120.3	0.3	1
1	A	65	LYS	H	8.31	0.02	1
1	A	65	LYS	HA	3.02	0.02	1
1	A	65	LYS	HB2	1.5	0.02	1
1	A	65	LYS	HB3	1.5	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	65	LYS	HD2	1.09	0.02	1
1	A	65	LYS	HD3	1.09	0.02	1
1	A	65	LYS	HE2	2.74	0.02	1
1	A	65	LYS	HE3	2.74	0.02	1
1	A	65	LYS	HG2	0.72	0.02	1
1	A	65	LYS	HG3	0.72	0.02	1
1	A	65	LYS	C	178.0	0.3	1
1	A	65	LYS	CA	59.9	0.3	1
1	A	65	LYS	CB	32.4	0.3	1
1	A	65	LYS	CD	29.8	0.3	1
1	A	65	LYS	CE	42.0	0.3	1
1	A	65	LYS	CG	24.5	0.3	1
1	A	65	LYS	N	120.2	0.3	1
1	A	66	ILE	H	6.78	0.02	1
1	A	66	ILE	HA	3.48	0.02	1
1	A	66	ILE	HB	1.81	0.02	1
1	A	66	ILE	HD11	0.84	0.02	1
1	A	66	ILE	HD12	0.84	0.02	1
1	A	66	ILE	HD13	0.84	0.02	1
1	A	66	ILE	HG12	1.04	0.02	1
1	A	66	ILE	HG13	1.04	0.02	1
1	A	66	ILE	HG21	0.95	0.02	1
1	A	66	ILE	HG22	0.95	0.02	1
1	A	66	ILE	HG23	0.95	0.02	1
1	A	66	ILE	C	178.3	0.3	1
1	A	66	ILE	CA	64.0	0.3	1
1	A	66	ILE	CB	37.9	0.3	1
1	A	66	ILE	CD1	13.3	0.3	1
1	A	66	ILE	CG1	27.9	0.3	1
1	A	66	ILE	CG2	17.7	0.3	1
1	A	66	ILE	N	119.2	0.3	1
1	A	67	ALA	H	7.0	0.02	1
1	A	67	ALA	HA	2.3	0.02	1
1	A	67	ALA	HB1	0.68	0.02	1
1	A	67	ALA	HB2	0.68	0.02	1
1	A	67	ALA	HB3	0.68	0.02	1
1	A	67	ALA	C	179.5	0.3	1
1	A	67	ALA	CA	54.3	0.3	1
1	A	67	ALA	CB	18.9	0.3	1
1	A	67	ALA	N	123.6	0.3	1
1	A	68	VAL	H	8.65	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	68	VAL	HA	3.12	0.02	1
1	A	68	VAL	HB	1.9	0.02	1
1	A	68	VAL	HG11	0.83	0.02	1
1	A	68	VAL	HG12	0.83	0.02	1
1	A	68	VAL	HG13	0.83	0.02	1
1	A	68	VAL	HG21	0.91	0.02	1
1	A	68	VAL	HG22	0.91	0.02	1
1	A	68	VAL	HG23	0.91	0.02	1
1	A	68	VAL	C	178.2	0.3	1
1	A	68	VAL	CA	66.1	0.3	1
1	A	68	VAL	CB	31.4	0.3	1
1	A	68	VAL	CG1	21.0	0.3	1
1	A	68	VAL	CG2	24.0	0.3	1
1	A	68	VAL	N	118.9	0.3	1
1	A	69	ALA	H	7.55	0.02	1
1	A	69	ALA	HA	3.94	0.02	1
1	A	69	ALA	HB1	1.33	0.02	1
1	A	69	ALA	HB2	1.33	0.02	1
1	A	69	ALA	HB3	1.33	0.02	1
1	A	69	ALA	C	178.9	0.3	1
1	A	69	ALA	CA	54.2	0.3	1
1	A	69	ALA	CB	17.6	0.3	1
1	A	69	ALA	N	122.7	0.3	1
1	A	70	SER	H	7.24	0.02	1
1	A	70	SER	HA	4.27	0.02	1
1	A	70	SER	HB2	3.83	0.02	1
1	A	70	SER	HB3	3.83	0.02	1
1	A	70	SER	C	174.8	0.3	1
1	A	70	SER	CA	60.0	0.3	1
1	A	70	SER	CB	63.9	0.3	1
1	A	70	SER	N	112.9	0.3	1
1	A	71	LEU	H	7.33	0.02	1
1	A	71	LEU	HA	4.11	0.02	1
1	A	71	LEU	HB2	1.44	0.02	1
1	A	71	LEU	HB3	1.44	0.02	1
1	A	71	LEU	HD11	0.18	0.02	1
1	A	71	LEU	HD12	0.18	0.02	1
1	A	71	LEU	HD13	0.18	0.02	1
1	A	71	LEU	HD21	0.47	0.02	1
1	A	71	LEU	HD22	0.47	0.02	1
1	A	71	LEU	HD23	0.47	0.02	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	71	LEU	HG	1.01	0.02	1
1	A	71	LEU	C	177.1	0.3	1
1	A	71	LEU	CA	55.1	0.3	1
1	A	71	LEU	CB	41.8	0.3	1
1	A	71	LEU	CD1	24.8	0.3	1
1	A	71	LEU	CD2	21.5	0.3	1
1	A	71	LEU	CG	24.6	0.3	1
1	A	71	LEU	N	121.2	0.3	1
1	A	72	THR	H	7.66	0.02	1
1	A	72	THR	HA	4.48	0.02	1
1	A	72	THR	HB	4.06	0.02	1
1	A	72	THR	HG21	1.07	0.02	1
1	A	72	THR	HG22	1.07	0.02	1
1	A	72	THR	HG23	1.07	0.02	1
1	A	72	THR	C	172.4	0.3	1
1	A	72	THR	CA	59.7	0.3	1
1	A	72	THR	CB	69.5	0.3	1
1	A	72	THR	N	115.3	0.3	1
1	A	73	PRO	HA	4.32	0.02	1
1	A	73	PRO	HB2	2.21	0.02	1
1	A	73	PRO	HB3	2.21	0.02	1
1	A	73	PRO	HD2	3.7	0.02	2
1	A	73	PRO	HD3	3.63	0.02	2
1	A	73	PRO	HG2	1.9	0.02	2
1	A	73	PRO	HG3	1.83	0.02	2
1	A	73	PRO	C	176.8	0.3	1
1	A	73	PRO	CA	63.3	0.3	1
1	A	73	PRO	CB	31.7	0.3	1
1	A	73	PRO	CD	50.7	0.3	1
1	A	73	PRO	CG	27.3	0.3	1
1	A	74	GLN	H	8.41	0.02	1
1	A	74	GLN	HA	4.28	0.02	1
1	A	74	GLN	HB2	1.89	0.02	2
1	A	74	GLN	HB3	2.04	0.02	2
1	A	74	GLN	HG2	2.28	0.02	1
1	A	74	GLN	HG3	2.28	0.02	1
1	A	74	GLN	C	175.7	0.3	1
1	A	74	GLN	CA	55.3	0.3	1
1	A	74	GLN	CB	29.4	0.3	1
1	A	74	GLN	CG	33.6	0.3	1
1	A	74	GLN	N	121.2	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	75	SER	H	8.3	0.02	1
1	A	75	SER	HA	4.78	0.02	1
1	A	75	SER	C	172.9	0.3	1
1	A	75	SER	CA	56.2	0.3	1
1	A	75	SER	CB	63.1	0.3	1
1	A	75	SER	N	119.2	0.3	1
1	A	76	PRO	HA	4.33	0.02	1
1	A	76	PRO	HB2	2.19	0.02	1
1	A	76	PRO	HB3	2.19	0.02	1
1	A	76	PRO	HD2	3.57	0.02	1
1	A	76	PRO	HD3	3.57	0.02	1
1	A	76	PRO	HG2	1.83	0.02	2
1	A	76	PRO	HG3	1.9	0.02	2
1	A	76	PRO	C	176.8	0.3	1
1	A	76	PRO	CA	63.4	0.3	1
1	A	76	PRO	CB	31.7	0.3	1
1	A	76	PRO	CG	27.3	0.3	1
1	A	77	GLU	H	8.38	0.02	1
1	A	77	GLU	HA	4.14	0.02	1
1	A	77	GLU	HB2	1.88	0.02	1
1	A	77	GLU	HB3	1.88	0.02	1
1	A	77	GLU	HG2	2.17	0.02	1
1	A	77	GLU	HG3	2.17	0.02	1
1	A	77	GLU	C	176.8	0.3	1
1	A	77	GLU	CA	56.7	0.3	1
1	A	77	GLU	CB	29.8	0.3	1
1	A	77	GLU	CG	36.2	0.3	1
1	A	77	GLU	N	121.0	0.3	1
1	A	78	GLY	H	8.21	0.02	1
1	A	78	GLY	HA2	3.83	0.02	1
1	A	78	GLY	HA3	3.83	0.02	1
1	A	78	GLY	C	174.0	0.3	1
1	A	78	GLY	CA	45.1	0.3	1
1	A	78	GLY	N	110.3	0.3	1
1	A	79	ILE	H	7.76	0.02	1
1	A	79	ILE	HA	4.03	0.02	1
1	A	79	ILE	HB	1.72	0.02	1
1	A	79	ILE	HD11	0.75	0.02	1
1	A	79	ILE	HD12	0.75	0.02	1
1	A	79	ILE	HD13	0.75	0.02	1
1	A	79	ILE	HG12	1.26	0.02	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	79	ILE	HG13	1.02	0.02	2
1	A	79	ILE	HG21	0.75	0.02	1
1	A	79	ILE	HG22	0.75	0.02	1
1	A	79	ILE	HG23	0.75	0.02	1
1	A	79	ILE	C	175.5	0.3	1
1	A	79	ILE	CA	61.0	0.3	1
1	A	79	ILE	CB	38.4	0.3	1
1	A	79	ILE	CD1	12.9	0.3	1
1	A	79	ILE	CG1	26.9	0.3	1
1	A	79	ILE	CG2	17.3	0.3	1
1	A	79	ILE	N	120.3	0.3	1
1	A	80	ASP	H	8.27	0.02	1
1	A	80	ASP	HA	4.49	0.02	1
1	A	80	ASP	HB2	2.52	0.02	1
1	A	80	ASP	HB3	2.52	0.02	1
1	A	80	ASP	C	175.6	0.3	1
1	A	80	ASP	CA	54.3	0.3	1
1	A	80	ASP	CB	40.7	0.3	1
1	A	80	ASP	N	124.2	0.3	1
1	A	81	VAL	H	7.58	0.02	1
1	A	152	ASN	H	8.18	0.02	1
1	A	152	ASN	HA	4.66	0.02	1
1	A	152	ASN	HB2	2.7	0.02	1
1	A	152	ASN	HB3	2.7	0.02	1
1	A	152	ASN	C	175.2	0.3	1
1	A	152	ASN	CA	53.0	0.3	1
1	A	152	ASN	CB	38.8	0.3	1
1	A	152	ASN	N	119.4	0.3	1
1	A	153	SER	H	8.19	0.02	1
1	A	153	SER	HA	4.3	0.02	1
1	A	153	SER	HB2	3.78	0.02	2
1	A	153	SER	HB3	3.82	0.02	2
1	A	153	SER	C	174.5	0.3	1
1	A	153	SER	CA	58.6	0.3	1
1	A	153	SER	CB	63.4	0.3	1
1	A	153	SER	N	116.8	0.3	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
$^{13}\text{C}_\alpha$	150	0.10 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	141	0.45 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}'$	150	0.07 ± 0.24	None needed (< 0.5 ppm)
^{15}N	139	-0.58 ± 0.28	Should be applied

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 86%, i.e. 757 atoms were assigned a chemical shift out of a possible 881. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	337/337 (100%)	136/136 (100%)	136/136 (100%)	65/65 (100%)
Sidechain	398/469 (85%)	278/309 (90%)	117/149 (79%)	3/11 (27%)
Aromatic	22/75 (29%)	22/37 (59%)	0/37 (0%)	0/1 (0%)
Overall	757/881 (86%)	436/482 (90%)	253/322 (79%)	68/77 (88%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 789 atoms were assigned a chemical shift out of a possible 914. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	353/353 (100%)	143/143 (100%)	142/142 (100%)	68/68 (100%)
Sidechain	414/486 (85%)	289/320 (90%)	121/154 (79%)	4/12 (33%)
Aromatic	22/75 (29%)	22/37 (59%)	0/37 (0%)	0/1 (0%)
Overall	789/914 (86%)	454/500 (91%)	263/333 (79%)	72/81 (89%)

7.1.4 Statistically unusual chemical shifts [i](#)

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.

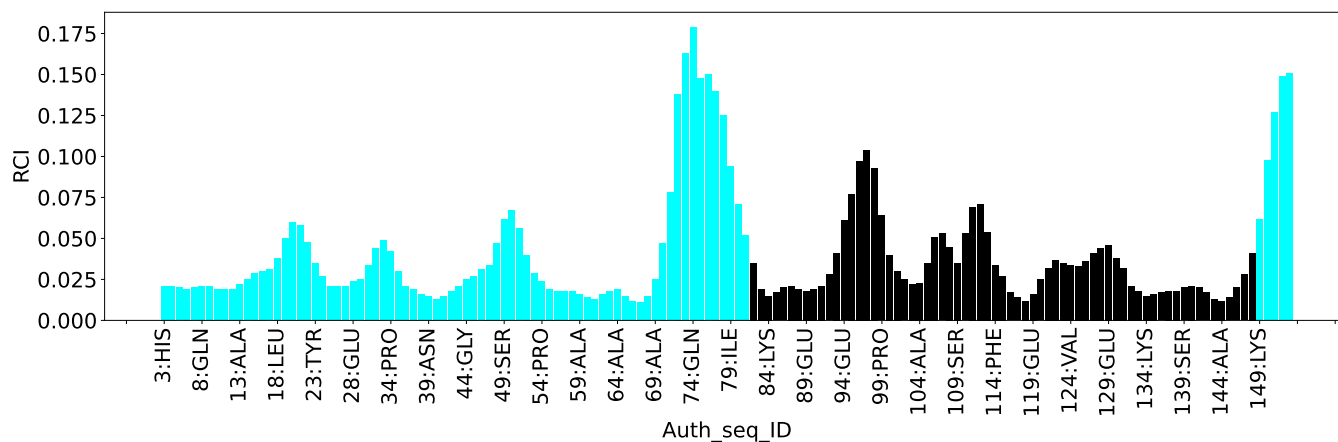
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	133	LYS	CE	37.30	37.57 – 46.21	-5.3

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	1321
Intra-residue ($ i-j =0$)	401
Sequential ($ i-j =1$)	322
Medium range ($ i-j >1$ and $ i-j <5$)	226
Long range ($ i-j \geq 5$)	310
Inter-chain	0
Hydrogen bond restraints	62
Disulfide bond restraints	0
Total dihedral-angle restraints	122
Number of unmapped restraints	0
Number of restraints per residue	9.4
Number of long range restraints per residue ¹	2.1

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)	9.9	0.2
0.2-0.5 (Medium)	9.3	0.5
>0.5 (Large)	48.1	3.99

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)	11.5	6.47
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis

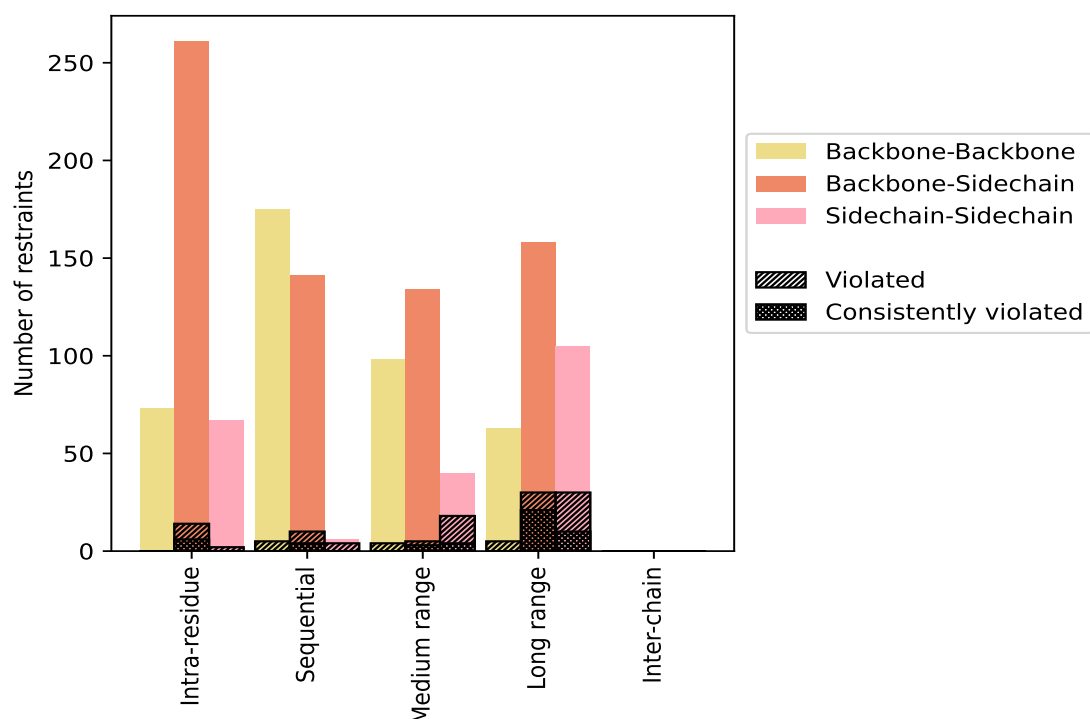
9.1 Summary of distance violations

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	401	30.4	16	4.0	1.2	6	1.5	0.5
Backbone-Backbone	73	5.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	261	19.8	14	5.4	1.1	6	2.3	0.5
Sidechain-Sidechain	67	5.1	2	3.0	0.2	0	0.0	0.0
Sequential (i-j =1)	322	24.4	19	5.9	1.4	4	1.2	0.3
Backbone-Backbone	175	13.2	5	2.9	0.4	0	0.0	0.0
Backbone-Sidechain	141	10.7	10	7.1	0.8	4	2.8	0.3
Sidechain-Sidechain	6	0.5	4	66.7	0.3	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	226	17.1	25	11.1	1.9	7	3.1	0.5
Backbone-Backbone	98	7.4	4	4.1	0.3	0	0.0	0.0
Backbone-Sidechain	88	6.7	3	3.4	0.2	3	3.4	0.2
Sidechain-Sidechain	40	3.0	18	45.0	1.4	4	10.0	0.3
Long range (i-j ≥5)	310	23.5	63	20.3	4.8	31	10.0	2.3
Backbone-Backbone	63	4.8	5	7.9	0.4	0	0.0	0.0
Backbone-Sidechain	142	10.7	28	19.7	2.1	21	14.8	1.6
Sidechain-Sidechain	105	7.9	30	28.6	2.3	10	9.5	0.8
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	62	4.7	4	6.5	0.3	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1321	100.0	127	9.6	9.6	48	3.6	3.6
Backbone-Backbone	409	31.0	14	3.4	1.1	0	0.0	0.0
Backbone-Sidechain	694	52.5	59	8.5	4.5	34	4.9	2.6
Sidechain-Sidechain	218	16.5	54	24.8	4.1	14	6.4	1.1

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 disulfide 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	10	10	10	38	0	68	1.59	3.92	1.25	1.34
2	10	8	7	40	0	65	1.66	3.94	1.22	1.49
3	9	7	8	32	0	56	1.7	3.83	1.26	1.8
4	10	9	11	39	0	69	1.59	3.53	1.16	1.4
5	8	7	9	34	0	58	1.71	3.59	1.22	2.3
6	9	7	9	31	0	56	1.74	3.91	1.3	1.96
7	12	9	9	38	0	68	1.65	3.66	1.19	1.62
8	11	9	9	39	0	68	1.63	3.59	1.21	1.74
9	8	8	12	41	0	69	1.58	3.52	1.16	1.52
10	9	11	9	40	0	69	1.58	3.99	1.23	1.39

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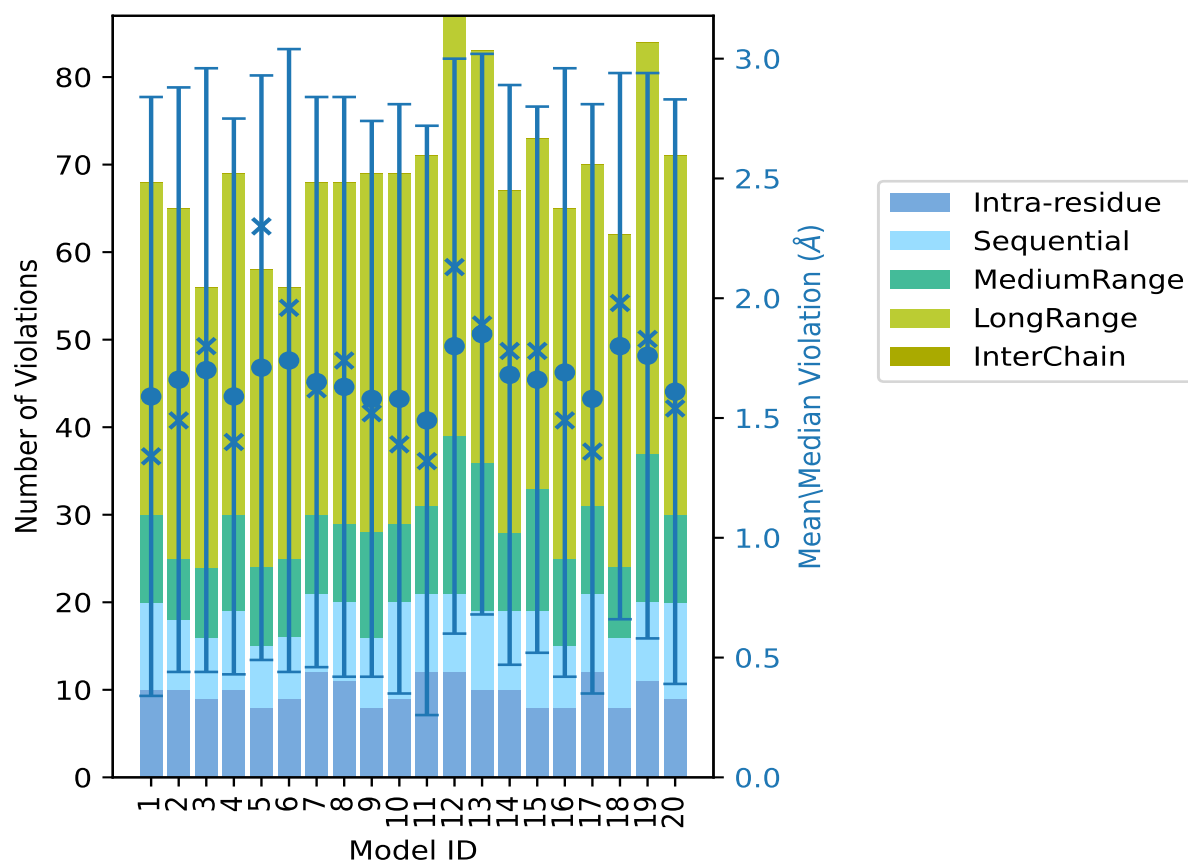
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	12	9	10	40	0	71	1.49	3.95	1.23	1.32
12	12	9	18	48	0	87	1.8	3.63	1.2	2.13
13	10	9	17	47	0	83	1.85	3.7	1.17	1.89
14	10	9	9	39	0	67	1.68	3.61	1.21	1.78
15	8	11	14	40	0	73	1.66	3.6	1.14	1.78
16	8	7	10	40	0	65	1.69	3.94	1.27	1.49
17	12	9	10	39	0	70	1.58	3.9	1.23	1.36
18	8	8	8	38	0	62	1.8	3.78	1.14	1.98
19	11	9	17	47	0	84	1.76	3.68	1.18	1.83
20	9	11	10	41	0	71	1.61	3.88	1.22	1.54

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

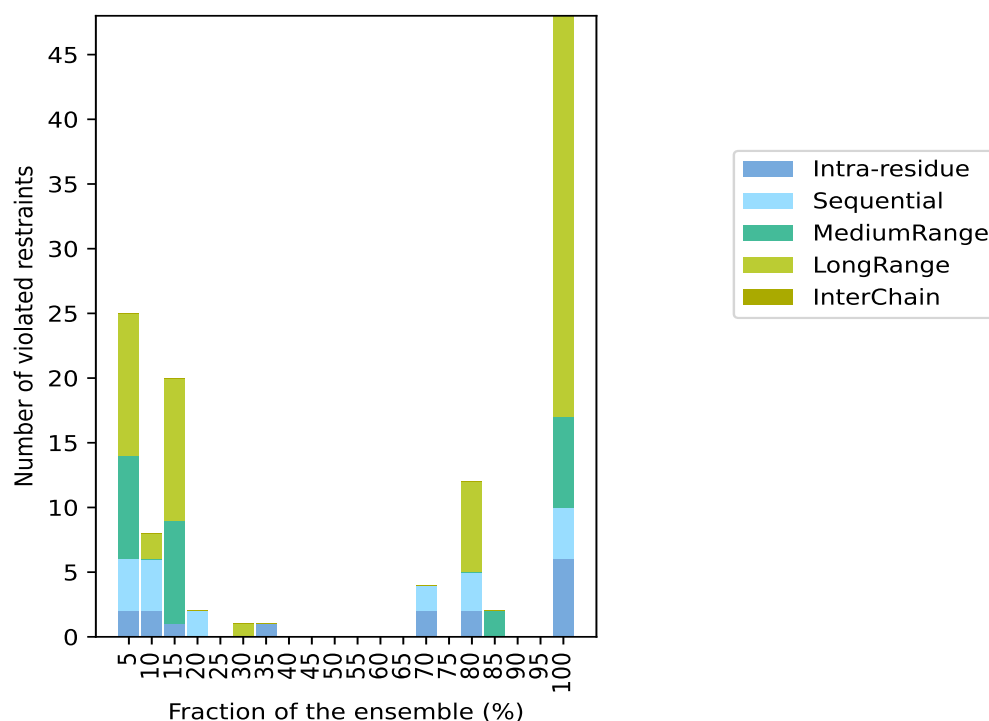
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1136(IR:385, SQ:303, MR:201, LR:247, IC:0) restraints are 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	%
2	4	8	11	0	25	1	5.0
2	4	0	2	0	8	2	10.0
1	0	8	11	0	20	3	15.0
0	2	0	0	0	2	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	1	0	1	6	30.0
1	0	0	0	0	1	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
2	2	0	0	0	4	14	70.0
0	0	0	0	0	0	15	75.0
2	3	0	7	0	12	16	80.0
0	0	2	0	0	2	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
6	4	7	31	0	48	20	100.0

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

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

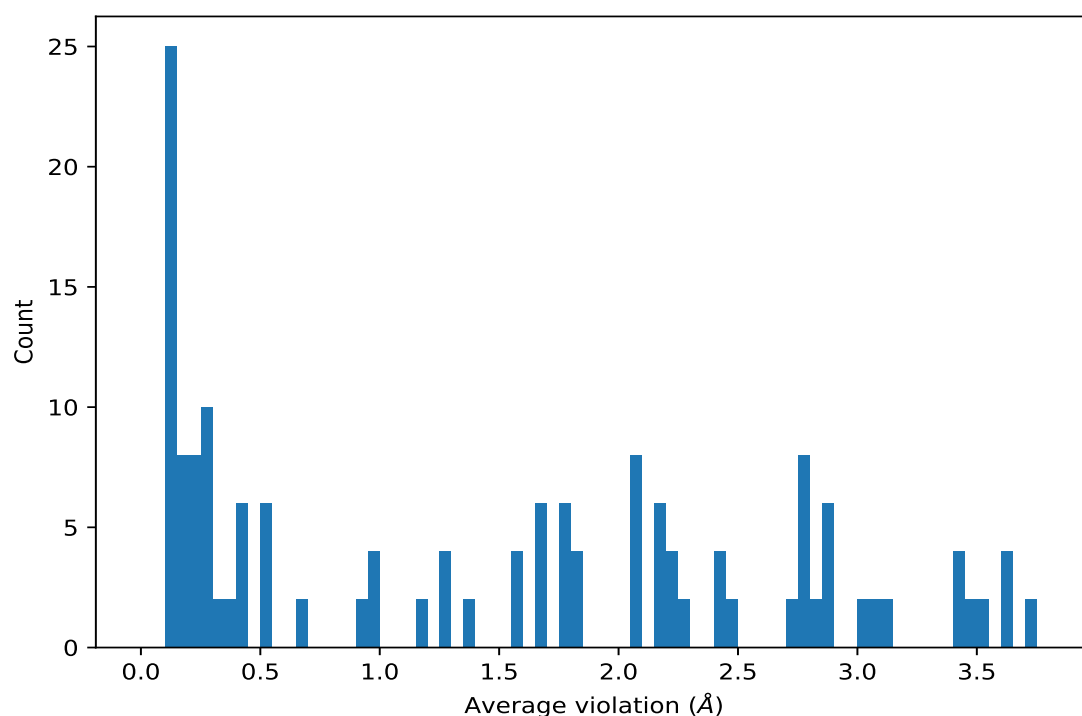
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,931)	1:105:A:THR:HB	1:114:A:PHE:HE2	20	3.74	0.18	3.74
(1,989)	1:114:A:PHE:HE2	1:105:A:THR:HB	20	3.74	0.18	3.74
(1,404)	1:114:A:PHE:HE1	1:132:A:THR:H	20	3.53	0.02	3.52
(1,581)	1:132:A:THR:H	1:114:A:PHE:HE1	20	3.53	0.02	3.52
(1,930)	1:105:A:THR:HB	1:114:A:PHE:HD2	20	3.48	0.19	3.46
(1,986)	1:114:A:PHE:HD2	1:105:A:THR:HB	20	3.48	0.19	3.46
(1,1001)	1:114:A:PHE:HD1	1:132:A:THR:HA	20	3.14	0.12	3.11
(1,1112)	1:132:A:THR:HA	1:114:A:PHE:HD1	20	3.14	0.12	3.11
(1,403)	1:114:A:PHE:HD1	1:132:A:THR:H	20	3.07	0.05	3.06
(1,580)	1:132:A:THR:H	1:114:A:PHE:HD1	20	3.07	0.05	3.06
(1,1002)	1:114:A:PHE:HE1	1:132:A:THR:HA	20	3.01	0.12	3.0
(1,1113)	1:132:A:THR:HA	1:114:A:PHE:HE1	20	3.01	0.12	3.0
(1,928)	1:105:A:THR:HA	1:114:A:PHE:HD2	20	2.8	0.05	2.8
(1,985)	1:114:A:PHE:HD2	1:105:A:THR:HA	20	2.8	0.05	2.8
(1,929)	1:105:A:THR:HA	1:114:A:PHE:HE2	20	2.78	0.04	2.78
(1,988)	1:114:A:PHE:HE2	1:105:A:THR:HA	20	2.78	0.04	2.78

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,406)	1:114:A:PHE:HE1	1:133:A:LYS:H	20	2.72	0.12	2.76
(1,588)	1:133:A:LYS:H	1:114:A:PHE:HE1	20	2.72	0.12	2.76
(1,147)	1:82:A:ALA:H	1:83:A:TYR:HD2	20	2.46	0.03	2.46
(1,150)	1:83:A:TYR:HD2	1:82:A:ALA:H	20	2.46	0.03	2.46
(1,998)	1:114:A:PHE:HD1	1:131:A:LYS:HA	20	2.44	0.08	2.46
(1,1109)	1:131:A:LYS:HA	1:114:A:PHE:HD1	20	2.44	0.08	2.46
(1,405)	1:114:A:PHE:HD1	1:133:A:LYS:H	20	2.41	0.1	2.4
(1,587)	1:133:A:LYS:H	1:114:A:PHE:HD1	20	2.41	0.1	2.4
(1,999)	1:114:A:PHE:HE1	1:131:A:LYS:HA	20	2.25	0.09	2.26
(1,1110)	1:131:A:LYS:HA	1:114:A:PHE:HE1	20	2.25	0.09	2.26
(1,932)	1:105:A:THR:HG21	1:114:A:PHE:HD2	20	2.17	0.23	2.27
(1,932)	1:105:A:THR:HG22	1:114:A:PHE:HD2	20	2.17	0.23	2.27
(1,932)	1:105:A:THR:HG23	1:114:A:PHE:HD2	20	2.17	0.23	2.27
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG21	20	2.17	0.23	2.27
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG22	20	2.17	0.23	2.27
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG23	20	2.17	0.23	2.27
(1,971)	1:112:A:PRO:HB2	1:114:A:PHE:HE2	20	2.05	0.54	2.35
(1,971)	1:112:A:PRO:HB3	1:114:A:PHE:HE2	20	2.05	0.54	2.35
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB2	20	2.05	0.54	2.35
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB3	20	2.05	0.54	2.35
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG2	20	1.84	0.92	1.77
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG3	20	1.84	0.92	1.77
(1,1111)	1:131:A:LYS:HG2	1:114:A:PHE:HE1	20	1.84	0.92	1.77
(1,1111)	1:131:A:LYS:HG3	1:114:A:PHE:HE1	20	1.84	0.92	1.77
(1,933)	1:105:A:THR:HG21	1:114:A:PHE:HE2	20	1.67	0.24	1.81
(1,933)	1:105:A:THR:HG22	1:114:A:PHE:HE2	20	1.67	0.24	1.81
(1,933)	1:105:A:THR:HG23	1:114:A:PHE:HE2	20	1.67	0.24	1.81
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG21	20	1.67	0.24	1.81
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG22	20	1.67	0.24	1.81
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG23	20	1.67	0.24	1.81
(1,970)	1:112:A:PRO:HB2	1:114:A:PHE:HD2	20	0.98	0.38	1.19
(1,970)	1:112:A:PRO:HB3	1:114:A:PHE:HD2	20	0.98	0.38	1.19
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB2	20	0.98	0.38	1.19
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB3	20	0.98	0.38	1.19
(1,393)	1:114:A:PHE:HE1	1:114:A:PHE:H	20	0.91	0.06	0.94
(1,397)	1:114:A:PHE:H	1:114:A:PHE:HE1	20	0.91	0.06	0.94
(1,392)	1:114:A:PHE:HD1	1:114:A:PHE:H	20	0.69	0.06	0.72
(1,396)	1:114:A:PHE:H	1:114:A:PHE:HD1	20	0.69	0.06	0.72
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB2	20	0.42	0.03	0.42
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB3	20	0.42	0.03	0.42
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB2	20	0.37	0.09	0.4
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB3	20	0.37	0.09	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,400)	1:114:A:PHE:HD2	1:115:A:THR:H	20	0.28	0.04	0.28
(1,411)	1:115:A:THR:H	1:114:A:PHE:HD2	20	0.28	0.04	0.28
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB2	20	0.26	0.02	0.25
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB3	20	0.26	0.02	0.25
(1,346)	1:105:A:THR:HB	1:105:A:THR:H	20	0.15	0.02	0.15
(1,348)	1:105:A:THR:H	1:105:A:THR:HB	20	0.15	0.02	0.15
(1,361)	1:108:A:PRO:HG2	1:110:A:HIS:H	20	0.15	0.02	0.15
(1,361)	1:108:A:PRO:HG3	1:110:A:HIS:H	20	0.15	0.02	0.15
(1,2)	1:82:A:ALA:H	1:84:A:LYS:H	17	0.11	0.01	0.1
(1,6)	1:84:A:LYS:H	1:82:A:ALA:H	17	0.11	0.01	0.1
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB1	16	1.75	0.28	1.72
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB2	16	1.75	0.28	1.72
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB3	16	1.75	0.28	1.72
(1,1194)	1:141:A:ALA:HB1	1:101:A:TYR:HE2	16	1.75	0.28	1.72
(1,1194)	1:141:A:ALA:HB2	1:101:A:TYR:HE2	16	1.75	0.28	1.72
(1,1194)	1:141:A:ALA:HB3	1:101:A:TYR:HE2	16	1.75	0.28	1.72
(1,316)	1:101:A:TYR:HD2	1:102:A:ALA:H	16	1.39	0.07	1.39
(1,320)	1:102:A:ALA:H	1:101:A:TYR:HD2	16	1.39	0.07	1.39
(1,311)	1:101:A:TYR:HD1	1:101:A:TYR:H	16	1.16	0.07	1.16
(1,313)	1:101:A:TYR:H	1:101:A:TYR:HD1	16	1.16	0.07	1.16
(1,811)	1:87:A:LEU:HD11	1:101:A:TYR:HE2	16	0.5	0.15	0.46
(1,811)	1:87:A:LEU:HD12	1:101:A:TYR:HE2	16	0.5	0.15	0.46
(1,811)	1:87:A:LEU:HD13	1:101:A:TYR:HE2	16	0.5	0.15	0.46
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD11	16	0.5	0.15	0.46
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD12	16	0.5	0.15	0.46
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD13	16	0.5	0.15	0.46
(1,1026)	1:118:A:VAL:HG21	1:101:A:TYR:HD2	16	0.4	0.13	0.37
(1,1026)	1:118:A:VAL:HG22	1:101:A:TYR:HD2	16	0.4	0.13	0.37
(1,1026)	1:118:A:VAL:HG23	1:101:A:TYR:HD2	16	0.4	0.13	0.37
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG21	16	0.29	0.11	0.3
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG22	16	0.29	0.11	0.3
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG23	16	0.29	0.11	0.3
(1,1027)	1:118:A:VAL:HG21	1:101:A:TYR:HE2	16	0.29	0.11	0.3
(1,1027)	1:118:A:VAL:HG22	1:101:A:TYR:HE2	16	0.29	0.11	0.3
(1,1027)	1:118:A:VAL:HG23	1:101:A:TYR:HE2	16	0.29	0.11	0.3
(1,333)	1:104:A:ALA:H	1:103:A:THR:HA	16	0.12	0.01	0.12
(1,302)	1:100:A:PHE:H	1:101:A:TYR:HA	14	0.2	0.02	0.19
(1,308)	1:101:A:TYR:HA	1:100:A:PHE:H	14	0.2	0.02	0.19
(1,619)	1:135:A:LEU:HD11	1:135:A:LEU:H	14	0.12	0.01	0.12
(1,619)	1:135:A:LEU:HD12	1:135:A:LEU:H	14	0.12	0.01	0.12
(1,619)	1:135:A:LEU:HD13	1:135:A:LEU:H	14	0.12	0.01	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD11	14	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD12	14	0.12	0.01	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD13	14	0.12	0.01	0.12
(1,546)	1:128:A:GLU:H	1:128:A:GLU:HG2	7	0.32	0.08	0.32
(1,546)	1:128:A:GLU:H	1:128:A:GLU:HG3	7	0.32	0.08	0.32
(2,15)	1:90:A:ILE:O	1:94:A:GLU:H	7	0.11	0.01	0.11
(1,666)	1:139:A:SER:HB2	1:128:A:GLU:H	6	0.14	0.02	0.14
(1,666)	1:139:A:SER:HB3	1:128:A:GLU:H	6	0.14	0.02	0.14
(1,548)	1:128:A:GLU:HB2	1:129:A:GLU:H	4	0.15	0.02	0.15
(1,548)	1:128:A:GLU:HB3	1:129:A:GLU:H	4	0.15	0.02	0.15
(1,553)	1:129:A:GLU:H	1:128:A:GLU:HB2	4	0.15	0.02	0.15
(1,553)	1:129:A:GLU:H	1:128:A:GLU:HB3	4	0.15	0.02	0.15
(1,787)	1:86:A:LEU:HB2	1:145:A:PHE:HD1	3	3.61	0.01	3.61
(1,787)	1:86:A:LEU:HB3	1:145:A:PHE:HD1	3	3.61	0.01	3.61
(1,1208)	1:145:A:PHE:HD1	1:86:A:LEU:HB2	3	3.61	0.01	3.61
(1,1208)	1:145:A:PHE:HD1	1:86:A:LEU:HB3	3	3.61	0.01	3.61
(1,788)	1:86:A:LEU:HB2	1:145:A:PHE:HE1	3	3.41	0.03	3.4
(1,788)	1:86:A:LEU:HB3	1:145:A:PHE:HE1	3	3.41	0.03	3.4
(1,1209)	1:145:A:PHE:HE1	1:86:A:LEU:HB2	3	3.41	0.03	3.4
(1,1209)	1:145:A:PHE:HE1	1:86:A:LEU:HB3	3	3.41	0.03	3.4
(1,859)	1:90:A:ILE:HG21	1:145:A:PHE:HE1	3	2.89	0.1	2.89
(1,859)	1:90:A:ILE:HG22	1:145:A:PHE:HE1	3	2.89	0.1	2.89
(1,859)	1:90:A:ILE:HG23	1:145:A:PHE:HE1	3	2.89	0.1	2.89
(1,1212)	1:145:A:PHE:HE1	1:90:A:ILE:HG21	3	2.89	0.1	2.89
(1,1212)	1:145:A:PHE:HE1	1:90:A:ILE:HG22	3	2.89	0.1	2.89
(1,1212)	1:145:A:PHE:HE1	1:90:A:ILE:HG23	3	2.89	0.1	2.89
(1,817)	1:87:A:LEU:HD21	1:145:A:PHE:HD1	3	2.77	0.07	2.82
(1,817)	1:87:A:LEU:HD22	1:145:A:PHE:HD1	3	2.77	0.07	2.82
(1,817)	1:87:A:LEU:HD23	1:145:A:PHE:HD1	3	2.77	0.07	2.82
(1,1211)	1:145:A:PHE:HD1	1:87:A:LEU:HD21	3	2.77	0.07	2.82
(1,1211)	1:145:A:PHE:HD1	1:87:A:LEU:HD22	3	2.77	0.07	2.82
(1,1211)	1:145:A:PHE:HD1	1:87:A:LEU:HD23	3	2.77	0.07	2.82
(1,1220)	1:145:A:PHE:HE2	1:149:A:LYS:HG2	3	2.23	0.46	2.48
(1,1220)	1:145:A:PHE:HE2	1:149:A:LYS:HG3	3	2.23	0.46	2.48
(1,1236)	1:149:A:LYS:HG2	1:145:A:PHE:HE2	3	2.23	0.46	2.48
(1,1236)	1:149:A:LYS:HG3	1:145:A:PHE:HE2	3	2.23	0.46	2.48
(1,1219)	1:145:A:PHE:HE2	1:149:A:LYS:HD2	3	2.05	0.25	2.13
(1,1219)	1:145:A:PHE:HE2	1:149:A:LYS:HD3	3	2.05	0.25	2.13
(1,1234)	1:149:A:LYS:HD2	1:145:A:PHE:HE2	3	2.05	0.25	2.13
(1,1234)	1:149:A:LYS:HD3	1:145:A:PHE:HE2	3	2.05	0.25	2.13
(1,1217)	1:145:A:PHE:HD2	1:149:A:LYS:HD2	3	1.55	0.2	1.58
(1,1217)	1:145:A:PHE:HD2	1:149:A:LYS:HD3	3	1.55	0.2	1.58
(1,1233)	1:149:A:LYS:HD2	1:145:A:PHE:HD2	3	1.55	0.2	1.58

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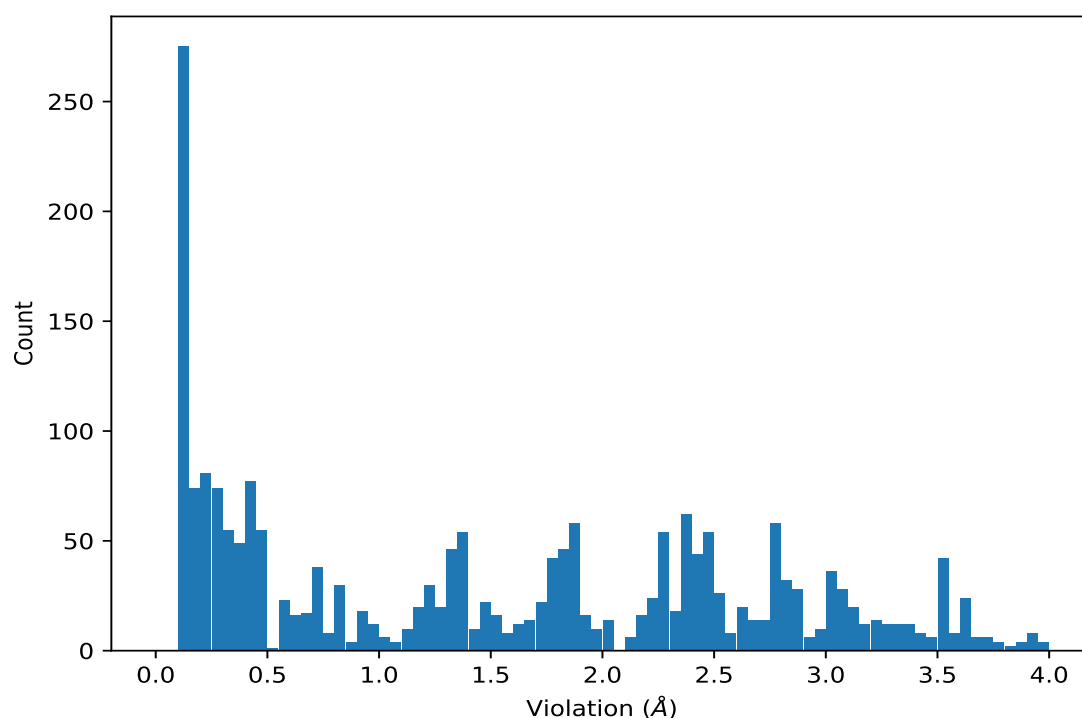
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1233)	1:149:A:LYS:HD3	1:145:A:PHE:HD2	3	1.55	0.2	1.58
(1,1218)	1:145:A:PHE:HD2	1:149:A:LYS:HG2	3	1.27	0.3	1.44
(1,1218)	1:145:A:PHE:HD2	1:149:A:LYS:HG3	3	1.27	0.3	1.44
(1,1235)	1:149:A:LYS:HG2	1:145:A:PHE:HD2	3	1.27	0.3	1.44
(1,1235)	1:149:A:LYS:HG3	1:145:A:PHE:HD2	3	1.27	0.3	1.44
(1,1213)	1:145:A:PHE:HA	1:145:A:PHE:HD1	3	0.43	0.05	0.41
(2,29)	1:120:A:PHE:O	1:123:A:LYS:H	3	0.12	0.01	0.11
(1,359)	1:107:A:GLY:HA2	1:113:A:THR:H	3	0.12	0.02	0.11
(1,359)	1:107:A:GLY:HA3	1:113:A:THR:H	3	0.12	0.02	0.11
(1,386)	1:113:A:THR:HA	1:132:A:THR:H	3	0.11	0.0	0.11
(1,579)	1:132:A:THR:H	1:113:A:THR:HA	3	0.11	0.0	0.11
(2,36)	1:125:A:PHE:O	1:118:A:VAL:N	3	0.11	0.0	0.11
(1,783)	1:86:A:LEU:HA	1:86:A:LEU:HD21	2	0.22	0.01	0.22
(1,783)	1:86:A:LEU:HA	1:86:A:LEU:HD22	2	0.22	0.01	0.22
(1,783)	1:86:A:LEU:HA	1:86:A:LEU:HD23	2	0.22	0.01	0.22
(1,785)	1:86:A:LEU:HD21	1:86:A:LEU:HA	2	0.22	0.01	0.22
(1,785)	1:86:A:LEU:HD22	1:86:A:LEU:HA	2	0.22	0.01	0.22
(1,785)	1:86:A:LEU:HD23	1:86:A:LEU:HA	2	0.22	0.01	0.22
(1,343)	1:104:A:ALA:H	1:116:A:SER:HA	2	0.12	0.01	0.12
(1,421)	1:116:A:SER:HA	1:104:A:ALA:H	2	0.12	0.01	0.12
(1,1)	1:82:A:ALA:H	1:83:A:TYR:H	2	0.11	0.0	0.11
(1,3)	1:83:A:TYR:H	1:82:A:ALA:H	2	0.11	0.0	0.11
(2,20)	1:102:A:ALA:O	1:117:A:THR:N	2	0.11	0.01	0.11
(1,975)	1:113:A:THR:HA	1:114:A:PHE:HD1	2	0.1	0.0	0.1
(1,993)	1:114:A:PHE:HD1	1:113:A:THR:HA	2	0.1	0.0	0.1

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)
(1,989)	1:114:A:PHE:HE2	1:105:A:THR:HB	10	3.99
(1,931)	1:105:A:THR:HB	1:114:A:PHE:HE2	10	3.99
(1,989)	1:114:A:PHE:HE2	1:105:A:THR:HB	11	3.95
(1,931)	1:105:A:THR:HB	1:114:A:PHE:HE2	11	3.95
(1,989)	1:114:A:PHE:HE2	1:105:A:THR:HB	2	3.94
(1,989)	1:114:A:PHE:HE2	1:105:A:THR:HB	16	3.94
(1,931)	1:105:A:THR:HB	1:114:A:PHE:HE2	2	3.94
(1,931)	1:105:A:THR:HB	1:114:A:PHE:HE2	16	3.94
(1,989)	1:114:A:PHE:HE2	1:105:A:THR:HB	1	3.92
(1,931)	1:105:A:THR:HB	1:114:A:PHE:HE2	1	3.92
(1,989)	1:114:A:PHE:HE2	1:105:A:THR:HB	6	3.91
(1,931)	1:105:A:THR:HB	1:114:A:PHE:HE2	6	3.91
(1,989)	1:114:A:PHE:HE2	1:105:A:THR:HB	17	3.9
(1,931)	1:105:A:THR:HB	1:114:A:PHE:HE2	17	3.9
(1,989)	1:114:A:PHE:HE2	1:105:A:THR:HB	20	3.88
(1,931)	1:105:A:THR:HB	1:114:A:PHE:HE2	20	3.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,989)	1:114:A:PHE:HE2	1:105:A:THR:HB	3	3.83
(1,931)	1:105:A:THR:HB	1:114:A:PHE:HE2	3	3.83
(1,989)	1:114:A:PHE:HE2	1:105:A:THR:HB	18	3.78
(1,931)	1:105:A:THR:HB	1:114:A:PHE:HE2	18	3.78
(1,986)	1:114:A:PHE:HD2	1:105:A:THR:HB	10	3.77
(1,930)	1:105:A:THR:HB	1:114:A:PHE:HD2	10	3.77
(1,986)	1:114:A:PHE:HD2	1:105:A:THR:HB	11	3.74
(1,930)	1:105:A:THR:HB	1:114:A:PHE:HD2	11	3.74
(1,989)	1:114:A:PHE:HE2	1:105:A:THR:HB	13	3.7
(1,986)	1:114:A:PHE:HD2	1:105:A:THR:HB	2	3.7
(1,931)	1:105:A:THR:HB	1:114:A:PHE:HE2	13	3.7
(1,930)	1:105:A:THR:HB	1:114:A:PHE:HD2	2	3.7
(1,986)	1:114:A:PHE:HD2	1:105:A:THR:HB	16	3.69
(1,930)	1:105:A:THR:HB	1:114:A:PHE:HD2	16	3.69
(1,989)	1:114:A:PHE:HE2	1:105:A:THR:HB	19	3.68
(1,931)	1:105:A:THR:HB	1:114:A:PHE:HE2	19	3.68
(1,989)	1:114:A:PHE:HE2	1:105:A:THR:HB	7	3.66
(1,931)	1:105:A:THR:HB	1:114:A:PHE:HE2	7	3.66
(1,986)	1:114:A:PHE:HD2	1:105:A:THR:HB	1	3.65
(1,930)	1:105:A:THR:HB	1:114:A:PHE:HD2	1	3.65
(1,986)	1:114:A:PHE:HD2	1:105:A:THR:HB	17	3.64
(1,930)	1:105:A:THR:HB	1:114:A:PHE:HD2	17	3.64
(1,1208)	1:145:A:PHE:HD1	1:86:A:LEU:HB2	12	3.63
(1,1208)	1:145:A:PHE:HD1	1:86:A:LEU:HB3	12	3.63
(1,986)	1:114:A:PHE:HD2	1:105:A:THR:HB	6	3.63
(1,986)	1:114:A:PHE:HD2	1:105:A:THR:HB	20	3.63
(1,930)	1:105:A:THR:HB	1:114:A:PHE:HD2	6	3.63
(1,930)	1:105:A:THR:HB	1:114:A:PHE:HD2	20	3.63
(1,787)	1:86:A:LEU:HB2	1:145:A:PHE:HD1	12	3.63
(1,787)	1:86:A:LEU:HB3	1:145:A:PHE:HD1	12	3.63
(1,1208)	1:145:A:PHE:HD1	1:86:A:LEU:HB2	13	3.61
(1,1208)	1:145:A:PHE:HD1	1:86:A:LEU:HB3	13	3.61
(1,989)	1:114:A:PHE:HE2	1:105:A:THR:HB	14	3.61
(1,931)	1:105:A:THR:HB	1:114:A:PHE:HE2	14	3.61
(1,787)	1:86:A:LEU:HB2	1:145:A:PHE:HD1	13	3.61
(1,787)	1:86:A:LEU:HB3	1:145:A:PHE:HD1	13	3.61
(1,1208)	1:145:A:PHE:HD1	1:86:A:LEU:HB2	19	3.6
(1,1208)	1:145:A:PHE:HD1	1:86:A:LEU:HB3	19	3.6
(1,989)	1:114:A:PHE:HE2	1:105:A:THR:HB	15	3.6
(1,931)	1:105:A:THR:HB	1:114:A:PHE:HE2	15	3.6
(1,787)	1:86:A:LEU:HB2	1:145:A:PHE:HD1	19	3.6
(1,787)	1:86:A:LEU:HB3	1:145:A:PHE:HD1	19	3.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,989)	1:114:A:PHE:HE2	1:105:A:THR:HB	5	3.59
(1,931)	1:105:A:THR:HB	1:114:A:PHE:HE2	5	3.59
(1,581)	1:132:A:THR:H	1:114:A:PHE:HE1	8	3.59
(1,581)	1:132:A:THR:H	1:114:A:PHE:HE1	13	3.59
(1,404)	1:114:A:PHE:HE1	1:132:A:THR:H	8	3.59
(1,404)	1:114:A:PHE:HE1	1:132:A:THR:H	13	3.59
(1,986)	1:114:A:PHE:HD2	1:105:A:THR:HB	3	3.58
(1,930)	1:105:A:THR:HB	1:114:A:PHE:HD2	3	3.58
(1,989)	1:114:A:PHE:HE2	1:105:A:THR:HB	12	3.55
(1,931)	1:105:A:THR:HB	1:114:A:PHE:HE2	12	3.55
(1,581)	1:132:A:THR:H	1:114:A:PHE:HE1	10	3.55
(1,581)	1:132:A:THR:H	1:114:A:PHE:HE1	19	3.55
(1,404)	1:114:A:PHE:HE1	1:132:A:THR:H	10	3.55
(1,404)	1:114:A:PHE:HE1	1:132:A:THR:H	19	3.55
(1,989)	1:114:A:PHE:HE2	1:105:A:THR:HB	8	3.54
(1,931)	1:105:A:THR:HB	1:114:A:PHE:HE2	8	3.54
(1,581)	1:132:A:THR:H	1:114:A:PHE:HE1	15	3.54
(1,581)	1:132:A:THR:H	1:114:A:PHE:HE1	16	3.54
(1,404)	1:114:A:PHE:HE1	1:132:A:THR:H	15	3.54
(1,404)	1:114:A:PHE:HE1	1:132:A:THR:H	16	3.54
(1,581)	1:132:A:THR:H	1:114:A:PHE:HE1	4	3.53
(1,581)	1:132:A:THR:H	1:114:A:PHE:HE1	12	3.53
(1,581)	1:132:A:THR:H	1:114:A:PHE:HE1	14	3.53
(1,581)	1:132:A:THR:H	1:114:A:PHE:HE1	17	3.53
(1,404)	1:114:A:PHE:HE1	1:132:A:THR:H	4	3.53
(1,404)	1:114:A:PHE:HE1	1:132:A:THR:H	12	3.53
(1,404)	1:114:A:PHE:HE1	1:132:A:THR:H	14	3.53
(1,404)	1:114:A:PHE:HE1	1:132:A:THR:H	17	3.53
(1,581)	1:132:A:THR:H	1:114:A:PHE:HE1	5	3.52
(1,581)	1:132:A:THR:H	1:114:A:PHE:HE1	7	3.52
(1,581)	1:132:A:THR:H	1:114:A:PHE:HE1	9	3.52
(1,581)	1:132:A:THR:H	1:114:A:PHE:HE1	20	3.52
(1,404)	1:114:A:PHE:HE1	1:132:A:THR:H	5	3.52
(1,404)	1:114:A:PHE:HE1	1:132:A:THR:H	7	3.52
(1,404)	1:114:A:PHE:HE1	1:132:A:THR:H	9	3.52
(1,404)	1:114:A:PHE:HE1	1:132:A:THR:H	20	3.52
(1,581)	1:132:A:THR:H	1:114:A:PHE:HE1	2	3.51
(1,581)	1:132:A:THR:H	1:114:A:PHE:HE1	3	3.51
(1,581)	1:132:A:THR:H	1:114:A:PHE:HE1	6	3.51
(1,404)	1:114:A:PHE:HE1	1:132:A:THR:H	2	3.51
(1,404)	1:114:A:PHE:HE1	1:132:A:THR:H	3	3.51
(1,404)	1:114:A:PHE:HE1	1:132:A:THR:H	6	3.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,986)	1:114:A:PHE:HD2	1:105:A:THR:HB	18	3.5
(1,930)	1:105:A:THR:HB	1:114:A:PHE:HD2	18	3.5
(1,581)	1:132:A:THR:H	1:114:A:PHE:HE1	1	3.5
(1,581)	1:132:A:THR:H	1:114:A:PHE:HE1	11	3.5
(1,581)	1:132:A:THR:H	1:114:A:PHE:HE1	18	3.5
(1,404)	1:114:A:PHE:HE1	1:132:A:THR:H	1	3.5
(1,404)	1:114:A:PHE:HE1	1:132:A:THR:H	11	3.5
(1,404)	1:114:A:PHE:HE1	1:132:A:THR:H	18	3.5
(1,989)	1:114:A:PHE:HE2	1:105:A:THR:HB	4	3.48
(1,931)	1:105:A:THR:HB	1:114:A:PHE:HE2	4	3.48
(1,1209)	1:145:A:PHE:HE1	1:86:A:LEU:HB2	13	3.45
(1,1209)	1:145:A:PHE:HE1	1:86:A:LEU:HB3	13	3.45
(1,788)	1:86:A:LEU:HB2	1:145:A:PHE:HE1	13	3.45
(1,788)	1:86:A:LEU:HB3	1:145:A:PHE:HE1	13	3.45
(1,986)	1:114:A:PHE:HD2	1:105:A:THR:HB	13	3.42
(1,930)	1:105:A:THR:HB	1:114:A:PHE:HD2	13	3.42
(1,1112)	1:132:A:THR:HA	1:114:A:PHE:HD1	8	3.41
(1,1112)	1:132:A:THR:HA	1:114:A:PHE:HD1	13	3.41
(1,1001)	1:114:A:PHE:HD1	1:132:A:THR:HA	8	3.41
(1,1001)	1:114:A:PHE:HD1	1:132:A:THR:HA	13	3.41
(1,986)	1:114:A:PHE:HD2	1:105:A:THR:HB	7	3.41
(1,930)	1:105:A:THR:HB	1:114:A:PHE:HD2	7	3.41
(1,1209)	1:145:A:PHE:HE1	1:86:A:LEU:HB2	12	3.4
(1,1209)	1:145:A:PHE:HE1	1:86:A:LEU:HB3	12	3.4
(1,788)	1:86:A:LEU:HB2	1:145:A:PHE:HE1	12	3.4
(1,788)	1:86:A:LEU:HB3	1:145:A:PHE:HE1	12	3.4
(1,989)	1:114:A:PHE:HE2	1:105:A:THR:HB	9	3.39
(1,986)	1:114:A:PHE:HD2	1:105:A:THR:HB	19	3.39
(1,931)	1:105:A:THR:HB	1:114:A:PHE:HE2	9	3.39
(1,930)	1:105:A:THR:HB	1:114:A:PHE:HD2	19	3.39
(1,1209)	1:145:A:PHE:HE1	1:86:A:LEU:HB2	19	3.38
(1,1209)	1:145:A:PHE:HE1	1:86:A:LEU:HB3	19	3.38
(1,788)	1:86:A:LEU:HB2	1:145:A:PHE:HE1	19	3.38
(1,788)	1:86:A:LEU:HB3	1:145:A:PHE:HE1	19	3.38
(1,986)	1:114:A:PHE:HD2	1:105:A:THR:HB	14	3.34
(1,930)	1:105:A:THR:HB	1:114:A:PHE:HD2	14	3.34
(1,1111)	1:131:A:LYS:HG2	1:114:A:PHE:HE1	12	3.33
(1,1111)	1:131:A:LYS:HG3	1:114:A:PHE:HE1	12	3.33
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG2	12	3.33
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG3	12	3.33
(1,986)	1:114:A:PHE:HD2	1:105:A:THR:HB	15	3.33
(1,930)	1:105:A:THR:HB	1:114:A:PHE:HD2	15	3.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,986)	1:114:A:PHE:HD2	1:105:A:THR:HB	5	3.32
(1,930)	1:105:A:THR:HB	1:114:A:PHE:HD2	5	3.32
(1,1112)	1:132:A:THR:HA	1:114:A:PHE:HD1	19	3.31
(1,1001)	1:114:A:PHE:HD1	1:132:A:THR:HA	19	3.31
(1,1111)	1:131:A:LYS:HG2	1:114:A:PHE:HE1	14	3.28
(1,1111)	1:131:A:LYS:HG3	1:114:A:PHE:HE1	14	3.28
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG2	14	3.28
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG3	14	3.28
(1,1113)	1:132:A:THR:HA	1:114:A:PHE:HE1	8	3.27
(1,1002)	1:114:A:PHE:HE1	1:132:A:THR:HA	8	3.27
(1,986)	1:114:A:PHE:HD2	1:105:A:THR:HB	12	3.27
(1,930)	1:105:A:THR:HB	1:114:A:PHE:HD2	12	3.27
(1,986)	1:114:A:PHE:HD2	1:105:A:THR:HB	8	3.26
(1,930)	1:105:A:THR:HB	1:114:A:PHE:HD2	8	3.26
(1,1113)	1:132:A:THR:HA	1:114:A:PHE:HE1	13	3.25
(1,1002)	1:114:A:PHE:HE1	1:132:A:THR:HA	13	3.25
(1,1112)	1:132:A:THR:HA	1:114:A:PHE:HD1	6	3.23
(1,1111)	1:131:A:LYS:HG2	1:114:A:PHE:HE1	1	3.23
(1,1111)	1:131:A:LYS:HG3	1:114:A:PHE:HE1	1	3.23
(1,1111)	1:131:A:LYS:HG2	1:114:A:PHE:HE1	16	3.23
(1,1111)	1:131:A:LYS:HG3	1:114:A:PHE:HE1	16	3.23
(1,1001)	1:114:A:PHE:HD1	1:132:A:THR:HA	6	3.23
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG2	1	3.23
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG3	1	3.23
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG2	16	3.23
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG3	16	3.23
(1,1112)	1:132:A:THR:HA	1:114:A:PHE:HD1	16	3.22
(1,1001)	1:114:A:PHE:HD1	1:132:A:THR:HA	16	3.22
(1,986)	1:114:A:PHE:HD2	1:105:A:THR:HB	4	3.21
(1,930)	1:105:A:THR:HB	1:114:A:PHE:HD2	4	3.21
(1,1111)	1:131:A:LYS:HG2	1:114:A:PHE:HE1	6	3.19
(1,1111)	1:131:A:LYS:HG3	1:114:A:PHE:HE1	6	3.19
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG2	6	3.19
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG3	6	3.19
(1,1112)	1:132:A:THR:HA	1:114:A:PHE:HD1	7	3.18
(1,1001)	1:114:A:PHE:HD1	1:132:A:THR:HA	7	3.18
(1,580)	1:132:A:THR:H	1:114:A:PHE:HD1	13	3.18
(1,403)	1:114:A:PHE:HD1	1:132:A:THR:H	13	3.18
(1,1112)	1:132:A:THR:HA	1:114:A:PHE:HD1	14	3.17
(1,1001)	1:114:A:PHE:HD1	1:132:A:THR:HA	14	3.17
(1,580)	1:132:A:THR:H	1:114:A:PHE:HD1	8	3.16
(1,403)	1:114:A:PHE:HD1	1:132:A:THR:H	8	3.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1112)	1:132:A:THR:HA	1:114:A:PHE:HD1	10	3.15
(1,1001)	1:114:A:PHE:HD1	1:132:A:THR:HA	10	3.15
(1,1112)	1:132:A:THR:HA	1:114:A:PHE:HD1	17	3.14
(1,1001)	1:114:A:PHE:HD1	1:132:A:THR:HA	17	3.14
(1,1113)	1:132:A:THR:HA	1:114:A:PHE:HE1	19	3.12
(1,1112)	1:132:A:THR:HA	1:114:A:PHE:HD1	12	3.12
(1,1002)	1:114:A:PHE:HE1	1:132:A:THR:HA	19	3.12
(1,1001)	1:114:A:PHE:HD1	1:132:A:THR:HA	12	3.12
(1,1113)	1:132:A:THR:HA	1:114:A:PHE:HE1	7	3.11
(1,1002)	1:114:A:PHE:HE1	1:132:A:THR:HA	7	3.11
(1,986)	1:114:A:PHE:HD2	1:105:A:THR:HB	9	3.11
(1,930)	1:105:A:THR:HB	1:114:A:PHE:HD2	9	3.11
(1,1112)	1:132:A:THR:HA	1:114:A:PHE:HD1	2	3.1
(1,1001)	1:114:A:PHE:HD1	1:132:A:THR:HA	2	3.1
(1,580)	1:132:A:THR:H	1:114:A:PHE:HD1	14	3.1
(1,580)	1:132:A:THR:H	1:114:A:PHE:HD1	16	3.1
(1,580)	1:132:A:THR:H	1:114:A:PHE:HD1	19	3.1
(1,403)	1:114:A:PHE:HD1	1:132:A:THR:H	14	3.1
(1,403)	1:114:A:PHE:HD1	1:132:A:THR:H	16	3.1
(1,403)	1:114:A:PHE:HD1	1:132:A:THR:H	19	3.1
(1,1113)	1:132:A:THR:HA	1:114:A:PHE:HE1	16	3.09
(1,1002)	1:114:A:PHE:HE1	1:132:A:THR:HA	16	3.09
(1,580)	1:132:A:THR:H	1:114:A:PHE:HD1	12	3.09
(1,403)	1:114:A:PHE:HD1	1:132:A:THR:H	12	3.09
(1,1113)	1:132:A:THR:HA	1:114:A:PHE:HE1	6	3.08
(1,1112)	1:132:A:THR:HA	1:114:A:PHE:HD1	1	3.08
(1,1112)	1:132:A:THR:HA	1:114:A:PHE:HD1	3	3.08
(1,1002)	1:114:A:PHE:HE1	1:132:A:THR:HA	6	3.08
(1,1001)	1:114:A:PHE:HD1	1:132:A:THR:HA	1	3.08
(1,1001)	1:114:A:PHE:HD1	1:132:A:THR:HA	3	3.08
(1,580)	1:132:A:THR:H	1:114:A:PHE:HD1	6	3.08
(1,580)	1:132:A:THR:H	1:114:A:PHE:HD1	10	3.08
(1,403)	1:114:A:PHE:HD1	1:132:A:THR:H	6	3.08
(1,403)	1:114:A:PHE:HD1	1:132:A:THR:H	10	3.08
(1,1113)	1:132:A:THR:HA	1:114:A:PHE:HE1	10	3.07
(1,1002)	1:114:A:PHE:HE1	1:132:A:THR:HA	10	3.07
(1,580)	1:132:A:THR:H	1:114:A:PHE:HD1	15	3.07
(1,403)	1:114:A:PHE:HD1	1:132:A:THR:H	15	3.07
(1,1112)	1:132:A:THR:HA	1:114:A:PHE:HD1	11	3.06
(1,1112)	1:132:A:THR:HA	1:114:A:PHE:HD1	15	3.06
(1,1112)	1:132:A:THR:HA	1:114:A:PHE:HD1	18	3.06
(1,1112)	1:132:A:THR:HA	1:114:A:PHE:HD1	20	3.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1001)	1:114:A:PHE:HD1	1:132:A:THR:HA	11	3.06
(1,1001)	1:114:A:PHE:HD1	1:132:A:THR:HA	15	3.06
(1,1001)	1:114:A:PHE:HD1	1:132:A:THR:HA	18	3.06
(1,1001)	1:114:A:PHE:HD1	1:132:A:THR:HA	20	3.06
(1,580)	1:132:A:THR:H	1:114:A:PHE:HD1	4	3.06
(1,403)	1:114:A:PHE:HD1	1:132:A:THR:H	4	3.06
(1,580)	1:132:A:THR:H	1:114:A:PHE:HD1	17	3.05
(1,403)	1:114:A:PHE:HD1	1:132:A:THR:H	17	3.05
(1,580)	1:132:A:THR:H	1:114:A:PHE:HD1	1	3.04
(1,580)	1:132:A:THR:H	1:114:A:PHE:HD1	2	3.04
(1,580)	1:132:A:THR:H	1:114:A:PHE:HD1	3	3.04
(1,580)	1:132:A:THR:H	1:114:A:PHE:HD1	9	3.04
(1,403)	1:114:A:PHE:HD1	1:132:A:THR:H	1	3.04
(1,403)	1:114:A:PHE:HD1	1:132:A:THR:H	2	3.04
(1,403)	1:114:A:PHE:HD1	1:132:A:THR:H	3	3.04
(1,403)	1:114:A:PHE:HD1	1:132:A:THR:H	9	3.04
(1,1112)	1:132:A:THR:HA	1:114:A:PHE:HD1	4	3.03
(1,1001)	1:114:A:PHE:HD1	1:132:A:THR:HA	4	3.03
(1,580)	1:132:A:THR:H	1:114:A:PHE:HD1	7	3.03
(1,580)	1:132:A:THR:H	1:114:A:PHE:HD1	20	3.03
(1,403)	1:114:A:PHE:HD1	1:132:A:THR:H	7	3.03
(1,403)	1:114:A:PHE:HD1	1:132:A:THR:H	20	3.03
(1,1113)	1:132:A:THR:HA	1:114:A:PHE:HE1	17	3.02
(1,1002)	1:114:A:PHE:HE1	1:132:A:THR:HA	17	3.02
(1,580)	1:132:A:THR:H	1:114:A:PHE:HD1	5	3.02
(1,403)	1:114:A:PHE:HD1	1:132:A:THR:H	5	3.02
(1,1212)	1:145:A:PHE:HE1	1:90:A:ILE:HG21	19	3.01
(1,1212)	1:145:A:PHE:HE1	1:90:A:ILE:HG22	19	3.01
(1,1212)	1:145:A:PHE:HE1	1:90:A:ILE:HG23	19	3.01
(1,1113)	1:132:A:THR:HA	1:114:A:PHE:HE1	18	3.01
(1,1002)	1:114:A:PHE:HE1	1:132:A:THR:HA	18	3.01
(1,859)	1:90:A:ILE:HG21	1:145:A:PHE:HE1	19	3.01
(1,859)	1:90:A:ILE:HG22	1:145:A:PHE:HE1	19	3.01
(1,859)	1:90:A:ILE:HG23	1:145:A:PHE:HE1	19	3.01
(1,580)	1:132:A:THR:H	1:114:A:PHE:HD1	11	3.01
(1,403)	1:114:A:PHE:HD1	1:132:A:THR:H	11	3.01
(1,1113)	1:132:A:THR:HA	1:114:A:PHE:HE1	2	3.0
(1,1113)	1:132:A:THR:HA	1:114:A:PHE:HE1	14	3.0
(1,1002)	1:114:A:PHE:HE1	1:132:A:THR:HA	2	3.0
(1,1002)	1:114:A:PHE:HE1	1:132:A:THR:HA	14	3.0
(1,580)	1:132:A:THR:H	1:114:A:PHE:HD1	18	3.0
(1,403)	1:114:A:PHE:HD1	1:132:A:THR:H	18	3.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1113)	1:132:A:THR:HA	1:114:A:PHE:HE1	11	2.99
(1,1002)	1:114:A:PHE:HE1	1:132:A:THR:HA	11	2.99
(1,1113)	1:132:A:THR:HA	1:114:A:PHE:HE1	3	2.98
(1,1113)	1:132:A:THR:HA	1:114:A:PHE:HE1	20	2.98
(1,1002)	1:114:A:PHE:HE1	1:132:A:THR:HA	3	2.98
(1,1002)	1:114:A:PHE:HE1	1:132:A:THR:HA	20	2.98
(1,1112)	1:132:A:THR:HA	1:114:A:PHE:HD1	9	2.96
(1,1001)	1:114:A:PHE:HD1	1:132:A:THR:HA	9	2.96
(1,1113)	1:132:A:THR:HA	1:114:A:PHE:HE1	12	2.95
(1,1002)	1:114:A:PHE:HE1	1:132:A:THR:HA	12	2.95
(1,1113)	1:132:A:THR:HA	1:114:A:PHE:HE1	1	2.94
(1,1112)	1:132:A:THR:HA	1:114:A:PHE:HD1	5	2.94
(1,1002)	1:114:A:PHE:HE1	1:132:A:THR:HA	1	2.94
(1,1001)	1:114:A:PHE:HD1	1:132:A:THR:HA	5	2.94
(1,1113)	1:132:A:THR:HA	1:114:A:PHE:HE1	15	2.93
(1,1002)	1:114:A:PHE:HE1	1:132:A:THR:HA	15	2.93
(1,985)	1:114:A:PHE:HD2	1:105:A:THR:HA	17	2.9
(1,928)	1:105:A:THR:HA	1:114:A:PHE:HD2	17	2.9
(1,588)	1:133:A:LYS:H	1:114:A:PHE:HE1	13	2.9
(1,406)	1:114:A:PHE:HE1	1:133:A:LYS:H	13	2.9
(1,1212)	1:145:A:PHE:HE1	1:90:A:ILE:HG21	13	2.89
(1,1212)	1:145:A:PHE:HE1	1:90:A:ILE:HG22	13	2.89
(1,1212)	1:145:A:PHE:HE1	1:90:A:ILE:HG23	13	2.89
(1,985)	1:114:A:PHE:HD2	1:105:A:THR:HA	10	2.89
(1,985)	1:114:A:PHE:HD2	1:105:A:THR:HA	20	2.89
(1,928)	1:105:A:THR:HA	1:114:A:PHE:HD2	10	2.89
(1,928)	1:105:A:THR:HA	1:114:A:PHE:HD2	20	2.89
(1,859)	1:90:A:ILE:HG21	1:145:A:PHE:HE1	13	2.89
(1,859)	1:90:A:ILE:HG22	1:145:A:PHE:HE1	13	2.89
(1,859)	1:90:A:ILE:HG23	1:145:A:PHE:HE1	13	2.89
(1,1113)	1:132:A:THR:HA	1:114:A:PHE:HE1	4	2.87
(1,1002)	1:114:A:PHE:HE1	1:132:A:THR:HA	4	2.87
(1,988)	1:114:A:PHE:HE2	1:105:A:THR:HA	17	2.86
(1,985)	1:114:A:PHE:HD2	1:105:A:THR:HA	2	2.86
(1,985)	1:114:A:PHE:HD2	1:105:A:THR:HA	11	2.86
(1,929)	1:105:A:THR:HA	1:114:A:PHE:HE2	17	2.86
(1,928)	1:105:A:THR:HA	1:114:A:PHE:HD2	2	2.86
(1,928)	1:105:A:THR:HA	1:114:A:PHE:HD2	11	2.86
(1,588)	1:133:A:LYS:H	1:114:A:PHE:HE1	7	2.86
(1,588)	1:133:A:LYS:H	1:114:A:PHE:HE1	8	2.86
(1,406)	1:114:A:PHE:HE1	1:133:A:LYS:H	7	2.86
(1,406)	1:114:A:PHE:HE1	1:133:A:LYS:H	8	2.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,988)	1:114:A:PHE:HE2	1:105:A:THR:HA	20	2.85
(1,929)	1:105:A:THR:HA	1:114:A:PHE:HE2	20	2.85
(1,588)	1:133:A:LYS:H	1:114:A:PHE:HE1	16	2.84
(1,406)	1:114:A:PHE:HE1	1:133:A:LYS:H	16	2.84
(1,1211)	1:145:A:PHE:HD1	1:87:A:LEU:HD21	19	2.83
(1,1211)	1:145:A:PHE:HD1	1:87:A:LEU:HD22	19	2.83
(1,1211)	1:145:A:PHE:HD1	1:87:A:LEU:HD23	19	2.83
(1,1113)	1:132:A:THR:HA	1:114:A:PHE:HE1	9	2.83
(1,1002)	1:114:A:PHE:HE1	1:132:A:THR:HA	9	2.83
(1,817)	1:87:A:LEU:HD21	1:145:A:PHE:HD1	19	2.83
(1,817)	1:87:A:LEU:HD22	1:145:A:PHE:HD1	19	2.83
(1,817)	1:87:A:LEU:HD23	1:145:A:PHE:HD1	19	2.83
(1,1211)	1:145:A:PHE:HD1	1:87:A:LEU:HD21	12	2.82
(1,1211)	1:145:A:PHE:HD1	1:87:A:LEU:HD22	12	2.82
(1,1211)	1:145:A:PHE:HD1	1:87:A:LEU:HD23	12	2.82
(1,988)	1:114:A:PHE:HE2	1:105:A:THR:HA	7	2.82
(1,985)	1:114:A:PHE:HD2	1:105:A:THR:HA	7	2.82
(1,929)	1:105:A:THR:HA	1:114:A:PHE:HE2	7	2.82
(1,928)	1:105:A:THR:HA	1:114:A:PHE:HD2	7	2.82
(1,817)	1:87:A:LEU:HD21	1:145:A:PHE:HD1	12	2.82
(1,817)	1:87:A:LEU:HD22	1:145:A:PHE:HD1	12	2.82
(1,817)	1:87:A:LEU:HD23	1:145:A:PHE:HD1	12	2.82
(1,588)	1:133:A:LYS:H	1:114:A:PHE:HE1	11	2.82
(1,406)	1:114:A:PHE:HE1	1:133:A:LYS:H	11	2.82
(1,988)	1:114:A:PHE:HE2	1:105:A:THR:HA	5	2.81
(1,988)	1:114:A:PHE:HE2	1:105:A:THR:HA	13	2.81
(1,985)	1:114:A:PHE:HD2	1:105:A:THR:HA	5	2.81
(1,985)	1:114:A:PHE:HD2	1:105:A:THR:HA	13	2.81
(1,985)	1:114:A:PHE:HD2	1:105:A:THR:HA	16	2.81
(1,929)	1:105:A:THR:HA	1:114:A:PHE:HE2	5	2.81
(1,929)	1:105:A:THR:HA	1:114:A:PHE:HE2	13	2.81
(1,928)	1:105:A:THR:HA	1:114:A:PHE:HD2	5	2.81
(1,928)	1:105:A:THR:HA	1:114:A:PHE:HD2	13	2.81
(1,928)	1:105:A:THR:HA	1:114:A:PHE:HD2	16	2.81
(1,1113)	1:132:A:THR:HA	1:114:A:PHE:HE1	5	2.8
(1,1002)	1:114:A:PHE:HE1	1:132:A:THR:HA	5	2.8
(1,988)	1:114:A:PHE:HE2	1:105:A:THR:HA	2	2.8
(1,988)	1:114:A:PHE:HE2	1:105:A:THR:HA	15	2.8
(1,985)	1:114:A:PHE:HD2	1:105:A:THR:HA	1	2.8
(1,985)	1:114:A:PHE:HD2	1:105:A:THR:HA	3	2.8
(1,929)	1:105:A:THR:HA	1:114:A:PHE:HE2	2	2.8
(1,929)	1:105:A:THR:HA	1:114:A:PHE:HE2	15	2.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,928)	1:105:A:THR:HA	1:114:A:PHE:HD2	1	2.8
(1,928)	1:105:A:THR:HA	1:114:A:PHE:HD2	3	2.8
(1,588)	1:133:A:LYS:H	1:114:A:PHE:HE1	1	2.8
(1,406)	1:114:A:PHE:HE1	1:133:A:LYS:H	1	2.8
(1,988)	1:114:A:PHE:HE2	1:105:A:THR:HA	14	2.79
(1,985)	1:114:A:PHE:HD2	1:105:A:THR:HA	14	2.79
(1,985)	1:114:A:PHE:HD2	1:105:A:THR:HA	15	2.79
(1,929)	1:105:A:THR:HA	1:114:A:PHE:HE2	14	2.79
(1,928)	1:105:A:THR:HA	1:114:A:PHE:HD2	14	2.79
(1,928)	1:105:A:THR:HA	1:114:A:PHE:HD2	15	2.79
(1,588)	1:133:A:LYS:H	1:114:A:PHE:HE1	10	2.79
(1,588)	1:133:A:LYS:H	1:114:A:PHE:HE1	18	2.79
(1,406)	1:114:A:PHE:HE1	1:133:A:LYS:H	10	2.79
(1,406)	1:114:A:PHE:HE1	1:133:A:LYS:H	18	2.79
(1,988)	1:114:A:PHE:HE2	1:105:A:THR:HA	9	2.78
(1,988)	1:114:A:PHE:HE2	1:105:A:THR:HA	10	2.78
(1,988)	1:114:A:PHE:HE2	1:105:A:THR:HA	12	2.78
(1,988)	1:114:A:PHE:HE2	1:105:A:THR:HA	18	2.78
(1,929)	1:105:A:THR:HA	1:114:A:PHE:HE2	9	2.78
(1,929)	1:105:A:THR:HA	1:114:A:PHE:HE2	10	2.78
(1,929)	1:105:A:THR:HA	1:114:A:PHE:HE2	12	2.78
(1,929)	1:105:A:THR:HA	1:114:A:PHE:HE2	18	2.78
(1,988)	1:114:A:PHE:HE2	1:105:A:THR:HA	4	2.77
(1,988)	1:114:A:PHE:HE2	1:105:A:THR:HA	11	2.77
(1,988)	1:114:A:PHE:HE2	1:105:A:THR:HA	19	2.77
(1,985)	1:114:A:PHE:HD2	1:105:A:THR:HA	12	2.77
(1,985)	1:114:A:PHE:HD2	1:105:A:THR:HA	18	2.77
(1,929)	1:105:A:THR:HA	1:114:A:PHE:HE2	4	2.77
(1,929)	1:105:A:THR:HA	1:114:A:PHE:HE2	11	2.77
(1,929)	1:105:A:THR:HA	1:114:A:PHE:HE2	19	2.77
(1,928)	1:105:A:THR:HA	1:114:A:PHE:HD2	12	2.77
(1,928)	1:105:A:THR:HA	1:114:A:PHE:HD2	18	2.77
(1,588)	1:133:A:LYS:H	1:114:A:PHE:HE1	3	2.77
(1,406)	1:114:A:PHE:HE1	1:133:A:LYS:H	3	2.77
(1,1212)	1:145:A:PHE:HE1	1:90:A:ILE:HG21	12	2.76
(1,1212)	1:145:A:PHE:HE1	1:90:A:ILE:HG22	12	2.76
(1,1212)	1:145:A:PHE:HE1	1:90:A:ILE:HG23	12	2.76
(1,988)	1:114:A:PHE:HE2	1:105:A:THR:HA	1	2.76
(1,929)	1:105:A:THR:HA	1:114:A:PHE:HE2	1	2.76
(1,859)	1:90:A:ILE:HG21	1:145:A:PHE:HE1	12	2.76
(1,859)	1:90:A:ILE:HG22	1:145:A:PHE:HE1	12	2.76
(1,859)	1:90:A:ILE:HG23	1:145:A:PHE:HE1	12	2.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,588)	1:133:A:LYS:H	1:114:A:PHE:HE1	2	2.76
(1,406)	1:114:A:PHE:HE1	1:133:A:LYS:H	2	2.76
(1,988)	1:114:A:PHE:HE2	1:105:A:THR:HA	8	2.75
(1,985)	1:114:A:PHE:HD2	1:105:A:THR:HA	4	2.75
(1,929)	1:105:A:THR:HA	1:114:A:PHE:HE2	8	2.75
(1,928)	1:105:A:THR:HA	1:114:A:PHE:HD2	4	2.75
(1,588)	1:133:A:LYS:H	1:114:A:PHE:HE1	20	2.75
(1,406)	1:114:A:PHE:HE1	1:133:A:LYS:H	20	2.75
(1,988)	1:114:A:PHE:HE2	1:105:A:THR:HA	3	2.74
(1,985)	1:114:A:PHE:HD2	1:105:A:THR:HA	6	2.74
(1,985)	1:114:A:PHE:HD2	1:105:A:THR:HA	9	2.74
(1,985)	1:114:A:PHE:HD2	1:105:A:THR:HA	19	2.74
(1,929)	1:105:A:THR:HA	1:114:A:PHE:HE2	3	2.74
(1,928)	1:105:A:THR:HA	1:114:A:PHE:HD2	6	2.74
(1,928)	1:105:A:THR:HA	1:114:A:PHE:HD2	9	2.74
(1,928)	1:105:A:THR:HA	1:114:A:PHE:HD2	19	2.74
(1,988)	1:114:A:PHE:HE2	1:105:A:THR:HA	6	2.73
(1,985)	1:114:A:PHE:HD2	1:105:A:THR:HA	8	2.73
(1,929)	1:105:A:THR:HA	1:114:A:PHE:HE2	6	2.73
(1,928)	1:105:A:THR:HA	1:114:A:PHE:HD2	8	2.73
(1,988)	1:114:A:PHE:HE2	1:105:A:THR:HA	16	2.72
(1,929)	1:105:A:THR:HA	1:114:A:PHE:HE2	16	2.72
(1,588)	1:133:A:LYS:H	1:114:A:PHE:HE1	6	2.68
(1,588)	1:133:A:LYS:H	1:114:A:PHE:HE1	15	2.68
(1,406)	1:114:A:PHE:HE1	1:133:A:LYS:H	6	2.68
(1,406)	1:114:A:PHE:HE1	1:133:A:LYS:H	15	2.68
(1,1211)	1:145:A:PHE:HD1	1:87:A:LEU:HD21	13	2.67
(1,1211)	1:145:A:PHE:HD1	1:87:A:LEU:HD22	13	2.67
(1,1211)	1:145:A:PHE:HD1	1:87:A:LEU:HD23	13	2.67
(1,817)	1:87:A:LEU:HD21	1:145:A:PHE:HD1	13	2.67
(1,817)	1:87:A:LEU:HD22	1:145:A:PHE:HD1	13	2.67
(1,817)	1:87:A:LEU:HD23	1:145:A:PHE:HD1	13	2.67
(1,588)	1:133:A:LYS:H	1:114:A:PHE:HE1	14	2.67
(1,406)	1:114:A:PHE:HE1	1:133:A:LYS:H	14	2.67
(1,588)	1:133:A:LYS:H	1:114:A:PHE:HE1	9	2.66
(1,406)	1:114:A:PHE:HE1	1:133:A:LYS:H	9	2.66
(1,588)	1:133:A:LYS:H	1:114:A:PHE:HE1	12	2.65
(1,406)	1:114:A:PHE:HE1	1:133:A:LYS:H	12	2.65
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB2	17	2.64
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB3	17	2.64
(1,971)	1:112:A:PRO:HB2	1:114:A:PHE:HE2	17	2.64
(1,971)	1:112:A:PRO:HB3	1:114:A:PHE:HE2	17	2.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,588)	1:133:A:LYS:H	1:114:A:PHE:HE1	5	2.64
(1,406)	1:114:A:PHE:HE1	1:133:A:LYS:H	5	2.64
(1,1236)	1:149:A:LYS:HG2	1:145:A:PHE:HE2	12	2.63
(1,1236)	1:149:A:LYS:HG3	1:145:A:PHE:HE2	12	2.63
(1,1220)	1:145:A:PHE:HE2	1:149:A:LYS:HG2	12	2.63
(1,1220)	1:145:A:PHE:HE2	1:149:A:LYS:HG3	12	2.63
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB2	4	2.63
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB3	4	2.63
(1,971)	1:112:A:PRO:HB2	1:114:A:PHE:HE2	4	2.63
(1,971)	1:112:A:PRO:HB3	1:114:A:PHE:HE2	4	2.63
(1,587)	1:133:A:LYS:H	1:114:A:PHE:HD1	13	2.63
(1,405)	1:114:A:PHE:HD1	1:133:A:LYS:H	13	2.63
(1,588)	1:133:A:LYS:H	1:114:A:PHE:HE1	4	2.62
(1,406)	1:114:A:PHE:HE1	1:133:A:LYS:H	4	2.62
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB2	15	2.58
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB3	15	2.58
(1,971)	1:112:A:PRO:HB2	1:114:A:PHE:HE2	15	2.58
(1,971)	1:112:A:PRO:HB3	1:114:A:PHE:HE2	15	2.58
(1,1109)	1:131:A:LYS:HA	1:114:A:PHE:HD1	5	2.56
(1,998)	1:114:A:PHE:HD1	1:131:A:LYS:HA	5	2.56
(1,587)	1:133:A:LYS:H	1:114:A:PHE:HD1	8	2.56
(1,405)	1:114:A:PHE:HD1	1:133:A:LYS:H	8	2.56
(1,587)	1:133:A:LYS:H	1:114:A:PHE:HD1	16	2.54
(1,405)	1:114:A:PHE:HD1	1:133:A:LYS:H	16	2.54
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB2	20	2.53
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB3	20	2.53
(1,971)	1:112:A:PRO:HB2	1:114:A:PHE:HE2	20	2.53
(1,971)	1:112:A:PRO:HB3	1:114:A:PHE:HE2	20	2.53
(1,150)	1:83:A:TYR:HD2	1:82:A:ALA:H	1	2.53
(1,147)	1:82:A:ALA:H	1:83:A:TYR:HD2	1	2.53
(1,1109)	1:131:A:LYS:HA	1:114:A:PHE:HD1	9	2.52
(1,998)	1:114:A:PHE:HD1	1:131:A:LYS:HA	9	2.52
(1,150)	1:83:A:TYR:HD2	1:82:A:ALA:H	3	2.52
(1,147)	1:82:A:ALA:H	1:83:A:TYR:HD2	3	2.52
(1,1109)	1:131:A:LYS:HA	1:114:A:PHE:HD1	18	2.51
(1,1109)	1:131:A:LYS:HA	1:114:A:PHE:HD1	20	2.51
(1,998)	1:114:A:PHE:HD1	1:131:A:LYS:HA	18	2.51
(1,998)	1:114:A:PHE:HD1	1:131:A:LYS:HA	20	2.51
(1,1109)	1:131:A:LYS:HA	1:114:A:PHE:HD1	10	2.5
(1,1109)	1:131:A:LYS:HA	1:114:A:PHE:HD1	15	2.5
(1,998)	1:114:A:PHE:HD1	1:131:A:LYS:HA	10	2.5
(1,998)	1:114:A:PHE:HD1	1:131:A:LYS:HA	15	2.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,588)	1:133:A:LYS:H	1:114:A:PHE:HE1	17	2.5
(1,587)	1:133:A:LYS:H	1:114:A:PHE:HD1	1	2.5
(1,406)	1:114:A:PHE:HE1	1:133:A:LYS:H	17	2.5
(1,405)	1:114:A:PHE:HD1	1:133:A:LYS:H	1	2.5
(1,150)	1:83:A:TYR:HD2	1:82:A:ALA:H	9	2.5
(1,147)	1:82:A:ALA:H	1:83:A:TYR:HD2	9	2.5
(1,1109)	1:131:A:LYS:HA	1:114:A:PHE:HD1	2	2.49
(1,998)	1:114:A:PHE:HD1	1:131:A:LYS:HA	2	2.49
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG21	18	2.49
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG22	18	2.49
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG23	18	2.49
(1,932)	1:105:A:THR:HG21	1:114:A:PHE:HD2	18	2.49
(1,932)	1:105:A:THR:HG22	1:114:A:PHE:HD2	18	2.49
(1,932)	1:105:A:THR:HG23	1:114:A:PHE:HD2	18	2.49
(1,150)	1:83:A:TYR:HD2	1:82:A:ALA:H	16	2.49
(1,147)	1:82:A:ALA:H	1:83:A:TYR:HD2	16	2.49
(1,1236)	1:149:A:LYS:HG2	1:145:A:PHE:HE2	13	2.48
(1,1236)	1:149:A:LYS:HG3	1:145:A:PHE:HE2	13	2.48
(1,1220)	1:145:A:PHE:HE2	1:149:A:LYS:HG2	13	2.48
(1,1220)	1:145:A:PHE:HE2	1:149:A:LYS:HG3	13	2.48
(1,1109)	1:131:A:LYS:HA	1:114:A:PHE:HD1	19	2.48
(1,998)	1:114:A:PHE:HD1	1:131:A:LYS:HA	19	2.48
(1,587)	1:133:A:LYS:H	1:114:A:PHE:HD1	7	2.48
(1,405)	1:114:A:PHE:HD1	1:133:A:LYS:H	7	2.48
(1,150)	1:83:A:TYR:HD2	1:82:A:ALA:H	10	2.48
(1,150)	1:83:A:TYR:HD2	1:82:A:ALA:H	11	2.48
(1,147)	1:82:A:ALA:H	1:83:A:TYR:HD2	10	2.48
(1,147)	1:82:A:ALA:H	1:83:A:TYR:HD2	11	2.48
(1,1109)	1:131:A:LYS:HA	1:114:A:PHE:HD1	4	2.47
(1,998)	1:114:A:PHE:HD1	1:131:A:LYS:HA	4	2.47
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB2	5	2.47
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB3	5	2.47
(1,971)	1:112:A:PRO:HB2	1:114:A:PHE:HE2	5	2.47
(1,971)	1:112:A:PRO:HB3	1:114:A:PHE:HE2	5	2.47
(1,150)	1:83:A:TYR:HD2	1:82:A:ALA:H	12	2.47
(1,150)	1:83:A:TYR:HD2	1:82:A:ALA:H	17	2.47
(1,150)	1:83:A:TYR:HD2	1:82:A:ALA:H	20	2.47
(1,147)	1:82:A:ALA:H	1:83:A:TYR:HD2	12	2.47
(1,147)	1:82:A:ALA:H	1:83:A:TYR:HD2	17	2.47
(1,147)	1:82:A:ALA:H	1:83:A:TYR:HD2	20	2.47
(1,1109)	1:131:A:LYS:HA	1:114:A:PHE:HD1	3	2.46
(1,998)	1:114:A:PHE:HD1	1:131:A:LYS:HA	3	2.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG21	20	2.46
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG22	20	2.46
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG23	20	2.46
(1,932)	1:105:A:THR:HG21	1:114:A:PHE:HD2	20	2.46
(1,932)	1:105:A:THR:HG22	1:114:A:PHE:HD2	20	2.46
(1,932)	1:105:A:THR:HG23	1:114:A:PHE:HD2	20	2.46
(1,150)	1:83:A:TYR:HD2	1:82:A:ALA:H	4	2.46
(1,150)	1:83:A:TYR:HD2	1:82:A:ALA:H	6	2.46
(1,147)	1:82:A:ALA:H	1:83:A:TYR:HD2	4	2.46
(1,147)	1:82:A:ALA:H	1:83:A:TYR:HD2	6	2.46
(1,1110)	1:131:A:LYS:HA	1:114:A:PHE:HE1	5	2.45
(1,1109)	1:131:A:LYS:HA	1:114:A:PHE:HD1	11	2.45
(1,999)	1:114:A:PHE:HE1	1:131:A:LYS:HA	5	2.45
(1,998)	1:114:A:PHE:HD1	1:131:A:LYS:HA	11	2.45
(1,150)	1:83:A:TYR:HD2	1:82:A:ALA:H	5	2.45
(1,150)	1:83:A:TYR:HD2	1:82:A:ALA:H	19	2.45
(1,147)	1:82:A:ALA:H	1:83:A:TYR:HD2	5	2.45
(1,147)	1:82:A:ALA:H	1:83:A:TYR:HD2	19	2.45
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB2	7	2.44
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB3	7	2.44
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB2	9	2.44
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB3	9	2.44
(1,971)	1:112:A:PRO:HB2	1:114:A:PHE:HE2	7	2.44
(1,971)	1:112:A:PRO:HB3	1:114:A:PHE:HE2	7	2.44
(1,971)	1:112:A:PRO:HB2	1:114:A:PHE:HE2	9	2.44
(1,971)	1:112:A:PRO:HB3	1:114:A:PHE:HE2	9	2.44
(1,150)	1:83:A:TYR:HD2	1:82:A:ALA:H	2	2.44
(1,150)	1:83:A:TYR:HD2	1:82:A:ALA:H	18	2.44
(1,147)	1:82:A:ALA:H	1:83:A:TYR:HD2	2	2.44
(1,147)	1:82:A:ALA:H	1:83:A:TYR:HD2	18	2.44
(1,1109)	1:131:A:LYS:HA	1:114:A:PHE:HD1	17	2.43
(1,998)	1:114:A:PHE:HD1	1:131:A:LYS:HA	17	2.43
(1,587)	1:133:A:LYS:H	1:114:A:PHE:HD1	11	2.43
(1,405)	1:114:A:PHE:HD1	1:133:A:LYS:H	11	2.43
(1,150)	1:83:A:TYR:HD2	1:82:A:ALA:H	13	2.43
(1,150)	1:83:A:TYR:HD2	1:82:A:ALA:H	14	2.43
(1,150)	1:83:A:TYR:HD2	1:82:A:ALA:H	15	2.43
(1,147)	1:82:A:ALA:H	1:83:A:TYR:HD2	13	2.43
(1,147)	1:82:A:ALA:H	1:83:A:TYR:HD2	14	2.43
(1,147)	1:82:A:ALA:H	1:83:A:TYR:HD2	15	2.43
(1,587)	1:133:A:LYS:H	1:114:A:PHE:HD1	14	2.42
(1,405)	1:114:A:PHE:HD1	1:133:A:LYS:H	14	2.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,150)	1:83:A:TYR:HD2	1:82:A:ALA:H	7	2.42
(1,147)	1:82:A:ALA:H	1:83:A:TYR:HD2	7	2.42
(1,1109)	1:131:A:LYS:HA	1:114:A:PHE:HD1	7	2.41
(1,1109)	1:131:A:LYS:HA	1:114:A:PHE:HD1	12	2.41
(1,1109)	1:131:A:LYS:HA	1:114:A:PHE:HD1	13	2.41
(1,998)	1:114:A:PHE:HD1	1:131:A:LYS:HA	7	2.41
(1,998)	1:114:A:PHE:HD1	1:131:A:LYS:HA	12	2.41
(1,998)	1:114:A:PHE:HD1	1:131:A:LYS:HA	13	2.41
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG21	17	2.41
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG22	17	2.41
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG23	17	2.41
(1,932)	1:105:A:THR:HG21	1:114:A:PHE:HD2	17	2.41
(1,932)	1:105:A:THR:HG22	1:114:A:PHE:HD2	17	2.41
(1,932)	1:105:A:THR:HG23	1:114:A:PHE:HD2	17	2.41
(1,588)	1:133:A:LYS:H	1:114:A:PHE:HE1	19	2.41
(1,587)	1:133:A:LYS:H	1:114:A:PHE:HD1	3	2.41
(1,406)	1:114:A:PHE:HE1	1:133:A:LYS:H	19	2.41
(1,405)	1:114:A:PHE:HD1	1:133:A:LYS:H	3	2.41
(1,150)	1:83:A:TYR:HD2	1:82:A:ALA:H	8	2.41
(1,147)	1:82:A:ALA:H	1:83:A:TYR:HD2	8	2.41
(1,1109)	1:131:A:LYS:HA	1:114:A:PHE:HD1	8	2.4
(1,1109)	1:131:A:LYS:HA	1:114:A:PHE:HD1	14	2.4
(1,998)	1:114:A:PHE:HD1	1:131:A:LYS:HA	8	2.4
(1,998)	1:114:A:PHE:HD1	1:131:A:LYS:HA	14	2.4
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB2	13	2.4
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB3	13	2.4
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG21	19	2.4
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG22	19	2.4
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG23	19	2.4
(1,971)	1:112:A:PRO:HB2	1:114:A:PHE:HE2	13	2.4
(1,971)	1:112:A:PRO:HB3	1:114:A:PHE:HE2	13	2.4
(1,932)	1:105:A:THR:HG21	1:114:A:PHE:HD2	19	2.4
(1,932)	1:105:A:THR:HG22	1:114:A:PHE:HD2	19	2.4
(1,932)	1:105:A:THR:HG23	1:114:A:PHE:HD2	19	2.4
(1,587)	1:133:A:LYS:H	1:114:A:PHE:HD1	2	2.4
(1,587)	1:133:A:LYS:H	1:114:A:PHE:HD1	10	2.4
(1,405)	1:114:A:PHE:HD1	1:133:A:LYS:H	2	2.4
(1,405)	1:114:A:PHE:HD1	1:133:A:LYS:H	10	2.4
(1,1110)	1:131:A:LYS:HA	1:114:A:PHE:HE1	9	2.39
(1,999)	1:114:A:PHE:HE1	1:131:A:LYS:HA	9	2.39
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB2	14	2.39
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB3	14	2.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,971)	1:112:A:PRO:HB2	1:114:A:PHE:HE2	14	2.39
(1,971)	1:112:A:PRO:HB3	1:114:A:PHE:HE2	14	2.39
(1,587)	1:133:A:LYS:H	1:114:A:PHE:HD1	6	2.39
(1,587)	1:133:A:LYS:H	1:114:A:PHE:HD1	12	2.39
(1,405)	1:114:A:PHE:HD1	1:133:A:LYS:H	6	2.39
(1,405)	1:114:A:PHE:HD1	1:133:A:LYS:H	12	2.39
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB2	12	2.38
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB3	12	2.38
(1,971)	1:112:A:PRO:HB2	1:114:A:PHE:HE2	12	2.38
(1,971)	1:112:A:PRO:HB3	1:114:A:PHE:HE2	12	2.38
(1,587)	1:133:A:LYS:H	1:114:A:PHE:HD1	18	2.38
(1,405)	1:114:A:PHE:HD1	1:133:A:LYS:H	18	2.38
(1,587)	1:133:A:LYS:H	1:114:A:PHE:HD1	15	2.37
(1,587)	1:133:A:LYS:H	1:114:A:PHE:HD1	20	2.37
(1,405)	1:114:A:PHE:HD1	1:133:A:LYS:H	15	2.37
(1,405)	1:114:A:PHE:HD1	1:133:A:LYS:H	20	2.37
(1,1194)	1:141:A:ALA:HB1	1:101:A:TYR:HE2	16	2.36
(1,1194)	1:141:A:ALA:HB2	1:101:A:TYR:HE2	16	2.36
(1,1194)	1:141:A:ALA:HB3	1:101:A:TYR:HE2	16	2.36
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG21	13	2.36
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG22	13	2.36
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG23	13	2.36
(1,932)	1:105:A:THR:HG21	1:114:A:PHE:HD2	13	2.36
(1,932)	1:105:A:THR:HG22	1:114:A:PHE:HD2	13	2.36
(1,932)	1:105:A:THR:HG23	1:114:A:PHE:HD2	13	2.36
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB1	16	2.36
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB2	16	2.36
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB3	16	2.36
(1,587)	1:133:A:LYS:H	1:114:A:PHE:HD1	4	2.36
(1,587)	1:133:A:LYS:H	1:114:A:PHE:HD1	5	2.36
(1,405)	1:114:A:PHE:HD1	1:133:A:LYS:H	4	2.36
(1,405)	1:114:A:PHE:HD1	1:133:A:LYS:H	5	2.36
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG21	7	2.35
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG22	7	2.35
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG23	7	2.35
(1,932)	1:105:A:THR:HG21	1:114:A:PHE:HD2	7	2.35
(1,932)	1:105:A:THR:HG22	1:114:A:PHE:HD2	7	2.35
(1,932)	1:105:A:THR:HG23	1:114:A:PHE:HD2	7	2.35
(1,587)	1:133:A:LYS:H	1:114:A:PHE:HD1	9	2.35
(1,405)	1:114:A:PHE:HD1	1:133:A:LYS:H	9	2.35
(1,1110)	1:131:A:LYS:HA	1:114:A:PHE:HE1	4	2.33
(1,1110)	1:131:A:LYS:HA	1:114:A:PHE:HE1	15	2.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,999)	1:114:A:PHE:HE1	1:131:A:LYS:HA	4	2.33
(1,999)	1:114:A:PHE:HE1	1:131:A:LYS:HA	15	2.33
(1,1109)	1:131:A:LYS:HA	1:114:A:PHE:HD1	16	2.32
(1,998)	1:114:A:PHE:HD1	1:131:A:LYS:HA	16	2.32
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB2	8	2.32
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB3	8	2.32
(1,971)	1:112:A:PRO:HB2	1:114:A:PHE:HE2	8	2.32
(1,971)	1:112:A:PRO:HB3	1:114:A:PHE:HE2	8	2.32
(1,1110)	1:131:A:LYS:HA	1:114:A:PHE:HE1	20	2.31
(1,999)	1:114:A:PHE:HE1	1:131:A:LYS:HA	20	2.31
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG21	12	2.31
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG22	12	2.31
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG23	12	2.31
(1,932)	1:105:A:THR:HG21	1:114:A:PHE:HD2	12	2.31
(1,932)	1:105:A:THR:HG22	1:114:A:PHE:HD2	12	2.31
(1,932)	1:105:A:THR:HG23	1:114:A:PHE:HD2	12	2.31
(1,1234)	1:149:A:LYS:HD2	1:145:A:PHE:HE2	19	2.3
(1,1234)	1:149:A:LYS:HD3	1:145:A:PHE:HE2	19	2.3
(1,1219)	1:145:A:PHE:HE2	1:149:A:LYS:HD2	19	2.3
(1,1219)	1:145:A:PHE:HE2	1:149:A:LYS:HD3	19	2.3
(1,1110)	1:131:A:LYS:HA	1:114:A:PHE:HE1	18	2.3
(1,1109)	1:131:A:LYS:HA	1:114:A:PHE:HD1	1	2.3
(1,999)	1:114:A:PHE:HE1	1:131:A:LYS:HA	18	2.3
(1,998)	1:114:A:PHE:HD1	1:131:A:LYS:HA	1	2.3
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG21	5	2.3
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG22	5	2.3
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG23	5	2.3
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG21	15	2.3
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG22	15	2.3
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG23	15	2.3
(1,932)	1:105:A:THR:HG21	1:114:A:PHE:HD2	5	2.3
(1,932)	1:105:A:THR:HG22	1:114:A:PHE:HD2	5	2.3
(1,932)	1:105:A:THR:HG23	1:114:A:PHE:HD2	5	2.3
(1,932)	1:105:A:THR:HG21	1:114:A:PHE:HD2	15	2.3
(1,932)	1:105:A:THR:HG22	1:114:A:PHE:HD2	15	2.3
(1,932)	1:105:A:THR:HG23	1:114:A:PHE:HD2	15	2.3
(1,1110)	1:131:A:LYS:HA	1:114:A:PHE:HE1	2	2.29
(1,1110)	1:131:A:LYS:HA	1:114:A:PHE:HE1	10	2.29
(1,1110)	1:131:A:LYS:HA	1:114:A:PHE:HE1	19	2.29
(1,999)	1:114:A:PHE:HE1	1:131:A:LYS:HA	2	2.29
(1,999)	1:114:A:PHE:HE1	1:131:A:LYS:HA	10	2.29
(1,999)	1:114:A:PHE:HE1	1:131:A:LYS:HA	19	2.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1194)	1:141:A:ALA:HB1	1:101:A:TYR:HE2	2	2.28
(1,1194)	1:141:A:ALA:HB2	1:101:A:TYR:HE2	2	2.28
(1,1194)	1:141:A:ALA:HB3	1:101:A:TYR:HE2	2	2.28
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB1	2	2.28
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB2	2	2.28
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB3	2	2.28
(1,1110)	1:131:A:LYS:HA	1:114:A:PHE:HE1	17	2.27
(1,999)	1:114:A:PHE:HE1	1:131:A:LYS:HA	17	2.27
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG21	4	2.27
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG22	4	2.27
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG23	4	2.27
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG21	9	2.27
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG22	9	2.27
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG23	9	2.27
(1,932)	1:105:A:THR:HG21	1:114:A:PHE:HD2	4	2.27
(1,932)	1:105:A:THR:HG22	1:114:A:PHE:HD2	4	2.27
(1,932)	1:105:A:THR:HG23	1:114:A:PHE:HD2	4	2.27
(1,932)	1:105:A:THR:HG21	1:114:A:PHE:HD2	9	2.27
(1,932)	1:105:A:THR:HG22	1:114:A:PHE:HD2	9	2.27
(1,932)	1:105:A:THR:HG23	1:114:A:PHE:HD2	9	2.27
(1,1110)	1:131:A:LYS:HA	1:114:A:PHE:HE1	3	2.25
(1,1109)	1:131:A:LYS:HA	1:114:A:PHE:HD1	6	2.25
(1,999)	1:114:A:PHE:HE1	1:131:A:LYS:HA	3	2.25
(1,998)	1:114:A:PHE:HD1	1:131:A:LYS:HA	6	2.25
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB2	18	2.25
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB3	18	2.25
(1,971)	1:112:A:PRO:HB2	1:114:A:PHE:HE2	18	2.25
(1,971)	1:112:A:PRO:HB3	1:114:A:PHE:HE2	18	2.25
(1,1110)	1:131:A:LYS:HA	1:114:A:PHE:HE1	11	2.24
(1,1110)	1:131:A:LYS:HA	1:114:A:PHE:HE1	12	2.24
(1,999)	1:114:A:PHE:HE1	1:131:A:LYS:HA	11	2.24
(1,999)	1:114:A:PHE:HE1	1:131:A:LYS:HA	12	2.24
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG21	8	2.23
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG22	8	2.23
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG23	8	2.23
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG21	14	2.23
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG22	14	2.23
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG23	14	2.23
(1,932)	1:105:A:THR:HG21	1:114:A:PHE:HD2	8	2.23
(1,932)	1:105:A:THR:HG22	1:114:A:PHE:HD2	8	2.23
(1,932)	1:105:A:THR:HG23	1:114:A:PHE:HD2	8	2.23
(1,932)	1:105:A:THR:HG21	1:114:A:PHE:HD2	14	2.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,932)	1:105:A:THR:HG22	1:114:A:PHE:HD2	14	2.23
(1,932)	1:105:A:THR:HG23	1:114:A:PHE:HD2	14	2.23
(1,1110)	1:131:A:LYS:HA	1:114:A:PHE:HE1	14	2.22
(1,999)	1:114:A:PHE:HE1	1:131:A:LYS:HA	14	2.22
(1,587)	1:133:A:LYS:H	1:114:A:PHE:HD1	19	2.22
(1,405)	1:114:A:PHE:HD1	1:133:A:LYS:H	19	2.22
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB2	19	2.21
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB3	19	2.21
(1,971)	1:112:A:PRO:HB2	1:114:A:PHE:HE2	19	2.21
(1,971)	1:112:A:PRO:HB3	1:114:A:PHE:HE2	19	2.21
(1,1110)	1:131:A:LYS:HA	1:114:A:PHE:HE1	13	2.19
(1,999)	1:114:A:PHE:HE1	1:131:A:LYS:HA	13	2.19
(1,1110)	1:131:A:LYS:HA	1:114:A:PHE:HE1	7	2.18
(1,1065)	1:121:A:ALA:HB1	1:120:A:PHE:HE1	15	2.18
(1,1065)	1:121:A:ALA:HB2	1:120:A:PHE:HE1	15	2.18
(1,1065)	1:121:A:ALA:HB3	1:120:A:PHE:HE1	15	2.18
(1,1058)	1:120:A:PHE:HE1	1:121:A:ALA:HB1	15	2.18
(1,1058)	1:120:A:PHE:HE1	1:121:A:ALA:HB2	15	2.18
(1,1058)	1:120:A:PHE:HE1	1:121:A:ALA:HB3	15	2.18
(1,999)	1:114:A:PHE:HE1	1:131:A:LYS:HA	7	2.18
(1,587)	1:133:A:LYS:H	1:114:A:PHE:HD1	17	2.18
(1,405)	1:114:A:PHE:HD1	1:133:A:LYS:H	17	2.18
(1,1110)	1:131:A:LYS:HA	1:114:A:PHE:HE1	8	2.17
(1,999)	1:114:A:PHE:HE1	1:131:A:LYS:HA	8	2.17
(1,1110)	1:131:A:LYS:HA	1:114:A:PHE:HE1	16	2.15
(1,999)	1:114:A:PHE:HE1	1:131:A:LYS:HA	16	2.15
(1,1110)	1:131:A:LYS:HA	1:114:A:PHE:HE1	1	2.14
(1,999)	1:114:A:PHE:HE1	1:131:A:LYS:HA	1	2.14
(1,1234)	1:149:A:LYS:HD2	1:145:A:PHE:HE2	12	2.13
(1,1234)	1:149:A:LYS:HD3	1:145:A:PHE:HE2	12	2.13
(1,1219)	1:145:A:PHE:HE2	1:149:A:LYS:HD2	12	2.13
(1,1219)	1:145:A:PHE:HE2	1:149:A:LYS:HD3	12	2.13
(1,1110)	1:131:A:LYS:HA	1:114:A:PHE:HE1	6	2.05
(1,999)	1:114:A:PHE:HE1	1:131:A:LYS:HA	6	2.05
(1,1194)	1:141:A:ALA:HB1	1:101:A:TYR:HE2	12	2.04
(1,1194)	1:141:A:ALA:HB2	1:101:A:TYR:HE2	12	2.04
(1,1194)	1:141:A:ALA:HB3	1:101:A:TYR:HE2	12	2.04
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB1	12	2.04
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB2	12	2.04
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB3	12	2.04
(1,1194)	1:141:A:ALA:HB1	1:101:A:TYR:HE2	9	2.01
(1,1194)	1:141:A:ALA:HB2	1:101:A:TYR:HE2	9	2.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1194)	1:141:A:ALA:HB3	1:101:A:TYR:HE2	9	2.01
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB1	9	2.01
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB2	9	2.01
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB3	9	2.01
(1,1111)	1:131:A:LYS:HG2	1:114:A:PHE:HE1	18	1.98
(1,1111)	1:131:A:LYS:HG3	1:114:A:PHE:HE1	18	1.98
(1,1055)	1:120:A:PHE:HE2	1:118:A:VAL:HG21	15	1.98
(1,1055)	1:120:A:PHE:HE2	1:118:A:VAL:HG22	15	1.98
(1,1055)	1:120:A:PHE:HE2	1:118:A:VAL:HG23	15	1.98
(1,1033)	1:118:A:VAL:HG21	1:120:A:PHE:HE2	15	1.98
(1,1033)	1:118:A:VAL:HG22	1:120:A:PHE:HE2	15	1.98
(1,1033)	1:118:A:VAL:HG23	1:120:A:PHE:HE2	15	1.98
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG2	18	1.98
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG3	18	1.98
(1,1111)	1:131:A:LYS:HG2	1:114:A:PHE:HE1	20	1.94
(1,1111)	1:131:A:LYS:HG3	1:114:A:PHE:HE1	20	1.94
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG2	20	1.94
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG3	20	1.94
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG21	10	1.94
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG22	10	1.94
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG23	10	1.94
(1,932)	1:105:A:THR:HG21	1:114:A:PHE:HD2	10	1.94
(1,932)	1:105:A:THR:HG22	1:114:A:PHE:HD2	10	1.94
(1,932)	1:105:A:THR:HG23	1:114:A:PHE:HD2	10	1.94
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG21	20	1.92
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG22	20	1.92
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG23	20	1.92
(1,933)	1:105:A:THR:HG21	1:114:A:PHE:HE2	20	1.92
(1,933)	1:105:A:THR:HG22	1:114:A:PHE:HE2	20	1.92
(1,933)	1:105:A:THR:HG23	1:114:A:PHE:HE2	20	1.92
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG21	18	1.9
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG22	18	1.9
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG23	18	1.9
(1,933)	1:105:A:THR:HG21	1:114:A:PHE:HE2	18	1.9
(1,933)	1:105:A:THR:HG22	1:114:A:PHE:HE2	18	1.9
(1,933)	1:105:A:THR:HG23	1:114:A:PHE:HE2	18	1.9
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG21	13	1.89
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG22	13	1.89
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG23	13	1.89
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG21	2	1.89
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG22	2	1.89
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG23	2	1.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,933)	1:105:A:THR:HG21	1:114:A:PHE:HE2	13	1.89
(1,933)	1:105:A:THR:HG22	1:114:A:PHE:HE2	13	1.89
(1,933)	1:105:A:THR:HG23	1:114:A:PHE:HE2	13	1.89
(1,932)	1:105:A:THR:HG21	1:114:A:PHE:HD2	2	1.89
(1,932)	1:105:A:THR:HG22	1:114:A:PHE:HD2	2	1.89
(1,932)	1:105:A:THR:HG23	1:114:A:PHE:HD2	2	1.89
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG21	17	1.88
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG22	17	1.88
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG23	17	1.88
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG21	11	1.88
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG22	11	1.88
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG23	11	1.88
(1,933)	1:105:A:THR:HG21	1:114:A:PHE:HE2	17	1.88
(1,933)	1:105:A:THR:HG22	1:114:A:PHE:HE2	17	1.88
(1,933)	1:105:A:THR:HG23	1:114:A:PHE:HE2	17	1.88
(1,932)	1:105:A:THR:HG21	1:114:A:PHE:HD2	11	1.88
(1,932)	1:105:A:THR:HG22	1:114:A:PHE:HD2	11	1.88
(1,932)	1:105:A:THR:HG23	1:114:A:PHE:HD2	11	1.88
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG21	19	1.87
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG22	19	1.87
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG23	19	1.87
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG21	6	1.87
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG22	6	1.87
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG23	6	1.87
(1,933)	1:105:A:THR:HG21	1:114:A:PHE:HE2	19	1.87
(1,933)	1:105:A:THR:HG22	1:114:A:PHE:HE2	19	1.87
(1,933)	1:105:A:THR:HG23	1:114:A:PHE:HE2	19	1.87
(1,932)	1:105:A:THR:HG21	1:114:A:PHE:HD2	6	1.87
(1,932)	1:105:A:THR:HG22	1:114:A:PHE:HD2	6	1.87
(1,932)	1:105:A:THR:HG23	1:114:A:PHE:HD2	6	1.87
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG21	1	1.86
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG22	1	1.86
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG23	1	1.86
(1,932)	1:105:A:THR:HG21	1:114:A:PHE:HD2	1	1.86
(1,932)	1:105:A:THR:HG22	1:114:A:PHE:HD2	1	1.86
(1,932)	1:105:A:THR:HG23	1:114:A:PHE:HD2	1	1.86
(1,1111)	1:131:A:LYS:HG2	1:114:A:PHE:HE1	2	1.85
(1,1111)	1:131:A:LYS:HG3	1:114:A:PHE:HE1	2	1.85
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG2	2	1.85
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG3	2	1.85
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG21	5	1.85
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG22	5	1.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG23	5	1.85
(1,933)	1:105:A:THR:HG21	1:114:A:PHE:HE2	5	1.85
(1,933)	1:105:A:THR:HG22	1:114:A:PHE:HE2	5	1.85
(1,933)	1:105:A:THR:HG23	1:114:A:PHE:HE2	5	1.85
(1,1111)	1:131:A:LYS:HG2	1:114:A:PHE:HE1	10	1.84
(1,1111)	1:131:A:LYS:HG3	1:114:A:PHE:HE1	10	1.84
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG2	10	1.84
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG3	10	1.84
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG21	16	1.84
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG22	16	1.84
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG23	16	1.84
(1,932)	1:105:A:THR:HG21	1:114:A:PHE:HD2	16	1.84
(1,932)	1:105:A:THR:HG22	1:114:A:PHE:HD2	16	1.84
(1,932)	1:105:A:THR:HG23	1:114:A:PHE:HD2	16	1.84
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG21	7	1.83
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG22	7	1.83
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG23	7	1.83
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG21	9	1.83
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG22	9	1.83
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG23	9	1.83
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG21	12	1.83
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG22	12	1.83
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG23	12	1.83
(1,933)	1:105:A:THR:HG21	1:114:A:PHE:HE2	7	1.83
(1,933)	1:105:A:THR:HG22	1:114:A:PHE:HE2	7	1.83
(1,933)	1:105:A:THR:HG23	1:114:A:PHE:HE2	7	1.83
(1,933)	1:105:A:THR:HG21	1:114:A:PHE:HE2	9	1.83
(1,933)	1:105:A:THR:HG22	1:114:A:PHE:HE2	9	1.83
(1,933)	1:105:A:THR:HG23	1:114:A:PHE:HE2	9	1.83
(1,933)	1:105:A:THR:HG21	1:114:A:PHE:HE2	12	1.83
(1,933)	1:105:A:THR:HG22	1:114:A:PHE:HE2	12	1.83
(1,933)	1:105:A:THR:HG23	1:114:A:PHE:HE2	12	1.83
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG21	3	1.82
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG22	3	1.82
(1,987)	1:114:A:PHE:HD2	1:105:A:THR:HG23	3	1.82
(1,932)	1:105:A:THR:HG21	1:114:A:PHE:HD2	3	1.82
(1,932)	1:105:A:THR:HG22	1:114:A:PHE:HD2	3	1.82
(1,932)	1:105:A:THR:HG23	1:114:A:PHE:HD2	3	1.82
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG21	15	1.81
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG22	15	1.81
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG23	15	1.81
(1,933)	1:105:A:THR:HG21	1:114:A:PHE:HE2	15	1.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,933)	1:105:A:THR:HG22	1:114:A:PHE:HE2	15	1.81
(1,933)	1:105:A:THR:HG23	1:114:A:PHE:HE2	15	1.81
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG21	8	1.8
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG22	8	1.8
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG23	8	1.8
(1,933)	1:105:A:THR:HG21	1:114:A:PHE:HE2	8	1.8
(1,933)	1:105:A:THR:HG22	1:114:A:PHE:HE2	8	1.8
(1,933)	1:105:A:THR:HG23	1:114:A:PHE:HE2	8	1.8
(1,1233)	1:149:A:LYS:HD2	1:145:A:PHE:HD2	19	1.79
(1,1233)	1:149:A:LYS:HD3	1:145:A:PHE:HD2	19	1.79
(1,1217)	1:145:A:PHE:HD2	1:149:A:LYS:HD2	19	1.79
(1,1217)	1:145:A:PHE:HD2	1:149:A:LYS:HD3	19	1.79
(1,1194)	1:141:A:ALA:HB1	1:101:A:TYR:HE2	8	1.79
(1,1194)	1:141:A:ALA:HB2	1:101:A:TYR:HE2	8	1.79
(1,1194)	1:141:A:ALA:HB3	1:101:A:TYR:HE2	8	1.79
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG21	4	1.79
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG22	4	1.79
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG23	4	1.79
(1,933)	1:105:A:THR:HG21	1:114:A:PHE:HE2	4	1.79
(1,933)	1:105:A:THR:HG22	1:114:A:PHE:HE2	4	1.79
(1,933)	1:105:A:THR:HG23	1:114:A:PHE:HE2	4	1.79
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB1	8	1.79
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB2	8	1.79
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB3	8	1.79
(1,1064)	1:121:A:ALA:HB1	1:120:A:PHE:HD1	15	1.78
(1,1064)	1:121:A:ALA:HB2	1:120:A:PHE:HD1	15	1.78
(1,1064)	1:121:A:ALA:HB3	1:120:A:PHE:HD1	15	1.78
(1,1057)	1:120:A:PHE:HD1	1:121:A:ALA:HB1	15	1.78
(1,1057)	1:120:A:PHE:HD1	1:121:A:ALA:HB2	15	1.78
(1,1057)	1:120:A:PHE:HD1	1:121:A:ALA:HB3	15	1.78
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG21	14	1.78
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG22	14	1.78
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG23	14	1.78
(1,933)	1:105:A:THR:HG21	1:114:A:PHE:HE2	14	1.78
(1,933)	1:105:A:THR:HG22	1:114:A:PHE:HE2	14	1.78
(1,933)	1:105:A:THR:HG23	1:114:A:PHE:HE2	14	1.78
(1,1111)	1:131:A:LYS:HG2	1:114:A:PHE:HE1	3	1.77
(1,1111)	1:131:A:LYS:HG3	1:114:A:PHE:HE1	3	1.77
(1,1111)	1:131:A:LYS:HG2	1:114:A:PHE:HE1	7	1.77
(1,1111)	1:131:A:LYS:HG3	1:114:A:PHE:HE1	7	1.77
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG2	3	1.77
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG3	3	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG2	7	1.77
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG3	7	1.77
(1,1194)	1:141:A:ALA:HB1	1:101:A:TYR:HE2	13	1.75
(1,1194)	1:141:A:ALA:HB2	1:101:A:TYR:HE2	13	1.75
(1,1194)	1:141:A:ALA:HB3	1:101:A:TYR:HE2	13	1.75
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB1	13	1.75
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB2	13	1.75
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB3	13	1.75
(1,1194)	1:141:A:ALA:HB1	1:101:A:TYR:HE2	1	1.74
(1,1194)	1:141:A:ALA:HB2	1:101:A:TYR:HE2	1	1.74
(1,1194)	1:141:A:ALA:HB3	1:101:A:TYR:HE2	1	1.74
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB1	1	1.74
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB2	1	1.74
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB3	1	1.74
(1,1194)	1:141:A:ALA:HB1	1:101:A:TYR:HE2	11	1.72
(1,1194)	1:141:A:ALA:HB2	1:101:A:TYR:HE2	11	1.72
(1,1194)	1:141:A:ALA:HB3	1:101:A:TYR:HE2	11	1.72
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB1	11	1.72
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB2	11	1.72
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB3	11	1.72
(1,1234)	1:149:A:LYS:HD2	1:145:A:PHE:HE2	13	1.71
(1,1234)	1:149:A:LYS:HD3	1:145:A:PHE:HE2	13	1.71
(1,1219)	1:145:A:PHE:HE2	1:149:A:LYS:HD2	13	1.71
(1,1219)	1:145:A:PHE:HE2	1:149:A:LYS:HD3	13	1.71
(1,1194)	1:141:A:ALA:HB1	1:101:A:TYR:HE2	4	1.71
(1,1194)	1:141:A:ALA:HB2	1:101:A:TYR:HE2	4	1.71
(1,1194)	1:141:A:ALA:HB3	1:101:A:TYR:HE2	4	1.71
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB1	4	1.71
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB2	4	1.71
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB3	4	1.71
(1,1111)	1:131:A:LYS:HG2	1:114:A:PHE:HE1	8	1.68
(1,1111)	1:131:A:LYS:HG3	1:114:A:PHE:HE1	8	1.68
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG2	8	1.68
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG3	8	1.68
(1,1111)	1:131:A:LYS:HG2	1:114:A:PHE:HE1	13	1.67
(1,1111)	1:131:A:LYS:HG3	1:114:A:PHE:HE1	13	1.67
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG2	13	1.67
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG3	13	1.67
(1,1194)	1:141:A:ALA:HB1	1:101:A:TYR:HE2	18	1.66
(1,1194)	1:141:A:ALA:HB2	1:101:A:TYR:HE2	18	1.66
(1,1194)	1:141:A:ALA:HB3	1:101:A:TYR:HE2	18	1.66
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB1	18	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB2	18	1.66
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB3	18	1.66
(1,1194)	1:141:A:ALA:HB1	1:101:A:TYR:HE2	19	1.64
(1,1194)	1:141:A:ALA:HB2	1:101:A:TYR:HE2	19	1.64
(1,1194)	1:141:A:ALA:HB3	1:101:A:TYR:HE2	19	1.64
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB1	19	1.64
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB2	19	1.64
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB3	19	1.64
(1,1194)	1:141:A:ALA:HB1	1:101:A:TYR:HE2	10	1.6
(1,1194)	1:141:A:ALA:HB2	1:101:A:TYR:HE2	10	1.6
(1,1194)	1:141:A:ALA:HB3	1:101:A:TYR:HE2	10	1.6
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB1	10	1.6
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB2	10	1.6
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB3	10	1.6
(1,1236)	1:149:A:LYS:HG2	1:145:A:PHE:HE2	19	1.59
(1,1236)	1:149:A:LYS:HG3	1:145:A:PHE:HE2	19	1.59
(1,1220)	1:145:A:PHE:HE2	1:149:A:LYS:HG2	19	1.59
(1,1220)	1:145:A:PHE:HE2	1:149:A:LYS:HG3	19	1.59
(1,1233)	1:149:A:LYS:HD2	1:145:A:PHE:HD2	12	1.58
(1,1233)	1:149:A:LYS:HD3	1:145:A:PHE:HD2	12	1.58
(1,1217)	1:145:A:PHE:HD2	1:149:A:LYS:HD2	12	1.58
(1,1217)	1:145:A:PHE:HD2	1:149:A:LYS:HD3	12	1.58
(1,1194)	1:141:A:ALA:HB1	1:101:A:TYR:HE2	20	1.54
(1,1194)	1:141:A:ALA:HB2	1:101:A:TYR:HE2	20	1.54
(1,1194)	1:141:A:ALA:HB3	1:101:A:TYR:HE2	20	1.54
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB1	20	1.54
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB2	20	1.54
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB3	20	1.54
(1,1235)	1:149:A:LYS:HG2	1:145:A:PHE:HD2	12	1.53
(1,1235)	1:149:A:LYS:HG3	1:145:A:PHE:HD2	12	1.53
(1,1218)	1:145:A:PHE:HD2	1:149:A:LYS:HG2	12	1.53
(1,1218)	1:145:A:PHE:HD2	1:149:A:LYS:HG3	12	1.53
(1,320)	1:102:A:ALA:H	1:101:A:TYR:HD2	9	1.52
(1,316)	1:101:A:TYR:HD2	1:102:A:ALA:H	9	1.52
(1,1230)	1:148:A:ILE:HG12	1:120:A:PHE:HE1	15	1.51
(1,1230)	1:148:A:ILE:HG13	1:120:A:PHE:HE1	15	1.51
(1,1061)	1:120:A:PHE:HE1	1:148:A:ILE:HG12	15	1.51
(1,1061)	1:120:A:PHE:HE1	1:148:A:ILE:HG13	15	1.51
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB2	11	1.49
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB3	11	1.49
(1,971)	1:112:A:PRO:HB2	1:114:A:PHE:HE2	11	1.49
(1,971)	1:112:A:PRO:HB3	1:114:A:PHE:HE2	11	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:102:A:ALA:H	1:101:A:TYR:HD2	2	1.49
(1,320)	1:102:A:ALA:H	1:101:A:TYR:HD2	16	1.49
(1,316)	1:101:A:TYR:HD2	1:102:A:ALA:H	2	1.49
(1,316)	1:101:A:TYR:HD2	1:102:A:ALA:H	16	1.49
(1,320)	1:102:A:ALA:H	1:101:A:TYR:HD2	12	1.48
(1,316)	1:101:A:TYR:HD2	1:102:A:ALA:H	12	1.48
(1,1194)	1:141:A:ALA:HB1	1:101:A:TYR:HE2	7	1.46
(1,1194)	1:141:A:ALA:HB2	1:101:A:TYR:HE2	7	1.46
(1,1194)	1:141:A:ALA:HB3	1:101:A:TYR:HE2	7	1.46
(1,1054)	1:120:A:PHE:HE2	1:118:A:VAL:HG11	15	1.46
(1,1054)	1:120:A:PHE:HE2	1:118:A:VAL:HG12	15	1.46
(1,1054)	1:120:A:PHE:HE2	1:118:A:VAL:HG13	15	1.46
(1,1032)	1:118:A:VAL:HG11	1:120:A:PHE:HE2	15	1.46
(1,1032)	1:118:A:VAL:HG12	1:120:A:PHE:HE2	15	1.46
(1,1032)	1:118:A:VAL:HG13	1:120:A:PHE:HE2	15	1.46
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB1	7	1.46
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB2	7	1.46
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB3	7	1.46
(1,1235)	1:149:A:LYS:HG2	1:145:A:PHE:HD2	13	1.44
(1,1235)	1:149:A:LYS:HG3	1:145:A:PHE:HD2	13	1.44
(1,1218)	1:145:A:PHE:HD2	1:149:A:LYS:HG2	13	1.44
(1,1218)	1:145:A:PHE:HD2	1:149:A:LYS:HG3	13	1.44
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG21	10	1.41
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG22	10	1.41
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG23	10	1.41
(1,933)	1:105:A:THR:HG21	1:114:A:PHE:HE2	10	1.41
(1,933)	1:105:A:THR:HG22	1:114:A:PHE:HE2	10	1.41
(1,933)	1:105:A:THR:HG23	1:114:A:PHE:HE2	10	1.41
(1,320)	1:102:A:ALA:H	1:101:A:TYR:HD2	4	1.4
(1,320)	1:102:A:ALA:H	1:101:A:TYR:HD2	7	1.4
(1,320)	1:102:A:ALA:H	1:101:A:TYR:HD2	19	1.4
(1,316)	1:101:A:TYR:HD2	1:102:A:ALA:H	4	1.4
(1,316)	1:101:A:TYR:HD2	1:102:A:ALA:H	7	1.4
(1,316)	1:101:A:TYR:HD2	1:102:A:ALA:H	19	1.4
(1,1194)	1:141:A:ALA:HB1	1:101:A:TYR:HE2	17	1.39
(1,1194)	1:141:A:ALA:HB2	1:101:A:TYR:HE2	17	1.39
(1,1194)	1:141:A:ALA:HB3	1:101:A:TYR:HE2	17	1.39
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB1	17	1.39
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB2	17	1.39
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB3	17	1.39
(1,320)	1:102:A:ALA:H	1:101:A:TYR:HD2	10	1.39
(1,320)	1:102:A:ALA:H	1:101:A:TYR:HD2	13	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,316)	1:101:A:TYR:HD2	1:102:A:ALA:H	10	1.39
(1,316)	1:101:A:TYR:HD2	1:102:A:ALA:H	13	1.39
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB2	10	1.37
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB3	10	1.37
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG21	2	1.37
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG22	2	1.37
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG23	2	1.37
(1,971)	1:112:A:PRO:HB2	1:114:A:PHE:HE2	10	1.37
(1,971)	1:112:A:PRO:HB3	1:114:A:PHE:HE2	10	1.37
(1,933)	1:105:A:THR:HG21	1:114:A:PHE:HE2	2	1.37
(1,933)	1:105:A:THR:HG22	1:114:A:PHE:HE2	2	1.37
(1,933)	1:105:A:THR:HG23	1:114:A:PHE:HE2	2	1.37
(1,320)	1:102:A:ALA:H	1:101:A:TYR:HD2	11	1.37
(1,316)	1:101:A:TYR:HD2	1:102:A:ALA:H	11	1.37
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB2	3	1.36
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB3	3	1.36
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB2	4	1.36
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB3	4	1.36
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB2	17	1.36
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB3	17	1.36
(1,971)	1:112:A:PRO:HB2	1:114:A:PHE:HE2	3	1.36
(1,971)	1:112:A:PRO:HB3	1:114:A:PHE:HE2	3	1.36
(1,970)	1:112:A:PRO:HB2	1:114:A:PHE:HD2	4	1.36
(1,970)	1:112:A:PRO:HB3	1:114:A:PHE:HD2	4	1.36
(1,970)	1:112:A:PRO:HB2	1:114:A:PHE:HD2	17	1.36
(1,970)	1:112:A:PRO:HB3	1:114:A:PHE:HD2	17	1.36
(1,320)	1:102:A:ALA:H	1:101:A:TYR:HD2	14	1.36
(1,316)	1:101:A:TYR:HD2	1:102:A:ALA:H	14	1.36
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG21	1	1.35
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG22	1	1.35
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG23	1	1.35
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG21	3	1.35
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG22	3	1.35
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG23	3	1.35
(1,933)	1:105:A:THR:HG21	1:114:A:PHE:HE2	1	1.35
(1,933)	1:105:A:THR:HG22	1:114:A:PHE:HE2	1	1.35
(1,933)	1:105:A:THR:HG23	1:114:A:PHE:HE2	1	1.35
(1,933)	1:105:A:THR:HG21	1:114:A:PHE:HE2	3	1.35
(1,933)	1:105:A:THR:HG22	1:114:A:PHE:HE2	3	1.35
(1,933)	1:105:A:THR:HG23	1:114:A:PHE:HE2	3	1.35
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB2	15	1.33
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB3	15	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,970)	1:112:A:PRO:HB2	1:114:A:PHE:HD2	15	1.33
(1,970)	1:112:A:PRO:HB3	1:114:A:PHE:HD2	15	1.33
(1,320)	1:102:A:ALA:H	1:101:A:TYR:HD2	8	1.33
(1,316)	1:101:A:TYR:HD2	1:102:A:ALA:H	8	1.33
(1,1204)	1:144:A:ALA:HA	1:120:A:PHE:HE2	15	1.32
(1,1194)	1:141:A:ALA:HB1	1:101:A:TYR:HE2	14	1.32
(1,1194)	1:141:A:ALA:HB2	1:101:A:TYR:HE2	14	1.32
(1,1194)	1:141:A:ALA:HB3	1:101:A:TYR:HE2	14	1.32
(1,1059)	1:120:A:PHE:HE2	1:144:A:ALA:HA	15	1.32
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB2	2	1.32
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB3	2	1.32
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG21	6	1.32
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG22	6	1.32
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG23	6	1.32
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG21	11	1.32
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG22	11	1.32
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG23	11	1.32
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG21	16	1.32
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG22	16	1.32
(1,990)	1:114:A:PHE:HE2	1:105:A:THR:HG23	16	1.32
(1,971)	1:112:A:PRO:HB2	1:114:A:PHE:HE2	2	1.32
(1,971)	1:112:A:PRO:HB3	1:114:A:PHE:HE2	2	1.32
(1,933)	1:105:A:THR:HG21	1:114:A:PHE:HE2	6	1.32
(1,933)	1:105:A:THR:HG22	1:114:A:PHE:HE2	6	1.32
(1,933)	1:105:A:THR:HG23	1:114:A:PHE:HE2	6	1.32
(1,933)	1:105:A:THR:HG21	1:114:A:PHE:HE2	11	1.32
(1,933)	1:105:A:THR:HG22	1:114:A:PHE:HE2	11	1.32
(1,933)	1:105:A:THR:HG23	1:114:A:PHE:HE2	11	1.32
(1,933)	1:105:A:THR:HG21	1:114:A:PHE:HE2	16	1.32
(1,933)	1:105:A:THR:HG22	1:114:A:PHE:HE2	16	1.32
(1,933)	1:105:A:THR:HG23	1:114:A:PHE:HE2	16	1.32
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB1	14	1.32
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB2	14	1.32
(1,907)	1:101:A:TYR:HE2	1:141:A:ALA:HB3	14	1.32
(1,320)	1:102:A:ALA:H	1:101:A:TYR:HD2	1	1.32
(1,316)	1:101:A:TYR:HD2	1:102:A:ALA:H	1	1.32
(1,320)	1:102:A:ALA:H	1:101:A:TYR:HD2	18	1.31
(1,316)	1:101:A:TYR:HD2	1:102:A:ALA:H	18	1.31
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB2	7	1.3
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB3	7	1.3
(1,970)	1:112:A:PRO:HB2	1:114:A:PHE:HD2	7	1.3
(1,970)	1:112:A:PRO:HB3	1:114:A:PHE:HD2	7	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:102:A:ALA:H	1:101:A:TYR:HD2	17	1.3
(1,316)	1:101:A:TYR:HD2	1:102:A:ALA:H	17	1.3
(1,1233)	1:149:A:LYS:HD2	1:145:A:PHE:HD2	13	1.29
(1,1233)	1:149:A:LYS:HD3	1:145:A:PHE:HD2	13	1.29
(1,1217)	1:145:A:PHE:HD2	1:149:A:LYS:HD2	13	1.29
(1,1217)	1:145:A:PHE:HD2	1:149:A:LYS:HD3	13	1.29
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB2	20	1.29
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB3	20	1.29
(1,970)	1:112:A:PRO:HB2	1:114:A:PHE:HD2	20	1.29
(1,970)	1:112:A:PRO:HB3	1:114:A:PHE:HD2	20	1.29
(1,313)	1:101:A:TYR:H	1:101:A:TYR:HD1	1	1.29
(1,311)	1:101:A:TYR:HD1	1:101:A:TYR:H	1	1.29
(1,320)	1:102:A:ALA:H	1:101:A:TYR:HD2	20	1.28
(1,316)	1:101:A:TYR:HD2	1:102:A:ALA:H	20	1.28
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB2	1	1.26
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB3	1	1.26
(1,971)	1:112:A:PRO:HB2	1:114:A:PHE:HE2	1	1.26
(1,971)	1:112:A:PRO:HB3	1:114:A:PHE:HE2	1	1.26
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB2	16	1.25
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB3	16	1.25
(1,971)	1:112:A:PRO:HB2	1:114:A:PHE:HE2	16	1.25
(1,971)	1:112:A:PRO:HB3	1:114:A:PHE:HE2	16	1.25
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB2	5	1.23
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB3	5	1.23
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB2	12	1.23
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB3	12	1.23
(1,970)	1:112:A:PRO:HB2	1:114:A:PHE:HD2	5	1.23
(1,970)	1:112:A:PRO:HB3	1:114:A:PHE:HD2	5	1.23
(1,970)	1:112:A:PRO:HB2	1:114:A:PHE:HD2	12	1.23
(1,970)	1:112:A:PRO:HB3	1:114:A:PHE:HD2	12	1.23
(1,313)	1:101:A:TYR:H	1:101:A:TYR:HD1	12	1.23
(1,313)	1:101:A:TYR:H	1:101:A:TYR:HD1	14	1.23
(1,311)	1:101:A:TYR:HD1	1:101:A:TYR:H	12	1.23
(1,311)	1:101:A:TYR:HD1	1:101:A:TYR:H	14	1.23
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB2	13	1.22
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB3	13	1.22
(1,970)	1:112:A:PRO:HB2	1:114:A:PHE:HD2	13	1.22
(1,970)	1:112:A:PRO:HB3	1:114:A:PHE:HD2	13	1.22
(1,313)	1:101:A:TYR:H	1:101:A:TYR:HD1	9	1.22
(1,313)	1:101:A:TYR:H	1:101:A:TYR:HD1	16	1.22
(1,311)	1:101:A:TYR:HD1	1:101:A:TYR:H	9	1.22
(1,311)	1:101:A:TYR:HD1	1:101:A:TYR:H	16	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB2	6	1.21
(1,992)	1:114:A:PHE:HE2	1:112:A:PRO:HB3	6	1.21
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB2	18	1.21
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB3	18	1.21
(1,971)	1:112:A:PRO:HB2	1:114:A:PHE:HE2	6	1.21
(1,971)	1:112:A:PRO:HB3	1:114:A:PHE:HE2	6	1.21
(1,970)	1:112:A:PRO:HB2	1:114:A:PHE:HD2	18	1.21
(1,970)	1:112:A:PRO:HB3	1:114:A:PHE:HD2	18	1.21
(1,313)	1:101:A:TYR:H	1:101:A:TYR:HD1	2	1.21
(1,311)	1:101:A:TYR:HD1	1:101:A:TYR:H	2	1.21
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB2	8	1.19
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB3	8	1.19
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB2	9	1.19
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB3	9	1.19
(1,970)	1:112:A:PRO:HB2	1:114:A:PHE:HD2	8	1.19
(1,970)	1:112:A:PRO:HB3	1:114:A:PHE:HD2	8	1.19
(1,970)	1:112:A:PRO:HB2	1:114:A:PHE:HD2	9	1.19
(1,970)	1:112:A:PRO:HB3	1:114:A:PHE:HD2	9	1.19
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB2	14	1.18
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB3	14	1.18
(1,970)	1:112:A:PRO:HB2	1:114:A:PHE:HD2	14	1.18
(1,970)	1:112:A:PRO:HB3	1:114:A:PHE:HD2	14	1.18
(1,313)	1:101:A:TYR:H	1:101:A:TYR:HD1	7	1.18
(1,313)	1:101:A:TYR:H	1:101:A:TYR:HD1	13	1.18
(1,311)	1:101:A:TYR:HD1	1:101:A:TYR:H	7	1.18
(1,311)	1:101:A:TYR:HD1	1:101:A:TYR:H	13	1.18
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB2	19	1.16
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB3	19	1.16
(1,970)	1:112:A:PRO:HB2	1:114:A:PHE:HD2	19	1.16
(1,970)	1:112:A:PRO:HB3	1:114:A:PHE:HD2	19	1.16
(1,313)	1:101:A:TYR:H	1:101:A:TYR:HD1	19	1.15
(1,311)	1:101:A:TYR:HD1	1:101:A:TYR:H	19	1.15
(1,313)	1:101:A:TYR:H	1:101:A:TYR:HD1	8	1.14
(1,311)	1:101:A:TYR:HD1	1:101:A:TYR:H	8	1.14
(1,313)	1:101:A:TYR:H	1:101:A:TYR:HD1	4	1.11
(1,313)	1:101:A:TYR:H	1:101:A:TYR:HD1	10	1.11
(1,313)	1:101:A:TYR:H	1:101:A:TYR:HD1	11	1.11
(1,311)	1:101:A:TYR:HD1	1:101:A:TYR:H	4	1.11
(1,311)	1:101:A:TYR:HD1	1:101:A:TYR:H	10	1.11
(1,311)	1:101:A:TYR:HD1	1:101:A:TYR:H	11	1.11
(1,313)	1:101:A:TYR:H	1:101:A:TYR:HD1	20	1.09
(1,311)	1:101:A:TYR:HD1	1:101:A:TYR:H	20	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,313)	1:101:A:TYR:H	1:101:A:TYR:HD1	17	1.06
(1,311)	1:101:A:TYR:HD1	1:101:A:TYR:H	17	1.06
(1,1111)	1:131:A:LYS:HG2	1:114:A:PHE:HE1	5	1.03
(1,1111)	1:131:A:LYS:HG3	1:114:A:PHE:HE1	5	1.03
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG2	5	1.03
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG3	5	1.03
(1,313)	1:101:A:TYR:H	1:101:A:TYR:HD1	18	1.0
(1,311)	1:101:A:TYR:HD1	1:101:A:TYR:H	18	1.0
(1,397)	1:114:A:PHE:H	1:114:A:PHE:HE1	5	0.98
(1,397)	1:114:A:PHE:H	1:114:A:PHE:HE1	13	0.98
(1,397)	1:114:A:PHE:H	1:114:A:PHE:HE1	20	0.98
(1,393)	1:114:A:PHE:HE1	1:114:A:PHE:H	5	0.98
(1,393)	1:114:A:PHE:HE1	1:114:A:PHE:H	13	0.98
(1,393)	1:114:A:PHE:HE1	1:114:A:PHE:H	20	0.98
(1,397)	1:114:A:PHE:H	1:114:A:PHE:HE1	18	0.97
(1,393)	1:114:A:PHE:HE1	1:114:A:PHE:H	18	0.97
(1,397)	1:114:A:PHE:H	1:114:A:PHE:HE1	9	0.96
(1,397)	1:114:A:PHE:H	1:114:A:PHE:HE1	19	0.96
(1,393)	1:114:A:PHE:HE1	1:114:A:PHE:H	9	0.96
(1,393)	1:114:A:PHE:HE1	1:114:A:PHE:H	19	0.96
(1,397)	1:114:A:PHE:H	1:114:A:PHE:HE1	4	0.95
(1,397)	1:114:A:PHE:H	1:114:A:PHE:HE1	8	0.95
(1,393)	1:114:A:PHE:HE1	1:114:A:PHE:H	4	0.95
(1,393)	1:114:A:PHE:HE1	1:114:A:PHE:H	8	0.95
(1,397)	1:114:A:PHE:H	1:114:A:PHE:HE1	7	0.94
(1,397)	1:114:A:PHE:H	1:114:A:PHE:HE1	17	0.94
(1,393)	1:114:A:PHE:HE1	1:114:A:PHE:H	7	0.94
(1,393)	1:114:A:PHE:HE1	1:114:A:PHE:H	17	0.94
(1,397)	1:114:A:PHE:H	1:114:A:PHE:HE1	12	0.93
(1,397)	1:114:A:PHE:H	1:114:A:PHE:HE1	15	0.93
(1,393)	1:114:A:PHE:HE1	1:114:A:PHE:H	12	0.93
(1,393)	1:114:A:PHE:HE1	1:114:A:PHE:H	15	0.93
(1,1111)	1:131:A:LYS:HG2	1:114:A:PHE:HE1	4	0.91
(1,1111)	1:131:A:LYS:HG3	1:114:A:PHE:HE1	4	0.91
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG2	4	0.91
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG3	4	0.91
(1,397)	1:114:A:PHE:H	1:114:A:PHE:HE1	14	0.9
(1,393)	1:114:A:PHE:HE1	1:114:A:PHE:H	14	0.9
(1,1111)	1:131:A:LYS:HG2	1:114:A:PHE:HE1	15	0.88
(1,1111)	1:131:A:LYS:HG3	1:114:A:PHE:HE1	15	0.88
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG2	15	0.88
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG3	15	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1235)	1:149:A:LYS:HG2	1:145:A:PHE:HD2	19	0.85
(1,1235)	1:149:A:LYS:HG3	1:145:A:PHE:HD2	19	0.85
(1,1218)	1:145:A:PHE:HD2	1:149:A:LYS:HG2	19	0.85
(1,1218)	1:145:A:PHE:HD2	1:149:A:LYS:HG3	19	0.85
(1,1111)	1:131:A:LYS:HG2	1:114:A:PHE:HE1	9	0.85
(1,1111)	1:131:A:LYS:HG3	1:114:A:PHE:HE1	9	0.85
(1,1111)	1:131:A:LYS:HG2	1:114:A:PHE:HE1	19	0.85
(1,1111)	1:131:A:LYS:HG3	1:114:A:PHE:HE1	19	0.85
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG2	9	0.85
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG3	9	0.85
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG2	19	0.85
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG3	19	0.85
(1,397)	1:114:A:PHE:H	1:114:A:PHE:HE1	2	0.85
(1,397)	1:114:A:PHE:H	1:114:A:PHE:HE1	10	0.85
(1,393)	1:114:A:PHE:HE1	1:114:A:PHE:H	2	0.85
(1,393)	1:114:A:PHE:HE1	1:114:A:PHE:H	10	0.85
(1,397)	1:114:A:PHE:H	1:114:A:PHE:HE1	11	0.83
(1,397)	1:114:A:PHE:H	1:114:A:PHE:HE1	16	0.83
(1,393)	1:114:A:PHE:HE1	1:114:A:PHE:H	11	0.83
(1,393)	1:114:A:PHE:HE1	1:114:A:PHE:H	16	0.83
(1,397)	1:114:A:PHE:H	1:114:A:PHE:HE1	3	0.82
(1,393)	1:114:A:PHE:HE1	1:114:A:PHE:H	3	0.82
(1,397)	1:114:A:PHE:H	1:114:A:PHE:HE1	1	0.81
(1,397)	1:114:A:PHE:H	1:114:A:PHE:HE1	6	0.81
(1,393)	1:114:A:PHE:HE1	1:114:A:PHE:H	1	0.81
(1,393)	1:114:A:PHE:HE1	1:114:A:PHE:H	6	0.81
(1,1111)	1:131:A:LYS:HG2	1:114:A:PHE:HE1	11	0.8
(1,1111)	1:131:A:LYS:HG3	1:114:A:PHE:HE1	11	0.8
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG2	11	0.8
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG3	11	0.8
(1,396)	1:114:A:PHE:H	1:114:A:PHE:HD1	5	0.76
(1,396)	1:114:A:PHE:H	1:114:A:PHE:HD1	13	0.76
(1,392)	1:114:A:PHE:HD1	1:114:A:PHE:H	5	0.76
(1,392)	1:114:A:PHE:HD1	1:114:A:PHE:H	13	0.76
(1,396)	1:114:A:PHE:H	1:114:A:PHE:HD1	9	0.75
(1,396)	1:114:A:PHE:H	1:114:A:PHE:HD1	20	0.75
(1,392)	1:114:A:PHE:HD1	1:114:A:PHE:H	9	0.75
(1,392)	1:114:A:PHE:HD1	1:114:A:PHE:H	20	0.75
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD11	17	0.74
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD12	17	0.74
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD13	17	0.74
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD11	18	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD12	18	0.74
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD13	18	0.74
(1,811)	1:87:A:LEU:HD11	1:101:A:TYR:HE2	17	0.74
(1,811)	1:87:A:LEU:HD12	1:101:A:TYR:HE2	17	0.74
(1,811)	1:87:A:LEU:HD13	1:101:A:TYR:HE2	17	0.74
(1,811)	1:87:A:LEU:HD11	1:101:A:TYR:HE2	18	0.74
(1,811)	1:87:A:LEU:HD12	1:101:A:TYR:HE2	18	0.74
(1,811)	1:87:A:LEU:HD13	1:101:A:TYR:HE2	18	0.74
(1,396)	1:114:A:PHE:H	1:114:A:PHE:HD1	8	0.74
(1,396)	1:114:A:PHE:H	1:114:A:PHE:HD1	18	0.74
(1,396)	1:114:A:PHE:H	1:114:A:PHE:HD1	19	0.74
(1,392)	1:114:A:PHE:HD1	1:114:A:PHE:H	8	0.74
(1,392)	1:114:A:PHE:HD1	1:114:A:PHE:H	18	0.74
(1,392)	1:114:A:PHE:HD1	1:114:A:PHE:H	19	0.74
(1,396)	1:114:A:PHE:H	1:114:A:PHE:HD1	4	0.73
(1,396)	1:114:A:PHE:H	1:114:A:PHE:HD1	7	0.73
(1,392)	1:114:A:PHE:HD1	1:114:A:PHE:H	4	0.73
(1,392)	1:114:A:PHE:HD1	1:114:A:PHE:H	7	0.73
(1,1111)	1:131:A:LYS:HG2	1:114:A:PHE:HE1	17	0.72
(1,1111)	1:131:A:LYS:HG3	1:114:A:PHE:HE1	17	0.72
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG2	17	0.72
(1,1000)	1:114:A:PHE:HE1	1:131:A:LYS:HG3	17	0.72
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD11	20	0.72
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD12	20	0.72
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD13	20	0.72
(1,811)	1:87:A:LEU:HD11	1:101:A:TYR:HE2	20	0.72
(1,811)	1:87:A:LEU:HD12	1:101:A:TYR:HE2	20	0.72
(1,811)	1:87:A:LEU:HD13	1:101:A:TYR:HE2	20	0.72
(1,396)	1:114:A:PHE:H	1:114:A:PHE:HD1	17	0.72
(1,392)	1:114:A:PHE:HD1	1:114:A:PHE:H	17	0.72
(1,396)	1:114:A:PHE:H	1:114:A:PHE:HD1	12	0.71
(1,396)	1:114:A:PHE:H	1:114:A:PHE:HD1	15	0.71
(1,392)	1:114:A:PHE:HD1	1:114:A:PHE:H	12	0.71
(1,392)	1:114:A:PHE:HD1	1:114:A:PHE:H	15	0.71
(1,1205)	1:144:A:ALA:HB1	1:120:A:PHE:HE2	15	0.68
(1,1205)	1:144:A:ALA:HB2	1:120:A:PHE:HE2	15	0.68
(1,1205)	1:144:A:ALA:HB3	1:120:A:PHE:HE2	15	0.68
(1,1060)	1:120:A:PHE:HE2	1:144:A:ALA:HB1	15	0.68
(1,1060)	1:120:A:PHE:HE2	1:144:A:ALA:HB2	15	0.68
(1,1060)	1:120:A:PHE:HE2	1:144:A:ALA:HB3	15	0.68
(1,1026)	1:118:A:VAL:HG21	1:101:A:TYR:HD2	4	0.68
(1,1026)	1:118:A:VAL:HG22	1:101:A:TYR:HD2	4	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1026)	1:118:A:VAL:HG23	1:101:A:TYR:HD2	4	0.68
(1,396)	1:114:A:PHE:H	1:114:A:PHE:HD1	14	0.68
(1,392)	1:114:A:PHE:HD1	1:114:A:PHE:H	14	0.68
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD11	10	0.65
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD12	10	0.65
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD13	10	0.65
(1,811)	1:87:A:LEU:HD11	1:101:A:TYR:HE2	10	0.65
(1,811)	1:87:A:LEU:HD12	1:101:A:TYR:HE2	10	0.65
(1,811)	1:87:A:LEU:HD13	1:101:A:TYR:HE2	10	0.65
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD11	7	0.63
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD12	7	0.63
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD13	7	0.63
(1,811)	1:87:A:LEU:HD11	1:101:A:TYR:HE2	7	0.63
(1,811)	1:87:A:LEU:HD12	1:101:A:TYR:HE2	7	0.63
(1,811)	1:87:A:LEU:HD13	1:101:A:TYR:HE2	7	0.63
(1,396)	1:114:A:PHE:H	1:114:A:PHE:HD1	2	0.63
(1,396)	1:114:A:PHE:H	1:114:A:PHE:HD1	10	0.63
(1,392)	1:114:A:PHE:HD1	1:114:A:PHE:H	2	0.63
(1,392)	1:114:A:PHE:HD1	1:114:A:PHE:H	10	0.63
(1,396)	1:114:A:PHE:H	1:114:A:PHE:HD1	1	0.62
(1,392)	1:114:A:PHE:HD1	1:114:A:PHE:H	1	0.62
(1,396)	1:114:A:PHE:H	1:114:A:PHE:HD1	3	0.61
(1,396)	1:114:A:PHE:H	1:114:A:PHE:HD1	16	0.61
(1,392)	1:114:A:PHE:HD1	1:114:A:PHE:H	3	0.61
(1,392)	1:114:A:PHE:HD1	1:114:A:PHE:H	16	0.61
(1,396)	1:114:A:PHE:H	1:114:A:PHE:HD1	11	0.6
(1,392)	1:114:A:PHE:HD1	1:114:A:PHE:H	11	0.6
(1,1026)	1:118:A:VAL:HG21	1:101:A:TYR:HD2	13	0.59
(1,1026)	1:118:A:VAL:HG22	1:101:A:TYR:HD2	13	0.59
(1,1026)	1:118:A:VAL:HG23	1:101:A:TYR:HD2	13	0.59
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB2	11	0.59
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB3	11	0.59
(1,970)	1:112:A:PRO:HB2	1:114:A:PHE:HD2	11	0.59
(1,970)	1:112:A:PRO:HB3	1:114:A:PHE:HD2	11	0.59
(1,396)	1:114:A:PHE:H	1:114:A:PHE:HD1	6	0.59
(1,392)	1:114:A:PHE:HD1	1:114:A:PHE:H	6	0.59
(1,1027)	1:118:A:VAL:HG21	1:101:A:TYR:HE2	4	0.57
(1,1027)	1:118:A:VAL:HG22	1:101:A:TYR:HE2	4	0.57
(1,1027)	1:118:A:VAL:HG23	1:101:A:TYR:HE2	4	0.57
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG21	4	0.57
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG22	4	0.57
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG23	4	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD11	13	0.57
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD12	13	0.57
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD13	13	0.57
(1,811)	1:87:A:LEU:HD11	1:101:A:TYR:HE2	13	0.57
(1,811)	1:87:A:LEU:HD12	1:101:A:TYR:HE2	13	0.57
(1,811)	1:87:A:LEU:HD13	1:101:A:TYR:HE2	13	0.57
(1,1213)	1:145:A:PHE:HA	1:145:A:PHE:HD1	19	0.5
(1,1026)	1:118:A:VAL:HG21	1:101:A:TYR:HD2	9	0.49
(1,1026)	1:118:A:VAL:HG22	1:101:A:TYR:HD2	9	0.49
(1,1026)	1:118:A:VAL:HG23	1:101:A:TYR:HD2	9	0.49
(1,1026)	1:118:A:VAL:HG21	1:101:A:TYR:HD2	12	0.49
(1,1026)	1:118:A:VAL:HG22	1:101:A:TYR:HD2	12	0.49
(1,1026)	1:118:A:VAL:HG23	1:101:A:TYR:HD2	12	0.49
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD11	4	0.49
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD12	4	0.49
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD13	4	0.49
(1,811)	1:87:A:LEU:HD11	1:101:A:TYR:HE2	4	0.49
(1,811)	1:87:A:LEU:HD12	1:101:A:TYR:HE2	4	0.49
(1,811)	1:87:A:LEU:HD13	1:101:A:TYR:HE2	4	0.49
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB2	9	0.49
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB3	9	0.49
(1,1026)	1:118:A:VAL:HG21	1:101:A:TYR:HD2	10	0.48
(1,1026)	1:118:A:VAL:HG22	1:101:A:TYR:HD2	10	0.48
(1,1026)	1:118:A:VAL:HG23	1:101:A:TYR:HD2	10	0.48
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB2	10	0.48
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB3	10	0.48
(1,970)	1:112:A:PRO:HB2	1:114:A:PHE:HD2	10	0.48
(1,970)	1:112:A:PRO:HB3	1:114:A:PHE:HD2	10	0.48
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB2	9	0.48
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB3	9	0.48
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB2	20	0.48
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB3	20	0.48
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB2	3	0.47
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB3	3	0.47
(1,970)	1:112:A:PRO:HB2	1:114:A:PHE:HD2	3	0.47
(1,970)	1:112:A:PRO:HB3	1:114:A:PHE:HD2	3	0.47
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD11	19	0.47
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD12	19	0.47
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD13	19	0.47
(1,811)	1:87:A:LEU:HD11	1:101:A:TYR:HE2	19	0.47
(1,811)	1:87:A:LEU:HD12	1:101:A:TYR:HE2	19	0.47
(1,811)	1:87:A:LEU:HD13	1:101:A:TYR:HE2	19	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB2	11	0.47
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB3	11	0.47
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB2	6	0.46
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB3	6	0.46
(1,970)	1:112:A:PRO:HB2	1:114:A:PHE:HD2	6	0.46
(1,970)	1:112:A:PRO:HB3	1:114:A:PHE:HD2	6	0.46
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB2	5	0.46
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB3	5	0.46
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB2	17	0.46
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB3	17	0.46
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB2	19	0.46
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB3	19	0.46
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB2	13	0.45
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB3	13	0.45
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD11	14	0.45
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD12	14	0.45
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD13	14	0.45
(1,811)	1:87:A:LEU:HD11	1:101:A:TYR:HE2	14	0.45
(1,811)	1:87:A:LEU:HD12	1:101:A:TYR:HE2	14	0.45
(1,811)	1:87:A:LEU:HD13	1:101:A:TYR:HE2	14	0.45
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB2	1	0.44
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB3	1	0.44
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB2	2	0.44
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB3	2	0.44
(1,970)	1:112:A:PRO:HB2	1:114:A:PHE:HD2	1	0.44
(1,970)	1:112:A:PRO:HB3	1:114:A:PHE:HD2	1	0.44
(1,970)	1:112:A:PRO:HB2	1:114:A:PHE:HD2	2	0.44
(1,970)	1:112:A:PRO:HB3	1:114:A:PHE:HD2	2	0.44
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB2	2	0.44
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB3	2	0.44
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB2	10	0.44
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB3	10	0.44
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB2	18	0.44
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB3	18	0.44
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB2	19	0.44
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB3	19	0.44
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD11	11	0.44
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD12	11	0.44
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD13	11	0.44
(1,811)	1:87:A:LEU:HD11	1:101:A:TYR:HE2	11	0.44
(1,811)	1:87:A:LEU:HD12	1:101:A:TYR:HE2	11	0.44
(1,811)	1:87:A:LEU:HD13	1:101:A:TYR:HE2	11	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB2	4	0.44
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB3	4	0.44
(1,1026)	1:118:A:VAL:HG21	1:101:A:TYR:HD2	2	0.43
(1,1026)	1:118:A:VAL:HG22	1:101:A:TYR:HD2	2	0.43
(1,1026)	1:118:A:VAL:HG23	1:101:A:TYR:HD2	2	0.43
(1,1026)	1:118:A:VAL:HG21	1:101:A:TYR:HD2	7	0.43
(1,1026)	1:118:A:VAL:HG22	1:101:A:TYR:HD2	7	0.43
(1,1026)	1:118:A:VAL:HG23	1:101:A:TYR:HD2	7	0.43
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB2	5	0.43
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB3	5	0.43
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB2	6	0.43
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB3	6	0.43
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB2	18	0.43
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB3	18	0.43
(1,546)	1:128:A:GLU:H	1:128:A:GLU:HG2	10	0.43
(1,546)	1:128:A:GLU:H	1:128:A:GLU:HG3	10	0.43
(1,1027)	1:118:A:VAL:HG21	1:101:A:TYR:HE2	13	0.42
(1,1027)	1:118:A:VAL:HG22	1:101:A:TYR:HE2	13	0.42
(1,1027)	1:118:A:VAL:HG23	1:101:A:TYR:HE2	13	0.42
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB2	11	0.42
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB3	11	0.42
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB2	15	0.42
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB3	15	0.42
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG21	13	0.42
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG22	13	0.42
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG23	13	0.42
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB2	2	0.42
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB3	2	0.42
(1,1213)	1:145:A:PHE:HA	1:145:A:PHE:HD1	13	0.41
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB2	16	0.41
(1,991)	1:114:A:PHE:HD2	1:112:A:PRO:HB3	16	0.41
(1,970)	1:112:A:PRO:HB2	1:114:A:PHE:HD2	16	0.41
(1,970)	1:112:A:PRO:HB3	1:114:A:PHE:HD2	16	0.41
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB2	1	0.41
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB3	1	0.41
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB2	3	0.41
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB3	3	0.41
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB2	4	0.41
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB3	4	0.41
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB2	12	0.41
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB3	12	0.41
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB2	16	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB3	16	0.41
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD11	8	0.41
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD12	8	0.41
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD13	8	0.41
(1,811)	1:87:A:LEU:HD11	1:101:A:TYR:HE2	8	0.41
(1,811)	1:87:A:LEU:HD12	1:101:A:TYR:HE2	8	0.41
(1,811)	1:87:A:LEU:HD13	1:101:A:TYR:HE2	8	0.41
(1,546)	1:128:A:GLU:H	1:128:A:GLU:HG2	13	0.41
(1,546)	1:128:A:GLU:H	1:128:A:GLU:HG3	13	0.41
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB2	1	0.4
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB3	1	0.4
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB2	14	0.4
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB3	14	0.4
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB2	17	0.39
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB3	17	0.39
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD11	1	0.39
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD12	1	0.39
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD13	1	0.39
(1,811)	1:87:A:LEU:HD11	1:101:A:TYR:HE2	1	0.39
(1,811)	1:87:A:LEU:HD12	1:101:A:TYR:HE2	1	0.39
(1,811)	1:87:A:LEU:HD13	1:101:A:TYR:HE2	1	0.39
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB2	15	0.39
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB3	15	0.39
(1,546)	1:128:A:GLU:H	1:128:A:GLU:HG2	8	0.39
(1,546)	1:128:A:GLU:H	1:128:A:GLU:HG3	8	0.39
(1,1027)	1:118:A:VAL:HG21	1:101:A:TYR:HE2	10	0.38
(1,1027)	1:118:A:VAL:HG22	1:101:A:TYR:HE2	10	0.38
(1,1027)	1:118:A:VAL:HG23	1:101:A:TYR:HE2	10	0.38
(1,1026)	1:118:A:VAL:HG21	1:101:A:TYR:HD2	20	0.38
(1,1026)	1:118:A:VAL:HG22	1:101:A:TYR:HD2	20	0.38
(1,1026)	1:118:A:VAL:HG23	1:101:A:TYR:HD2	20	0.38
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB2	14	0.38
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB3	14	0.38
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG21	10	0.38
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG22	10	0.38
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG23	10	0.38
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB2	3	0.38
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB3	3	0.38
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB2	20	0.38
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB3	20	0.38
(1,1213)	1:145:A:PHE:HA	1:145:A:PHE:HD1	12	0.37
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD11	16	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD12	16	0.37
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD13	16	0.37
(1,811)	1:87:A:LEU:HD11	1:101:A:TYR:HE2	16	0.37
(1,811)	1:87:A:LEU:HD12	1:101:A:TYR:HE2	16	0.37
(1,811)	1:87:A:LEU:HD13	1:101:A:TYR:HE2	16	0.37
(1,1027)	1:118:A:VAL:HG21	1:101:A:TYR:HE2	7	0.36
(1,1027)	1:118:A:VAL:HG22	1:101:A:TYR:HE2	7	0.36
(1,1027)	1:118:A:VAL:HG23	1:101:A:TYR:HE2	7	0.36
(1,1026)	1:118:A:VAL:HG21	1:101:A:TYR:HD2	16	0.36
(1,1026)	1:118:A:VAL:HG22	1:101:A:TYR:HD2	16	0.36
(1,1026)	1:118:A:VAL:HG23	1:101:A:TYR:HD2	16	0.36
(1,1026)	1:118:A:VAL:HG21	1:101:A:TYR:HD2	17	0.36
(1,1026)	1:118:A:VAL:HG22	1:101:A:TYR:HD2	17	0.36
(1,1026)	1:118:A:VAL:HG23	1:101:A:TYR:HD2	17	0.36
(1,1026)	1:118:A:VAL:HG21	1:101:A:TYR:HD2	18	0.36
(1,1026)	1:118:A:VAL:HG22	1:101:A:TYR:HD2	18	0.36
(1,1026)	1:118:A:VAL:HG23	1:101:A:TYR:HD2	18	0.36
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG21	7	0.36
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG22	7	0.36
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG23	7	0.36
(1,1026)	1:118:A:VAL:HG21	1:101:A:TYR:HD2	11	0.35
(1,1026)	1:118:A:VAL:HG22	1:101:A:TYR:HD2	11	0.35
(1,1026)	1:118:A:VAL:HG23	1:101:A:TYR:HD2	11	0.35
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB2	7	0.35
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB3	7	0.35
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD11	12	0.35
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD12	12	0.35
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD13	12	0.35
(1,811)	1:87:A:LEU:HD11	1:101:A:TYR:HE2	12	0.35
(1,811)	1:87:A:LEU:HD12	1:101:A:TYR:HE2	12	0.35
(1,811)	1:87:A:LEU:HD13	1:101:A:TYR:HE2	12	0.35
(1,1027)	1:118:A:VAL:HG21	1:101:A:TYR:HE2	9	0.34
(1,1027)	1:118:A:VAL:HG22	1:101:A:TYR:HE2	9	0.34
(1,1027)	1:118:A:VAL:HG23	1:101:A:TYR:HE2	9	0.34
(1,1027)	1:118:A:VAL:HG21	1:101:A:TYR:HE2	11	0.34
(1,1027)	1:118:A:VAL:HG22	1:101:A:TYR:HE2	11	0.34
(1,1027)	1:118:A:VAL:HG23	1:101:A:TYR:HE2	11	0.34
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB2	8	0.34
(1,953)	1:111:A:ALA:HA	1:108:A:PRO:HB3	8	0.34
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG21	9	0.34
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG22	9	0.34
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG23	9	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG21	11	0.34
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG22	11	0.34
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG23	11	0.34
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB2	7	0.34
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB3	7	0.34
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB2	12	0.34
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB3	12	0.34
(1,411)	1:115:A:THR:H	1:114:A:PHE:HD2	12	0.34
(1,400)	1:114:A:PHE:HD2	1:115:A:THR:H	12	0.34
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD11	9	0.33
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD12	9	0.33
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD13	9	0.33
(1,811)	1:87:A:LEU:HD11	1:101:A:TYR:HE2	9	0.33
(1,811)	1:87:A:LEU:HD12	1:101:A:TYR:HE2	9	0.33
(1,811)	1:87:A:LEU:HD13	1:101:A:TYR:HE2	9	0.33
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB2	6	0.33
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB3	6	0.33
(1,411)	1:115:A:THR:H	1:114:A:PHE:HD2	15	0.33
(1,400)	1:114:A:PHE:HD2	1:115:A:THR:H	15	0.33
(1,1027)	1:118:A:VAL:HG21	1:101:A:TYR:HE2	2	0.32
(1,1027)	1:118:A:VAL:HG22	1:101:A:TYR:HE2	2	0.32
(1,1027)	1:118:A:VAL:HG23	1:101:A:TYR:HE2	2	0.32
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG21	2	0.32
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG22	2	0.32
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG23	2	0.32
(1,546)	1:128:A:GLU:H	1:128:A:GLU:HG2	12	0.32
(1,546)	1:128:A:GLU:H	1:128:A:GLU:HG3	12	0.32
(1,411)	1:115:A:THR:H	1:114:A:PHE:HD2	11	0.32
(1,400)	1:114:A:PHE:HD2	1:115:A:THR:H	11	0.32
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB2	9	0.31
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB3	9	0.31
(1,411)	1:115:A:THR:H	1:114:A:PHE:HD2	18	0.31
(1,400)	1:114:A:PHE:HD2	1:115:A:THR:H	18	0.31
(1,1027)	1:118:A:VAL:HG21	1:101:A:TYR:HE2	19	0.3
(1,1027)	1:118:A:VAL:HG22	1:101:A:TYR:HE2	19	0.3
(1,1027)	1:118:A:VAL:HG23	1:101:A:TYR:HE2	19	0.3
(1,1026)	1:118:A:VAL:HG21	1:101:A:TYR:HD2	19	0.3
(1,1026)	1:118:A:VAL:HG22	1:101:A:TYR:HD2	19	0.3
(1,1026)	1:118:A:VAL:HG23	1:101:A:TYR:HD2	19	0.3
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG21	19	0.3
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG22	19	0.3
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG23	19	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB2	1	0.3
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB3	1	0.3
(1,411)	1:115:A:THR:H	1:114:A:PHE:HD2	4	0.3
(1,411)	1:115:A:THR:H	1:114:A:PHE:HD2	14	0.3
(1,411)	1:115:A:THR:H	1:114:A:PHE:HD2	20	0.3
(1,400)	1:114:A:PHE:HD2	1:115:A:THR:H	4	0.3
(1,400)	1:114:A:PHE:HD2	1:115:A:THR:H	14	0.3
(1,400)	1:114:A:PHE:HD2	1:115:A:THR:H	20	0.3
(1,1027)	1:118:A:VAL:HG21	1:101:A:TYR:HE2	12	0.29
(1,1027)	1:118:A:VAL:HG22	1:101:A:TYR:HE2	12	0.29
(1,1027)	1:118:A:VAL:HG23	1:101:A:TYR:HE2	12	0.29
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG21	12	0.29
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG22	12	0.29
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG23	12	0.29
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB2	5	0.29
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB3	5	0.29
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB2	10	0.29
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB3	10	0.29
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB2	16	0.29
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB3	16	0.29
(1,411)	1:115:A:THR:H	1:114:A:PHE:HD2	3	0.29
(1,411)	1:115:A:THR:H	1:114:A:PHE:HD2	10	0.29
(1,400)	1:114:A:PHE:HD2	1:115:A:THR:H	3	0.29
(1,400)	1:114:A:PHE:HD2	1:115:A:THR:H	10	0.29
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD11	2	0.28
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD12	2	0.28
(1,902)	1:101:A:TYR:HE2	1:87:A:LEU:HD13	2	0.28
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB2	20	0.28
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB3	20	0.28
(1,811)	1:87:A:LEU:HD11	1:101:A:TYR:HE2	2	0.28
(1,811)	1:87:A:LEU:HD12	1:101:A:TYR:HE2	2	0.28
(1,811)	1:87:A:LEU:HD13	1:101:A:TYR:HE2	2	0.28
(1,411)	1:115:A:THR:H	1:114:A:PHE:HD2	17	0.28
(1,400)	1:114:A:PHE:HD2	1:115:A:THR:H	17	0.28
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB2	6	0.27
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB3	6	0.27
(1,411)	1:115:A:THR:H	1:114:A:PHE:HD2	2	0.27
(1,411)	1:115:A:THR:H	1:114:A:PHE:HD2	19	0.27
(1,400)	1:114:A:PHE:HD2	1:115:A:THR:H	2	0.27
(1,400)	1:114:A:PHE:HD2	1:115:A:THR:H	19	0.27
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB2	8	0.26
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB3	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB2	13	0.26
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB3	13	0.26
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB2	18	0.26
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB3	18	0.26
(1,546)	1:128:A:GLU:H	1:128:A:GLU:HG2	20	0.26
(1,546)	1:128:A:GLU:H	1:128:A:GLU:HG3	20	0.26
(1,411)	1:115:A:THR:H	1:114:A:PHE:HD2	6	0.26
(1,411)	1:115:A:THR:H	1:114:A:PHE:HD2	7	0.26
(1,411)	1:115:A:THR:H	1:114:A:PHE:HD2	16	0.26
(1,400)	1:114:A:PHE:HD2	1:115:A:THR:H	6	0.26
(1,400)	1:114:A:PHE:HD2	1:115:A:THR:H	7	0.26
(1,400)	1:114:A:PHE:HD2	1:115:A:THR:H	16	0.26
(1,1026)	1:118:A:VAL:HG21	1:101:A:TYR:HD2	8	0.25
(1,1026)	1:118:A:VAL:HG22	1:101:A:TYR:HD2	8	0.25
(1,1026)	1:118:A:VAL:HG23	1:101:A:TYR:HD2	8	0.25
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB2	4	0.25
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB3	4	0.25
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB2	7	0.25
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB3	7	0.25
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB2	16	0.25
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB3	16	0.25
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB2	19	0.25
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB3	19	0.25
(1,1027)	1:118:A:VAL:HG21	1:101:A:TYR:HE2	18	0.24
(1,1027)	1:118:A:VAL:HG22	1:101:A:TYR:HE2	18	0.24
(1,1027)	1:118:A:VAL:HG23	1:101:A:TYR:HE2	18	0.24
(1,1026)	1:118:A:VAL:HG21	1:101:A:TYR:HD2	14	0.24
(1,1026)	1:118:A:VAL:HG22	1:101:A:TYR:HD2	14	0.24
(1,1026)	1:118:A:VAL:HG23	1:101:A:TYR:HD2	14	0.24
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG21	18	0.24
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG22	18	0.24
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG23	18	0.24
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB2	2	0.24
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB3	2	0.24
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB2	3	0.24
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB3	3	0.24
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB2	11	0.24
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB3	11	0.24
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB2	12	0.24
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB3	12	0.24
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB2	14	0.24
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB3	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB2	15	0.24
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB3	15	0.24
(1,411)	1:115:A:THR:H	1:114:A:PHE:HD2	9	0.24
(1,400)	1:114:A:PHE:HD2	1:115:A:THR:H	9	0.24
(1,308)	1:101:A:TYR:HA	1:100:A:PHE:H	1	0.24
(1,302)	1:100:A:PHE:H	1:101:A:TYR:HA	1	0.24
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB2	17	0.23
(1,833)	1:89:A:GLU:H	1:86:A:LEU:HB3	17	0.23
(1,546)	1:128:A:GLU:H	1:128:A:GLU:HG2	6	0.23
(1,546)	1:128:A:GLU:H	1:128:A:GLU:HG3	6	0.23
(1,411)	1:115:A:THR:H	1:114:A:PHE:HD2	5	0.23
(1,411)	1:115:A:THR:H	1:114:A:PHE:HD2	13	0.23
(1,400)	1:114:A:PHE:HD2	1:115:A:THR:H	5	0.23
(1,400)	1:114:A:PHE:HD2	1:115:A:THR:H	13	0.23
(1,348)	1:105:A:THR:H	1:105:A:THR:HB	9	0.23
(1,346)	1:105:A:THR:HB	1:105:A:THR:H	9	0.23
(1,785)	1:86:A:LEU:HD21	1:86:A:LEU:HA	11	0.22
(1,785)	1:86:A:LEU:HD22	1:86:A:LEU:HA	11	0.22
(1,785)	1:86:A:LEU:HD23	1:86:A:LEU:HA	11	0.22
(1,783)	1:86:A:LEU:HA	1:86:A:LEU:HD21	11	0.22
(1,783)	1:86:A:LEU:HA	1:86:A:LEU:HD22	11	0.22
(1,783)	1:86:A:LEU:HA	1:86:A:LEU:HD23	11	0.22
(1,546)	1:128:A:GLU:H	1:128:A:GLU:HG2	3	0.22
(1,546)	1:128:A:GLU:H	1:128:A:GLU:HG3	3	0.22
(1,411)	1:115:A:THR:H	1:114:A:PHE:HD2	8	0.22
(1,400)	1:114:A:PHE:HD2	1:115:A:THR:H	8	0.22
(1,308)	1:101:A:TYR:HA	1:100:A:PHE:H	10	0.22
(1,308)	1:101:A:TYR:HA	1:100:A:PHE:H	20	0.22
(1,302)	1:100:A:PHE:H	1:101:A:TYR:HA	10	0.22
(1,302)	1:100:A:PHE:H	1:101:A:TYR:HA	20	0.22
(1,1027)	1:118:A:VAL:HG21	1:101:A:TYR:HE2	17	0.21
(1,1027)	1:118:A:VAL:HG22	1:101:A:TYR:HE2	17	0.21
(1,1027)	1:118:A:VAL:HG23	1:101:A:TYR:HE2	17	0.21
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG21	17	0.21
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG22	17	0.21
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG23	17	0.21
(1,785)	1:86:A:LEU:HD21	1:86:A:LEU:HA	17	0.21
(1,785)	1:86:A:LEU:HD22	1:86:A:LEU:HA	17	0.21
(1,785)	1:86:A:LEU:HD23	1:86:A:LEU:HA	17	0.21
(1,783)	1:86:A:LEU:HA	1:86:A:LEU:HD21	17	0.21
(1,783)	1:86:A:LEU:HA	1:86:A:LEU:HD22	17	0.21
(1,783)	1:86:A:LEU:HA	1:86:A:LEU:HD23	17	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,411)	1:115:A:THR:H	1:114:A:PHE:HD2	1	0.21
(1,400)	1:114:A:PHE:HD2	1:115:A:THR:H	1	0.21
(1,308)	1:101:A:TYR:HA	1:100:A:PHE:H	13	0.21
(1,302)	1:100:A:PHE:H	1:101:A:TYR:HA	13	0.21
(1,1027)	1:118:A:VAL:HG21	1:101:A:TYR:HE2	14	0.2
(1,1027)	1:118:A:VAL:HG22	1:101:A:TYR:HE2	14	0.2
(1,1027)	1:118:A:VAL:HG23	1:101:A:TYR:HE2	14	0.2
(1,1027)	1:118:A:VAL:HG21	1:101:A:TYR:HE2	16	0.2
(1,1027)	1:118:A:VAL:HG22	1:101:A:TYR:HE2	16	0.2
(1,1027)	1:118:A:VAL:HG23	1:101:A:TYR:HE2	16	0.2
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG21	14	0.2
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG22	14	0.2
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG23	14	0.2
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG21	16	0.2
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG22	16	0.2
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG23	16	0.2
(1,308)	1:101:A:TYR:HA	1:100:A:PHE:H	5	0.2
(1,308)	1:101:A:TYR:HA	1:100:A:PHE:H	11	0.2
(1,302)	1:100:A:PHE:H	1:101:A:TYR:HA	5	0.2
(1,302)	1:100:A:PHE:H	1:101:A:TYR:HA	11	0.2
(1,1027)	1:118:A:VAL:HG21	1:101:A:TYR:HE2	8	0.19
(1,1027)	1:118:A:VAL:HG22	1:101:A:TYR:HE2	8	0.19
(1,1027)	1:118:A:VAL:HG23	1:101:A:TYR:HE2	8	0.19
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG21	8	0.19
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG22	8	0.19
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG23	8	0.19
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB2	8	0.19
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB3	8	0.19
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB2	13	0.19
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB3	13	0.19
(1,361)	1:108:A:PRO:HG2	1:110:A:HIS:H	18	0.19
(1,361)	1:108:A:PRO:HG3	1:110:A:HIS:H	18	0.19
(1,361)	1:108:A:PRO:HG2	1:110:A:HIS:H	19	0.19
(1,361)	1:108:A:PRO:HG3	1:110:A:HIS:H	19	0.19
(1,308)	1:101:A:TYR:HA	1:100:A:PHE:H	17	0.19
(1,308)	1:101:A:TYR:HA	1:100:A:PHE:H	18	0.19
(1,308)	1:101:A:TYR:HA	1:100:A:PHE:H	19	0.19
(1,302)	1:100:A:PHE:H	1:101:A:TYR:HA	17	0.19
(1,302)	1:100:A:PHE:H	1:101:A:TYR:HA	18	0.19
(1,302)	1:100:A:PHE:H	1:101:A:TYR:HA	19	0.19
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB2	10	0.18
(1,550)	1:128:A:GLU:HA	1:139:A:SER:HB3	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,308)	1:101:A:TYR:HA	1:100:A:PHE:H	4	0.18
(1,308)	1:101:A:TYR:HA	1:100:A:PHE:H	7	0.18
(1,302)	1:100:A:PHE:H	1:101:A:TYR:HA	4	0.18
(1,302)	1:100:A:PHE:H	1:101:A:TYR:HA	7	0.18
(1,1027)	1:118:A:VAL:HG21	1:101:A:TYR:HE2	20	0.17
(1,1027)	1:118:A:VAL:HG22	1:101:A:TYR:HE2	20	0.17
(1,1027)	1:118:A:VAL:HG23	1:101:A:TYR:HE2	20	0.17
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG21	20	0.17
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG22	20	0.17
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG23	20	0.17
(1,666)	1:139:A:SER:HB2	1:128:A:GLU:H	12	0.17
(1,666)	1:139:A:SER:HB3	1:128:A:GLU:H	12	0.17
(1,553)	1:129:A:GLU:H	1:128:A:GLU:HB2	6	0.17
(1,553)	1:129:A:GLU:H	1:128:A:GLU:HB3	6	0.17
(1,548)	1:128:A:GLU:HB2	1:129:A:GLU:H	6	0.17
(1,548)	1:128:A:GLU:HB3	1:129:A:GLU:H	6	0.17
(1,361)	1:108:A:PRO:HG2	1:110:A:HIS:H	14	0.17
(1,361)	1:108:A:PRO:HG3	1:110:A:HIS:H	14	0.17
(1,348)	1:105:A:THR:H	1:105:A:THR:HB	4	0.17
(1,348)	1:105:A:THR:H	1:105:A:THR:HB	5	0.17
(1,348)	1:105:A:THR:H	1:105:A:THR:HB	12	0.17
(1,348)	1:105:A:THR:H	1:105:A:THR:HB	14	0.17
(1,346)	1:105:A:THR:HB	1:105:A:THR:H	4	0.17
(1,346)	1:105:A:THR:HB	1:105:A:THR:H	5	0.17
(1,346)	1:105:A:THR:HB	1:105:A:THR:H	12	0.17
(1,346)	1:105:A:THR:HB	1:105:A:THR:H	14	0.17
(1,308)	1:101:A:TYR:HA	1:100:A:PHE:H	8	0.17
(1,308)	1:101:A:TYR:HA	1:100:A:PHE:H	14	0.17
(1,308)	1:101:A:TYR:HA	1:100:A:PHE:H	15	0.17
(1,302)	1:100:A:PHE:H	1:101:A:TYR:HA	8	0.17
(1,302)	1:100:A:PHE:H	1:101:A:TYR:HA	14	0.17
(1,302)	1:100:A:PHE:H	1:101:A:TYR:HA	15	0.17
(1,666)	1:139:A:SER:HB2	1:128:A:GLU:H	15	0.16
(1,666)	1:139:A:SER:HB3	1:128:A:GLU:H	15	0.16
(1,553)	1:129:A:GLU:H	1:128:A:GLU:HB2	12	0.16
(1,553)	1:129:A:GLU:H	1:128:A:GLU:HB3	12	0.16
(1,548)	1:128:A:GLU:HB2	1:129:A:GLU:H	12	0.16
(1,548)	1:128:A:GLU:HB3	1:129:A:GLU:H	12	0.16
(1,361)	1:108:A:PRO:HG2	1:110:A:HIS:H	1	0.16
(1,361)	1:108:A:PRO:HG3	1:110:A:HIS:H	1	0.16
(1,361)	1:108:A:PRO:HG2	1:110:A:HIS:H	4	0.16
(1,361)	1:108:A:PRO:HG3	1:110:A:HIS:H	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,361)	1:108:A:PRO:HG2	1:110:A:HIS:H	20	0.16
(1,361)	1:108:A:PRO:HG3	1:110:A:HIS:H	20	0.16
(1,348)	1:105:A:THR:H	1:105:A:THR:HB	1	0.16
(1,348)	1:105:A:THR:H	1:105:A:THR:HB	13	0.16
(1,348)	1:105:A:THR:H	1:105:A:THR:HB	15	0.16
(1,348)	1:105:A:THR:H	1:105:A:THR:HB	20	0.16
(1,346)	1:105:A:THR:HB	1:105:A:THR:H	1	0.16
(1,346)	1:105:A:THR:HB	1:105:A:THR:H	13	0.16
(1,346)	1:105:A:THR:HB	1:105:A:THR:H	15	0.16
(1,346)	1:105:A:THR:HB	1:105:A:THR:H	20	0.16
(1,1253)	1:149:A:LYS:HE2	1:149:A:LYS:HB2	7	0.15
(1,1253)	1:149:A:LYS:HE2	1:149:A:LYS:HB3	7	0.15
(1,1253)	1:149:A:LYS:HE3	1:149:A:LYS:HB2	7	0.15
(1,1253)	1:149:A:LYS:HE3	1:149:A:LYS:HB3	7	0.15
(1,1246)	1:149:A:LYS:HB2	1:149:A:LYS:HE2	7	0.15
(1,1246)	1:149:A:LYS:HB2	1:149:A:LYS:HE3	7	0.15
(1,1246)	1:149:A:LYS:HB3	1:149:A:LYS:HE2	7	0.15
(1,1246)	1:149:A:LYS:HB3	1:149:A:LYS:HE3	7	0.15
(1,1175)	1:136:A:ALA:HA	1:128:A:GLU:HG2	16	0.15
(1,1175)	1:136:A:ALA:HA	1:128:A:GLU:HG3	16	0.15
(1,1100)	1:128:A:GLU:HG2	1:136:A:ALA:HA	16	0.15
(1,1100)	1:128:A:GLU:HG3	1:136:A:ALA:HA	16	0.15
(1,666)	1:139:A:SER:HB2	1:128:A:GLU:H	14	0.15
(1,666)	1:139:A:SER:HB3	1:128:A:GLU:H	14	0.15
(1,361)	1:108:A:PRO:HG2	1:110:A:HIS:H	6	0.15
(1,361)	1:108:A:PRO:HG3	1:110:A:HIS:H	6	0.15
(1,361)	1:108:A:PRO:HG2	1:110:A:HIS:H	7	0.15
(1,361)	1:108:A:PRO:HG3	1:110:A:HIS:H	7	0.15
(1,361)	1:108:A:PRO:HG2	1:110:A:HIS:H	8	0.15
(1,361)	1:108:A:PRO:HG3	1:110:A:HIS:H	8	0.15
(1,361)	1:108:A:PRO:HG2	1:110:A:HIS:H	9	0.15
(1,361)	1:108:A:PRO:HG3	1:110:A:HIS:H	9	0.15
(1,361)	1:108:A:PRO:HG2	1:110:A:HIS:H	11	0.15
(1,361)	1:108:A:PRO:HG3	1:110:A:HIS:H	11	0.15
(1,361)	1:108:A:PRO:HG2	1:110:A:HIS:H	13	0.15
(1,361)	1:108:A:PRO:HG3	1:110:A:HIS:H	13	0.15
(1,361)	1:108:A:PRO:HG2	1:110:A:HIS:H	15	0.15
(1,361)	1:108:A:PRO:HG3	1:110:A:HIS:H	15	0.15
(1,361)	1:108:A:PRO:HG2	1:110:A:HIS:H	16	0.15
(1,361)	1:108:A:PRO:HG3	1:110:A:HIS:H	16	0.15
(1,361)	1:108:A:PRO:HG2	1:110:A:HIS:H	17	0.15
(1,361)	1:108:A:PRO:HG3	1:110:A:HIS:H	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,348)	1:105:A:THR:H	1:105:A:THR:HB	7	0.15
(1,348)	1:105:A:THR:H	1:105:A:THR:HB	8	0.15
(1,348)	1:105:A:THR:H	1:105:A:THR:HB	17	0.15
(1,346)	1:105:A:THR:HB	1:105:A:THR:H	7	0.15
(1,346)	1:105:A:THR:HB	1:105:A:THR:H	8	0.15
(1,346)	1:105:A:THR:HB	1:105:A:THR:H	17	0.15
(1,6)	1:84:A:LYS:H	1:82:A:ALA:H	9	0.15
(1,2)	1:82:A:ALA:H	1:84:A:LYS:H	9	0.15
(2,29)	1:120:A:PHE:O	1:123:A:LYS:H	9	0.14
(1,1035)	1:118:A:VAL:HG21	1:125:A:PHE:HD1	4	0.14
(1,1035)	1:118:A:VAL:HG22	1:125:A:PHE:HD1	4	0.14
(1,1035)	1:118:A:VAL:HG23	1:125:A:PHE:HD1	4	0.14
(1,1027)	1:118:A:VAL:HG21	1:101:A:TYR:HE2	1	0.14
(1,1027)	1:118:A:VAL:HG22	1:101:A:TYR:HE2	1	0.14
(1,1027)	1:118:A:VAL:HG23	1:101:A:TYR:HE2	1	0.14
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG21	1	0.14
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG22	1	0.14
(1,906)	1:101:A:TYR:HE2	1:118:A:VAL:HG23	1	0.14
(1,553)	1:129:A:GLU:H	1:128:A:GLU:HB2	20	0.14
(1,553)	1:129:A:GLU:H	1:128:A:GLU:HB3	20	0.14
(1,548)	1:128:A:GLU:HB2	1:129:A:GLU:H	20	0.14
(1,548)	1:128:A:GLU:HB3	1:129:A:GLU:H	20	0.14
(1,361)	1:108:A:PRO:HG2	1:110:A:HIS:H	3	0.14
(1,361)	1:108:A:PRO:HG3	1:110:A:HIS:H	3	0.14
(1,361)	1:108:A:PRO:HG2	1:110:A:HIS:H	5	0.14
(1,361)	1:108:A:PRO:HG3	1:110:A:HIS:H	5	0.14
(1,361)	1:108:A:PRO:HG2	1:110:A:HIS:H	12	0.14
(1,361)	1:108:A:PRO:HG3	1:110:A:HIS:H	12	0.14
(1,359)	1:107:A:GLY:HA2	1:113:A:THR:H	9	0.14
(1,359)	1:107:A:GLY:HA3	1:113:A:THR:H	9	0.14
(1,348)	1:105:A:THR:H	1:105:A:THR:HB	3	0.14
(1,348)	1:105:A:THR:H	1:105:A:THR:HB	10	0.14
(1,348)	1:105:A:THR:H	1:105:A:THR:HB	18	0.14
(1,348)	1:105:A:THR:H	1:105:A:THR:HB	19	0.14
(1,346)	1:105:A:THR:HB	1:105:A:THR:H	3	0.14
(1,346)	1:105:A:THR:HB	1:105:A:THR:H	10	0.14
(1,346)	1:105:A:THR:HB	1:105:A:THR:H	18	0.14
(1,346)	1:105:A:THR:HB	1:105:A:THR:H	19	0.14
(1,333)	1:104:A:ALA:H	1:103:A:THR:HA	10	0.14
(1,333)	1:104:A:ALA:H	1:103:A:THR:HA	16	0.14
(2,15)	1:90:A:ILE:O	1:94:A:GLU:H	1	0.13
(1,1026)	1:118:A:VAL:HG21	1:101:A:TYR:HD2	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1026)	1:118:A:VAL:HG22	1:101:A:TYR:HD2	1	0.13
(1,1026)	1:118:A:VAL:HG23	1:101:A:TYR:HD2	1	0.13
(1,666)	1:139:A:SER:HB2	1:128:A:GLU:H	20	0.13
(1,666)	1:139:A:SER:HB3	1:128:A:GLU:H	20	0.13
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD11	17	0.13
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD12	17	0.13
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD13	17	0.13
(1,619)	1:135:A:LEU:HD11	1:135:A:LEU:H	17	0.13
(1,619)	1:135:A:LEU:HD12	1:135:A:LEU:H	17	0.13
(1,619)	1:135:A:LEU:HD13	1:135:A:LEU:H	17	0.13
(1,421)	1:116:A:SER:HA	1:104:A:ALA:H	9	0.13
(1,361)	1:108:A:PRO:HG2	1:110:A:HIS:H	2	0.13
(1,361)	1:108:A:PRO:HG3	1:110:A:HIS:H	2	0.13
(1,361)	1:108:A:PRO:HG2	1:110:A:HIS:H	10	0.13
(1,361)	1:108:A:PRO:HG3	1:110:A:HIS:H	10	0.13
(1,348)	1:105:A:THR:H	1:105:A:THR:HB	6	0.13
(1,348)	1:105:A:THR:H	1:105:A:THR:HB	11	0.13
(1,348)	1:105:A:THR:H	1:105:A:THR:HB	16	0.13
(1,346)	1:105:A:THR:HB	1:105:A:THR:H	6	0.13
(1,346)	1:105:A:THR:HB	1:105:A:THR:H	11	0.13
(1,346)	1:105:A:THR:HB	1:105:A:THR:H	16	0.13
(1,343)	1:104:A:ALA:H	1:116:A:SER:HA	9	0.13
(1,333)	1:104:A:ALA:H	1:103:A:THR:HA	6	0.13
(1,333)	1:104:A:ALA:H	1:103:A:THR:HA	7	0.13
(1,333)	1:104:A:ALA:H	1:103:A:THR:HA	11	0.13
(1,333)	1:104:A:ALA:H	1:103:A:THR:HA	13	0.13
(1,333)	1:104:A:ALA:H	1:103:A:THR:HA	19	0.13
(1,6)	1:84:A:LYS:H	1:82:A:ALA:H	1	0.13
(1,2)	1:82:A:ALA:H	1:84:A:LYS:H	1	0.13
(2,20)	1:102:A:ALA:O	1:117:A:THR:N	20	0.12
(2,15)	1:90:A:ILE:O	1:94:A:GLU:H	17	0.12
(2,15)	1:90:A:ILE:O	1:94:A:GLU:H	20	0.12
(1,666)	1:139:A:SER:HB2	1:128:A:GLU:H	3	0.12
(1,666)	1:139:A:SER:HB3	1:128:A:GLU:H	3	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD11	1	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD12	1	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD13	1	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD11	2	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD12	2	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD13	2	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD11	4	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD12	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD13	4	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD11	5	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD12	5	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD13	5	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD11	7	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD12	7	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD13	7	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD11	14	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD12	14	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD13	14	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD11	15	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD12	15	0.12
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD13	15	0.12
(1,619)	1:135:A:LEU:HD11	1:135:A:LEU:H	1	0.12
(1,619)	1:135:A:LEU:HD12	1:135:A:LEU:H	1	0.12
(1,619)	1:135:A:LEU:HD13	1:135:A:LEU:H	1	0.12
(1,619)	1:135:A:LEU:HD11	1:135:A:LEU:H	2	0.12
(1,619)	1:135:A:LEU:HD12	1:135:A:LEU:H	2	0.12
(1,619)	1:135:A:LEU:HD13	1:135:A:LEU:H	2	0.12
(1,619)	1:135:A:LEU:HD11	1:135:A:LEU:H	4	0.12
(1,619)	1:135:A:LEU:HD12	1:135:A:LEU:H	4	0.12
(1,619)	1:135:A:LEU:HD13	1:135:A:LEU:H	4	0.12
(1,619)	1:135:A:LEU:HD11	1:135:A:LEU:H	5	0.12
(1,619)	1:135:A:LEU:HD12	1:135:A:LEU:H	5	0.12
(1,619)	1:135:A:LEU:HD13	1:135:A:LEU:H	5	0.12
(1,619)	1:135:A:LEU:HD11	1:135:A:LEU:H	7	0.12
(1,619)	1:135:A:LEU:HD12	1:135:A:LEU:H	7	0.12
(1,619)	1:135:A:LEU:HD13	1:135:A:LEU:H	7	0.12
(1,619)	1:135:A:LEU:HD11	1:135:A:LEU:H	14	0.12
(1,619)	1:135:A:LEU:HD12	1:135:A:LEU:H	14	0.12
(1,619)	1:135:A:LEU:HD13	1:135:A:LEU:H	14	0.12
(1,619)	1:135:A:LEU:HD11	1:135:A:LEU:H	15	0.12
(1,619)	1:135:A:LEU:HD12	1:135:A:LEU:H	15	0.12
(1,619)	1:135:A:LEU:HD13	1:135:A:LEU:H	15	0.12
(1,553)	1:129:A:GLU:H	1:128:A:GLU:HB2	3	0.12
(1,553)	1:129:A:GLU:H	1:128:A:GLU:HB3	3	0.12
(1,548)	1:128:A:GLU:HB2	1:129:A:GLU:H	3	0.12
(1,548)	1:128:A:GLU:HB3	1:129:A:GLU:H	3	0.12
(1,348)	1:105:A:THR:H	1:105:A:THR:HB	2	0.12
(1,346)	1:105:A:THR:HB	1:105:A:THR:H	2	0.12
(1,333)	1:104:A:ALA:H	1:103:A:THR:HA	3	0.12
(1,333)	1:104:A:ALA:H	1:103:A:THR:HA	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,333)	1:104:A:ALA:H	1:103:A:THR:HA	5	0.12
(1,333)	1:104:A:ALA:H	1:103:A:THR:HA	8	0.12
(1,333)	1:104:A:ALA:H	1:103:A:THR:HA	12	0.12
(1,333)	1:104:A:ALA:H	1:103:A:THR:HA	14	0.12
(1,333)	1:104:A:ALA:H	1:103:A:THR:HA	15	0.12
(2,36)	1:125:A:PHE:O	1:118:A:VAL:N	13	0.11
(2,36)	1:125:A:PHE:O	1:118:A:VAL:N	20	0.11
(2,29)	1:120:A:PHE:O	1:123:A:LYS:H	15	0.11
(2,29)	1:120:A:PHE:O	1:123:A:LYS:H	16	0.11
(2,15)	1:90:A:ILE:O	1:94:A:GLU:H	3	0.11
(2,15)	1:90:A:ILE:O	1:94:A:GLU:H	18	0.11
(1,1198)	1:143:A:VAL:HG21	1:125:A:PHE:HA	15	0.11
(1,1198)	1:143:A:VAL:HG22	1:125:A:PHE:HA	15	0.11
(1,1198)	1:143:A:VAL:HG23	1:125:A:PHE:HA	15	0.11
(1,1089)	1:125:A:PHE:HA	1:143:A:VAL:HG21	15	0.11
(1,1089)	1:125:A:PHE:HA	1:143:A:VAL:HG22	15	0.11
(1,1089)	1:125:A:PHE:HA	1:143:A:VAL:HG23	15	0.11
(1,1086)	1:125:A:PHE:HE1	1:123:A:LYS:HD2	4	0.11
(1,1086)	1:125:A:PHE:HE1	1:123:A:LYS:HD3	4	0.11
(1,1075)	1:123:A:LYS:HD2	1:125:A:PHE:HE1	4	0.11
(1,1075)	1:123:A:LYS:HD3	1:125:A:PHE:HE1	4	0.11
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD11	3	0.11
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD12	3	0.11
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD13	3	0.11
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD11	8	0.11
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD12	8	0.11
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD13	8	0.11
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD11	11	0.11
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD12	11	0.11
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD13	11	0.11
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD11	12	0.11
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD12	12	0.11
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD13	12	0.11
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD11	19	0.11
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD12	19	0.11
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD13	19	0.11
(1,619)	1:135:A:LEU:HD11	1:135:A:LEU:H	3	0.11
(1,619)	1:135:A:LEU:HD12	1:135:A:LEU:H	3	0.11
(1,619)	1:135:A:LEU:HD13	1:135:A:LEU:H	3	0.11
(1,619)	1:135:A:LEU:HD11	1:135:A:LEU:H	8	0.11
(1,619)	1:135:A:LEU:HD12	1:135:A:LEU:H	8	0.11
(1,619)	1:135:A:LEU:HD13	1:135:A:LEU:H	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,619)	1:135:A:LEU:HD11	1:135:A:LEU:H	11	0.11
(1,619)	1:135:A:LEU:HD12	1:135:A:LEU:H	11	0.11
(1,619)	1:135:A:LEU:HD13	1:135:A:LEU:H	11	0.11
(1,619)	1:135:A:LEU:HD11	1:135:A:LEU:H	12	0.11
(1,619)	1:135:A:LEU:HD12	1:135:A:LEU:H	12	0.11
(1,619)	1:135:A:LEU:HD13	1:135:A:LEU:H	12	0.11
(1,619)	1:135:A:LEU:HD11	1:135:A:LEU:H	19	0.11
(1,619)	1:135:A:LEU:HD12	1:135:A:LEU:H	19	0.11
(1,619)	1:135:A:LEU:HD13	1:135:A:LEU:H	19	0.11
(1,579)	1:132:A:THR:H	1:113:A:THR:HA	10	0.11
(1,579)	1:132:A:THR:H	1:113:A:THR:HA	11	0.11
(1,421)	1:116:A:SER:HA	1:104:A:ALA:H	5	0.11
(1,386)	1:113:A:THR:HA	1:132:A:THR:H	10	0.11
(1,386)	1:113:A:THR:HA	1:132:A:THR:H	11	0.11
(1,359)	1:107:A:GLY:HA2	1:113:A:THR:H	5	0.11
(1,359)	1:107:A:GLY:HA3	1:113:A:THR:H	5	0.11
(1,343)	1:104:A:ALA:H	1:116:A:SER:HA	5	0.11
(1,333)	1:104:A:ALA:H	1:103:A:THR:HA	20	0.11
(1,10)	1:85:A:ASN:H	1:83:A:TYR:H	9	0.11
(1,6)	1:84:A:LYS:H	1:82:A:ALA:H	7	0.11
(1,6)	1:84:A:LYS:H	1:82:A:ALA:H	10	0.11
(1,6)	1:84:A:LYS:H	1:82:A:ALA:H	11	0.11
(1,6)	1:84:A:LYS:H	1:82:A:ALA:H	12	0.11
(1,6)	1:84:A:LYS:H	1:82:A:ALA:H	13	0.11
(1,6)	1:84:A:LYS:H	1:82:A:ALA:H	20	0.11
(1,5)	1:83:A:TYR:H	1:85:A:ASN:H	9	0.11
(1,3)	1:83:A:TYR:H	1:82:A:ALA:H	1	0.11
(1,3)	1:83:A:TYR:H	1:82:A:ALA:H	9	0.11
(1,2)	1:82:A:ALA:H	1:84:A:LYS:H	7	0.11
(1,2)	1:82:A:ALA:H	1:84:A:LYS:H	10	0.11
(1,2)	1:82:A:ALA:H	1:84:A:LYS:H	11	0.11
(1,2)	1:82:A:ALA:H	1:84:A:LYS:H	12	0.11
(1,2)	1:82:A:ALA:H	1:84:A:LYS:H	13	0.11
(1,2)	1:82:A:ALA:H	1:84:A:LYS:H	20	0.11
(1,1)	1:82:A:ALA:H	1:83:A:TYR:H	1	0.11
(1,1)	1:82:A:ALA:H	1:83:A:TYR:H	9	0.11
(2,36)	1:125:A:PHE:O	1:118:A:VAL:N	8	0.1
(2,20)	1:102:A:ALA:O	1:117:A:THR:N	17	0.1
(2,15)	1:90:A:ILE:O	1:94:A:GLU:H	11	0.1
(2,15)	1:90:A:ILE:O	1:94:A:GLU:H	12	0.1
(1,993)	1:114:A:PHE:HD1	1:113:A:THR:HA	2	0.1
(1,993)	1:114:A:PHE:HD1	1:113:A:THR:HA	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,975)	1:113:A:THR:HA	1:114:A:PHE:HD1	2	0.1
(1,975)	1:113:A:THR:HA	1:114:A:PHE:HD1	10	0.1
(1,666)	1:139:A:SER:HB2	1:128:A:GLU:H	19	0.1
(1,666)	1:139:A:SER:HB3	1:128:A:GLU:H	19	0.1
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD11	6	0.1
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD12	6	0.1
(1,623)	1:135:A:LEU:H	1:135:A:LEU:HD13	6	0.1
(1,619)	1:135:A:LEU:HD11	1:135:A:LEU:H	6	0.1
(1,619)	1:135:A:LEU:HD12	1:135:A:LEU:H	6	0.1
(1,619)	1:135:A:LEU:HD13	1:135:A:LEU:H	6	0.1
(1,579)	1:132:A:THR:H	1:113:A:THR:HA	2	0.1
(1,386)	1:113:A:THR:HA	1:132:A:THR:H	2	0.1
(1,359)	1:107:A:GLY:HA2	1:113:A:THR:H	12	0.1
(1,359)	1:107:A:GLY:HA3	1:113:A:THR:H	12	0.1
(1,333)	1:104:A:ALA:H	1:103:A:THR:HA	17	0.1
(1,6)	1:84:A:LYS:H	1:82:A:ALA:H	4	0.1
(1,6)	1:84:A:LYS:H	1:82:A:ALA:H	5	0.1
(1,6)	1:84:A:LYS:H	1:82:A:ALA:H	6	0.1
(1,6)	1:84:A:LYS:H	1:82:A:ALA:H	8	0.1
(1,6)	1:84:A:LYS:H	1:82:A:ALA:H	14	0.1
(1,6)	1:84:A:LYS:H	1:82:A:ALA:H	15	0.1
(1,6)	1:84:A:LYS:H	1:82:A:ALA:H	16	0.1
(1,6)	1:84:A:LYS:H	1:82:A:ALA:H	17	0.1
(1,6)	1:84:A:LYS:H	1:82:A:ALA:H	19	0.1
(1,2)	1:82:A:ALA:H	1:84:A:LYS:H	4	0.1
(1,2)	1:82:A:ALA:H	1:84:A:LYS:H	5	0.1
(1,2)	1:82:A:ALA:H	1:84:A:LYS:H	6	0.1
(1,2)	1:82:A:ALA:H	1:84:A:LYS:H	8	0.1
(1,2)	1:82:A:ALA:H	1:84:A:LYS:H	14	0.1
(1,2)	1:82:A:ALA:H	1:84:A:LYS:H	15	0.1
(1,2)	1:82:A:ALA:H	1:84:A:LYS:H	16	0.1
(1,2)	1:82:A:ALA:H	1:84:A:LYS:H	17	0.1
(1,2)	1:82:A:ALA:H	1:84:A:LYS:H	19	0.1

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

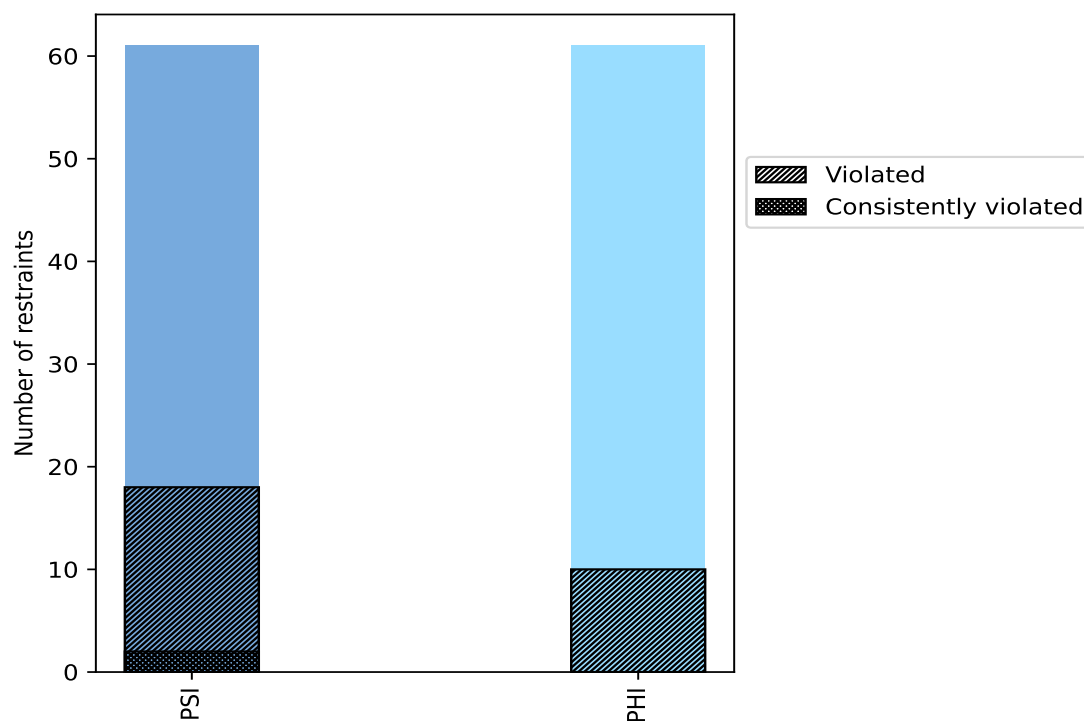
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	61	50.0	18	29.5	14.8	2	3.3	1.6
PHI	61	50.0	10	16.4	8.2	0	0.0	0.0
Total	122	100.0	28	23.0	23.0	2	1.6	1.6

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

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



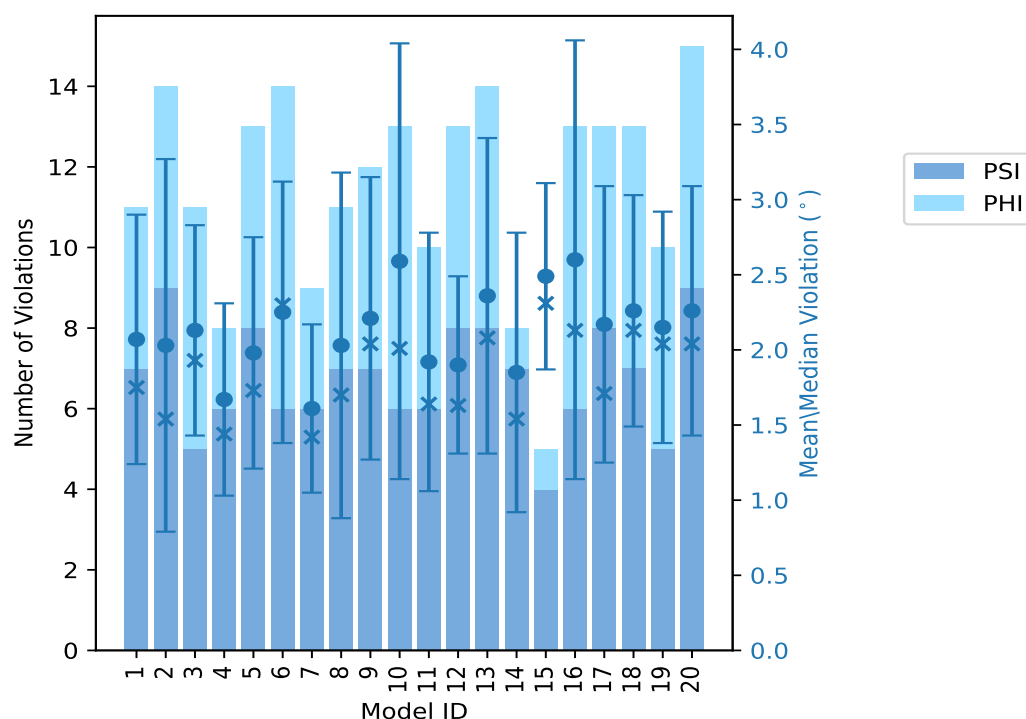
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	7	4	11	2.07	3.78	0.83	1.75
2	9	5	14	2.03	5.44	1.24	1.54
3	5	6	11	2.13	3.48	0.7	1.93
4	6	2	8	1.67	3.12	0.64	1.44
5	8	5	13	1.98	3.83	0.77	1.73
6	6	8	14	2.25	3.75	0.87	2.3
7	6	3	9	1.61	2.97	0.56	1.42
8	7	4	11	2.03	5.49	1.15	1.7
9	7	5	12	2.21	4.44	0.94	2.04
10	6	7	13	2.59	6.26	1.45	2.01
11	6	4	10	1.92	3.89	0.86	1.64
12	8	5	13	1.9	2.89	0.59	1.63
13	8	6	14	2.36	5.33	1.05	2.08
14	7	1	8	1.85	4.12	0.93	1.54
15	4	1	5	2.49	3.57	0.62	2.31
16	6	7	13	2.6	6.47	1.46	2.13
17	8	5	13	2.17	4.04	0.92	1.71
18	7	6	13	2.26	3.35	0.77	2.13
19	5	5	10	2.15	3.31	0.77	2.04
20	9	6	15	2.26	3.89	0.83	2.04

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

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

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
3	1	4	1	5.0
4	0	4	2	10.0
1	0	1	3	15.0
1	1	2	4	20.0
1	1	2	5	25.0
0	0	0	6	30.0
0	1	1	7	35.0
1	1	2	8	40.0
2	1	3	9	45.0
0	0	0	10	50.0
1	1	2	11	55.0

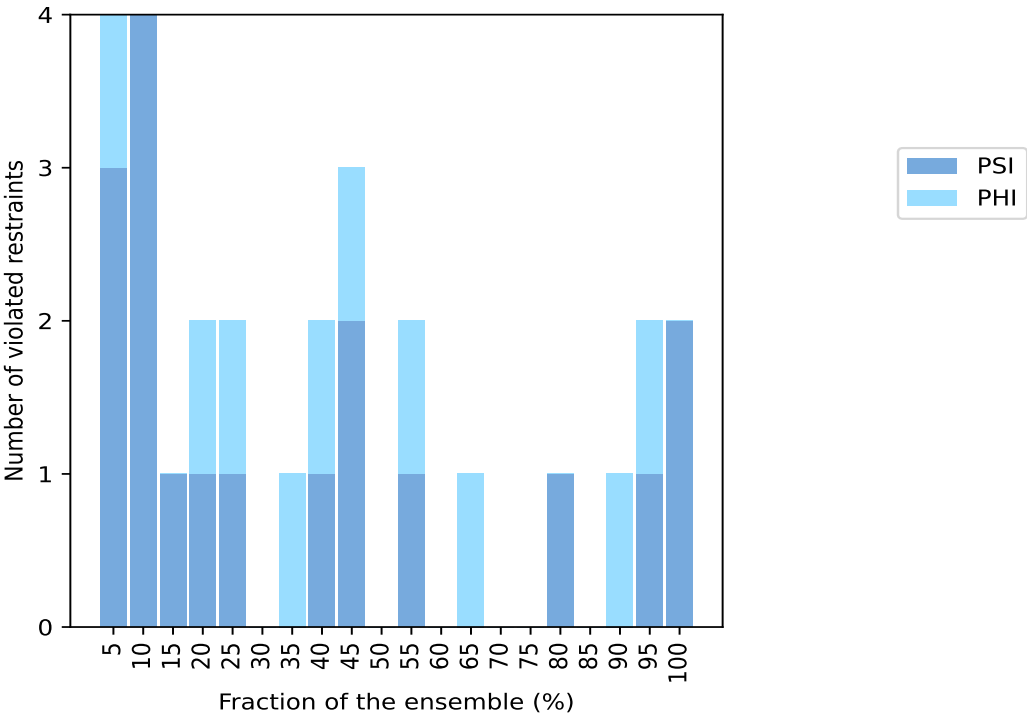
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	0	0	12	60.0
0	1	1	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
1	0	1	16	80.0
0	0	0	17	85.0
0	1	1	18	90.0
1	1	2	19	95.0
2	0	2	20	100.0

¹ Number of models with violations

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

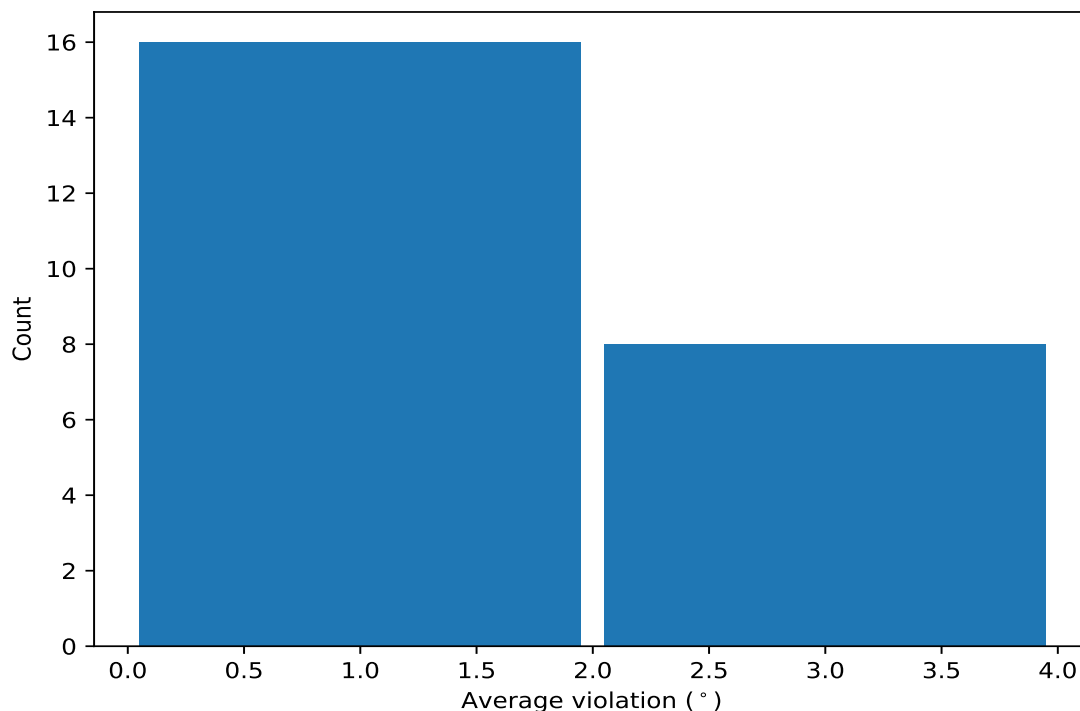


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints [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
(1,104)	1:131:A:LYS:N	1:131:A:LYS:CA	1:131:A:LYS:C	1:132:A:THR:N	20	3.77	1.35	3.6
(1,63)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:LYS:N	20	1.84	0.33	1.83
(1,87)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:PRO:N	19	3.27	0.71	3.41
(1,1)	1:81:A:VAL:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	19	1.68	0.34	1.67
(1,54)	1:141:A:ALA:C	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	18	2.2	0.58	2.28
(1,62)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:TYR:N	16	1.57	0.32	1.64
(1,2)	1:82:A:ALA:C	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	13	1.87	0.44	1.78
(1,42)	1:129:A:GLU:C	1:130:A:ALA:N	1:130:A:ALA:CA	1:130:A:ALA:C	11	2.63	1.14	2.45
(1,114)	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	1:142:A:LYS:N	11	1.81	0.47	1.71
(1,26)	1:110:A:HIS:C	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	9	2.03	0.83	1.73
(1,115)	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	1:143:A:VAL:N	9	1.57	0.53	1.3
(1,109)	1:136:A:ALA:N	1:136:A:ALA:CA	1:136:A:ALA:C	1:137:A:GLU:N	9	1.19	0.11	1.16
(1,79)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:THR:N	8	1.9	0.67	1.89
(1,14)	1:97:A:LEU:C	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	8	1.57	0.27	1.47
(1,45)	1:132:A:THR:C	1:133:A:LYS:N	1:133:A:LYS:CA	1:133:A:LYS:C	7	1.96	0.68	1.66
(1,91)	1:116:A:SER:N	1:116:A:SER:CA	1:116:A:SER:C	1:117:A:THR:N	5	1.95	0.76	2.04
(1,36)	1:122:A:GLY:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	5	1.19	0.24	1.08
(1,78)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:ALA:N	4	2.96	0.88	3.35
(1,16)	1:99:A:PRO:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	4	1.7	0.47	1.57
(1,76)	1:99:A:PRO:N	1:99:A:PRO:CA	1:99:A:PRO:C	1:100:A:PHE:N	3	1.84	0.32	1.77

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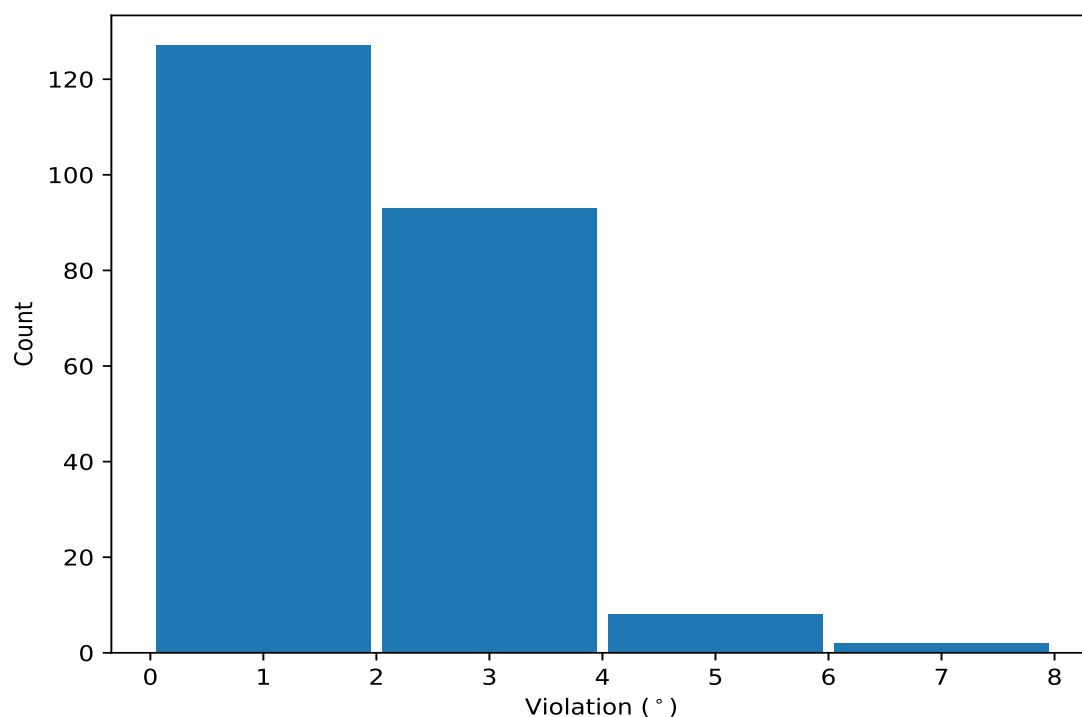
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,98)	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	1:125:A:PHE:N	2	2.76	0.04	2.76
(1,70)	1:90:A:ILE:N	1:90:A:ILE:CA	1:90:A:ILE:C	1:91:A:ALA:N	2	2.64	0.3	2.64
(1,105)	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	1:133:A:LYS:N	2	1.99	0.96	1.99
(1,86)	1:110:A:HIS:N	1:110:A:HIS:CA	1:110:A:HIS:C	1:111:A:ALA:N	2	1.14	0.04	1.14

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 (°)
(1,104)	1:131:A:LYS:N	1:131:A:LYS:CA	1:131:A:LYS:C	1:132:A:THR:N	16	6.47
(1,104)	1:131:A:LYS:N	1:131:A:LYS:CA	1:131:A:LYS:C	1:132:A:THR:N	10	6.26
(1,104)	1:131:A:LYS:N	1:131:A:LYS:CA	1:131:A:LYS:C	1:132:A:THR:N	8	5.49

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,104)	1:131:A:LYS:N	1:131:A:LYS:CA	1:131:A:LYS:C	1:132:A:THR:N	2	5.44
(1,104)	1:131:A:LYS:N	1:131:A:LYS:CA	1:131:A:LYS:C	1:132:A:THR:N	13	5.33
(1,42)	1:129:A:GLU:C	1:130:A:ALA:N	1:130:A:ALA:CA	1:130:A:ALA:C	10	4.98
(1,87)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:PRO:N	9	4.44
(1,104)	1:131:A:LYS:N	1:131:A:LYS:CA	1:131:A:LYS:C	1:132:A:THR:N	14	4.12
(1,87)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:PRO:N	2	4.08
(1,104)	1:131:A:LYS:N	1:131:A:LYS:CA	1:131:A:LYS:C	1:132:A:THR:N	17	4.04
(1,42)	1:129:A:GLU:C	1:130:A:ALA:N	1:130:A:ALA:CA	1:130:A:ALA:C	16	3.99
(1,87)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:PRO:N	11	3.89
(1,87)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:PRO:N	20	3.89
(1,87)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:PRO:N	5	3.83
(1,87)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:PRO:N	16	3.79
(1,104)	1:131:A:LYS:N	1:131:A:LYS:CA	1:131:A:LYS:C	1:132:A:THR:N	1	3.78
(1,42)	1:129:A:GLU:C	1:130:A:ALA:N	1:130:A:ALA:CA	1:130:A:ALA:C	6	3.75
(1,104)	1:131:A:LYS:N	1:131:A:LYS:CA	1:131:A:LYS:C	1:132:A:THR:N	9	3.69
(1,104)	1:131:A:LYS:N	1:131:A:LYS:CA	1:131:A:LYS:C	1:132:A:THR:N	20	3.68
(1,78)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:ALA:N	20	3.68
(1,87)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:PRO:N	10	3.62
(1,87)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:PRO:N	15	3.57
(1,104)	1:131:A:LYS:N	1:131:A:LYS:CA	1:131:A:LYS:C	1:132:A:THR:N	6	3.51
(1,87)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:PRO:N	3	3.48
(1,78)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:ALA:N	17	3.47
(1,87)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:PRO:N	13	3.41
(1,87)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:PRO:N	18	3.35
(1,87)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:PRO:N	19	3.31
(1,78)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:ALA:N	18	3.23
(1,104)	1:131:A:LYS:N	1:131:A:LYS:CA	1:131:A:LYS:C	1:132:A:THR:N	3	3.2
(1,45)	1:132:A:THR:C	1:133:A:LYS:N	1:133:A:LYS:CA	1:133:A:LYS:C	16	3.2
(1,104)	1:131:A:LYS:N	1:131:A:LYS:CA	1:131:A:LYS:C	1:132:A:THR:N	11	3.16
(1,79)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:THR:N	18	3.15
(1,87)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:PRO:N	4	3.12
(1,26)	1:110:A:HIS:C	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	19	3.11
(1,26)	1:110:A:HIS:C	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	6	3.08
(1,91)	1:116:A:SER:N	1:116:A:SER:CA	1:116:A:SER:C	1:117:A:THR:N	17	3.07
(1,54)	1:141:A:ALA:C	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	16	3.06
(1,26)	1:110:A:HIS:C	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	18	3.06
(1,2)	1:82:A:ALA:C	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1	2.98
(1,104)	1:131:A:LYS:N	1:131:A:LYS:CA	1:131:A:LYS:C	1:132:A:THR:N	7	2.97
(1,87)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:PRO:N	17	2.97
(1,105)	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	1:133:A:LYS:N	19	2.95
(1,70)	1:90:A:ILE:N	1:90:A:ILE:CA	1:90:A:ILE:C	1:91:A:ALA:N	1	2.93
(1,54)	1:141:A:ALA:C	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	13	2.93
(1,104)	1:131:A:LYS:N	1:131:A:LYS:CA	1:131:A:LYS:C	1:132:A:THR:N	18	2.92
(1,42)	1:129:A:GLU:C	1:130:A:ALA:N	1:130:A:ALA:CA	1:130:A:ALA:C	13	2.9
(1,54)	1:141:A:ALA:C	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	12	2.89
(1,54)	1:141:A:ALA:C	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	6	2.88
(1,87)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:PRO:N	6	2.82
(1,98)	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	1:125:A:PHE:N	5	2.8
(1,104)	1:131:A:LYS:N	1:131:A:LYS:CA	1:131:A:LYS:C	1:132:A:THR:N	12	2.77
(1,45)	1:132:A:THR:C	1:133:A:LYS:N	1:133:A:LYS:CA	1:133:A:LYS:C	13	2.77
(1,98)	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	1:125:A:PHE:N	15	2.71

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,54)	1:141:A:ALA:C	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	2	2.67
(1,114)	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	1:142:A:LYS:N	20	2.65
(1,87)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:PRO:N	1	2.64
(1,104)	1:131:A:LYS:N	1:131:A:LYS:CA	1:131:A:LYS:C	1:132:A:THR:N	19	2.61
(1,63)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:LYS:N	6	2.59
(1,107)	1:134:A:LYS:N	1:134:A:LYS:CA	1:134:A:LYS:C	1:135:A:LEU:N	12	2.57
(1,54)	1:141:A:ALA:C	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	5	2.57
(1,42)	1:129:A:GLU:C	1:130:A:ALA:N	1:130:A:ALA:CA	1:130:A:ALA:C	12	2.57
(1,54)	1:141:A:ALA:C	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	20	2.56
(1,54)	1:141:A:ALA:C	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	10	2.54
(1,114)	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	1:142:A:LYS:N	10	2.51
(1,115)	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	1:143:A:VAL:N	6	2.47
(1,104)	1:131:A:LYS:N	1:131:A:LYS:CA	1:131:A:LYS:C	1:132:A:THR:N	5	2.46
(1,16)	1:99:A:PRO:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	3	2.46
(1,42)	1:129:A:GLU:C	1:130:A:ALA:N	1:130:A:ALA:CA	1:130:A:ALA:C	17	2.45
(1,115)	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	1:143:A:VAL:N	16	2.42
(1,91)	1:116:A:SER:N	1:116:A:SER:CA	1:116:A:SER:C	1:117:A:THR:N	13	2.41
(1,63)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:LYS:N	2	2.38
(1,54)	1:141:A:ALA:C	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	3	2.37
(1,42)	1:129:A:GLU:C	1:130:A:ALA:N	1:130:A:ALA:CA	1:130:A:ALA:C	8	2.36
(1,26)	1:110:A:HIS:C	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	9	2.36
(1,70)	1:90:A:ILE:N	1:90:A:ILE:CA	1:90:A:ILE:C	1:91:A:ALA:N	3	2.34
(1,2)	1:82:A:ALA:C	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	9	2.34
(1,79)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:THR:N	9	2.33
(1,104)	1:131:A:LYS:N	1:131:A:LYS:CA	1:131:A:LYS:C	1:132:A:THR:N	15	2.31
(1,79)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:THR:N	5	2.31
(1,1)	1:81:A:VAL:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	18	2.31
(1,76)	1:99:A:PRO:N	1:99:A:PRO:CA	1:99:A:PRO:C	1:100:A:PHE:N	12	2.26
(1,2)	1:82:A:ALA:C	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	10	2.26
(1,54)	1:141:A:ALA:C	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	19	2.18
(1,114)	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	1:142:A:LYS:N	4	2.15
(1,114)	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	1:142:A:LYS:N	18	2.13
(1,63)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:LYS:N	5	2.13
(1,1)	1:81:A:VAL:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	16	2.13
(1,62)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:TYR:N	6	2.12
(1,63)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:LYS:N	8	2.11
(1,63)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:LYS:N	13	2.09
(1,14)	1:97:A:LEU:C	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	9	2.09
(1,1)	1:81:A:VAL:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	15	2.08
(1,99)	1:125:A:PHE:N	1:125:A:PHE:CA	1:125:A:PHE:C	1:126:A:SER:N	14	2.06
(1,1)	1:81:A:VAL:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	13	2.06
(1,63)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:LYS:N	20	2.05
(1,54)	1:141:A:ALA:C	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	17	2.05
(1,91)	1:116:A:SER:N	1:116:A:SER:CA	1:116:A:SER:C	1:117:A:THR:N	20	2.04
(1,1)	1:81:A:VAL:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	20	2.04
(1,87)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:PRO:N	8	2.03
(1,79)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:THR:N	2	2.03
(1,63)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:LYS:N	10	2.01
(1,87)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:PRO:N	14	2.0
(1,63)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:LYS:N	9	1.99
(1,42)	1:129:A:GLU:C	1:130:A:ALA:N	1:130:A:ALA:CA	1:130:A:ALA:C	20	1.96

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1)	1:81:A:VAL:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	7	1.96
(1,14)	1:97:A:LEU:C	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	10	1.94
(1,115)	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	1:143:A:VAL:N	13	1.93
(1,2)	1:82:A:ALA:C	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	3	1.93
(1,114)	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	1:142:A:LYS:N	11	1.91
(1,2)	1:82:A:ALA:C	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	11	1.9
(1,63)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:LYS:N	19	1.89
(1,54)	1:141:A:ALA:C	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	1	1.88
(1,87)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:PRO:N	7	1.87
(1,62)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:TYR:N	9	1.87
(1,62)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:TYR:N	18	1.85
(1,62)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:TYR:N	20	1.85
(1,63)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:LYS:N	16	1.84
(1,2)	1:82:A:ALA:C	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	6	1.84
(1,63)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:LYS:N	18	1.82
(1,1)	1:81:A:VAL:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	19	1.82
(1,62)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:TYR:N	10	1.81
(1,46)	1:133:A:LYS:C	1:134:A:LYS:N	1:134:A:LYS:CA	1:134:A:LYS:C	12	1.81
(1,1)	1:81:A:VAL:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	8	1.8
(1,63)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:LYS:N	3	1.79
(1,63)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:LYS:N	15	1.79
(1,2)	1:82:A:ALA:C	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	16	1.78
(1,76)	1:99:A:PRO:N	1:99:A:PRO:CA	1:99:A:PRO:C	1:100:A:PHE:N	9	1.77
(1,2)	1:82:A:ALA:C	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	20	1.76
(1,79)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:THR:N	1	1.75
(1,62)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:TYR:N	11	1.75
(1,54)	1:141:A:ALA:C	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	4	1.75
(1,26)	1:110:A:HIS:C	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	5	1.73
(1,114)	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	1:142:A:LYS:N	13	1.71
(1,2)	1:82:A:ALA:C	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	17	1.71
(1,62)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:TYR:N	13	1.7
(1,54)	1:141:A:ALA:C	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	8	1.7
(1,45)	1:132:A:THR:C	1:133:A:LYS:N	1:133:A:LYS:CA	1:133:A:LYS:C	3	1.7
(1,2)	1:82:A:ALA:C	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	18	1.69
(1,1)	1:81:A:VAL:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	2	1.67
(1,1)	1:81:A:VAL:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	17	1.67
(1,45)	1:132:A:THR:C	1:133:A:LYS:N	1:133:A:LYS:CA	1:133:A:LYS:C	8	1.66
(1,45)	1:132:A:THR:C	1:133:A:LYS:N	1:133:A:LYS:CA	1:133:A:LYS:C	10	1.66
(1,36)	1:122:A:GLY:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	20	1.66
(1,1)	1:81:A:VAL:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	14	1.66
(1,62)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:TYR:N	17	1.65
(1,62)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:TYR:N	12	1.63
(1,16)	1:99:A:PRO:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	6	1.61
(1,62)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:TYR:N	2	1.6
(1,1)	1:81:A:VAL:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	3	1.6
(1,63)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:LYS:N	17	1.58
(1,42)	1:129:A:GLU:C	1:130:A:ALA:N	1:130:A:ALA:CA	1:130:A:ALA:C	18	1.57
(1,62)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:TYR:N	5	1.56
(1,54)	1:141:A:ALA:C	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	7	1.56
(1,79)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:THR:N	20	1.54
(1,63)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:LYS:N	4	1.53

Continued on next page...

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,45)	1:132:A:THR:C	1:133:A:LYS:N	1:133:A:LYS:CA	1:133:A:LYS:C	20	1.53
(1,16)	1:99:A:PRO:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	16	1.53
(1,14)	1:97:A:LEU:C	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	6	1.53
(1,63)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:LYS:N	11	1.52
(1,63)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:LYS:N	1	1.51
(1,63)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:LYS:N	12	1.5
(1,1)	1:81:A:VAL:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1	1.5
(1,76)	1:99:A:PRO:N	1:99:A:PRO:CA	1:99:A:PRO:C	1:100:A:PHE:N	2	1.49
(1,14)	1:97:A:LEU:C	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	3	1.49
(1,54)	1:141:A:ALA:C	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	11	1.48
(1,115)	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	1:143:A:VAL:N	10	1.47
(1,78)	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	1:102:A:ALA:N	8	1.47
(1,114)	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	1:142:A:LYS:N	17	1.46
(1,14)	1:97:A:LEU:C	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	16	1.45
(1,63)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:LYS:N	14	1.42
(1,42)	1:129:A:GLU:C	1:130:A:ALA:N	1:130:A:ALA:CA	1:130:A:ALA:C	7	1.42
(1,114)	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	1:142:A:LYS:N	12	1.41
(1,62)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:TYR:N	1	1.4
(1,14)	1:97:A:LEU:C	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	5	1.39
(1,114)	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	1:142:A:LYS:N	8	1.38
(1,2)	1:82:A:ALA:C	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	12	1.38
(1,2)	1:82:A:ALA:C	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	13	1.38
(1,1)	1:81:A:VAL:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	5	1.37
(1,1)	1:81:A:VAL:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	10	1.37
(1,114)	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	1:142:A:LYS:N	14	1.36
(1,26)	1:110:A:HIS:C	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1	1.36
(1,14)	1:97:A:LEU:C	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	2	1.36
(1,1)	1:81:A:VAL:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	12	1.36
(1,109)	1:136:A:ALA:N	1:136:A:ALA:CA	1:136:A:ALA:C	1:137:A:GLU:N	4	1.35
(1,109)	1:136:A:ALA:N	1:136:A:ALA:CA	1:136:A:ALA:C	1:137:A:GLU:N	11	1.34
(1,26)	1:110:A:HIS:C	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	13	1.32
(1,2)	1:82:A:ALA:C	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	5	1.32
(1,14)	1:97:A:LEU:C	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	19	1.31
(1,115)	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	1:143:A:VAL:N	12	1.3
(1,63)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:LYS:N	7	1.3
(1,109)	1:136:A:ALA:N	1:136:A:ALA:CA	1:136:A:ALA:C	1:137:A:GLU:N	12	1.29
(1,54)	1:141:A:ALA:C	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	18	1.29
(1,115)	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	1:143:A:VAL:N	8	1.26
(1,62)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:TYR:N	19	1.26
(1,54)	1:141:A:ALA:C	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	9	1.25
(1,114)	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	1:142:A:LYS:N	7	1.22
(1,104)	1:131:A:LYS:N	1:131:A:LYS:CA	1:131:A:LYS:C	1:132:A:THR:N	4	1.22
(1,91)	1:116:A:SER:N	1:116:A:SER:CA	1:116:A:SER:C	1:117:A:THR:N	7	1.21
(1,109)	1:136:A:ALA:N	1:136:A:ALA:CA	1:136:A:ALA:C	1:137:A:GLU:N	9	1.2
(1,1)	1:81:A:VAL:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	4	1.2
(1,86)	1:110:A:HIS:N	1:110:A:HIS:CA	1:110:A:HIS:C	1:111:A:ALA:N	2	1.19
(1,26)	1:110:A:HIS:C	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	10	1.19
(1,1)	1:81:A:VAL:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	6	1.19
(1,45)	1:132:A:THR:C	1:133:A:LYS:N	1:133:A:LYS:CA	1:133:A:LYS:C	2	1.18
(1,16)	1:99:A:PRO:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	9	1.18
(1,115)	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	1:143:A:VAL:N	5	1.17

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Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,109)	1:136:A:ALA:N	1:136:A:ALA:CA	1:136:A:ALA:C	1:137:A:GLU:N	13	1.16
(1,69)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:ILE:N	2	1.14
(1,36)	1:122:A:GLY:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	11	1.14
(1,1)	1:81:A:VAL:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	11	1.14
(1,115)	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	1:143:A:VAL:N	2	1.11
(1,109)	1:136:A:ALA:N	1:136:A:ALA:CA	1:136:A:ALA:C	1:137:A:GLU:N	14	1.11
(1,86)	1:110:A:HIS:N	1:110:A:HIS:CA	1:110:A:HIS:C	1:111:A:ALA:N	5	1.1
(1,109)	1:136:A:ALA:N	1:136:A:ALA:CA	1:136:A:ALA:C	1:137:A:GLU:N	16	1.09
(1,109)	1:136:A:ALA:N	1:136:A:ALA:CA	1:136:A:ALA:C	1:137:A:GLU:N	1	1.08
(1,109)	1:136:A:ALA:N	1:136:A:ALA:CA	1:136:A:ALA:C	1:137:A:GLU:N	20	1.08
(1,36)	1:122:A:GLY:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	6	1.08
(1,36)	1:122:A:GLY:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	19	1.08
(1,79)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:THR:N	8	1.06
(1,115)	1:142:A:LYS:N	1:142:A:LYS:CA	1:142:A:LYS:C	1:143:A:VAL:N	3	1.04
(1,62)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:TYR:N	4	1.04
(1,26)	1:110:A:HIS:C	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	17	1.04
(1,105)	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	1:133:A:LYS:N	6	1.03
(1,91)	1:116:A:SER:N	1:116:A:SER:CA	1:116:A:SER:C	1:117:A:THR:N	14	1.03
(1,79)	1:102:A:ALA:N	1:102:A:ALA:CA	1:102:A:ALA:C	1:103:A:THR:N	17	1.03
(1,62)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:TYR:N	16	1.03
(1,42)	1:129:A:GLU:C	1:130:A:ALA:N	1:130:A:ALA:CA	1:130:A:ALA:C	2	1.03
(1,62)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:TYR:N	7	1.01
(1,36)	1:122:A:GLY:C	1:123:A:LYS:N	1:123:A:LYS:CA	1:123:A:LYS:C	18	1.01