wwPDB NMR Structure Validation Summary Report

Dec 25, 2024 – 07:59 PM EST

PDB ID	:	8S8O
BMRB ID	:	34908
Title	:	Solution Structure of cAMP-dependent Protein Kinase RII-alpha Subunit Dimerization and Docking Domain Complex with Microtubule Associated Protein 2c (84-111)
Authors	:	Bartosik, V.; Lanikova, A.; Janackova, Z.; Padrta, P.; Zidek, L.
Deposited on	:	2024-03-06

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 (1)) were used in the production of this report:

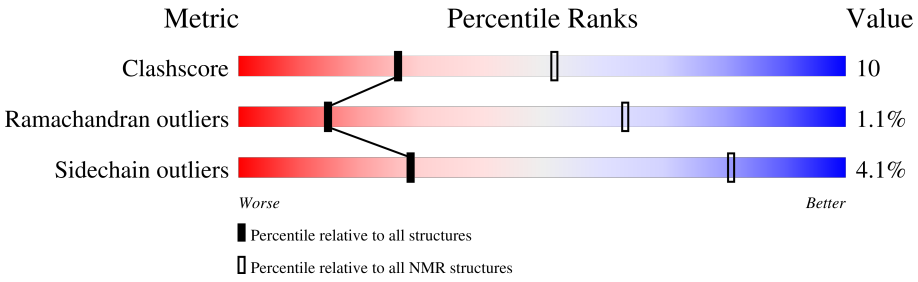
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 66%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	52	63% 17% 19%
1	B	52	60% 12% 29%
2	C	28	57% 29% 14%

2 Ensemble composition and analysis

This entry contains 20 models. Model 20 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:7-A:48, B:10-B:46, C:86-C:109 (103)	0.88	20

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. No single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2050 atoms, of which 1028 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called cAMP-dependent protein kinase type II-alpha regulatory subunit.

Mol	Chain	Residues	Atoms						Trace
1	A	52	Total	C	H	N	O	S	0
			814	259	408	70	75	2	
1	B	52	Total	C	H	N	O	S	0
			812	259	406	70	75	2	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P13861
A	2	ALA	-	expression tag	UNP P13861
A	3	MET	-	expression tag	UNP P13861
A	4	GLY	-	expression tag	UNP P13861
B	1	GLY	-	expression tag	UNP P13861
B	2	ALA	-	expression tag	UNP P13861
B	3	MET	-	expression tag	UNP P13861
B	4	GLY	-	expression tag	UNP P13861

- Molecule 2 is a protein called Isoform 3 of Microtubule-associated protein 2.

Mol	Chain	Residues	Atoms					Trace
2	C	28	Total	C	H	N	O	0
			424	128	214	37	45	

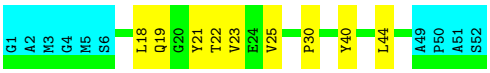
4 Residue-property plots

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.

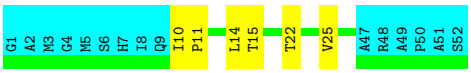
• Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit

Chain A:



• Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit

Chain B:



• Molecule 2: Isoform 3 of Microtubule-associated protein 2

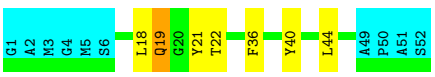
Chain C:

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

The representative model is number 20. Colouring as in section 4.1 above.

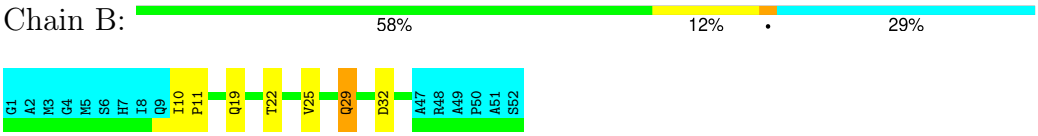
• Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit

Chain A:



• Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit

Chain B:



• Molecule 2: Isoform 3 of Microtubule-associated protein 2

Chain C:

5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CNS	structure calculation	1.21
SCULPTOR	structure calculation	3.1
CNS	refinement	1.21
SCULPTOR	refinement	3.1

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1760
Number of shifts mapped to atoms	1217
Number of unparsed shifts	0
Number of shifts with mapping errors	543
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	66%

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	B	0.0±0.0	0.1±0.4
1	A	0.0±0.0	0.1±0.4
All	All	0	6

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	45	ARG	Sidechain	2
1	B	45	ARG	Sidechain	2
1	A	43	ARG	Sidechain	1
1	B	43	ARG	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	348	350	350	9±2
1	B	305	306	306	5±3
2	C	172	181	181	4±2
All	All	16500	16740	16740	329

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 10.

5 of 104 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:103:VAL:O	2:C:106:LEU:HG	0.65	1.91	13	14
2:C:97:VAL:O	2:C:101:GLU:HG3	0.63	1.94	14	2
1:A:14:LEU:HG	1:B:33:LEU:HD22	0.62	1.72	3	2
1:A:36:PHE:O	1:A:40:TYR:HB2	0.61	1.95	12	2
1:A:22:THR:HB	1:A:40:TYR:CE1	0.60	2.31	10	8

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	42/52 (81%)	40±1 (95±2%)	2±1 (5±2%)	0±0 (0±1%)	32 76
1	B	37/52 (71%)	34±1 (93±3%)	2±1 (4±3%)	1±0 (3±1%)	6 42
2	C	24/28 (86%)	24±0 (99±2%)	0±0 (1±2%)	0±0 (0±1%)	45 81
All	All	2060/2640 (78%)	1959 (95%)	78 (4%)	23 (1%)	15 64

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

Mol	Chain	Res	Type	Models (Total)
1	B	11	PRO	17
1	A	11	PRO	2
1	B	12	PRO	2
1	A	31	PRO	1
2	C	108	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	38/43 (88%)	37±1 (97±2%)	1±1 (2±2%)	43 90
1	B	34/43 (79%)	32±1 (94±4%)	2±1 (6±4%)	17 68
2	C	18/22 (82%)	17±1 (97±4%)	1±1 (3±4%)	37 86
All	All	1800/2160 (83%)	1726 (96%)	74 (4%)	28 81

5 of 27 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	B	10	ILE	15
1	A	19	GLN	10
1	B	14	LEU	8
1	B	21	TYR	3
1	B	28	GLN	3

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 (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 66% for the well-defined parts and 67% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_ output*

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	1760
Number of shifts mapped to atoms	1217
Number of unparsed shifts	0
Number of shifts with mapping errors	543
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- No matching atom found in the structure. First 5 (of 543) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	10	LYS	H	7.932	0.003	1
1	C	10	LYS	CA	55.766	0.078	1
1	C	10	LYS	CB	33.233	0.005	1
1	C	10	LYS	N	120.212	0.022	1
1	C	11	ALA	H	8.189	0.004	1
1	C	11	ALA	HA	4.525	0.000	1
1	C	11	ALA	HB1	1.33	0.000	1
1	C	11	ALA	HB2	1.33	0.000	1
1	C	11	ALA	HB3	1.33	0.000	1
1	C	11	ALA	CA	50.598	0.000	1
1	C	11	ALA	CB	18.158	0.000	1
1	C	11	ALA	N	126.193	0.056	1
1	C	13	HIS	CA	56.215	0.064	1
1	C	13	HIS	CB	30.383	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	14	TRP	H	7.832	0.004	1
1	C	14	TRP	HA	4.697	0.000	1
1	C	14	TRP	HB2	3.246	0.000	2
1	C	14	TRP	HB3	3.246	0.000	2
1	C	14	TRP	CA	57.565	0.013	1
1	C	14	TRP	CB	29.594	0.071	1
1	C	14	TRP	N	122.146	0.075	1
1	C	15	THR	H	7.803	0.004	1
1	C	15	THR	HG21	1.024	0.000	1
1	C	15	THR	HG22	1.024	0.000	1
1	C	15	THR	HG23	1.024	0.000	1
1	C	15	THR	CA	61.501	0.121	1
1	C	15	THR	CB	70.172	0.045	1
1	C	15	THR	N	115.431	0.046	1
1	C	16	SER	H	8.122	0.005	1
1	C	16	SER	CA	58.689	0.048	1
1	C	16	SER	CB	63.773	0.090	1
1	C	16	SER	N	117.493	0.034	1
1	C	17	ALA	H	8.232	0.002	1
1	C	17	ALA	HB1	1.393	0.000	1
1	C	17	ALA	HB2	1.393	0.000	1
1	C	17	ALA	HB3	1.393	0.000	1
1	C	17	ALA	CA	52.931	0.032	1
1	C	17	ALA	CB	19.171	0.026	1
1	C	17	ALA	N	125.873	0.030	1
1	C	18	SER	H	8.147	0.002	1
1	C	18	SER	CA	58.674	0.020	1
1	C	18	SER	CB	63.631	0.018	1
1	C	18	SER	N	114.521	0.018	1
1	C	19	LEU	H	8.182	0.004	1
1	C	19	LEU	CA	55.689	0.058	1
1	C	19	LEU	CB	42.224	0.030	1
1	C	19	LEU	N	123.857	0.028	1
1	C	20	THR	H	7.984	0.004	1
1	C	20	THR	HG21	1.19	0.000	1
1	C	20	THR	HG22	1.19	0.000	1
1	C	20	THR	HG23	1.19	0.000	1
1	C	20	THR	CA	62.24	0.094	1
1	C	20	THR	CB	69.746	0.026	1
1	C	20	THR	N	113.807	0.023	1
1	C	21	GLU	H	8.243	0.003	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	21	GLU	CA	56.901	0.068	1
1	C	21	GLU	CB	30.174	0.043	1
1	C	21	GLU	N	122.99	0.045	1
1	C	22	ALA	H	8.185	0.002	1
1	C	22	ALA	CA	52.878	0.011	1
1	C	22	ALA	CB	19.099	0.060	1
1	C	22	ALA	N	124.508	0.063	1
1	C	23	ALA	H	8.038	0.003	1
1	C	23	ALA	CA	52.52	0.078	1
1	C	23	ALA	CB	19.168	0.004	1
1	C	23	ALA	N	122.333	0.029	1
1	C	24	ALA	H	7.999	0.004	1
1	C	24	ALA	CA	52.319	0.063	1
1	C	24	ALA	CB	19.25	0.009	1
1	C	24	ALA	N	122.349	0.032	1
1	C	25	HIS	H	8.118	0.004	1
1	C	25	HIS	CA	53.947	0.000	1
1	C	25	HIS	CB	29.892	0.000	1
1	C	25	HIS	N	118.968	0.017	1
1	C	29	PRO	CB	31.999	0.029	1
1	C	30	GLU	H	8.494	0.002	1
1	C	30	GLU	CA	56.889	0.000	1
1	C	30	GLU	CB	30.02	0.000	1
1	C	30	GLU	N	120.133	0.012	1
1	C	35	GLY	CA	45.465	0.000	1
1	C	36	GLY	H	8.262	0.003	1
1	C	36	GLY	CA	45.36	0.055	1
1	C	36	GLY	N	108.858	0.030	1
1	C	37	SER	H	8.342	0.003	1
1	C	37	SER	HA	4.491	0.000	1
1	C	37	SER	HB2	3.919	0.000	2
1	C	37	SER	HB3	3.919	0.000	2
1	C	37	SER	CA	58.599	0.055	1
1	C	37	SER	CB	63.938	0.026	1
1	C	37	SER	N	115.567	0.102	1
1	C	38	GLY	H	8.498	0.004	1
1	C	38	GLY	HA2	3.98	0.000	2
1	C	38	GLY	HA3	3.98	0.000	2
1	C	38	GLY	CA	45.545	0.000	1
1	C	38	GLY	N	110.974	0.024	1
1	C	39	GLU	CA	56.127	0.085	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	39	GLU	CB	29.303	0.078	1
1	C	40	GLY	H	8.468	0.003	1
1	C	40	GLY	CA	45.576	0.066	1
1	C	40	GLY	N	109.548	0.033	1
1	C	41	LEU	H	8.032	0.004	1
1	C	41	LEU	HA	4.377	0.000	1
1	C	41	LEU	CA	55.319	0.023	1
1	C	41	LEU	CB	42.414	0.033	1
1	C	41	LEU	N	121.491	0.024	1
1	C	42	SER	H	8.283	0.003	1
1	C	42	SER	HA	4.443	0.000	1
1	C	42	SER	CA	58.537	0.000	1
1	C	42	SER	CB	63.74	0.000	1
1	C	42	SER	N	116.324	0.033	1
1	C	43	ARG	CA	56.193	0.002	1
1	C	43	ARG	CB	30.834	0.055	1
1	C	44	SER	H	8.264	0.003	1
1	C	44	SER	CA	58.394	0.067	1
1	C	44	SER	CB	63.908	0.032	1
1	C	44	SER	N	116.496	0.028	1
1	C	45	ALA	H	8.357	0.004	1
1	C	45	ALA	HB1	1.399	0.000	1
1	C	45	ALA	HB2	1.399	0.000	1
1	C	45	ALA	HB3	1.399	0.000	1
1	C	45	ALA	CA	52.912	0.015	1
1	C	45	ALA	CB	19.166	0.048	1
1	C	45	ALA	N	125.9	0.034	1
1	C	46	ASN	H	8.247	0.004	1
1	C	46	ASN	CA	53.228	0.052	1
1	C	46	ASN	CB	38.908	0.050	1
1	C	46	ASN	N	116.936	0.027	1
1	C	47	GLY	H	8.127	0.006	1
1	C	47	GLY	HA2	3.846	0.000	2
1	C	47	GLY	HA3	3.846	0.000	2
1	C	47	GLY	CA	45.171	0.039	1
1	C	47	GLY	N	108.297	0.030	1
1	C	48	PHE	H	7.995	0.005	1
1	C	48	PHE	HA	4.845	0.000	1
1	C	48	PHE	HB2	2.996	0.000	2
1	C	48	PHE	HB3	2.996	0.000	2
1	C	48	PHE	CA	55.795	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	48	PHE	CB	39.079	0.000	1
1	C	48	PHE	N	120.855	0.027	1
1	C	49	PRO	CA	63.177	0.019	1
1	C	49	PRO	CB	31.672	0.030	1
1	C	50	TYR	H	8.043	0.004	1
1	C	50	TYR	CA	57.953	0.052	1
1	C	50	TYR	CB	38.848	0.041	1
1	C	50	TYR	N	120.752	0.032	1
1	C	51	ARG	H	8.091	0.006	1
1	C	51	ARG	HA	4.322	0.000	1
1	C	51	ARG	HD2	3.163	0.000	2
1	C	51	ARG	HD3	3.163	0.000	2
1	C	51	ARG	CA	55.552	0.057	1
1	C	51	ARG	CB	31.296	0.041	1
1	C	51	ARG	N	123.699	0.048	1
1	C	52	GLU	H	8.472	0.006	1
1	C	52	GLU	HA	4.177	0.000	1
1	C	52	GLU	HB2	1.965	0.000	2
1	C	52	GLU	HB3	1.965	0.000	2
1	C	52	GLU	HG2	2.285	0.000	2
1	C	52	GLU	HG3	2.285	0.000	2
1	C	52	GLU	CA	57.055	0.101	1
1	C	52	GLU	CB	30.162	0.050	1
1	C	52	GLU	N	122.91	0.033	1
1	C	53	GLU	H	8.515	0.004	1
1	C	53	GLU	HA	4.248	0.000	1
1	C	53	GLU	HB2	1.956	0.000	2
1	C	53	GLU	HB3	1.956	0.000	2
1	C	53	GLU	HG2	2.252	0.000	2
1	C	53	GLU	HG3	2.252	0.000	2
1	C	53	GLU	CA	56.906	0.000	1
1	C	53	GLU	N	121.243	0.030	1
1	C	55	GLU	CA	57.073	0.087	1
1	C	55	GLU	CB	30.217	0.039	1
1	C	56	GLY	H	8.372	0.003	1
1	C	56	GLY	CA	45.382	0.045	1
1	C	56	GLY	N	110.002	0.040	1
1	C	57	ALA	H	8.005	0.003	1
1	C	57	ALA	CA	52.589	0.059	1
1	C	57	ALA	CB	19.181	0.016	1
1	C	57	ALA	N	123.533	0.043	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	58	PHE	H	8.199	0.003	1
1	C	58	PHE	HA	4.588	0.000	1
1	C	58	PHE	HB2	3.088	0.000	2
1	C	58	PHE	HB3	3.088	0.000	2
1	C	58	PHE	CA	57.772	0.013	1
1	C	58	PHE	CB	39.336	0.045	1
1	C	58	PHE	N	118.997	0.024	1
1	C	59	GLY	H	8.17	0.004	1
1	C	59	GLY	HA2	3.886	0.000	2
1	C	59	GLY	HA3	3.886	0.000	2
1	C	59	GLY	CA	45.28	0.050	1
1	C	59	GLY	N	110.023	0.033	1
1	C	60	GLU	H	8.253	0.004	1
1	C	60	GLU	CA	56.667	0.032	1
1	C	60	GLU	CB	30.168	0.078	1
1	C	60	GLU	N	120.669	0.020	1
1	C	61	HIS	H	8.445	0.006	1
1	C	61	HIS	HB2	3.17	0.000	2
1	C	61	HIS	HB3	3.17	0.000	2
1	C	61	HIS	CA	56.193	0.140	1
1	C	61	HIS	CB	30.022	0.065	1
1	C	61	HIS	N	119.659	0.033	1
1	C	62	GLY	H	8.313	0.003	1
1	C	62	GLY	CA	45.461	0.055	1
1	C	62	GLY	N	109.78	0.017	1
1	C	63	SER	H	8.283	0.003	1
1	C	63	SER	CA	58.534	0.040	1
1	C	63	SER	CB	63.82	0.011	1
1	C	63	SER	N	115.699	0.032	1
1	C	64	GLN	H	8.475	0.007	1
1	C	64	GLN	CA	56.239	0.028	1
1	C	64	GLN	CB	29.396	0.021	1
1	C	64	GLN	N	121.934	0.046	1
1	C	65	GLY	H	8.349	0.003	1
1	C	65	GLY	CA	45.454	0.000	1
1	C	65	GLY	N	109.669	0.027	1
1	C	66	THR	H	7.982	0.006	1
1	C	66	THR	HG21	1.155	0.000	1
1	C	66	THR	HG22	1.155	0.000	1
1	C	66	THR	HG23	1.155	0.000	1
1	C	66	THR	CA	61.895	0.108	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	66	THR	CB	69.832	0.078	1
1	C	66	THR	N	113.791	0.048	1
1	C	67	TYR	H	8.256	0.004	1
1	C	67	TYR	CA	58.011	0.109	1
1	C	67	TYR	CB	38.852	0.035	1
1	C	67	TYR	N	122.686	0.049	1
1	C	68	SER	H	8.093	0.007	1
1	C	68	SER	HA	4.413	0.000	1
1	C	68	SER	HB2	3.806	0.000	2
1	C	68	SER	HB3	3.806	0.000	2
1	C	68	SER	CA	58.132	0.022	1
1	C	68	SER	CB	63.996	0.073	1
1	C	68	SER	N	117.468	0.032	1
1	C	69	ASP	H	8.313	0.004	1
1	C	69	ASP	CA	54.326	0.046	1
1	C	69	ASP	CB	41.253	0.029	1
1	C	69	ASP	N	122.845	0.017	1
1	C	70	THR	H	8.066	0.004	1
1	C	70	THR	CA	62.062	0.052	1
1	C	70	THR	CB	69.686	0.051	1
1	C	70	THR	N	114.328	0.030	1
1	C	71	LYS	H	8.286	0.004	1
1	C	71	LYS	HA	4.33	0.000	1
1	C	71	LYS	CA	56.583	0.000	1
1	C	71	LYS	CB	32.82	0.000	1
1	C	71	LYS	N	123.394	0.041	1
1	C	72	GLU	CA	56.724	0.064	1
1	C	72	GLU	CB	30.11	0.110	1
1	C	73	ASN	H	8.388	0.003	1
1	C	73	ASN	CA	53.289	0.014	1
1	C	73	ASN	CB	39.059	0.031	1
1	C	73	ASN	N	119.385	0.026	1
1	C	74	GLY	H	8.313	0.004	1
1	C	74	GLY	HA2	3.978	0.000	2
1	C	74	GLY	HA3	3.978	0.000	2
1	C	74	GLY	CA	45.533	0.066	1
1	C	74	GLY	N	109.119	0.025	1
1	C	75	ILE	H	8.022	0.003	1
1	C	75	ILE	HA	4.155	0.018	1
1	C	75	ILE	HB	1.813	0.010	1
1	C	75	ILE	HD11	0.811	0.006	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	75	ILE	HD12	0.811	0.006	1
1	C	75	ILE	HD13	0.811	0.006	1
1	C	75	ILE	HG12	1.426	0.029	1
1	C	75	ILE	HG13	1.107	0.014	1
1	C	75	ILE	HG21	0.885	0.013	1
1	C	75	ILE	HG22	0.885	0.013	1
1	C	75	ILE	HG23	0.885	0.013	1
1	C	75	ILE	CA	61.345	0.056	1
1	C	75	ILE	CB	38.686	0.071	1
1	C	75	ILE	CD1	12.915	0.065	1
1	C	75	ILE	CG1	27.143	0.193	1
1	C	75	ILE	CG2	17.215	0.102	1
1	C	75	ILE	N	119.822	0.024	1
1	C	76	ASN	H	8.528	0.004	1
1	C	76	ASN	HA	4.724	0.000	1
1	C	76	ASN	HB2	2.816	0.000	2
1	C	76	ASN	HB3	2.816	0.000	2
1	C	76	ASN	CA	53.424	0.083	1
1	C	76	ASN	CB	38.9	0.030	1
1	C	76	ASN	N	122.07	0.016	1
1	C	77	GLY	H	8.275	0.003	1
1	C	77	GLY	CA	45.533	0.000	1
1	C	77	GLY	N	109.431	0.028	1
1	C	79	LEU	H	8.269	0.003	1
1	C	79	LEU	CA	55.288	0.005	1
1	C	79	LEU	CB	42.301	0.036	1
1	C	79	LEU	N	122.763	0.042	1
1	C	80	THR	H	8.168	0.016	1
1	C	80	THR	HA	4.394	0.007	1
1	C	80	THR	HB	4.247	0.005	1
1	C	80	THR	HG21	1.177	0.010	1
1	C	80	THR	HG22	1.177	0.010	1
1	C	80	THR	HG23	1.177	0.010	1
1	C	80	THR	CA	61.581	0.000	1
1	C	80	THR	CB	70.027	0.023	1
1	C	80	THR	CG2	21.608	0.015	1
1	C	80	THR	N	114.341	0.010	1
1	C	81	SER	H	8.3	0.006	1
1	C	81	SER	HA	4.399	0.001	1
1	C	81	SER	HB2	3.824	0.012	2
1	C	81	SER	HB3	3.824	0.012	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	81	SER	CA	58.419	0.041	1
1	C	81	SER	CB	63.716	0.063	1
1	C	81	SER	N	117.698	0.049	1
1	C	82	ALA	H	8.188	0.012	1
1	C	82	ALA	HA	4.27	0.024	1
1	C	82	ALA	HB1	1.34	0.011	1
1	C	82	ALA	HB2	1.34	0.011	1
1	C	82	ALA	HB3	1.34	0.011	1
1	C	82	ALA	CA	52.519	0.127	1
1	C	82	ALA	CB	19.207	0.046	1
1	C	82	ALA	N	124.612	0.012	1
1	C	83	ASP	H	8.174	0.008	1
1	C	83	ASP	HA	4.52	0.005	1
1	C	83	ASP	HB2	2.644	0.020	2
1	C	83	ASP	HB3	2.644	0.020	2
1	C	83	ASP	CA	54.743	0.083	1
1	C	83	ASP	CB	41.166	0.039	1
1	C	83	ASP	N	118.873	0.016	1
1	C	84	ARG	H	8.048	0.013	1
1	C	113	GLU	H	8.066	0.003	1
1	C	113	GLU	HA	4.161	0.000	1
1	C	113	GLU	HB2	2.007	0.012	2
1	C	113	GLU	HB3	2.007	0.012	2
1	C	113	GLU	HG2	2.316	0.019	2
1	C	113	GLU	HG3	2.316	0.019	2
1	C	113	GLU	CB	29.876	0.000	1
1	C	113	GLU	N	120.143	0.011	1
1	C	114	ALA	H	8.007	0.004	1
1	C	114	ALA	HA	4.201	0.008	1
1	C	114	ALA	HB1	1.381	0.009	1
1	C	114	ALA	HB2	1.381	0.009	1
1	C	114	ALA	HB3	1.381	0.009	1
1	C	114	ALA	CA	52.82	0.086	1
1	C	114	ALA	CB	18.935	0.004	1
1	C	114	ALA	N	123.121	0.028	1
1	C	115	GLN	H	8.003	0.006	1
1	C	115	GLN	HA	4.194	0.018	1
1	C	115	GLN	HB2	1.977	0.003	2
1	C	115	GLN	HB3	1.977	0.003	2
1	C	115	GLN	HG2	2.322	0.016	2
1	C	115	GLN	HG3	2.322	0.016	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	115	GLN	CA	56.569	0.017	1
1	C	115	GLN	CG	33.709	0.032	1
1	C	115	GLN	N	117.87	0.004	1
1	C	116	HIS	H	8.131	0.013	1
1	C	116	HIS	HA	4.591	0.005	1
1	C	116	HIS	HB2	3.173	0.005	1
1	C	116	HIS	HB3	3.104	0.018	1
1	C	116	HIS	CA	56.381	0.121	1
1	C	116	HIS	CB	30.084	0.091	1
1	C	116	HIS	N	119.534	0.000	1
1	C	120	PRO	HA	4.38	0.016	1
1	C	120	PRO	HB2	1.876	0.003	1
1	C	120	PRO	HB3	2.258	0.010	1
1	C	120	PRO	HD2	3.646	0.013	1
1	C	120	PRO	HD3	3.817	0.022	1
1	C	120	PRO	HG2	1.907	0.002	1
1	C	120	PRO	HG3	1.999	0.005	1
1	C	120	PRO	CA	63.308	0.036	1
1	C	120	PRO	CB	31.543	0.339	1
1	C	120	PRO	CD	50.942	0.110	1
1	C	120	PRO	CG	27.315	0.024	1
1	C	121	ALA	H	8.33	0.003	1
1	C	121	ALA	HA	4.365	0.000	1
1	C	121	ALA	HB1	1.351	0.000	1
1	C	121	ALA	HB2	1.351	0.000	1
1	C	121	ALA	HB3	1.351	0.000	1
1	C	121	ALA	CA	52.404	0.000	1
1	C	121	ALA	CB	19.219	0.000	1
1	C	121	ALA	N	124.37	0.047	1
1	C	122	ALA	H	8.186	0.001	1
1	C	122	ALA	CA	51.921	0.101	1
1	C	122	ALA	CB	19.295	0.002	1
1	C	122	ALA	N	123.432	0.000	1
1	C	123	LEU	H	8.15	0.004	1
1	C	123	LEU	CA	52.857	0.000	1
1	C	123	LEU	CB	41.72	0.000	1
1	C	124	PRO	CA	62.892	0.066	1
1	C	124	PRO	CB	31.915	0.031	1
1	C	125	LEU	H	8.226	0.003	1
1	C	125	LEU	CA	55.116	0.025	1
1	C	125	LEU	CB	42.452	0.028	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	125	LEU	N	122.551	0.037	1
1	C	126	ALA	H	8.266	0.002	1
1	C	126	ALA	HA	4.317	0.000	1
1	C	126	ALA	HB1	1.399	0.000	1
1	C	126	ALA	HB2	1.399	0.000	1
1	C	126	ALA	HB3	1.399	0.000	1
1	C	126	ALA	CA	52.242	0.069	1
1	C	126	ALA	CB	19.271	0.020	1
1	C	126	ALA	N	125.189	0.041	1
1	C	127	ALA	H	8.244	0.002	1
1	C	127	ALA	HA	4.279	0.000	1
1	C	127	ALA	HB1	1.4	0.000	1
1	C	127	ALA	HB2	1.4	0.000	1
1	C	127	ALA	HB3	1.4	0.000	1
1	C	127	ALA	CA	52.574	0.000	1
1	C	127	ALA	CB	19.296	0.000	1
1	C	127	ALA	N	123.661	0.030	1
1	C	128	GLU	H	8.392	0.003	1
1	C	128	GLU	N	119.908	0.029	1
1	C	129	GLU	CA	56.608	0.026	1
1	C	129	GLU	CB	30.413	0.031	1
1	C	130	THR	H	8.189	0.003	1
1	C	130	THR	HG21	1.19	0.000	1
1	C	130	THR	HG22	1.19	0.000	1
1	C	130	THR	HG23	1.19	0.000	1
1	C	130	THR	CA	62.066	0.027	1
1	C	130	THR	CB	69.823	0.002	1
1	C	130	THR	N	115.823	0.033	1
1	C	131	VAL	H	8.089	0.003	1
1	C	131	VAL	HA	4.095	0.011	1
1	C	131	VAL	HB	2.041	0.010	1
1	C	131	VAL	HG11	0.896	0.011	2
1	C	131	VAL	HG12	0.896	0.011	2
1	C	131	VAL	HG13	0.896	0.011	2
1	C	131	VAL	HG21	0.896	0.011	2
1	C	131	VAL	HG22	0.896	0.011	2
1	C	131	VAL	HG23	0.896	0.011	2
1	C	131	VAL	CA	62.248	0.039	1
1	C	131	VAL	CB	32.822	0.101	1
1	C	131	VAL	CG1	20.866	0.082	1
1	C	131	VAL	N	122.399	0.037	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	132	ASN	H	8.451	0.004	1
1	C	132	ASN	HA	4.751	0.000	1
1	C	132	ASN	CA	52.942	0.027	1
1	C	132	ASN	CB	39.07	0.030	1
1	C	132	ASN	N	122.555	0.030	1
1	C	133	LEU	H	8.146	0.004	1
1	C	133	LEU	CA	52.957	0.000	1
1	C	133	LEU	CB	41.815	0.000	1
1	C	133	LEU	N	124.33	0.038	1
1	C	135	PRO	CA	62.747	0.000	1
1	C	135	PRO	CB	31.968	0.032	1
1	C	136	SER	H	8.338	0.003	1
1	C	136	SER	HA	4.748	0.000	1
1	C	136	SER	HB2	3.851	0.000	2
1	C	136	SER	HB3	3.851	0.000	2
1	C	136	SER	CA	56.502	0.000	1
1	C	136	SER	CB	63.539	0.000	1
1	C	136	SER	N	117.564	0.057	1
1	C	139	PRO	CA	62.744	0.000	1
1	C	139	PRO	CB	31.963	0.032	1
1	C	140	SER	H	8.378	0.003	1
1	C	140	SER	HA	4.763	0.000	1
1	C	140	SER	HB2	3.872	0.000	2
1	C	140	SER	HB3	3.872	0.000	2
1	C	140	SER	CA	56.408	0.000	1
1	C	140	SER	CB	63.5	0.000	1
1	C	140	SER	N	117.473	0.033	1
1	C	141	PRO	CA	63.283	0.005	1
1	C	141	PRO	CB	32.016	0.047	1
1	C	142	ALA	H	8.357	0.003	1
1	C	142	ALA	HA	4.324	0.000	1
1	C	142	ALA	HB1	1.423	0.000	1
1	C	142	ALA	HB2	1.423	0.000	1
1	C	142	ALA	HB3	1.423	0.000	1
1	C	142	ALA	CA	52.773	0.035	1
1	C	142	ALA	CB	19.093	0.038	1
1	C	142	ALA	N	124.224	0.031	1
1	C	143	SER	H	8.211	0.003	1
1	C	143	SER	HA	4.395	0.000	1
1	C	143	SER	HB2	3.894	0.000	2
1	C	143	SER	HB3	3.894	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	143	SER	CA	58.607	0.019	1
1	C	143	SER	CB	63.822	0.024	1
1	C	143	SER	N	114.828	0.033	1
1	C	144	GLU	H	8.381	0.004	1
1	C	144	GLU	CA	56.963	0.000	1
1	C	144	GLU	CB	30.249	0.000	1
1	C	144	GLU	N	122.533	0.021	1
1	C	145	GLN	CA	56.112	0.052	1
1	C	145	GLN	CB	29.364	0.020	1
1	C	146	THR	H	8.125	0.004	1
1	C	146	THR	HG21	1.217	0.000	1
1	C	146	THR	HG22	1.217	0.000	1
1	C	146	THR	HG23	1.217	0.000	1
1	C	146	THR	CA	62.179	0.004	1
1	C	146	THR	CB	69.734	0.032	1
1	C	146	THR	N	115.788	0.034	1
1	C	147	ALA	H	8.259	0.002	1
1	C	147	ALA	HA	4.309	0.016	1
1	C	147	ALA	CA	52.58	0.125	1
1	C	147	ALA	CB	19.215	0.021	1
1	C	147	ALA	N	126.607	0.028	1
1	C	148	ALA	H	8.192	0.003	1
1	C	148	ALA	CA	52.493	0.038	1
1	C	148	ALA	CB	19.127	0.073	1
1	C	148	ALA	N	123.37	0.036	1
1	C	149	LEU	H	8.127	0.003	1
1	C	149	LEU	CA	55.331	0.000	1
1	C	149	LEU	CB	42.333	0.000	1
1	C	149	LEU	N	121.57	0.026	1
1	C	151	GLU	CA	56.593	0.052	1
1	C	151	GLU	CB	30.422	0.043	1
1	C	152	ALA	H	8.326	0.003	1
1	C	152	ALA	HA	4.408	0.000	1
1	C	152	ALA	HB1	1.436	0.000	1
1	C	152	ALA	HB2	1.436	0.000	1
1	C	152	ALA	HB3	1.436	0.000	1
1	C	152	ALA	CA	52.749	0.042	1
1	C	152	ALA	CB	19.241	0.029	1
1	C	152	ALA	N	125.168	0.033	1
1	C	153	THR	H	8.123	0.004	1
1	C	153	THR	HG21	1.233	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	153	THR	HG22	1.233	0.000	1
1	C	153	THR	HG23	1.233	0.000	1
1	C	153	THR	CA	61.726	0.055	1
1	C	153	THR	CB	69.905	0.045	1
1	C	153	THR	N	112.989	0.028	1
1	C	154	SER	H	8.312	0.003	1
1	C	154	SER	CA	58.557	0.026	1
1	C	154	SER	CB	63.956	0.022	1
1	C	154	SER	N	117.896	0.043	1
1	C	155	GLY	H	8.404	0.005	1
1	C	155	GLY	HA2	4.017	0.000	2
1	C	155	GLY	HA3	4.017	0.000	2
1	C	155	GLY	CA	45.346	0.027	1
1	C	155	GLY	N	110.902	0.032	1
1	C	156	GLU	H	8.273	0.002	1
1	C	156	GLU	CA	56.6	0.032	1
1	C	156	GLU	CB	30.413	0.028	1
1	C	156	GLU	N	120.624	0.043	1
1	C	157	SER	H	8.344	0.003	1
1	C	157	SER	HA	4.478	0.000	1
1	C	157	SER	HB2	3.89	0.000	2
1	C	157	SER	HB3	3.89	0.000	2
1	C	157	SER	CA	58.339	0.066	1
1	C	157	SER	CB	63.925	0.042	1
1	C	157	SER	N	116.872	0.036	1
1	C	158	ALA	H	8.301	0.003	1
1	C	158	ALA	HA	4.383	0.000	1
1	C	158	ALA	HB1	1.404	0.000	1
1	C	158	ALA	HB2	1.404	0.000	1
1	C	158	ALA	HB3	1.404	0.000	1
1	C	158	ALA	CA	52.639	0.043	1
1	C	158	ALA	CB	19.316	0.026	1
1	C	158	ALA	N	126.702	0.038	1
1	C	159	GLN	H	8.288	0.006	1
1	C	159	GLN	CA	55.48	0.000	1
1	C	159	GLN	CB	32.897	0.000	1
1	C	159	GLN	N	119.165	0.018	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	212	-0.44 ± 0.18	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	184	0.17 ± 0.09	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	205	-0.11 ± 0.14	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 66%, i.e. 970 atoms were assigned a chemical shift out of a possible 1473. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	364/504 (72%)	187/203 (92%)	84/206 (41%)	93/95 (98%)
Sidechain	606/886 (68%)	427/579 (74%)	179/274 (65%)	0/33 (0%)
Aromatic	0/83 (0%)	0/40 (0%)	0/42 (0%)	0/1 (0%)
Overall	970/1473 (66%)	614/822 (75%)	263/522 (50%)	93/129 (72%)

7.1.4 Statistically unusual chemical shifts

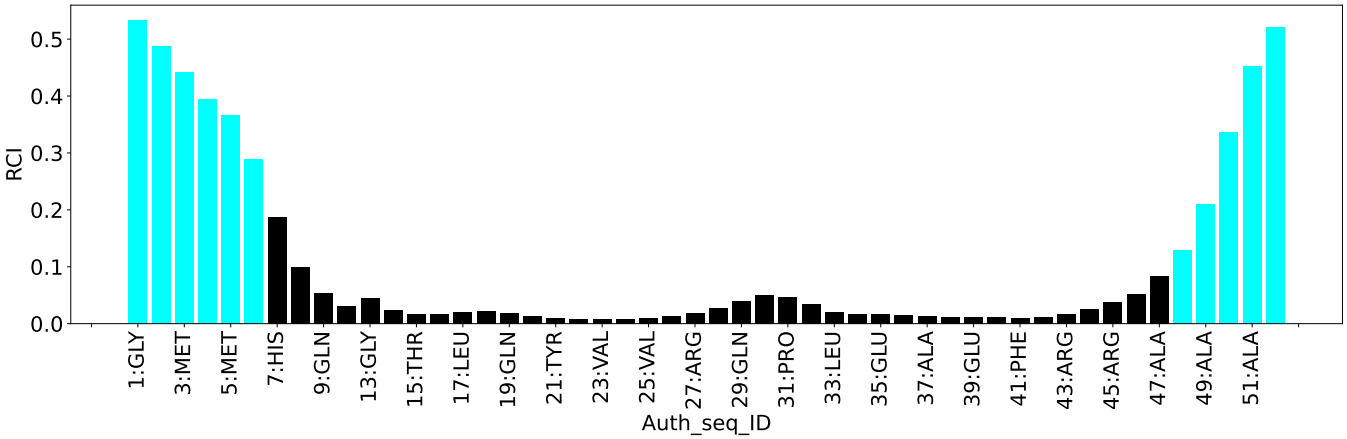
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	B	8	ILE	CG2	28.02	10.93 – 24.12	8.0

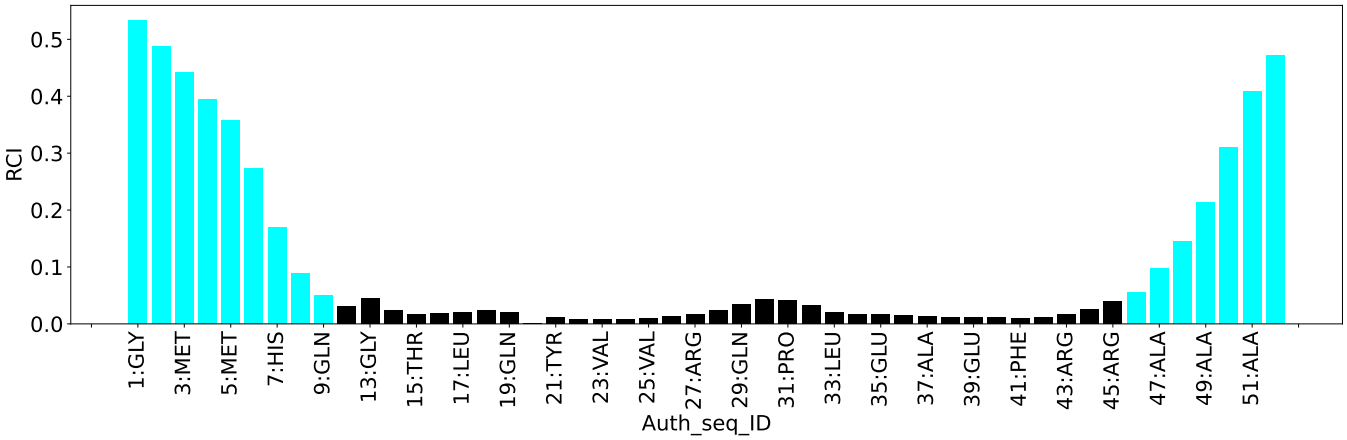
7.1.5 Random Coil Index (RCI) plots

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

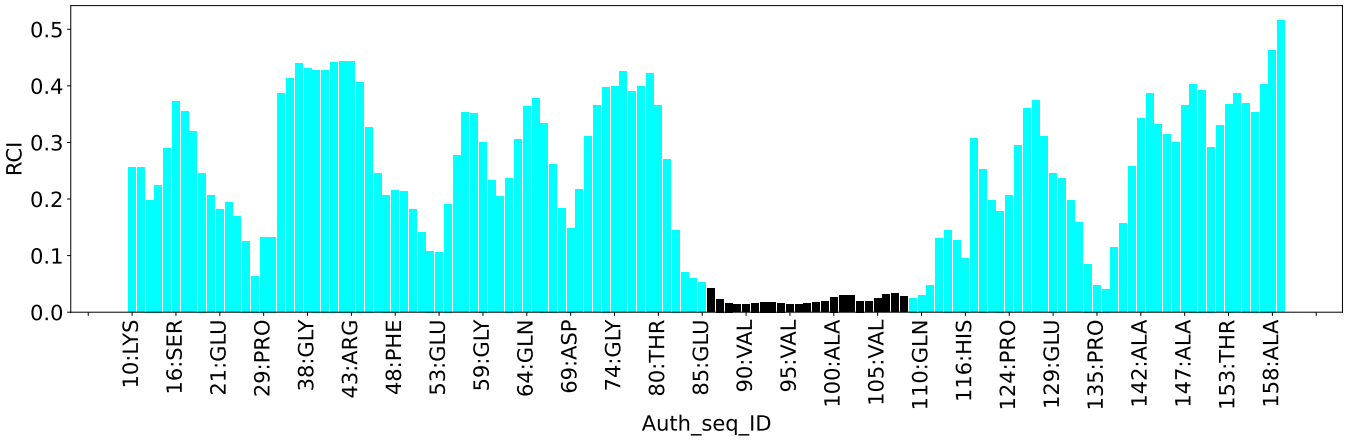
Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



Random coil index (RCI) for chain C:



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	0
Intra-residue (|i-j|=0)	0
Sequential (|i-j|=1)	0
Medium range (|i-j|>1 and |i-j|<5)	0
Long range (|i-j|≥5)	0
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	174
Number of unmapped restraints	0
Number of restraints per residue	0
Number of long range restraints per residue[1]	0

[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.There are no distance restraints

8.2.2 Average number of dihedral-angle violations per model

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)	11.7	7.14

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Bins (°)	Average number of violations per model	Max (°)
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

No distance restraints data found

10 Dihedral-angle violation analysis

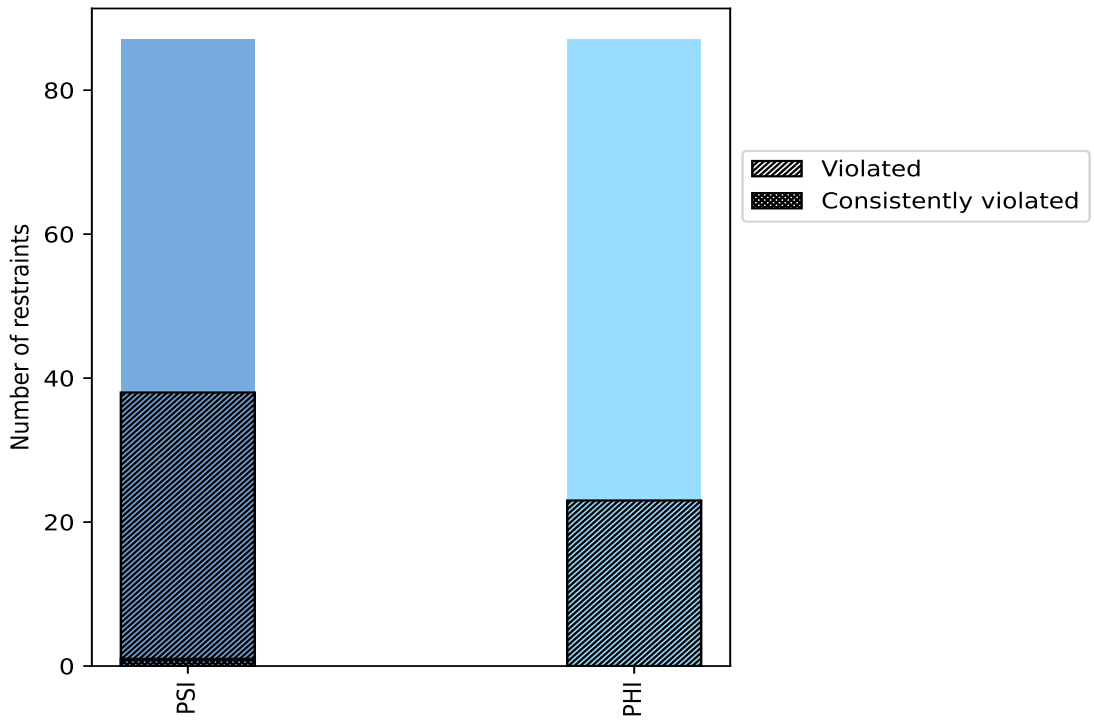
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	87	50.0	38	43.7	21.8	1	1.1	0.6
PHI	87	50.0	23	26.4	13.2	0	0.0	0.0
Total	174	100.0	61	35.1	35.1	1	0.6	0.6

[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



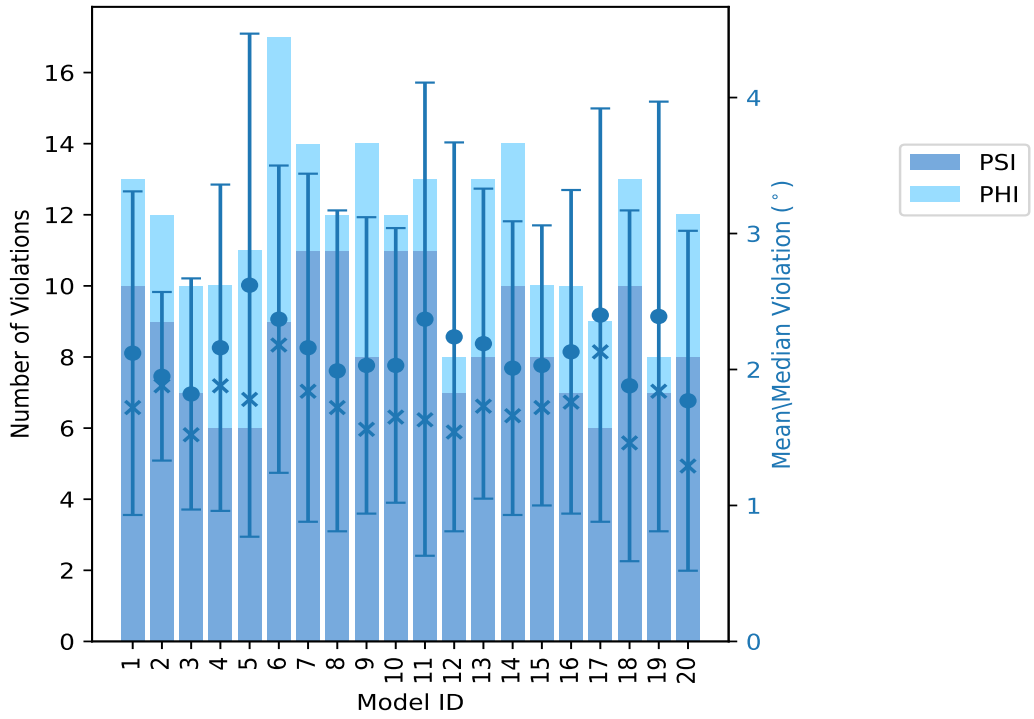
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PSI	PHI	Total				
1	10	3	13	2.12	5.34	1.19	1.72
2	9	3	12	1.95	3.12	0.62	1.88
3	7	3	10	1.82	4.05	0.85	1.52
4	6	4	10	2.16	5.2	1.2	1.88
5	6	5	11	2.62	7.14	1.85	1.78
6	9	8	17	2.37	4.59	1.13	2.18
7	11	3	14	2.16	5.3	1.28	1.84
8	11	1	12	1.99	5.75	1.18	1.72
9	8	6	14	2.03	4.63	1.09	1.56
10	11	1	12	2.03	4.49	1.01	1.65
11	11	2	13	2.37	6.34	1.74	1.63
12	7	1	8	2.24	5.45	1.43	1.54
13	8	5	13	2.19	5.4	1.14	1.73
14	10	4	14	2.01	5.07	1.08	1.66
15	8	2	10	2.03	4.79	1.03	1.72
16	7	3	10	2.13	5.37	1.19	1.76
17	6	3	9	2.4	6.44	1.52	2.13
18	10	3	13	1.88	5.84	1.29	1.46
19	7	1	8	2.39	6.11	1.58	1.84
20	8	4	12	1.77	5.74	1.25	1.29

10.2.1 Bar graph : Dihedral violation statistics for each model



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

10.3 Dihedral-angle violation statistics for the ensemble

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
8	9	17	1	5.0
11	9	20	2	10.0
6	1	7	3	15.0
1	2	3	4	20.0
4	0	4	5	25.0
0	0	0	6	30.0
2	0	2	7	35.0
0	1	1	8	40.0
0	0	0	9	45.0
1	0	1	10	50.0
0	0	0	11	55.0

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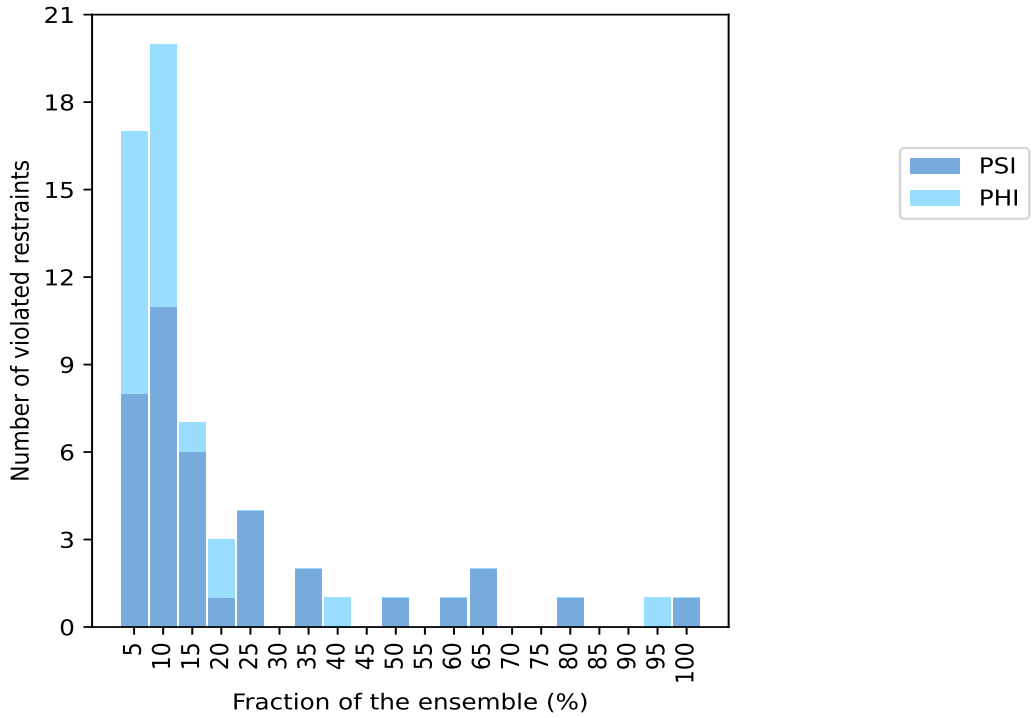
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
1	0	1	12	60.0
2	0	2	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
1	0	1	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	1	1	19	95.0
1	0	1	20	100.0

[1] Number of models with violations

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

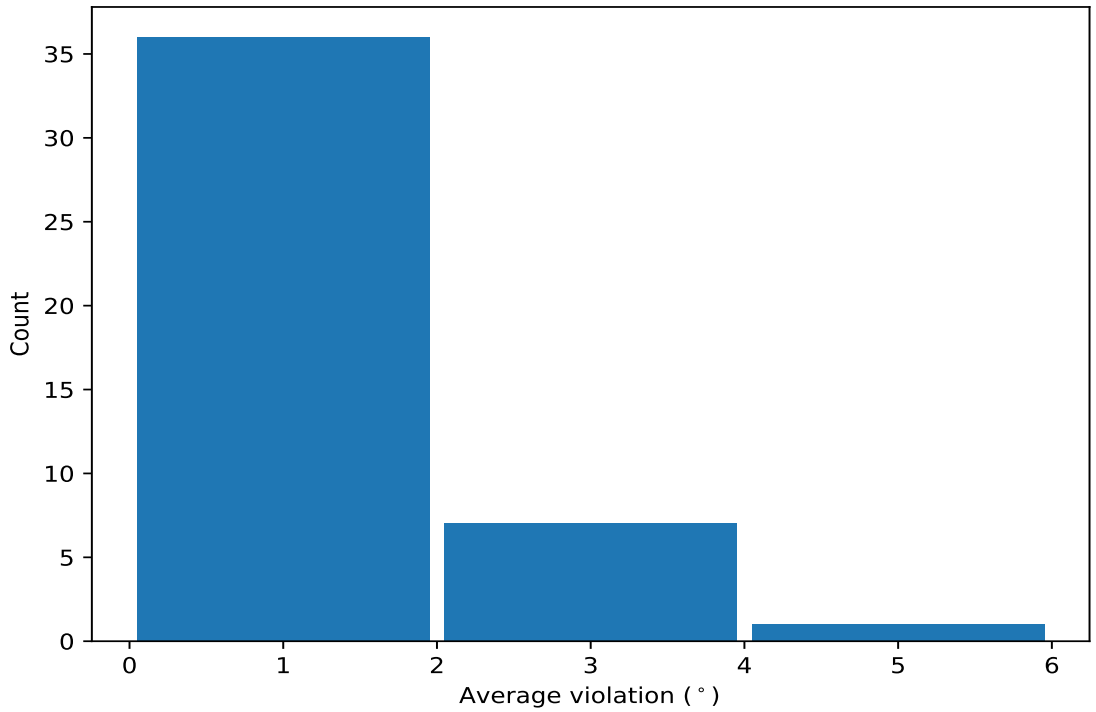


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints

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

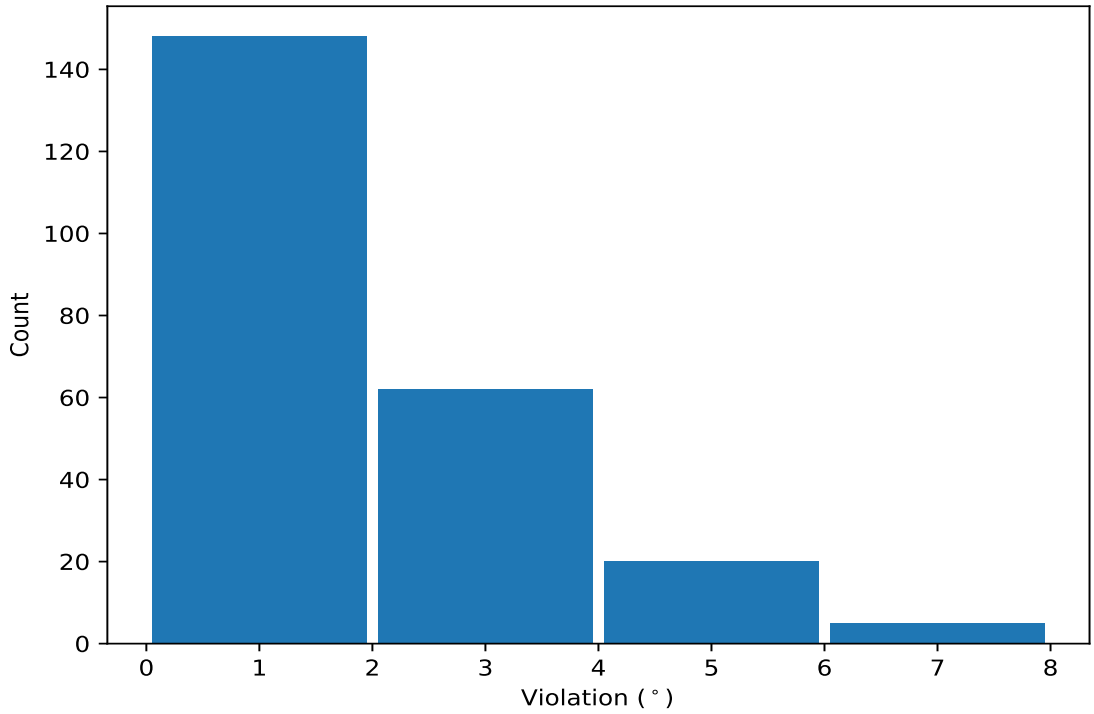
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	20	5.31	0.88	5.36
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	19	1.81	0.68	1.67
(1,74)	1:10:B:ILE:N	1:10:B:ILE:CA	1:10:B:ILE:C	1:11:B:PRO:N	16	2.03	0.62	2.02
(1,56)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:PHE:N	13	2.67	0.76	2.9
(1,48)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ALA:N	13	1.86	0.46	1.89
(1,132)	2:86:C:THR:N	2:86:C:THR:CA	2:86:C:THR:C	2:87:C:ALA:N	12	3.14	1.67	2.61
(1,76)	1:13:B:GLY:N	1:13:B:GLY:CA	1:13:B:GLY:C	1:14:B:LEU:N	10	1.96	0.83	1.7
(1,63)	1:44:A:LEU:C	1:45:A:ARG:N	1:45:A:ARG:CA	1:45:A:ARG:C	8	1.78	0.63	1.56
(1,170)	2:105:C:VAL:N	2:105:C:VAL:CA	2:105:C:VAL:C	2:106:C:LEU:N	7	1.61	0.49	1.56
(1,14)	1:16:A:GLU:N	1:16:A:GLU:CA	1:16:A:GLU:C	1:17:A:LEU:N	7	1.55	0.23	1.53

[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 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 (°)
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	5	7.14
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	17	6.44
(1,132)	2:86:C:THR:N	2:86:C:THR:CA	2:86:C:THR:C	2:87:C:ALA:N	11	6.34
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	11	6.33
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	19	6.11
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	18	5.84
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	8	5.75
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	20	5.74
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	12	5.45
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	13	5.4