



wwPDB NMR Structure Validation Summary Report ⓘ

Dec 25, 2024 – 03:31 AM EST

PDB ID : 5ID3
BMRB ID : 30021
Title : Solution structure of the pore-forming region of *C. elegans* Mitochondrial Calcium Uniporter (MCU)
Authors : Oxenoid, K.; Dong, Y.; Cao, C.; Cui, T.; Sancak, Y.; Markhard, A.L.; Grabarek, Z.; Kong, L.; Liu, Z.; Ouyang, B.; Cong, Y.; Mootha, V.K.; Chou, J.J.; Membrane Protein Structures by Solution NMR (MPSbyNMR)
Deposited on : 2016-02-23

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.40

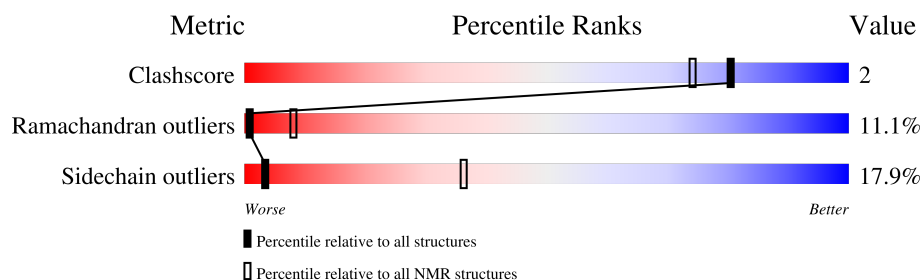
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 6%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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

Mol	Chain	Length	Quality of chain
1	A	159	50% 21% 6% 19% .
1	B	159	56% 16% . . 19% .
1	C	159	51% 19% 5% 21% .
1	D	159	50% 21% . 21% .
1	E	159	53% 18% . . 19% .

2 Ensemble composition and analysis

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

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:179-A:271, A:289-A:318, B:178-B:271, B:290-B:318, C:179-C:269, C:290-C:317, D:178-D:269, D:291-D:317, E:177-E:269, E:290-E:318 (606)	1.03	1

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

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

The models can be grouped into 1 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12675 atoms, of which 6270 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mitochondrial Calcium Uniporter.

Mol	Chain	Residues	Atoms						Trace
1	A	153	Total	C	H	N	O	S	0
			2535	822	1254	219	239	1	
1	B	153	Total	C	H	N	O	S	0
			2535	822	1254	219	239	1	
1	C	153	Total	C	H	N	O	S	0
			2535	822	1254	219	239	1	
1	D	153	Total	C	H	N	O	S	0
			2535	822	1254	219	239	1	
1	E	153	Total	C	H	N	O	S	0
			2535	822	1254	219	239	1	

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	MET	-	initiating methionine	UNP Q21121
A	170	SER	CYS	engineered mutation	UNP Q21121
A	207	ALA	CYS	engineered mutation	UNP Q21121
A	215	ALA	MET	engineered mutation	UNP Q21121
A	222	SER	MET	engineered mutation	UNP Q21121
A	242	VAL	MET	engineered mutation	UNP Q21121
A	255	ALA	CYS	engineered mutation	UNP Q21121
A	313	LEU	MET	engineered mutation	UNP Q21121
A	318	GLU	PHE	engineered mutation	UNP Q21121
A	319	HIS	-	expression tag	UNP Q21121
A	320	HIS	-	expression tag	UNP Q21121
A	321	HIS	-	expression tag	UNP Q21121
A	322	HIS	-	expression tag	UNP Q21121
A	323	HIS	-	expression tag	UNP Q21121
A	324	HIS	-	expression tag	UNP Q21121
B	166	MET	-	initiating methionine	UNP Q21121
B	170	SER	CYS	engineered mutation	UNP Q21121
B	207	ALA	CYS	engineered mutation	UNP Q21121
B	215	ALA	MET	engineered mutation	UNP Q21121
B	222	SER	MET	engineered mutation	UNP Q21121
B	242	VAL	MET	engineered mutation	UNP Q21121
B	255	ALA	CYS	engineered mutation	UNP Q21121
B	313	LEU	MET	engineered mutation	UNP Q21121

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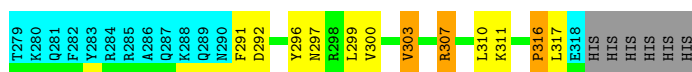
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Chain	Residue	Modelled	Actual	Comment	Reference
B	318	GLU	PHE	engineered mutation	UNP Q21121
B	319	HIS	-	expression tag	UNP Q21121
B	320	HIS	-	expression tag	UNP Q21121
B	321	HIS	-	expression tag	UNP Q21121
B	322	HIS	-	expression tag	UNP Q21121
B	323	HIS	-	expression tag	UNP Q21121
B	324	HIS	-	expression tag	UNP Q21121
C	166	MET	-	initiating methionine	UNP Q21121
C	170	SER	CYS	engineered mutation	UNP Q21121
C	207	ALA	CYS	engineered mutation	UNP Q21121
C	215	ALA	MET	engineered mutation	UNP Q21121
C	222	SER	MET	engineered mutation	UNP Q21121
C	242	VAL	MET	engineered mutation	UNP Q21121
C	255	ALA	CYS	engineered mutation	UNP Q21121
C	313	LEU	MET	engineered mutation	UNP Q21121
C	318	GLU	PHE	engineered mutation	UNP Q21121
C	319	HIS	-	expression tag	UNP Q21121
C	320	HIS	-	expression tag	UNP Q21121
C	321	HIS	-	expression tag	UNP Q21121
C	322	HIS	-	expression tag	UNP Q21121
C	323	HIS	-	expression tag	UNP Q21121
C	324	HIS	-	expression tag	UNP Q21121
D	166	MET	-	initiating methionine	UNP Q21121
D	170	SER	CYS	engineered mutation	UNP Q21121
D	207	ALA	CYS	engineered mutation	UNP Q21121
D	215	ALA	MET	engineered mutation	UNP Q21121
D	222	SER	MET	engineered mutation	UNP Q21121
D	242	VAL	MET	engineered mutation	UNP Q21121
D	255	ALA	CYS	engineered mutation	UNP Q21121
D	313	LEU	MET	engineered mutation	UNP Q21121
D	318	GLU	PHE	engineered mutation	UNP Q21121
D	319	HIS	-	expression tag	UNP Q21121
D	320	HIS	-	expression tag	UNP Q21121
D	321	HIS	-	expression tag	UNP Q21121
D	322	HIS	-	expression tag	UNP Q21121
D	323	HIS	-	expression tag	UNP Q21121
D	324	HIS	-	expression tag	UNP Q21121
E	166	MET	-	initiating methionine	UNP Q21121
E	170	SER	CYS	engineered mutation	UNP Q21121
E	207	ALA	CYS	engineered mutation	UNP Q21121
E	215	ALA	MET	engineered mutation	UNP Q21121
E	222	SER	MET	engineered mutation	UNP Q21121

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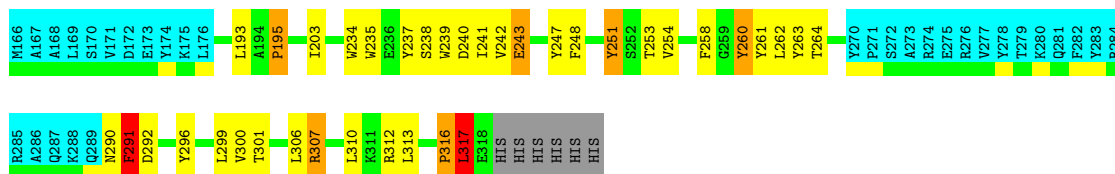
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Chain	Residue	Modelled	Actual	Comment	Reference
E	242	VAL	MET	engineered mutation	UNP Q21121
E	255	ALA	CYS	engineered mutation	UNP Q21121
E	313	LEU	MET	engineered mutation	UNP Q21121
E	318	GLU	PHE	engineered mutation	UNP Q21121
E	319	HIS	-	expression tag	UNP Q21121
E	320	HIS	-	expression tag	UNP Q21121
E	321	HIS	-	expression tag	UNP Q21121
E	322	HIS	-	expression tag	UNP Q21121
E	323	HIS	-	expression tag	UNP Q21121
E	324	HIS	-	expression tag	UNP Q21121



• Molecule 1: Mitochondrial Calcium Uniporter

Chain E: 53% 18% 19%

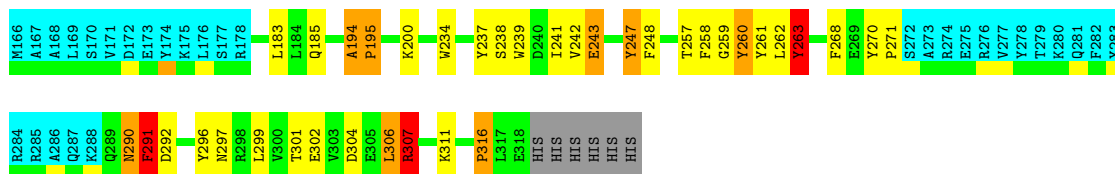


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

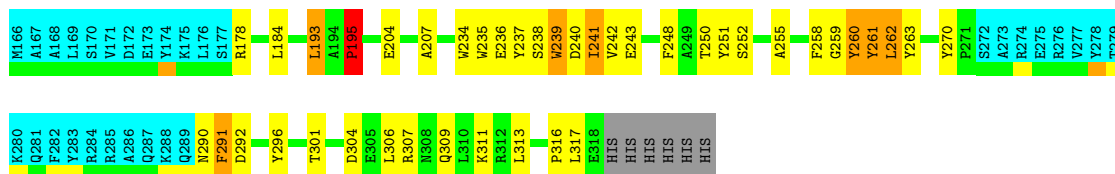
• Molecule 1: Mitochondrial Calcium Uniporter

Chain A: 54% 16% 5% 19%



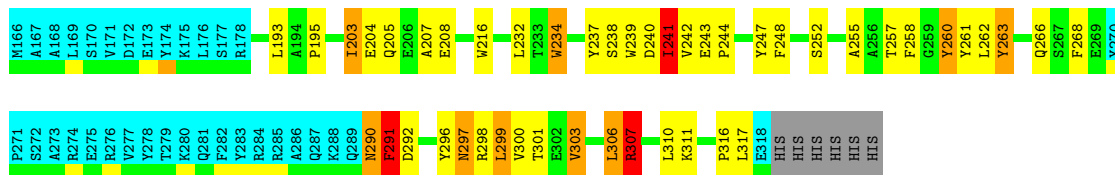
• Molecule 1: Mitochondrial Calcium Uniporter

Chain B: 52% 21% 19%



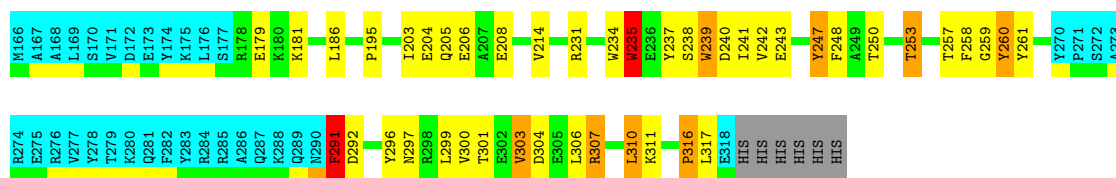
• Molecule 1: Mitochondrial Calcium Uniporter

Chain C: 46% 21% 6% 21%



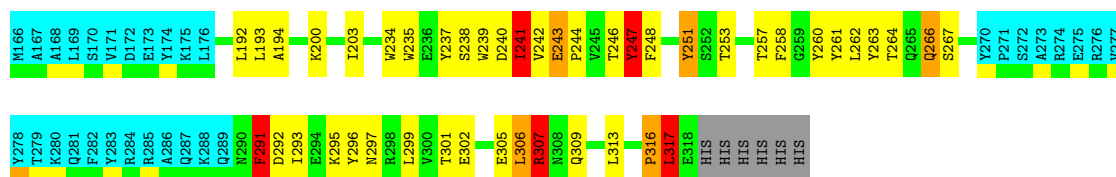
• Molecule 1: Mitochondrial Calcium Uniporter

Chain D:  47% 21% 5% 21%



● Molecule 1: Mitochondrial Calcium Uniporter

Chain E:  48% 22% 19%



5 Refinement protocol and experimental data overview

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

Of the 150 calculated structures, 15 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
XPLOR-NIH	structure calculation	
XPLOR-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	657
Number of shifts mapped to atoms	657
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	6%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	2.27±0.01	15±2/1052 (1.4± 0.2%)	0.99±0.02	2±1/1432 (0.1± 0.1%)
1	B	2.27±0.01	14±2/1054 (1.3± 0.2%)	0.99±0.02	2±1/1434 (0.1± 0.1%)
1	C	2.27±0.02	14±2/1014 (1.4± 0.2%)	1.02±0.03	3±2/1381 (0.2± 0.1%)
1	D	2.27±0.01	12±2/1017 (1.2± 0.2%)	1.01±0.02	1±1/1384 (0.1± 0.1%)
1	E	2.28±0.01	14±2/1039 (1.3± 0.2%)	1.02±0.02	2±1/1412 (0.1± 0.1%)
All	All	2.27	1031/77640 (1.3%)	1.01	151/105645 (0.1%)

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	D	0.0±0.0	0.2±0.4
1	C	0.0±0.0	0.2±0.4
1	E	0.0±0.0	0.1±0.2
All	All	0	7

5 of 168 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	E	296	TYR	CB-CG	6.90	1.62	1.51	12	15
1	C	248	PHE	CB-CG	6.84	1.62	1.51	10	15
1	B	237	TYR	CB-CG	6.80	1.61	1.51	12	14
1	C	296	TYR	CB-CG	6.78	1.61	1.51	12	13
1	D	243	GLU	CB-CG	6.76	1.65	1.52	8	6

5 of 48 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	263	TYR	CB-CG-CD1	7.42	125.45	121.00	15	1
1	C	263	TYR	CB-CG-CD2	6.84	125.10	121.00	15	2
1	B	195	PRO	N-CA-CB	-6.79	95.14	102.60	1	8
1	E	251	TYR	CB-CG-CD1	6.74	125.05	121.00	15	1
1	D	237	TYR	CB-CG-CD2	6.56	124.93	121.00	11	11

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	D	247	TYR	Sidechain	2
1	C	307	ARG	Sidechain	2
1	D	261	TYR	Sidechain	1
1	E	307	ARG	Sidechain	1
1	C	261	TYR	Sidechain	1

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	1025	989	987	6±2
1	B	1027	994	992	5±2
1	C	988	959	957	5±2
1	D	991	966	964	6±2
1	E	1014	983	981	6±2
All	All	75675	73365	73215	367

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 2.

5 of 175 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:299:LEU:HD12	1:B:300:VAL:N	0.78	1.93	6	1
1:D:262:LEU:H	1:D:262:LEU:HD23	0.73	1.44	13	4
1:B:262:LEU:HD23	1:B:262:LEU:H	0.72	1.43	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:317:LEU:H	1:B:317:LEU:HD13	0.70	1.46	10	1
1:A:262:LEU:H	1:A:262:LEU:HD23	0.69	1.48	15	2

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	122/159 (77%)	99±2 (81±1%)	8±2 (7±1%)	15±2 (12±1%)	1	6
1	B	122/159 (77%)	100±2 (82±2%)	8±3 (7±2%)	14±2 (11±2%)	1	8
1	C	119/159 (75%)	95±2 (80±2%)	10±2 (8±2%)	14±2 (12±2%)	1	7
1	D	119/159 (75%)	97±2 (81±2%)	12±3 (10±2%)	11±2 (9±1%)	1	12
1	E	121/159 (76%)	99±3 (82±2%)	9±2 (7±2%)	13±2 (11±2%)	1	8
All	All	9045/11925 (76%)	7352 (81%)	692 (8%)	1001 (11%)	1	8

5 of 114 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	194	ALA	15
1	A	238	SER	15
1	A	242	VAL	15
1	A	243	GLU	15
1	A	291	PHE	15

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	106/138 (77%)	86±2 (81±2%)	20±2 (19±2%)	3	34
1	B	106/138 (77%)	90±3 (85±3%)	16±3 (15±3%)	4	42
1	C	102/138 (74%)	84±2 (82±2%)	18±2 (18±2%)	3	37
1	D	102/138 (74%)	85±3 (83±3%)	17±3 (17±3%)	4	39
1	E	105/138 (76%)	83±4 (79±4%)	22±4 (21±4%)	2	30
All	All	7815/10350 (76%)	6416 (82%)	1399 (18%)	3	36

5 of 318 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	307	ARG	15
1	B	195	PRO	15
1	C	195	PRO	15
1	C	307	ARG	15
1	D	195	PRO	15

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 6% for the well-defined parts and 6% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *CS.bmrB*

7.1.1 Bookkeeping [i](#)

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

Total number of shifts	657
Number of shifts mapped to atoms	657
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	143	-0.44 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	103	-1.96 ± 0.11	Should be checked
$^{13}\text{C}'$	139	-0.47 ± 0.11	None needed (< 0.5 ppm)
^{15}N	136	0.27 ± 0.35	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 6%, i.e. 545 atoms were assigned a chemical shift out of a possible 8634. 0 out of 110 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	460/3016 (15%)	113/1215 (9%)	234/1212 (19%)	113/589 (19%)
Sidechain	85/4665 (2%)	0/3020 (0%)	85/1451 (6%)	0/194 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/953 (0%)	0/458 (0%)	0/455 (0%)	0/40 (0%)
Overall	545/8634 (6%)	113/4693 (2%)	319/3118 (10%)	113/823 (14%)

7.1.4 Statistically unusual chemical shifts [i](#)

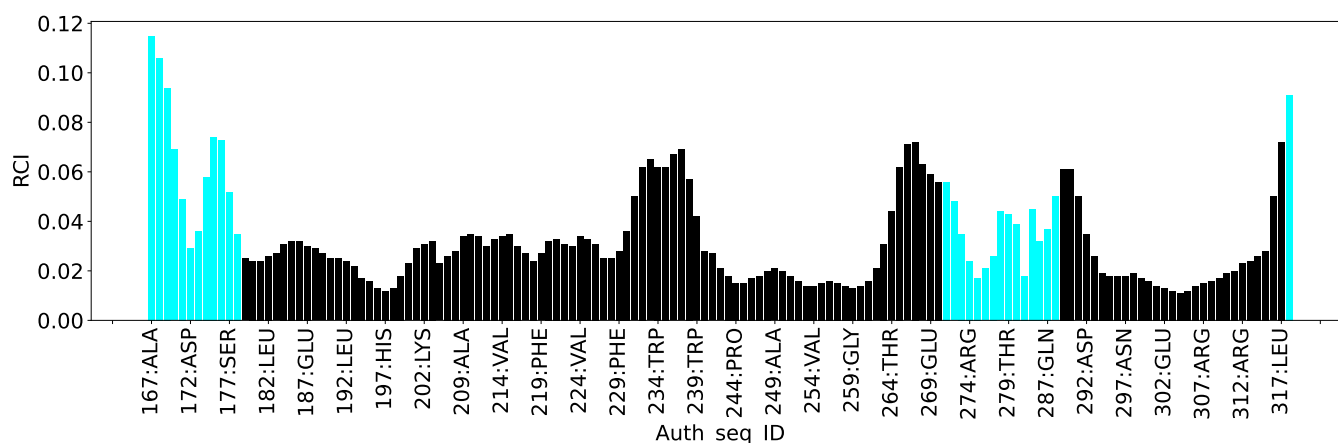
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	315	ASP	CB	32.94	32.98 – 48.76	-5.0

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	2430
Intra-residue ($ i-j =0$)	165
Sequential ($ i-j =1$)	1350
Medium range ($ i-j >1$ and $ i-j <5$)	755
Long range ($ i-j \geq 5$)	160
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	198
Number of unmapped restraints	0
Number of restraints per residue	3.3
Number of long range restraints per residue ¹	0.2

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	170.7	0.2
0.2-0.5 (Medium)	239.0	0.5
>0.5 (Large)	244.7	10.47

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)	67.9	9.57
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

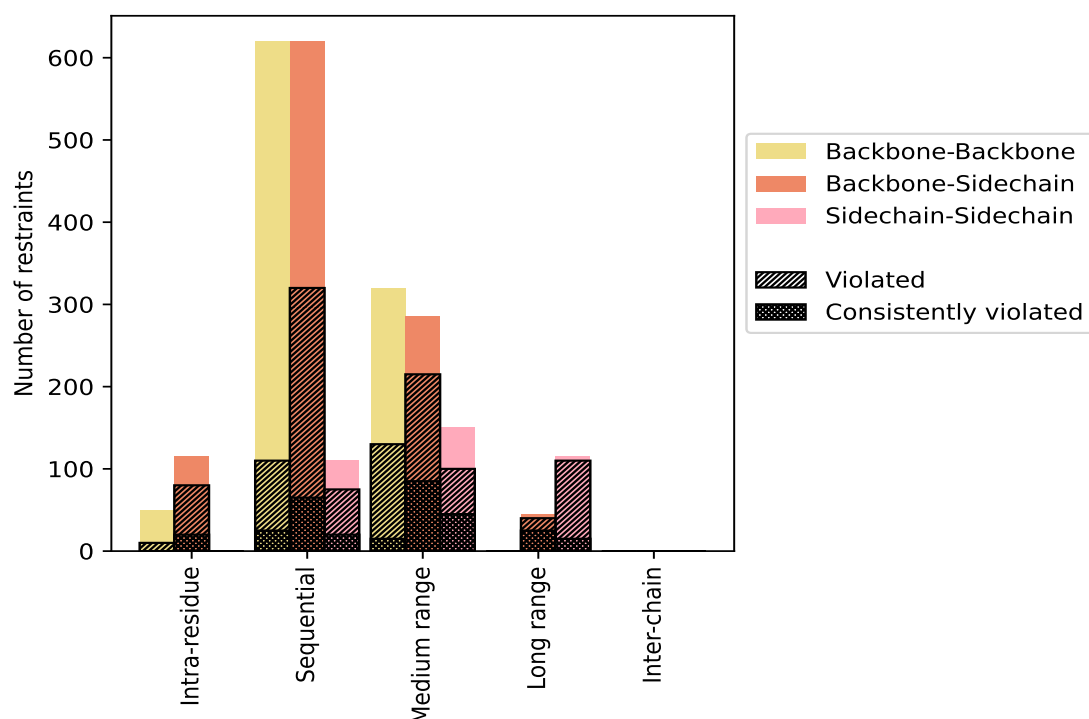
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	165	6.8	90	54.5	3.7	20	12.1	0.8
Backbone-Backbone	50	2.1	10	20.0	0.4	0	0.0	0.0
Backbone-Sidechain	115	4.7	80	69.6	3.3	20	17.4	0.8
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	1350	55.6	505	37.4	20.8	110	8.1	4.5
Backbone-Backbone	620	25.5	110	17.7	4.5	25	4.0	1.0
Backbone-Sidechain	620	25.5	320	51.6	13.2	65	10.5	2.7
Sidechain-Sidechain	110	4.5	75	68.2	3.1	20	18.2	0.8
Medium range ($i-j >1$ & $i-j <5$)	755	31.1	445	58.9	18.3	145	19.2	6.0
Backbone-Backbone	320	13.2	130	40.6	5.3	15	4.7	0.6
Backbone-Sidechain	285	11.7	215	75.4	8.8	85	29.8	3.5
Sidechain-Sidechain	150	6.2	100	66.7	4.1	45	30.0	1.9
Long range ($i-j \geq 5$)	160	6.6	150	93.8	6.2	40	25.0	1.6
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	45	1.9	40	88.9	1.6	25	55.6	1.0
Sidechain-Sidechain	115	4.7	110	95.7	4.5	15	13.0	0.6
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	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2430	100.0	1190	49.0	49.0	315	13.0	13.0
Backbone-Backbone	990	40.7	250	25.3	10.3	40	4.0	1.6
Backbone-Sidechain	1065	43.8	655	61.5	27.0	195	18.3	8.0
Sidechain-Sidechain	375	15.4	285	76.0	11.7	80	21.3	3.3

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

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



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

9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	50	265	290	100	0	705	0.97	9.78	1.52	0.31
2	45	245	285	85	0	660	1.02	10.47	1.52	0.4
3	45	250	280	90	0	665	1.04	9.78	1.61	0.34
4	45	270	250	105	0	670	1.01	9.82	1.52	0.39
5	55	230	280	95	0	660	0.99	10.02	1.51	0.35
6	45	255	295	100	0	695	0.97	9.47	1.53	0.31
7	55	255	285	110	0	705	0.98	10.22	1.56	0.35
8	65	235	285	90	0	675	1.02	9.73	1.58	0.34
9	40	270	235	120	0	665	1.03	10.04	1.61	0.34
10	35	205	275	90	0	605	1.07	9.65	1.55	0.38

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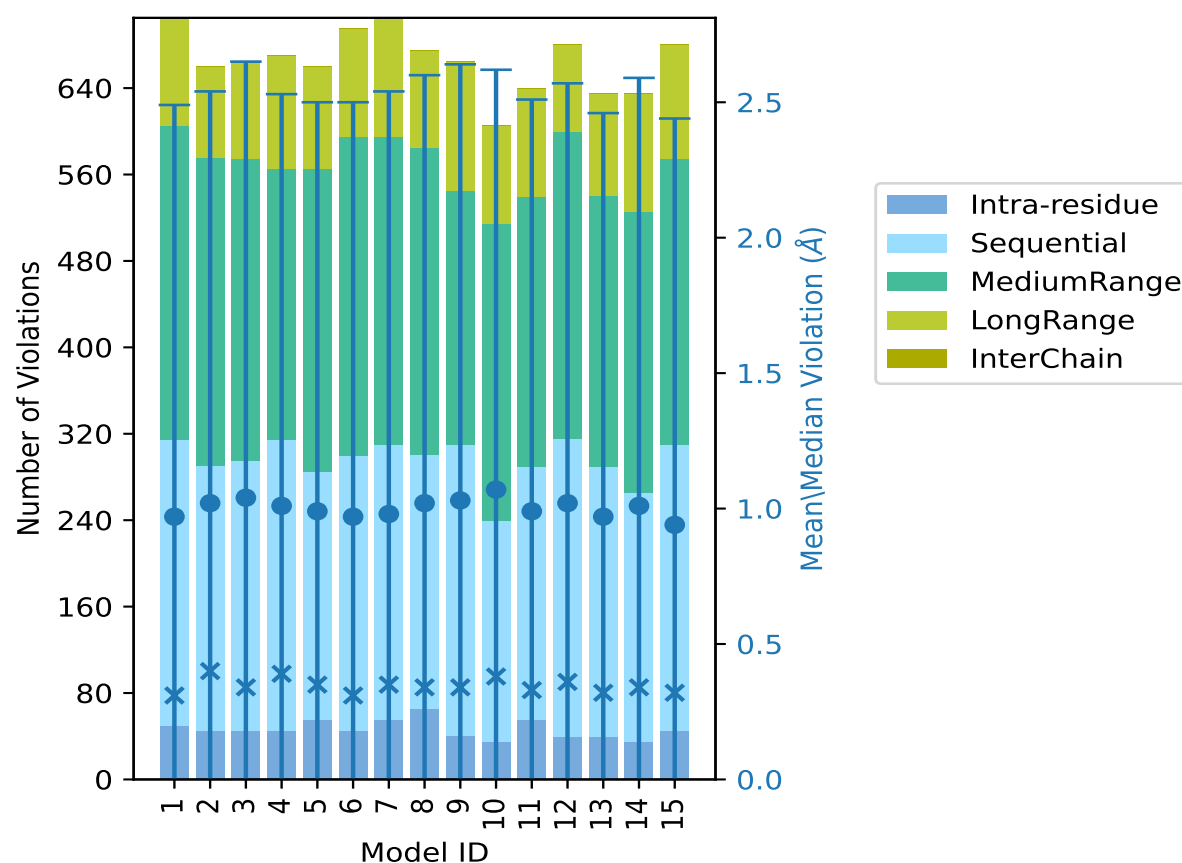
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	55	235	250	100	0	640	0.99	9.83	1.52	0.33
12	40	275	285	80	0	680	1.02	9.62	1.55	0.36
13	40	250	250	95	0	635	0.97	9.38	1.49	0.32
14	35	230	260	110	0	635	1.01	9.54	1.58	0.34
15	45	265	265	105	0	680	0.94	9.42	1.5	0.32

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

9.3 Distance violation statistics for the ensemble ⓘ

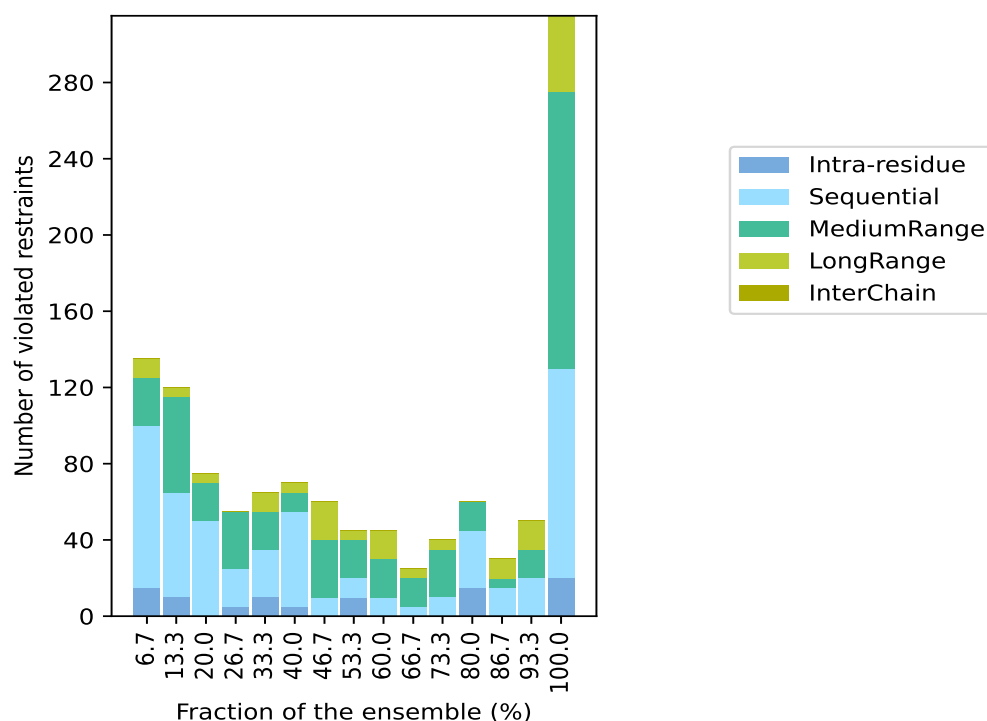
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1240(IR:75, SQ:845, MR:310, LR:10, IC:0) restraints are not 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	%
15	85	25	10	0	135	1	6.7
10	55	50	5	0	120	2	13.3
0	50	20	5	0	75	3	20.0
5	20	30	0	0	55	4	26.7
10	25	20	10	0	65	5	33.3
5	50	10	5	0	70	6	40.0
0	10	30	20	0	60	7	46.7
10	10	20	5	0	45	8	53.3
0	10	20	15	0	45	9	60.0
0	5	15	5	0	25	10	66.7
0	10	25	5	0	40	11	73.3
15	30	15	0	0	60	12	80.0
0	15	5	10	0	30	13	86.7
0	20	15	15	0	50	14	93.3
20	110	145	40	0	315	15	100.0

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

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

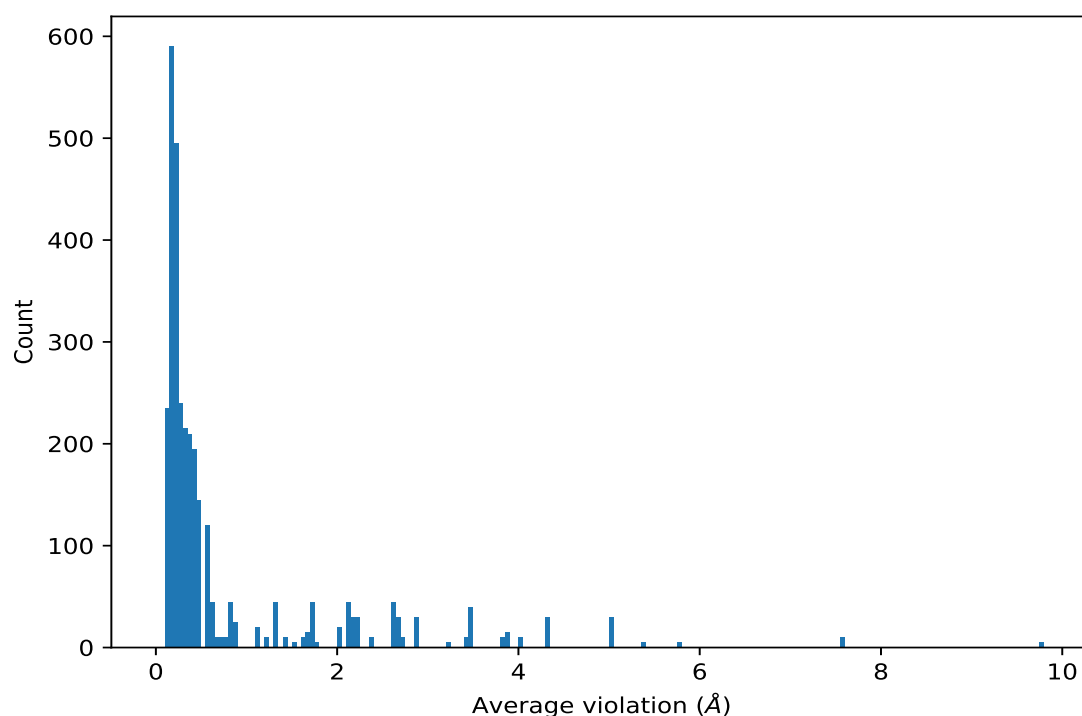
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

The following table provides the mean and the standard deviation of the 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.

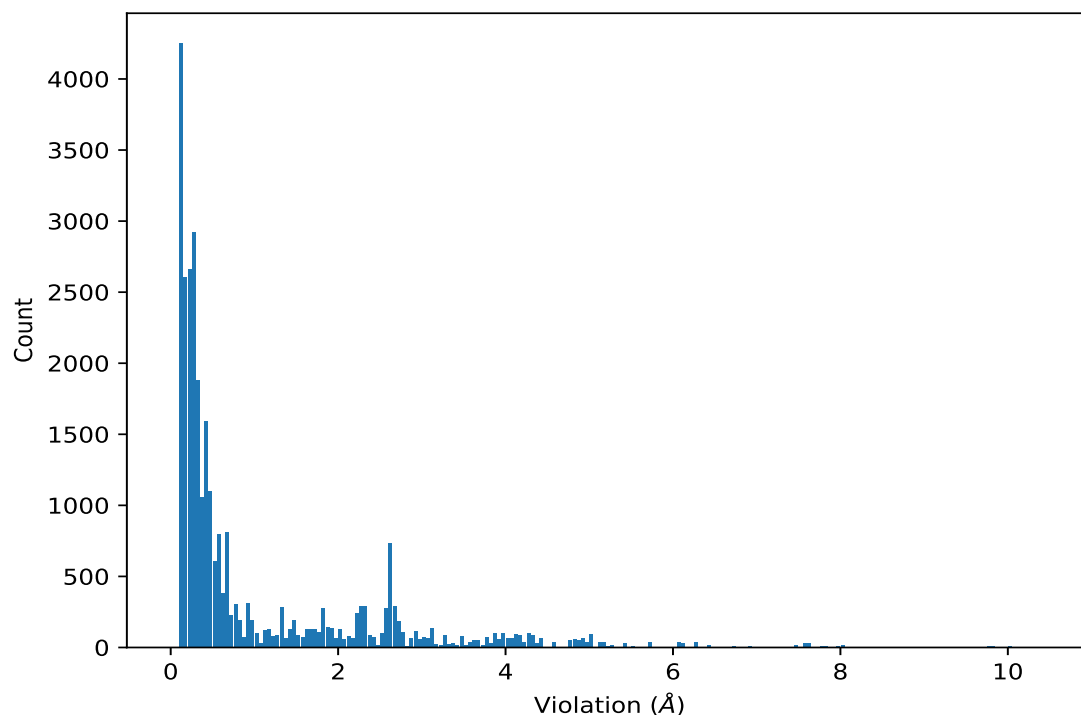
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2216)	1:235:A:TRP:HE1	1:237:A:TYR:HH	15	9.78	0.29	9.78
(1,2217)	1:235:A:TRP:HE1	1:237:A:TYR:HH	15	9.78	0.29	9.78
(1,2218)	1:235:A:TRP:HE1	1:237:A:TYR:HH	15	9.78	0.29	9.78
(1,2219)	1:235:A:TRP:HE1	1:237:A:TYR:HH	15	9.78	0.29	9.78
(1,2220)	1:235:A:TRP:HE1	1:237:A:TYR:HH	15	9.78	0.29	9.78
(1,2211)	1:185:A:GLN:H	1:308:A:ASN:HD21	15	7.59	0.35	7.63
(1,2211)	1:185:A:GLN:H	1:308:A:ASN:HD22	15	7.59	0.35	7.63
(1,2212)	1:185:A:GLN:H	1:308:A:ASN:HD21	15	7.59	0.35	7.63
(1,2212)	1:185:A:GLN:H	1:308:A:ASN:HD22	15	7.59	0.35	7.63
(1,2213)	1:185:A:GLN:H	1:308:A:ASN:HD21	15	7.59	0.35	7.63
(1,2213)	1:185:A:GLN:H	1:308:A:ASN:HD22	15	7.59	0.35	7.63
(1,2214)	1:185:A:GLN:H	1:308:A:ASN:HD21	15	7.59	0.35	7.63
(1,2214)	1:185:A:GLN:H	1:308:A:ASN:HD22	15	7.59	0.35	7.63
(1,2215)	1:185:A:GLN:H	1:308:A:ASN:HD21	15	7.59	0.35	7.63

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



9.5.2 Table : All distance violations [i](#)

The following table 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)
(1,2220)	1:235:A:TRP:HE1	1:237:A:TYR:HH	2	10.47
(1,2219)	1:235:A:TRP:HE1	1:237:A:TYR:HH	2	10.47
(1,2218)	1:235:A:TRP:HE1	1:237:A:TYR:HH	2	10.47
(1,2217)	1:235:A:TRP:HE1	1:237:A:TYR:HH	2	10.47
(1,2216)	1:235:A:TRP:HE1	1:237:A:TYR:HH	2	10.47
(1,2220)	1:235:A:TRP:HE1	1:237:A:TYR:HH	7	10.22
(1,2219)	1:235:A:TRP:HE1	1:237:A:TYR:HH	7	10.22
(1,2218)	1:235:A:TRP:HE1	1:237:A:TYR:HH	7	10.22
(1,2217)	1:235:A:TRP:HE1	1:237:A:TYR:HH	7	10.22
(1,2216)	1:235:A:TRP:HE1	1:237:A:TYR:HH	7	10.22

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

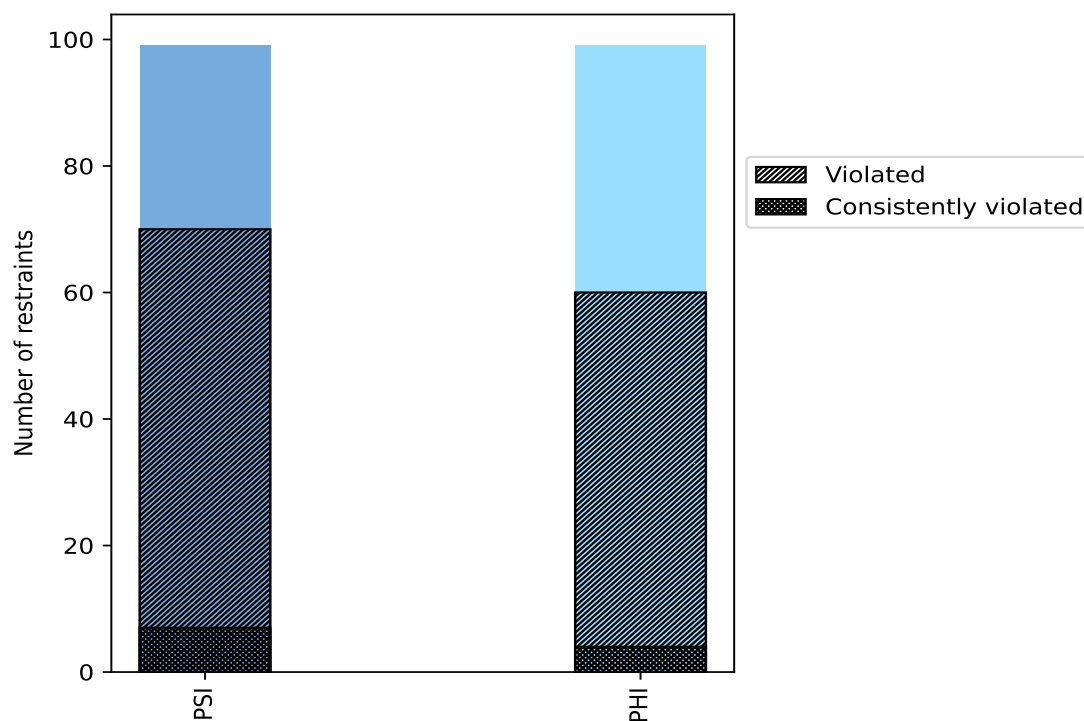
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	99	50.0	70	70.7	35.4	7	7.1	3.5
PHI	99	50.0	60	60.6	30.3	4	4.0	2.0
Total	198	100.0	130	65.7	65.7	11	5.6	5.6

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

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



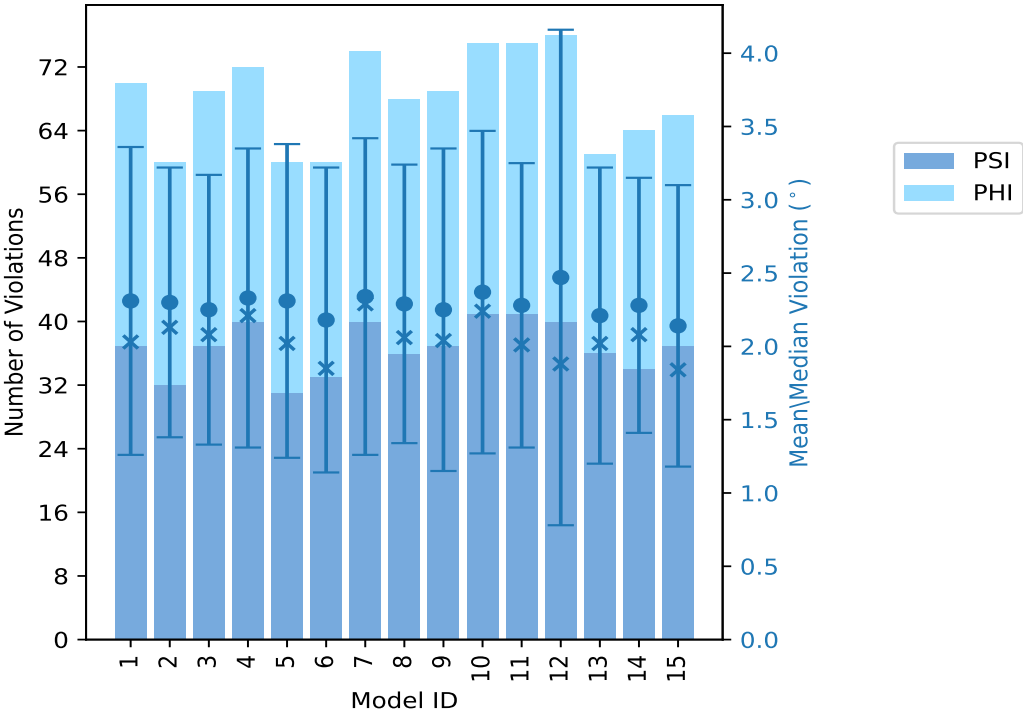
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	37	33	70	2.31	5.36	1.05	2.03
2	32	28	60	2.3	4.39	0.92	2.13
3	37	32	69	2.25	4.82	0.92	2.08
4	40	32	72	2.33	5.4	1.02	2.21
5	31	29	60	2.31	5.73	1.07	2.02
6	33	27	60	2.18	5.17	1.04	1.85
7	40	34	74	2.34	5.42	1.08	2.29
8	36	32	68	2.29	5.23	0.95	2.06
9	37	32	69	2.25	5.89	1.1	2.04
10	41	34	75	2.37	5.98	1.1	2.24
11	41	34	75	2.28	5.57	0.97	2.01
12	40	36	76	2.47	9.57	1.69	1.88
13	36	25	61	2.21	6.48	1.01	2.02
14	34	30	64	2.28	4.71	0.87	2.08
15	37	29	66	2.14	5.0	0.96	1.84

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

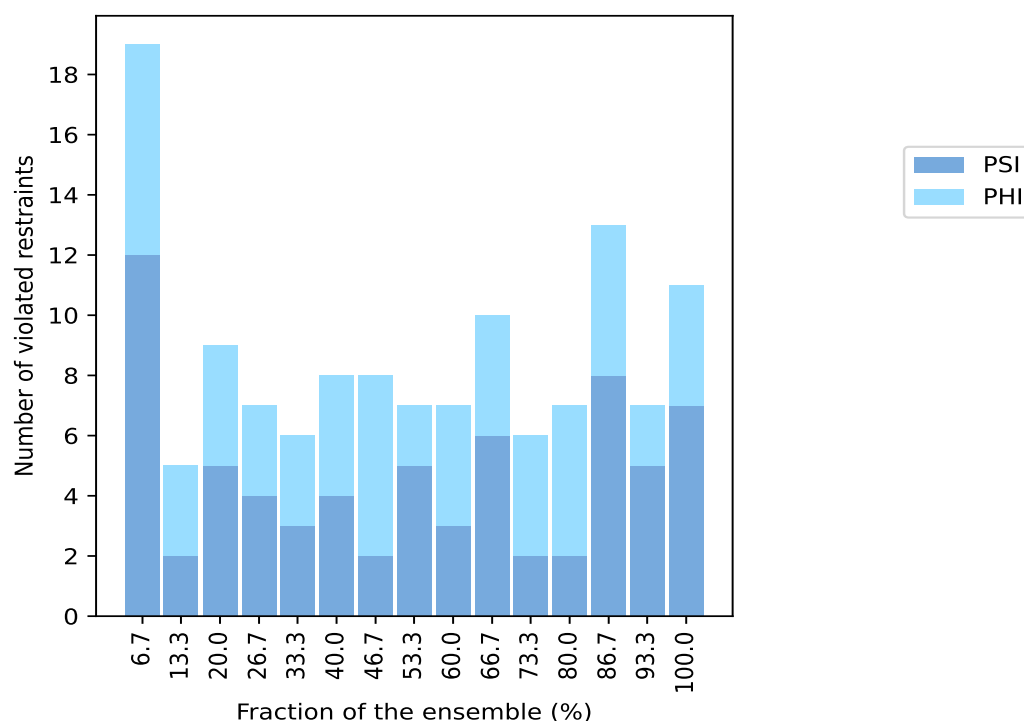
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
12	7	19	1	6.7
2	3	5	2	13.3
5	4	9	3	20.0
4	3	7	4	26.7
3	3	6	5	33.3
4	4	8	6	40.0
2	6	8	7	46.7
5	2	7	8	53.3
3	4	7	9	60.0
6	4	10	10	66.7
2	4	6	11	73.3
2	5	7	12	80.0
8	5	13	13	86.7
5	2	7	14	93.3
7	4	11	15	100.0

¹ Number of models with violations

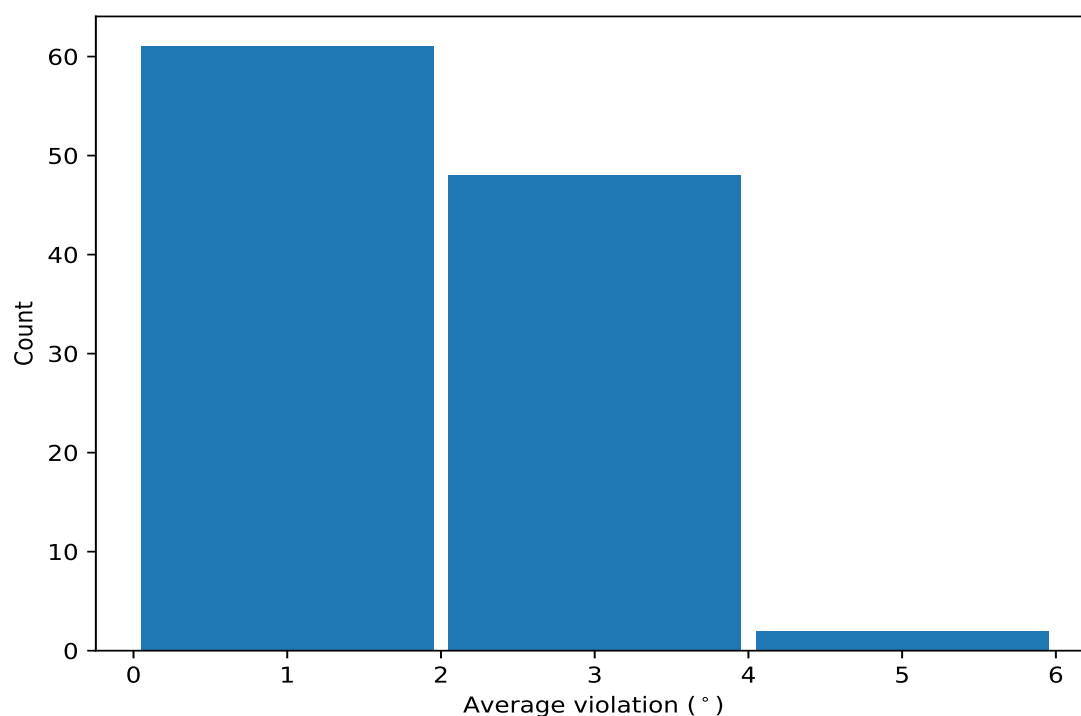
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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



10.4.2 Table: Most violated dihedral-angle 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.

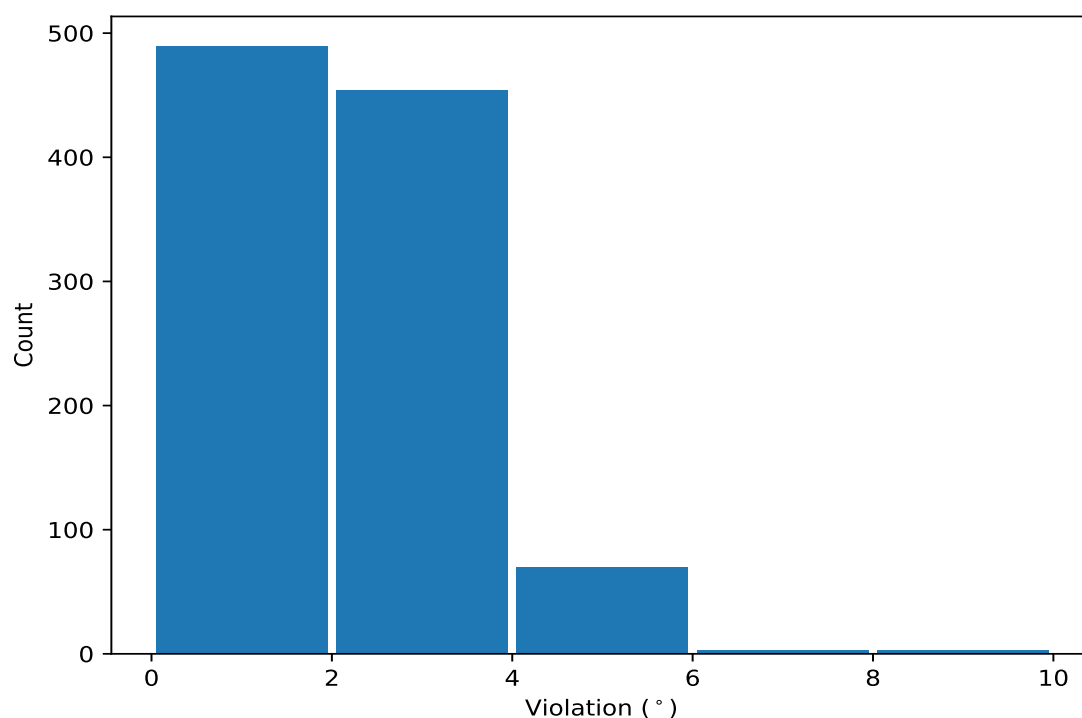
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(2,60)	1:265:A:GLN:N	1:265:A:GLN:CA	1:265:A:GLN:C	1:266:A:GLN:N	15	4.6	1.01	4.87
(2,61)	1:265:A:GLN:C	1:266:A:GLN:N	1:266:A:GLN:CA	1:266:A:GLN:C	15	4.57	0.94	4.53
(2,56)	1:263:A:TYR:N	1:263:A:TYR:CA	1:263:A:TYR:C	1:264:A:THR:N	15	3.79	1.3	3.99
(1,74)	1:254:A:VAL:N	1:254:A:VAL:CA	1:254:A:VAL:C	1:255:A:ALA:N	15	3.34	0.75	3.44
(1,8)	1:183:A:LEU:N	1:183:A:LEU:CA	1:183:A:LEU:C	1:184:A:LEU:N	15	3.2	0.84	3.24
(1,32)	1:198:A:ASP:N	1:198:A:ASP:CA	1:198:A:ASP:C	1:199:A:ALA:N	15	2.87	0.53	2.76
(1,2)	1:180:A:LYS:N	1:180:A:LYS:CA	1:180:A:LYS:C	1:181:A:LYS:N	15	2.81	0.58	2.95
(1,21)	1:189:A:ALA:C	1:190:A:GLU:N	1:190:A:GLU:CA	1:190:A:GLU:C	15	2.73	0.66	2.68
(1,9)	1:183:A:LEU:C	1:184:A:LEU:N	1:184:A:LEU:CA	1:184:A:LEU:C	15	2.72	0.73	2.74
(1,75)	1:254:A:VAL:C	1:255:A:ALA:N	1:255:A:ALA:CA	1:255:A:ALA:C	15	2.33	0.61	2.38

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

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table provides the list of violations for 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 (°)
(2,4)	1:204:A:GLU:N	1:204:A:GLU:CA	1:204:A:GLU:C	1:205:A:GLN:N	12	9.57
(2,3)	1:203:A:ILE:C	1:204:A:GLU:N	1:204:A:GLU:CA	1:204:A:GLU:C	12	8.12
(2,5)	1:204:A:GLU:C	1:205:A:GLN:N	1:205:A:GLN:CA	1:205:A:GLN:C	12	8.11
(2,2)	1:203:A:ILE:N	1:203:A:ILE:CA	1:203:A:ILE:C	1:204:A:GLU:N	12	7.84
(1,82)	1:258:A:PHE:N	1:258:A:PHE:CA	1:258:A:PHE:C	1:259:A:GLY:N	13	6.48
(2,56)	1:263:A:TYR:N	1:263:A:TYR:CA	1:263:A:TYR:C	1:264:A:THR:N	12	6.19
(2,61)	1:265:A:GLN:C	1:266:A:GLN:N	1:266:A:GLN:CA	1:266:A:GLN:C	10	5.98
(2,60)	1:265:A:GLN:N	1:265:A:GLN:CA	1:265:A:GLN:C	1:266:A:GLN:N	10	5.96
(2,56)	1:263:A:TYR:N	1:263:A:TYR:CA	1:263:A:TYR:C	1:264:A:THR:N	9	5.89
(2,60)	1:265:A:GLN:N	1:265:A:GLN:CA	1:265:A:GLN:C	1:266:A:GLN:N	5	5.73