



Full wwPDB NMR Structure Validation Report ⓘ

Jun 3, 2023 – 09:56 AM EDT

PDB ID : 1IYM
BMRB ID : 5459
Title : RING-H2 finger domain of EL5
Authors : Katoh, E.; Katoh, S.; Minami, E.; Yamazaki, T.
Deposited on : 2002-08-30

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
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) : 2.33

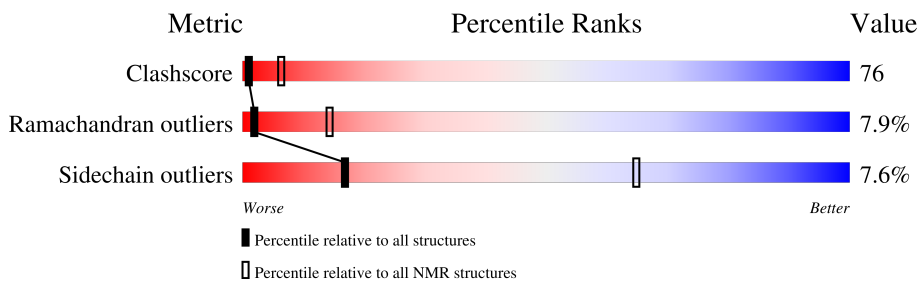
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 92%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	55	

2 Ensemble composition and analysis

This entry contains 15 models. Model 1 is the overall representative, medoid model (most similar to other models). The authors have identified model 15 as representative.

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:133-A:177 (45)	0.32	1

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

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

The models can be grouped into 2 clusters and 4 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 795 atoms, of which 380 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called EL5.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	55	793	254	380	71	80	8	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	ALA	-	cloning artifact	UNP Q9LRB7
A	128	MET	-	cloning artifact	UNP Q9LRB7

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

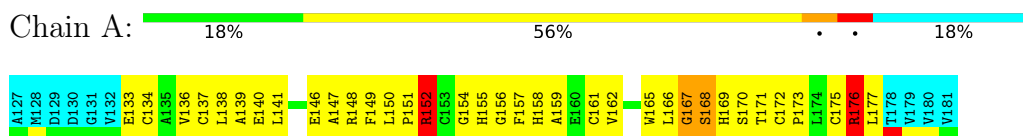
Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	2	2	2

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: EL5

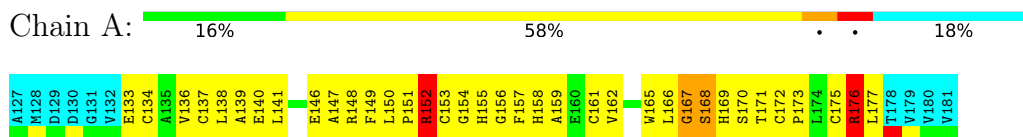


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

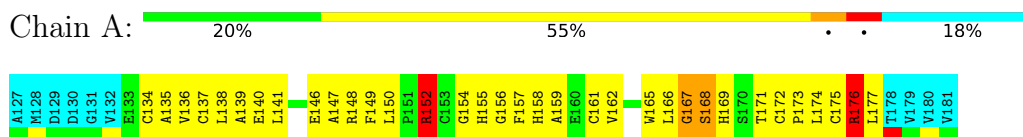
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: EL5



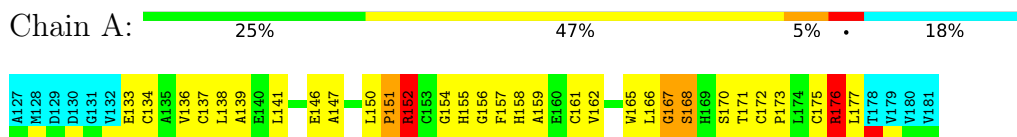
4.2.2 Score per residue for model 2

- Molecule 1: EL5



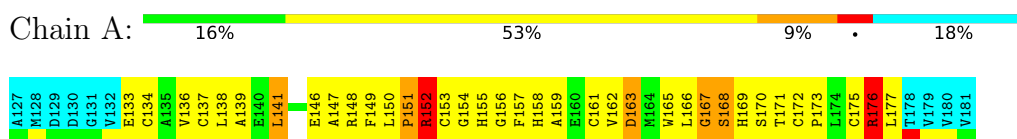
4.2.3 Score per residue for model 3

- Molecule 1: EL5



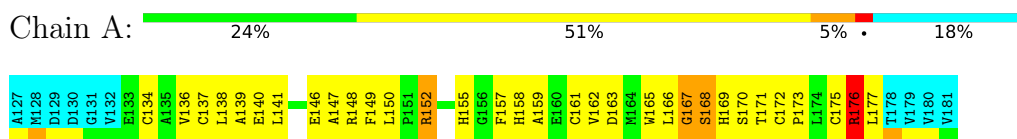
4.2.4 Score per residue for model 4

- Molecule 1: EL5



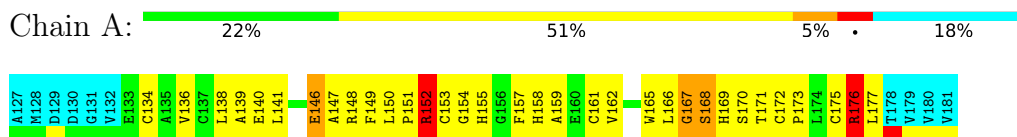
4.2.5 Score per residue for model 5

- Molecule 1: EL5



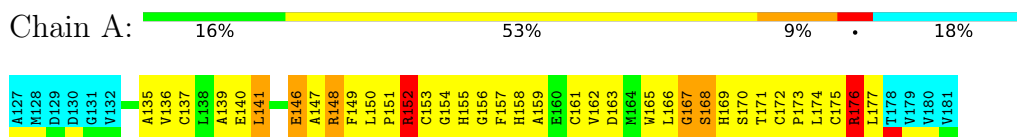
4.2.6 Score per residue for model 6

- Molecule 1: EL5



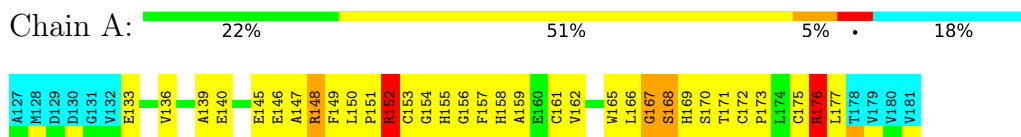
4.2.7 Score per residue for model 7

- Molecule 1: EL5



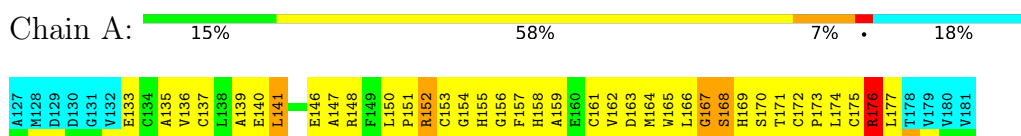
4.2.8 Score per residue for model 8

- Molecule 1: EL5



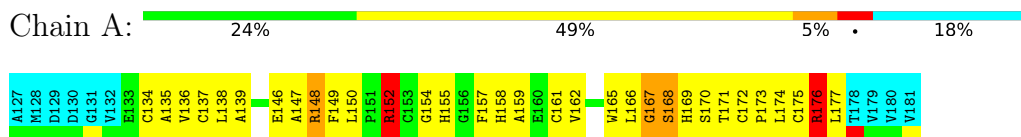
4.2.9 Score per residue for model 9

- Molecule 1: EL5



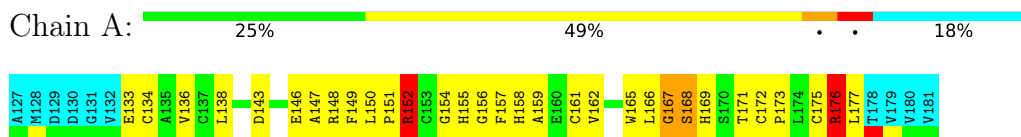
4.2.10 Score per residue for model 10

- Molecule 1: EL5



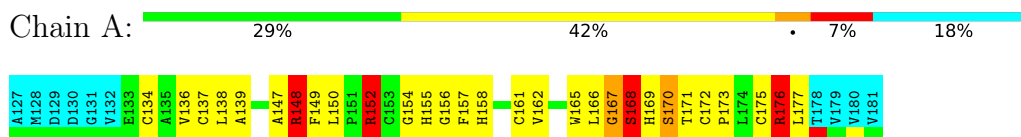
4.2.11 Score per residue for model 11

- Molecule 1: EL5



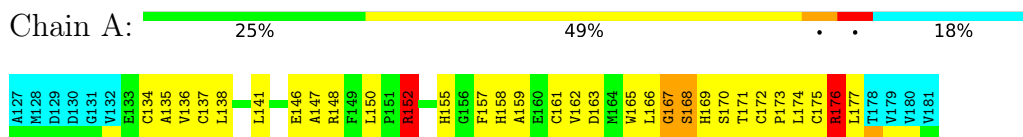
4.2.12 Score per residue for model 12

- Molecule 1: EL5



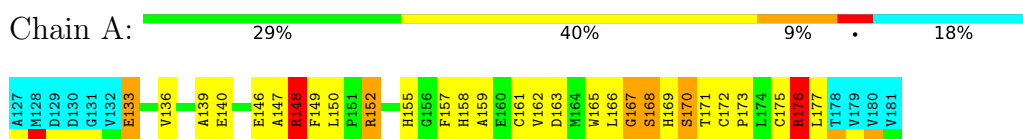
4.2.13 Score per residue for model 13

- Molecule 1: EL5



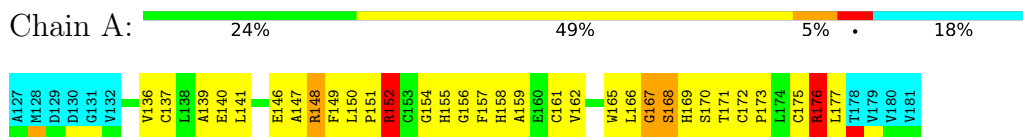
4.2.14 Score per residue for model 14

- Molecule 1: EL5



4.2.15 Score per residue for model 15

- Molecule 1: EL5



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 15 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	refinement	3.1

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	633
Number of shifts mapped to atoms	628
Number of unparsed shifts	0
Number of shifts with mapping errors	5
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.9±0.3
All	All	0	43

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	176	ARG	Sidechain	15
1	A	148	ARG	Sidechain	14
1	A	152	ARG	Sidechain	14

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	344	310	312	50±3
All	All	5190	4650	4680	750

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 76.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:134:CYS:O	1:A:138:LEU:HD23	0.96	1.61	1	8
1:A:166:LEU:HD23	1:A:169:HIS:O	0.87	1.70	13	9
1:A:146:GLU:O	1:A:159:ALA:HB2	0.85	1.71	7	14
1:A:150:LEU:HD12	1:A:172:CYS:HB2	0.80	1.53	1	11
1:A:141:LEU:HD23	1:A:158:HIS:NE2	0.77	1.94	2	4
1:A:141:LEU:HD22	1:A:147:ALA:HB2	0.75	1.59	13	3
1:A:150:LEU:HD12	1:A:172:CYS:SG	0.71	2.26	3	4
1:A:167:GLY:O	1:A:168:SER:CB	0.68	2.41	3	15
1:A:175:CYS:SG	1:A:177:LEU:HD12	0.67	2.29	2	15
1:A:166:LEU:O	1:A:168:SER:N	0.66	2.28	4	10
1:A:141:LEU:CD2	1:A:147:ALA:HB2	0.65	2.21	13	1
1:A:163:ASP:HA	1:A:166:LEU:HD12	0.64	1.68	13	6
1:A:165:TRP:CD1	1:A:173:PRO:HB3	0.63	2.29	15	15
1:A:152:ARG:CD	1:A:177:LEU:HB3	0.61	2.25	9	12
1:A:147:ALA:HB1	1:A:157:PHE:O	0.61	1.95	5	11
1:A:150:LEU:HD12	1:A:172:CYS:CB	0.60	2.25	1	12
1:A:175:CYS:O	1:A:176:ARG:CB	0.60	2.50	13	15
1:A:135:ALA:HB2	1:A:174:LEU:HD13	0.59	1.73	9	5
1:A:135:ALA:CB	1:A:174:LEU:HD13	0.58	2.28	13	1
1:A:155:HIS:HB3	1:A:157:PHE:CE1	0.57	2.34	3	8
1:A:155:HIS:HB3	1:A:157:PHE:CE2	0.56	2.35	13	6
1:A:166:LEU:O	1:A:167:GLY:C	0.56	2.44	12	15
1:A:145:GLU:OE1	1:A:158:HIS:CD2	0.56	2.59	8	1
1:A:152:ARG:CB	1:A:177:LEU:HB3	0.56	2.31	1	12
1:A:175:CYS:O	1:A:176:ARG:HB2	0.56	2.00	4	15
1:A:155:HIS:HB3	1:A:157:PHE:CZ	0.55	2.36	8	14
1:A:166:LEU:O	1:A:169:HIS:N	0.55	2.39	6	5
1:A:147:ALA:CB	1:A:157:PHE:O	0.55	2.55	2	11
1:A:165:TRP:CE2	1:A:173:PRO:HB3	0.55	2.37	6	15
1:A:158:HIS:O	1:A:162:VAL:CG1	0.55	2.55	6	15
1:A:146:GLU:O	1:A:159:ALA:CB	0.54	2.56	9	11
1:A:175:CYS:SG	1:A:177:LEU:CD1	0.54	2.96	13	15
1:A:152:ARG:CD	1:A:177:LEU:O	0.54	2.55	5	3
1:A:158:HIS:O	1:A:162:VAL:HG12	0.54	2.03	9	15
1:A:150:LEU:CD1	1:A:172:CYS:SG	0.53	2.97	4	3
1:A:147:ALA:CA	1:A:157:PHE:O	0.52	2.58	13	11
1:A:157:PHE:CE1	1:A:173:PRO:HG2	0.51	2.40	13	6
1:A:137:CYS:SG	1:A:139:ALA:HB3	0.51	2.46	9	6
1:A:150:LEU:CD1	1:A:172:CYS:CB	0.51	2.88	9	4
1:A:148:ARG:HD2	1:A:162:VAL:HG11	0.51	1.82	15	1
1:A:157:PHE:CD2	1:A:173:PRO:HG2	0.51	2.41	14	5
1:A:137:CYS:SG	1:A:139:ALA:CB	0.50	3.00	4	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:157:PHE:CD1	1:A:173:PRO:HG2	0.50	2.41	5	4
1:A:157:PHE:CE2	1:A:173:PRO:HG2	0.50	2.42	7	9
1:A:150:LEU:CD1	1:A:172:CYS:HB2	0.50	2.36	5	9
1:A:149:PHE:CD1	1:A:149:PHE:N	0.50	2.80	10	8
1:A:165:TRP:CG	1:A:173:PRO:HB3	0.50	2.41	4	15
1:A:141:LEU:HD23	1:A:158:HIS:CE1	0.49	2.41	2	1
1:A:165:TRP:CD2	1:A:173:PRO:HB3	0.49	2.42	12	15
1:A:152:ARG:HD3	1:A:177:LEU:O	0.49	2.07	5	3
1:A:150:LEU:HD23	1:A:150:LEU:N	0.49	2.22	10	2
1:A:166:LEU:CD2	1:A:169:HIS:O	0.49	2.58	10	4
1:A:165:TRP:NE1	1:A:173:PRO:HB3	0.49	2.23	15	15
1:A:149:PHE:CD2	1:A:156:GLY:HA3	0.49	2.43	2	2
1:A:158:HIS:O	1:A:162:VAL:HB	0.49	2.08	14	15
1:A:175:CYS:SG	1:A:176:ARG:N	0.49	2.86	2	15
1:A:137:CYS:O	1:A:138:LEU:CB	0.49	2.60	13	2
1:A:152:ARG:HD3	1:A:177:LEU:HD22	0.49	1.85	9	1
1:A:149:PHE:CE2	1:A:156:GLY:HA3	0.48	2.43	7	4
1:A:155:HIS:CB	1:A:157:PHE:CE2	0.48	2.96	4	6
1:A:155:HIS:CB	1:A:157:PHE:CE1	0.48	2.96	7	6
1:A:157:PHE:CE1	1:A:173:PRO:HD2	0.48	2.43	8	2
1:A:152:ARG:HD3	1:A:177:LEU:CB	0.48	2.39	14	3
1:A:152:ARG:HD3	1:A:177:LEU:HB3	0.47	1.85	14	11
1:A:167:GLY:O	1:A:168:SER:OG	0.47	2.33	4	7
1:A:175:CYS:SG	1:A:177:LEU:CG	0.47	3.03	3	12
1:A:149:PHE:C	1:A:150:LEU:HD23	0.47	2.30	10	2
1:A:147:ALA:HA	1:A:157:PHE:O	0.47	2.10	1	11
1:A:136:VAL:HB	1:A:161:CYS:HB3	0.46	1.87	2	15
1:A:149:PHE:CD1	1:A:156:GLY:HA3	0.46	2.45	8	2
1:A:158:HIS:O	1:A:162:VAL:CB	0.46	2.64	2	15
1:A:136:VAL:CG1	1:A:161:CYS:HB3	0.46	2.41	13	15
1:A:149:PHE:CE1	1:A:156:GLY:HA3	0.46	2.45	4	2
1:A:136:VAL:CB	1:A:161:CYS:HB3	0.46	2.41	13	15
1:A:167:GLY:O	1:A:168:SER:HB3	0.44	2.12	3	4
1:A:159:ALA:O	1:A:163:ASP:OD2	0.44	2.35	7	1
1:A:154:GLY:O	1:A:155:HIS:C	0.44	2.55	10	3
1:A:152:ARG:HB2	1:A:177:LEU:HB3	0.44	1.89	12	5
1:A:153:CYS:HB3	1:A:177:LEU:CD1	0.44	2.42	9	6
1:A:146:GLU:O	1:A:159:ALA:N	0.44	2.49	8	3
1:A:175:CYS:SG	1:A:177:LEU:HG	0.44	2.53	11	13
1:A:167:GLY:O	1:A:168:SER:HB2	0.44	2.12	5	5
1:A:166:LEU:C	1:A:168:SER:N	0.44	2.71	13	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:162:VAL:CG1	1:A:163:ASP:N	0.43	2.80	9	1
1:A:166:LEU:HD22	1:A:170:SER:HA	0.43	1.90	10	2
1:A:137:CYS:O	1:A:138:LEU:HB2	0.43	2.12	13	2
1:A:141:LEU:HD11	1:A:156:GLY:O	0.43	2.14	3	1
1:A:165:TRP:NE1	1:A:173:PRO:HA	0.43	2.28	4	15
1:A:150:LEU:O	1:A:154:GLY:HA2	0.42	2.14	4	10
1:A:172:CYS:O	1:A:176:ARG:HA	0.42	2.14	11	8
1:A:175:CYS:O	1:A:176:ARG:HG3	0.42	2.15	5	8
1:A:147:ALA:O	1:A:148:ARG:HG2	0.42	2.14	8	4
1:A:146:GLU:N	1:A:146:GLU:CD	0.42	2.73	15	1
1:A:149:PHE:CD2	1:A:156:GLY:CA	0.42	3.03	2	1
1:A:152:ARG:HD2	1:A:177:LEU:C	0.42	2.34	11	8
1:A:152:ARG:NH1	1:A:152:ARG:HG2	0.42	2.29	15	1
1:A:139:ALA:O	1:A:140:GLU:C	0.42	2.58	14	8
1:A:166:LEU:CD2	1:A:170:SER:HA	0.42	2.45	8	3
1:A:165:TRP:CE2	1:A:173:PRO:CB	0.41	3.04	4	5
1:A:150:LEU:N	1:A:150:LEU:HD23	0.41	2.30	8	1
1:A:152:ARG:HD2	1:A:177:LEU:O	0.41	2.16	13	2
1:A:165:TRP:O	1:A:166:LEU:C	0.41	2.59	11	1
1:A:136:VAL:HG22	1:A:165:TRP:CE3	0.40	2.51	7	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	45/55 (82%)	36±1 (79±3%)	6±1 (13±2%)	4±1 (8±1%)	2	14
All	All	675/825 (82%)	533 (79%)	89 (13%)	53 (8%)	2	14

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	167	GLY	15
1	A	168	SER	15

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Mol	Chain	Res	Type	Models (Total)
1	A	176	ARG	15
1	A	141	LEU	6
1	A	151	PRO	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	37/45 (82%)	34±1 (92±3%)	3±1 (8±3%)	17 65
All	All	555/675 (82%)	513 (92%)	42 (8%)	17 65

All 11 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	152	ARG	13
1	A	170	SER	11
1	A	133	GLU	6
1	A	148	ARG	3
1	A	134	CYS	2
1	A	146	GLU	2
1	A	140	GLU	1
1	A	163	ASP	1
1	A	164	MET	1
1	A	143	ASP	1
1	A	168	SER	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 monosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 92% 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 [i](#)

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	633
Number of shifts mapped to atoms	628
Number of unparsed shifts	0
Number of shifts with mapping errors	5
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 5 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	155	HIS	HD1	7.38	.	1
1	A	155	HIS	HE2	7.97	.	1
1	A	158	HIS	HD1	7.39	.	1
1	A	158	HIS	HE2	7.43	.	1
1	A	169	HIS	HE2	7.74	.	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	55	-1.19 ± 0.25	Should be checked
$^{13}\text{C}_\beta$	49	0.38 ± 0.25	None needed (< 0.5 ppm)
$^{13}\text{C}'$	55	-0.57 ± 0.17	Should be applied

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Nucleus	# values	Correction \pm precision, ppm	Suggested action
^{15}N	50	0.95 \pm 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 92%, i.e. 523 atoms were assigned a chemical shift out of a possible 570. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	223/225 (99%)	91/92 (99%)	90/90 (100%)	42/43 (98%)
Sidechain	262/294 (89%)	174/192 (91%)	88/93 (95%)	0/9 (0%)
Aromatic	38/51 (75%)	22/28 (79%)	15/21 (71%)	1/2 (50%)
Overall	523/570 (92%)	287/312 (92%)	193/204 (95%)	43/54 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 92%, i.e. 632 atoms were assigned a chemical shift out of a possible 689. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	270/276 (98%)	110/113 (97%)	110/110 (100%)	50/53 (94%)
Sidechain	324/362 (90%)	217/238 (91%)	107/115 (93%)	0/9 (0%)
Aromatic	38/51 (75%)	22/28 (79%)	15/21 (71%)	1/2 (50%)
Overall	632/689 (92%)	349/379 (92%)	232/246 (94%)	51/64 (80%)

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.

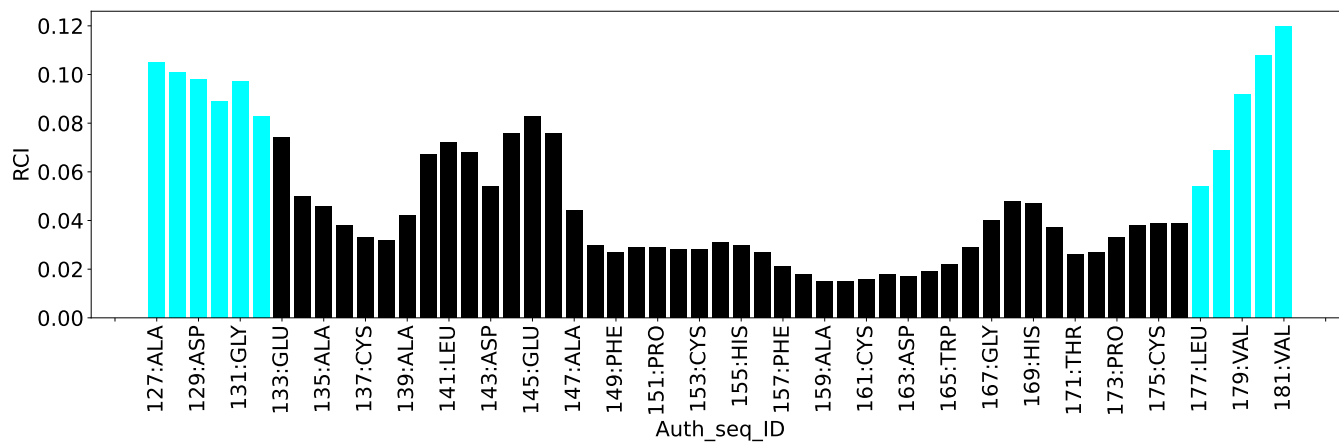
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	173	PRO	HG3	0.20	0.33 – 3.48	-5.4

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	773
Intra-residue ($ i-j =0$)	290
Sequential ($ i-j =1$)	185
Medium range ($ i-j >1$ and $ i-j <5$)	73
Long range ($ i-j \geq 5$)	207
Inter-chain	0
Hydrogen bond restraints	18
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	14.1
Number of long range restraints per residue ¹	3.9

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)	11.0	0.2
0.2-0.5 (Medium)	5.6	0.49
>0.5 (Large)	9.9	4.17

8.2.2 Average number of dihedral-angle violations per model

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

9 Distance violation analysis [i](#)

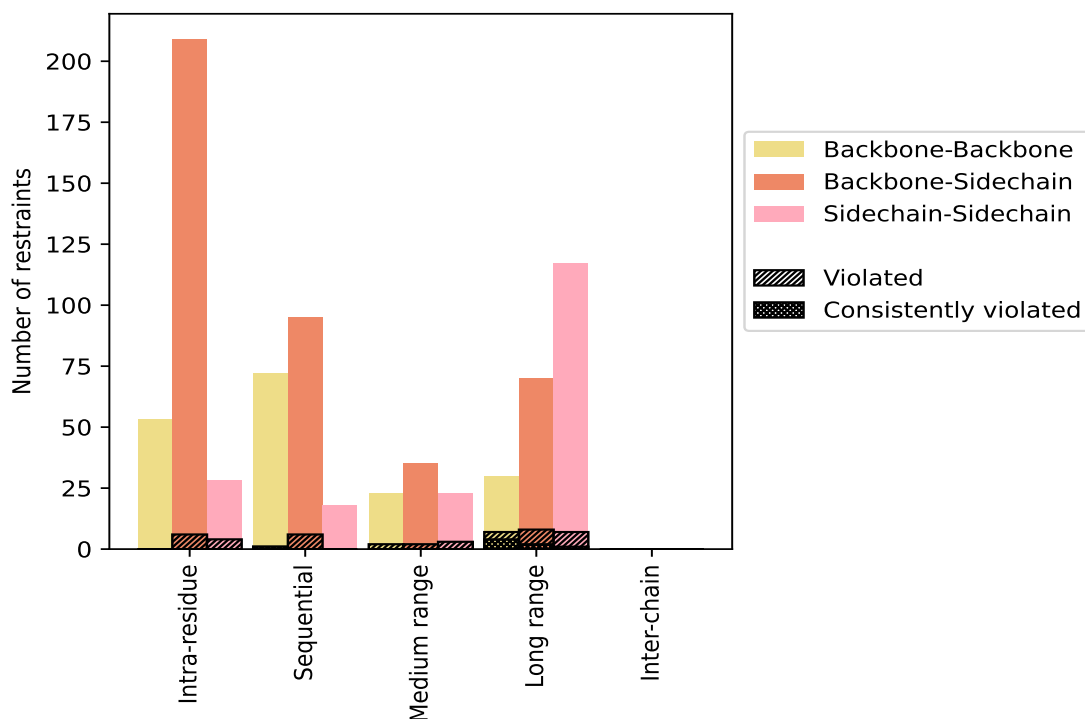
9.1 Summary of distance violations [i](#)

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 ($i-j =0$)	290	37.5	10	3.4	1.3	0	0.0	0.0
Backbone-Backbone	53	6.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	209	27.0	6	2.9	0.8	0	0.0	0.0
Sidechain-Sidechain	28	3.6	4	14.3	0.5	0	0.0	0.0
Sequential ($i-j =1$)	185	23.9	7	3.8	0.9	1	0.5	0.1
Backbone-Backbone	72	9.3	1	1.4	0.1	1	1.4	0.1
Backbone-Sidechain	95	12.3	6	6.3	0.8	0	0.0	0.0
Sidechain-Sidechain	18	2.3	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	73	9.4	5	6.8	0.6	0	0.0	0.0
Backbone-Backbone	15	1.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	35	4.5	2	5.7	0.3	0	0.0	0.0
Sidechain-Sidechain	23	3.0	3	13.0	0.4	0	0.0	0.0
Long range ($i-j \geq 5$)	207	26.8	16	7.7	2.1	3	1.4	0.4
Backbone-Backbone	20	2.6	1	5.0	0.1	0	0.0	0.0
Backbone-Sidechain	70	9.1	8	11.4	1.0	2	2.9	0.3
Sidechain-Sidechain	117	15.1	7	6.0	0.9	1	0.9	0.1
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	18	2.3	8	44.4	1.0	4	22.2	0.5
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	773	100.0	46	6.0	6.0	8	1.0	1.0
Backbone-Backbone	178	23.0	10	5.6	1.3	5	2.8	0.6
Backbone-Sidechain	409	52.9	22	5.4	2.8	2	0.5	0.3
Sidechain-Sidechain	186	24.1	14	7.5	1.8	1	0.5	0.1

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 disulfid 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	5	2	4	9	0	20	0.39	1.06	0.31	0.24
2	8	4	3	15	0	30	0.86	3.66	0.92	0.48
3	8	4	2	16	0	30	0.91	4.03	0.97	0.7
4	0	2	5	11	0	18	0.24	0.73	0.17	0.17
5	5	4	6	10	0	25	0.32	1.03	0.28	0.18
6	8	4	3	17	0	32	0.86	4.13	0.99	0.44
7	8	4	3	14	0	29	0.89	4.0	0.99	0.41
8	5	4	6	14	0	29	0.8	3.87	0.98	0.37
9	4	2	4	13	0	23	0.33	1.67	0.37	0.18
10	8	5	3	15	0	31	0.83	3.91	0.94	0.36
11	10	4	2	16	0	32	0.89	4.17	1.02	0.32

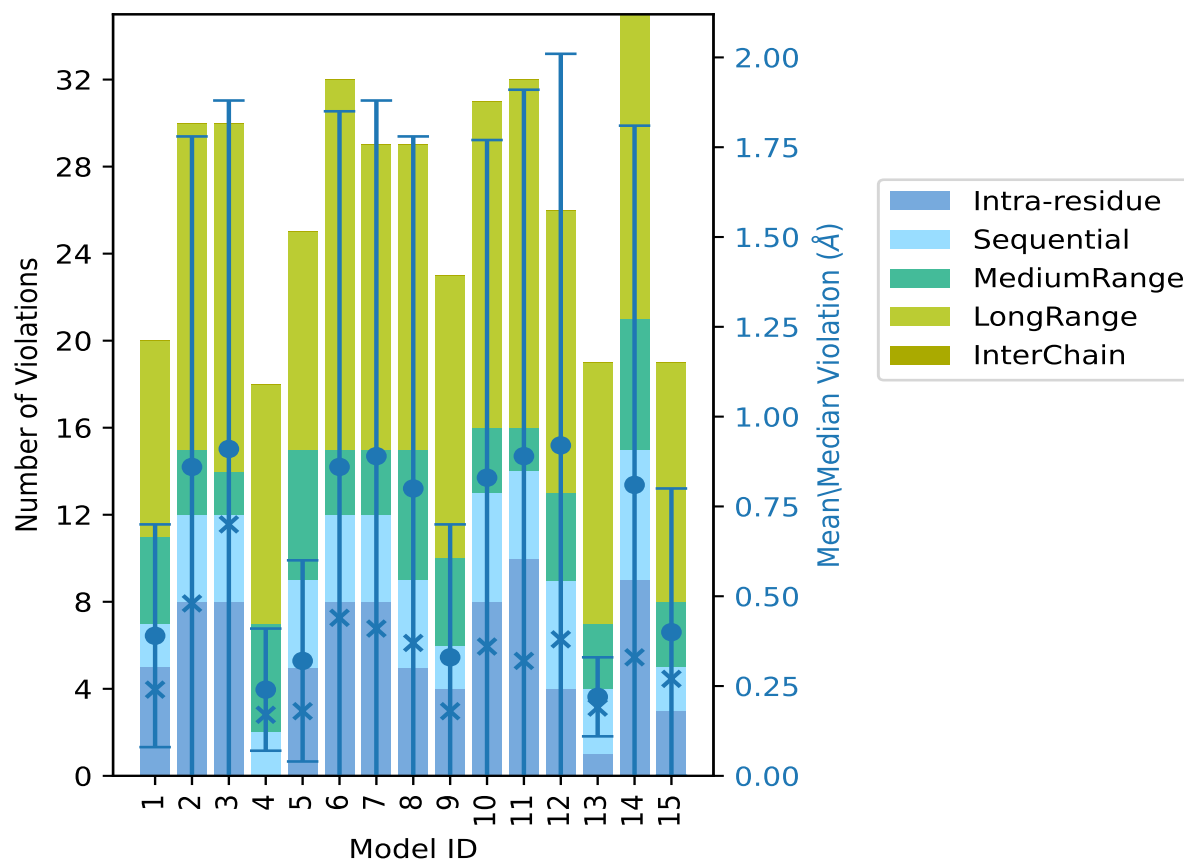
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
12	4	5	4	13	0	26	0.92	4.1	1.09	0.38
13	1	3	3	12	0	19	0.22	0.55	0.11	0.19
14	9	6	6	14	0	35	0.81	4.14	1.0	0.33
15	3	2	3	11	0	19	0.4	1.69	0.4	0.27

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

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



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

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

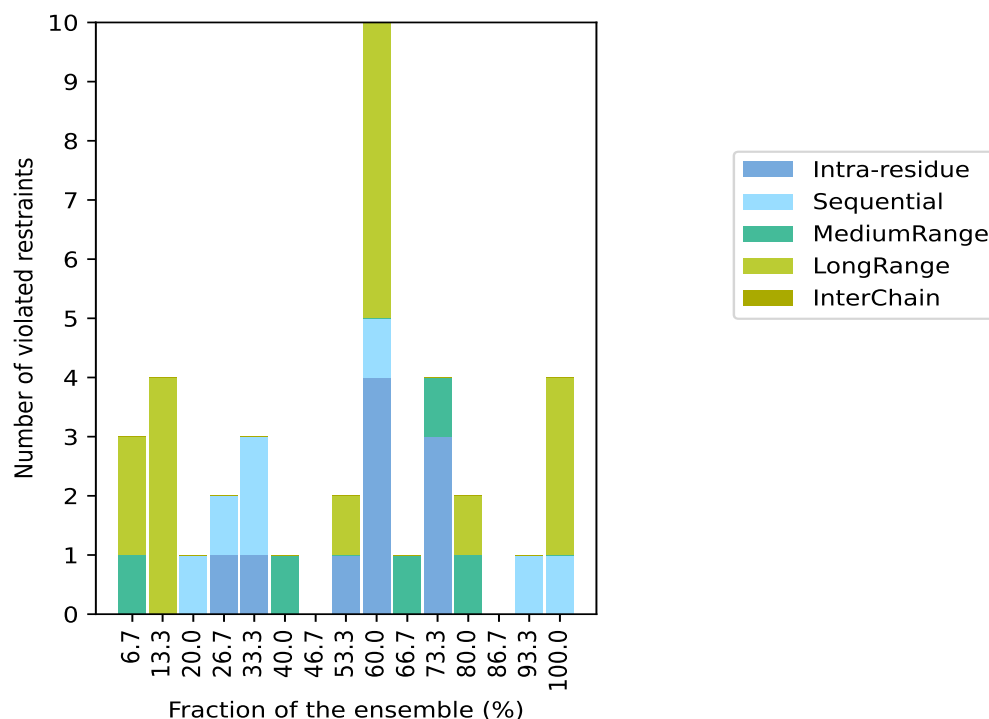
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints

for a given fraction of the ensemble. In total, 717(IR:280, SQ:178, MR:68, LR:191, 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	%
0	0	1	2	0	3	1	6.7
0	0	0	4	0	4	2	13.3
0	1	0	0	0	1	3	20.0
1	1	0	0	0	2	4	26.7
1	2	0	0	0	3	5	33.3
0	0	1	0	0	1	6	40.0
0	0	0	0	0	0	7	46.7
1	0	0	1	0	2	8	53.3
4	1	0	5	0	10	9	60.0
0	0	1	0	0	1	10	66.7
3	0	1	0	0	4	11	73.3
0	0	1	1	0	2	12	80.0
0	0	0	0	0	0	13	86.7
0	1	0	0	0	1	14	93.3
0	1	0	3	0	4	15	100.0

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

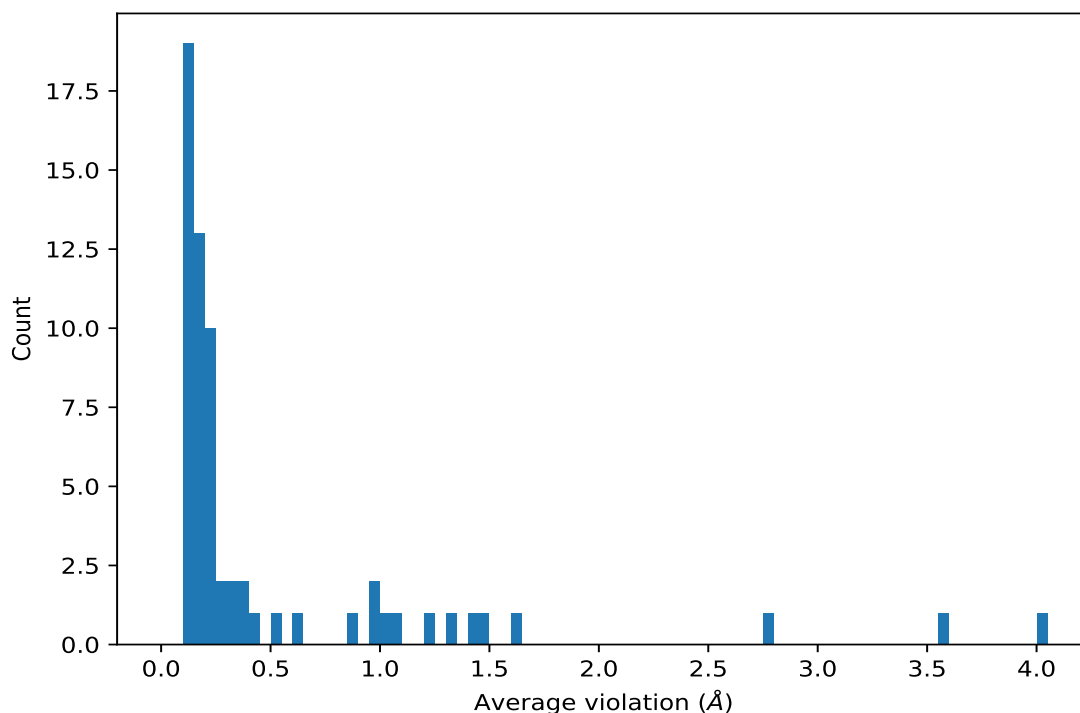
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,10)	1:A:179:VAL:H	1:A:170:SER:O	15	0.6	0.26	0.69
(2,9)	1:A:179:VAL:N	1:A:170:SER:O	15	0.54	0.25	0.61
(2,8)	1:A:172:CYS:H	1:A:177:LEU:O	15	0.39	0.14	0.41
(1,16)	1:A:165:TRP:HE1	1:A:174:LEU:HA	15	0.33	0.01	0.33
(1,545)	1:A:161:CYS:HB2	1:A:137:CYS:HA	15	0.28	0.02	0.28
(2,4)	1:A:150:LEU:H	1:A:155:HIS:O	15	0.27	0.09	0.27
(1,316)	1:A:167:GLY:H	1:A:166:LEU:H	15	0.19	0.01	0.18
(1,505)	1:A:157:PHE:HB3	1:A:173:PRO:HD3	15	0.16	0.01	0.16
(1,502)	1:A:157:PHE:HA	1:A:158:HIS:HE1	14	0.15	0.03	0.13
(2,7)	1:A:172:CYS:N	1:A:177:LEU:O	12	0.3	0.12	0.29
(1,473)	1:A:152:ARG:HG3	1:A:177:LEU:HB2	12	0.14	0.01	0.14
(1,546)	1:A:161:CYS:HB2	1:A:158:HIS:HB3	12	0.12	0.01	0.12
(1,168)	1:A:149:PHE:H	1:A:149:PHE:HD2	11	1.41	0.23	1.42
(1,669)	1:A:149:PHE:HB3	1:A:149:PHE:HD1	11	1.04	0.02	1.04
(1,670)	1:A:149:PHE:HB2	1:A:149:PHE:HD2	11	0.88	0.04	0.88
(1,13)	1:A:165:TRP:HE1	1:A:169:HIS:HB2	11	0.12	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,12)	1:A:163:ASP:H	1:A:159:ALA:O	10	0.24	0.09	0.22
(1,274)	1:A:162:VAL:H	1:A:158:HIS:HB2	10	0.12	0.01	0.11
(1,70)	1:A:136:VAL:H	1:A:157:PHE:HD1	9	4.0	0.16	4.03
(1,59)	1:A:135:ALA:H	1:A:157:PHE:HD1	9	3.56	0.14	3.49
(1,60)	1:A:135:ALA:H	1:A:157:PHE:HE1	9	2.78	0.18	2.81
(1,71)	1:A:136:VAL:H	1:A:157:PHE:HE1	9	1.6	0.18	1.61
(1,221)	1:A:157:PHE:H	1:A:157:PHE:HD2	9	1.46	0.03	1.45
(1,216)	1:A:156:GLY:H	1:A:157:PHE:HD2	9	1.31	0.27	1.44
(1,399)	1:A:134:CYS:HA	1:A:157:PHE:HD1	9	1.2	0.28	1.24
(1,693)	1:A:157:PHE:HA	1:A:157:PHE:HD1	9	1.05	0.05	1.04
(1,694)	1:A:157:PHE:HB3	1:A:157:PHE:HD1	9	0.98	0.01	0.98
(1,695)	1:A:157:PHE:HB2	1:A:157:PHE:HD2	9	0.97	0.01	0.97
(1,668)	1:A:149:PHE:HA	1:A:149:PHE:HD1	8	0.39	0.18	0.38
(2,3)	1:A:150:LEU:N	1:A:155:HIS:O	8	0.16	0.04	0.16
(1,582)	1:A:165:TRP:HD1	1:A:173:PRO:HD2	8	0.11	0.0	0.11
(2,18)	1:A:166:LEU:H	1:A:162:VAL:O	7	0.18	0.04	0.17
(1,12)	1:A:165:TRP:HE1	1:A:169:HIS:HB3	6	0.12	0.0	0.12
(1,217)	1:A:156:GLY:H	1:A:157:PHE:HE2	5	0.42	0.16	0.33
(1,191)	1:A:153:CYS:H	1:A:152:ARG:HB3	5	0.14	0.03	0.16
(1,388)	1:A:180:VAL:H	1:A:180:VAL:HB	5	0.11	0.0	0.11
(1,233)	1:A:158:HIS:H	1:A:157:PHE:HB2	4	0.16	0.03	0.15
(1,365)	1:A:177:LEU:H	1:A:177:LEU:HB3	4	0.12	0.01	0.12
(1,384)	1:A:179:VAL:H	1:A:178:THR:HB	3	0.18	0.02	0.19
(1,428)	1:A:141:LEU:HD11	1:A:132:VAL:HG11	2	0.22	0.01	0.22
(1,428)	1:A:141:LEU:HD11	1:A:132:VAL:HG12	2	0.22	0.01	0.22
(1,428)	1:A:141:LEU:HD11	1:A:132:VAL:HG13	2	0.22	0.01	0.22
(1,428)	1:A:141:LEU:HD12	1:A:132:VAL:HG11	2	0.22	0.01	0.22
(1,428)	1:A:141:LEU:HD12	1:A:132:VAL:HG12	2	0.22	0.01	0.22
(1,428)	1:A:141:LEU:HD12	1:A:132:VAL:HG13	2	0.22	0.01	0.22
(1,428)	1:A:141:LEU:HD13	1:A:132:VAL:HG11	2	0.22	0.01	0.22
(1,428)	1:A:141:LEU:HD13	1:A:132:VAL:HG12	2	0.22	0.01	0.22
(1,428)	1:A:141:LEU:HD13	1:A:132:VAL:HG13	2	0.22	0.01	0.22
(1,469)	1:A:151:PRO:HD2	1:A:179:VAL:HG11	2	0.16	0.01	0.16
(1,469)	1:A:151:PRO:HD2	1:A:179:VAL:HG12	2	0.16	0.01	0.16
(1,469)	1:A:151:PRO:HD2	1:A:179:VAL:HG13	2	0.16	0.01	0.16
(1,469)	1:A:151:PRO:HD3	1:A:179:VAL:HG11	2	0.16	0.01	0.16
(1,469)	1:A:151:PRO:HD3	1:A:179:VAL:HG12	2	0.16	0.01	0.16
(1,469)	1:A:151:PRO:HD3	1:A:179:VAL:HG13	2	0.16	0.01	0.16
(1,445)	1:A:149:PHE:HA	1:A:156:GLY:HA3	2	0.12	0.01	0.12
(1,406)	1:A:135:ALA:HB1	1:A:174:LEU:HD11	2	0.12	0.0	0.12
(1,406)	1:A:135:ALA:HB1	1:A:174:LEU:HD12	2	0.12	0.0	0.12
(1,406)	1:A:135:ALA:HB1	1:A:174:LEU:HD13	2	0.12	0.0	0.12

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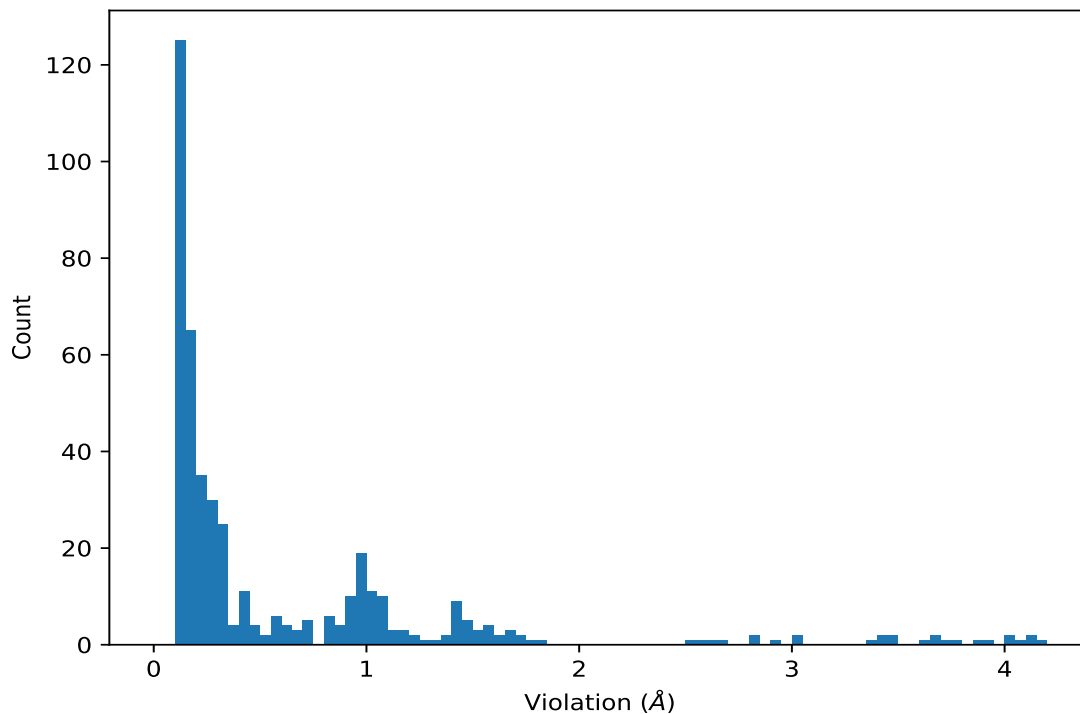
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,406)	1:A:135:ALA:HB2	1:A:174:LEU:HD11	2	0.12	0.0	0.12
(1,406)	1:A:135:ALA:HB2	1:A:174:LEU:HD12	2	0.12	0.0	0.12
(1,406)	1:A:135:ALA:HB2	1:A:174:LEU:HD13	2	0.12	0.0	0.12
(1,406)	1:A:135:ALA:HB3	1:A:174:LEU:HD11	2	0.12	0.0	0.12
(1,406)	1:A:135:ALA:HB3	1:A:174:LEU:HD12	2	0.12	0.0	0.12
(1,406)	1:A:135:ALA:HB3	1:A:174:LEU:HD13	2	0.12	0.0	0.12

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)
(1,70)	1:A:136:VAL:H	1:A:157:PHE:HD1	11	4.17
(1,70)	1:A:136:VAL:H	1:A:157:PHE:HD1	14	4.14
(1,70)	1:A:136:VAL:H	1:A:157:PHE:HD1	6	4.13
(1,70)	1:A:136:VAL:H	1:A:157:PHE:HD1	12	4.1
(1,70)	1:A:136:VAL:H	1:A:157:PHE:HD1	3	4.03
(1,70)	1:A:136:VAL:H	1:A:157:PHE:HD1	7	4.0
(1,70)	1:A:136:VAL:H	1:A:157:PHE:HD1	10	3.91
(1,70)	1:A:136:VAL:H	1:A:157:PHE:HD1	8	3.87
(1,59)	1:A:135:ALA:H	1:A:157:PHE:HD1	14	3.76
(1,59)	1:A:135:ALA:H	1:A:157:PHE:HD1	11	3.71
(1,59)	1:A:135:ALA:H	1:A:157:PHE:HD1	12	3.69
(1,70)	1:A:136:VAL:H	1:A:157:PHE:HD1	2	3.66
(1,59)	1:A:135:ALA:H	1:A:157:PHE:HD1	6	3.64
(1,59)	1:A:135:ALA:H	1:A:157:PHE:HD1	3	3.49
(1,59)	1:A:135:ALA:H	1:A:157:PHE:HD1	7	3.48
(1,59)	1:A:135:ALA:H	1:A:157:PHE:HD1	2	3.44
(1,59)	1:A:135:ALA:H	1:A:157:PHE:HD1	8	3.44
(1,59)	1:A:135:ALA:H	1:A:157:PHE:HD1	10	3.35
(1,60)	1:A:135:ALA:H	1:A:157:PHE:HE1	14	3.04
(1,60)	1:A:135:ALA:H	1:A:157:PHE:HE1	12	3.02
(1,60)	1:A:135:ALA:H	1:A:157:PHE:HE1	11	2.93
(1,60)	1:A:135:ALA:H	1:A:157:PHE:HE1	6	2.83
(1,60)	1:A:135:ALA:H	1:A:157:PHE:HE1	8	2.81
(1,60)	1:A:135:ALA:H	1:A:157:PHE:HE1	7	2.69
(1,60)	1:A:135:ALA:H	1:A:157:PHE:HE1	10	2.63
(1,60)	1:A:135:ALA:H	1:A:157:PHE:HE1	2	2.56
(1,60)	1:A:135:ALA:H	1:A:157:PHE:HE1	3	2.53
(1,71)	1:A:136:VAL:H	1:A:157:PHE:HE1	12	1.8
(1,71)	1:A:136:VAL:H	1:A:157:PHE:HE1	14	1.79
(1,216)	1:A:156:GLY:H	1:A:157:PHE:HD2	3	1.73
(1,71)	1:A:136:VAL:H	1:A:157:PHE:HE1	11	1.72
(1,168)	1:A:149:PHE:H	1:A:149:PHE:HD2	15	1.69
(1,71)	1:A:136:VAL:H	1:A:157:PHE:HE1	6	1.68
(1,168)	1:A:149:PHE:H	1:A:149:PHE:HD2	9	1.67
(1,168)	1:A:149:PHE:H	1:A:149:PHE:HD2	3	1.64
(1,71)	1:A:136:VAL:H	1:A:157:PHE:HE1	8	1.61
(1,71)	1:A:136:VAL:H	1:A:157:PHE:HE1	10	1.57
(1,71)	1:A:136:VAL:H	1:A:157:PHE:HE1	7	1.56
(1,216)	1:A:156:GLY:H	1:A:157:PHE:HD2	2	1.56
(1,168)	1:A:149:PHE:H	1:A:149:PHE:HD2	11	1.55
(1,168)	1:A:149:PHE:H	1:A:149:PHE:HD2	7	1.54
(1,399)	1:A:134:CYS:HA	1:A:157:PHE:HD1	14	1.52
(1,221)	1:A:157:PHE:H	1:A:157:PHE:HD2	11	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,221)	1:A:157:PHE:H	1:A:157:PHE:HD2	6	1.49
(1,221)	1:A:157:PHE:H	1:A:157:PHE:HD2	3	1.48
(1,216)	1:A:156:GLY:H	1:A:157:PHE:HD2	6	1.48
(1,221)	1:A:157:PHE:H	1:A:157:PHE:HD2	2	1.47
(1,216)	1:A:156:GLY:H	1:A:157:PHE:HD2	7	1.46
(1,399)	1:A:134:CYS:HA	1:A:157:PHE:HD1	12	1.45
(1,221)	1:A:157:PHE:H	1:A:157:PHE:HD2	12	1.45
(1,221)	1:A:157:PHE:H	1:A:157:PHE:HD2	14	1.45
(1,221)	1:A:157:PHE:H	1:A:157:PHE:HD2	10	1.44
(1,216)	1:A:156:GLY:H	1:A:157:PHE:HD2	11	1.44
(1,221)	1:A:157:PHE:H	1:A:157:PHE:HD2	7	1.43
(1,71)	1:A:136:VAL:H	1:A:157:PHE:HE1	3	1.42
(1,221)	1:A:157:PHE:H	1:A:157:PHE:HD2	8	1.42
(1,168)	1:A:149:PHE:H	1:A:149:PHE:HD2	2	1.42
(1,399)	1:A:134:CYS:HA	1:A:157:PHE:HD1	11	1.37
(1,168)	1:A:149:PHE:H	1:A:149:PHE:HD2	10	1.36
(1,168)	1:A:149:PHE:H	1:A:149:PHE:HD2	14	1.33
(1,399)	1:A:134:CYS:HA	1:A:157:PHE:HD1	8	1.28
(1,399)	1:A:134:CYS:HA	1:A:157:PHE:HD1	6	1.24
(1,71)	1:A:136:VAL:H	1:A:157:PHE:HE1	2	1.21
(1,168)	1:A:149:PHE:H	1:A:149:PHE:HD2	6	1.19
(1,399)	1:A:134:CYS:HA	1:A:157:PHE:HD1	3	1.18
(1,399)	1:A:134:CYS:HA	1:A:157:PHE:HD1	7	1.18
(1,216)	1:A:156:GLY:H	1:A:157:PHE:HD2	14	1.15
(1,693)	1:A:157:PHE:HA	1:A:157:PHE:HD1	8	1.13
(1,693)	1:A:157:PHE:HA	1:A:157:PHE:HD1	14	1.11
(1,399)	1:A:134:CYS:HA	1:A:157:PHE:HD1	10	1.09
(1,216)	1:A:156:GLY:H	1:A:157:PHE:HD2	10	1.08
(1,693)	1:A:157:PHE:HA	1:A:157:PHE:HD1	12	1.07
(1,693)	1:A:157:PHE:HA	1:A:157:PHE:HD1	10	1.06
(1,669)	1:A:149:PHE:HB3	1:A:149:PHE:HD1	3	1.06
(1,669)	1:A:149:PHE:HB3	1:A:149:PHE:HD1	9	1.06
(1,669)	1:A:149:PHE:HB3	1:A:149:PHE:HD1	15	1.06
(1,168)	1:A:149:PHE:H	1:A:149:PHE:HD2	1	1.06
(1,669)	1:A:149:PHE:HB3	1:A:149:PHE:HD1	7	1.05
(1,669)	1:A:149:PHE:HB3	1:A:149:PHE:HD1	11	1.05
(1,693)	1:A:157:PHE:HA	1:A:157:PHE:HD1	11	1.04
(1,669)	1:A:149:PHE:HB3	1:A:149:PHE:HD1	2	1.04
(1,669)	1:A:149:PHE:HB3	1:A:149:PHE:HD1	10	1.04
(1,669)	1:A:149:PHE:HB3	1:A:149:PHE:HD1	14	1.04
(1,693)	1:A:157:PHE:HA	1:A:157:PHE:HD1	6	1.03
(1,693)	1:A:157:PHE:HA	1:A:157:PHE:HD1	7	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,168)	1:A:149:PHE:H	1:A:149:PHE:HD2	5	1.03
(1,669)	1:A:149:PHE:HB3	1:A:149:PHE:HD1	1	1.02
(1,669)	1:A:149:PHE:HB3	1:A:149:PHE:HD1	6	1.02
(1,216)	1:A:156:GLY:H	1:A:157:PHE:HD2	12	1.01
(1,669)	1:A:149:PHE:HB3	1:A:149:PHE:HD1	5	1.0
(1,694)	1:A:157:PHE:HB3	1:A:157:PHE:HD1	8	0.99
(1,694)	1:A:157:PHE:HB3	1:A:157:PHE:HD1	10	0.99
(1,694)	1:A:157:PHE:HB3	1:A:157:PHE:HD1	12	0.99
(2,10)	1:A:179:VAL:H	1:A:170:SER:O	11	0.98
(1,695)	1:A:157:PHE:HB2	1:A:157:PHE:HD2	3	0.98
(1,695)	1:A:157:PHE:HB2	1:A:157:PHE:HD2	6	0.98
(1,695)	1:A:157:PHE:HB2	1:A:157:PHE:HD2	7	0.98
(1,695)	1:A:157:PHE:HB2	1:A:157:PHE:HD2	11	0.98
(1,694)	1:A:157:PHE:HB3	1:A:157:PHE:HD1	2	0.98
(1,694)	1:A:157:PHE:HB3	1:A:157:PHE:HD1	6	0.98
(1,694)	1:A:157:PHE:HB3	1:A:157:PHE:HD1	11	0.98
(1,694)	1:A:157:PHE:HB3	1:A:157:PHE:HD1	14	0.98
(1,693)	1:A:157:PHE:HA	1:A:157:PHE:HD1	2	0.98
(1,695)	1:A:157:PHE:HB2	1:A:157:PHE:HD2	2	0.97
(1,695)	1:A:157:PHE:HB2	1:A:157:PHE:HD2	14	0.97
(1,694)	1:A:157:PHE:HB3	1:A:157:PHE:HD1	3	0.97
(1,694)	1:A:157:PHE:HB3	1:A:157:PHE:HD1	7	0.97
(1,693)	1:A:157:PHE:HA	1:A:157:PHE:HD1	3	0.97
(1,695)	1:A:157:PHE:HB2	1:A:157:PHE:HD2	8	0.96
(2,10)	1:A:179:VAL:H	1:A:170:SER:O	2	0.95
(1,695)	1:A:157:PHE:HB2	1:A:157:PHE:HD2	10	0.95
(1,695)	1:A:157:PHE:HB2	1:A:157:PHE:HD2	12	0.95
(1,670)	1:A:149:PHE:HB2	1:A:149:PHE:HD2	5	0.95
(1,670)	1:A:149:PHE:HB2	1:A:149:PHE:HD2	1	0.94
(1,670)	1:A:149:PHE:HB2	1:A:149:PHE:HD2	6	0.92
(2,9)	1:A:179:VAL:N	1:A:170:SER:O	11	0.9
(2,10)	1:A:179:VAL:H	1:A:170:SER:O	12	0.9
(1,670)	1:A:149:PHE:HB2	1:A:149:PHE:HD2	14	0.9
(1,216)	1:A:156:GLY:H	1:A:157:PHE:HD2	8	0.9
(2,9)	1:A:179:VAL:N	1:A:170:SER:O	2	0.89
(1,670)	1:A:149:PHE:HB2	1:A:149:PHE:HD2	10	0.89
(1,670)	1:A:149:PHE:HB2	1:A:149:PHE:HD2	2	0.88
(1,670)	1:A:149:PHE:HB2	1:A:149:PHE:HD2	11	0.87
(1,670)	1:A:149:PHE:HB2	1:A:149:PHE:HD2	7	0.84
(1,670)	1:A:149:PHE:HB2	1:A:149:PHE:HD2	3	0.83
(2,9)	1:A:179:VAL:N	1:A:170:SER:O	12	0.82
(1,670)	1:A:149:PHE:HB2	1:A:149:PHE:HD2	9	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,670)	1:A:149:PHE:HB2	1:A:149:PHE:HD2	15	0.82
(2,10)	1:A:179:VAL:H	1:A:170:SER:O	10	0.81
(2,10)	1:A:179:VAL:H	1:A:170:SER:O	3	0.74
(2,9)	1:A:179:VAL:N	1:A:170:SER:O	10	0.73
(2,10)	1:A:179:VAL:H	1:A:170:SER:O	4	0.73
(1,217)	1:A:156:GLY:H	1:A:157:PHE:HE2	3	0.73
(2,10)	1:A:179:VAL:H	1:A:170:SER:O	1	0.71
(2,10)	1:A:179:VAL:H	1:A:170:SER:O	15	0.69
(2,9)	1:A:179:VAL:N	1:A:170:SER:O	3	0.67
(2,9)	1:A:179:VAL:N	1:A:170:SER:O	4	0.65
(2,9)	1:A:179:VAL:N	1:A:170:SER:O	1	0.64
(2,10)	1:A:179:VAL:H	1:A:170:SER:O	8	0.63
(1,668)	1:A:149:PHE:HA	1:A:149:PHE:HD1	5	0.63
(2,9)	1:A:179:VAL:N	1:A:170:SER:O	15	0.61
(2,8)	1:A:172:CYS:H	1:A:177:LEU:O	14	0.6
(1,668)	1:A:149:PHE:HA	1:A:149:PHE:HD1	1	0.6
(2,9)	1:A:179:VAL:N	1:A:170:SER:O	8	0.59
(2,8)	1:A:172:CYS:H	1:A:177:LEU:O	8	0.57
(2,8)	1:A:172:CYS:H	1:A:177:LEU:O	5	0.55
(2,8)	1:A:172:CYS:H	1:A:177:LEU:O	13	0.55
(1,668)	1:A:149:PHE:HA	1:A:149:PHE:HD1	6	0.52
(1,399)	1:A:134:CYS:HA	1:A:157:PHE:HD1	2	0.51
(2,7)	1:A:172:CYS:N	1:A:177:LEU:O	14	0.49
(2,10)	1:A:179:VAL:H	1:A:170:SER:O	6	0.49
(2,8)	1:A:172:CYS:H	1:A:177:LEU:O	6	0.46
(1,217)	1:A:156:GLY:H	1:A:157:PHE:HE2	2	0.45
(2,8)	1:A:172:CYS:H	1:A:177:LEU:O	7	0.44
(2,7)	1:A:172:CYS:N	1:A:177:LEU:O	5	0.44
(2,7)	1:A:172:CYS:N	1:A:177:LEU:O	8	0.44
(2,7)	1:A:172:CYS:N	1:A:177:LEU:O	13	0.44
(2,9)	1:A:179:VAL:N	1:A:170:SER:O	6	0.43
(2,4)	1:A:150:LEU:H	1:A:155:HIS:O	9	0.43
(2,12)	1:A:163:ASP:H	1:A:159:ALA:O	12	0.42
(2,8)	1:A:172:CYS:H	1:A:177:LEU:O	9	0.41
(2,8)	1:A:172:CYS:H	1:A:177:LEU:O	15	0.41
(2,10)	1:A:179:VAL:H	1:A:170:SER:O	7	0.41
(1,668)	1:A:149:PHE:HA	1:A:149:PHE:HD1	14	0.4
(2,4)	1:A:150:LEU:H	1:A:155:HIS:O	3	0.39
(2,4)	1:A:150:LEU:H	1:A:155:HIS:O	14	0.39
(2,12)	1:A:163:ASP:H	1:A:159:ALA:O	8	0.37
(1,668)	1:A:149:PHE:HA	1:A:149:PHE:HD1	10	0.36
(2,9)	1:A:179:VAL:N	1:A:170:SER:O	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4)	1:A:150:LEU:H	1:A:155:HIS:O	4	0.35
(1,16)	1:A:165:TRP:HE1	1:A:174:LEU:HA	6	0.35
(1,16)	1:A:165:TRP:HE1	1:A:174:LEU:HA	8	0.35
(2,4)	1:A:150:LEU:H	1:A:155:HIS:O	5	0.34
(1,16)	1:A:165:TRP:HE1	1:A:174:LEU:HA	2	0.34
(1,16)	1:A:165:TRP:HE1	1:A:174:LEU:HA	3	0.34
(1,16)	1:A:165:TRP:HE1	1:A:174:LEU:HA	12	0.34
(2,8)	1:A:172:CYS:H	1:A:177:LEU:O	1	0.33
(2,7)	1:A:172:CYS:N	1:A:177:LEU:O	6	0.33
(2,10)	1:A:179:VAL:H	1:A:170:SER:O	9	0.33
(1,217)	1:A:156:GLY:H	1:A:157:PHE:HE2	6	0.33
(1,217)	1:A:156:GLY:H	1:A:157:PHE:HE2	7	0.33
(1,16)	1:A:165:TRP:HE1	1:A:174:LEU:HA	1	0.33
(1,16)	1:A:165:TRP:HE1	1:A:174:LEU:HA	9	0.33
(1,16)	1:A:165:TRP:HE1	1:A:174:LEU:HA	11	0.33
(1,16)	1:A:165:TRP:HE1	1:A:174:LEU:HA	14	0.33
(1,16)	1:A:165:TRP:HE1	1:A:174:LEU:HA	15	0.33
(2,8)	1:A:172:CYS:H	1:A:177:LEU:O	11	0.32
(1,668)	1:A:149:PHE:HA	1:A:149:PHE:HD1	2	0.32
(1,16)	1:A:165:TRP:HE1	1:A:174:LEU:HA	5	0.32
(1,16)	1:A:165:TRP:HE1	1:A:174:LEU:HA	7	0.32
(1,16)	1:A:165:TRP:HE1	1:A:174:LEU:HA	10	0.32
(1,16)	1:A:165:TRP:HE1	1:A:174:LEU:HA	13	0.32
(1,545)	1:A:161:CYS:HB2	1:A:137:CYS:HA	5	0.31
(2,8)	1:A:172:CYS:H	1:A:177:LEU:O	2	0.3
(2,7)	1:A:172:CYS:N	1:A:177:LEU:O	7	0.3
(2,4)	1:A:150:LEU:H	1:A:155:HIS:O	6	0.3
(1,545)	1:A:161:CYS:HB2	1:A:137:CYS:HA	12	0.3
(1,545)	1:A:161:CYS:HB2	1:A:137:CYS:HA	14	0.3
(1,545)	1:A:161:CYS:HB2	1:A:137:CYS:HA	1	0.29
(1,545)	1:A:161:CYS:HB2	1:A:137:CYS:HA	3	0.29
(1,545)	1:A:161:CYS:HB2	1:A:137:CYS:HA	6	0.29
(1,545)	1:A:161:CYS:HB2	1:A:137:CYS:HA	11	0.29
(1,16)	1:A:165:TRP:HE1	1:A:174:LEU:HA	4	0.29
(2,4)	1:A:150:LEU:H	1:A:155:HIS:O	13	0.28
(2,12)	1:A:163:ASP:H	1:A:159:ALA:O	4	0.28
(1,545)	1:A:161:CYS:HB2	1:A:137:CYS:HA	7	0.28
(1,545)	1:A:161:CYS:HB2	1:A:137:CYS:HA	9	0.28
(1,545)	1:A:161:CYS:HB2	1:A:137:CYS:HA	10	0.28
(1,217)	1:A:156:GLY:H	1:A:157:PHE:HE2	11	0.28
(2,9)	1:A:179:VAL:N	1:A:170:SER:O	9	0.27
(2,7)	1:A:172:CYS:N	1:A:177:LEU:O	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:A:172:CYS:N	1:A:177:LEU:O	15	0.27
(2,4)	1:A:150:LEU:H	1:A:155:HIS:O	15	0.27
(1,545)	1:A:161:CYS:HB2	1:A:137:CYS:HA	13	0.27
(1,545)	1:A:161:CYS:HB2	1:A:137:CYS:HA	15	0.27
(2,8)	1:A:172:CYS:H	1:A:177:LEU:O	3	0.26
(2,12)	1:A:163:ASP:H	1:A:159:ALA:O	11	0.26
(2,10)	1:A:179:VAL:H	1:A:170:SER:O	13	0.26
(1,545)	1:A:161:CYS:HB2	1:A:137:CYS:HA	4	0.26
(1,545)	1:A:161:CYS:HB2	1:A:137:CYS:HA	8	0.26
(2,8)	1:A:172:CYS:H	1:A:177:LEU:O	4	0.25
(2,4)	1:A:150:LEU:H	1:A:155:HIS:O	2	0.25
(2,12)	1:A:163:ASP:H	1:A:159:ALA:O	1	0.25
(1,545)	1:A:161:CYS:HB2	1:A:137:CYS:HA	2	0.24
(2,9)	1:A:179:VAL:N	1:A:170:SER:O	13	0.23
(2,18)	1:A:166:LEU:H	1:A:162:VAL:O	12	0.23
(1,428)	1:A:141:LEU:HD11	1:A:132:VAL:HG11	3	0.23
(1,428)	1:A:141:LEU:HD11	1:A:132:VAL:HG12	3	0.23
(1,428)	1:A:141:LEU:HD11	1:A:132:VAL:HG13	3	0.23
(1,428)	1:A:141:LEU:HD12	1:A:132:VAL:HG11	3	0.23
(1,428)	1:A:141:LEU:HD12	1:A:132:VAL:HG12	3	0.23
(1,428)	1:A:141:LEU:HD12	1:A:132:VAL:HG13	3	0.23
(1,428)	1:A:141:LEU:HD13	1:A:132:VAL:HG11	3	0.23
(1,428)	1:A:141:LEU:HD13	1:A:132:VAL:HG12	3	0.23
(1,428)	1:A:141:LEU:HD13	1:A:132:VAL:HG13	3	0.23
(2,3)	1:A:150:LEU:N	1:A:155:HIS:O	9	0.22
(2,18)	1:A:166:LEU:H	1:A:162:VAL:O	1	0.22
(2,18)	1:A:166:LEU:H	1:A:162:VAL:O	10	0.22
(2,4)	1:A:150:LEU:H	1:A:155:HIS:O	7	0.21
(1,428)	1:A:141:LEU:HD11	1:A:132:VAL:HG11	13	0.21
(1,428)	1:A:141:LEU:HD11	1:A:132:VAL:HG12	13	0.21
(1,428)	1:A:141:LEU:HD11	1:A:132:VAL:HG13	13	0.21
(1,428)	1:A:141:LEU:HD12	1:A:132:VAL:HG11	13	0.21
(1,428)	1:A:141:LEU:HD12	1:A:132:VAL:HG12	13	0.21
(1,428)	1:A:141:LEU:HD12	1:A:132:VAL:HG13	13	0.21
(1,428)	1:A:141:LEU:HD13	1:A:132:VAL:HG11	13	0.21
(1,428)	1:A:141:LEU:HD13	1:A:132:VAL:HG12	13	0.21
(1,428)	1:A:141:LEU:HD13	1:A:132:VAL:HG13	13	0.21
(1,384)	1:A:179:VAL:H	1:A:178:THR:HB	13	0.21
(2,7)	1:A:172:CYS:N	1:A:177:LEU:O	1	0.2
(2,10)	1:A:179:VAL:H	1:A:170:SER:O	5	0.2
(1,502)	1:A:157:PHE:HA	1:A:158:HIS:HE1	12	0.2
(1,316)	1:A:167:GLY:H	1:A:166:LEU:H	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,316)	1:A:167:GLY:H	1:A:166:LEU:H	2	0.2
(1,316)	1:A:167:GLY:H	1:A:166:LEU:H	3	0.2
(1,316)	1:A:167:GLY:H	1:A:166:LEU:H	4	0.2
(1,316)	1:A:167:GLY:H	1:A:166:LEU:H	10	0.2
(1,233)	1:A:158:HIS:H	1:A:157:PHE:HB2	14	0.2
(2,4)	1:A:150:LEU:H	1:A:155:HIS:O	1	0.19
(2,3)	1:A:150:LEU:N	1:A:155:HIS:O	5	0.19
(2,12)	1:A:163:ASP:H	1:A:159:ALA:O	6	0.19
(2,10)	1:A:179:VAL:H	1:A:170:SER:O	14	0.19
(1,505)	1:A:157:PHE:HB3	1:A:173:PRO:HD3	6	0.19
(1,502)	1:A:157:PHE:HA	1:A:158:HIS:HE1	14	0.19
(1,441)	1:A:147:ALA:HB1	1:A:141:LEU:HD21	13	0.19
(1,441)	1:A:147:ALA:HB1	1:A:141:LEU:HD22	13	0.19
(1,441)	1:A:147:ALA:HB1	1:A:141:LEU:HD23	13	0.19
(1,441)	1:A:147:ALA:HB2	1:A:141:LEU:HD21	13	0.19
(1,441)	1:A:147:ALA:HB2	1:A:141:LEU:HD22	13	0.19
(1,441)	1:A:147:ALA:HB2	1:A:141:LEU:HD23	13	0.19
(1,441)	1:A:147:ALA:HB3	1:A:141:LEU:HD21	13	0.19
(1,441)	1:A:147:ALA:HB3	1:A:141:LEU:HD22	13	0.19
(1,441)	1:A:147:ALA:HB3	1:A:141:LEU:HD23	13	0.19
(1,384)	1:A:179:VAL:H	1:A:178:THR:HB	5	0.19
(1,316)	1:A:167:GLY:H	1:A:166:LEU:H	6	0.19
(1,316)	1:A:167:GLY:H	1:A:166:LEU:H	8	0.19
(2,8)	1:A:172:CYS:H	1:A:177:LEU:O	12	0.18
(2,7)	1:A:172:CYS:N	1:A:177:LEU:O	11	0.18
(2,4)	1:A:150:LEU:H	1:A:155:HIS:O	10	0.18
(2,3)	1:A:150:LEU:N	1:A:155:HIS:O	3	0.18
(2,3)	1:A:150:LEU:N	1:A:155:HIS:O	14	0.18
(1,505)	1:A:157:PHE:HB3	1:A:173:PRO:HD3	5	0.18
(1,505)	1:A:157:PHE:HB3	1:A:173:PRO:HD3	9	0.18
(1,505)	1:A:157:PHE:HB3	1:A:173:PRO:HD3	14	0.18
(1,502)	1:A:157:PHE:HA	1:A:158:HIS:HE1	8	0.18
(1,502)	1:A:157:PHE:HA	1:A:158:HIS:HE1	10	0.18
(1,316)	1:A:167:GLY:H	1:A:166:LEU:H	9	0.18
(1,316)	1:A:167:GLY:H	1:A:166:LEU:H	12	0.18
(1,316)	1:A:167:GLY:H	1:A:166:LEU:H	13	0.18
(1,316)	1:A:167:GLY:H	1:A:166:LEU:H	14	0.18
(1,316)	1:A:167:GLY:H	1:A:166:LEU:H	15	0.18
(2,9)	1:A:179:VAL:N	1:A:170:SER:O	5	0.17
(2,18)	1:A:166:LEU:H	1:A:162:VAL:O	8	0.17
(2,12)	1:A:163:ASP:H	1:A:159:ALA:O	10	0.17
(2,12)	1:A:163:ASP:H	1:A:159:ALA:O	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:A:149:PHE:HA	1:A:149:PHE:HD1	11	0.17
(1,505)	1:A:157:PHE:HB3	1:A:173:PRO:HD3	2	0.17
(1,505)	1:A:157:PHE:HB3	1:A:173:PRO:HD3	4	0.17
(1,505)	1:A:157:PHE:HB3	1:A:173:PRO:HD3	7	0.17
(1,473)	1:A:152:ARG:HG3	1:A:177:LEU:HB2	9	0.17
(1,469)	1:A:151:PRO:HD2	1:A:179:VAL:HG11	4	0.17
(1,469)	1:A:151:PRO:HD2	1:A:179:VAL:HG12	4	0.17
(1,469)	1:A:151:PRO:HD2	1:A:179:VAL:HG13	4	0.17
(1,469)	1:A:151:PRO:HD3	1:A:179:VAL:HG11	4	0.17
(1,469)	1:A:151:PRO:HD3	1:A:179:VAL:HG12	4	0.17
(1,469)	1:A:151:PRO:HD3	1:A:179:VAL:HG13	4	0.17
(1,316)	1:A:167:GLY:H	1:A:166:LEU:H	5	0.17
(1,316)	1:A:167:GLY:H	1:A:166:LEU:H	7	0.17
(1,316)	1:A:167:GLY:H	1:A:166:LEU:H	11	0.17
(1,191)	1:A:153:CYS:H	1:A:152:ARG:HB3	13	0.17
(2,9)	1:A:179:VAL:N	1:A:170:SER:O	14	0.16
(2,4)	1:A:150:LEU:H	1:A:155:HIS:O	8	0.16
(2,4)	1:A:150:LEU:H	1:A:155:HIS:O	11	0.16
(2,18)	1:A:166:LEU:H	1:A:162:VAL:O	14	0.16
(2,12)	1:A:163:ASP:H	1:A:159:ALA:O	2	0.16
(1,505)	1:A:157:PHE:HB3	1:A:173:PRO:HD3	1	0.16
(1,505)	1:A:157:PHE:HB3	1:A:173:PRO:HD3	8	0.16
(1,505)	1:A:157:PHE:HB3	1:A:173:PRO:HD3	13	0.16
(1,505)	1:A:157:PHE:HB3	1:A:173:PRO:HD3	15	0.16
(1,473)	1:A:152:ARG:HG3	1:A:177:LEU:HB2	1	0.16
(1,233)	1:A:158:HIS:H	1:A:157:PHE:HB2	10	0.16
(1,191)	1:A:153:CYS:H	1:A:152:ARG:HB3	5	0.16
(1,191)	1:A:153:CYS:H	1:A:152:ARG:HB3	14	0.16
(2,8)	1:A:172:CYS:H	1:A:177:LEU:O	10	0.15
(2,7)	1:A:172:CYS:N	1:A:177:LEU:O	2	0.15
(2,18)	1:A:166:LEU:H	1:A:162:VAL:O	4	0.15
(2,12)	1:A:163:ASP:H	1:A:159:ALA:O	5	0.15
(1,546)	1:A:161:CYS:HB2	1:A:158:HIS:HB3	10	0.15
(1,505)	1:A:157:PHE:HB3	1:A:173:PRO:HD3	3	0.15
(1,505)	1:A:157:PHE:HB3	1:A:173:PRO:HD3	12	0.15
(1,473)	1:A:152:ARG:HG3	1:A:177:LEU:HB2	2	0.15
(1,473)	1:A:152:ARG:HG3	1:A:177:LEU:HB2	7	0.15
(1,473)	1:A:152:ARG:HG3	1:A:177:LEU:HB2	15	0.15
(1,469)	1:A:151:PRO:HD2	1:A:179:VAL:HG11	11	0.15
(1,469)	1:A:151:PRO:HD2	1:A:179:VAL:HG12	11	0.15
(1,469)	1:A:151:PRO:HD2	1:A:179:VAL:HG13	11	0.15
(1,469)	1:A:151:PRO:HD3	1:A:179:VAL:HG11	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,469)	1:A:151:PRO:HD3	1:A:179:VAL:HG12	11	0.15
(1,469)	1:A:151:PRO:HD3	1:A:179:VAL:HG13	11	0.15
(1,384)	1:A:179:VAL:H	1:A:178:THR:HB	14	0.15
(2,4)	1:A:150:LEU:H	1:A:155:HIS:O	12	0.14
(2,3)	1:A:150:LEU:N	1:A:155:HIS:O	4	0.14
(2,3)	1:A:150:LEU:N	1:A:155:HIS:O	13	0.14
(1,505)	1:A:157:PHE:HB3	1:A:173:PRO:HD3	10	0.14
(1,505)	1:A:157:PHE:HB3	1:A:173:PRO:HD3	11	0.14
(1,502)	1:A:157:PHE:HA	1:A:158:HIS:HE1	5	0.14
(1,473)	1:A:152:ARG:HG3	1:A:177:LEU:HB2	3	0.14
(1,473)	1:A:152:ARG:HG3	1:A:177:LEU:HB2	4	0.14
(1,473)	1:A:152:ARG:HG3	1:A:177:LEU:HB2	6	0.14
(1,473)	1:A:152:ARG:HG3	1:A:177:LEU:HB2	11	0.14
(1,274)	1:A:162:VAL:H	1:A:158:HIS:HB2	7	0.14
(1,233)	1:A:158:HIS:H	1:A:157:PHE:HB2	8	0.14
(1,546)	1:A:161:CYS:HB2	1:A:158:HIS:HB3	9	0.13
(1,546)	1:A:161:CYS:HB2	1:A:158:HIS:HB3	14	0.13
(1,502)	1:A:157:PHE:HA	1:A:158:HIS:HE1	1	0.13
(1,502)	1:A:157:PHE:HA	1:A:158:HIS:HE1	2	0.13
(1,502)	1:A:157:PHE:HA	1:A:158:HIS:HE1	7	0.13
(1,502)	1:A:157:PHE:HA	1:A:158:HIS:HE1	9	0.13
(1,502)	1:A:157:PHE:HA	1:A:158:HIS:HE1	11	0.13
(1,502)	1:A:157:PHE:HA	1:A:158:HIS:HE1	15	0.13
(1,473)	1:A:152:ARG:HG3	1:A:177:LEU:HB2	8	0.13
(1,473)	1:A:152:ARG:HG3	1:A:177:LEU:HB2	12	0.13
(1,445)	1:A:149:PHE:HA	1:A:156:GLY:HA3	9	0.13
(1,365)	1:A:177:LEU:H	1:A:177:LEU:HB3	13	0.13
(1,274)	1:A:162:VAL:H	1:A:158:HIS:HB2	5	0.13
(1,13)	1:A:165:TRP:HE1	1:A:169:HIS:HB2	11	0.13
(2,7)	1:A:172:CYS:N	1:A:177:LEU:O	3	0.12
(2,3)	1:A:150:LEU:N	1:A:155:HIS:O	6	0.12
(1,582)	1:A:165:TRP:HD1	1:A:173:PRO:HD2	13	0.12
(1,546)	1:A:161:CYS:HB2	1:A:158:HIS:HB3	1	0.12
(1,546)	1:A:161:CYS:HB2	1:A:158:HIS:HB3	3	0.12
(1,546)	1:A:161:CYS:HB2	1:A:158:HIS:HB3	4	0.12
(1,546)	1:A:161:CYS:HB2	1:A:158:HIS:HB3	8	0.12
(1,546)	1:A:161:CYS:HB2	1:A:158:HIS:HB3	12	0.12
(1,546)	1:A:161:CYS:HB2	1:A:158:HIS:HB3	15	0.12
(1,502)	1:A:157:PHE:HA	1:A:158:HIS:HE1	3	0.12
(1,502)	1:A:157:PHE:HA	1:A:158:HIS:HE1	4	0.12
(1,502)	1:A:157:PHE:HA	1:A:158:HIS:HE1	6	0.12
(1,473)	1:A:152:ARG:HG3	1:A:177:LEU:HB2	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,406)	1:A:135:ALA:HB1	1:A:174:LEU:HD11	10	0.12
(1,406)	1:A:135:ALA:HB1	1:A:174:LEU:HD12	10	0.12
(1,406)	1:A:135:ALA:HB1	1:A:174:LEU:HD13	10	0.12
(1,406)	1:A:135:ALA:HB2	1:A:174:LEU:HD11	10	0.12
(1,406)	1:A:135:ALA:HB2	1:A:174:LEU:HD12	10	0.12
(1,406)	1:A:135:ALA:HB2	1:A:174:LEU:HD13	10	0.12
(1,406)	1:A:135:ALA:HB3	1:A:174:LEU:HD11	10	0.12
(1,406)	1:A:135:ALA:HB3	1:A:174:LEU:HD12	10	0.12
(1,406)	1:A:135:ALA:HB3	1:A:174:LEU:HD13	10	0.12
(1,388)	1:A:180:VAL:H	1:A:180:VAL:HB	8	0.12
(1,365)	1:A:177:LEU:H	1:A:177:LEU:HB3	5	0.12
(1,365)	1:A:177:LEU:H	1:A:177:LEU:HB3	14	0.12
(1,233)	1:A:158:HIS:H	1:A:157:PHE:HB2	12	0.12
(1,13)	1:A:165:TRP:HE1	1:A:169:HIS:HB2	8	0.12
(1,13)	1:A:165:TRP:HE1	1:A:169:HIS:HB2	12	0.12
(1,13)	1:A:165:TRP:HE1	1:A:169:HIS:HB2	13	0.12
(1,13)	1:A:165:TRP:HE1	1:A:169:HIS:HB2	15	0.12
(1,12)	1:A:165:TRP:HE1	1:A:169:HIS:HB3	6	0.12
(1,12)	1:A:165:TRP:HE1	1:A:169:HIS:HB3	9	0.12
(1,12)	1:A:165:TRP:HE1	1:A:169:HIS:HB3	13	0.12
(2,3)	1:A:150:LEU:N	1:A:155:HIS:O	15	0.11
(2,18)	1:A:166:LEU:H	1:A:162:VAL:O	5	0.11
(1,668)	1:A:149:PHE:HA	1:A:149:PHE:HD1	7	0.11
(1,582)	1:A:165:TRP:HD1	1:A:173:PRO:HD2	2	0.11
(1,582)	1:A:165:TRP:HD1	1:A:173:PRO:HD2	4	0.11
(1,582)	1:A:165:TRP:HD1	1:A:173:PRO:HD2	5	0.11
(1,582)	1:A:165:TRP:HD1	1:A:173:PRO:HD2	9	0.11
(1,582)	1:A:165:TRP:HD1	1:A:173:PRO:HD2	10	0.11
(1,582)	1:A:165:TRP:HD1	1:A:173:PRO:HD2	11	0.11
(1,582)	1:A:165:TRP:HD1	1:A:173:PRO:HD2	15	0.11
(1,549)	1:A:162:VAL:HB	1:A:147:ALA:HA	6	0.11
(1,546)	1:A:161:CYS:HB2	1:A:158:HIS:HB3	2	0.11
(1,546)	1:A:161:CYS:HB2	1:A:158:HIS:HB3	5	0.11
(1,546)	1:A:161:CYS:HB2	1:A:158:HIS:HB3	7	0.11
(1,445)	1:A:149:PHE:HA	1:A:156:GLY:HA3	6	0.11
(1,406)	1:A:135:ALA:HB1	1:A:174:LEU:HD11	9	0.11
(1,406)	1:A:135:ALA:HB1	1:A:174:LEU:HD12	9	0.11
(1,406)	1:A:135:ALA:HB1	1:A:174:LEU:HD13	9	0.11
(1,406)	1:A:135:ALA:HB2	1:A:174:LEU:HD11	9	0.11
(1,406)	1:A:135:ALA:HB2	1:A:174:LEU:HD12	9	0.11
(1,406)	1:A:135:ALA:HB2	1:A:174:LEU:HD13	9	0.11
(1,406)	1:A:135:ALA:HB3	1:A:174:LEU:HD11	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,406)	1:A:135:ALA:HB3	1:A:174:LEU:HD12	9	0.11
(1,406)	1:A:135:ALA:HB3	1:A:174:LEU:HD13	9	0.11
(1,388)	1:A:180:VAL:H	1:A:180:VAL:HB	1	0.11
(1,388)	1:A:180:VAL:H	1:A:180:VAL:HB	3	0.11
(1,388)	1:A:180:VAL:H	1:A:180:VAL:HB	9	0.11
(1,388)	1:A:180:VAL:H	1:A:180:VAL:HB	11	0.11
(1,365)	1:A:177:LEU:H	1:A:177:LEU:HB3	11	0.11
(1,274)	1:A:162:VAL:H	1:A:158:HIS:HB2	1	0.11
(1,274)	1:A:162:VAL:H	1:A:158:HIS:HB2	4	0.11
(1,274)	1:A:162:VAL:H	1:A:158:HIS:HB2	6	0.11
(1,274)	1:A:162:VAL:H	1:A:158:HIS:HB2	8	0.11
(1,274)	1:A:162:VAL:H	1:A:158:HIS:HB2	9	0.11
(1,274)	1:A:162:VAL:H	1:A:158:HIS:HB2	13	0.11
(1,274)	1:A:162:VAL:H	1:A:158:HIS:HB2	14	0.11
(1,274)	1:A:162:VAL:H	1:A:158:HIS:HB2	15	0.11
(1,273)	1:A:162:VAL:H	1:A:158:HIS:HB3	8	0.11
(1,191)	1:A:153:CYS:H	1:A:152:ARG:HB3	10	0.11
(1,191)	1:A:153:CYS:H	1:A:152:ARG:HB3	12	0.11
(1,13)	1:A:165:TRP:HE1	1:A:169:HIS:HB2	3	0.11
(1,13)	1:A:165:TRP:HE1	1:A:169:HIS:HB2	4	0.11
(1,13)	1:A:165:TRP:HE1	1:A:169:HIS:HB2	5	0.11
(1,13)	1:A:165:TRP:HE1	1:A:169:HIS:HB2	7	0.11
(1,13)	1:A:165:TRP:HE1	1:A:169:HIS:HB2	9	0.11
(1,13)	1:A:165:TRP:HE1	1:A:169:HIS:HB2	14	0.11
(1,12)	1:A:165:TRP:HE1	1:A:169:HIS:HB3	2	0.11
(1,12)	1:A:165:TRP:HE1	1:A:169:HIS:HB3	5	0.11
(1,12)	1:A:165:TRP:HE1	1:A:169:HIS:HB3	14	0.11

10 Dihedral-angle violation analysis

No dihedral-angle restraints found