wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2MTP
BMRB ID	:	25176
Title	:	The structure of Filamin repeat 21 bound to integrin
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Deposited on	:	2014-08-28

This is a wwPDB NMR Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

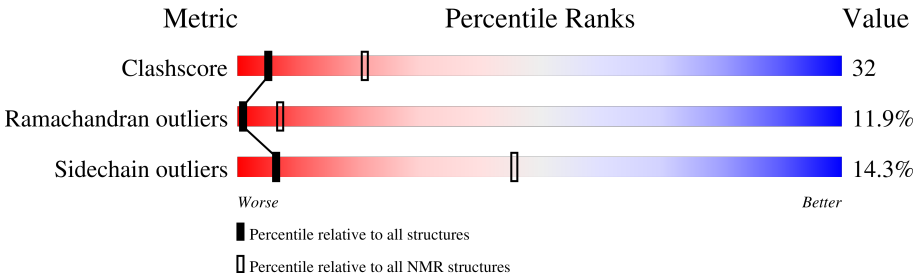
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 71%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	95	53% 40% 6%
2	B	21	24% 19% 5% 52%
3	C	47	9% 87%

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 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:2237-A:2330, B:988-B:997, C:746-C:751 (110)	0.82	17

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

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2464 atoms, of which 1195 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Filamin-A.

Mol	Chain	Residues	Atoms						Trace
1	A	95	Total	C	H	N	O	S	0
			1332	431	643	118	139	1	

- Molecule 2 is a protein called Integrin alpha-IIb.

Mol	Chain	Residues	Atoms					Trace
2	B	21	Total	C	H	N	O	0
			347	115	164	31	37	

- Molecule 3 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					Trace
3	C	47	Total	C	H	N	O	0
			785	250	388	72	75	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	717	LYS	LEU	engineered mutation	UNP P05106
C	718	LYS	LEU	engineered mutation	UNP P05106

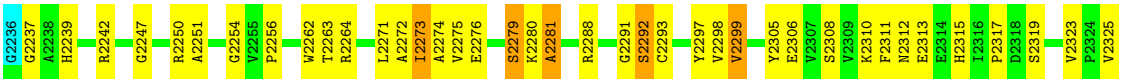
4 Residue-property plots

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.

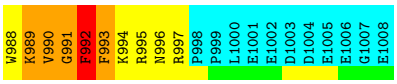
• Molecule 1: Filamin-A

Chain A:



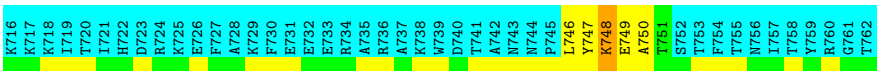
• Molecule 2: Integrin alpha-IIb

Chain B:



• Molecule 3: Integrin beta-3

Chain C:



4.2 Residue scores for the representative (medoid) model from the NMR ensemble

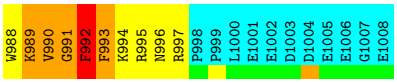
The representative model is number 17. Colouring as in section 4.1 above.

• Molecule 1: Filamin-A

Chain A:

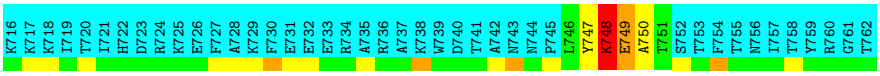
- Molecule 2: Integrin alpha-IIb

Chain B:



- Molecule 3: Integrin beta-3

Chain C:



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
X-PLOR NIH	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	1430
Number of shifts mapped to atoms	1429
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	71%

6 Model quality

6.1 Standard geometry

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	3.2±0.7
All	All	0	65

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	2288	ARG	Sidechain	20
1	A	2264	ARG	Sidechain	18
1	A	2242	ARG	Sidechain	14
1	A	2250	ARG	Sidechain	13

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	685	640	650	34±4
2	B	95	98	97	19±2
3	C	50	50	51	4±1
All	All	16600	15760	15960	1054

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 32.

5 of 248 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:989:LYS:O	2:B:991:GLY:N	1.02	1.92	2	20
2:B:993:PHE:CD1	2:B:994:LYS:N	0.72	2.58	15	20
2:B:992:PHE:CD1	2:B:993:PHE:N	0.69	2.60	1	20
2:B:992:PHE:CE1	2:B:993:PHE:CD1	0.67	2.83	7	20
2:B:992:PHE:CG	2:B:993:PHE:N	0.66	2.63	7	20

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	93/95 (98%)	73±2 (79±2%)	13±2 (14±2%)	7±1 (7±1%)	2	17
2	B	9/21 (43%)	4±0 (40±5%)	1±1 (9±8%)	5±1 (51±9%)	0	0
3	C	6/47 (13%)	3±1 (47±15%)	1±1 (24±12%)	2±1 (29±12%)	0	1
All	All	2160/3260 (66%)	1596 (74%)	306 (14%)	258 (12%)	1	7

5 of 25 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	2256	PRO	20
1	A	2281	ALA	20
1	A	2329	SER	20
2	B	990	VAL	20
2	B	991	GLY	20

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	69/69 (100%)	61±2 (89±3%)	8±2 (11±3%)	10 54
2	B	9/19 (47%)	6±1 (64±9%)	3±1 (36±9%)	1 8
3	C	5/41 (12%)	4±1 (80±11%)	1±1 (20±11%)	4 34
All	All	1660/2580 (64%)	1423 (86%)	237 (14%)	6 46

5 of 37 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	2279	SER	20
2	B	993	PHE	20
1	A	2273	ILE	18
2	B	992	PHE	18
3	C	748	LYS	17

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)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 71% for the well-defined parts and 67% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	1430
Number of shifts mapped to atoms	1429
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	148

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

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2315	HIS	HE2	7.103	.	.

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	142	-0.18 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	127	-0.21 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	133	0.00 ± 0.00	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 71%, i.e. 1004 atoms were assigned a chemical shift out of a possible 1407. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	417/548 (76%)	225/226 (100%)	100/220 (45%)	92/102 (90%)
Sidechain	559/736 (76%)	378/478 (79%)	181/230 (79%)	0/28 (0%)
Aromatic	28/123 (23%)	27/62 (44%)	1/59 (2%)	0/2 (0%)
Overall	1004/1407 (71%)	630/766 (82%)	282/509 (55%)	92/132 (70%)

7.1.4 Statistically unusual chemical shifts

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

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	2321	PHE	CE2	51.05	124.80 – 136.72	-66.9
1	A	2313	GLU	N	17.84	103.74 – 137.78	-30.2
1	A	2247	GLY	N	12.01	91.59 – 127.52	-27.1
1	A	2279	SER	N	26.47	99.14 – 133.45	-26.2
1	C	761	GLY	N	17.20	91.59 – 127.52	-25.7
1	A	2267	GLY	N	17.46	91.59 – 127.52	-25.6
1	A	2270	GLY	N	17.79	91.59 – 127.52	-25.5
1	A	2319	SER	N	29.28	99.14 – 133.45	-25.4
1	A	2244	GLY	N	18.65	91.59 – 127.52	-25.3
1	A	2303	GLY	N	19.32	91.59 – 127.52	-25.1
1	A	2301	GLU	N	37.06	103.74 – 137.78	-24.6
1	A	2265	GLU	N	37.59	103.74 – 137.78	-24.4
1	A	2237	GLY	N	22.00	91.59 – 127.52	-24.4
1	A	2254	GLY	N	22.89	91.59 – 127.52	-24.1
1	A	2291	GLY	N	23.41	91.59 – 127.52	-24.0
1	A	2236	GLY	N	23.65	91.59 – 127.52	-23.9
1	A	2260	SER	N	35.00	99.14 – 133.45	-23.7
1	A	2250	ARG	N	35.91	102.91 – 138.82	-23.7
1	A	2269	GLY	N	24.73	91.59 – 127.52	-23.6
1	A	2258	GLU	N	42.47	103.74 – 137.78	-23.0
1	A	2318	ASP	N	35.40	102.08 – 139.36	-22.9
1	A	2327	SER	N	37.84	99.14 – 133.45	-22.9
1	A	2300	GLN	N	41.20	102.61 – 137.42	-22.6
1	A	2249	GLU	N	44.26	103.74 – 137.78	-22.5

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List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	2239	HIS	N	29.47	99.59 – 139.87	-22.4
1	A	2329	SER	N	39.93	99.14 – 133.45	-22.3
1	C	752	SER	N	40.29	99.14 – 133.45	-22.2
1	A	2292	SER	N	40.26	99.14 – 133.45	-22.2
1	A	2314	GLU	N	45.32	103.74 – 137.78	-22.2
1	A	2248	LEU	N	37.83	102.77 – 140.89	-22.0
1	A	2245	GLY	N	30.39	91.59 – 127.52	-22.0
1	A	2266	ALA	N	47.76	106.13 – 140.55	-22.0
1	A	2251	ALA	N	47.79	106.13 – 140.55	-21.9
1	A	2277	GLY	N	30.98	91.59 – 127.52	-21.9
1	A	2306	GLU	N	46.48	103.74 – 137.78	-21.8
1	C	743	ASN	N	35.10	99.66 – 138.23	-21.7
1	A	2290	ASP	N	39.77	102.08 – 139.36	-21.7
1	A	2240	LYS	N	41.60	102.74 – 139.42	-21.7
1	C	736	ARG	N	43.35	102.91 – 138.82	-21.6
1	A	2252	GLU	N	47.30	103.74 – 137.78	-21.6
1	A	2294	GLY	N	32.30	91.59 – 127.52	-21.5
1	A	2268	ALA	N	50.07	106.13 – 140.55	-21.3
1	C	732	GLU	N	48.46	103.74 – 137.78	-21.2
1	A	2238	ALA	N	50.29	106.13 – 140.55	-21.2
1	C	738	LYS	N	43.35	102.74 – 139.42	-21.2
1	C	726	GLU	N	48.65	103.74 – 137.78	-21.2
1	C	731	GLU	N	49.24	103.74 – 137.78	-21.0
1	C	733	GLU	N	49.96	103.74 – 137.78	-20.8
1	C	729	LYS	N	45.31	102.74 – 139.42	-20.7
1	A	2282	GLU	N	50.59	103.74 – 137.78	-20.6
1	A	2289	LYS	N	45.71	102.74 – 139.42	-20.6
1	A	2259	PHE	N	36.48	99.93 – 140.82	-20.5
1	C	734	ARG	N	47.85	102.91 – 138.82	-20.3
1	C	749	GLU	N	51.60	103.74 – 137.78	-20.3
1	A	2280	LYS	N	46.78	102.74 – 139.42	-20.3
1	C	735	ALA	N	53.95	106.13 – 140.55	-20.2
1	A	2243	ALA	N	54.00	106.13 – 140.55	-20.1
1	A	2286	GLU	N	52.23	103.74 – 137.78	-20.1
1	A	2304	ASP	N	46.08	102.08 – 139.36	-20.0
1	C	746	LEU	N	45.76	102.77 – 140.89	-20.0
1	A	2264	ARG	N	49.34	102.91 – 138.82	-19.9
1	C	737	ALA	N	55.49	106.13 – 140.55	-19.7
1	C	724	ARG	N	50.63	102.91 – 138.82	-19.6
1	A	2272	ALA	N	56.20	106.13 – 140.55	-19.5
1	A	2297	TYR	N	41.14	100.12 – 140.79	-19.5
1	A	2330	GLY	N	39.48	91.59 – 127.52	-19.5

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List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	C	728	ALA	N	57.03	106.13 – 140.55	-19.3
1	A	2316	ILE	N	41.20	100.55 – 142.30	-19.2
1	A	2242	ARG	N	51.90	102.91 – 138.82	-19.2
1	A	2308	SER	N	50.88	99.14 – 133.45	-19.1
1	C	723	ASP	N	49.65	102.08 – 139.36	-19.1
1	C	751	THR	N	26.10	91.89 – 138.78	-19.0
1	C	744	ASN	N	45.76	99.66 – 138.23	-19.0
1	A	2310	LYS	N	51.59	102.74 – 139.42	-18.9
1	C	725	LYS	N	51.71	102.74 – 139.42	-18.9
1	A	2281	ALA	N	58.65	106.13 – 140.55	-18.8
1	C	740	ASP	N	50.85	102.08 – 139.36	-18.7
1	C	742	ALA	N	58.82	106.13 – 140.55	-18.7
1	A	2284	SER	N	52.20	99.14 – 133.45	-18.7
1	C	739	TRP	N	47.20	101.51 – 141.60	-18.6
1	C	747	TYR	N	45.30	100.12 – 140.79	-18.5
1	A	2288	ARG	N	54.62	102.91 – 138.82	-18.4
1	C	716	LYS	N	53.66	102.74 – 139.42	-18.4
1	A	2253	ALA	N	60.10	106.13 – 140.55	-18.4
1	A	2296	ALA	N	60.10	106.13 – 140.55	-18.4
1	C	717	LYS	N	53.77	102.74 – 139.42	-18.4
1	A	2298	VAL	N	41.09	99.23 – 142.92	-18.3
1	A	2276	GLU	N	58.49	103.74 – 137.78	-18.3
1	C	741	THR	N	29.61	91.89 – 138.78	-18.3
1	C	750	ALA	N	60.48	106.13 – 140.55	-18.3
1	A	2261	ILE	N	45.26	100.55 – 142.30	-18.2
1	C	748	LYS	N	54.75	102.74 – 139.42	-18.1
1	C	756	ASN	N	49.59	99.66 – 138.23	-18.0
1	C	727	PHE	N	47.07	99.93 – 140.82	-17.9
1	A	2293	CYS	N	41.57	98.14 – 142.06	-17.9
1	A	2271	LEU	N	53.76	102.77 – 140.89	-17.9
1	C	730	PHE	N	47.72	99.93 – 140.82	-17.8
1	C	718	LYS	N	56.29	102.74 – 139.42	-17.7
1	A	2274	ALA	N	62.57	106.13 – 140.55	-17.7
1	C	760	ARG	N	58.14	102.91 – 138.82	-17.5
1	A	2321	PHE	N	48.97	99.93 – 140.82	-17.5
1	C	755	THR	N	33.93	91.89 – 138.78	-17.4
1	C	753	THR	N	34.07	91.89 – 138.78	-17.3
1	A	2285	PHE	N	49.50	99.93 – 140.82	-17.3
1	A	2311	PHE	N	49.73	99.93 – 140.82	-17.3
1	A	2263	THR	N	34.39	91.89 – 138.78	-17.3
1	A	2305	TYR	N	50.29	100.12 – 140.79	-17.2
1	C	757	ILE	N	49.44	100.55 – 142.30	-17.2

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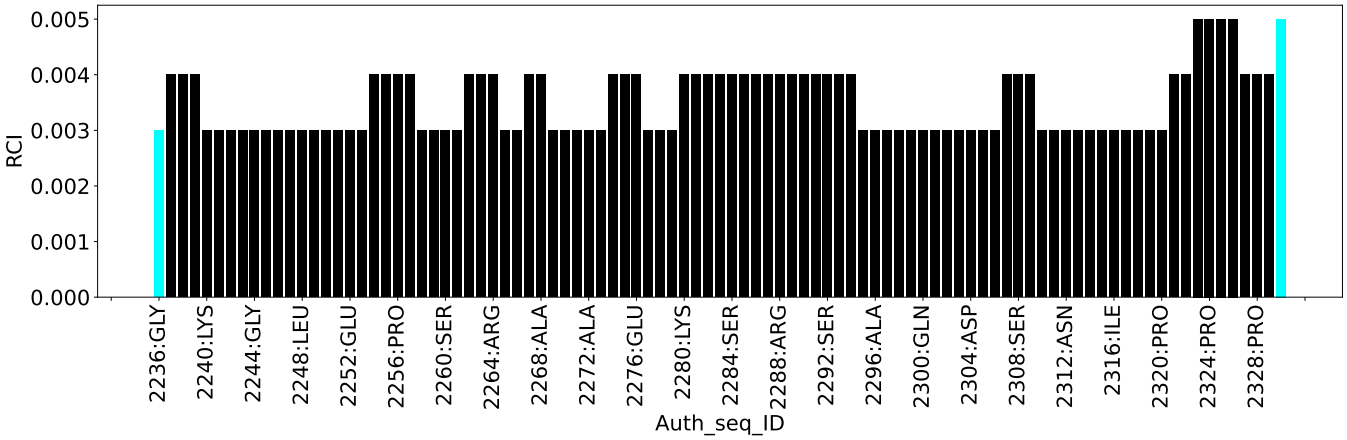
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	2315	HIS	N	51.59	99.59 – 139.87	-16.9
1	A	2299	VAL	N	47.91	99.23 – 142.92	-16.8
1	C	754	PHE	N	51.97	99.93 – 140.82	-16.7
1	A	2275	VAL	N	48.20	99.23 – 142.92	-16.7
1	A	2287	ASP	N	58.65	102.08 – 139.36	-16.6
1	A	2257	ALA	N	67.07	106.13 – 140.55	-16.4
1	A	2273	ILE	N	53.38	100.55 – 142.30	-16.3
1	C	722	HIS	N	54.39	99.59 – 139.87	-16.2
1	A	2326	ALA	N	67.77	106.13 – 140.55	-16.1
1	A	2255	VAL	N	51.02	99.23 – 142.92	-16.0
1	C	721	ILE	N	54.59	100.55 – 142.30	-16.0
1	C	762	THR	N	41.00	91.89 – 138.78	-15.8
1	C	758	THR	N	41.13	91.89 – 138.78	-15.8
1	A	2241	VAL	N	51.95	99.23 – 142.92	-15.8
1	C	759	TYR	N	56.19	100.12 – 140.79	-15.8
1	C	719	ILE	N	55.91	100.55 – 142.30	-15.7
1	A	2295	VAL	N	54.21	99.23 – 142.92	-15.3
1	A	2283	ILE	N	57.63	100.55 – 142.30	-15.3
1	A	2309	VAL	N	54.87	99.23 – 142.92	-15.2
1	A	2322	VAL	N	55.13	99.23 – 142.92	-15.1
1	A	2312	ASN	N	60.81	99.66 – 138.23	-15.1
1	A	2262	TRP	N	61.30	101.51 – 141.60	-15.0
1	C	720	THR	N	45.51	91.89 – 138.78	-14.9
1	A	2325	VAL	N	57.87	99.23 – 142.92	-14.5
1	C	729	LYS	CD	43.08	23.50 – 34.42	12.9
1	C	738	LYS	CD	43.08	23.50 – 34.42	12.9
1	A	2307	VAL	N	66.60	99.23 – 142.92	-12.5
1	A	2323	VAL	N	68.80	99.23 – 142.92	-12.0
1	A	2273	ILE	CG2	29.60	10.93 – 24.12	9.2
1	A	2261	ILE	CG2	27.81	10.93 – 24.12	7.8
1	A	2283	ILE	CG2	27.81	10.93 – 24.12	7.8
1	C	719	ILE	CG2	26.99	10.93 – 24.12	7.2
1	C	721	ILE	CG2	26.99	10.93 – 24.12	7.2
1	C	757	ILE	CG2	26.99	10.93 – 24.12	7.2
1	A	2273	ILE	CD1	25.14	5.18 – 21.60	7.2
1	A	2264	ARG	CD	49.65	38.57 – 47.75	7.1
1	A	2278	PRO	CD	43.01	45.11 – 55.58	-7.0
1	A	2310	LYS	CG	32.61	19.35 – 30.45	7.0
1	C	729	LYS	HD2	3.02	0.58 – 2.64	6.9
1	C	738	LYS	HD2	3.02	0.58 – 2.64	6.9

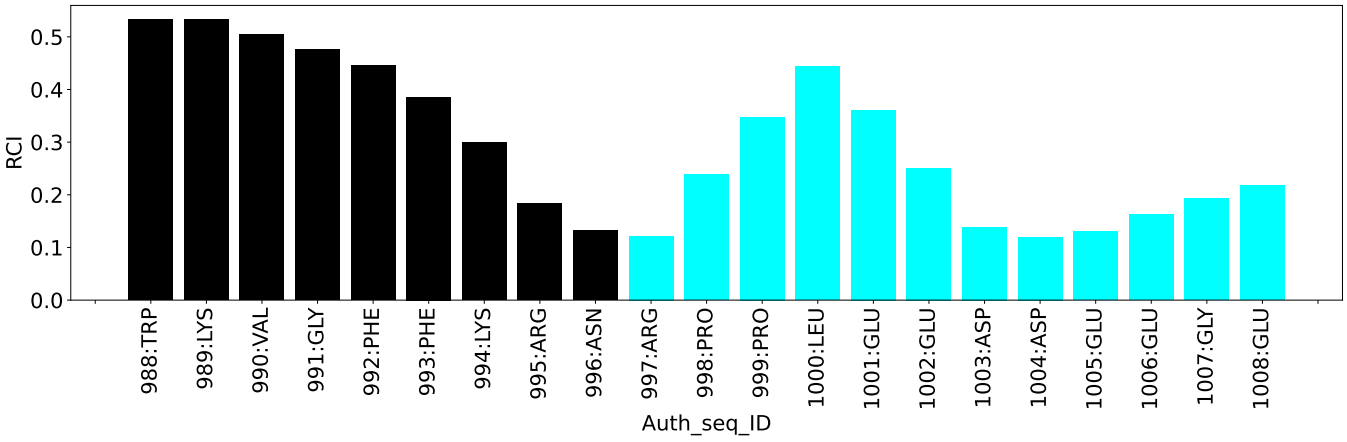
7.1.5 Random Coil Index (RCI) plots

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

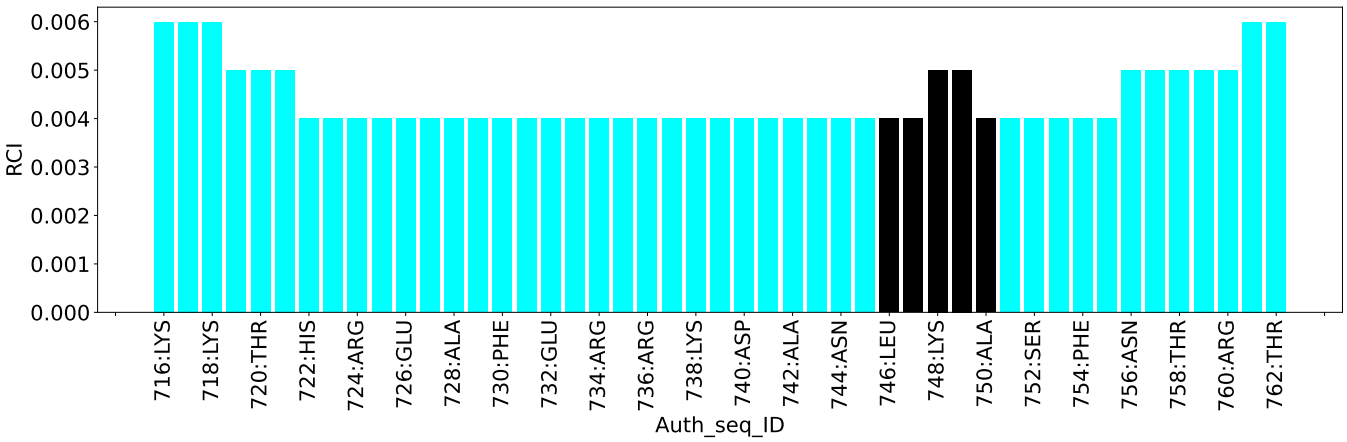
Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



Random coil index (RCI) for chain C:


RCI
0.006
0.005
0.004
0.003
0.002
0.001
0.000
716:LYS
718:LYS
720:THR
722:HIS
724:ARG
726:GLU
728:ALA
730:PHE
732:GLU
734:ARG
736:ARG
738:LYS
740:ASP
742:ALA
744:ASN
746:LEU
748:LYS
750:ALA
752:SER
754:PHE
756:ASN
758:THR
760:ARG
762:THR
Auth_seq_ID

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	1341
Intra-residue (|i-j|=0)	425
Sequential (|i-j|=1)	483
Medium range (|i-j|>1 and |i-j|<5)	172
Long range (|i-j|≥5)	230
Inter-chain	31
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	122
Number of unmapped restraints	6
Number of restraints per residue	9.0
Number of long range restraints per residue[1]	1.4

[1]Long 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)	48.0	0.2
0.2-0.5 (Medium)	26.0	0.5
>0.5 (Large)	13.8	3.55

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)	15.9	10.0
10.0-20.0 (Medium)	6.4	19.8
>20.0 (Large)	5.3	87.4

9 Distance violation analysis (i)

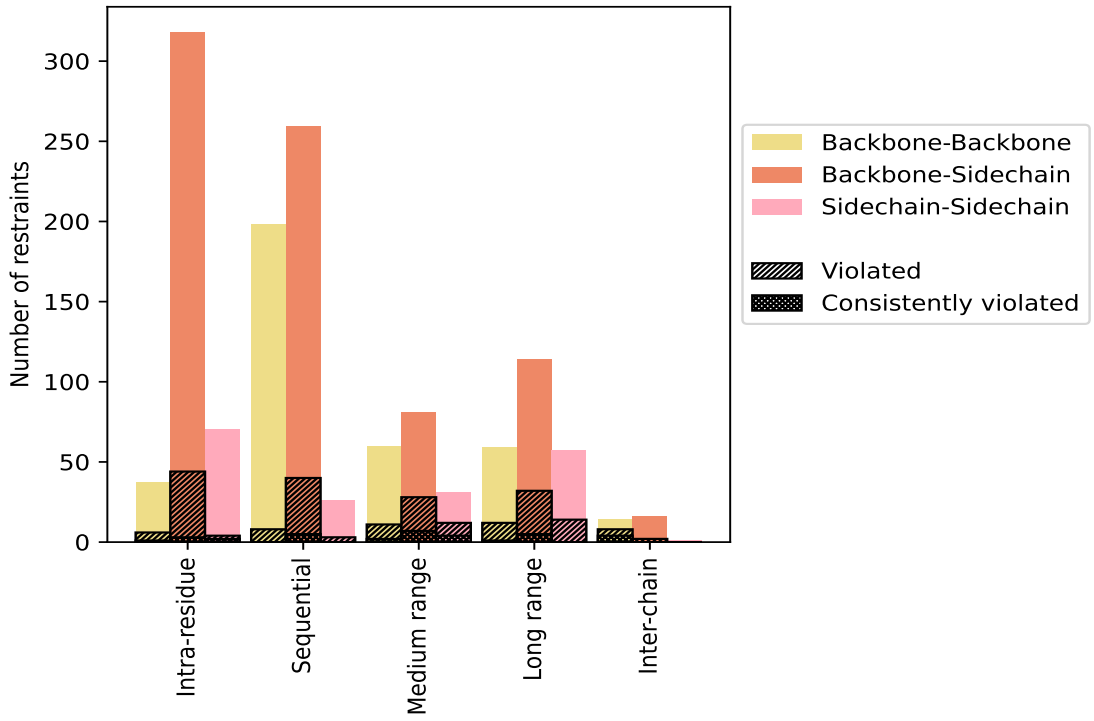
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	425	31.7	54	12.7	4.0	6	1.4	0.4
Backbone-Backbone	37	2.8	6	16.2	0.4	1	2.7	0.1
Backbone-Sidechain	318	23.7	44	13.8	3.3	3	0.9	0.2
Sidechain-Sidechain	70	5.2	4	5.7	0.3	2	2.9	0.1
Sequential (|i-j|=1)	483	36.0	51	10.6	3.8	5	1.0	0.4
Backbone-Backbone	198	14.8	8	4.0	0.6	0	0.0	0.0
Backbone-Sidechain	259	19.3	40	15.4	3.0	5	1.9	0.4
Sidechain-Sidechain	26	1.9	3	11.5	0.2	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	172	12.8	51	29.7	3.8	13	7.6	1.0
Backbone-Backbone	60	4.5	11	18.3	0.8	2	3.3	0.1
Backbone-Sidechain	81	6.0	28	34.6	2.1	7	8.6	0.5
Sidechain-Sidechain	31	2.3	12	38.7	0.9	4	12.9	0.3
Long range (|i-j|≥5)	230	17.2	58	25.2	4.3	6	2.6	0.4
Backbone-Backbone	59	4.4	12	20.3	0.9	1	1.7	0.1
Backbone-Sidechain	114	8.5	32	28.1	2.4	5	4.4	0.4
Sidechain-Sidechain	57	4.3	14	24.6	1.0	0	0.0	0.0
Inter-chain	31	2.3	10	32.3	0.7	4	12.9	0.3
Backbone-Backbone	14	1.0	8	57.1	0.6	4	28.6	0.3
Backbone-Sidechain	16	1.2	2	12.5	0.1	0	0.0	0.0
Sidechain-Sidechain	1	0.1	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1341	100.0	224	16.7	16.7	34	2.5	2.5
Backbone-Backbone	368	27.4	45	12.2	3.4	8	2.2	0.6
Backbone-Sidechain	788	58.8	146	18.5	10.9	20	2.5	1.5
Sidechain-Sidechain	185	13.8	33	17.8	2.5	6	3.2	0.4

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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	18	15	21	26	6	86	0.38	3.09	0.56	0.19
2	17	19	27	23	8	94	0.46	2.92	0.64	0.2
3	17	16	19	23	8	83	0.34	2.92	0.45	0.18
4	14	14	19	26	7	80	0.45	3.16	0.65	0.2
5	12	20	26	28	6	92	0.42	3.11	0.59	0.2
6	19	17	22	25	6	89	0.38	3.08	0.57	0.18
7	14	20	21	20	7	82	0.41	3.11	0.6	0.21
8	18	18	18	23	9	86	0.32	2.51	0.42	0.18
9	17	21	23	25	7	93	0.36	2.52	0.47	0.19
10	17	18	19	26	8	88	0.41	3.55	0.6	0.21
11	16	22	23	26	7	94	0.46	3.14	0.65	0.2

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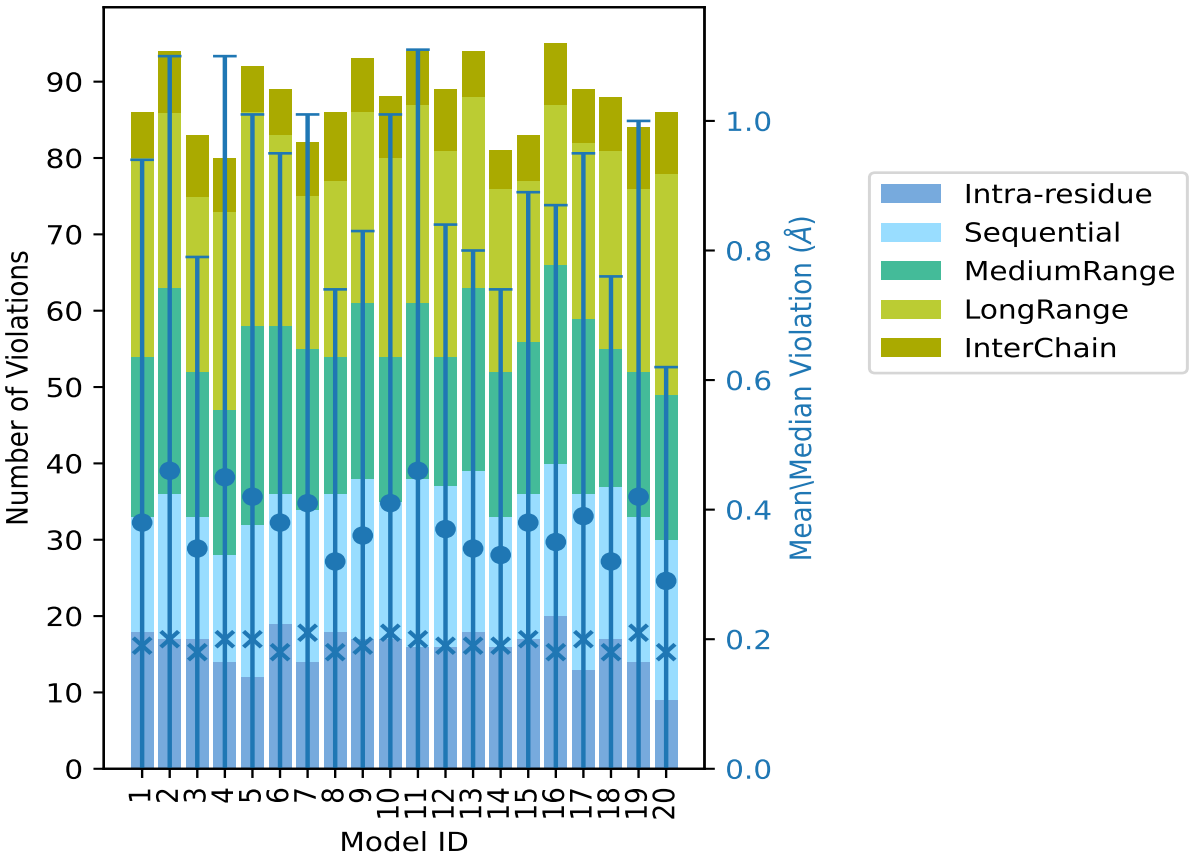
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	16	21	17	27	8	89	0.37	2.78	0.47	0.19
13	18	21	24	25	6	94	0.34	2.95	0.46	0.19
14	16	17	19	24	5	81	0.33	2.87	0.41	0.19
15	17	19	20	21	6	83	0.38	3.04	0.51	0.2
16	20	20	26	21	8	95	0.35	3.09	0.52	0.18
17	13	23	23	23	7	89	0.39	3.02	0.56	0.2
18	17	20	18	26	7	88	0.32	3.08	0.44	0.18
19	14	19	19	24	8	84	0.42	3.03	0.58	0.21
20	9	21	19	29	8	86	0.29	1.8	0.33	0.18

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

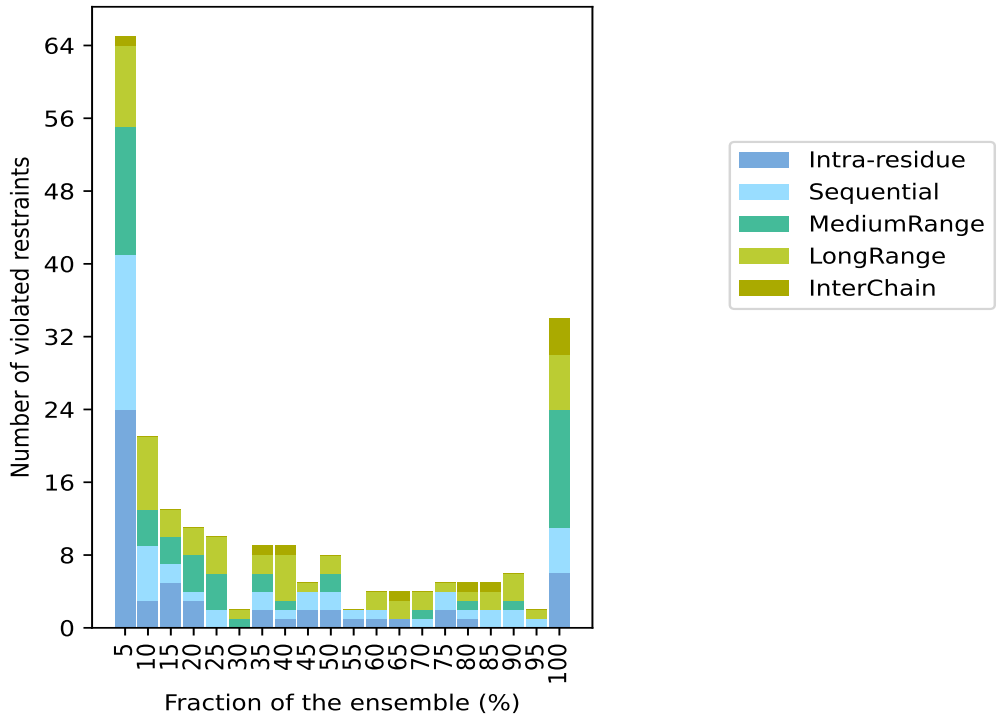
9.3 Distance violation statistics for the ensemble (i)

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, 1117(IR:371, SQ:432, MR:121, LR:172, IC:21) 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]	%
24	17	14	9	1	65	1	5.0
3	6	4	8	0	21	2	10.0
5	2	3	3	0	13	3	15.0
3	1	4	3	0	11	4	20.0
0	2	4	4	0	10	5	25.0
0	0	1	1	0	2	6	30.0
2	2	2	2	1	9	7	35.0
1	1	1	5	1	9	8	40.0
2	2	0	1	0	5	9	45.0
2	2	2	2	0	8	10	50.0
1	1	0	0	0	2	11	55.0
1	1	0	2	0	4	12	60.0
1	0	0	2	1	4	13	65.0
0	1	1	2	0	4	14	70.0
2	2	0	1	0	5	15	75.0
1	1	1	1	1	5	16	80.0
0	2	0	2	1	5	17	85.0
0	2	1	3	0	6	18	90.0
0	1	0	1	0	2	19	95.0
6	5	13	6	4	34	20	100.0

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

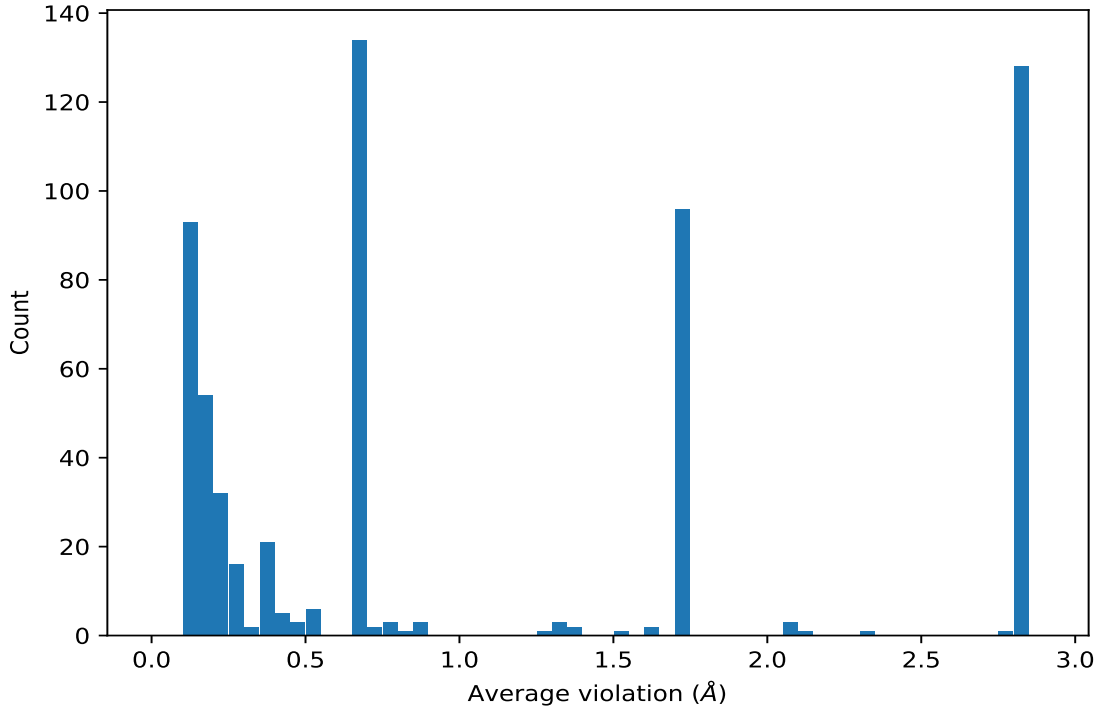
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance 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



9.4.2 Table: Most violated distance restraints

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation 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)
(2,1)	3:C:716:LYS:N	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:716:LYS:N	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:716:LYS:N	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:716:LYS:N	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:716:LYS:NZ	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:716:LYS:NZ	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:716:LYS:NZ	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:716:LYS:NZ	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:716:LYS:O	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:716:LYS:O	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:716:LYS:O	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:716:LYS:O	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:717:LYS:N	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:717:LYS:N	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:717:LYS:N	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:717:LYS:N	1:A:2239:HIS:O	20	2.82	0.31	2.92

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,1)	3:C:717:LYS:NZ	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:717:LYS:NZ	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:717:LYS:NZ	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:717:LYS:NZ	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:717:LYS:O	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:717:LYS:O	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:717:LYS:O	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:717:LYS:O	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:718:LYS:N	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:718:LYS:N	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:718:LYS:N	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:718:LYS:N	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:718:LYS:NZ	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:718:LYS:NZ	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:718:LYS:NZ	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:718:LYS:NZ	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:718:LYS:O	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:718:LYS:O	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:718:LYS:O	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:718:LYS:O	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:719:ILE:N	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:719:ILE:N	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:719:ILE:N	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:719:ILE:N	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:719:ILE:O	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:719:ILE:O	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:719:ILE:O	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:719:ILE:O	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:720:THR:N	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:720:THR:N	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:720:THR:N	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:720:THR:N	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:720:THR:O	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:720:THR:O	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:720:THR:O	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:720:THR:O	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:720:THR:OG1	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:720:THR:OG1	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:720:THR:OG1	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:720:THR:OG1	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:721:ILE:N	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:721:ILE:N	1:A:2239:HIS:ND1	20	2.82	0.31	2.92

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,1)	3:C:721:ILE:N	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:721:ILE:N	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:721:ILE:O	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:721:ILE:O	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:721:ILE:O	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:721:ILE:O	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:722:HIS:N	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:722:HIS:N	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:722:HIS:N	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:722:HIS:N	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:722:HIS:ND1	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:722:HIS:ND1	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:722:HIS:ND1	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:722:HIS:ND1	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:722:HIS:NE2	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:722:HIS:NE2	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:722:HIS:NE2	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:722:HIS:NE2	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:722:HIS:O	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:722:HIS:O	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:722:HIS:O	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:722:HIS:O	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:723:ASP:N	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:723:ASP:N	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:723:ASP:N	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:723:ASP:N	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:723:ASP:O	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:723:ASP:O	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:723:ASP:O	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:723:ASP:O	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:723:ASP:OD1	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:723:ASP:OD1	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:723:ASP:OD1	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:723:ASP:OD1	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:723:ASP:OD2	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:723:ASP:OD2	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:723:ASP:OD2	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:723:ASP:OD2	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:724:ARG:N	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:724:ARG:N	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:724:ARG:N	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:724:ARG:N	1:A:2239:HIS:O	20	2.82	0.31	2.92

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,1)	3:C:724:ARG:NE	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:724:ARG:NE	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:724:ARG:NE	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:724:ARG:NE	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:724:ARG:NH1	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:724:ARG:NH1	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:724:ARG:NH1	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:724:ARG:NH1	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:724:ARG:NH2	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:724:ARG:NH2	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:724:ARG:NH2	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:724:ARG:NH2	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:724:ARG:O	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:724:ARG:O	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:724:ARG:O	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:724:ARG:O	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:725:LYS:N	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:725:LYS:N	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:725:LYS:N	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:725:LYS:N	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:725:LYS:NZ	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:725:LYS:NZ	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:725:LYS:NZ	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:725:LYS:NZ	1:A:2239:HIS:O	20	2.82	0.31	2.92
(2,1)	3:C:725:LYS:O	1:A:2239:HIS:N	20	2.82	0.31	2.92
(2,1)	3:C:725:LYS:O	1:A:2239:HIS:ND1	20	2.82	0.31	2.92
(2,1)	3:C:725:LYS:O	1:A:2239:HIS:NE2	20	2.82	0.31	2.92
(2,1)	3:C:725:LYS:O	1:A:2239:HIS:O	20	2.82	0.31	2.92
(1,927)	2:B:995:ARG:HB2	2:B:992:PHE:HE1	20	0.85	0.02	0.85
(1,927)	2:B:995:ARG:HB2	2:B:992:PHE:HE2	20	0.85	0.02	0.85
(1,921)	2:B:995:ARG:HG2	2:B:996:ASN:H	20	0.78	0.1	0.78
(1,921)	2:B:995:ARG:HG3	2:B:996:ASN:H	20	0.78	0.1	0.78
(1,928)	2:B:995:ARG:HB3	2:B:996:ASN:H	20	0.71	0.05	0.72
(1,894)	2:B:993:PHE:HE1	2:B:989:LYS:HA	20	0.51	0.03	0.5
(1,894)	2:B:993:PHE:HE2	2:B:989:LYS:HA	20	0.51	0.03	0.5
(1,909)	2:B:993:PHE:HE1	2:B:995:ARG:HB2	20	0.5	0.02	0.51
(1,909)	2:B:993:PHE:HE2	2:B:995:ARG:HB2	20	0.5	0.02	0.51
(1,913)	2:B:994:LYS:HA	2:B:992:PHE:HE1	20	0.5	0.03	0.5
(1,913)	2:B:994:LYS:HA	2:B:992:PHE:HE2	20	0.5	0.03	0.5
(1,888)	2:B:993:PHE:HE1	2:B:995:ARG:HA	20	0.48	0.04	0.48
(1,888)	2:B:993:PHE:HE2	2:B:995:ARG:HA	20	0.48	0.04	0.48
(1,814)	2:B:988:TRP:HZ2	2:B:988:TRP:HB3	20	0.41	0.04	0.44

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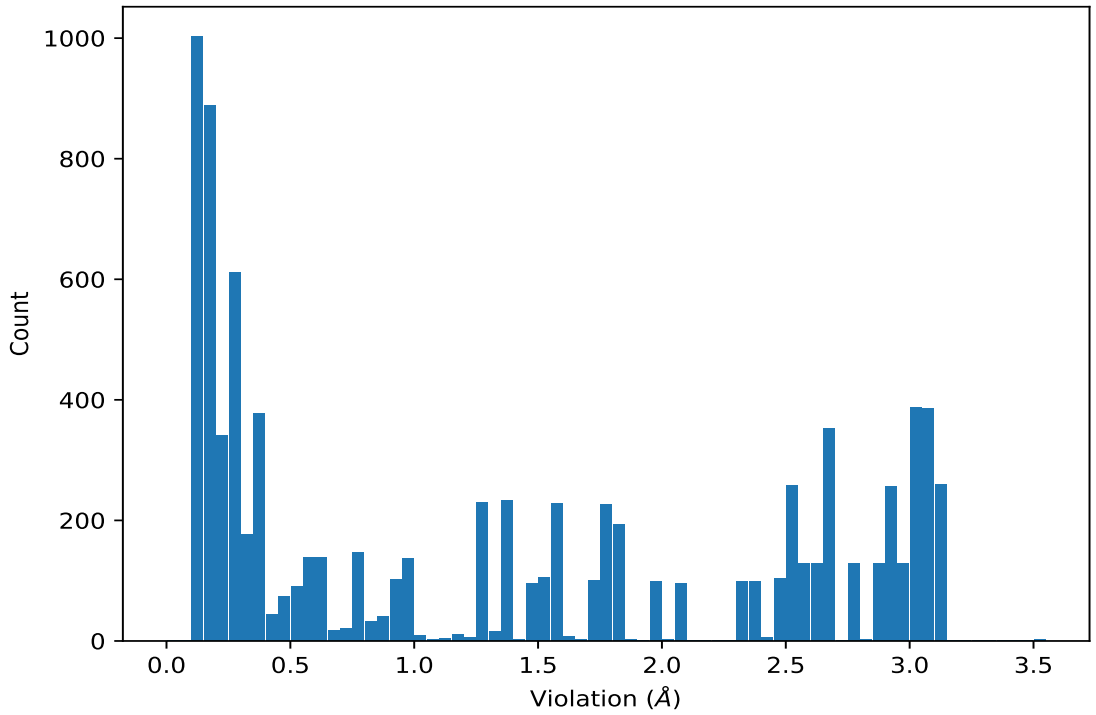
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,864)	2:B:992:PHE:HB2	2:B:995:ARG:HA	20	0.41	0.04	0.42

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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



9.5.2 Table : All distance violations

The following table provides the 10 worst performing restraints, sorted by the violation 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)
(1,365)	1:A:2273:ILE:HD11	1:A:2285:PHE:HE2	10	3.55
(1,365)	1:A:2273:ILE:HD12	1:A:2285:PHE:HE2	10	3.55
(1,365)	1:A:2273:ILE:HD13	1:A:2285:PHE:HE2	10	3.55
(1,754)	1:A:2319:SER:HB2	1:A:2321:PHE:HD2	4	3.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,365)	1:A:2273:ILE:HD11	1:A:2285:PHE:HE2	11	3.14
(1,365)	1:A:2273:ILE:HD12	1:A:2285:PHE:HE2	11	3.14
(1,365)	1:A:2273:ILE:HD13	1:A:2285:PHE:HE2	11	3.14
(2,1)	3:C:716:LYS:N	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:716:LYS:N	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:716:LYS:N	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:716:LYS:N	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:716:LYS:NZ	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:716:LYS:NZ	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:716:LYS:NZ	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:716:LYS:NZ	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:716:LYS:O	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:716:LYS:O	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:716:LYS:O	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:716:LYS:O	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:717:LYS:N	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:717:LYS:N	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:717:LYS:N	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:717:LYS:N	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:717:LYS:NZ	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:717:LYS:NZ	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:717:LYS:NZ	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:717:LYS:NZ	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:717:LYS:O	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:717:LYS:O	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:717:LYS:O	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:717:LYS:O	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:718:LYS:N	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:718:LYS:N	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:718:LYS:N	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:718:LYS:N	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:718:LYS:NZ	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:718:LYS:NZ	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:718:LYS:NZ	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:718:LYS:NZ	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:718:LYS:O	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:718:LYS:O	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:718:LYS:O	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:718:LYS:O	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:719:ILE:N	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:719:ILE:N	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:719:ILE:N	1:A:2239:HIS:NE2	10	3.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	3:C:719:ILE:N	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:719:ILE:O	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:719:ILE:O	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:719:ILE:O	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:719:ILE:O	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:720:THR:N	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:720:THR:N	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:720:THR:N	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:720:THR:N	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:720:THR:O	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:720:THR:O	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:720:THR:O	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:720:THR:O	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:720:THR:OG1	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:720:THR:OG1	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:720:THR:OG1	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:720:THR:OG1	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:721:ILE:N	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:721:ILE:N	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:721:ILE:N	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:721:ILE:N	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:721:ILE:O	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:721:ILE:O	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:721:ILE:O	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:721:ILE:O	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:722:HIS:N	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:722:HIS:N	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:722:HIS:N	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:722:HIS:N	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:722:HIS:ND1	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:722:HIS:ND1	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:722:HIS:ND1	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:722:HIS:ND1	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:722:HIS:NE2	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:722:HIS:NE2	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:722:HIS:NE2	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:722:HIS:NE2	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:722:HIS:O	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:722:HIS:O	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:722:HIS:O	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:722:HIS:O	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:723:ASP:N	1:A:2239:HIS:N	10	3.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	3:C:723:ASP:N	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:723:ASP:N	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:723:ASP:N	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:723:ASP:O	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:723:ASP:O	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:723:ASP:O	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:723:ASP:O	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:723:ASP:OD1	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:723:ASP:OD1	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:723:ASP:OD1	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:723:ASP:OD1	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:723:ASP:OD2	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:723:ASP:OD2	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:723:ASP:OD2	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:723:ASP:OD2	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:724:ARG:N	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:724:ARG:N	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:724:ARG:N	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:724:ARG:N	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:724:ARG:NE	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:724:ARG:NE	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:724:ARG:NE	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:724:ARG:NE	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:724:ARG:NH1	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:724:ARG:NH1	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:724:ARG:NH1	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:724:ARG:NH1	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:724:ARG:NH2	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:724:ARG:NH2	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:724:ARG:NH2	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:724:ARG:NH2	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:724:ARG:O	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:724:ARG:O	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:724:ARG:O	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:724:ARG:O	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:725:LYS:N	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:725:LYS:N	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:725:LYS:N	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:725:LYS:N	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:725:LYS:NZ	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:725:LYS:NZ	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:725:LYS:NZ	1:A:2239:HIS:NE2	10	3.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	3:C:725:LYS:NZ	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:725:LYS:O	1:A:2239:HIS:N	10	3.12
(2,1)	3:C:725:LYS:O	1:A:2239:HIS:ND1	10	3.12
(2,1)	3:C:725:LYS:O	1:A:2239:HIS:NE2	10	3.12
(2,1)	3:C:725:LYS:O	1:A:2239:HIS:O	10	3.12
(2,1)	3:C:716:LYS:N	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:716:LYS:N	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:716:LYS:N	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:716:LYS:N	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:716:LYS:NZ	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:716:LYS:NZ	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:716:LYS:NZ	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:716:LYS:NZ	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:716:LYS:O	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:716:LYS:O	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:716:LYS:O	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:716:LYS:O	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:717:LYS:N	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:717:LYS:N	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:717:LYS:N	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:717:LYS:N	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:717:LYS:NZ	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:717:LYS:NZ	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:717:LYS:NZ	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:717:LYS:NZ	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:717:LYS:O	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:717:LYS:O	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:717:LYS:O	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:717:LYS:O	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:718:LYS:N	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:718:LYS:N	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:718:LYS:N	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:718:LYS:N	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:718:LYS:NZ	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:718:LYS:NZ	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:718:LYS:NZ	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:718:LYS:NZ	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:718:LYS:O	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:718:LYS:O	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:718:LYS:O	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:718:LYS:O	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:719:ILE:N	1:A:2239:HIS:N	7	3.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	3:C:719:ILE:N	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:719:ILE:N	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:719:ILE:N	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:719:ILE:O	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:719:ILE:O	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:719:ILE:O	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:719:ILE:O	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:720:THR:N	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:720:THR:N	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:720:THR:N	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:720:THR:N	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:720:THR:O	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:720:THR:O	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:720:THR:O	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:720:THR:O	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:720:THR:OG1	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:720:THR:OG1	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:720:THR:OG1	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:720:THR:OG1	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:721:ILE:N	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:721:ILE:N	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:721:ILE:N	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:721:ILE:N	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:721:ILE:O	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:721:ILE:O	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:721:ILE:O	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:721:ILE:O	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:722:HIS:N	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:722:HIS:N	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:722:HIS:N	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:722:HIS:N	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:722:HIS:ND1	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:722:HIS:ND1	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:722:HIS:ND1	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:722:HIS:ND1	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:722:HIS:NE2	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:722:HIS:NE2	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:722:HIS:NE2	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:722:HIS:NE2	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:722:HIS:O	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:722:HIS:O	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:722:HIS:O	1:A:2239:HIS:NE2	7	3.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	3:C:722:HIS:O	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:723:ASP:N	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:723:ASP:N	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:723:ASP:N	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:723:ASP:N	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:723:ASP:O	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:723:ASP:O	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:723:ASP:O	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:723:ASP:O	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:723:ASP:OD1	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:723:ASP:OD1	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:723:ASP:OD1	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:723:ASP:OD1	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:723:ASP:OD2	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:723:ASP:OD2	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:723:ASP:OD2	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:723:ASP:OD2	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:724:ARG:N	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:724:ARG:N	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:724:ARG:N	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:724:ARG:N	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:724:ARG:NE	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:724:ARG:NE	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:724:ARG:NE	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:724:ARG:NE	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:724:ARG:NH1	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:724:ARG:NH1	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:724:ARG:NH1	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:724:ARG:NH1	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:724:ARG:NH2	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:724:ARG:NH2	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:724:ARG:NH2	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:724:ARG:NH2	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:724:ARG:O	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:724:ARG:O	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:724:ARG:O	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:724:ARG:O	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:725:LYS:N	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:725:LYS:N	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:725:LYS:N	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:725:LYS:N	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:725:LYS:NZ	1:A:2239:HIS:N	7	3.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	3:C:725:LYS:NZ	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:725:LYS:NZ	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:725:LYS:NZ	1:A:2239:HIS:O	7	3.11
(2,1)	3:C:725:LYS:O	1:A:2239:HIS:N	7	3.11
(2,1)	3:C:725:LYS:O	1:A:2239:HIS:ND1	7	3.11
(2,1)	3:C:725:LYS:O	1:A:2239:HIS:NE2	7	3.11
(2,1)	3:C:725:LYS:O	1:A:2239:HIS:O	7	3.11
(1,754)	1:A:2319:SER:HB2	1:A:2321:PHE:HD2	5	3.11
(2,1)	3:C:716:LYS:N	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:716:LYS:N	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:716:LYS:N	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:716:LYS:N	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:716:LYS:NZ	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:716:LYS:NZ	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:716:LYS:NZ	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:716:LYS:NZ	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:716:LYS:O	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:716:LYS:O	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:716:LYS:O	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:716:LYS:O	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:717:LYS:N	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:717:LYS:N	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:717:LYS:N	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:717:LYS:N	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:717:LYS:NZ	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:717:LYS:NZ	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:717:LYS:NZ	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:717:LYS:NZ	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:717:LYS:O	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:717:LYS:O	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:717:LYS:O	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:717:LYS:O	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:718:LYS:N	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:718:LYS:N	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:718:LYS:N	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:718:LYS:N	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:718:LYS:NZ	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:718:LYS:NZ	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:718:LYS:NZ	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:718:LYS:NZ	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:718:LYS:O	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:718:LYS:O	1:A:2239:HIS:ND1	16	3.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	3:C:718:LYS:O	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:718:LYS:O	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:719:ILE:N	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:719:ILE:N	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:719:ILE:N	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:719:ILE:N	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:719:ILE:O	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:719:ILE:O	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:719:ILE:O	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:719:ILE:O	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:720:THR:N	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:720:THR:N	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:720:THR:N	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:720:THR:N	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:720:THR:O	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:720:THR:O	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:720:THR:O	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:720:THR:O	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:720:THR:OG1	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:720:THR:OG1	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:720:THR:OG1	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:720:THR:OG1	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:721:ILE:N	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:721:ILE:N	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:721:ILE:N	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:721:ILE:N	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:721:ILE:O	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:721:ILE:O	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:721:ILE:O	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:721:ILE:O	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:722:HIS:N	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:722:HIS:N	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:722:HIS:N	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:722:HIS:N	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:722:HIS:ND1	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:722:HIS:ND1	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:722:HIS:ND1	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:722:HIS:ND1	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:722:HIS:NE2	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:722:HIS:NE2	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:722:HIS:NE2	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:722:HIS:NE2	1:A:2239:HIS:O	16	3.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	3:C:722:HIS:O	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:722:HIS:O	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:722:HIS:O	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:722:HIS:O	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:723:ASP:N	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:723:ASP:N	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:723:ASP:N	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:723:ASP:N	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:723:ASP:O	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:723:ASP:O	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:723:ASP:O	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:723:ASP:O	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:723:ASP:OD1	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:723:ASP:OD1	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:723:ASP:OD1	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:723:ASP:OD1	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:723:ASP:OD2	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:723:ASP:OD2	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:723:ASP:OD2	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:723:ASP:OD2	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:724:ARG:N	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:724:ARG:N	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:724:ARG:N	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:724:ARG:N	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:724:ARG:NE	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:724:ARG:NE	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:724:ARG:NE	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:724:ARG:NE	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:724:ARG:NH1	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:724:ARG:NH1	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:724:ARG:NH1	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:724:ARG:NH1	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:724:ARG:NH2	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:724:ARG:NH2	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:724:ARG:NH2	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:724:ARG:NH2	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:724:ARG:O	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:724:ARG:O	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:724:ARG:O	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:724:ARG:O	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:725:LYS:N	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:725:LYS:N	1:A:2239:HIS:ND1	16	3.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	3:C:725:LYS:N	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:725:LYS:N	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:725:LYS:NZ	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:725:LYS:NZ	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:725:LYS:NZ	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:725:LYS:NZ	1:A:2239:HIS:O	16	3.09
(2,1)	3:C:725:LYS:O	1:A:2239:HIS:N	16	3.09
(2,1)	3:C:725:LYS:O	1:A:2239:HIS:ND1	16	3.09
(2,1)	3:C:725:LYS:O	1:A:2239:HIS:NE2	16	3.09
(2,1)	3:C:725:LYS:O	1:A:2239:HIS:O	16	3.09
(1,754)	1:A:2319:SER:HB2	1:A:2321:PHE:HD2	1	3.09
(2,1)	3:C:716:LYS:N	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:716:LYS:N	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:716:LYS:N	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:716:LYS:N	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:716:LYS:NZ	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:716:LYS:NZ	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:716:LYS:NZ	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:716:LYS:NZ	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:716:LYS:O	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:716:LYS:O	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:716:LYS:O	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:716:LYS:O	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:717:LYS:N	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:717:LYS:N	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:717:LYS:N	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:717:LYS:N	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:717:LYS:NZ	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:717:LYS:NZ	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:717:LYS:NZ	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:717:LYS:NZ	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:717:LYS:O	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:717:LYS:O	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:717:LYS:O	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:717:LYS:O	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:718:LYS:N	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:718:LYS:N	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:718:LYS:N	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:718:LYS:N	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:718:LYS:NZ	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:718:LYS:NZ	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:718:LYS:NZ	1:A:2239:HIS:NE2	6	3.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	3:C:718:LYS:NZ	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:718:LYS:O	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:718:LYS:O	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:718:LYS:O	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:718:LYS:O	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:719:ILE:N	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:719:ILE:N	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:719:ILE:N	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:719:ILE:N	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:719:ILE:O	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:719:ILE:O	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:719:ILE:O	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:719:ILE:O	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:720:THR:N	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:720:THR:N	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:720:THR:N	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:720:THR:N	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:720:THR:O	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:720:THR:O	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:720:THR:O	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:720:THR:O	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:720:THR:OG1	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:720:THR:OG1	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:720:THR:OG1	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:720:THR:OG1	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:721:ILE:N	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:721:ILE:N	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:721:ILE:N	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:721:ILE:N	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:721:ILE:O	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:721:ILE:O	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:721:ILE:O	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:721:ILE:O	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:722:HIS:N	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:722:HIS:N	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:722:HIS:N	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:722:HIS:N	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:722:HIS:ND1	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:722:HIS:ND1	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:722:HIS:ND1	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:722:HIS:ND1	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:722:HIS:NE2	1:A:2239:HIS:N	6	3.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	3:C:722:HIS:NE2	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:722:HIS:NE2	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:722:HIS:NE2	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:722:HIS:O	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:722:HIS:O	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:722:HIS:O	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:722:HIS:O	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:723:ASP:N	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:723:ASP:N	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:723:ASP:N	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:723:ASP:N	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:723:ASP:O	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:723:ASP:O	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:723:ASP:O	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:723:ASP:O	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:723:ASP:OD1	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:723:ASP:OD1	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:723:ASP:OD1	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:723:ASP:OD1	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:723:ASP:OD2	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:723:ASP:OD2	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:723:ASP:OD2	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:723:ASP:OD2	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:724:ARG:N	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:724:ARG:N	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:724:ARG:N	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:724:ARG:N	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:724:ARG:NE	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:724:ARG:NE	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:724:ARG:NE	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:724:ARG:NE	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:724:ARG:NH1	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:724:ARG:NH1	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:724:ARG:NH1	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:724:ARG:NH1	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:724:ARG:NH2	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:724:ARG:NH2	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:724:ARG:NH2	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:724:ARG:NH2	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:724:ARG:O	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:724:ARG:O	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:724:ARG:O	1:A:2239:HIS:NE2	6	3.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	3:C:724:ARG:O	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:725:LYS:N	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:725:LYS:N	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:725:LYS:N	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:725:LYS:N	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:725:LYS:NZ	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:725:LYS:NZ	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:725:LYS:NZ	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:725:LYS:NZ	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:725:LYS:O	1:A:2239:HIS:N	6	3.08
(2,1)	3:C:725:LYS:O	1:A:2239:HIS:ND1	6	3.08
(2,1)	3:C:725:LYS:O	1:A:2239:HIS:NE2	6	3.08
(2,1)	3:C:725:LYS:O	1:A:2239:HIS:O	6	3.08
(2,1)	3:C:716:LYS:N	1:A:2239:HIS:N	18	3.08

10 Dihedral-angle violation analysis

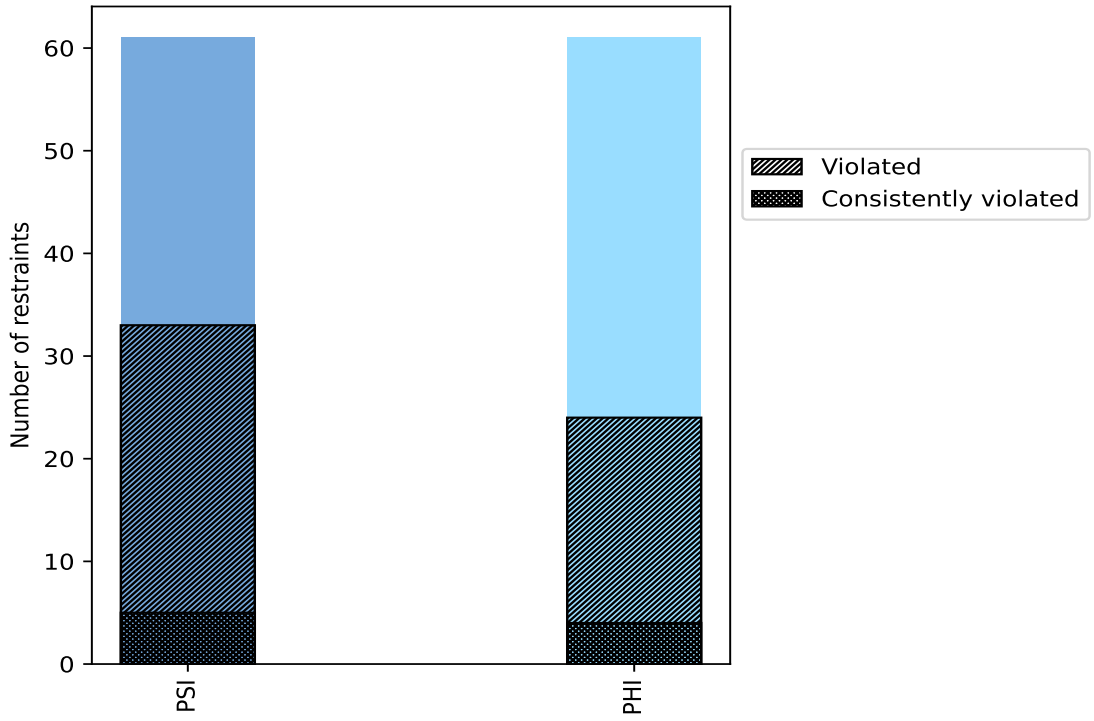
10.1 Summary of dihedral-angle violations

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	33	54.1	27.0	5	8.2	4.1
PHI	61	50.0	24	39.3	19.7	4	6.6	3.3
Total	122	100.0	57	46.7	46.7	9	7.4	7.4

[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



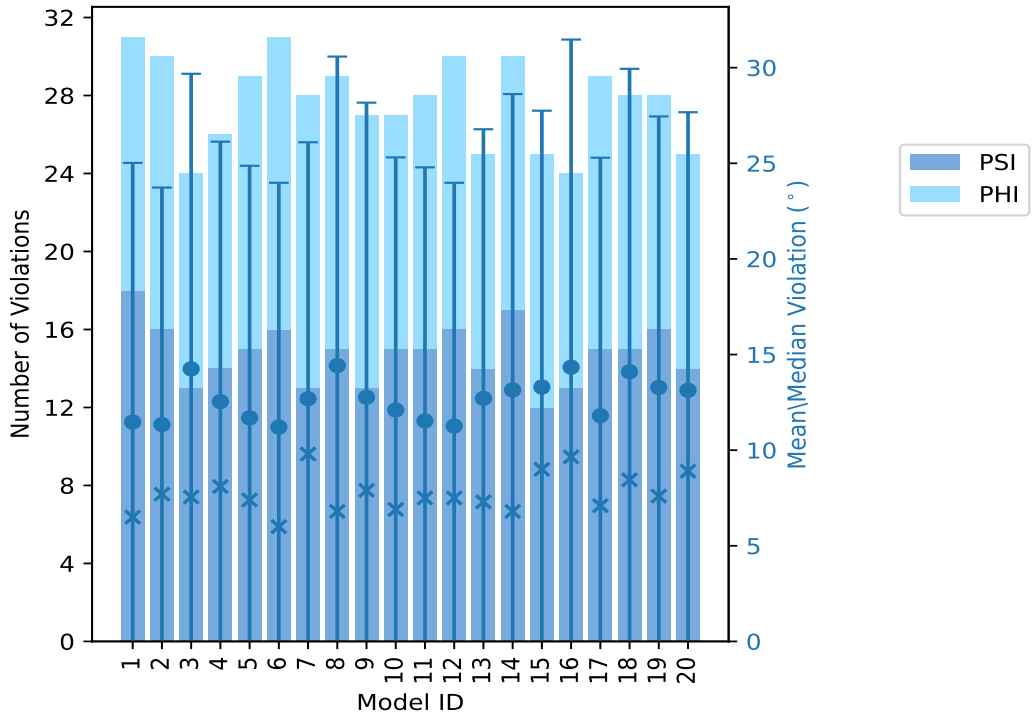
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

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	18	13	31	11.47	73.0	13.55	6.5
2	16	14	30	11.34	64.6	12.39	7.7
3	13	11	24	14.25	64.7	15.43	7.55
4	14	12	26	12.54	67.3	13.59	8.1
5	15	14	29	11.69	68.5	13.18	7.4
6	16	15	31	11.21	66.4	12.77	6.0
7	13	15	28	12.69	69.0	13.41	9.8
8	15	14	29	14.42	79.9	16.16	6.8
9	13	14	27	12.77	79.9	15.4	7.9
10	15	12	27	12.1	64.6	13.21	6.9
11	15	13	28	11.53	67.5	13.26	7.5
12	16	14	30	11.26	65.8	12.72	7.5
13	14	11	25	12.71	66.2	14.07	7.3
14	17	13	30	13.15	75.4	15.47	6.8
15	12	13	25	13.3	71.6	14.45	9.0
16	13	11	24	14.34	87.4	17.13	9.65
17	15	14	29	11.8	69.5	13.49	7.1
18	15	13	28	14.1	74.8	15.84	8.45
19	16	12	28	13.28	64.8	14.17	7.6
20	14	11	25	13.13	74.3	14.54	8.9

10.2.1 Bar graph : Dihedral violation statistics for each model



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

10.3 Dihedral-angle violation statistics for the ensemble

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]	%
6	5	11	1	5.0
3	1	4	2	10.0
3	1	4	3	15.0
1	0	1	4	20.0
2	1	3	5	25.0
2	1	3	6	30.0
1	1	2	7	35.0
1	0	1	8	40.0
1	2	3	9	45.0
1	0	1	10	50.0
0	1	1	11	55.0

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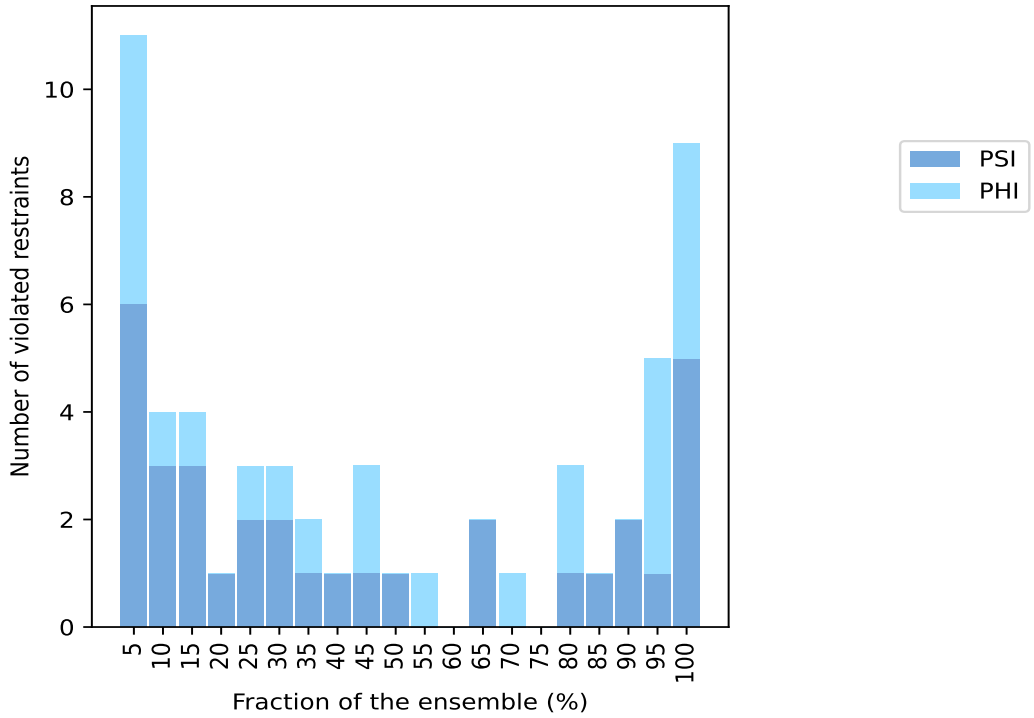
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	60.0
2	0	2	13	65.0
0	1	1	14	70.0
0	0	0	15	75.0
1	2	3	16	80.0
1	0	1	17	85.0
2	0	2	18	90.0
1	4	5	19	95.0
5	4	9	20	100.0

[1] Number of models with violations

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

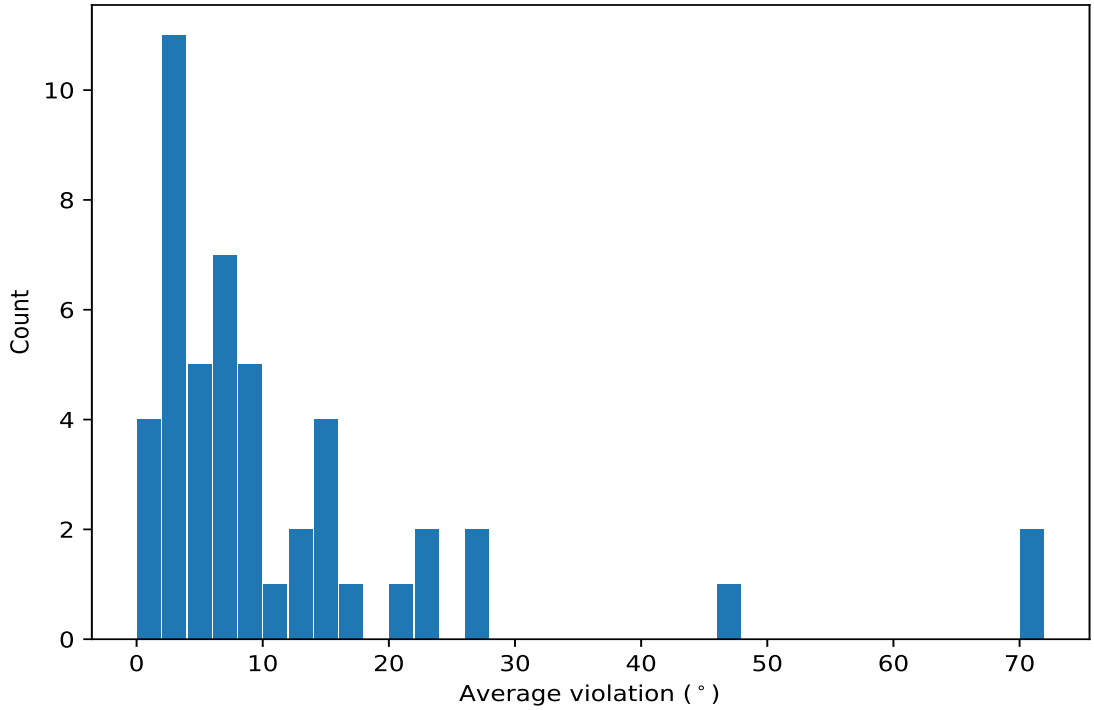


10.4 Most violated dihedral-angle restraints in the ensemble

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

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

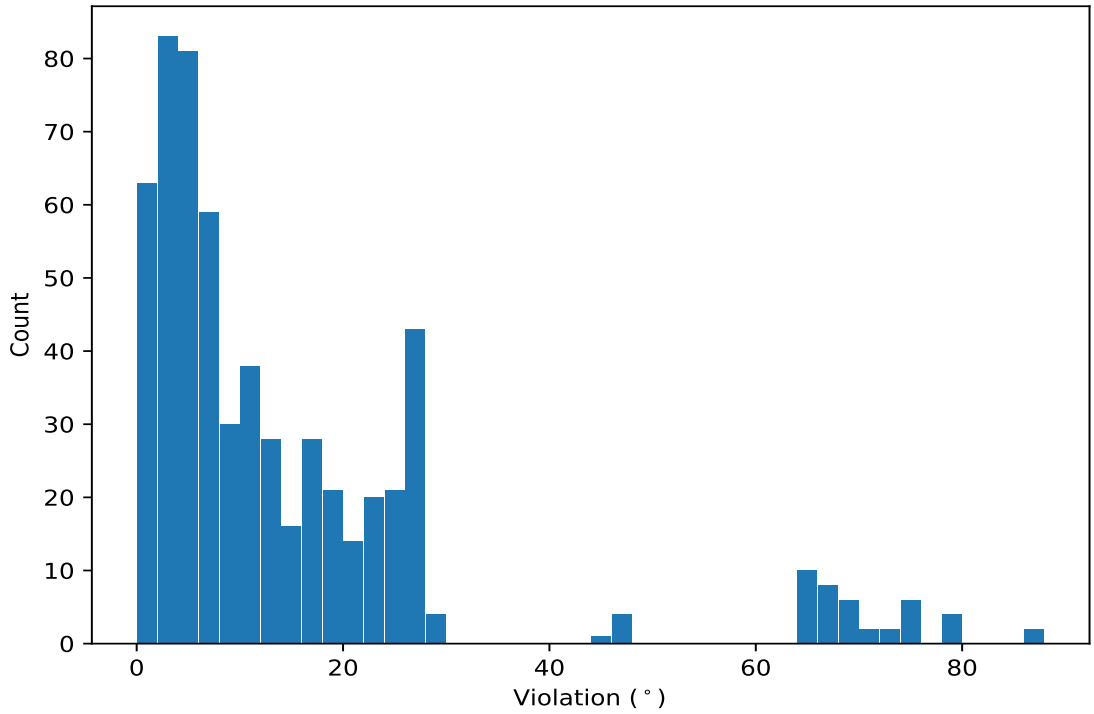
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Media
(1,30)	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	1:A:2262:TRP:N	20	70.76	6.1	68.75
(1,30)	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	1:A:2262:TRP:N	20	70.76	6.1	68.75
(1,14)	1:A:2251:ALA:N	1:A:2251:ALA:CA	1:A:2251:ALA:C	1:A:2252:GLU:N	20	27.66	0.41	27.6
(1,51)	1:A:2280:LYS:C	1:A:2281:ALA:N	1:A:2281:ALA:CA	1:A:2281:ALA:C	20	26.83	0.66	27.0
(1,29)	1:A:2260:SER:C	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	20	23.81	1.44	23.9
(1,29)	1:A:2260:SER:C	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	20	23.81	1.44	23.9
(1,72)	1:A:2293:CYS:N	1:A:2293:CYS:CA	1:A:2293:CYS:C	1:A:2294:GLY:N	20	21.77	4.89	21.8
(1,57)	1:A:2283:ILE:C	1:A:2284:SER:N	1:A:2284:SER:CA	1:A:2284:SER:C	20	15.25	3.42	16.45
(1,114)	1:A:2326:ALA:N	1:A:2326:ALA:CA	1:A:2326:ALA:C	1:A:2327:SER:N	20	14.69	3.41	14.55
(1,17)	1:A:2254:GLY:C	1:A:2255:VAL:N	1:A:2255:VAL:CA	1:A:2255:VAL:C	20	6.13	1.71	6.05
(1,118)	1:A:2329:SER:N	1:A:2329:SER:CA	1:A:2329:SER:C	1:A:2330:GLY:N	20	1.34	0.15	1.35
(1,69)	1:A:2291:GLY:C	1:A:2292:SER:N	1:A:2292:SER:CA	1:A:2292:SER:C	19	14.63	4.05	15.0

[1] Number of violated models, [2]Standard 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 provides the list of violationsfor the 10 worst performing restraints, sorted by the violation 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 (°)
(1,30)	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	1:A:2262:TRP:N	16	87.4
(1,30)	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	1:A:2262:TRP:N	16	87.4
(1,30)	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	1:A:2262:TRP:N	8	79.9
(1,30)	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	1:A:2262:TRP:N	8	79.9
(1,30)	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	1:A:2262:TRP:N	9	79.9
(1,30)	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	1:A:2262:TRP:N	9	79.9
(1,30)	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	1:A:2262:TRP:N	14	75.4
(1,30)	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	1:A:2262:TRP:N	14	75.4
(1,30)	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	1:A:2262:TRP:N	18	74.8
(1,30)	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	1:A:2262:TRP:N	18	74.8
(1,30)	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	1:A:2262:TRP:N	20	74.3
(1,30)	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	1:A:2262:TRP:N	20	74.3
(1,30)	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	1:A:2262:TRP:N	1	73.0
(1,30)	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	1:A:2262:TRP:N	1	73.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,30)	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	1:A:2262:TRP:N	15	71.6
(1,30)	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	1:A:2262:TRP:N	15	71.6
(1,30)	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	1:A:2262:TRP:N	17	69.5
(1,30)	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	1:A:2262:TRP:N	17	69.5
(1,30)	1:A:2261:ILE:N	1:A:2261:ILE:CA	1:A:2261:ILE:C	1:A:2262:TRP:N	7	69.0