wwPDB NMR Structure Validation Summary Report

Jun 4, 2023 – 10:54 AM EDT

PDB ID	:	2LC6
BMRB ID	:	17599
Title	:	Solution structure of Par-6 Q144C/L164C
Authors	:	Volkman, B.F.; Whitney, D.S.; Peterson, F.C.
Deposited on	:	2011-04-25

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:

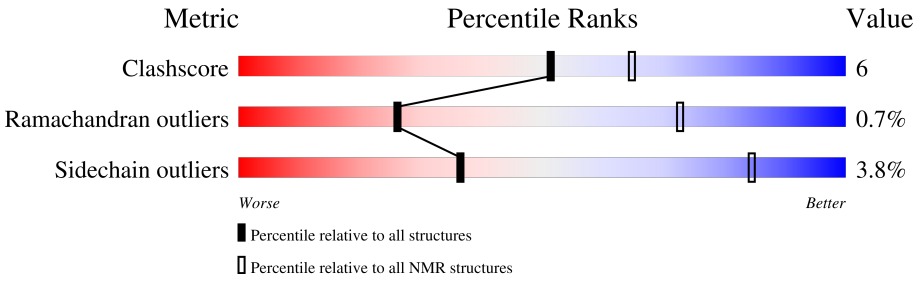
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	128	63% 6% 30%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 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:147-A:164, A:171-A:181, A:192-A:251 (89)	0.62	3

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. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1764 atoms, of which 803 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Par-6.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	128	1764	599	803	173	185	4	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	GLY	-	expression tag	UNP O97111
A	129	SER	-	expression tag	UNP O97111
A	144	CYS	GLN	engineered mutation	UNP O97111
A	164	CYS	LEU	engineered mutation	UNP O97111

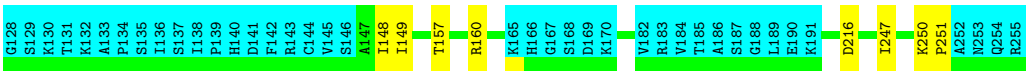
4 Residue-property plots

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: Par-6

Chain A:

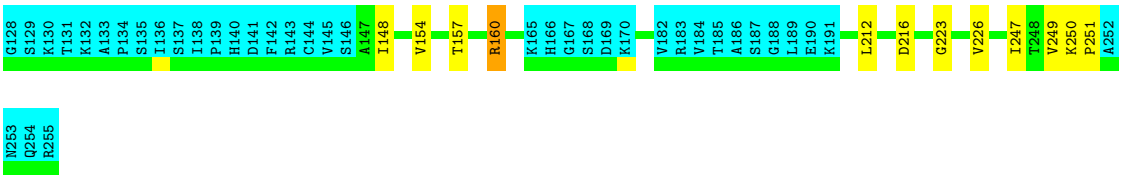


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 3. Colouring as in section 4.1 above.

- Molecule 1: Par-6

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
Xplor-NIH	refinement	2.9.3

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	1521
Number of shifts mapped to atoms	1347
Number of unparsed shifts	0
Number of shifts with mapping errors	174
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

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	0.1±0.4
All	All	0	3

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	160	ARG	Sidechain	3

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	667	536	689	8±2
All	All	13340	10720	13780	156

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 6.

5 of 51 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:148:ILE:HA	1:A:160:ARG:O	0.61	1.96	1	13
1:A:172:LEU:HD21	1:A:238:MET:HB3	0.57	1.77	8	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:216:ASP:OD1	1:A:251:PRO:HA	0.57	2.00	6	17
1:A:239:VAL:HA	1:A:242:SER:OG	0.57	2.00	20	1
1:A:157:THR:O	1:A:251:PRO:HD2	0.56	2.00	10	15

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	89/128 (70%)	86±2 (97±2%)	2±1 (3±2%)	1±1 (1±1%)	26	73
All	All	1780/2560 (70%)	1723 (97%)	45 (3%)	12 (1%)	26	73

All 4 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	226	VAL	7
1	A	223	GLY	3
1	A	150	ASP	1
1	A	173	GLY	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	76/109 (70%)	73±1 (96±2%)	3±1 (4±2%)	36	84
All	All	1520/2180 (70%)	1462 (96%)	58 (4%)	36	84

5 of 13 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	250	LYS	16
1	A	149	ILE	11
1	A	207	GLU	7
1	A	241	ASN	7
1	A	212	LEU	3

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 89% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1521
Number of shifts mapped to atoms	1347
Number of unparsed shifts	0
Number of shifts with mapping errors	174
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. First 5 (of 174) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	131	THR	HG22	1.204	0.000	1
1	A	131	THR	HG23	1.204	0.000	1
1	A	136	ILE	HG21	0.924	0.013	1
1	A	136	ILE	HG22	0.924	0.013	1
1	A	136	ILE	HG13	1.181	0.012	2
1	A	136	ILE	HD12	0.883	0.011	1
1	A	136	ILE	HD13	0.883	0.011	1
1	A	138	ILE	HG21	0.883	0.011	1
1	A	138	ILE	HG22	0.883	0.011	1
1	A	138	ILE	HG13	1.47	0.000	2
1	A	138	ILE	HD12	0.833	0.008	1
1	A	138	ILE	HD13	0.833	0.008	1
1	A	145	VAL	HG11	0.953	0.020	2
1	A	145	VAL	HG12	0.953	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	145	VAL	HG22	0.928	0.000	2
1	A	145	VAL	HG23	0.928	0.000	2
1	A	148	ILE	HG21	1.012	0.001	1
1	A	148	ILE	HG22	1.012	0.001	1
1	A	148	ILE	HG13	1.774	0.001	1
1	A	148	ILE	HD12	0.901	0.011	1
1	A	148	ILE	HD13	0.901	0.011	1
1	A	149	ILE	HG21	0.866	0.000	1
1	A	149	ILE	HG22	0.866	0.000	1
1	A	149	ILE	HD12	0.752	0.001	1
1	A	149	ILE	HD13	0.752	0.001	1
1	A	151	VAL	HG11	0.97	0.001	2
1	A	151	VAL	HG12	0.97	0.001	2
1	A	151	VAL	HG22	0.994	0.002	2
1	A	151	VAL	HG23	0.994	0.002	2
1	A	153	ILE	HG21	0.845	0.000	1
1	A	153	ILE	HG22	0.845	0.000	1
1	A	153	ILE	HG13	1.008	0.006	2
1	A	153	ILE	HD12	0.798	0.003	1
1	A	153	ILE	HD13	0.798	0.003	1
1	A	154	VAL	HG11	1.052	0.000	2
1	A	154	VAL	HG12	1.052	0.000	2
1	A	154	VAL	HG22	1.013	0.000	2
1	A	154	VAL	HG23	1.013	0.000	2
1	A	157	THR	HG22	1.29	0.000	1
1	A	157	THR	HG23	1.29	0.000	1
1	A	161	VAL	HG11	0.87	0.009	2
1	A	161	VAL	HG12	0.87	0.009	2
1	A	161	VAL	HG22	0.784	0.006	2
1	A	161	VAL	HG23	0.784	0.006	2
1	A	163	LEU	HD11	0.817	0.007	1
1	A	163	LEU	HD12	0.817	0.007	1
1	A	163	LEU	HD22	0.817	0.000	1
1	A	163	LEU	HD23	0.817	0.000	1
1	A	172	LEU	HD11	0.894	0.012	2
1	A	172	LEU	HD12	0.894	0.012	2
1	A	172	LEU	HD22	0.883	0.002	2
1	A	172	LEU	HD23	0.883	0.002	2
1	A	176	ILE	HG21	0.914	0.007	1
1	A	176	ILE	HG22	0.914	0.007	1
1	A	176	ILE	HG13	1.509	0.013	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	176	ILE	HD12	0.862	0.000	1
1	A	176	ILE	HD13	0.862	0.000	1
1	A	180	THR	HG22	1.094	0.005	1
1	A	180	THR	HG23	1.094	0.005	1
1	A	182	VAL	HG11	0.92	0.012	2
1	A	182	VAL	HG12	0.92	0.012	2
1	A	182	VAL	HG22	0.868	0.000	2
1	A	182	VAL	HG23	0.868	0.000	2
1	A	184	VAL	HG11	0.918	0.000	2
1	A	184	VAL	HG12	0.918	0.000	2
1	A	184	VAL	HG22	0.975	0.000	2
1	A	184	VAL	HG23	0.975	0.000	2
1	A	185	THR	HG22	1.143	0.004	1
1	A	185	THR	HG23	1.143	0.004	1
1	A	189	LEU	HD11	0.892	0.004	2
1	A	189	LEU	HD12	0.892	0.004	2
1	A	189	LEU	HD22	0.811	0.011	2
1	A	189	LEU	HD23	0.811	0.011	2
1	A	192	GLN	HE22	6.764	0.000	2
1	A	195	ILE	HG21	0.788	0.009	1
1	A	195	ILE	HG22	0.788	0.009	1
1	A	195	ILE	HG13	1.413	0.000	2
1	A	195	ILE	HD12	0.777	0.009	1
1	A	195	ILE	HD13	0.777	0.009	1
1	A	197	ILE	HG21	0.79	0.007	1
1	A	197	ILE	HG22	0.79	0.007	1
1	A	197	ILE	HG13	1.203	0.007	2
1	A	197	ILE	HD12	0.42	0.007	1
1	A	197	ILE	HD13	0.42	0.007	1
1	A	200	LEU	HD11	0.906	0.004	2
1	A	200	LEU	HD12	0.906	0.004	2
1	A	200	LEU	HD22	0.706	0.009	2
1	A	200	LEU	HD23	0.706	0.009	2
1	A	201	VAL	HG11	1.014	0.004	2
1	A	201	VAL	HG12	1.014	0.004	2
1	A	201	VAL	HG22	0.908	0.000	2
1	A	201	VAL	HG23	0.908	0.000	2
1	A	205	LEU	HD11	0.884	0.000	2
1	A	205	LEU	HD12	0.884	0.000	2
1	A	205	LEU	HD22	0.831	0.003	2
1	A	205	LEU	HD23	0.831	0.003	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	209	THR	HG22	1.439	0.007	1
1	A	209	THR	HG23	1.439	0.007	1
1	A	211	LEU	HD11	0.735	0.000	2
1	A	211	LEU	HD12	0.735	0.000	2
1	A	211	LEU	HD22	0.824	0.005	2
1	A	211	LEU	HD23	0.824	0.005	2
1	A	212	LEU	HD11	0.108	0.005	2
1	A	212	LEU	HD12	0.108	0.005	2
1	A	212	LEU	HD22	0.623	0.008	2
1	A	212	LEU	HD23	0.623	0.008	2
1	A	214	VAL	HG11	0.961	0.015	2
1	A	214	VAL	HG12	0.961	0.015	2
1	A	214	VAL	HG22	0.932	0.000	2
1	A	214	VAL	HG23	0.932	0.000	2
1	A	215	ASN	HD22	6.956	0.000	2
1	A	218	VAL	HG11	0.69	0.000	2
1	A	218	VAL	HG12	0.69	0.000	2
1	A	218	VAL	HG22	0.7	0.000	2
1	A	218	VAL	HG23	0.7	0.000	2
1	A	219	ILE	HG21	0.916	0.001	1
1	A	219	ILE	HG22	0.916	0.001	1
1	A	219	ILE	HG13	0.836	0.000	2
1	A	219	ILE	HD12	0.411	0.000	1
1	A	219	ILE	HD13	0.411	0.000	1
1	A	221	VAL	HG11	0.794	0.008	2
1	A	221	VAL	HG12	0.794	0.008	2
1	A	221	VAL	HG22	0.766	0.001	2
1	A	221	VAL	HG23	0.766	0.001	2
1	A	222	ASN	HD22	7.319	0.003	2
1	A	224	ILE	HG21	0.94	0.009	1
1	A	224	ILE	HG22	0.94	0.009	1
1	A	224	ILE	HG13	1.192	0.000	2
1	A	224	ILE	HD12	0.854	0.008	1
1	A	224	ILE	HD13	0.854	0.008	1
1	A	226	VAL	HG11	0.765	0.004	2
1	A	226	VAL	HG12	0.765	0.004	2
1	A	226	VAL	HG22	0.701	0.000	2
1	A	226	VAL	HG23	0.701	0.000	2
1	A	230	THR	HG22	1.338	0.000	1
1	A	230	THR	HG23	1.338	0.000	1
1	A	231	LEU	HD11	0.913	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	231	LEU	HD12	0.913	0.000	2
1	A	231	LEU	HD22	0.93	0.000	2
1	A	231	LEU	HD23	0.93	0.000	2
1	A	234	VAL	HG11	0.902	0.007	2
1	A	234	VAL	HG12	0.902	0.007	2
1	A	234	VAL	HG22	0.997	0.007	2
1	A	234	VAL	HG23	0.997	0.007	2
1	A	235	THR	HG22	1.238	0.009	1
1	A	235	THR	HG23	1.238	0.009	1
1	A	239	VAL	HG11	0.935	0.001	2
1	A	239	VAL	HG12	0.935	0.001	2
1	A	239	VAL	HG22	1.029	0.000	2
1	A	239	VAL	HG23	1.029	0.000	2
1	A	241	ASN	HD22	6.99	0.000	2
1	A	244	ASN	HD22	6.812	0.000	2
1	A	245	LEU	HD11	1.113	0.009	2
1	A	245	LEU	HD12	1.113	0.009	2
1	A	245	LEU	HD22	1.095	0.003	2
1	A	245	LEU	HD23	1.095	0.003	2
1	A	246	ILE	HG21	0.787	0.000	1
1	A	246	ILE	HG22	0.787	0.000	1
1	A	246	ILE	HG13	1.592	0.000	1
1	A	246	ILE	HD12	0.803	0.003	1
1	A	246	ILE	HD13	0.803	0.003	1
1	A	247	ILE	HG21	0.916	0.012	1
1	A	247	ILE	HG22	0.916	0.012	1
1	A	247	ILE	HG13	1.716	0.000	1
1	A	247	ILE	HD12	0.776	0.000	1
1	A	247	ILE	HD13	0.776	0.000	1
1	A	248	THR	HG22	1.15	0.000	1
1	A	248	THR	HG23	1.15	0.000	1
1	A	249	VAL	HG11	0.699	0.000	2
1	A	249	VAL	HG12	0.699	0.000	2
1	A	249	VAL	HG22	0.779	0.009	2
1	A	249	VAL	HG23	0.779	0.009	2
1	A	253	ASN	HD22	6.884	0.000	2
1	A	254	GLN	HE22	6.961	0.004	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	123	-0.50 ± 0.08	Should be checked
$^{13}C_{\beta}$	114	-0.20 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	124	-0.14 ± 0.14	None needed (< 0.5 ppm)
^{15}N	117	0.11 ± 0.53	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 92%, i.e. 1100 atoms were assigned a chemical shift out of a possible 1198. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	441/443 (100%)	181/181 (100%)	176/178 (99%)	84/84 (100%)
Sidechain	635/718 (88%)	437/473 (92%)	194/222 (87%)	4/23 (17%)
Aromatic	24/37 (65%)	15/18 (83%)	9/17 (53%)	0/2 (0%)
Overall	1100/1198 (92%)	633/672 (94%)	379/417 (91%)	88/109 (81%)

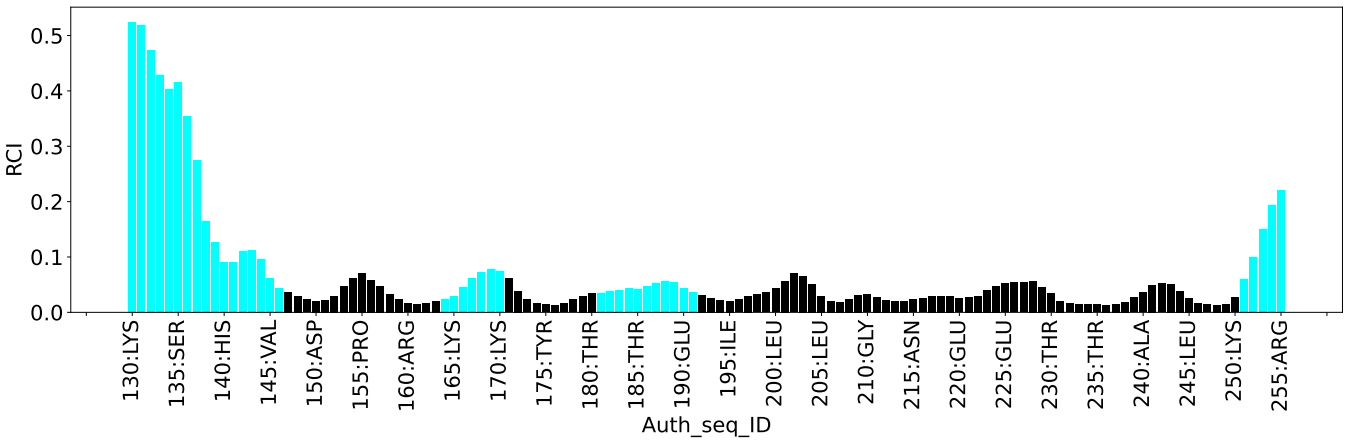
7.1.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

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:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
130:LYS
135:SER
140:HIS
145:VAL
150:ASP
155:PRO
160:ARG
165:LYS
170:LYS
175:TYR
180:THR
185:THR
190:GLU
195:ILE
200:LEU
205:LEU
210:GLY
215:ASN
220:GLU
225:GLU
230:THR
235:THR
240:ALA
245:LEU
250:LYS
255:ARG
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	1381
Intra-residue (|i-j|=0)	313
Sequential (|i-j|=1)	347
Medium range (|i-j|>1 and |i-j|<5)	197
Long range (|i-j|≥5)	521
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	3
Total dihedral-angle restraints	0
Number of unmapped restraints	576
Number of restraints per residue	10.8
Number of long range restraints per residue[1]	4.1

[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)	29.9	0.2
0.2-0.5 (Medium)	68.0	0.5
>0.5 (Large)	153.3	3.66

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

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

9 Distance violation analysis (i)

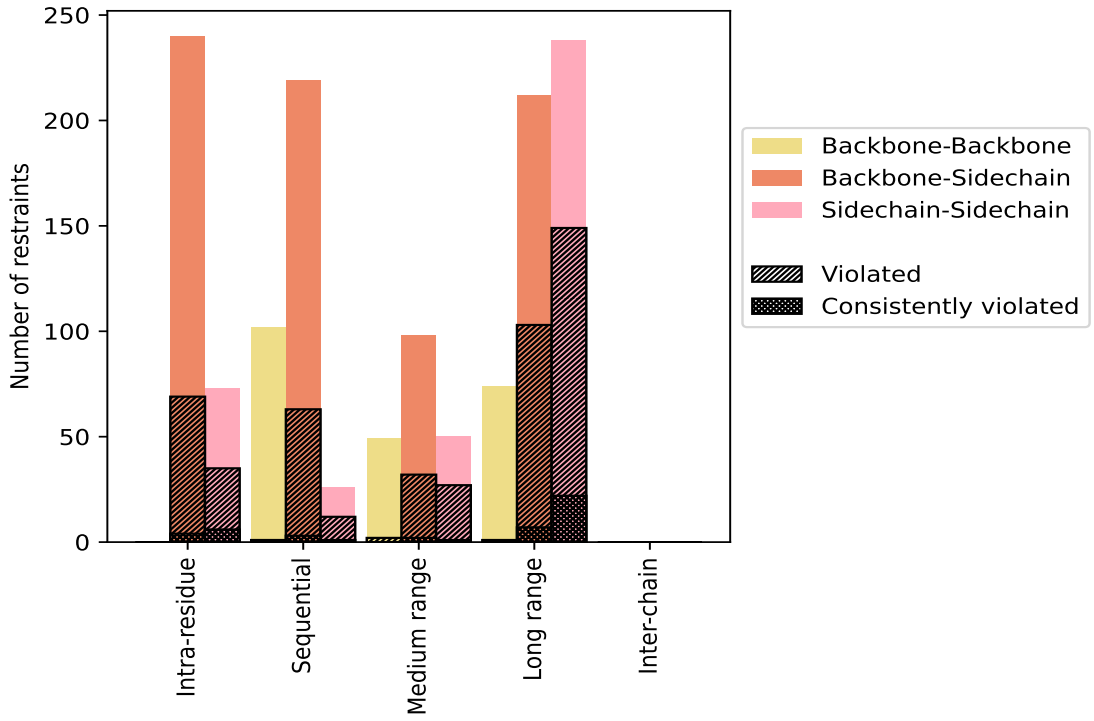
9.1 Summary of distance violations (i)

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)	313	22.7	104	33.2	7.5	10	3.2	0.7
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	240	17.4	69	28.7	5.0	4	1.7	0.3
Sidechain-Sidechain	73	5.3	35	47.9	2.5	6	8.2	0.4
Sequential (|i-j|=1)	347	25.1	76	21.9	5.5	4	1.2	0.3
Backbone-Backbone	102	7.4	1	1.0	0.1	0	0.0	0.0
Backbone-Sidechain	219	15.9	63	28.8	4.6	3	1.4	0.2
Sidechain-Sidechain	26	1.9	12	46.2	0.9	1	3.8	0.1
Medium range (|i-j|>1 & |i-j|<5)	197	14.3	61	31.0	4.4	3	1.5	0.2
Backbone-Backbone	49	3.5	2	4.1	0.1	0	0.0	0.0
Backbone-Sidechain	98	7.1	32	32.7	2.3	2	2.0	0.1
Sidechain-Sidechain	50	3.6	27	54.0	2.0	1	2.0	0.1
Long range (|i-j|≥5)	521	37.7	253	48.6	18.3	29	5.6	2.1
Backbone-Backbone	74	5.4	1	1.4	0.1	0	0.0	0.0
Backbone-Sidechain	212	15.4	103	48.6	7.5	7	3.3	0.5
Sidechain-Sidechain	235	17.0	149	63.4	10.8	22	9.4	1.6
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	3	0.2	0	0.0	0.0	0	0.0	0.0
Total	1381	100.0	494	35.8	35.8	46	3.3	3.3
Backbone-Backbone	225	16.3	4	1.8	0.3	0	0.0	0.0
Backbone-Sidechain	769	55.7	267	34.7	19.3	16	2.1	1.2
Sidechain-Sidechain	387	28.0	223	57.6	16.1	30	7.8	2.2

[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	43	51	34	143	0	271	0.85	2.72	0.57	0.71
2	45	32	24	133	0	234	0.82	3.04	0.58	0.69
3	53	38	31	127	0	249	0.78	3.12	0.59	0.61
4	43	35	27	125	0	230	0.8	2.98	0.57	0.66
5	44	40	28	136	0	248	0.8	2.66	0.56	0.63
6	47	39	33	135	0	254	0.82	3.05	0.59	0.66
7	56	47	30	137	0	270	0.76	3.14	0.57	0.63
8	45	31	31	129	0	236	0.83	3.58	0.6	0.69
9	51	41	25	135	0	252	0.8	2.71	0.6	0.61
10	43	40	36	136	0	255	0.78	2.99	0.53	0.69
11	48	39	29	139	0	255	0.84	2.66	0.56	0.69

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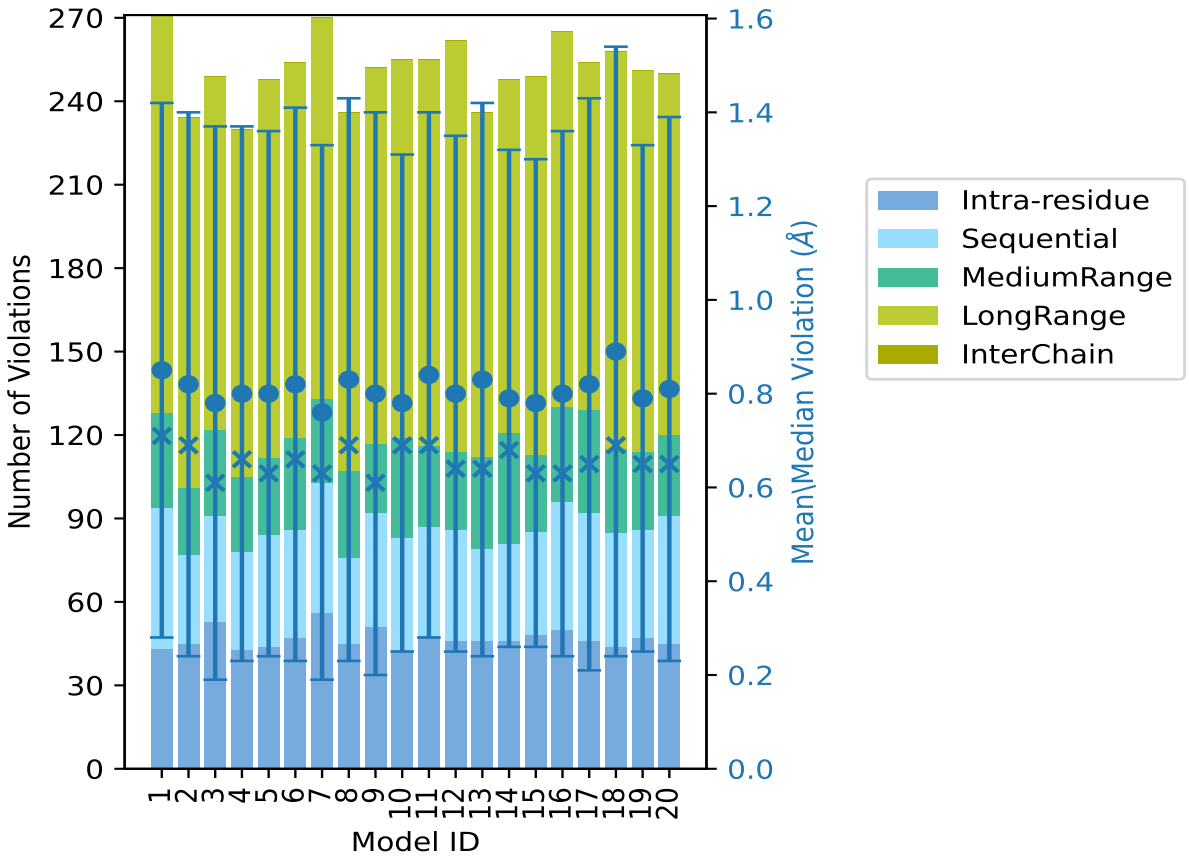
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	46	40	28	148	0	262	0.8	2.59	0.55	0.64
13	46	33	33	124	0	236	0.83	2.66	0.59	0.64
14	46	35	40	127	0	248	0.79	3.02	0.53	0.68
15	48	37	28	136	0	249	0.78	2.46	0.52	0.63
16	50	46	34	135	0	265	0.8	2.88	0.56	0.63
17	46	46	37	125	0	254	0.82	3.49	0.61	0.65
18	44	41	30	143	0	258	0.89	3.19	0.65	0.69
19	47	39	28	137	0	251	0.79	2.57	0.54	0.65
20	45	46	29	130	0	250	0.81	3.66	0.58	0.65

[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

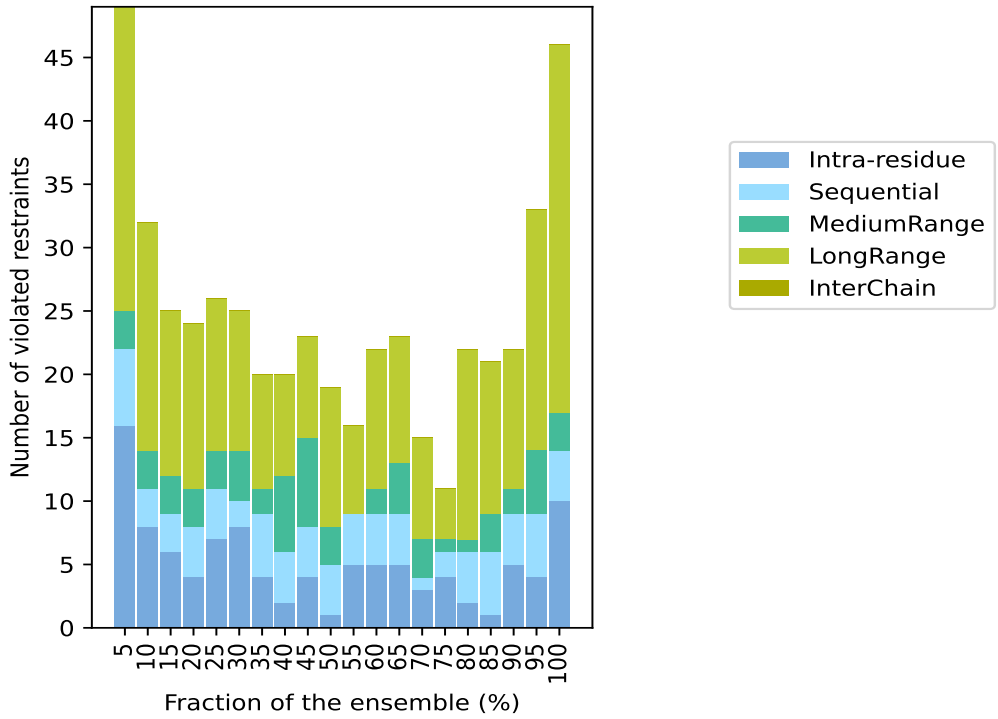
9.3 Distance violation statistics for the ensemble (i)

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, 884(IR:209, SQ:271, MR:136, LR:268, 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]	%
16	6	3	24	0	49	1	5.0
8	3	3	18	0	32	2	10.0
6	3	3	13	0	25	3	15.0
4	4	3	13	0	24	4	20.0
7	4	3	12	0	26	5	25.0
8	2	4	11	0	25	6	30.0
4	5	2	9	0	20	7	35.0
2	4	6	8	0	20	8	40.0
4	4	7	8	0	23	9	45.0
1	4	3	11	0	19	10	50.0
5	4	0	7	0	16	11	55.0
5	4	2	11	0	22	12	60.0
5	4	4	10	0	23	13	65.0
3	1	3	8	0	15	14	70.0
4	2	1	4	0	11	15	75.0
2	4	1	15	0	22	16	80.0
1	5	3	12	0	21	17	85.0
5	4	2	11	0	22	18	90.0
4	5	5	19	0	33	19	95.0
10	4	3	29	0	46	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

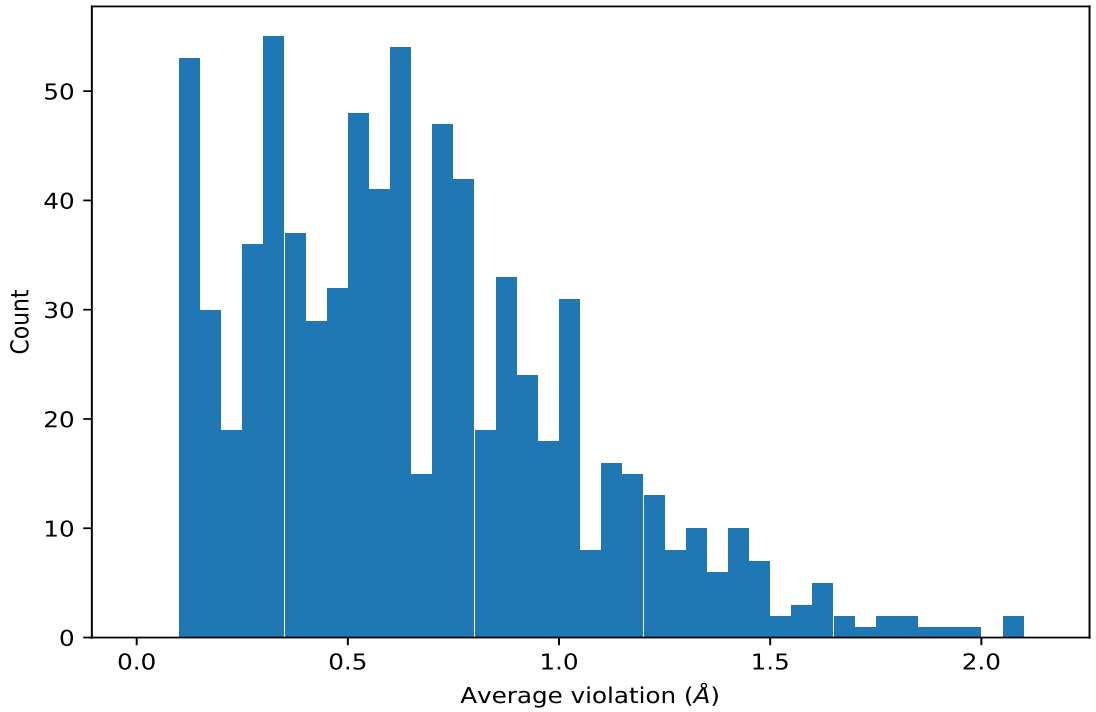
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 (i)

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.

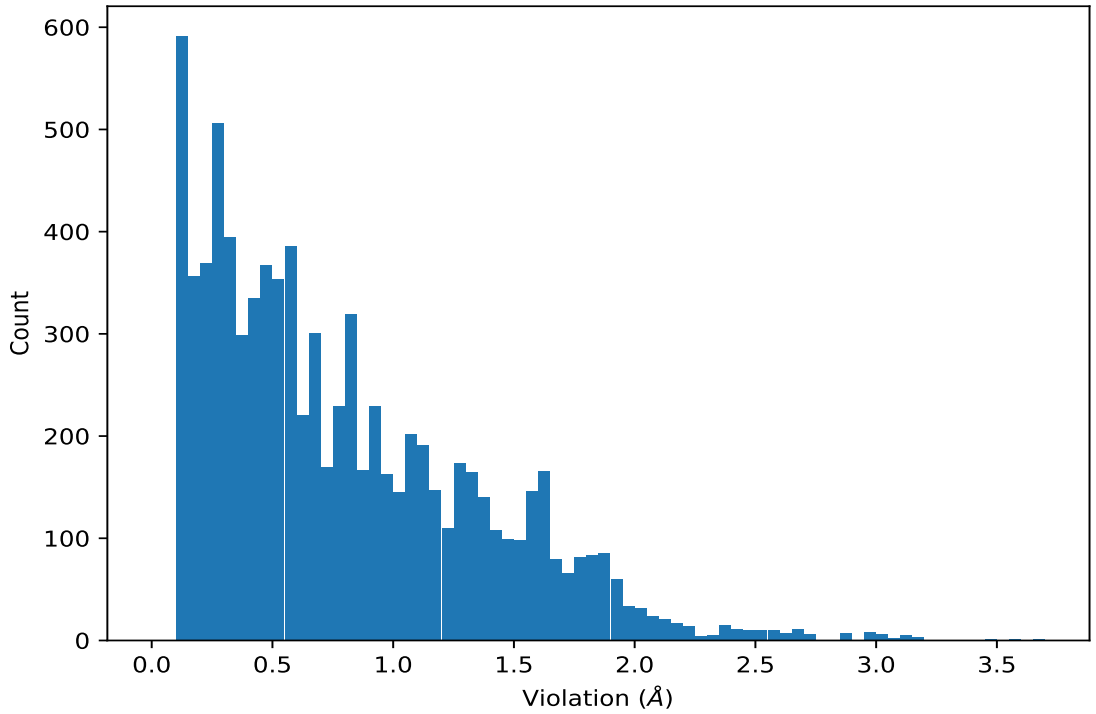
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,361)	1:A:172:LEU:HD13	1:A:247:ILE:HD11	20	2.08	0.76	2.12
(1,361)	1:A:172:LEU:HD21	1:A:247:ILE:HD11	20	2.08	0.76	2.12
(1,689)	1:A:195:ILE:HD11	1:A:234:VAL:HG21	20	1.96	0.94	1.98
(1,1115)	1:A:226:VAL:HG21	1:A:234:VAL:HG21	20	1.9	0.66	1.83
(1,1040)	1:A:221:VAL:HG13	1:A:247:ILE:HG12	20	1.88	0.61	1.84
(1,967)	1:A:219:ILE:HD11	1:A:248:THR:HG21	20	1.82	0.61	1.46
(1,262)	1:A:161:VAL:HG13	1:A:247:ILE:HG23	20	1.78	0.76	1.88
(1,262)	1:A:161:VAL:HG21	1:A:247:ILE:HG23	20	1.78	0.76	1.88
(1,90)	1:A:148:ILE:HG23	1:A:148:ILE:HD11	20	1.74	0.67	1.66
(1,365)	1:A:173:GLY:HA2	1:A:200:LEU:HD13	20	1.65	0.5	1.58
(1,365)	1:A:173:GLY:HA2	1:A:200:LEU:HD21	20	1.65	0.5	1.58
(1,691)	1:A:195:ILE:HG12	1:A:234:VAL:HG21	20	1.6	0.51	1.72
(1,466)	1:A:176:ILE:HG12	1:A:218:VAL:HG13	20	1.53	0.7	1.52

[1]Number of violated models, [2]Standard 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 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)
(1,689)	1:A:195:ILE:HD11	1:A:234:VAL:HG21	20	3.66
(1,689)	1:A:195:ILE:HD11	1:A:234:VAL:HG21	8	3.58
(1,689)	1:A:195:ILE:HD11	1:A:234:VAL:HG21	17	3.49
(1,689)	1:A:195:ILE:HD11	1:A:234:VAL:HG21	18	3.19
(1,361)	1:A:172:LEU:HD13	1:A:247:ILE:HD11	18	3.18
(1,361)	1:A:172:LEU:HD21	1:A:247:ILE:HD11	18	3.18
(1,967)	1:A:219:ILE:HD11	1:A:248:THR:HG21	7	3.14
(1,1040)	1:A:221:VAL:HG13	1:A:247:ILE:HG12	18	3.13
(1,1115)	1:A:226:VAL:HG21	1:A:234:VAL:HG21	3	3.12
(1,262)	1:A:161:VAL:HG13	1:A:247:ILE:HG23	17	3.11
(1,262)	1:A:161:VAL:HG21	1:A:247:ILE:HG23	17	3.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:A:197:ILE:HG23	1:A:212:LEU:HD13	17	3.08

10 Dihedral-angle violation analysis (i)

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value