



Full wwPDB NMR Structure Validation Report ⓘ

Jun 6, 2023 – 08:20 pm BST

PDB ID : 6TDN
BMRB ID : 34448
Title : Bam_5925cDD 5924nDD docking domains
Authors : Risser, F.; Chagot, B.
Deposited on : 2019-11-08

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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.33

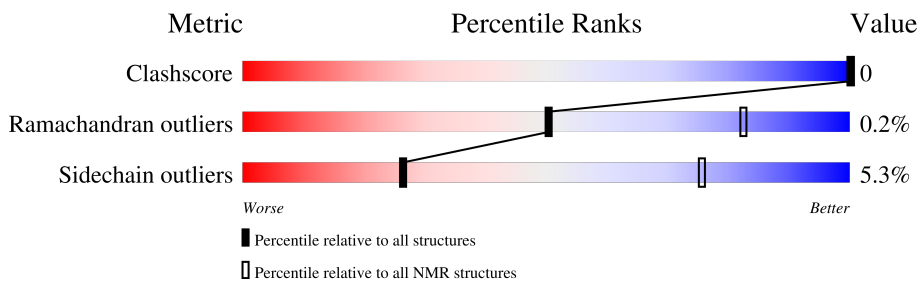
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 93%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	87	
1	B	87	

2 Ensemble composition and analysis i

This entry contains 25 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:11-A:32, A:56-A:82, B:111-B:132, B:156-B:182 (98)	0.53	3

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 5 clusters and 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2540 atoms, of which 1258 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Beta-ketoacyl synthase, Beta-ketoacyl synthase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	87	1270	392	629	111	136	2	0
1	B	87	1270	392	629	111	136	2	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q0B303
A	2	PRO	-	expression tag	UNP Q0B303
A	3	GLY	-	expression tag	UNP Q0B303
A	4	SER	-	expression tag	UNP Q0B303
A	5	TYR	-	expression tag	UNP Q0B303
A	35	GLY	-	linker	UNP Q0B303
A	36	GLY	-	linker	UNP Q0B303
A	37	GLY	-	linker	UNP Q0B303
A	38	SER	-	linker	UNP Q0B303
A	39	GLY	-	linker	UNP Q0B303
A	40	GLY	-	linker	UNP Q0B303
A	41	GLY	-	linker	UNP Q0B303
A	42	SER	-	linker	UNP Q0B303
A	43	GLY	-	linker	UNP Q0B303
A	44	GLY	-	linker	UNP Q0B303
A	45	GLY	-	linker	UNP Q0B303
A	46	SER	-	linker	UNP Q0B303
B	101	GLY	-	expression tag	UNP Q0B303
B	102	PRO	-	expression tag	UNP Q0B303
B	103	GLY	-	expression tag	UNP Q0B303
B	104	SER	-	expression tag	UNP Q0B303
B	105	TYR	-	expression tag	UNP Q0B303
B	135	GLY	-	linker	UNP Q0B303
B	136	GLY	-	linker	UNP Q0B303
B	137	GLY	-	linker	UNP Q0B303
B	138	SER	-	linker	UNP Q0B303
B	139	GLY	-	linker	UNP Q0B303
B	140	GLY	-	linker	UNP Q0B303
B	141	GLY	-	linker	UNP Q0B303

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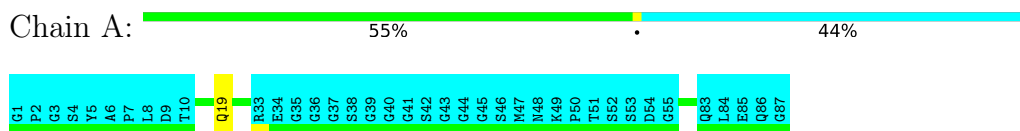
Chain	Residue	Modelled	Actual	Comment	Reference
B	142	SER	-	linker	UNP Q0B303
B	143	GLY	-	linker	UNP Q0B303
B	144	GLY	-	linker	UNP Q0B303
B	145	GLY	-	linker	UNP Q0B303
B	146	SER	-	linker	UNP Q0B303

4 Residue-property plots [i](#)

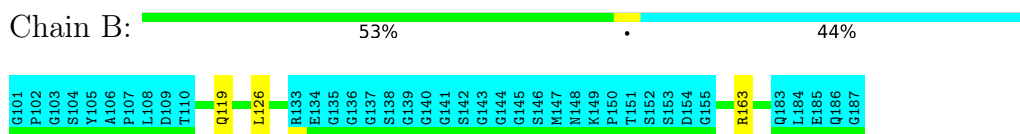
4.1 Average score per residue in the NMR ensemble

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: Beta-ketoacyl synthase,Beta-ketoacyl synthase



- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

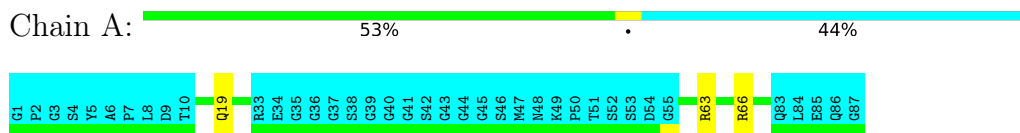


4.2 Scores per residue for each member of the ensemble

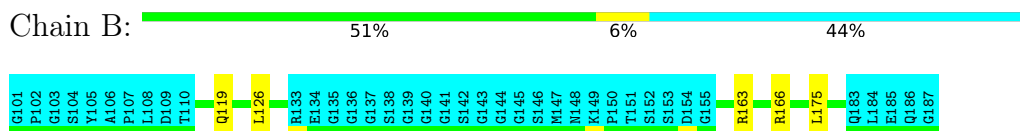
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

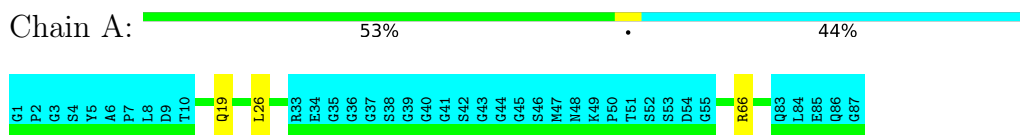


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

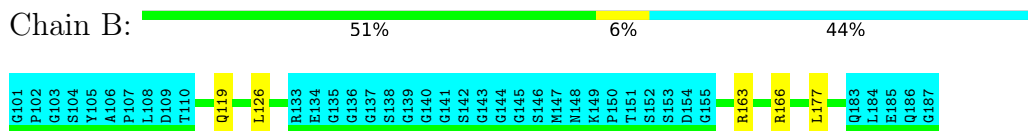


4.2.2 Score per residue for model 2

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

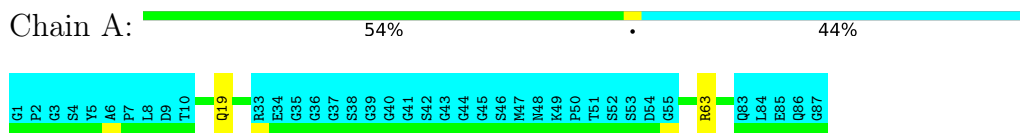


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

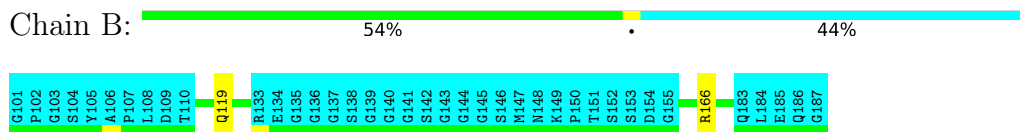


4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

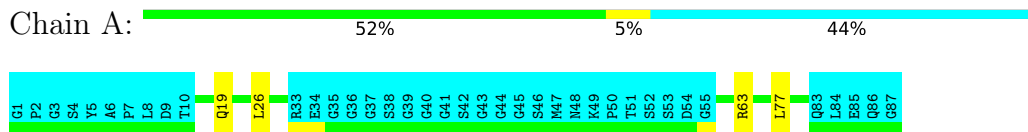


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

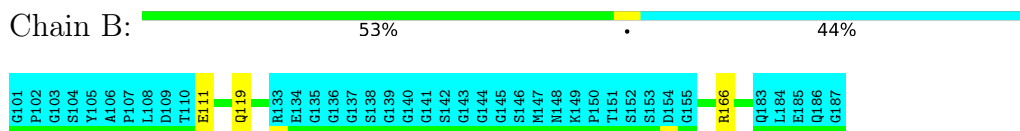


4.2.4 Score per residue for model 4

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

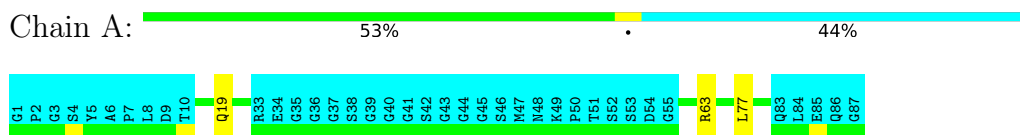


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

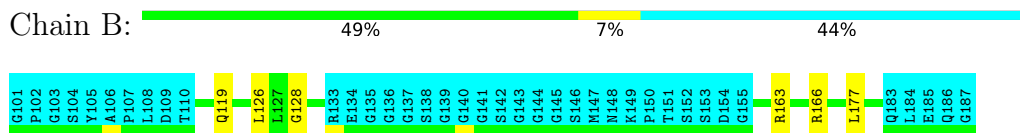


4.2.5 Score per residue for model 5

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

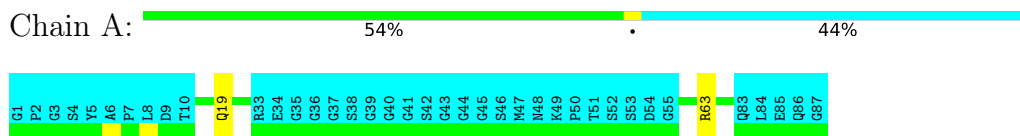


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

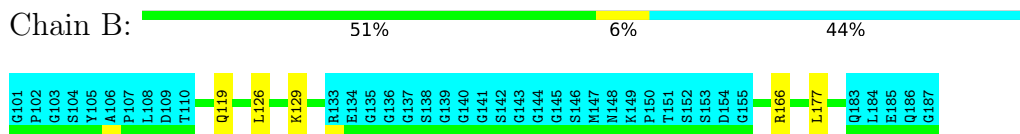


4.2.6 Score per residue for model 6

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

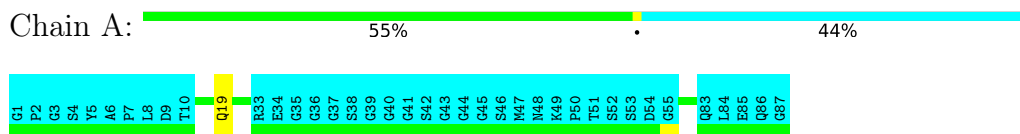


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

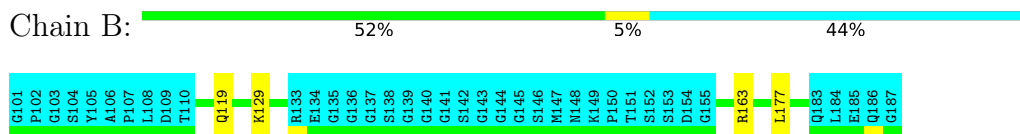


4.2.7 Score per residue for model 7

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

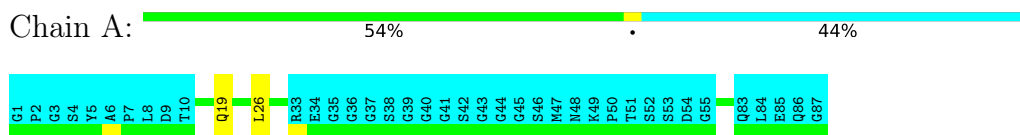


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

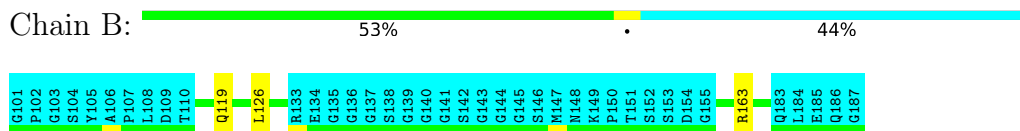


4.2.8 Score per residue for model 8

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

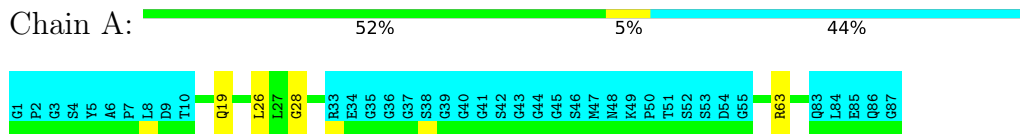


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

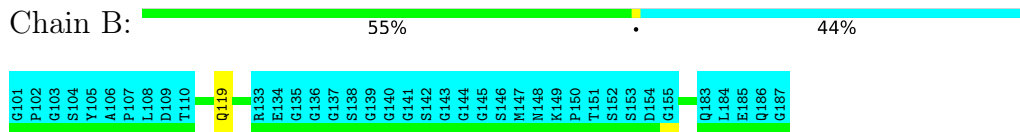


4.2.9 Score per residue for model 9

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

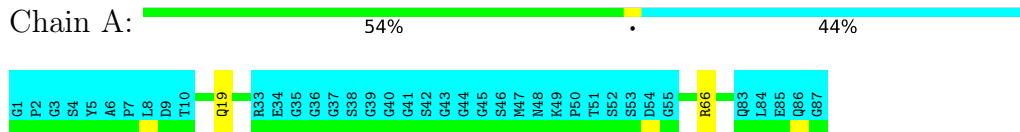


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

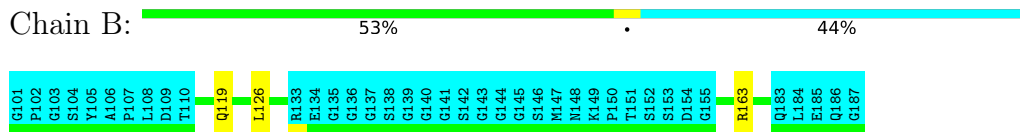


4.2.10 Score per residue for model 10

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

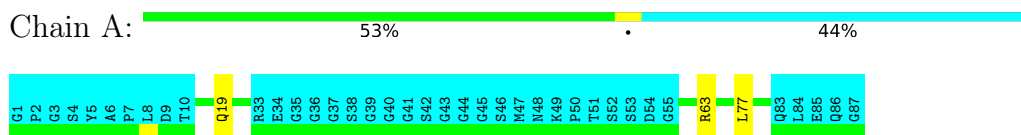


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

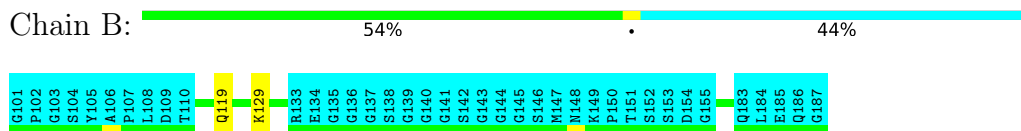


4.2.11 Score per residue for model 11

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

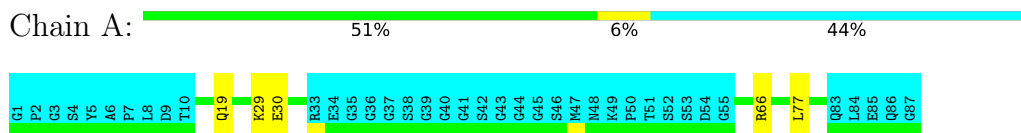


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

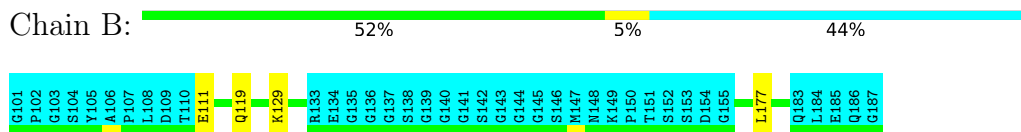


4.2.12 Score per residue for model 12

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

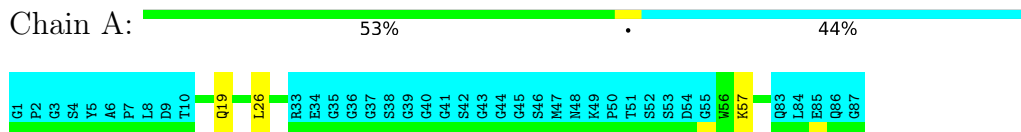


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

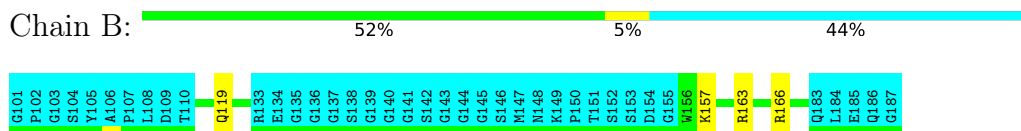


4.2.13 Score per residue for model 13

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

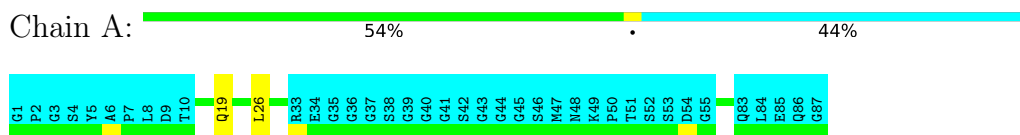


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

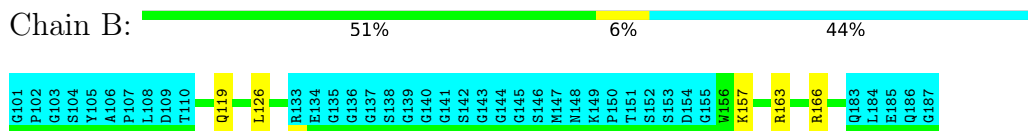


4.2.14 Score per residue for model 14

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

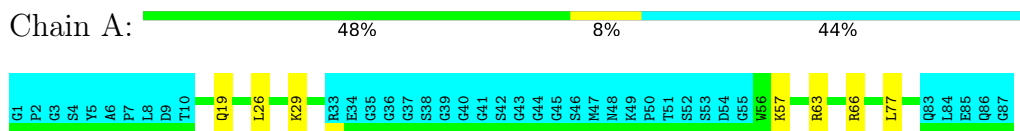


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

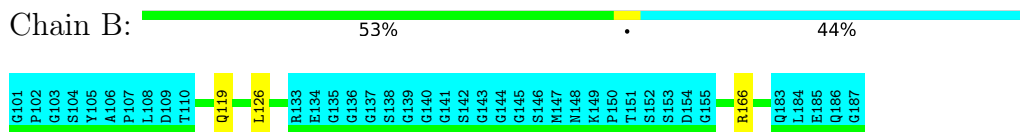


4.2.15 Score per residue for model 15

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

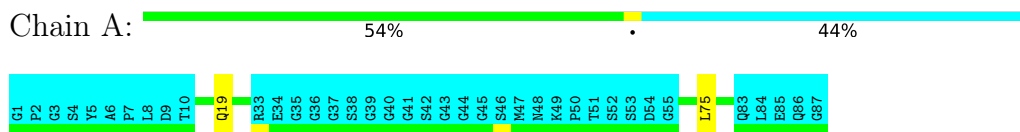


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

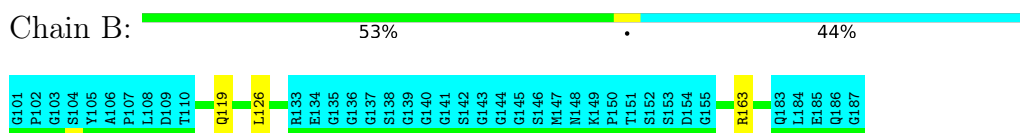


4.2.16 Score per residue for model 16

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

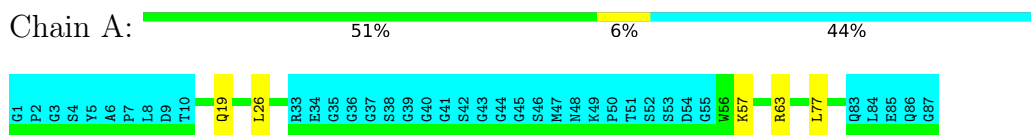


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

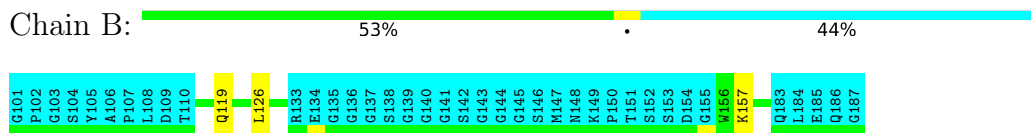


4.2.17 Score per residue for model 17

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

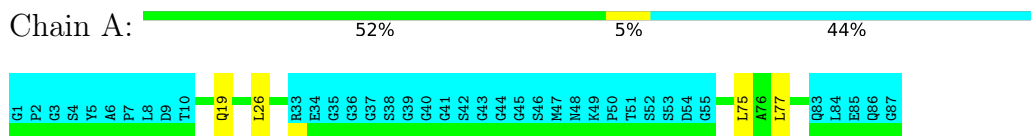


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

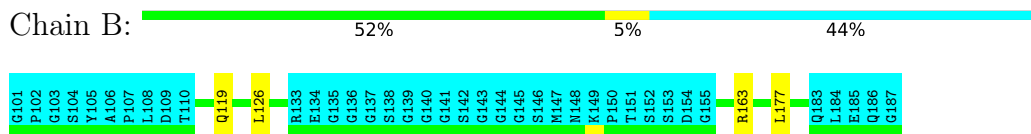


4.2.18 Score per residue for model 18

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

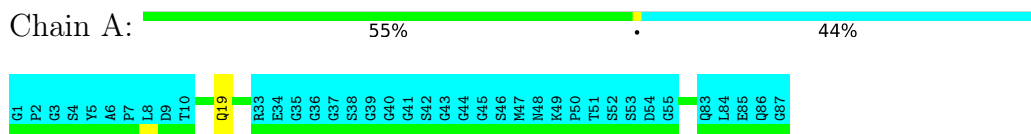


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

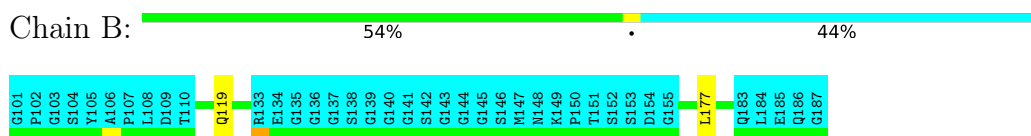


4.2.19 Score per residue for model 19

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

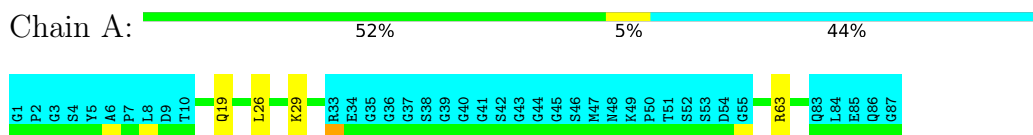


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

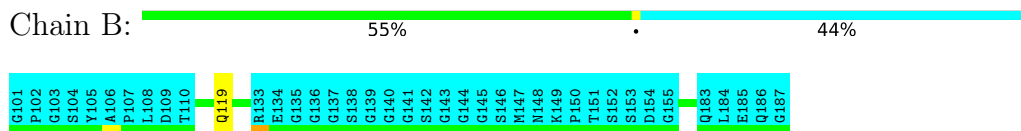


4.2.20 Score per residue for model 20

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

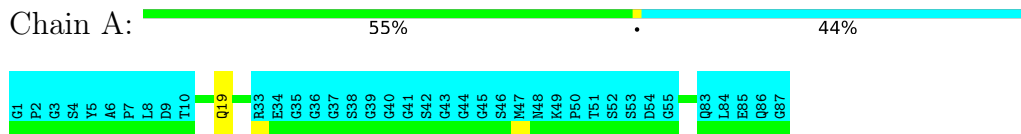


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

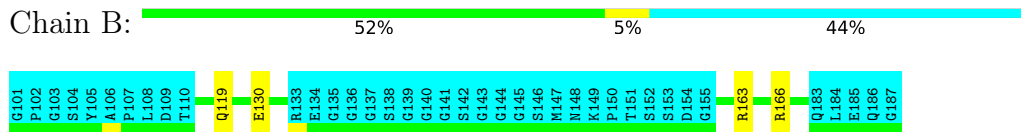


4.2.21 Score per residue for model 21

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

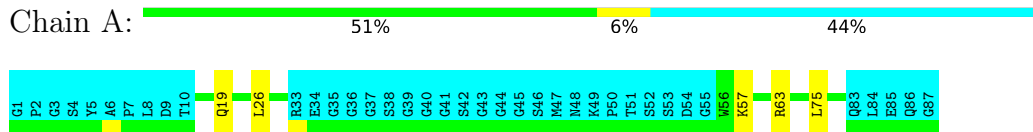


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

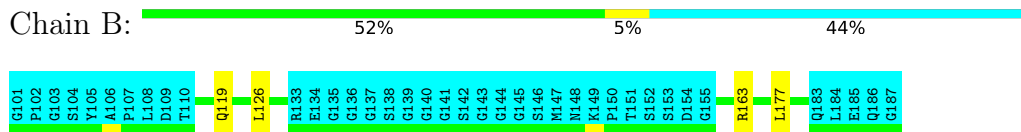


4.2.22 Score per residue for model 22

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

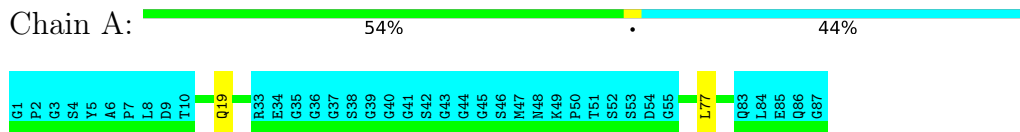


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

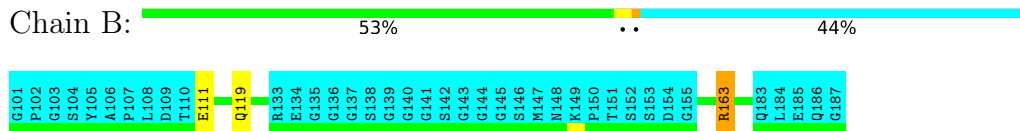


4.2.23 Score per residue for model 23

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

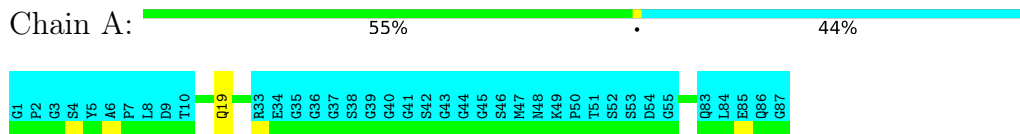


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

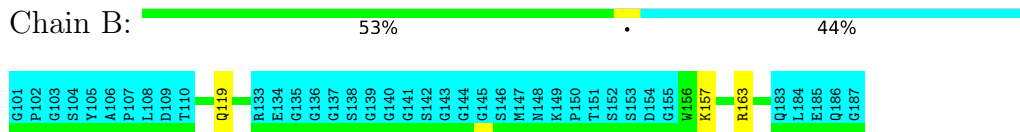


4.2.24 Score per residue for model 24

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

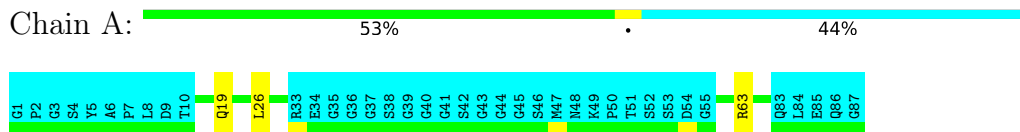


- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase

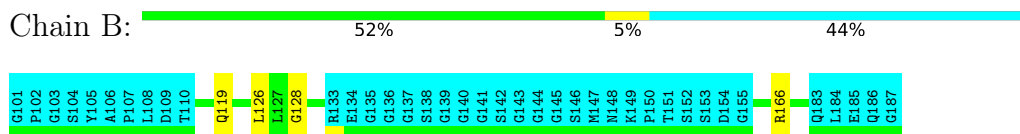


4.2.25 Score per residue for model 25

- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase



- Molecule 1: Beta-ketoacyl synthase,Beta-ketoacyl synthase



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 25 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
Amber	refinement	
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	1938
Number of shifts mapped to atoms	1938
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.68±0.01	0±0/400 (0.0± 0.0%)	0.97±0.03	1±1/536 (0.1± 0.1%)
1	B	0.68±0.01	0±0/400 (0.0± 0.0%)	0.97±0.04	1±1/536 (0.2± 0.1%)
All	All	0.68	0/20000 (0.0%)	0.97	43/26800 (0.2%)

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±0.3
All	All	0	2

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	63	ARG	NE-CZ-NH2	9.10	124.85	120.30	22	2
1	A	63	ARG	NE-CZ-NH1	8.36	124.48	120.30	4	10
1	B	163	ARG	NE-CZ-NH1	7.76	124.18	120.30	1	14
1	B	166	ARG	NE-CZ-NH2	7.75	124.18	120.30	3	2
1	B	166	ARG	NE-CZ-NH1	7.34	123.97	120.30	25	8
1	A	66	ARG	NE-CZ-NH2	6.46	123.53	120.30	1	1
1	B	163	ARG	NE-CZ-NH2	-6.39	117.10	120.30	10	2
1	A	66	ARG	NE-CZ-NH1	6.12	123.36	120.30	10	4

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	B	166	ARG	Sidechain	1
1	B	163	ARG	Sidechain	1

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
All	All	19800	20500	20500	-

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 -.

There are no clashes.

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	49/87 (56%)	49±0 (100±1%)	0±0 (0±1%)	0±0 (0±0%)	54 85
1	B	49/87 (56%)	49±1 (99±1%)	0±0 (0±1%)	0±0 (0±1%)	50 82
All	All	2450/4350 (56%)	2438 (100%)	8 (0%)	4 (0%)	50 82

All 3 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	128	GLY	2
1	A	28	GLY	1
1	B	129	LYS	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	43/67 (64%)	41±1 (95±3%)	2±1 (5±3%)	27 76
1	B	43/67 (64%)	41±1 (95±2%)	2±1 (5±2%)	26 75
All	All	2150/3350 (64%)	2036 (95%)	114 (5%)	26 75

All 15 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	19	GLN	25
1	B	119	GLN	25
1	B	126	LEU	13
1	A	26	LEU	12
1	B	177	LEU	8
1	A	77	LEU	8
1	A	57	LYS	4
1	B	157	LYS	4
1	B	111	GLU	3
1	B	129	LYS	3
1	A	29	LYS	3
1	A	75	LEU	3
1	B	175	LEU	1
1	A	30	GLU	1
1	B	130	GLU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [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 93% for the well-defined parts and 89% 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 [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	1938
Number of shifts mapped to atoms	1938
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
$^{13}\text{C}_\alpha$	152	-0.46 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	140	0.06 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}'$	152	-0.47 ± 0.05	None needed (< 0.5 ppm)
^{15}N	154	0.12 ± 0.12	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 93%, i.e. 1308 atoms were assigned a chemical shift out of a possible 1406. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	494/494 (100%)	200/200 (100%)	196/196 (100%)	98/98 (100%)
Sidechain	762/850 (90%)	518/550 (94%)	230/268 (86%)	14/32 (44%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	52/62 (84%)	30/30 (100%)	20/30 (67%)	2/2 (100%)
Overall	1308/1406 (93%)	748/780 (96%)	446/494 (90%)	114/132 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 1938 atoms were assigned a chemical shift out of a possible 2178. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	794/888 (89%)	336/372 (90%)	304/348 (87%)	154/168 (92%)
Sidechain	1080/1210 (89%)	732/780 (94%)	326/384 (85%)	22/46 (48%)
Aromatic	64/80 (80%)	38/38 (100%)	24/40 (60%)	2/2 (100%)
Overall	1938/2178 (89%)	1106/1190 (93%)	654/772 (85%)	178/216 (82%)

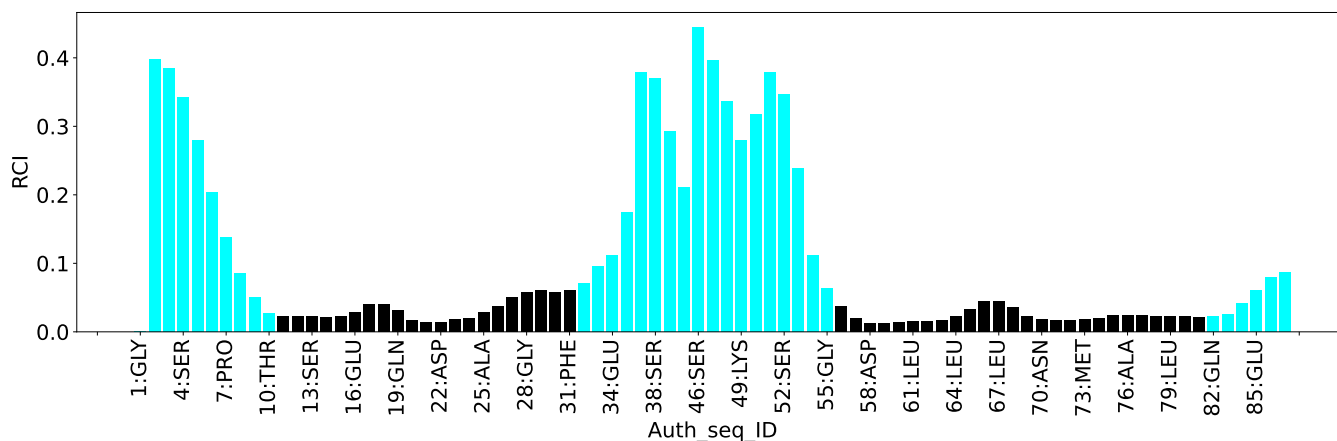
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

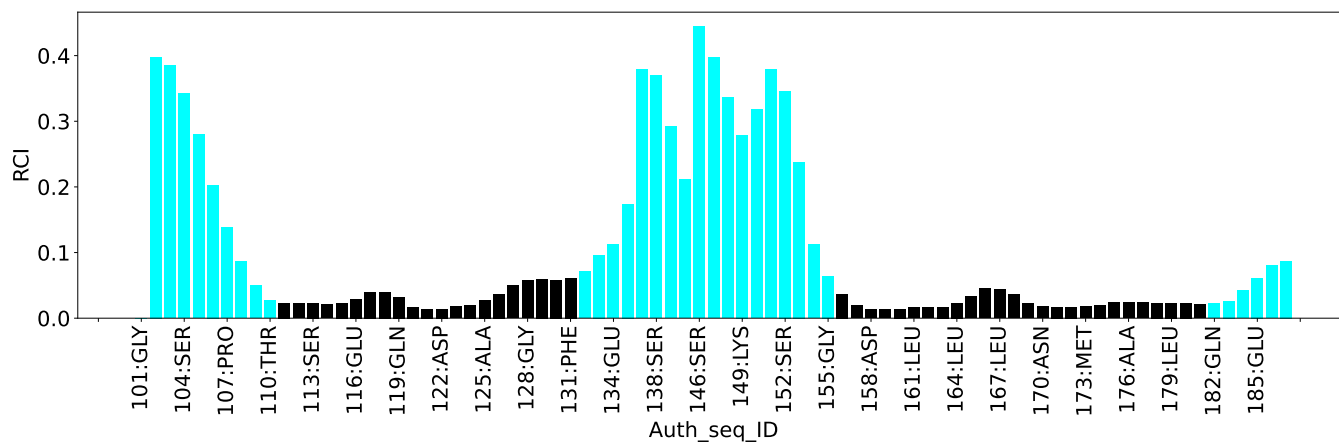
7.1.5 Random Coil Index (RCI) plots [i](#)

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:



Random coil index (RCI) for chain B:



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	2860
Intra-residue ($ i-j =0$)	751
Sequential ($ i-j =1$)	808
Medium range ($ i-j >1$ and $ i-j <5$)	709
Long range ($ i-j \geq 5$)	424
Inter-chain	168
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	16.4
Number of long range restraints per residue ¹	2.4

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)	0.7	0.2
0.2-0.5 (Medium)	None	None
>0.5 (Large)	None	None

8.2.2 Average number of dihedral-angle violations per model

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

9 Distance violation analysis [i](#)

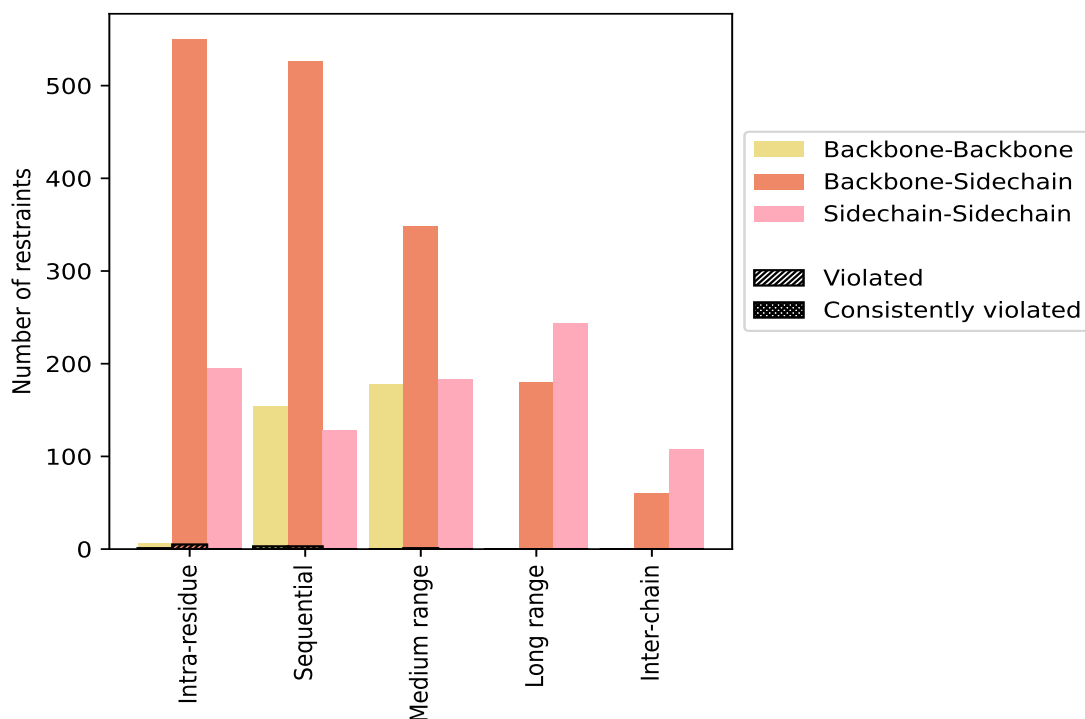
9.1 Summary of distance violations [i](#)

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	751	26.3	6	0.8	0.2	0	0.0	0.0
Backbone-Backbone	6	0.2	1	16.7	0.0	0	0.0	0.0
Backbone-Sidechain	550	19.2	5	0.9	0.2	0	0.0	0.0
Sidechain-Sidechain	195	6.8	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	808	28.3	6	0.7	0.2	0	0.0	0.0
Backbone-Backbone	154	5.4	3	1.9	0.1	0	0.0	0.0
Backbone-Sidechain	526	18.4	3	0.6	0.1	0	0.0	0.0
Sidechain-Sidechain	128	4.5	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	709	24.8	1	0.1	0.0	0	0.0	0.0
Backbone-Backbone	178	6.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	348	12.2	1	0.3	0.0	0	0.0	0.0
Sidechain-Sidechain	183	6.4	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	424	14.8	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	180	6.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	244	8.5	0	0.0	0.0	0	0.0	0.0
Inter-chain	168	5.9	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	60	2.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	108	3.8	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	2860	100.0	13	0.5	0.5	0	0.0	0.0
Backbone-Backbone	338	11.8	4	1.2	0.1	0	0.0	0.0
Backbone-Sidechain	1664	58.2	9	0.5	0.3	0	0.0	0.0
Sidechain-Sidechain	858	30.0	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 [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	0	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0	0	0	0.0	0.0	0.0	0.0
7	1	0	0	0	0	1	0.12	0.12	0.0	0.12
8	0	0	0	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0	0	0	0.0	0.0	0.0	0.0
10	1	0	0	0	0	1	0.12	0.12	0.0	0.12
11	0	0	1	0	0	1	0.12	0.12	0.0	0.12

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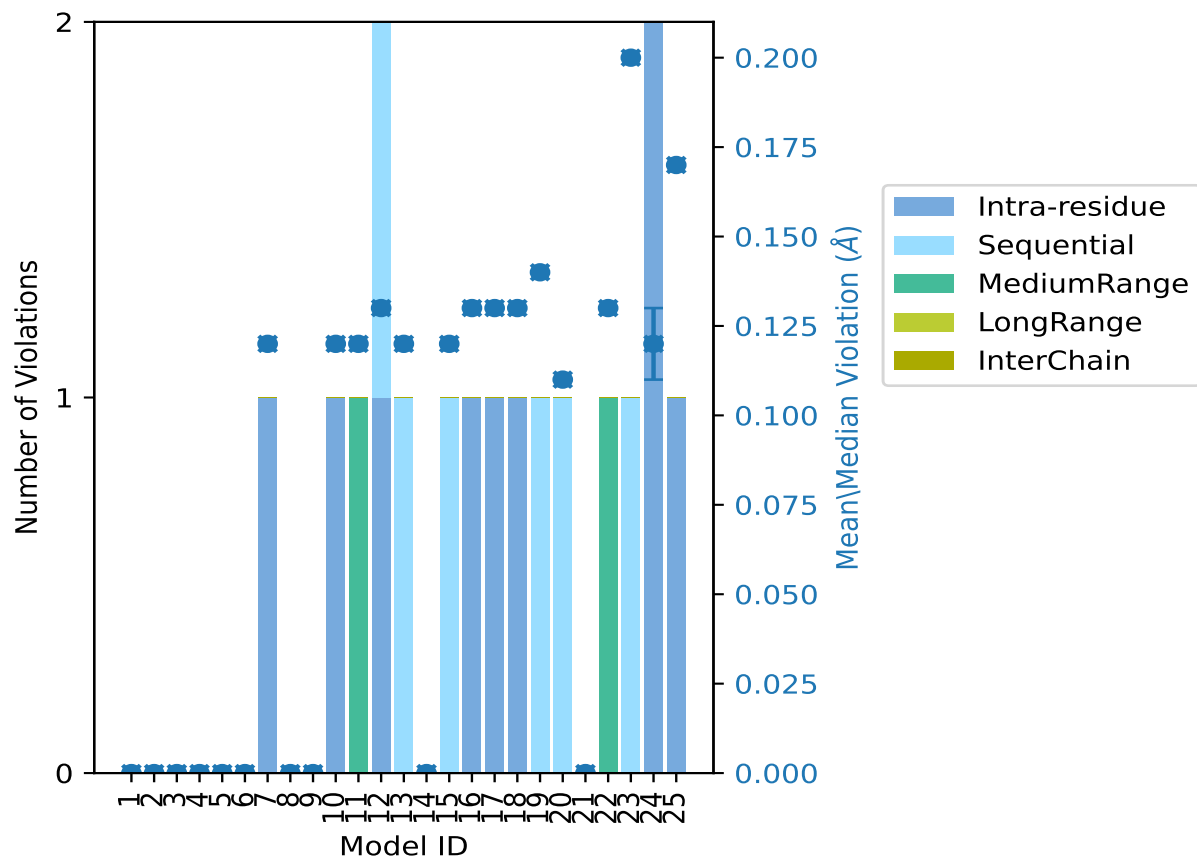
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
12	1	1	0	0	0	2	0.13	0.13	0.0	0.13
13	0	1	0	0	0	1	0.12	0.12	0.0	0.12
14	0	0	0	0	0	0	0.0	0.0	0.0	0.0
15	0	1	0	0	0	1	0.12	0.12	0.0	0.12
16	1	0	0	0	0	1	0.13	0.13	0.0	0.13
17	1	0	0	0	0	1	0.13	0.13	0.0	0.13
18	1	0	0	0	0	1	0.13	0.13	0.0	0.13
19	0	1	0	0	0	1	0.14	0.14	0.0	0.14
20	0	1	0	0	0	1	0.11	0.11	0.0	0.11
21	0	0	0	0	0	0	0.0	0.0	0.0	0.0
22	0	0	1	0	0	1	0.13	0.13	0.0	0.13
23	0	1	0	0	0	1	0.2	0.2	0.0	0.2
24	2	0	0	0	0	2	0.12	0.13	0.01	0.12
25	1	0	0	0	0	1	0.17	0.17	0.0	0.17

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, 2847(IR:745, SQ:802, MR:708, LR:424, IC:168) 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	%
4	6	0	0	0	10	1	4.0
1	0	1	0	0	2	2	8.0
1	0	0	0	0	1	3	12.0
0	0	0	0	0	0	4	16.0
0	0	0	0	0	0	5	20.0
0	0	0	0	0	0	6	24.0

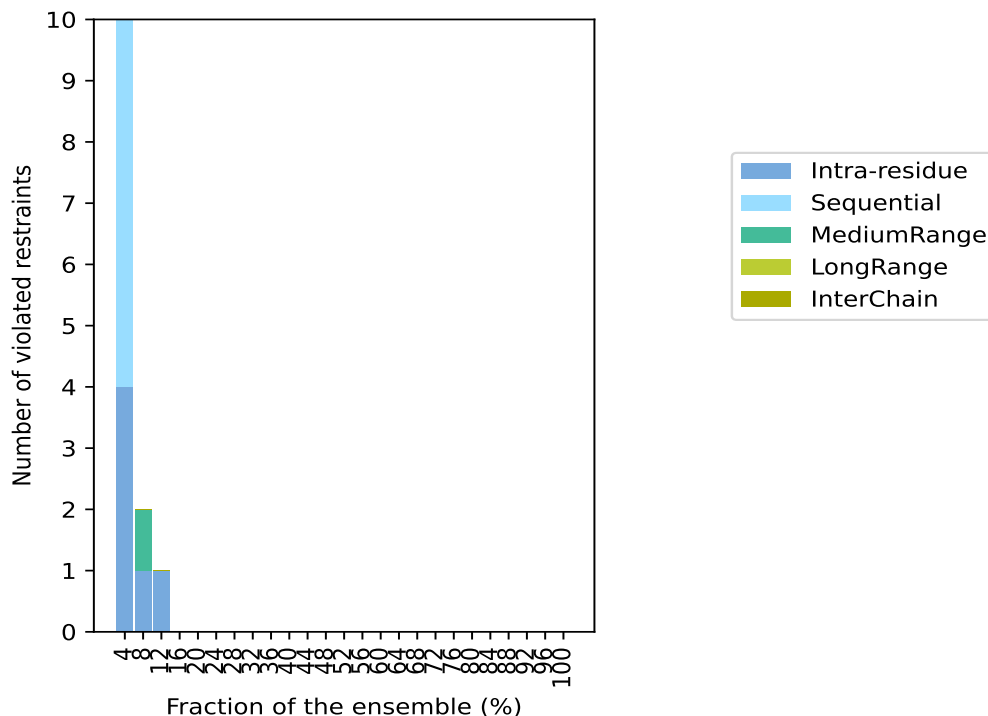
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	7	28.0
0	0	0	0	0	0	8	32.0
0	0	0	0	0	0	9	36.0
0	0	0	0	0	0	10	40.0
0	0	0	0	0	0	11	44.0
0	0	0	0	0	0	12	48.0
0	0	0	0	0	0	13	52.0
0	0	0	0	0	0	14	56.0
0	0	0	0	0	0	15	60.0
0	0	0	0	0	0	16	64.0
0	0	0	0	0	0	17	68.0
0	0	0	0	0	0	18	72.0
0	0	0	0	0	0	19	76.0
0	0	0	0	0	0	20	80.0
0	0	0	0	0	0	21	84.0
0	0	0	0	0	0	22	88.0
0	0	0	0	0	0	23	92.0
0	0	0	0	0	0	24	96.0
0	0	0	0	0	0	25	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶ Number of models with violations

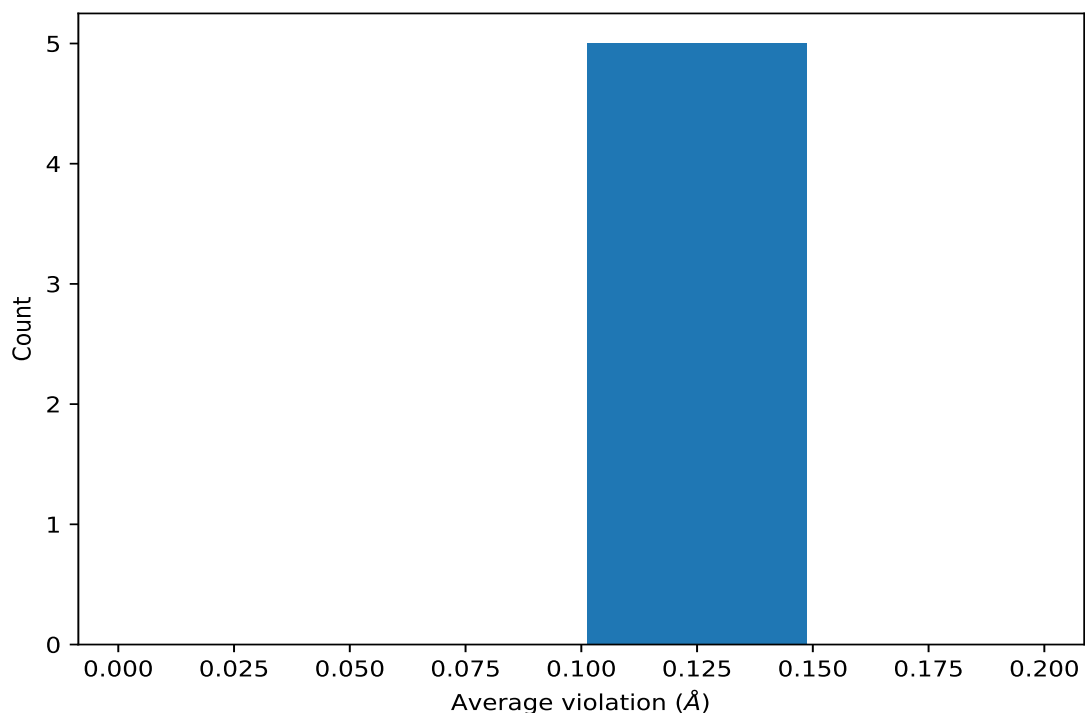
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 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. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

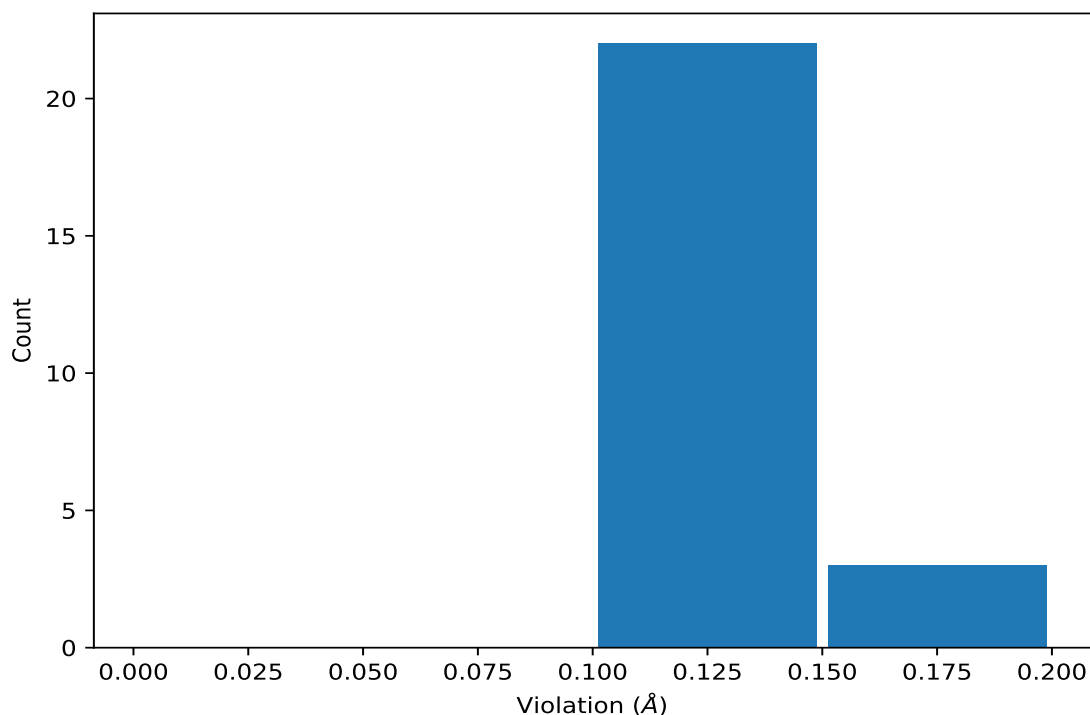
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2693)	1:B:186:GLN:H	1:B:186:GLN:HB2	3	0.12	0.0	0.12
(1,2693)	1:B:186:GLN:H	1:B:186:GLN:HB3	3	0.12	0.0	0.12
(1,211)	1:A:19:GLN:HA	1:A:19:GLN:HE21	2	0.13	0.0	0.13
(2,23)	1:A:29:LYS:HD2	1:A:31:PHE:H	2	0.12	0.01	0.12
(2,23)	1:A:29:LYS:HD3	1:A:31:PHE:H	2	0.12	0.01	0.12

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 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. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1131)	1:A:54:ASP:HB3	1:A:55:GLY:H	23	0.2
(1,2303)	1:A:5:TYR:HA	1:A:5:TYR:HD1	25	0.17
(1,2303)	1:A:5:TYR:HA	1:A:5:TYR:HD2	25	0.17
(1,1132)	1:B:154:ASP:HB3	1:B:155:GLY:H	19	0.14
(2,23)	1:A:29:LYS:HD2	1:A:31:PHE:H	22	0.13
(2,23)	1:A:29:LYS:HD3	1:A:31:PHE:H	22	0.13
(1,46)	1:B:106:ALA:H	1:B:106:ALA:HA	17	0.13
(1,2693)	1:B:186:GLN:H	1:B:186:GLN:HB2	18	0.13
(1,2693)	1:B:186:GLN:H	1:B:186:GLN:HB3	18	0.13
(1,212)	1:B:119:GLN:HA	1:B:119:GLN:HE21	16	0.13
(1,211)	1:A:19:GLN:HA	1:A:19:GLN:HE21	12	0.13
(1,211)	1:A:19:GLN:HA	1:A:19:GLN:HE21	24	0.13
(1,1092)	1:B:186:GLN:HA	1:B:187:GLY:H	12	0.13
(2,23)	1:A:29:LYS:HD2	1:A:31:PHE:H	11	0.12
(2,23)	1:A:29:LYS:HD3	1:A:31:PHE:H	11	0.12
(1,506)	1:A:48:ASN:HA	1:A:49:LYS:H	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,480)	1:A:34:GLU:H	1:A:34:GLU:HG2	10	0.12
(1,480)	1:A:34:GLU:H	1:A:34:GLU:HG3	10	0.12
(1,35)	1:A:4:SER:HA	1:A:5:TYR:H	13	0.12
(1,2693)	1:B:186:GLN:H	1:B:186:GLN:HB2	7	0.12
(1,2693)	1:B:186:GLN:H	1:B:186:GLN:HB3	7	0.12
(1,2693)	1:B:186:GLN:H	1:B:186:GLN:HB2	24	0.12
(1,2693)	1:B:186:GLN:H	1:B:186:GLN:HB3	24	0.12
(1,2591)	1:B:134:GLU:HB2	1:B:135:GLY:H	20	0.11
(1,2591)	1:B:134:GLU:HB3	1:B:135:GLY:H	20	0.11

10 Dihedral-angle violation analysis

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value