wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2LO0
BMRB ID	:	18187
Title	:	Solution structure of the Get5 carboxyl domain from A. fumigatus
Authors	:	Chartron, J.W.; Vandervelde, D.G.; Rao, M.; Clemons Jr., W.M.
Deposited on	:	2012-01-08

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:

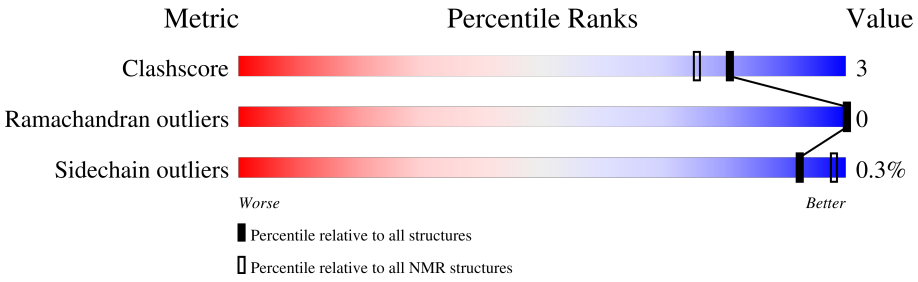
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 44%.

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	75	55% 5% 40%
1	B	75	55% 5% 40%

2 Ensemble composition and analysis

This entry contains 10 models. Model 4 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:190-A:230, B:190-B:230 (82)	0.30	4

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

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

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

Cluster number	Models
1	2, 5, 6, 7
2	1, 4, 8
3	3, 10
Single-model clusters	9

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1456 atoms, of which 706 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					Trace
1	A	45	Total	C	H	N	O	0
			728	240	353	62	73	
1	B	45	Total	C	H	N	O	0
			728	240	353	62	73	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	SER	-	expression tag	UNP Q4WE50
A	157	VAL	-	expression tag	UNP Q4WE50
A	158	ASP	-	expression tag	UNP Q4WE50
B	156	SER	-	expression tag	UNP Q4WE50
B	157	VAL	-	expression tag	UNP Q4WE50
B	158	ASP	-	expression tag	UNP Q4WE50

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Uncharacterized protein

Chain A:

• Molecule 1: Uncharacterized protein

Chain B:

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

The representative model is number 4. Colouring as in section 4.1 above.

• Molecule 1: Uncharacterized protein

Chain A:

• Molecule 1: Uncharacterized protein

Chain B:

5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
ARIA	structure solution	2.3
CNS	refinement	1.21

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	832
Number of shifts mapped to atoms	555
Number of unparsed shifts	0
Number of shifts with mapping errors	277
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	44%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	349	332	332	2±1
1	B	349	332	332	2±1
All	All	6980	6640	6640	36

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 3.

5 of 15 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:203:GLY:O	1:A:207:GLN:HG3	0.53	2.04	1	2
1:A:220:VAL:O	1:A:224:GLU:HG3	0.52	2.05	10	4
1:B:220:VAL:O	1:B:224:GLU:HG3	0.52	2.04	10	4
1:A:205:LEU:O	1:A:209:LEU:HB2	0.51	2.05	3	4
1:B:203:GLY:O	1:B:207:GLN:HG3	0.51	2.05	1	1

6.3 Torsion angles

6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	40/75 (53%)	40±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
1	B	40/75 (53%)	40±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	800/1500 (53%)	800 (100%)	0 (0%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	36/60 (60%)	36±0 (100±1%)	0±0 (0±1%)	92	98
1	B	36/60 (60%)	36±0 (100±1%)	0±0 (0±1%)	92	98
All	All	720/1200 (60%)	718 (100%)	2 (0%)	92	98

All 2 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	216	ASN	1
1	B	216	ASN	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry

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 44% for the well-defined parts and 44% 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	832
Number of shifts mapped to atoms	555
Number of unparsed shifts	0
Number of shifts with mapping errors	277
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 277) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	157	VAL	HA	4.212	0	1
1	A	157	VAL	HB	2.09	0	1
1	A	157	VAL	HG21	0.95	0	1
1	A	157	VAL	HG22	0.95	0	1
1	A	157	VAL	HG23	0.95	0	1
1	A	157	VAL	C	175.51	0.002	1
1	A	157	VAL	CA	62.256	0.046	1
1	A	157	VAL	CB	32.791	0.083	1
1	A	157	VAL	CG1	21.106	0	2
1	A	157	VAL	CG2	20.232	0	2
1	A	158	ASP	H	8.459	0.003	1
1	A	158	ASP	HA	4.65	0.006	1
1	A	158	ASP	HB2	2.699	0.006	2
1	A	158	ASP	HB3	2.553	0.019	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	158	ASP	C	176.159	0.015	1
1	A	158	ASP	CA	54.338	0.044	1
1	A	158	ASP	CB	41.364	0.012	1
1	A	158	ASP	N	124.622	0.046	1
1	A	159	VAL	H	8.105	0.002	1
1	A	159	VAL	HA	4.1	0.001	1
1	A	159	VAL	HB	2.104	0.011	1
1	A	159	VAL	HG21	0.94	0	1
1	A	159	VAL	HG22	0.94	0	1
1	A	159	VAL	HG23	0.94	0	1
1	A	159	VAL	C	175.809	0.011	1
1	A	159	VAL	CA	62.224	0.059	1
1	A	159	VAL	CB	32.793	0.018	1
1	A	159	VAL	CG1	20.295	0	2
1	A	159	VAL	CG2	21.157	0	2
1	A	159	VAL	N	120.675	0.06	1
1	A	160	ALA	H	8.386	0.003	1
1	A	160	ALA	HA	4.345	0.008	1
1	A	160	ALA	HB1	1.384	0.004	1
1	A	160	ALA	HB2	1.384	0.004	1
1	A	160	ALA	HB3	1.384	0.004	1
1	A	160	ALA	C	177.88	0.001	1
1	A	160	ALA	CA	52.553	0.048	1
1	A	160	ALA	CB	19.206	0.022	1
1	A	160	ALA	N	127.491	0.043	1
1	A	161	VAL	H	8.091	0.002	1
1	A	161	VAL	HA	4.118	0.007	1
1	A	161	VAL	HB	2.103	0.004	1
1	A	161	VAL	HG21	0.955	0.006	1
1	A	161	VAL	HG22	0.955	0.006	1
1	A	161	VAL	HG23	0.955	0.006	1
1	A	161	VAL	C	176.39	0.021	1
1	A	161	VAL	CA	62.353	0.074	1
1	A	161	VAL	CB	32.851	0.018	1
1	A	161	VAL	CG1	21.184	0	2
1	A	161	VAL	CG2	20.407	0	2
1	A	161	VAL	N	119.395	0.057	1
1	A	162	SER	H	8.328	0.002	1
1	A	162	SER	HA	4.44	0.002	1
1	A	162	SER	HB3	3.866	0.002	1
1	A	162	SER	C	174.399	0.002	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	162	SER	CA	58.202	0.091	1
1	A	162	SER	CB	63.827	0.068	1
1	A	162	SER	N	119.208	0.048	1
1	A	163	ALA	H	8.391	0.002	1
1	A	163	ALA	HA	4.35	0.006	1
1	A	163	ALA	HB1	1.405	0.001	1
1	A	163	ALA	HB2	1.405	0.001	1
1	A	163	ALA	HB3	1.405	0.001	1
1	A	163	ALA	C	178.257	0.002	1
1	A	163	ALA	CA	52.811	0.07	1
1	A	163	ALA	CB	19.242	0.032	1
1	A	163	ALA	N	126.394	0.063	1
1	A	164	GLY	H	8.388	0.002	1
1	A	164	GLY	HA3	3.947	0.01	1
1	A	164	GLY	C	174.142	0.009	1
1	A	164	GLY	CA	45.363	0.027	1
1	A	164	GLY	N	108.263	0.044	1
1	A	165	ALA	H	8.225	0.004	1
1	A	165	ALA	HA	4.326	0.005	1
1	A	165	ALA	HB1	1.404	0.005	1
1	A	165	ALA	HB2	1.404	0.005	1
1	A	165	ALA	HB3	1.404	0.005	1
1	A	165	ALA	C	178.468	0.003	1
1	A	165	ALA	CA	52.876	0.06	1
1	A	165	ALA	CB	19.265	0.032	1
1	A	165	ALA	N	123.793	0.062	1
1	A	166	GLY	H	8.431	0.003	1
1	A	166	GLY	HA3	3.918	0.003	1
1	A	166	GLY	C	174.235	0	1
1	A	166	GLY	CA	45.828	0.035	1
1	A	166	GLY	N	108.116	0.11	1
1	A	167	GLU	H	8.433	0.003	1
1	A	167	GLU	HA	4.268	0.007	1
1	A	167	GLU	C	176.785	0.015	1
1	A	167	GLU	CA	56.85	0.083	1
1	A	167	GLU	CB	30.31	0.063	1
1	A	167	GLU	CG	36.296	0	1
1	A	167	GLU	N	120.703	0.052	1
1	A	168	ARG	H	8.367	0.002	1
1	A	168	ARG	HA	4.329	0.004	1
1	A	168	ARG	HB3	1.874	0	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	168	ARG	HG3	1.653	0	1
1	A	168	ARG	HD3	3.201	0.006	1
1	A	168	ARG	C	176.189	0.008	1
1	A	168	ARG	CA	56.158	0.05	1
1	A	168	ARG	CB	30.754	0.005	1
1	A	168	ARG	CG	27.042	0	1
1	A	168	ARG	CD	43.369	0.088	1
1	A	168	ARG	N	121.815	0.032	1
1	A	169	ALA	H	8.333	0.002	1
1	A	169	ALA	HA	4.33	0.003	1
1	A	169	ALA	HB1	1.402	0.005	1
1	A	169	ALA	HB2	1.402	0.005	1
1	A	169	ALA	HB3	1.402	0.005	1
1	A	169	ALA	C	177.994	0.005	1
1	A	169	ALA	CA	52.753	0.069	1
1	A	169	ALA	CB	19.23	0.029	1
1	A	169	ALA	N	125.167	0.043	1
1	A	170	SER	H	8.277	0.002	1
1	A	170	SER	HA	4.409	0.005	1
1	A	170	SER	HB3	3.892	0.004	1
1	A	170	SER	C	174.64	0.002	1
1	A	170	SER	CA	58.441	0.07	1
1	A	170	SER	CB	63.823	0.054	1
1	A	170	SER	N	115.108	0.052	1
1	A	171	ALA	H	8.343	0.002	1
1	A	171	ALA	HA	4.328	0.001	1
1	A	171	ALA	HB1	1.406	0.005	1
1	A	171	ALA	HB2	1.406	0.005	1
1	A	171	ALA	HB3	1.406	0.005	1
1	A	171	ALA	C	177.861	0.004	1
1	A	171	ALA	CA	52.844	0.057	1
1	A	171	ALA	CB	19.235	0.044	1
1	A	171	ALA	N	125.701	0.027	1
1	A	172	GLU	H	8.304	0.002	1
1	A	172	GLU	HA	4.226	0.007	1
1	A	172	GLU	HB2	2.042	0	2
1	A	172	GLU	HB3	1.939	0	2
1	A	172	GLU	HG3	2.257	0.012	1
1	A	172	GLU	C	176.537	0.021	1
1	A	172	GLU	CA	56.818	0.034	1
1	A	172	GLU	CB	30.238	0.014	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	172	GLU	CG	36.344	0.038	1
1	A	172	GLU	N	119.404	0.046	1
1	A	173	GLN	H	8.305	0.002	1
1	A	173	GLN	HA	4.337	0.004	1
1	A	173	GLN	HB2	2.016	0	2
1	A	173	GLN	HB3	2.117	0	2
1	A	173	GLN	HG3	2.366	0.004	1
1	A	173	GLN	HE21	7.541	0	1
1	A	173	GLN	HE22	6.842	0	1
1	A	173	GLN	C	175.869	0.004	1
1	A	173	GLN	CA	55.809	0.07	1
1	A	173	GLN	CB	29.318	0.012	1
1	A	173	GLN	CG	33.825	0.024	1
1	A	173	GLN	N	121.529	0.036	1
1	A	173	GLN	NE2	112.402	0.001	1
1	A	174	LYS	H	8.329	0.001	1
1	A	174	LYS	HA	4.322	0.006	1
1	A	174	LYS	HB2	1.845	0.015	2
1	A	174	LYS	HB3	1.762	0.007	2
1	A	174	LYS	HG3	1.441	0.012	1
1	A	174	LYS	HE3	2.998	0.001	1
1	A	174	LYS	C	176.613	0.008	1
1	A	174	LYS	CA	56.386	0.071	1
1	A	174	LYS	CB	33.265	0.052	1
1	A	174	LYS	CG	24.639	0.028	1
1	A	174	LYS	CD	28.935	0	1
1	A	174	LYS	CE	42.213	0	1
1	A	174	LYS	N	122.956	0.046	1
1	A	175	GLU	H	8.514	0.003	1
1	A	175	GLU	HA	4.284	0.008	1
1	A	175	GLU	HB2	2.049	0	2
1	A	175	GLU	HB3	1.951	0	2
1	A	175	GLU	HG3	2.275	0	1
1	A	175	GLU	C	176.365	0.005	1
1	A	175	GLU	CA	56.789	0.122	1
1	A	175	GLU	CB	30.252	0.004	1
1	A	175	GLU	CG	36.269	0	1
1	A	175	GLU	N	121.874	0.042	1
1	A	176	SER	H	8.278	0.002	1
1	A	176	SER	HA	4.427	0.003	1
1	A	176	SER	HB3	3.827	0.002	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	176	SER	C	173.851	0.005	1
1	A	176	SER	CA	58.104	0.039	1
1	A	176	SER	CB	63.884	0.076	1
1	A	176	SER	N	116.411	0.049	1
1	A	177	TYR	H	8.216	0.002	1
1	A	177	TYR	HA	4.587	0.006	1
1	A	177	TYR	HB2	3.109	0	2
1	A	177	TYR	HB3	2.98	0.005	2
1	A	177	TYR	HD1	7.101	0	3
1	A	177	TYR	HD2	7.101	0	3
1	A	177	TYR	HE1	6.794	0	3
1	A	177	TYR	HE2	6.794	0	3
1	A	177	TYR	C	174.979	0.003	1
1	A	177	TYR	CA	57.802	0.075	1
1	A	177	TYR	CB	39.068	0.045	1
1	A	177	TYR	CD1	133.253	0	3
1	A	177	TYR	CD2	133.253	0	3
1	A	177	TYR	CE1	118.129	0	3
1	A	177	TYR	CE2	118.129	0	3
1	A	177	TYR	N	122.709	0.064	1
1	A	178	GLU	H	8.047	0.002	1
1	A	178	GLU	HA	4.572	0.004	1
1	A	178	GLU	HB2	1.917	0.011	2
1	A	178	GLU	HB3	1.8	0.007	2
1	A	178	GLU	HG3	2.204	0.004	1
1	A	178	GLU	C	173.149	0	1
1	A	178	GLU	CA	53.428	0.07	1
1	A	178	GLU	CB	30.551	0	1
1	A	178	GLU	N	125.637	0.055	1
1	A	179	PRO	HA	4.594	0.003	1
1	A	179	PRO	HB2	2.377	0.001	2
1	A	179	PRO	HB3	1.917	0	2
1	A	179	PRO	HG3	2.039	0	1
1	A	179	PRO	HD2	3.65	0	2
1	A	179	PRO	HD3	3.684	0	2
1	A	179	PRO	CA	61.315	0.025	1
1	A	179	PRO	CB	30.82	0	1
1	A	179	PRO	CG	27.236	0	1
1	A	179	PRO	CD	50.666	0	1
1	A	180	PRO	HA	4.413	0.006	1
1	A	180	PRO	HB2	2.301	0.004	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	180	PRO	HB3	1.885	0.014	2
1	A	180	PRO	HG3	2.043	0.001	1
1	A	180	PRO	HD2	3.843	0.005	2
1	A	180	PRO	HD3	3.651	0	2
1	A	180	PRO	C	176.659	0.001	1
1	A	180	PRO	CA	62.841	0.085	1
1	A	180	PRO	CB	32.155	0.05	1
1	A	180	PRO	CG	27.334	0.012	1
1	A	180	PRO	CD	50.567	0.058	1
1	A	181	LYS	H	8.407	0.003	1
1	A	181	LYS	HA	4.595	0.001	1
1	A	181	LYS	HB2	1.714	0.012	2
1	A	181	LYS	HB3	1.844	0.009	2
1	A	181	LYS	HG2	1.527	0	2
1	A	181	LYS	HG3	1.496	0	2
1	A	181	LYS	HD3	1.713	0	1
1	A	181	LYS	HE3	3.016	0.005	1
1	A	181	LYS	C	174.66	0	1
1	A	181	LYS	CA	54.117	0.048	1
1	A	181	LYS	CB	32.372	0.031	1
1	A	181	LYS	CG	24.601	0	1
1	A	181	LYS	CD	29.077	0	1
1	A	181	LYS	CE	42.181	0	1
1	A	181	LYS	N	122.926	0.053	1
1	A	182	PRO	HA	4.41	0	1
1	A	182	PRO	HB2	2.306	0.002	2
1	A	182	PRO	HB3	1.902	0.003	2
1	A	182	PRO	HD3	3.841	0	1
1	A	182	PRO	C	176.489	0.004	1
1	A	182	PRO	CA	62.97	0	1
1	A	182	PRO	CB	32.138	0.056	1
1	A	182	PRO	CD	50.582	0	1
1	A	183	ALA	H	8.438	0.003	1
1	A	183	ALA	HA	4.349	0.003	1
1	A	183	ALA	HB1	1.396	0.001	1
1	A	183	ALA	HB2	1.396	0.001	1
1	A	183	ALA	HB3	1.396	0.001	1
1	A	183	ALA	C	177.674	0.015	1
1	A	183	ALA	CA	52.387	0.075	1
1	A	183	ALA	CB	19.234	0.022	1
1	A	183	ALA	N	124.907	0.046	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	184	VAL	H	8.12	0.002	1
1	A	184	VAL	HA	4.216	0.001	1
1	A	184	VAL	HB	2.095	0.004	1
1	A	184	VAL	HG21	0.956	0	1
1	A	184	VAL	HG22	0.956	0	1
1	A	184	VAL	HG23	0.956	0	1
1	A	184	VAL	C	176.291	0.046	1
1	A	184	VAL	CA	61.935	0.028	1
1	A	184	VAL	CB	33.222	0.034	1
1	A	184	VAL	CG2	21.158	0.037	1
1	A	184	VAL	N	118.963	0.068	1
1	A	185	GLY	H	8.334	0.002	1
1	A	185	GLY	HA2	4.169	0.007	2
1	A	185	GLY	HA3	4.012	0.009	2
1	A	185	GLY	C	176.715	0	1
1	A	185	GLY	CA	44.5	0.04	1
1	A	185	GLY	N	112.379	0.057	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	74	-0.39 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	69	0.18 ± 0.19	None needed (< 0.5 ppm)
$^{13}C'$	72	-0.23 ± 0.18	None needed (< 0.5 ppm)
^{15}N	69	-0.09 ± 0.73	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 44%, i.e. 522 atoms were assigned a chemical shift out of a possible 1180. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	203/412 (49%)	81/166 (49%)	81/164 (49%)	41/82 (50%)
Sidechain	247/622 (40%)	163/398 (41%)	81/194 (42%)	3/30 (10%)
Aromatic	72/146 (49%)	36/72 (50%)	34/70 (49%)	2/4 (50%)
Overall	522/1180 (44%)	280/636 (44%)	196/428 (46%)	46/116 (40%)

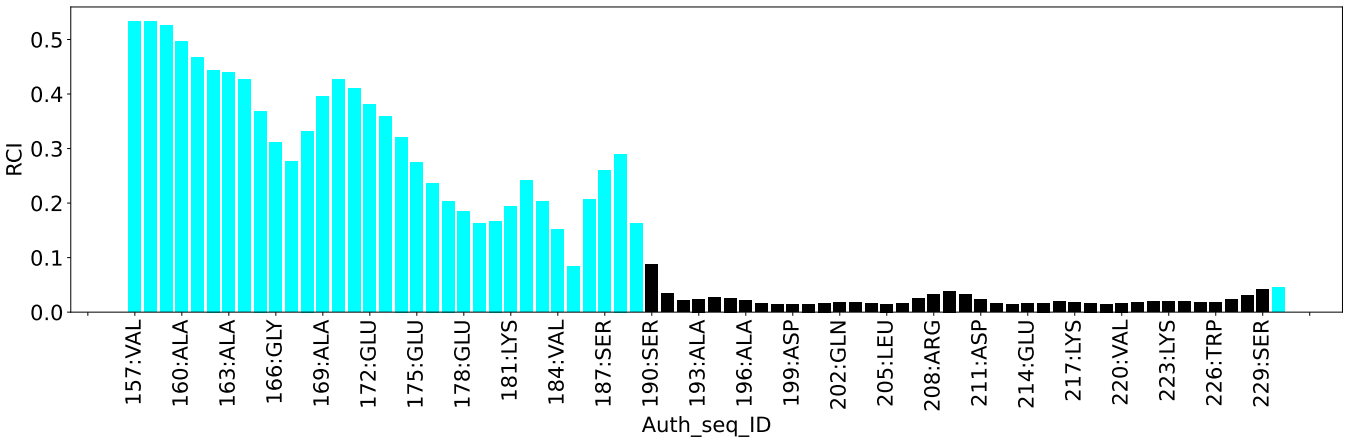
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2240
Intra-residue (|i-j|=0)	692
Sequential (|i-j|=1)	442
Medium range (|i-j|>1 and |i-j|<5)	574
Long range (|i-j|≥5)	270
Inter-chain	166
Hydrogen bond restraints	96
Disulfide bond restraints	0
Total dihedral-angle restraints	152
Number of unmapped restraints	0
Number of restraints per residue	15.9
Number of long range restraints per residue[1]	1.8

[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)	46.7	0.2
0.2-0.5 (Medium)	68.8	0.5
>0.5 (Large)	50.0	4.44

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)	12.9	3.8
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

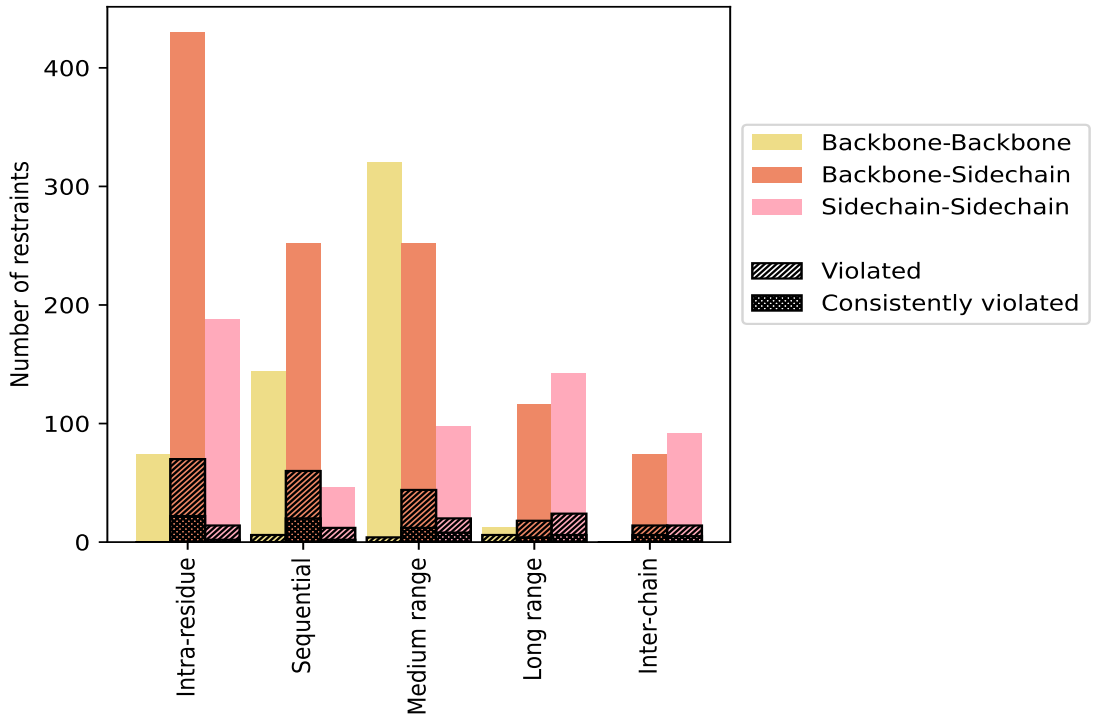
9.1 Summary of distance violations (i)

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)	692	30.9	84	12.1	3.8	24	3.5	1.1
Backbone-Backbone	74	3.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	430	19.2	70	16.3	3.1	22	5.1	1.0
Sidechain-Sidechain	188	8.4	14	7.4	0.6	2	1.1	0.1
Sequential (|i-j|=1)	442	19.7	78	17.6	3.5	22	5.0	1.0
Backbone-Backbone	144	6.4	6	4.2	0.3	0	0.0	0.0
Backbone-Sidechain	252	11.2	60	23.8	2.7	20	7.9	0.9
Sidechain-Sidechain	46	2.1	12	26.1	0.5	2	4.3	0.1
Medium range (|i-j|>1 & |i-j|<5)	574	25.6	68	11.8	3.0	20	3.5	0.9
Backbone-Backbone	224	10.0	4	1.8	0.2	0	0.0	0.0
Backbone-Sidechain	252	11.2	44	17.5	2.0	12	4.8	0.5
Sidechain-Sidechain	98	4.4	20	20.4	0.9	8	8.2	0.4
Long range (|i-j|≥5)	270	12.1	48	17.8	2.1	10	3.7	0.4
Backbone-Backbone	12	0.5	6	50.0	0.3	0	0.0	0.0
Backbone-Sidechain	116	5.2	18	15.5	0.8	4	3.4	0.2
Sidechain-Sidechain	142	6.3	24	16.9	1.1	6	4.2	0.3
Inter-chain	166	7.4	28	16.9	1.2	11	6.6	0.5
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	74	3.3	14	18.9	0.6	6	8.1	0.3
Sidechain-Sidechain	92	4.1	14	15.2	0.6	5	5.4	0.2
Hydrogen bond	96	4.3	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	2240	100.0	306	13.7	13.7	87	3.9	3.9
Backbone-Backbone	550	24.6	16	2.9	0.7	0	0.0	0.0
Backbone-Sidechain	1124	50.2	206	18.3	9.2	64	5.7	2.9
Sidechain-Sidechain	566	25.3	84	14.8	3.8	23	4.1	1.0

[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

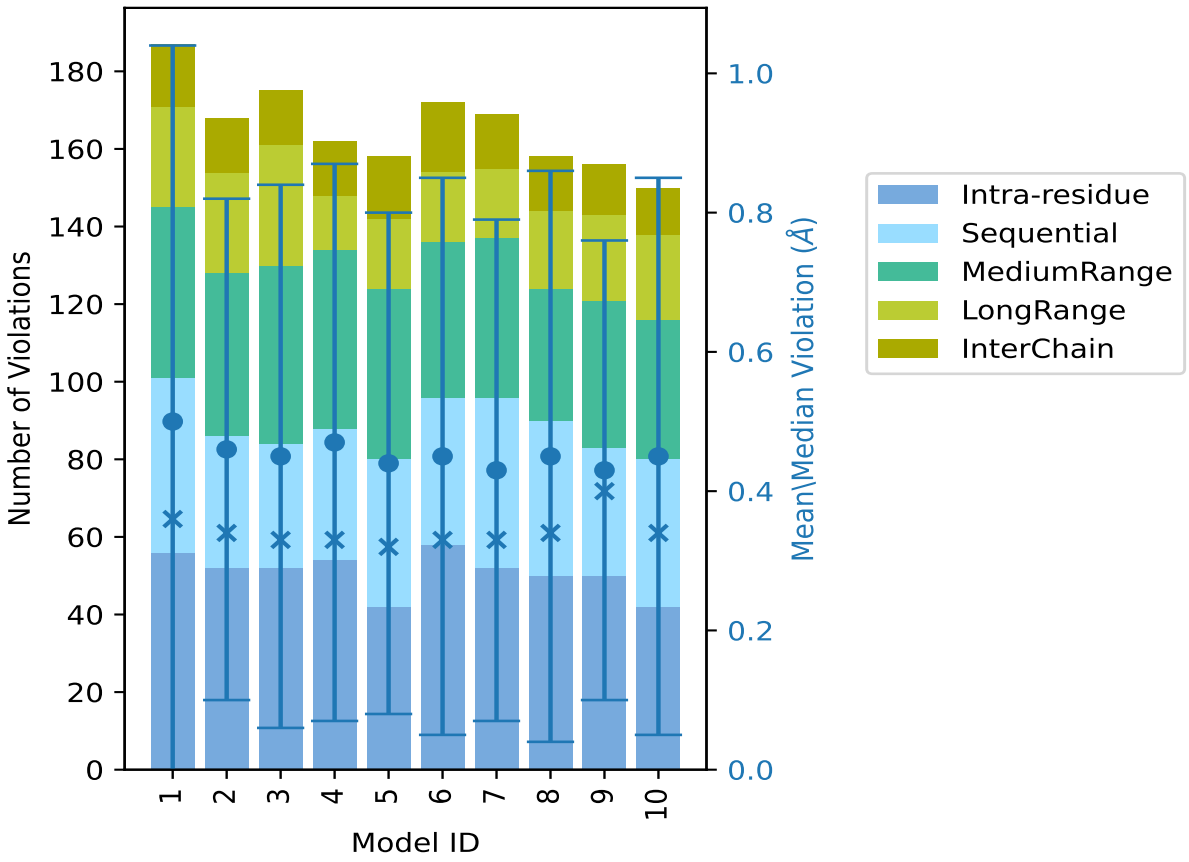
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

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	56	45	44	26	16	187	0.5	4.44	0.54	0.36
2	52	34	42	26	14	168	0.46	2.0	0.36	0.34
3	52	32	46	31	14	175	0.45	2.27	0.39	0.33
4	54	34	46	14	14	162	0.47	2.17	0.4	0.33
5	42	38	44	18	16	158	0.44	2.15	0.36	0.32
6	58	38	40	18	18	172	0.45	2.29	0.4	0.33
7	52	44	41	18	14	169	0.43	2.12	0.36	0.33
8	50	40	34	20	14	158	0.45	2.57	0.41	0.34
9	50	33	38	22	13	156	0.43	2.2	0.33	0.4
10	42	38	36	22	12	150	0.45	2.16	0.4	0.34

[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

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, 1838(IR:608, SQ:364, MR:506, LR:222, IC:138) 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]	%
12	24	12	15	7	70	1	10.0
4	6	4	11	8	33	2	20.0
10	6	7	2	1	26	3	30.0
4	6	3	0	0	13	4	40.0

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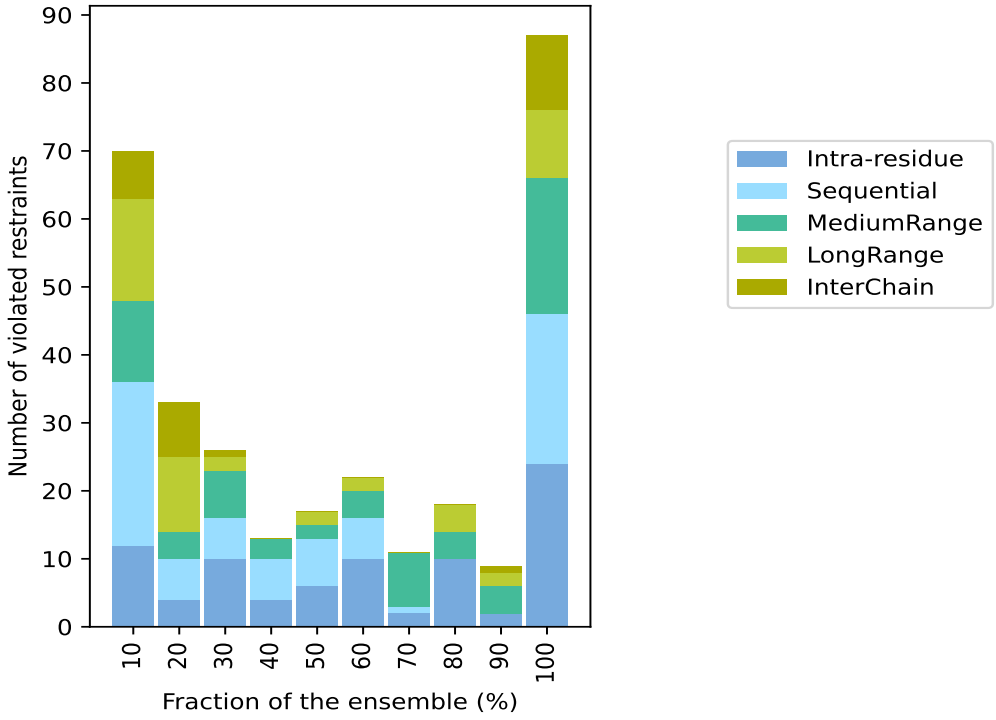
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
6	7	2	2	0	17	5	50.0
10	6	4	2	0	22	6	60.0
2	1	8	0	0	11	7	70.0
10	0	4	4	0	18	8	80.0
2	0	4	2	1	9	9	90.0
24	22	20	10	11	87	10	100.0

[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

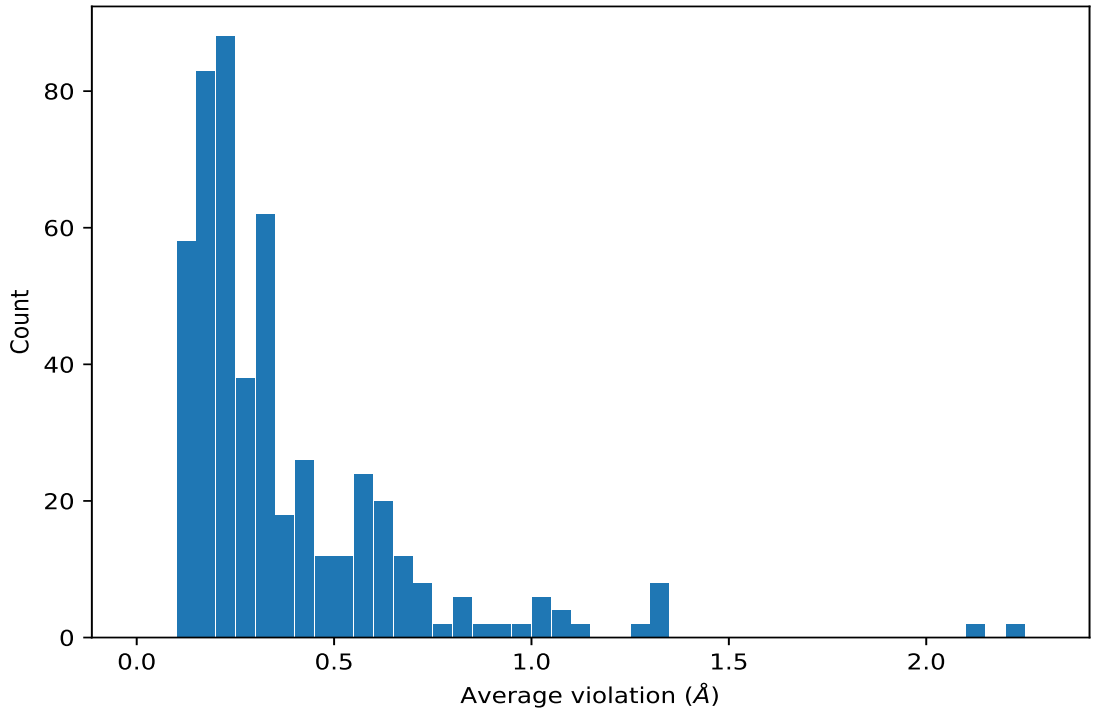
9.3.1 Bar graph : Distance violation statistics for the ensemble



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.

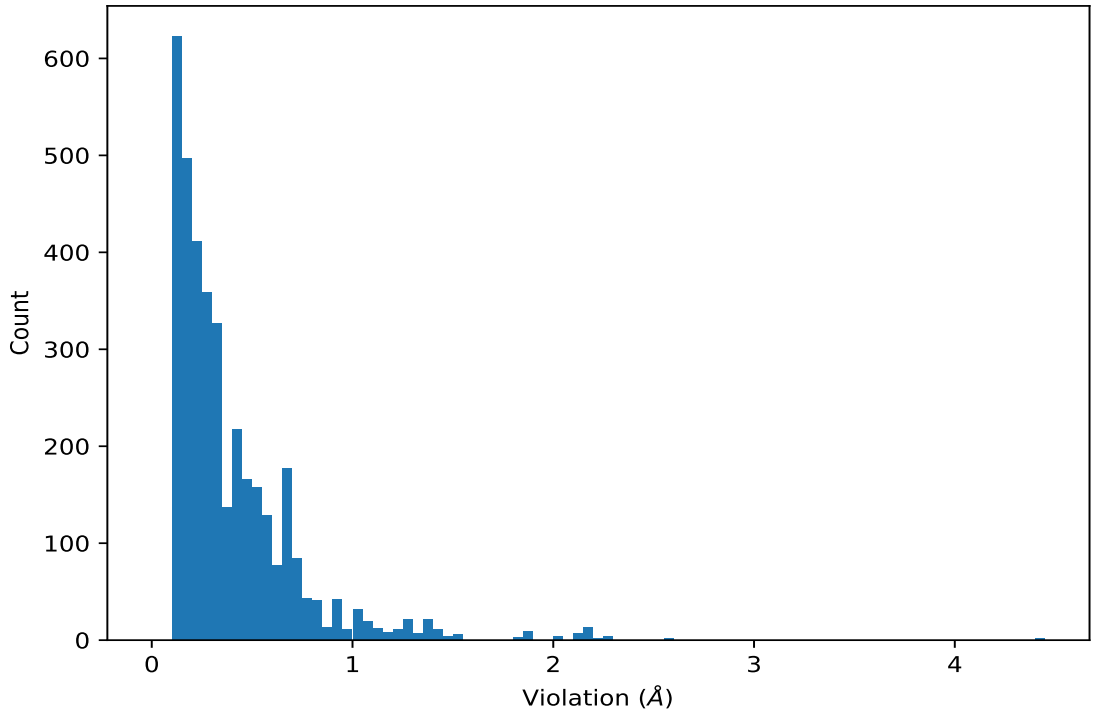
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,908)	1:B:206:GLU:HB3	1:B:203:GLY:HA3	10	2.13	0.08	2.13
(1,907)	1:A:206:GLU:HB3	1:A:203:GLY:HA3	10	2.13	0.08	2.13
(1,837)	1:A:209:LEU:HD12	1:B:188:GLY:HA3	10	1.34	0.33	1.35
(1,837)	1:A:209:LEU:HD11	1:B:188:GLY:HA3	10	1.34	0.33	1.35
(1,837)	1:A:209:LEU:HD13	1:B:188:GLY:HA3	10	1.34	0.33	1.35
(1,838)	1:B:209:LEU:HD12	1:A:188:GLY:HA3	10	1.34	0.33	1.34
(1,838)	1:B:209:LEU:HD11	1:A:188:GLY:HA3	10	1.34	0.33	1.34
(1,838)	1:B:209:LEU:HD13	1:A:188:GLY:HA3	10	1.34	0.33	1.34
(1,558)	1:B:215:ALA:HA	1:B:214:GLU:HB2	10	1.33	0.05	1.36
(1,557)	1:A:215:ALA:HA	1:A:214:GLU:HB2	10	1.33	0.06	1.36
(1,608)	1:B:207:GLN:HB3	1:B:204:PHE:HA	10	1.1	0.09	1.06
(1,607)	1:A:207:GLN:HB3	1:A:204:PHE:HA	10	1.1	0.09	1.06
(1,1810)	1:B:186:PRO:HB3	1:B:187:SER:HA	10	1.09	0.49	1.08
(1,1810)	1:B:187:SER:HA	1:A:210:LYS:HB3	10	1.09	0.49	1.08
(1,1809)	1:A:186:PRO:HB3	1:A:187:SER:HA	10	1.08	0.5	1.08

[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)
(1,147)	1:A:186:PRO:HB2	1:A:190:SER:HB3	1	4.44
(1,148)	1:B:186:PRO:HB2	1:B:190:SER:HB3	1	4.43
(1,147)	1:A:186:PRO:HB2	1:A:190:SER:HB3	8	2.57
(1,148)	1:B:186:PRO:HB2	1:B:190:SER:HB3	8	2.56
(1,907)	1:A:206:GLU:HB3	1:A:203:GLY:HA3	6	2.29
(1,908)	1:B:206:GLU:HB3	1:B:203:GLY:HA3	6	2.28
(1,148)	1:B:186:PRO:HB2	1:B:190:SER:HB3	3	2.27
(1,147)	1:A:186:PRO:HB2	1:A:190:SER:HB3	3	2.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,908)	1:B:206:GLU:HB3	1:B:203:GLY:HA3	9	2.2
(1,907)	1:A:206:GLU:HB3	1:A:203:GLY:HA3	9	2.2

10 Dihedral-angle violation analysis

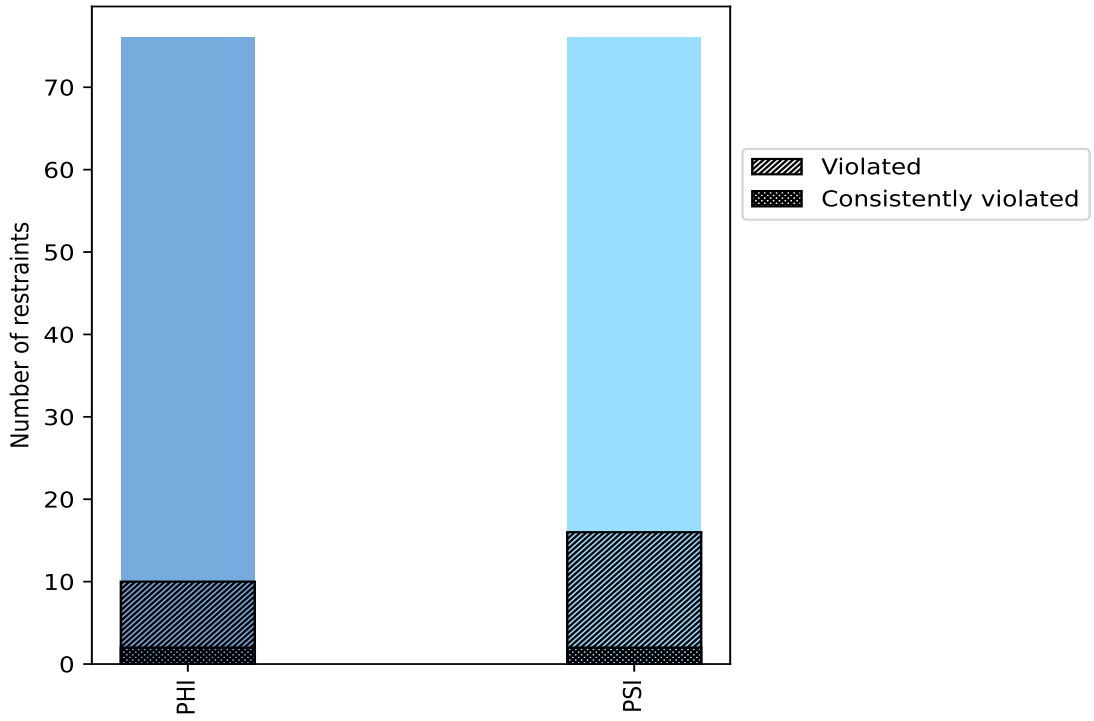
10.1 Summary of dihedral-angle violations

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]
PHI	76	50.0	10	13.2	6.6	2	2.6	1.3
PSI	76	50.0	16	21.1	10.5	2	2.6	1.3
Total	152	100.0	26	17.1	17.1	4	2.6	2.6

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



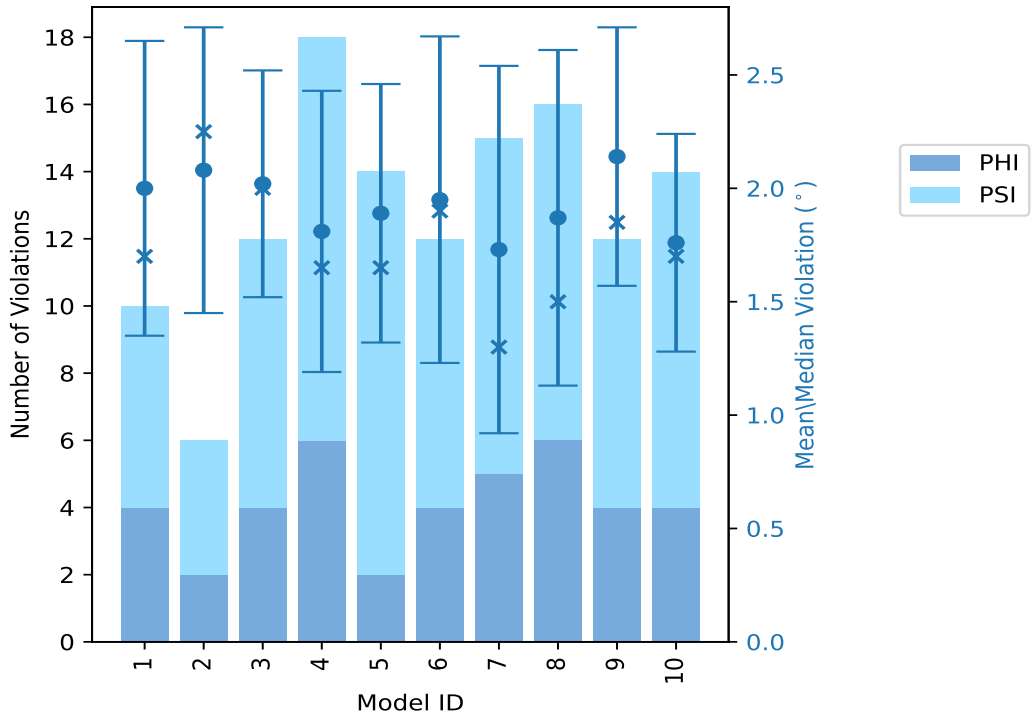
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PHI	PSI	Total				
1	4	6	10	2.0	2.9	0.65	1.7
2	2	4	6	2.08	2.8	0.63	2.25
3	4	8	12	2.02	3.0	0.5	2.0
4	6	12	18	1.81	3.1	0.62	1.65
5	2	12	14	1.89	2.9	0.57	1.65
6	4	8	12	1.95	3.1	0.72	1.9
7	5	10	15	1.73	3.3	0.81	1.3
8	6	10	16	1.87	3.8	0.74	1.5
9	4	8	12	2.14	3.1	0.57	1.85
10	4	10	14	1.76	2.6	0.48	1.7

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



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

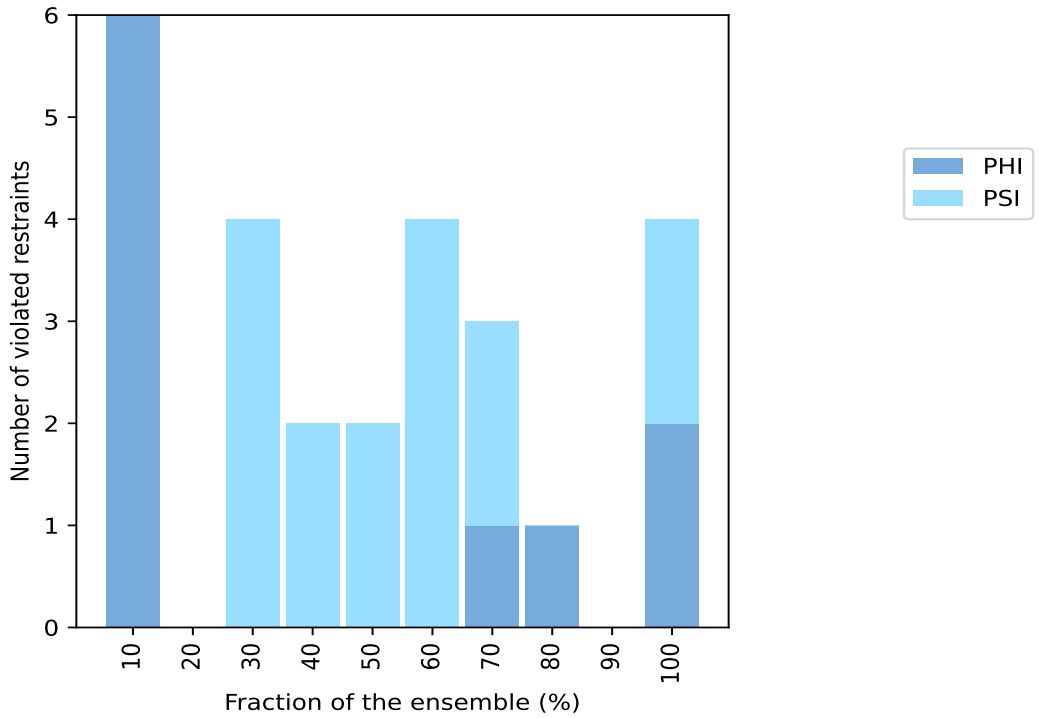
10.3 Dihedral-angle violation statistics for the ensemble

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
6	0	6	1	10.0
0	0	0	2	20.0
0	4	4	3	30.0
0	2	2	4	40.0
0	2	2	5	50.0
0	4	4	6	60.0
1	2	3	7	70.0
1	0	1	8	80.0
0	0	0	9	90.0
2	2	4	10	100.0

[1] Number of models with violations

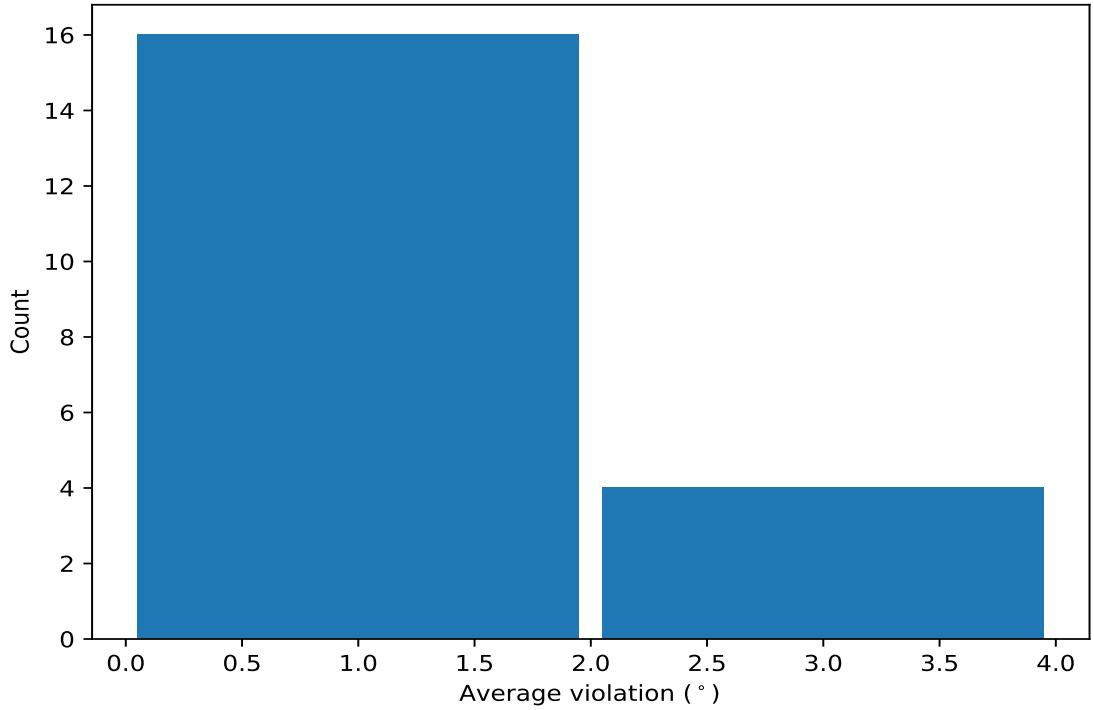
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



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.

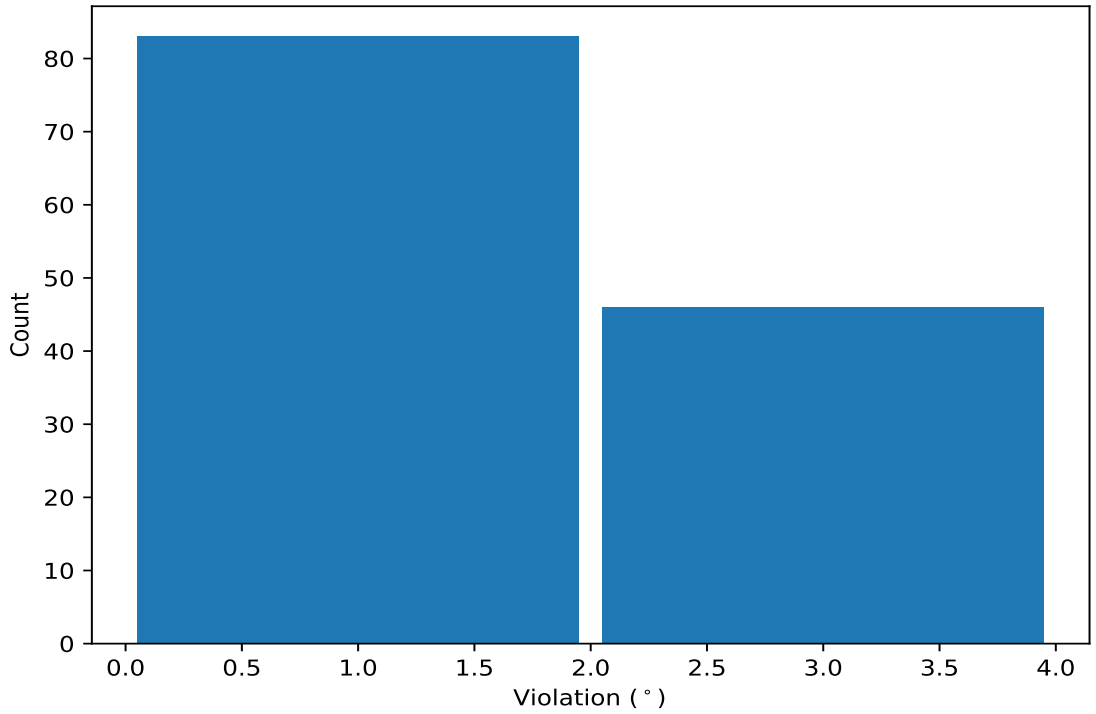
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,53)	1:A:217:LYS:C	1:A:218:LEU:N	1:A:218:LEU:CA	1:A:218:LEU:C	10	2.93	0.34	2.85
(1,129)	1:B:217:LYS:C	1:B:218:LEU:N	1:B:218:LEU:CA	1:B:218:LEU:C	10	2.9	0.3	2.9
(1,6)	1:A:193:ALA:N	1:A:193:ALA:CA	1:A:193:ALA:C	1:A:194:THR:N	10	2.59	0.47	2.75
(1,82)	1:B:193:ALA:N	1:B:193:ALA:CA	1:B:193:ALA:C	1:B:194:THR:N	10	2.5	0.4	2.5
(1,133)	1:B:219:ARG:C	1:B:220:VAL:N	1:B:220:VAL:CA	1:B:220:VAL:C	8	1.64	0.32	1.75
(1,57)	1:A:219:ARG:C	1:A:220:VAL:N	1:A:220:VAL:CA	1:A:220:VAL:C	7	1.7	0.31	1.7
(1,114)	1:B:209:LEU:N	1:B:209:LEU:CA	1:B:209:LEU:C	1:B:210:LYS:N	7	1.63	0.4	1.5
(1,98)	1:B:201:LEU:N	1:B:201:LEU:CA	1:B:201:LEU:C	1:B:202:GLN:N	7	1.57	0.25	1.6
(1,38)	1:A:209:LEU:N	1:A:209:LEU:CA	1:A:209:LEU:C	1:A:210:LYS:N	6	1.67	0.33	1.7
(1,22)	1:A:201:LEU:N	1:A:201:LEU:CA	1:A:201:LEU:C	1:A:202:GLN:N	6	1.62	0.16	1.6

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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

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 (°)
(1,53)	1:A:217:LYS:C	1:A:218:LEU:N	1:A:218:LEU:CA	1:A:218:LEU:C	8	3.8
(1,129)	1:B:217:LYS:C	1:B:218:LEU:N	1:B:218:LEU:CA	1:B:218:LEU:C	8	3.5
(1,129)	1:B:217:LYS:C	1:B:218:LEU:N	1:B:218:LEU:CA	1:B:218:LEU:C	7	3.3
(1,53)	1:A:217:LYS:C	1:A:218:LEU:N	1:A:218:LEU:CA	1:A:218:LEU:C	7	3.2
(1,82)	1:B:193:ALA:N	1:B:193:ALA:CA	1:B:193:ALA:C	1:B:194:THR:N	4	3.1
(1,6)	1:A:193:ALA:N	1:A:193:ALA:CA	1:A:193:ALA:C	1:A:194:THR:N	6	3.1
(1,6)	1:A:193:ALA:N	1:A:193:ALA:CA	1:A:193:ALA:C	1:A:194:THR:N	9	3.1
(1,6)	1:A:193:ALA:N	1:A:193:ALA:CA	1:A:193:ALA:C	1:A:194:THR:N	7	3.0
(1,53)	1:A:217:LYS:C	1:A:218:LEU:N	1:A:218:LEU:CA	1:A:218:LEU:C	3	3.0
(1,129)	1:B:217:LYS:C	1:B:218:LEU:N	1:B:218:LEU:CA	1:B:218:LEU:C	3	3.0