Full wwPDB NMR Structure Validation Report (i)

Dec 25, 2024 – 07:54 PM EST

PDB ID	:	8R6T
BMRB ID	:	34883
Title	:	NMR solution structure of thyropin IrThy-Cd from the hard tick Ixodes ricinus
Authors	:	Srb, P.; Veverka, V.; Matouskova, Z.; Orsaghova, K.; Mares, M.
Deposited on	:	2023-11-23

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

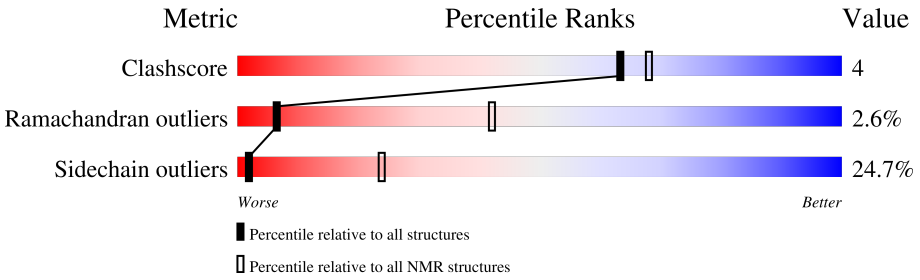
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 84%.

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	72	60% 15% 19% 6%

2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:80-A:85, A:100-A:147 (54)	1.07	11

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 4 clusters and 4 single-model clusters were found.

Cluster number	Models
1	5, 8, 12, 15, 16, 17, 20, 22, 23, 24, 28, 30
2	4, 6, 7, 10, 11, 18, 25
3	1, 3, 14, 19, 21
4	27, 29
Single-model clusters	2; 9; 13; 26

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 989 atoms, of which 468 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative two thyropin protein (Fragment).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	68	989	308	468	99	107	7	0

There are 6 discrepancies between the modelled and reference sequences:

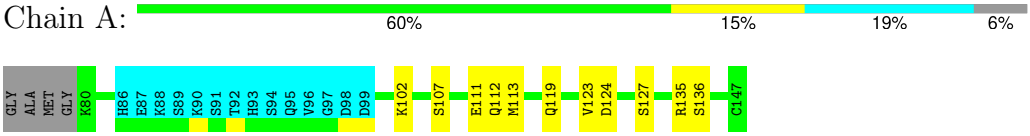
Chain	Residue	Modelled	Actual	Comment	Reference
A	76	GLY	-	expression tag	UNP A0A131Y7Z7
A	77	ALA	-	expression tag	UNP A0A131Y7Z7
A	78	MET	-	expression tag	UNP A0A131Y7Z7
A	79	GLY	-	expression tag	UNP A0A131Y7Z7
A	98	ASP	VAL	conflict	UNP A0A131Y7Z7
A	106	ALA	THR	conflict	UNP A0A131Y7Z7

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: Putative two thyropin protein (Fragment)

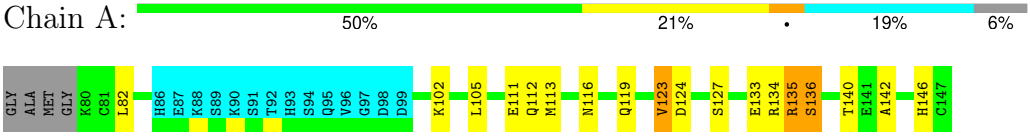


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

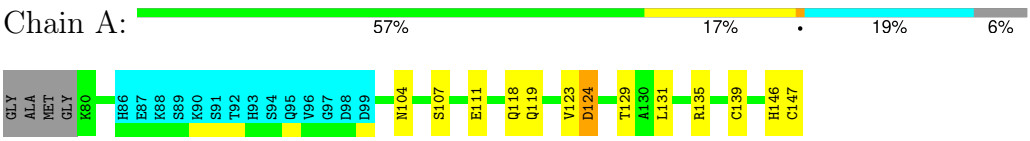
4.2.1 Score per residue for model 1

• Molecule 1: Putative two thyropin protein (Fragment)



4.2.2 Score per residue for model 2

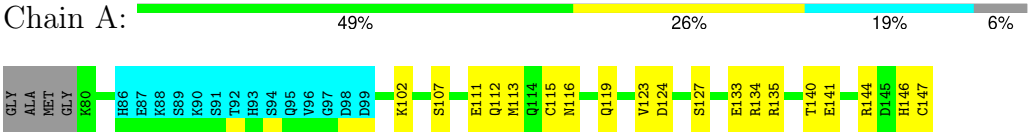
• Molecule 1: Putative two thyropin protein (Fragment)



4.2.3 Score per residue for model 3

• Molecule 1: Putative two thyropin protein (Fragment)

Chain A:



4.2.4 Score per residue for model 4

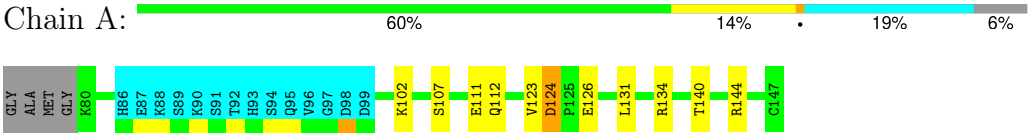
• Molecule 1: Putative two thyropin protein (Fragment)

Chain A:

4.2.5 Score per residue for model 5

• Molecule 1: Putative two thyropin protein (Fragment)

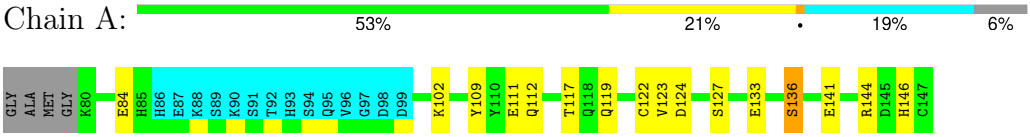
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Putative two thyropin protein (Fragment)

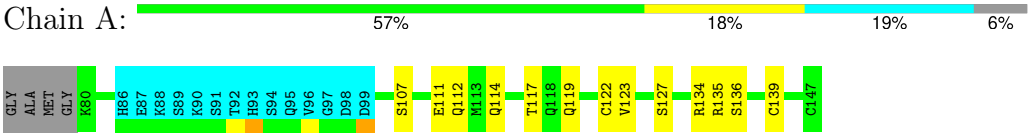
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Putative two thyropin protein (Fragment)

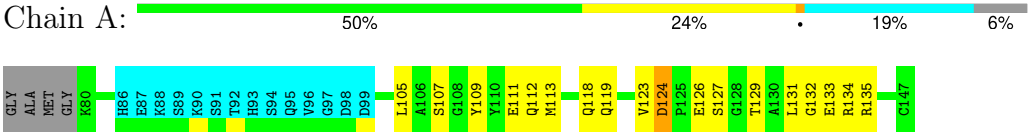
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Putative two thyropin protein (Fragment)

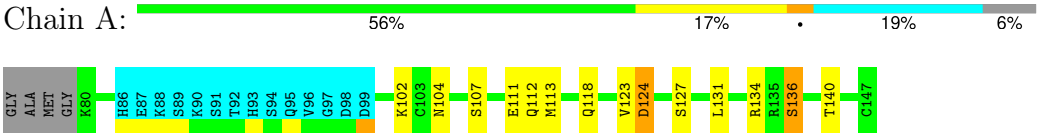
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Putative two thyropin protein (Fragment)

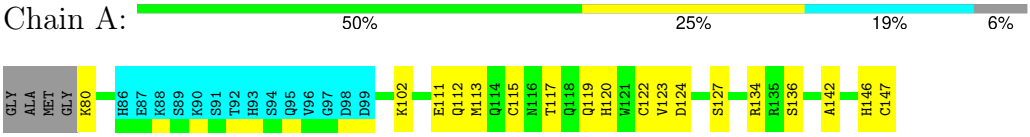
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Putative two thyropin protein (Fragment)

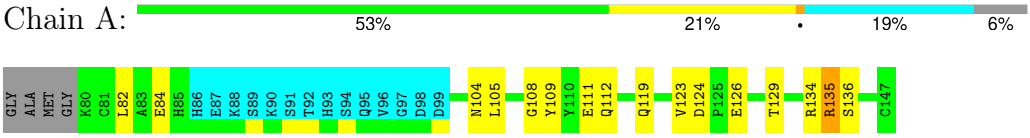
Chain A:



4.2.11 Score per residue for model 11 (medoid)

• Molecule 1: Putative two thyropin protein (Fragment)

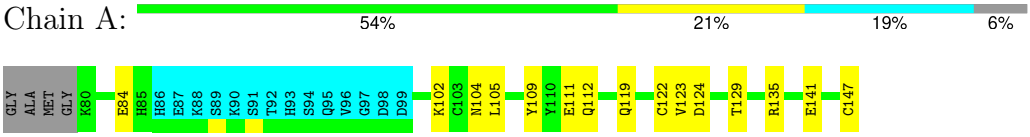
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Putative two thyropin protein (Fragment)

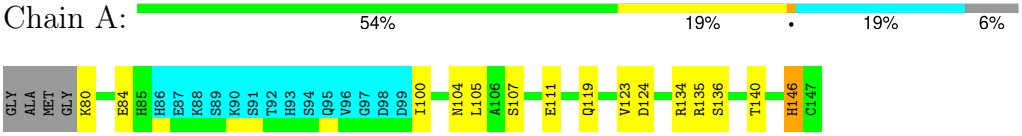
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Putative two thyropin protein (Fragment)

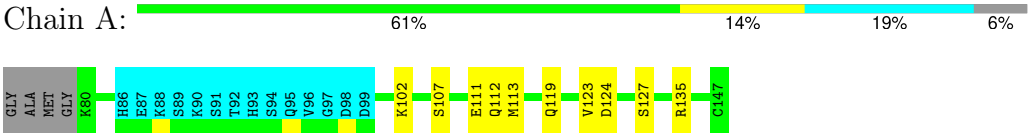
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Putative two thyropin protein (Fragment)

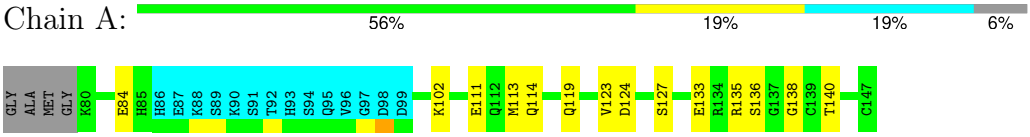
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Putative two thyropin protein (Fragment)

Chain A:



4.2.16 Score per residue for model 16

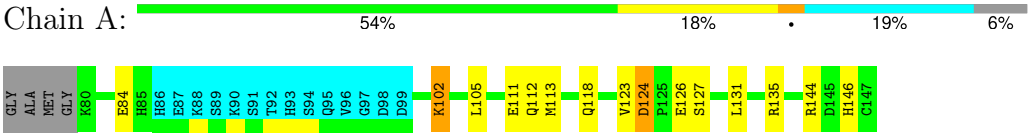
• Molecule 1: Putative two thyropin protein (Fragment)

Chain A:

4.2.17 Score per residue for model 17

• Molecule 1: Putative two thyropin protein (Fragment)

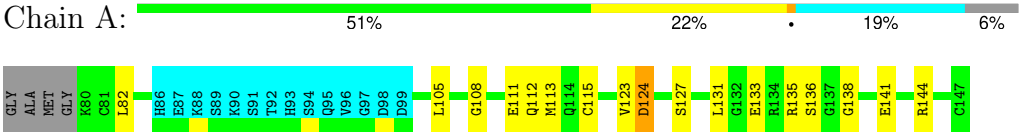
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Putative two thyropin protein (Fragment)

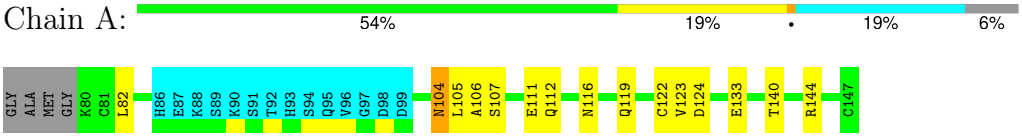
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Putative two thyropin protein (Fragment)

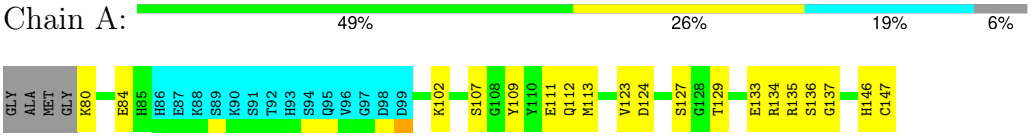
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Putative two thyropin protein (Fragment)

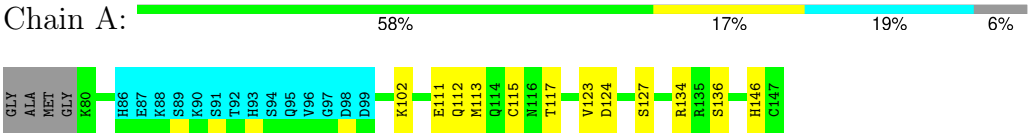
Chain A:



4.2.21 Score per residue for model 21

• Molecule 1: Putative two thyropin protein (Fragment)

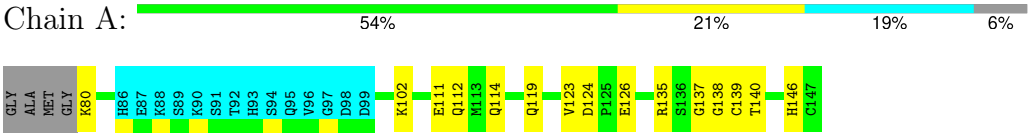
Chain A:



4.2.22 Score per residue for model 22

• Molecule 1: Putative two thyropin protein (Fragment)

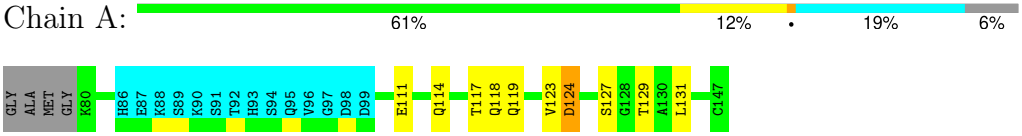
Chain A:



4.2.23 Score per residue for model 23

• Molecule 1: Putative two thyropin protein (Fragment)

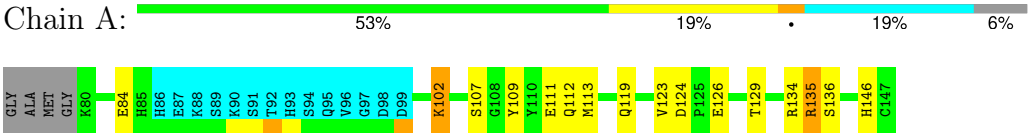
Chain A:



4.2.24 Score per residue for model 24

• Molecule 1: Putative two thyropin protein (Fragment)

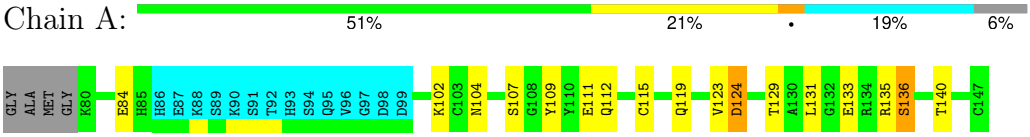
Chain A:



4.2.25 Score per residue for model 25

• Molecule 1: Putative two thyropin protein (Fragment)

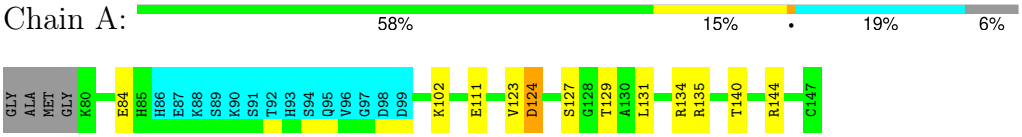
Chain A:



4.2.26 Score per residue for model 26

• Molecule 1: Putative two thyropin protein (Fragment)

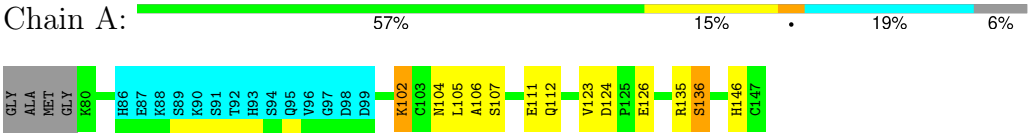
Chain A:



4.2.27 Score per residue for model 27

• Molecule 1: Putative two thyropin protein (Fragment)

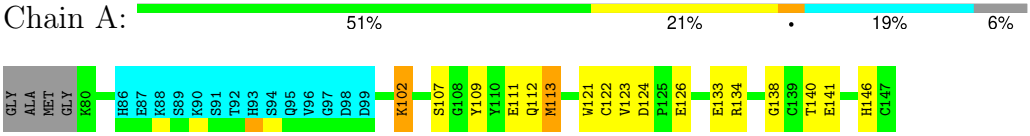
Chain A:



4.2.28 Score per residue for model 28

• Molecule 1: Putative two thyropin protein (Fragment)

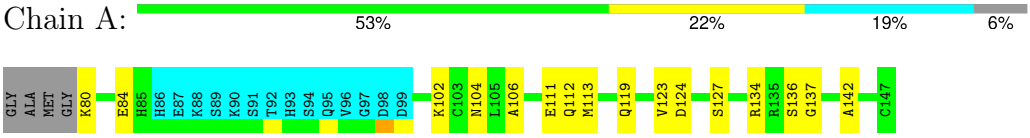
Chain A:



4.2.29 Score per residue for model 29

• Molecule 1: Putative two thyropin protein (Fragment)

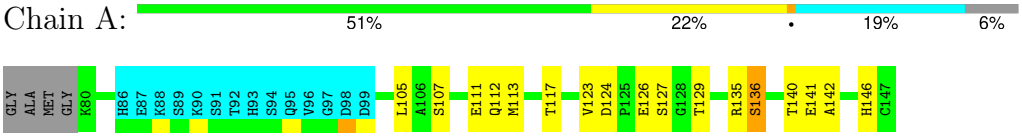
Chain A:



4.2.30 Score per residue for model 30

• Molecule 1: Putative two thyropin protein (Fragment)

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 30 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure calculation	

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	618
Number of shifts mapped to atoms	618
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	413	372	371	3±1
All	All	12390	11160	11130	94

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 4.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:LEU:HD11	1:A:105:LEU:HD23	0.72	1.62	19	1
1:A:104:ASN:ND2	1:A:106:ALA:HB3	0.63	2.09	27	2
1:A:104:ASN:OD1	1:A:106:ALA:HB3	0.61	1.96	19	1
1:A:82:LEU:HD11	1:A:105:LEU:CD1	0.59	2.28	16	1
1:A:111:GLU:C	1:A:123:VAL:HG23	0.56	2.20	9	30
1:A:123:VAL:HG12	1:A:129:THR:C	0.52	2.25	8	12
1:A:124:ASP:HB2	1:A:131:LEU:HD21	0.51	1.82	23	9
1:A:120:HIS:CD2	1:A:142:ALA:HB3	0.50	2.41	10	1
1:A:136:SER:HB3	1:A:142:ALA:HB2	0.49	1.84	1	1
1:A:82:LEU:HD21	1:A:108:GLY:HA2	0.49	1.84	11	1
1:A:111:GLU:O	1:A:123:VAL:HG23	0.48	2.08	6	29
1:A:113:MET:HE2	1:A:121:TRP:O	0.46	2.10	28	1
1:A:114:GLN:OE1	1:A:123:VAL:HG11	0.43	2.14	15	1
1:A:82:LEU:HD11	1:A:105:LEU:HD12	0.43	1.90	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:GLY:HA3	1:A:142:ALA:HB2	0.42	1.89	29	1
1:A:82:LEU:HD11	1:A:108:GLY:HA2	0.42	1.91	18	1
1:A:136:SER:CB	1:A:142:ALA:HB1	0.41	2.45	30	1

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	52/72 (72%)	44±2 (85±4%)	6±2 (12±3%)	1±1 (3±2%)	6	42
All	All	1560/2160 (72%)	1330 (85%)	190 (12%)	40 (3%)	6	42

All 8 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	146	HIS	12
1	A	136	SER	8
1	A	135	ARG	6
1	A	102	LYS	6
1	A	138	GLY	4
1	A	137	GLY	2
1	A	134	ARG	1
1	A	132	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	44/58 (76%)	33±2 (75±6%)	11±2 (25±6%)	2	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1320/1740 (76%)	994 (75%)	326 (25%)	2 24

All 32 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	124	ASP	29
1	A	112	GLN	25
1	A	119	GLN	20
1	A	127	SER	19
1	A	102	LYS	18
1	A	113	MET	17
1	A	135	ARG	17
1	A	107	SER	17
1	A	136	SER	16
1	A	134	ARG	14
1	A	140	THR	12
1	A	84	GLU	11
1	A	105	LEU	10
1	A	133	GLU	10
1	A	109	TYR	10
1	A	144	ARG	9
1	A	126	GLU	9
1	A	104	ASN	7
1	A	141	GLU	7
1	A	115	CYS	6
1	A	117	THR	6
1	A	122	CYS	6
1	A	118	GLN	5
1	A	147	CYS	5
1	A	80	LYS	5
1	A	139	CYS	4
1	A	116	ASN	3
1	A	114	GLN	3
1	A	146	HIS	3
1	A	82	LEU	1
1	A	123	VAL	1
1	A	100	ILE	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 74% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	618
Number of shifts mapped to atoms	618
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	58	-0.04 ± 0.27	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	53	0.02 ± 0.18	None needed (< 0.5 ppm)
$^{13}C'$	53	-0.28 ± 0.16	None needed (< 0.5 ppm)
^{15}N	51	0.60 ± 0.39	None needed (imprecise)

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 84%, i.e. 562 atoms were assigned a chemical shift out of a possible 672. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	243/271 (90%)	102/111 (92%)	96/108 (89%)	45/52 (87%)
Sidechain	292/350 (83%)	198/224 (88%)	91/109 (83%)	3/17 (18%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	27/51 (53%)	17/26 (65%)	9/21 (43%)	1/4 (25%)
Overall	562/672 (84%)	317/361 (88%)	196/238 (82%)	49/73 (67%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 74%, i.e. 618 atoms were assigned a chemical shift out of a possible 839. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	278/342 (81%)	116/140 (83%)	111/136 (82%)	51/66 (77%)
Sidechain	312/432 (72%)	211/275 (77%)	98/137 (72%)	3/20 (15%)
Aromatic	28/65 (43%)	18/34 (53%)	9/25 (36%)	1/6 (17%)
Overall	618/839 (74%)	345/449 (77%)	218/298 (73%)	55/92 (60%)

7.1.4 Statistically unusual chemical shifts (i)

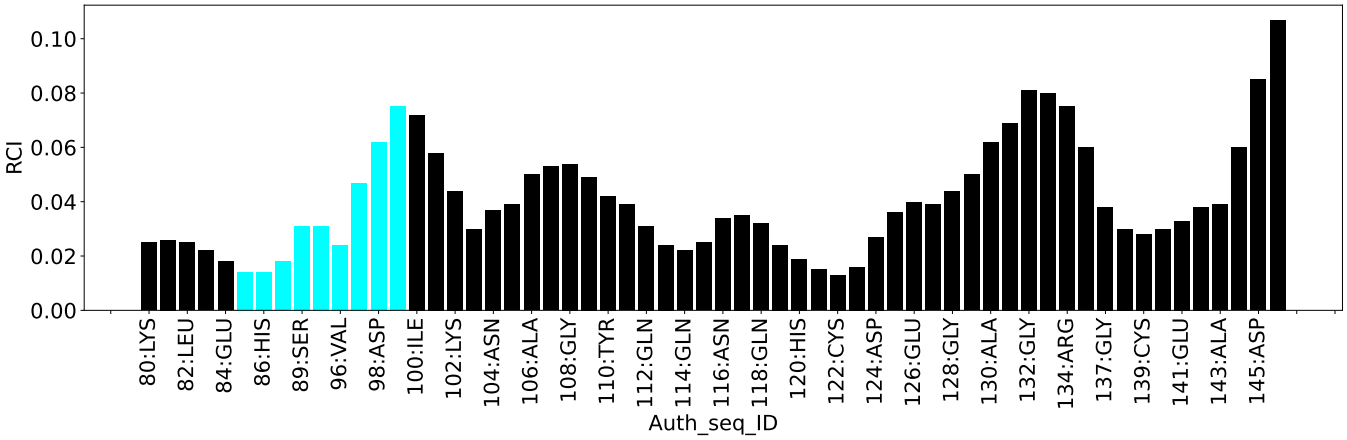
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	114	GLN	HB2	-0.17	0.80 – 3.29	-8.9
1	A	135	ARG	HB2	0.38	0.52 – 3.08	-5.5

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:


RCI
0.00
0.02
0.04
0.06
0.08
0.10
80:LYS
82:LEU
84:GLU
86:HIS
89:SER
96:VAL
98:ASP
100:ILE
102:LYS
104:ASN
106:ALA
108:GLY
110:TYR
112:GLN
114:GLN
116:ASN
118:GLN
120:HIS
122:CYS
124:ASP
126:GLU
128:GLY
130:ALA
132:GLY
134:ARG
137:GLY
139:CYS
141:GLU
143:ALA
145:ASP
Auth_seq_ID

8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	331
Intra-residue (|i-j|=0)	110
Sequential (|i-j|=1)	96
Medium range (|i-j|>1 and |i-j|<5)	30
Long range (|i-j|≥5)	95
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	203
Number of unmapped restraints	0
Number of restraints per residue	7.9
Number of long range restraints per residue[1]	1.4

[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 violations

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)	1.5	5.89

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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)

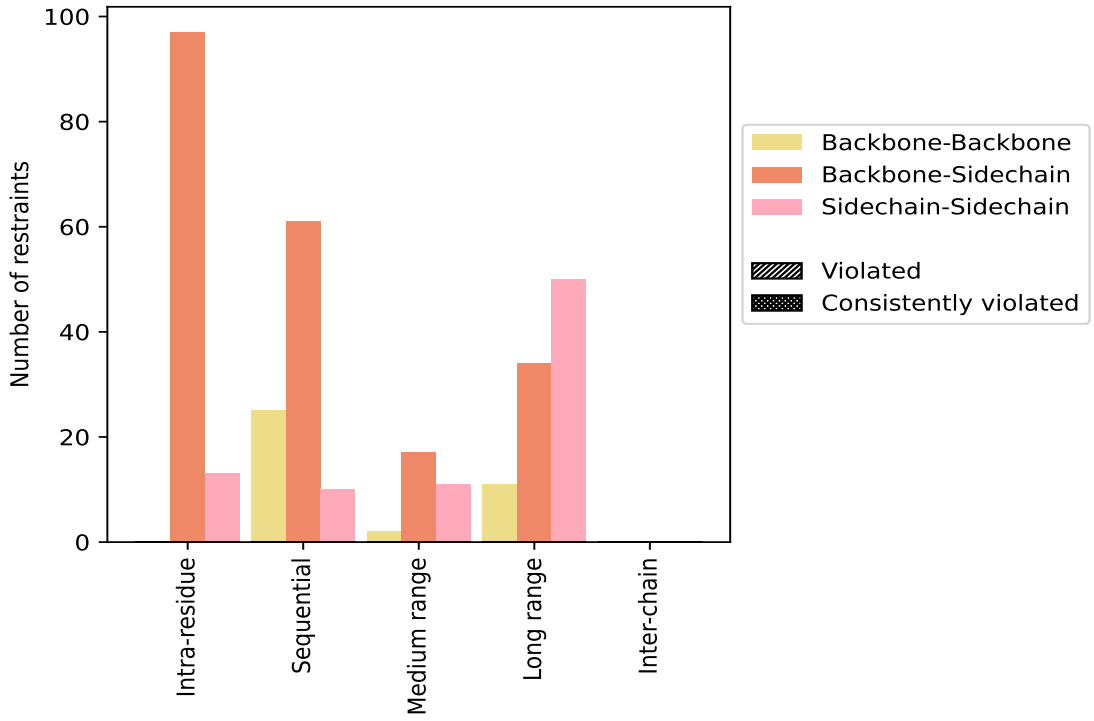
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	110	33.2	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	97	29.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	13	3.9	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	96	29.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	25	7.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	61	18.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	10	3.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	30	9.1	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	2	0.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	17	5.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	11	3.3	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	95	28.7	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	11	3.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	34	10.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	50	15.1	0	0.0	0.0	0	0.0	0.0
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	331	100.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	38	11.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	209	63.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	84	25.4	0	0.0	0.0	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

No violations found

9.3 Distance violation statistics for the ensemble

No violations found

9.4 Most violated distance restraints in the ensemble

No violations found

9.5 All violated distance restraints

No violations found

10 Dihedral-angle violation analysis

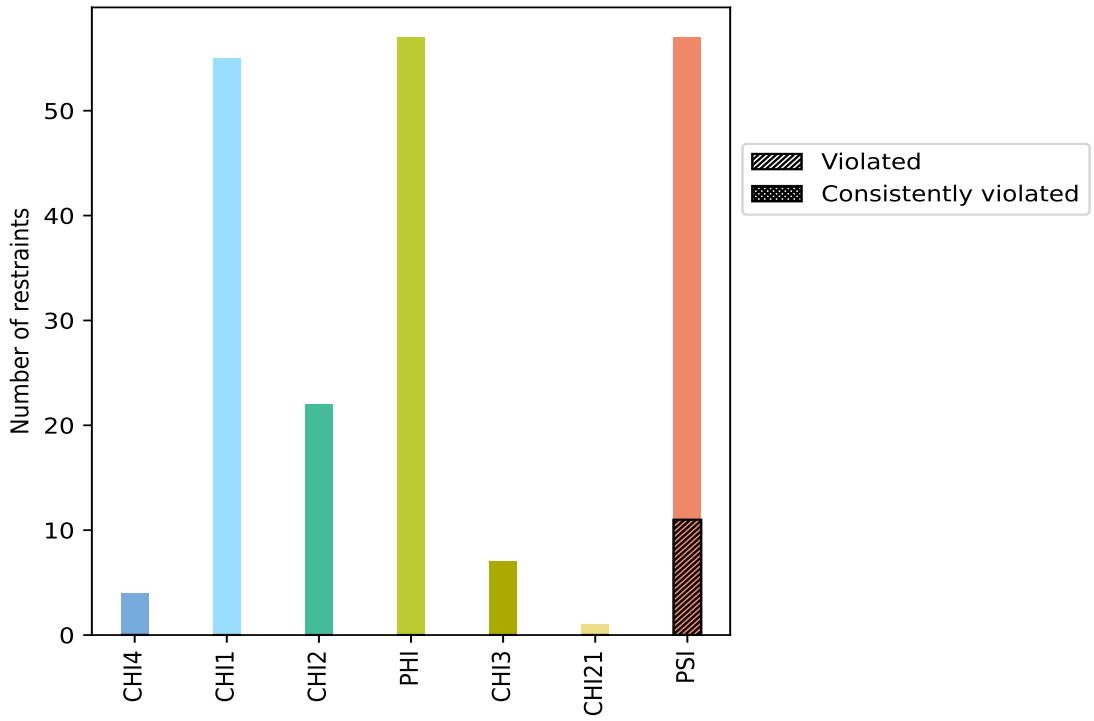
10.1 Summary of dihedral-angle violations

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]
CHI4	4	2.0	0	0.0	0.0	0	0.0	0.0
CHI1	55	27.1	0	0.0	0.0	0	0.0	0.0
CHI2	22	10.8	0	0.0	0.0	0	0.0	0.0
PHI	57	28.1	0	0.0	0.0	0	0.0	0.0
CHI3	7	3.4	0	0.0	0.0	0	0.0	0.0
CHI21	1	0.5	0	0.0	0.0	0	0.0	0.0
PSI	57	28.1	11	19.3	5.4	0	0.0	0.0
Total	203	100.0	11	5.4	5.4	0	0.0	0.0

[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



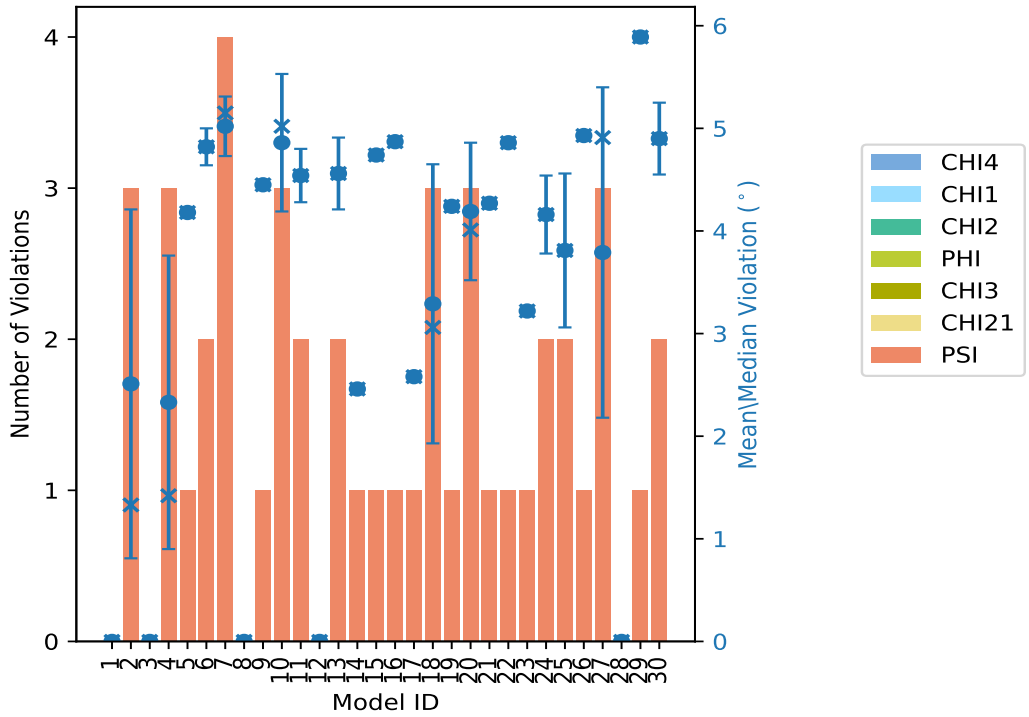
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	CHI4	CHI1	CHI2	PHI	CHI3	CHI21	PSI	Total				
1	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0	0	0	3	3	2.51	4.91	1.7	1.33
3	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0	0	0	3	3	2.33	4.35	1.43	1.42
5	0	0	0	0	0	0	1	1	4.18	4.18	0.0	4.18
6	0	0	0	0	0	0	2	2	4.82	5.0	0.18	4.82
7	0	0	0	0	0	0	4	4	5.02	5.26	0.29	5.15
8	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0	0	0	1	1	4.45	4.45	0.0	4.45
10	0	0	0	0	0	0	3	3	4.86	5.59	0.67	5.02
11	0	0	0	0	0	0	2	2	4.54	4.8	0.26	4.54
12	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0	0	0	2	2	4.56	4.91	0.35	4.56
14	0	0	0	0	0	0	1	1	2.46	2.46	0.0	2.46
15	0	0	0	0	0	0	1	1	4.74	4.74	0.0	4.74
16	0	0	0	0	0	0	1	1	4.87	4.87	0.0	4.87
17	0	0	0	0	0	0	1	1	2.58	2.58	0.0	2.58
18	0	0	0	0	0	0	3	3	3.29	5.06	1.36	3.06
19	0	0	0	0	0	0	1	1	4.24	4.24	0.0	4.24
20	0	0	0	0	0	0	3	3	4.19	5.08	0.67	4.01
21	0	0	0	0	0	0	1	1	4.27	4.27	0.0	4.27
22	0	0	0	0	0	0	1	1	4.86	4.86	0.0	4.86
23	0	0	0	0	0	0	1	1	3.22	3.22	0.0	3.22
24	0	0	0	0	0	0	2	2	4.16	4.54	0.38	4.16
25	0	0	0	0	0	0	2	2	3.81	4.56	0.75	3.81
26	0	0	0	0	0	0	1	1	4.93	4.93	0.0	4.93
27	0	0	0	0	0	0	3	3	3.79	4.95	1.61	4.91
28	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
29	0	0	0	0	0	0	1	1	5.89	5.89	0.0	5.89
30	0	0	0	0	0	0	2	2	4.9	5.25	0.35	4.9

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	
CHI4	CHI1	CHI2	PHI	CHI3	CHI21	PSI	Total	Count[1]	%
0	0	0	0	0	0	3	3	1	3.3
0	0	0	0	0	0	2	2	2	6.7
0	0	0	0	0	0	2	2	3	10.0
0	0	0	0	0	0	1	1	4	13.3
0	0	0	0	0	0	1	1	5	16.7
0	0	0	0	0	0	1	1	6	20.0
0	0	0	0	0	0	0	0	7	23.3
0	0	0	0	0	0	0	0	8	26.7
0	0	0	0	0	0	0	0	9	30.0
0	0	0	0	0	0	0	0	10	33.3
0	0	0	0	0	0	0	0	11	36.7
0	0	0	0	0	0	0	0	12	40.0
0	0	0	0	0	0	0	0	13	43.3
0	0	0	0	0	0	0	0	14	46.7
0	0	0	0	0	0	0	0	15	50.0

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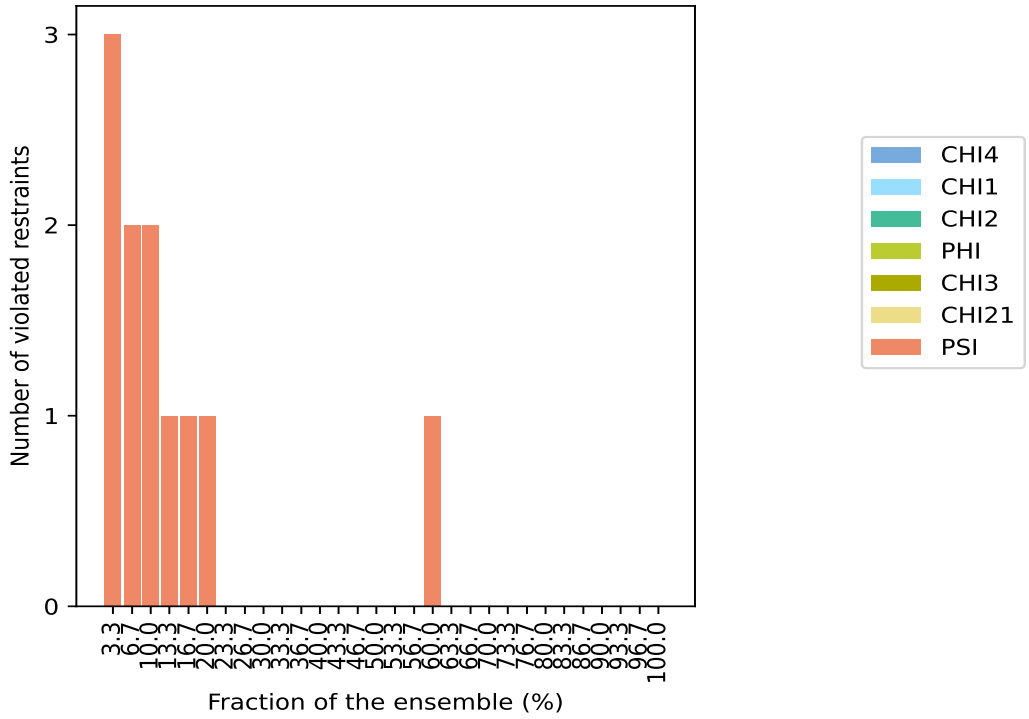
Number of violated restraints								Fraction of the ensemble	
CHI4	CHI1	CHI2	PHI	CHI3	CHI21	PSI	Total	Count[1]	%
0	0	0	0	0	0	0	0	16	53.3
0	0	0	0	0	0	0	0	17	56.7
0	0	0	0	0	0	1	1	18	60.0
0	0	0	0	0	0	0	0	19	63.3
0	0	0	0	0	0	0	0	20	66.7
0	0	0	0	0	0	0	0	21	70.0
0	0	0	0	0	0	0	0	22	73.3
0	0	0	0	0	0	0	0	23	76.7
0	0	0	0	0	0	0	0	24	80.0
0	0	0	0	0	0	0	0	25	83.3
0	0	0	0	0	0	0	0	26	86.7
0	0	0	0	0	0	0	0	27	90.0
0	0	0	0	0	0	0	0	28	93.3
0	0	0	0	0	0	0	0	29	96.7
0	0	0	0	0	0	0	0	30	100.0

[1] Number of models with violations

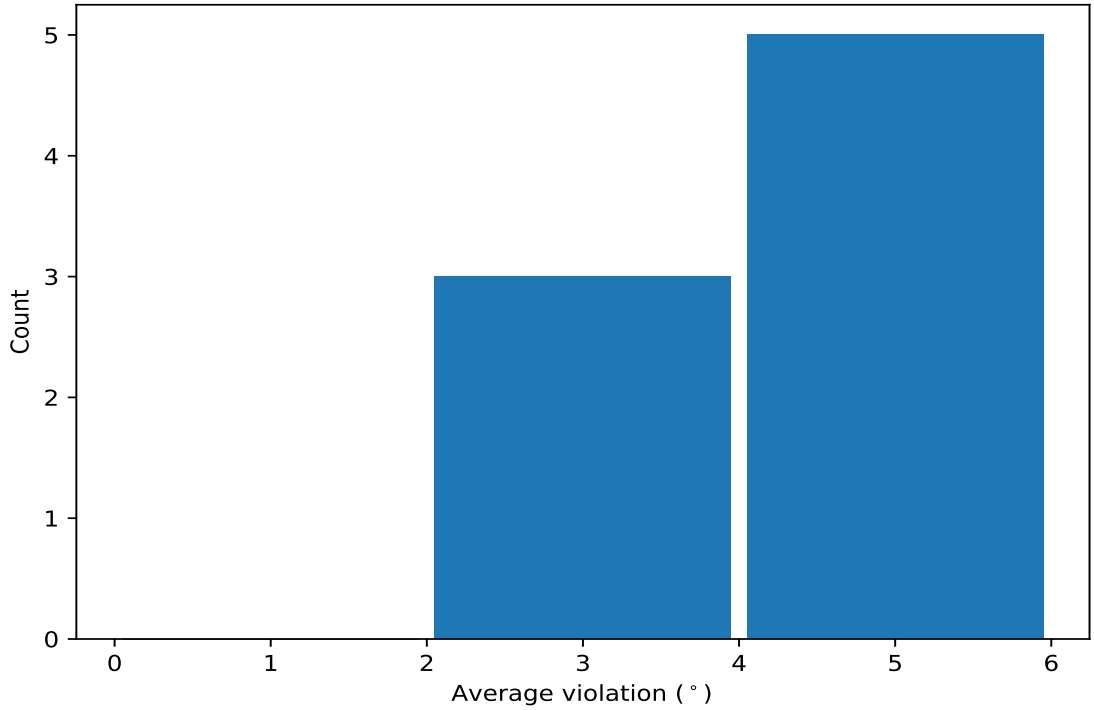
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



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 violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

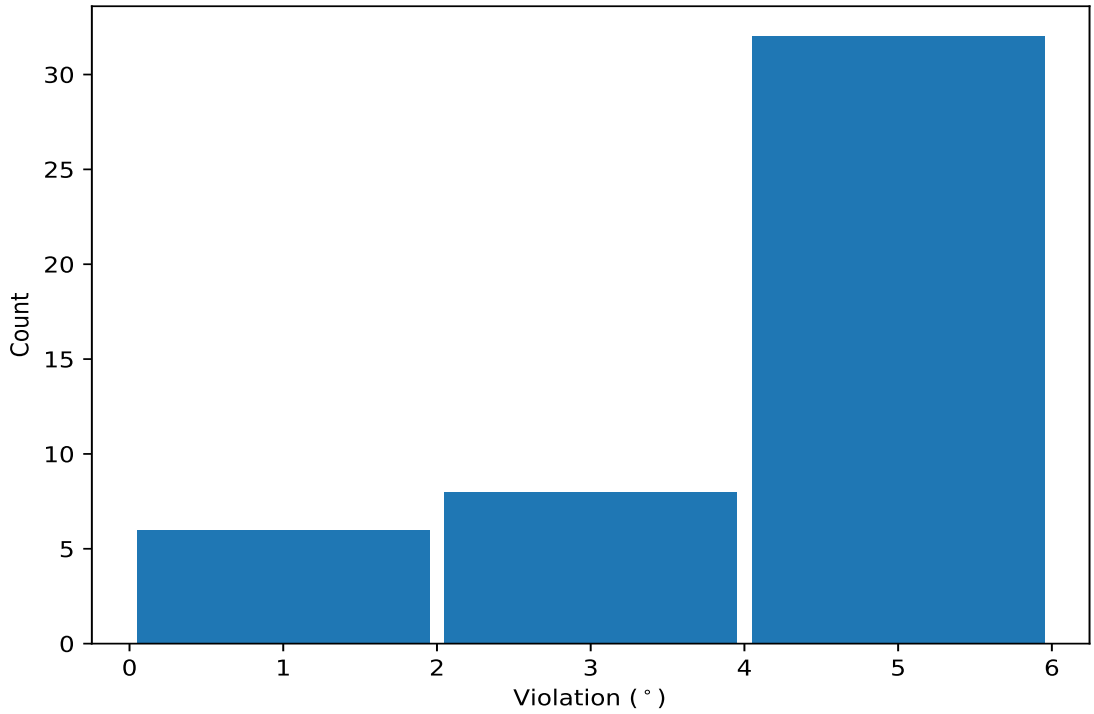
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,91)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:ARG:N	18	3.78	1.24	4.22
(1,97)	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1:137:A:GLY:N	6	4.14	1.47	4.97
(1,37)	1:99:A:ASP:N	1:99:A:ASP:CA	1:99:A:ASP:C	1:100:A:ILE:N	5	5.07	0.5	5.02
(1,29)	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1:95:A:GLN:N	4	3.53	1.44	4.0
(1,31)	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	1:96:A:VAL:N	3	4.89	0.06	4.91
(1,23)	1:91:A:SER:N	1:91:A:SER:CA	1:91:A:SER:C	1:92:A:THR:N	3	4.49	0.16	4.56
(1,93)	1:134:A:ARG:N	1:134:A:ARG:CA	1:134:A:ARG:C	1:135:A:ARG:N	2	5.08	0.03	5.08
(1,95)	1:135:A:ARG:N	1:135:A:ARG:CA	1:135:A:ARG:C	1:136:A:SER:N	2	3.7	1.23	3.7

[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 lists the absolute value of the violation for each restraint in the ensemble sorted by its 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 (°)
(1,37)	1:99:A:ASP:N	1:99:A:ASP:CA	1:99:A:ASP:C	1:100:A:ILE:N	29	5.89
(1,91)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:ARG:N	10	5.59
(1,97)	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1:137:A:GLY:N	7	5.26
(1,97)	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1:137:A:GLY:N	30	5.25
(1,37)	1:99:A:ASP:N	1:99:A:ASP:CA	1:99:A:ASP:C	1:100:A:ILE:N	7	5.19
(1,93)	1:134:A:ARG:N	1:134:A:ARG:CA	1:134:A:ARG:C	1:135:A:ARG:N	7	5.11
(1,97)	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1:137:A:GLY:N	20	5.08
(1,93)	1:134:A:ARG:N	1:134:A:ARG:CA	1:134:A:ARG:C	1:135:A:ARG:N	18	5.06
(1,37)	1:99:A:ASP:N	1:99:A:ASP:CA	1:99:A:ASP:C	1:100:A:ILE:N	10	5.02
(1,91)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:ARG:N	6	5.0
(1,31)	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	1:96:A:VAL:N	27	4.95
(1,95)	1:135:A:ARG:N	1:135:A:ARG:CA	1:135:A:ARG:C	1:136:A:SER:N	26	4.93
(1,37)	1:99:A:ASP:N	1:99:A:ASP:CA	1:99:A:ASP:C	1:100:A:ILE:N	2	4.91
(1,31)	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	1:96:A:VAL:N	13	4.91

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,29)	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1:95:A:GLN:N	27	4.91
(1,91)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:ARG:N	16	4.87
(1,97)	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1:137:A:GLY:N	22	4.86
(1,31)	1:95:A:GLN:N	1:95:A:GLN:CA	1:95:A:GLN:C	1:96:A:VAL:N	11	4.8
(1,91)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:ARG:N	15	4.74
(1,23)	1:91:A:SER:N	1:91:A:SER:CA	1:91:A:SER:C	1:92:A:THR:N	6	4.64
(1,91)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:ARG:N	30	4.56
(1,23)	1:91:A:SER:N	1:91:A:SER:CA	1:91:A:SER:C	1:92:A:THR:N	25	4.56
(1,91)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:ARG:N	24	4.54
(1,29)	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1:95:A:GLN:N	7	4.52
(1,91)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:ARG:N	9	4.45
(1,37)	1:99:A:ASP:N	1:99:A:ASP:CA	1:99:A:ASP:C	1:100:A:ILE:N	4	4.35
(1,91)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:ARG:N	11	4.28
(1,23)	1:91:A:SER:N	1:91:A:SER:CA	1:91:A:SER:C	1:92:A:THR:N	21	4.27
(1,91)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:ARG:N	19	4.24
(1,91)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:ARG:N	13	4.21
(1,91)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:ARG:N	5	4.18
(1,91)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:ARG:N	20	4.01
(1,35)	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	1:99:A:ASP:N	10	3.98
(1,27)	1:93:A:HIS:N	1:93:A:HIS:CA	1:93:A:HIS:C	1:94:A:SER:N	24	3.77
(1,29)	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1:95:A:GLN:N	20	3.47
(1,91)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:ARG:N	23	3.22
(1,97)	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1:137:A:GLY:N	18	3.06
(1,91)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:ARG:N	25	3.06
(1,91)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:ARG:N	17	2.58
(1,95)	1:135:A:ARG:N	1:135:A:ARG:CA	1:135:A:ARG:C	1:136:A:SER:N	14	2.46
(1,91)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:ARG:N	18	1.74
(1,33)	1:96:A:VAL:N	1:96:A:VAL:CA	1:96:A:VAL:C	1:97:A:GLY:N	27	1.51
(1,91)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:ARG:N	4	1.42
(1,97)	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1:137:A:GLY:N	2	1.33
(1,91)	1:133:A:GLU:N	1:133:A:GLU:CA	1:133:A:GLU:C	1:134:A:ARG:N	2	1.28
(1,29)	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1:95:A:GLN:N	4	1.21