



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:50 AM UTC

PDB ID : 7WKC / pdb_00007wkc
BMRB ID : 36468
Title : A prototype protein nanocage minimized from carboxysomes with gated oxygen permeability
Authors : Tan, H.; Yang, J.
Deposited on : 2022-01-08

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We welcome your comments at validation@mail.wwpdb.org

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<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

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 : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

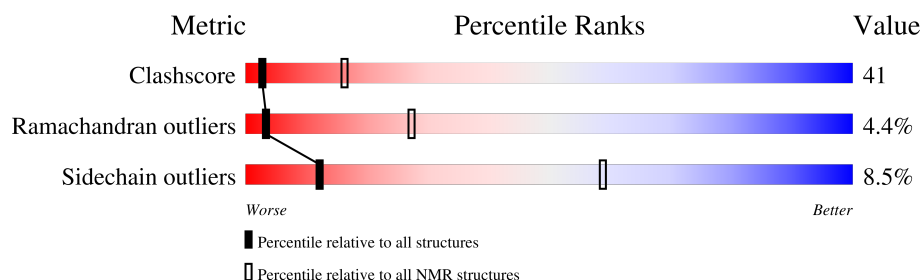
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE 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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	104	
1	B	104	
1	C	104	
1	D	104	
1	E	104	

2 Ensemble composition and analysis

This entry contains 5 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:1-A:92, B:1-B:92, C:1-C:92, D:1-D:92, E:1-E:92 (460)	0.17	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 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	2, 4
2	3, 5
Single-model clusters	1

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6960 atoms, of which 3450 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Carboxysome shell vertex protein CcmL.

Mol	Chain	Residues	Atoms						Trace
1	A	92	Total	C	H	N	O	S	0
			1392	439	690	125	136	2	
1	B	92	Total	C	H	N	O	S	0
			1392	439	690	125	136	2	
1	C	92	Total	C	H	N	O	S	0
			1392	439	690	125	136	2	
1	D	92	Total	C	H	N	O	S	0
			1392	439	690	125	136	2	
1	E	92	Total	C	H	N	O	S	0
			1392	439	690	125	136	2	

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	HIS	-	insertion	UNP Q8DKB4
A	35	HIS	-	insertion	UNP Q8DKB4
A	36	HIS	-	insertion	UNP Q8DKB4
A	37	HIS	-	insertion	UNP Q8DKB4
A	38	HIS	-	insertion	UNP Q8DKB4
B	34	HIS	-	insertion	UNP Q8DKB4
B	35	HIS	-	insertion	UNP Q8DKB4
B	36	HIS	-	insertion	UNP Q8DKB4
B	37	HIS	-	insertion	UNP Q8DKB4
B	38	HIS	-	insertion	UNP Q8DKB4
C	34	HIS	-	insertion	UNP Q8DKB4
C	35	HIS	-	insertion	UNP Q8DKB4
C	36	HIS	-	insertion	UNP Q8DKB4
C	37	HIS	-	insertion	UNP Q8DKB4
C	38	HIS	-	insertion	UNP Q8DKB4
D	34	HIS	-	insertion	UNP Q8DKB4
D	35	HIS	-	insertion	UNP Q8DKB4
D	36	HIS	-	insertion	UNP Q8DKB4
D	37	HIS	-	insertion	UNP Q8DKB4
D	38	HIS	-	insertion	UNP Q8DKB4
E	34	HIS	-	insertion	UNP Q8DKB4
E	35	HIS	-	insertion	UNP Q8DKB4
E	36	HIS	-	insertion	UNP Q8DKB4

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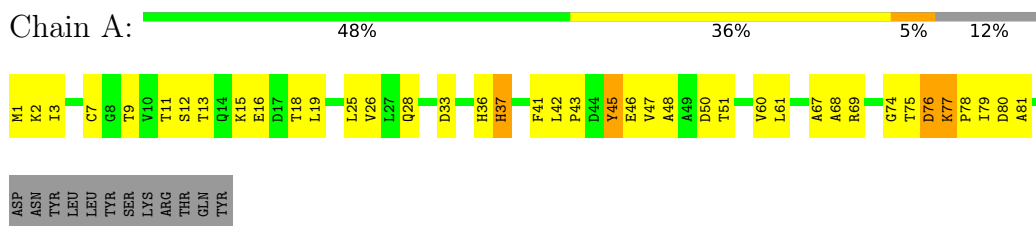
Chain	Residue	Modelled	Actual	Comment	Reference
E	37	HIS	-	insertion	UNP Q8DKB4
E	38	HIS	-	insertion	UNP Q8DKB4

4 Residue-property plots [i](#)

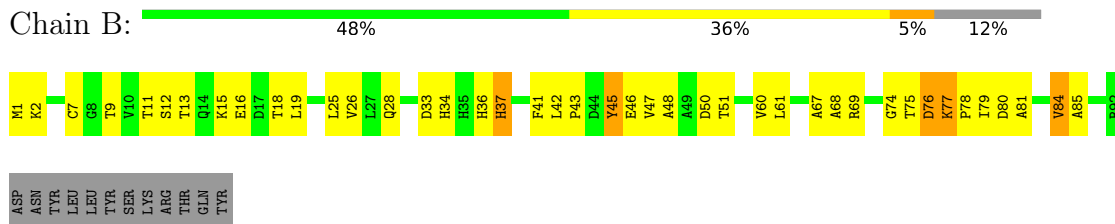
4.1 Average score per residue in the NMR ensemble

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.

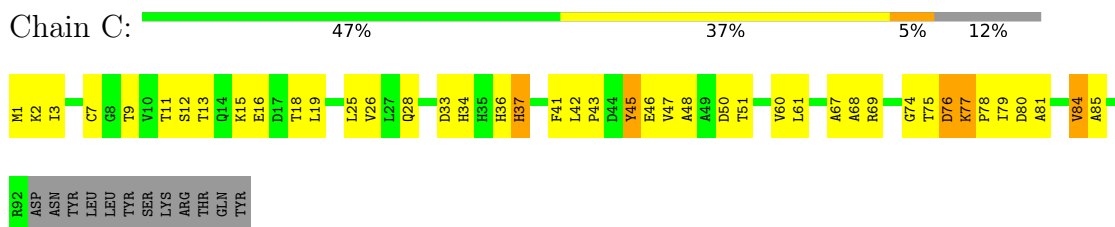
- Molecule 1: Carboxysome shell vertex protein CcmL



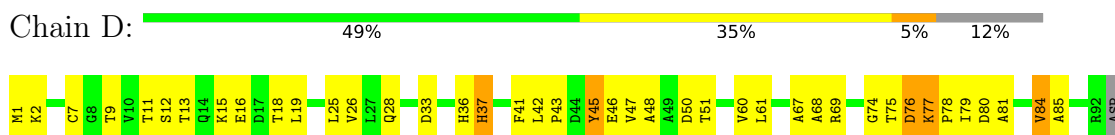
- Molecule 1: Carboxysome shell vertex protein CcmL



- Molecule 1: Carboxysome shell vertex protein CcmL



- Molecule 1: Carboxysome shell vertex protein CcmL



ASN
TYR
LEU
LEU
TYR
SER
LYS
ARG
THR
GLN
TYR

- Molecule 1: Carboxysome shell vertex protein CcmL

Chain E: 

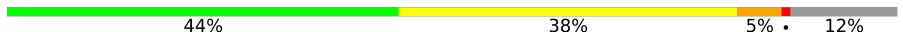
M1 K2 C7 G8 T9 V10 T11 S12 T13 Q14 K15 E16 D17 T18 L19 L25 V26 L27 Q28 D33 H36 H37 F41 L42 P43 D44 Y45 E46 V47 A48 A49 D50 T51 V60 L61 A67 A68 R69 G74 T75 D76 K77 P78 I79 D80 A81 V84 A85 R92 ASP

ASN
TYR
LEU
LEU
TYR
SER
LYS
ARG
THR
GLN
TYR

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.

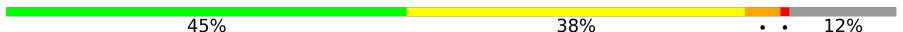
- Molecule 1: Carboxysome shell vertex protein CcmL

Chain A: 

M1 K2 C7 G8 T9 V10 T11 S12 T13 Q14 K15 E16 D17 T18 L19 F24 L25 V26 L27 Q28 D33 H34 H35 H36 H37 F41 L42 P43 D44 Y45 E46 V47 A48 A49 D50 T51 V60 L61 A67 A68 R69 G74 T75 D76 K77 P78 I79 D80 A81 V84 A85

D88 R92 ASP ASN TYR LEU LEU TYR SER LYS ARG THR GLN TYR

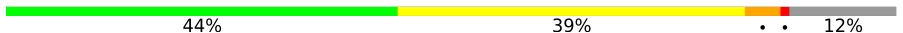
- Molecule 1: Carboxysome shell vertex protein CcmL

Chain B: 

M1 K2 C7 G8 T9 V10 T11 S12 T13 Q14 K15 E16 D17 T18 L19 F24 L25 V26 L27 Q28 D33 H34 H35 H36 H37 F41 L42 P43 D44 Y45 E46 V47 A48 A49 D50 T51 V60 L61 A67 A68 R69 G74 T75 D76 K77 P78 I79 D80 A81 V84 A85 D88

R92 ASP ASN TYR LEU LEU TYR SER LYS ARG THR GLN TYR

- Molecule 1: Carboxysome shell vertex protein CcmL

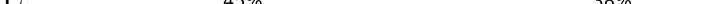
Chain C: 

M1 K2 C7 G8 T9 V10 T11 S12 T13 Q14 K15 E16 D17 T18 L19 F24 L25 V26 L27 Q28 D33 H34 H35 H36 H37 F41 L42 P43 D44 Y45 E46 V47 A48 A49 D50 T51 V60 L61 A67 A68 R69 G74 T75 D76 K77 P78 I79 D80 A81 V84 A85

D88 R92 ASP ASN TYR LEU LEU TYR SER LYS ARG THR GLN TYR

- Molecule 1: Carboxysome shell vertex protein CcmL

A85	D88	A92	ASP	ASN	TYR	LEU	LEU	TYR	SER	LYS	ARG	THR	GLN	TYR	M1	K2	C7	G8	T9	V10	T11	S12	T13	Q14	K15	E16	D17	T18	L19	F24	L25	V26	L27	Q28	D33	H34	H35	H36	H37	F41	L42	P43	L44	Y45	E46	V47	A48	A49	D50	T51	V60	L61	G65	S66	A67	A68	R69	G74	T75	D76	K77	P78	I79	D80	A81	V82
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Chain E:  45% 38% . . 12%

R92	ASP	M1
ASN	TYR	K2
LEU	TYR	C7
LEU	TYR	G8
SER	TYR	T9
LYS	ARG	V10
ARG	THR	S12
GLN	THR	S13
TYR	TYR	Q14
		K15
		E16
		D17
		T18
		L19
		F24
		L25
		V26
		L27
		Q28
		D33
		H34
		H35
		H36
		H37
		F41
		L43
		P43
		D44
		Y45
		E46
		V47
		A48
		A49
		D50
		T51
		V60
		A67
		A68
		R69
		G74
		T75
		D76
		K77
		P78
		I79
		D80
		A81
		V84
		A85
		T88

5 Refinement protocol and experimental data overview

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

Of the 500 calculated structures, 5 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR	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	349
Number of shifts mapped to atoms	349
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%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 [i](#)

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	702	690	690	85±7
1	B	702	690	690	82±5
1	C	702	690	690	85±8
1	D	702	690	690	81±6
1	E	702	690	690	82±8
All	All	17550	17250	17250	1424

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 41.

5 of 510 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:77:LYS:O	1:E:67:ALA:HB2	1.08	1.47	1	5
1:A:67:ALA:HB2	1:D:77:LYS:O	1.07	1.49	1	5
1:B:77:LYS:O	1:D:67:ALA:HB2	1.06	1.51	1	5
1:A:77:LYS:O	1:C:67:ALA:HB2	1.05	1.51	1	5
1:A:2:LYS:HG2	1:D:47:VAL:HG21	1.04	1.04	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	90/104 (87%)	78±0 (87±0%)	8±0 (9±0%)	4±0 (4±0%)	3	27
1	B	90/104 (87%)	78±0 (87±0%)	8±0 (9±0%)	4±0 (4±0%)	3	27
1	C	90/104 (87%)	78±0 (87±0%)	8±0 (9±0%)	4±0 (4±0%)	3	27
1	D	90/104 (87%)	78±0 (87±0%)	8±0 (9±0%)	4±0 (4±0%)	3	27
1	E	90/104 (87%)	78±0 (87±0%)	8±0 (9±0%)	4±0 (4±0%)	3	27
All	All	2250/2600 (87%)	1950 (87%)	200 (9%)	100 (4%)	3	27

5 of 20 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	13	THR	5
1	A	37	HIS	5
1	A	76	ASP	5
1	A	77	LYS	5
1	B	13	THR	5

6.3.2 Protein sidechains

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	75/87 (86%)	69±1 (91±2%)	6±1 (9±2%)	12	59
1	B	75/87 (86%)	69±1 (91±2%)	6±1 (9±2%)	12	59
1	C	75/87 (86%)	69±1 (91±2%)	6±1 (9±2%)	12	59
1	D	75/87 (86%)	69±1 (91±2%)	6±1 (9±2%)	12	59
1	E	75/87 (86%)	69±1 (91±2%)	6±1 (9±2%)	12	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1875/2175 (86%)	1715 (91%)	160 (9%)	12 59

5 of 65 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	7	CYS	5
1	A	60	VAL	5
1	B	7	CYS	5
1	B	60	VAL	5
1	C	7	CYS	5

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 [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_HCcmL@QD.star*

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	349
Number of shifts mapped to atoms	349
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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
$^{13}\text{C}_\alpha$	70	-0.62 ± 0.33	None needed (imprecise)
$^{13}\text{C}_\beta$	61	-0.64 ± 0.31	Should be applied
$^{13}\text{C}'$	69	-0.59 ± 0.14	Should be applied
^{15}N	69	0.84 ± 0.62	None needed (imprecise)

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. 348 atoms were assigned a chemical shift out of a possible 6050. 0 out of 85 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	207/2320 (9%)	0/950 (0%)	139/920 (15%)	68/450 (15%)
Sidechain	141/3270 (4%)	0/2145 (0%)	141/1025 (14%)	0/100 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/460 (0%)	0/240 (0%)	0/185 (0%)	0/35 (0%)
Overall	348/6050 (6%)	0/3335 (0%)	280/2130 (13%)	68/585 (12%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

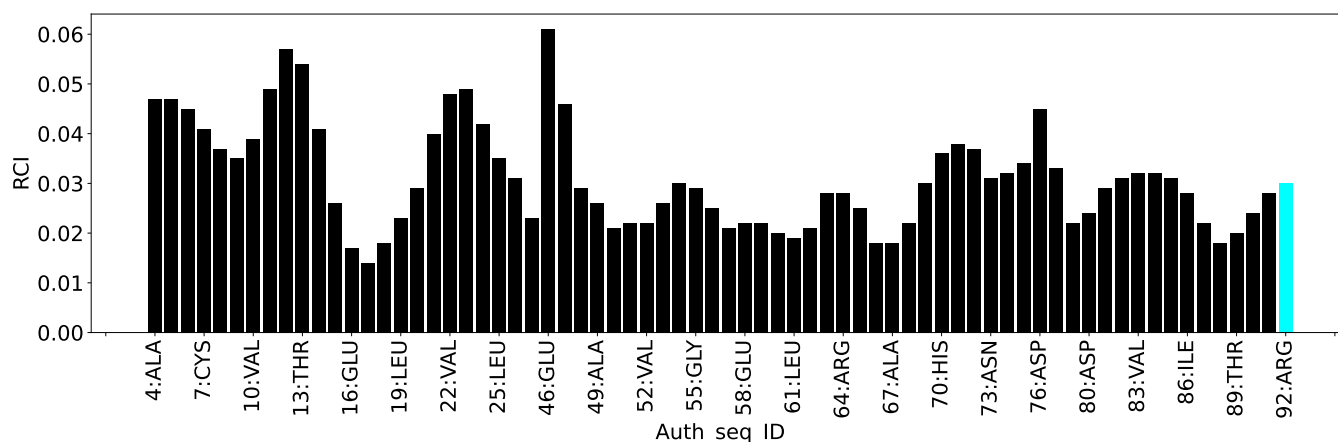
7.1.4 Statistically unusual chemical shifts [i](#)

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	511
Intra-residue ($ i-j =0$)	143
Sequential ($ i-j =1$)	54
Medium range ($ i-j >1$ and $ i-j <5$)	57
Long range ($ i-j \geq 5$)	162
Inter-chain	95
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	1.0
Number of long range restraints per residue ¹	0.3

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)	4.6	0.17
0.2-0.5 (Medium)	8.2	0.49
>0.5 (Large)	126.2	34.51

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

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

9 Distance violation analysis ⓘ

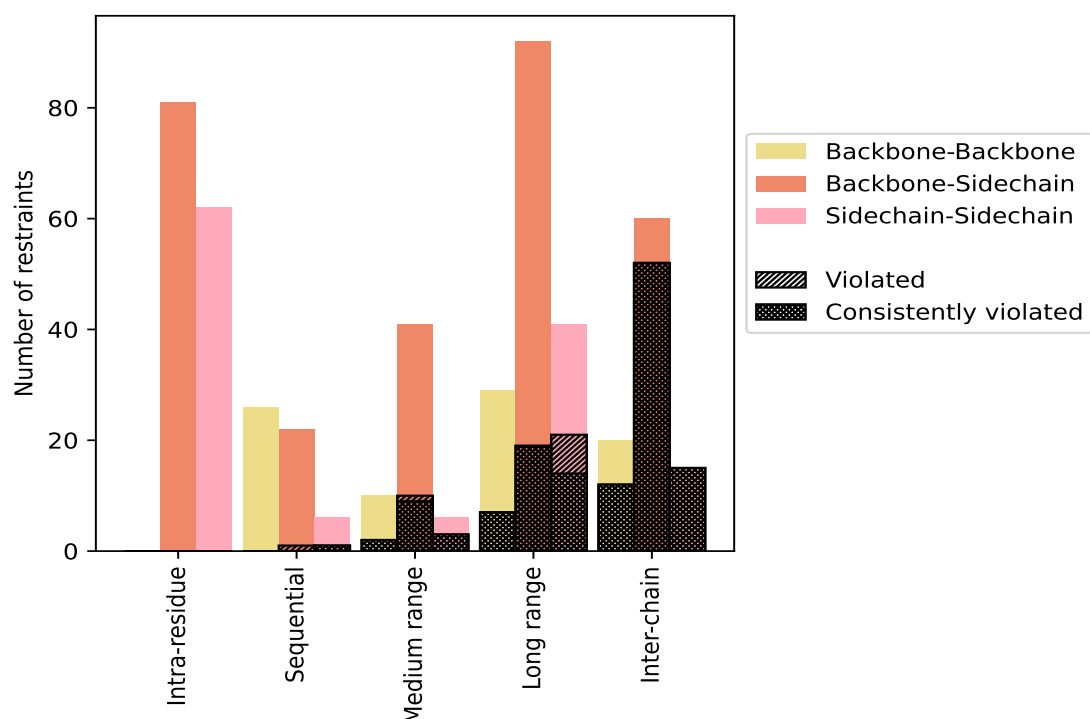
9.1 Summary of distance violations ⓘ

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)	143	28.0	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	81	15.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	62	12.1	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	54	10.6	2	3.7	0.4	1	1.9	0.2
Backbone-Backbone	26	5.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	22	4.3	1	4.5	0.2	0	0.0	0.0
Sidechain-Sidechain	6	1.2	1	16.7	0.2	1	16.7	0.2
Medium range (i-j >1 & i-j <5)	57	11.2	15	26.3	2.9	14	24.6	2.7
Backbone-Backbone	10	2.0	2	20.0	0.4	2	20.0	0.4
Backbone-Sidechain	41	8.0	10	24.4	2.0	9	22.0	1.8
Sidechain-Sidechain	6	1.2	3	50.0	0.6	3	50.0	0.6
Long range (i-j ≥5)	162	31.7	47	29.0	9.2	40	24.7	7.8
Backbone-Backbone	29	5.7	7	24.1	1.4	7	24.1	1.4
Backbone-Sidechain	92	18.0	19	20.7	3.7	19	20.7	3.7
Sidechain-Sidechain	41	8.0	21	51.2	4.1	14	34.1	2.7
Inter-chain	95	18.6	79	83.2	15.5	79	83.2	15.5
Backbone-Backbone	20	3.9	12	60.0	2.3	12	60.0	2.3
Backbone-Sidechain	60	11.7	52	86.7	10.2	52	86.7	10.2
Sidechain-Sidechain	15	2.9	15	100.0	2.9	15	100.0	2.9
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	511	100.0	143	28.0	28.0	134	26.2	26.2
Backbone-Backbone	85	16.6	21	24.7	4.1	21	24.7	4.1
Backbone-Sidechain	296	57.9	82	27.7	16.0	80	27.0	15.7
Sidechain-Sidechain	130	25.4	40	30.8	7.8	33	25.4	6.5

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 disulfid bonds are counted in their appropriate category on the x-axis

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

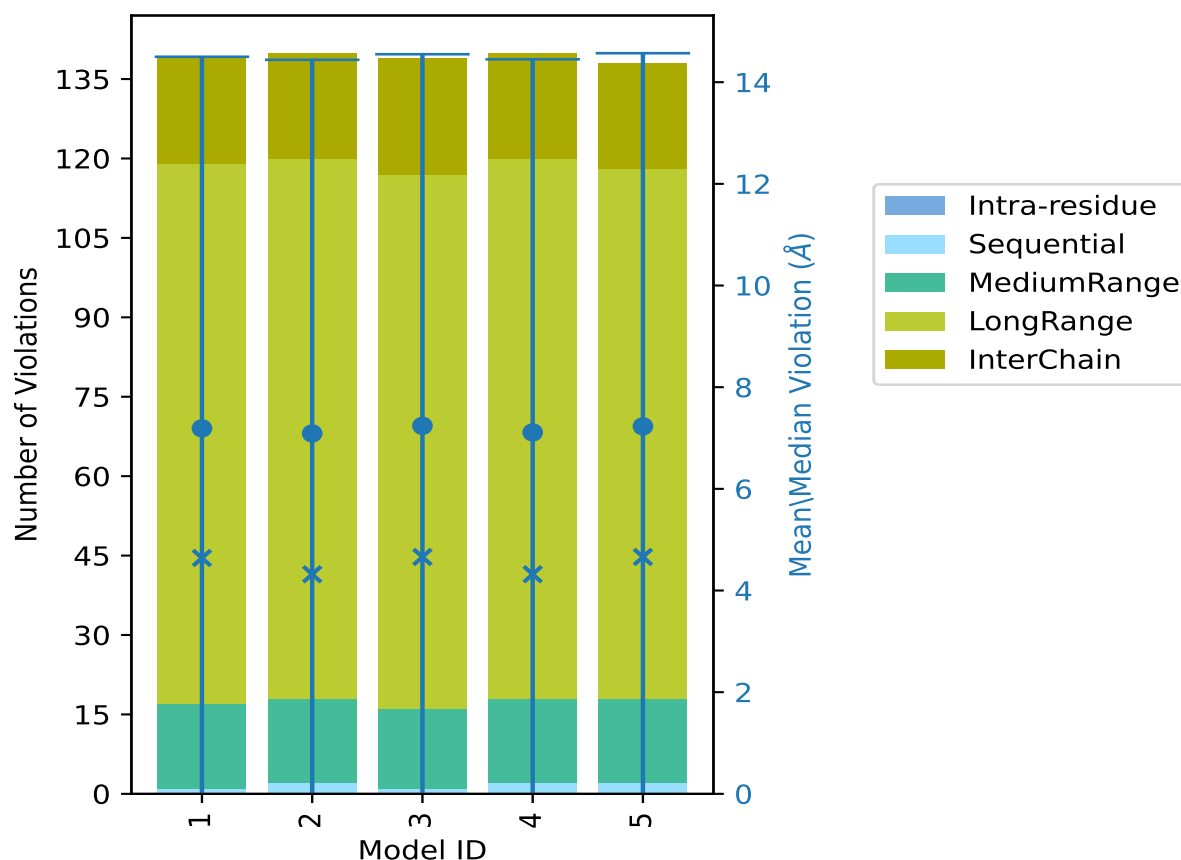
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

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	0	1	16	102	20	139	7.19	34.38	7.31	4.64
2	0	2	16	102	20	140	7.09	34.43	7.35	4.32
3	0	1	15	101	22	139	7.24	34.51	7.31	4.66
4	0	2	16	102	20	140	7.11	34.39	7.34	4.32
5	0	2	16	100	20	138	7.23	34.42	7.34	4.66

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 [i](#)

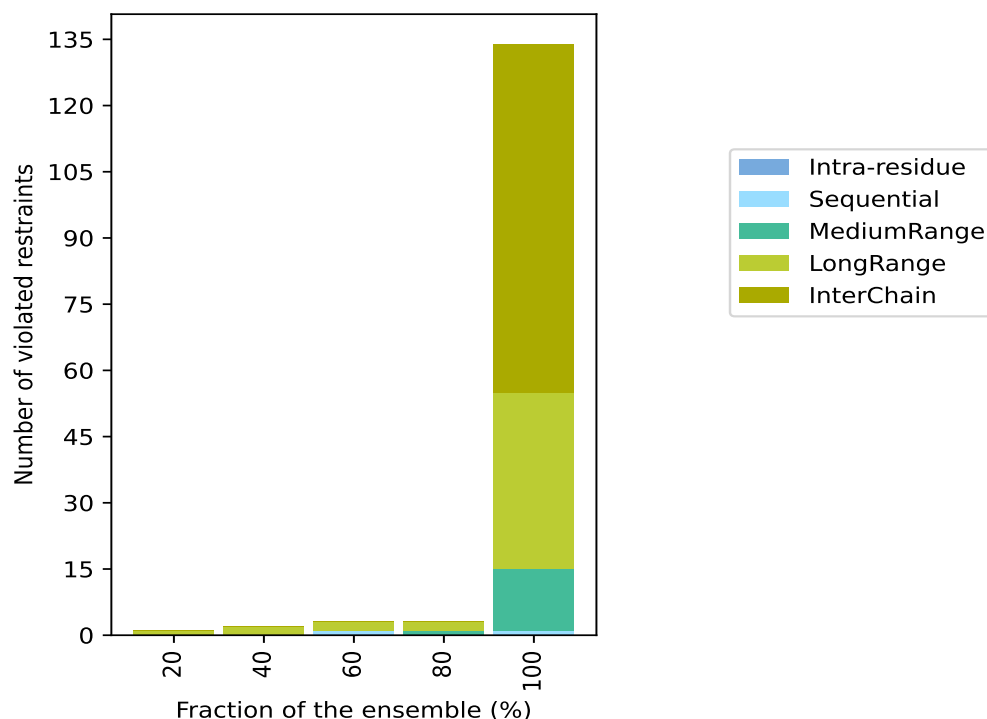
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 368(IR:143, SQ:52, MR:42, LR:115, IC:16) restraints are not 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	%
0	0	0	1	0	1	1	20.0
0	0	0	2	0	2	2	40.0
0	1	0	2	0	3	3	60.0
0	0	1	2	0	3	4	80.0
0	1	14	40	79	134	5	100.0

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

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

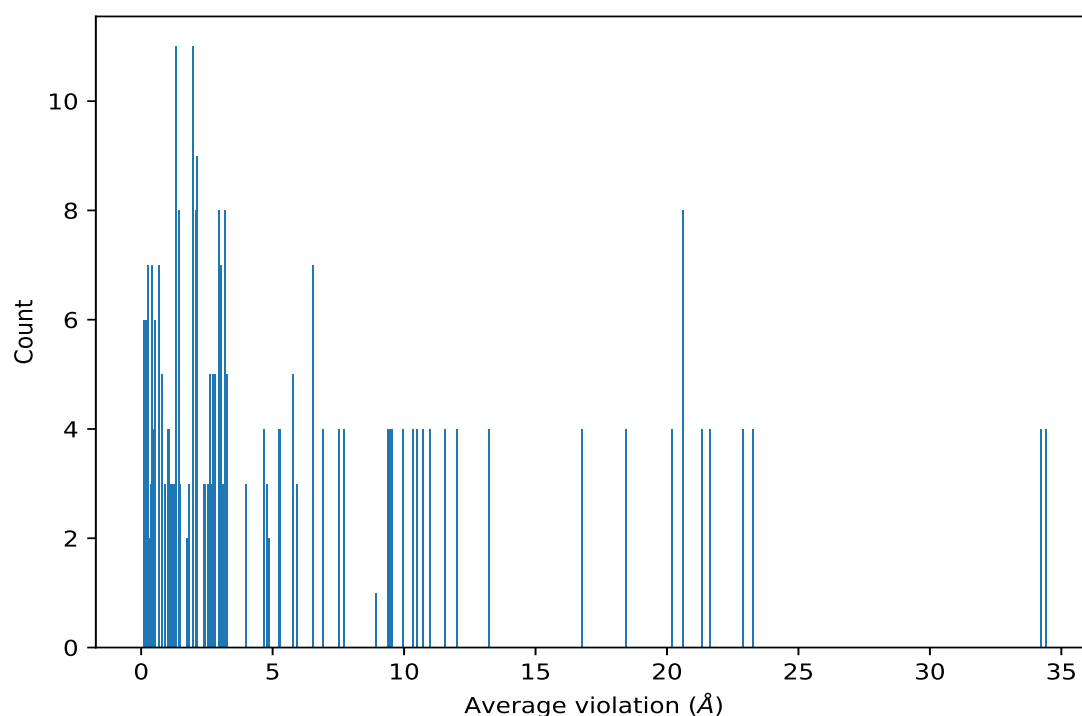
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	5	34.43	0.05	34.42
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	5	34.43	0.05	34.42
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	5	34.43	0.05	34.42
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	5	34.43	0.05	34.42
(3,6)	1:12:A:SER:CB	1:87:B:ILE:CD1	5	34.2	0.02	34.22
(3,6)	1:12:A:SER:CB	1:87:B:ILE:CD1	5	34.2	0.02	34.22
(3,6)	1:12:A:SER:CB	1:87:B:ILE:CD1	5	34.2	0.02	34.22
(3,6)	1:12:A:SER:CB	1:87:B:ILE:CD1	5	34.2	0.02	34.22
(3,86)	1:89:A:THR:CB	1:9:B:THR:C	5	23.25	0.07	23.27
(3,86)	1:89:A:THR:CB	1:9:B:THR:C	5	23.25	0.07	23.27
(3,86)	1:89:A:THR:CB	1:9:B:THR:C	5	23.25	0.07	23.27
(3,86)	1:89:A:THR:CB	1:9:B:THR:C	5	23.25	0.07	23.27
(3,91)	1:89:A:THR:CB	1:10:B:VAL:C	5	22.86	0.03	22.87
(3,91)	1:89:A:THR:CB	1:10:B:VAL:C	5	22.86	0.03	22.87
(3,91)	1:89:A:THR:CB	1:10:B:VAL:C	5	22.86	0.03	22.87
(3,91)	1:89:A:THR:CB	1:10:B:VAL:C	5	22.86	0.03	22.87

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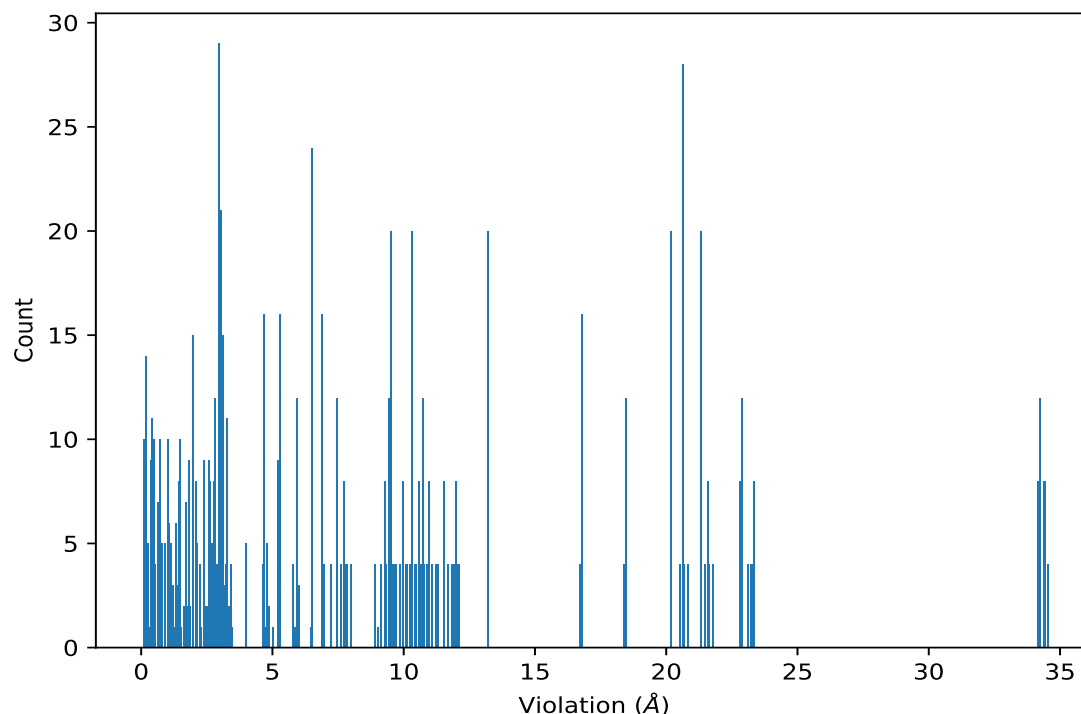
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,11)	1:15:A:LYS:CA	1:84:B:VAL:CA	5	21.6	0.09	21.58
(3,11)	1:15:A:LYS:CA	1:84:B:VAL:CA	5	21.6	0.09	21.58
(3,11)	1:15:A:LYS:CA	1:84:B:VAL:CA	5	21.6	0.09	21.58
(3,11)	1:15:A:LYS:CA	1:84:B:VAL:CA	5	21.6	0.09	21.58
(3,82)	1:88:B:ASP:CA	1:14:B:GLN:CB	5	21.34	0.0	21.34
(3,83)	1:88:B:ASP:CA	1:14:B:GLN:CB	5	21.34	0.0	21.34
(3,84)	1:88:B:ASP:CA	1:14:B:GLN:CB	5	21.34	0.0	21.34
(3,85)	1:88:B:ASP:CA	1:14:B:GLN:CB	5	21.34	0.0	21.34
(3,16)	1:15:A:LYS:CA	1:84:B:VAL:CB	5	20.65	0.09	20.64

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)
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	3	34.51
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	3	34.51
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	3	34.51
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	3	34.51
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	2	34.43
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	2	34.43
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	2	34.43
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	2	34.43
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	5	34.42
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	5	34.42
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	5	34.42
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	5	34.42
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	4	34.39
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	4	34.39
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	4	34.39
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	4	34.39
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	1	34.38
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	1	34.38
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	1	34.38
(3,1)	1:12:A:SER:CB	1:87:B:ILE:CB	1	34.38
(3,6)	1:12:A:SER:CB	1:87:B:ILE:CD1	3	34.23
(3,6)	1:12:A:SER:CB	1:87:B:ILE:CD1	3	34.23
(3,6)	1:12:A:SER:CB	1:87:B:ILE:CD1	3	34.23
(3,6)	1:12:A:SER:CB	1:87:B:ILE:CD1	3	34.23
(3,6)	1:12:A:SER:CB	1:87:B:ILE:CD1	1	34.22
(3,6)	1:12:A:SER:CB	1:87:B:ILE:CD1	1	34.22
(3,6)	1:12:A:SER:CB	1:87:B:ILE:CD1	1	34.22
(3,6)	1:12:A:SER:CB	1:87:B:ILE:CD1	1	34.22
(3,6)	1:12:A:SER:CB	1:87:B:ILE:CD1	2	34.22
(3,6)	1:12:A:SER:CB	1:87:B:ILE:CD1	2	34.22
(3,6)	1:12:A:SER:CB	1:87:B:ILE:CD1	2	34.22
(3,6)	1:12:A:SER:CB	1:87:B:ILE:CD1	2	34.22
(3,6)	1:12:A:SER:CB	1:87:B:ILE:CD1	4	34.18
(3,6)	1:12:A:SER:CB	1:87:B:ILE:CD1	4	34.18
(3,6)	1:12:A:SER:CB	1:87:B:ILE:CD1	4	34.18
(3,6)	1:12:A:SER:CB	1:87:B:ILE:CD1	4	34.18
(3,6)	1:12:A:SER:CB	1:87:B:ILE:CD1	5	34.17

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found