Full wwPDB NMR Structure Validation Report (i)

Dec 25, 2024 – 07:54 PM EST

PDB ID	:	8RAJ
BMRB ID	:	34886
Title	:	NMR structure of PKS docking domains
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Deposited on	:	2023-12-01

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:

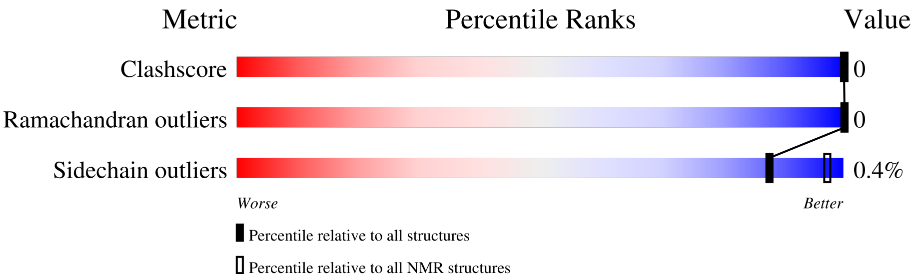
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 97%.

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	62	39% • 58%
2	B	49	20% 80%

2 Ensemble composition and analysis

This entry contains 20 models. Model 14 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:2253-A:2278, B:20-B:29 (36)	0.26	14

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1602 atoms, of which 786 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	62	935	287	470	81	95	2	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2217	GLY	-	expression tag	UNP C5B3B7
A	2218	PRO	-	expression tag	UNP C5B3B7
A	2219	GLY	-	expression tag	UNP C5B3B7
A	2220	SER	-	expression tag	UNP C5B3B7
A	2221	PRO	-	expression tag	UNP C5B3B7
A	2222	ASN	-	expression tag	UNP C5B3B7
A	2223	SER	-	expression tag	UNP C5B3B7
A	2224	TYR	-	expression tag	UNP C5B3B7

- Molecule 2 is a protein called Trimethylamine monooxygenase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	49	667	208	316	60	81	2	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	expression tag	UNP C5B3B9
B	-4	PRO	-	expression tag	UNP C5B3B9
B	-3	GLY	-	expression tag	UNP C5B3B9
B	-2	SER	-	expression tag	UNP C5B3B9
B	-1	TYR	-	expression tag	UNP C5B3B9

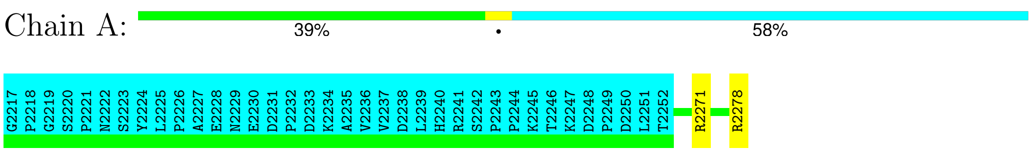
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

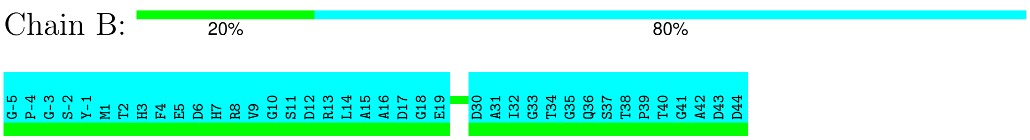
- Molecule 1: Beta-ketoacyl synthase

Chain A:



- Molecule 2: Trimethylamine monooxygenase

Chain B:



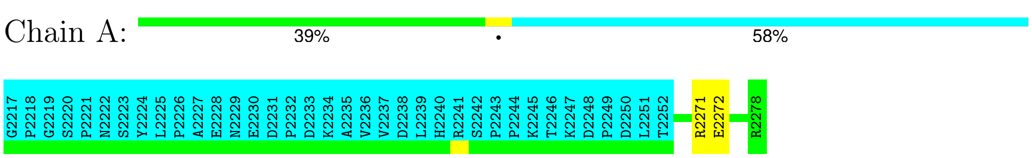
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

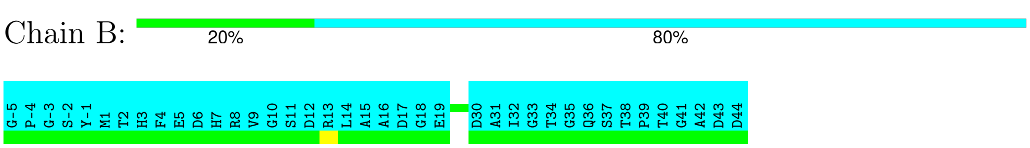
- Molecule 1: Beta-ketoacyl synthase

Chain A:



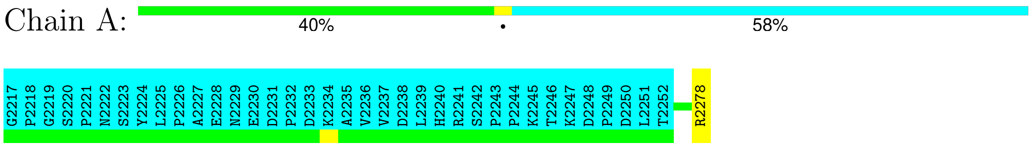
- Molecule 2: Trimethylamine monooxygenase

Chain B:

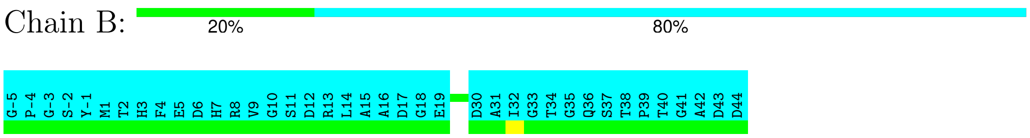


4.2.2 Score per residue for model 2

• Molecule 1: Beta-ketoacyl synthase

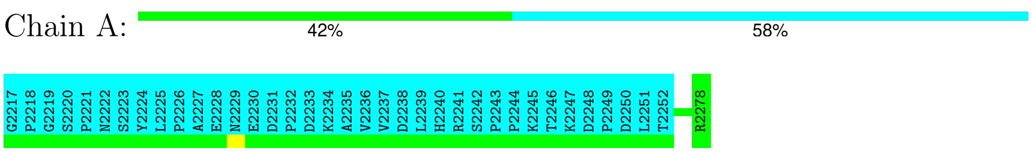


• Molecule 2: Trimethylamine monooxygenase

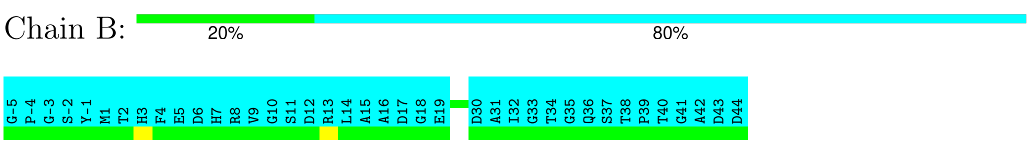


4.2.3 Score per residue for model 3

• Molecule 1: Beta-ketoacyl synthase

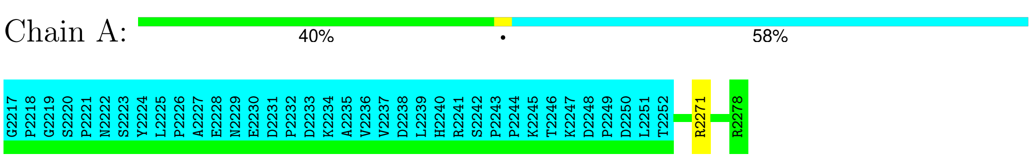


• Molecule 2: Trimethylamine monooxygenase

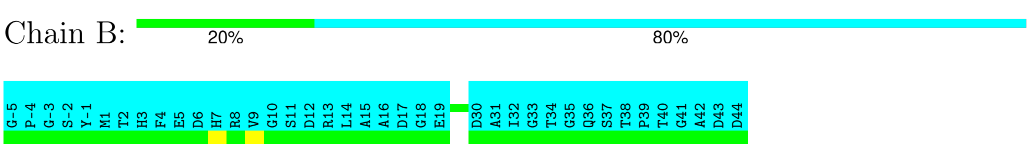


4.2.4 Score per residue for model 4

• Molecule 1: Beta-ketoacyl synthase

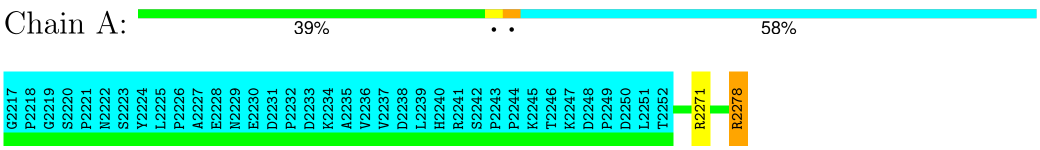


• Molecule 2: Trimethylamine monooxygenase

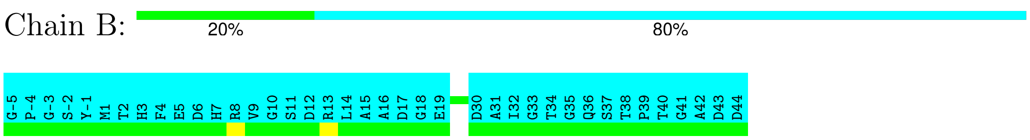


4.2.5 Score per residue for model 5

- Molecule 1: Beta-ketoacyl synthase

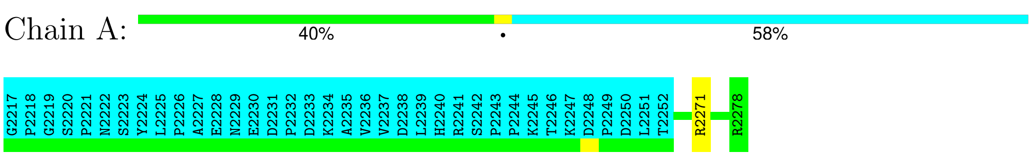


- Molecule 2: Trimethylamine monooxygenase

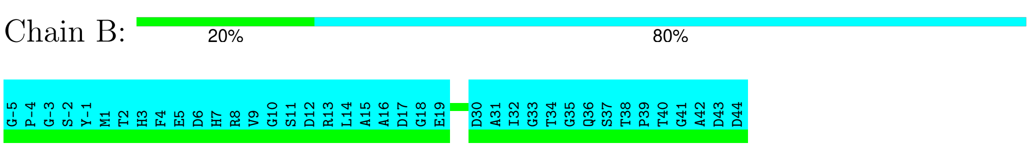


4.2.6 Score per residue for model 6

- Molecule 1: Beta-ketoacyl synthase

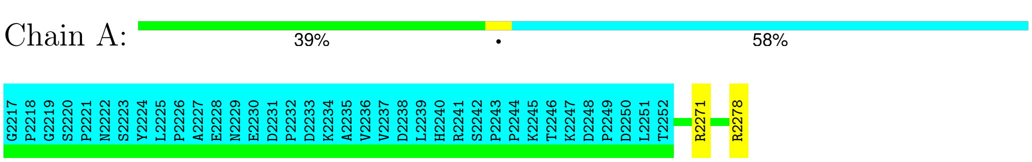


- Molecule 2: Trimethylamine monooxygenase

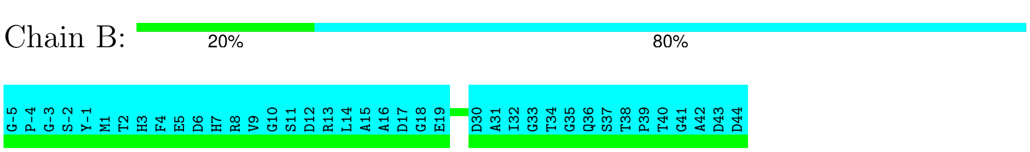


4.2.7 Score per residue for model 7

- Molecule 1: Beta-ketoacyl synthase



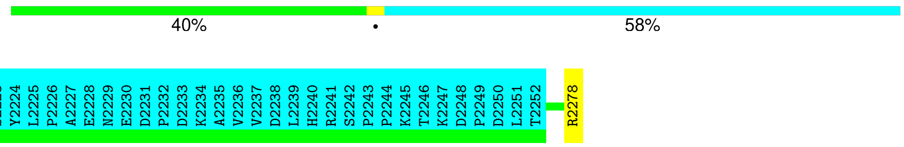
- Molecule 2: Trimethylamine monooxygenase



4.2.8 Score per residue for model 8

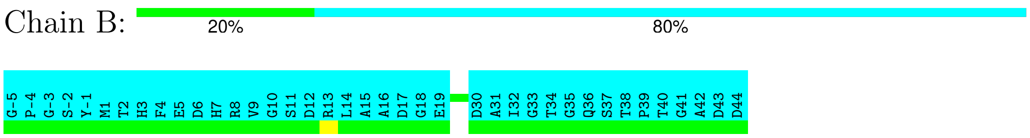
- Molecule 1: Beta-ketoacyl synthase

Chain A:



- Molecule 2: Trimethylamine monooxygenase

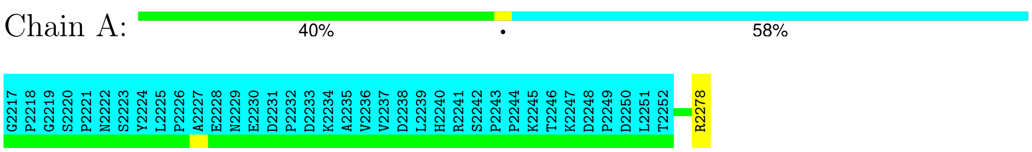
Chain B:



4.2.9 Score per residue for model 9

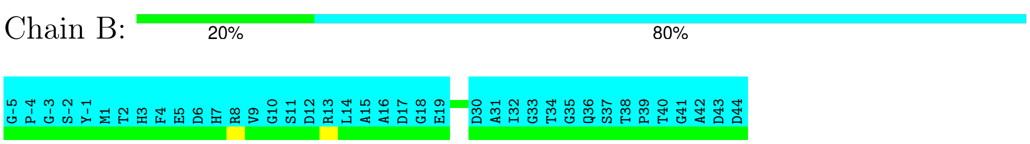
- Molecule 1: Beta-ketoacyl synthase

Chain A:



- Molecule 2: Trimethylamine monooxygenase

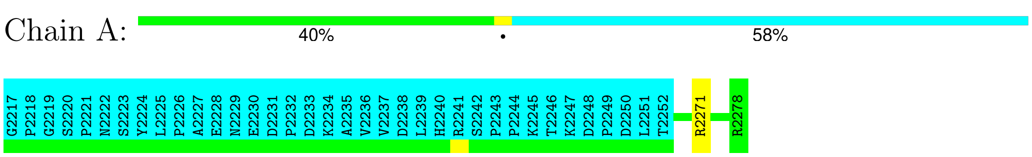
Chain B:



4.2.10 Score per residue for model 10

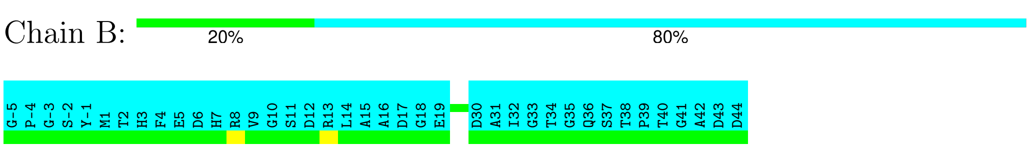
- Molecule 1: Beta-ketoacyl synthase

Chain A:



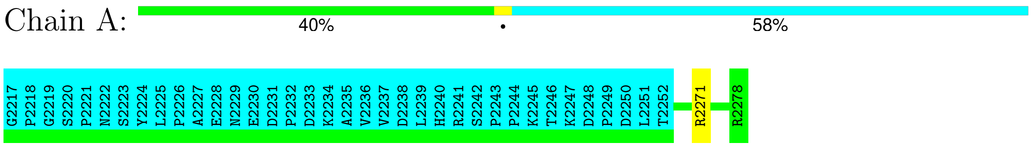
- Molecule 2: Trimethylamine monooxygenase

Chain B:

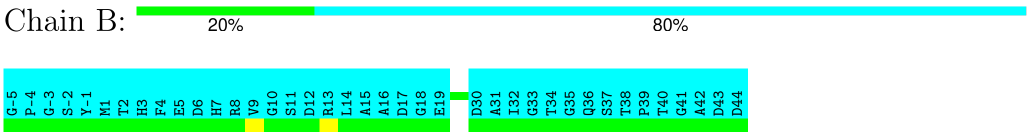


4.2.11 Score per residue for model 11

• Molecule 1: Beta-ketoacyl synthase

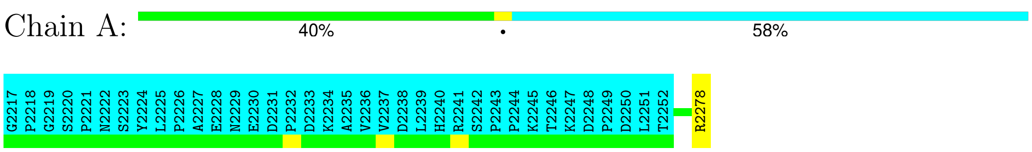


• Molecule 2: Trimethylamine monooxygenase

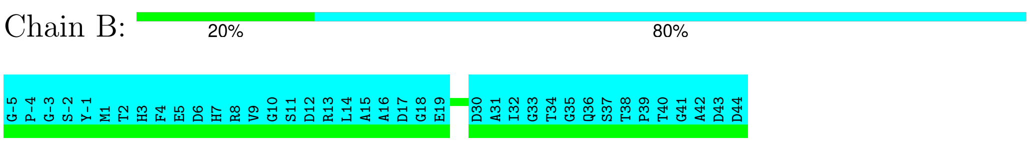


4.2.12 Score per residue for model 12

• Molecule 1: Beta-ketoacyl synthase

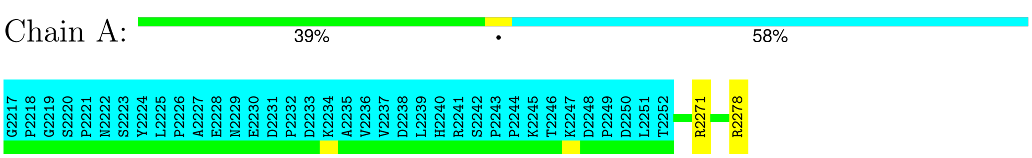


• Molecule 2: Trimethylamine monooxygenase

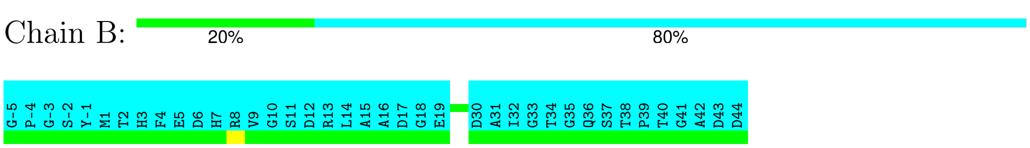


4.2.13 Score per residue for model 13

• Molecule 1: Beta-ketoacyl synthase

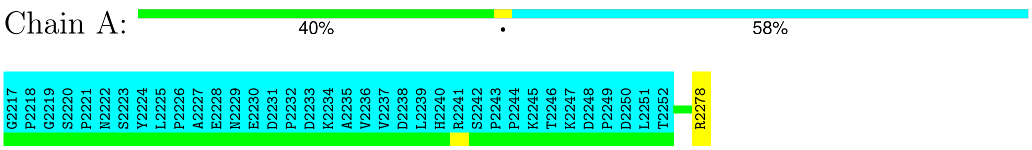


• Molecule 2: Trimethylamine monooxygenase

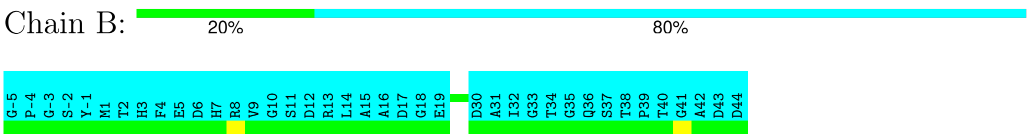


4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Beta-ketoacyl synthase

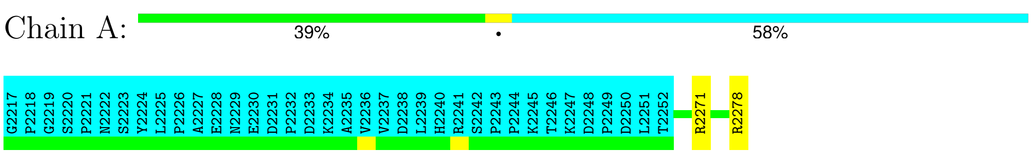


- Molecule 2: Trimethylamine monooxygenase

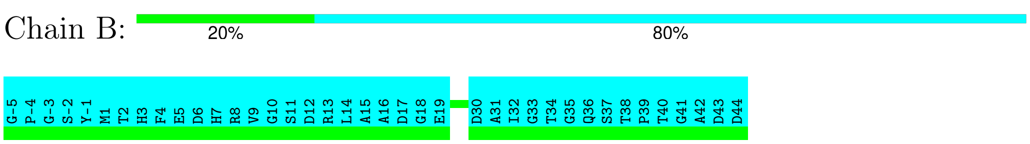


4.2.15 Score per residue for model 15

- Molecule 1: Beta-ketoacyl synthase

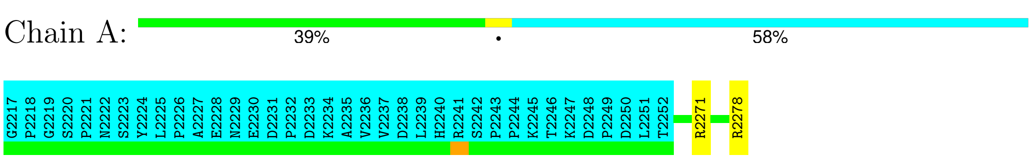


- Molecule 2: Trimethylamine monooxygenase

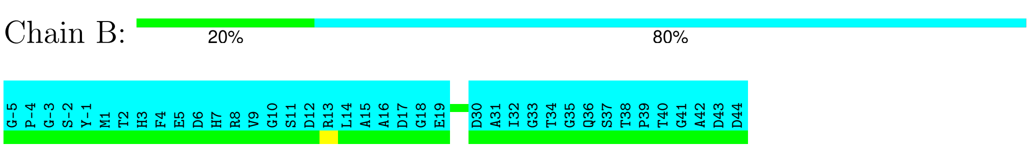


4.2.16 Score per residue for model 16

- Molecule 1: Beta-ketoacyl synthase



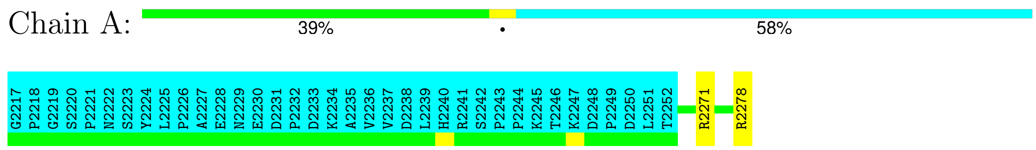
- Molecule 2: Trimethylamine monooxygenase



4.2.17 Score per residue for model 17

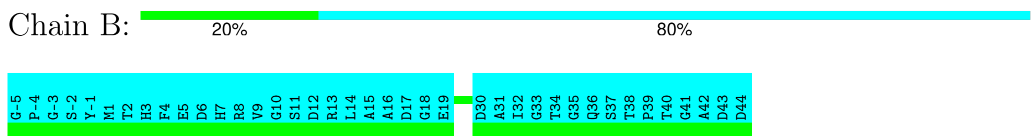
• Molecule 1: Beta-ketoacyl synthase

Chain A:



• Molecule 2: Trimethylamine monooxygenase

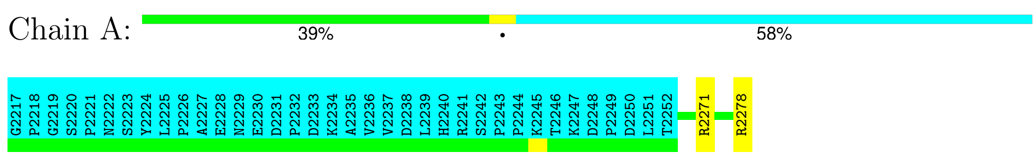
Chain B:



4.2.18 Score per residue for model 18

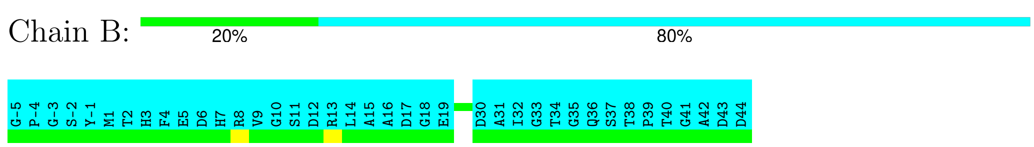
• Molecule 1: Beta-ketoacyl synthase

Chain A:



• Molecule 2: Trimethylamine monooxygenase

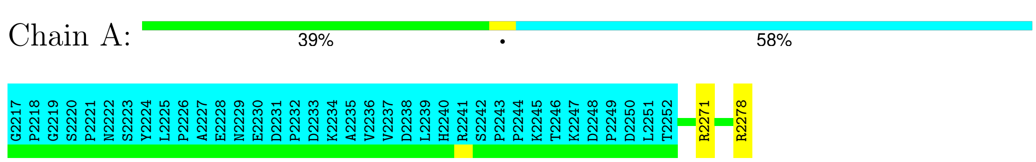
Chain B:



4.2.19 Score per residue for model 19

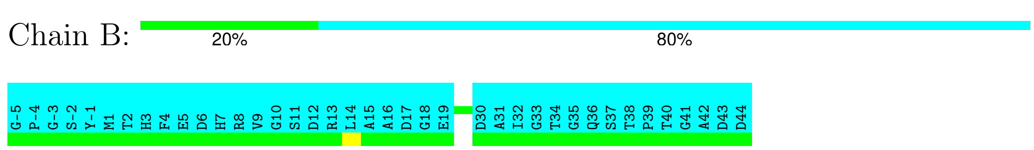
• Molecule 1: Beta-ketoacyl synthase

Chain A:



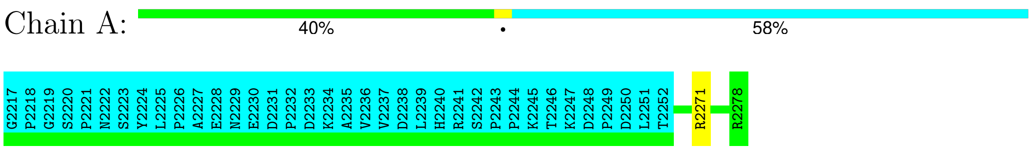
• Molecule 2: Trimethylamine monooxygenase

Chain B:

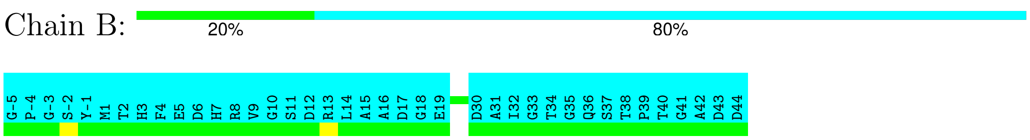


4.2.20 Score per residue for model 20

• Molecule 1: Beta-ketoacyl synthase



• Molecule 2: Trimethylamine monooxygenase



5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 20 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	1290
Number of shifts mapped to atoms	1290
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	97%

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	0.65±0.01	0±0/194 (0.0± 0.0%)	0.99±0.04	1±1/256 (0.5± 0.2%)
2	B	0.55±0.02	0±0/71 (0.0± 0.0%)	0.72±0.05	0±0/96 (0.0± 0.0%)
All	All	0.62	0/5300 (0.0%)	0.93	28/7040 (0.4%)

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	2271	ARG	NE-CZ-NH1	7.53	124.07	120.30	5	11
1	A	2278	ARG	NE-CZ-NH1	6.88	123.74	120.30	9	10
1	A	2278	ARG	NE-CZ-NH2	6.42	123.51	120.30	16	4
1	A	2271	ARG	NE-CZ-NH2	6.05	123.33	120.30	16	3

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
All	All	5300	5640	5640	-

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	25/62 (40%)	25±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
2	B	10/49 (20%)	10±0 (99±2%)	0±0 (0±2%)	0±0 (0±0%)	100	100
All	All	700/2220 (32%)	699 (100%)	1 (0%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	20/52 (38%)	20±0 (99±1%)	0±0 (0±2%)	85	97
2	B	8/36 (22%)	8±0 (100±0%)	0±0 (0±0%)	100	100
All	All	560/1760 (32%)	558 (100%)	2 (0%)	88	97

All 2 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	2272	GLU	1
1	A	2278	ARG	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 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 97% for the well-defined parts and 94% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

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	1290
Number of shifts mapped to atoms	1290
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 ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	111	-0.14 ± 0.22	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	100	0.06 ± 0.05	None needed (< 0.5 ppm)
$^{13}C'$	106	-0.19 ± 0.08	None needed (< 0.5 ppm)
^{15}N	99	-0.41 ± 0.19	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 97%, i.e. 465 atoms were assigned a chemical shift out of a possible 479. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	180/180 (100%)	73/73 (100%)	72/72 (100%)	35/35 (100%)
Sidechain	285/299 (95%)	196/198 (99%)	86/92 (93%)	3/9 (33%)

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	Total	^{1}H	^{13}C	^{15}N
Overall	465/479 (97%)	269/271 (99%)	158/164 (96%)	38/44 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 94%, i.e. 1290 atoms were assigned a chemical shift out of a possible 1368. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	537/546 (98%)	221/223 (99%)	217/222 (98%)	99/101 (98%)
Sidechain	715/770 (93%)	486/500 (97%)	220/246 (89%)	9/24 (38%)
Aromatic	38/52 (73%)	19/25 (76%)	13/21 (62%)	6/6 (100%)
Overall	1290/1368 (94%)	726/748 (97%)	450/489 (92%)	114/131 (87%)

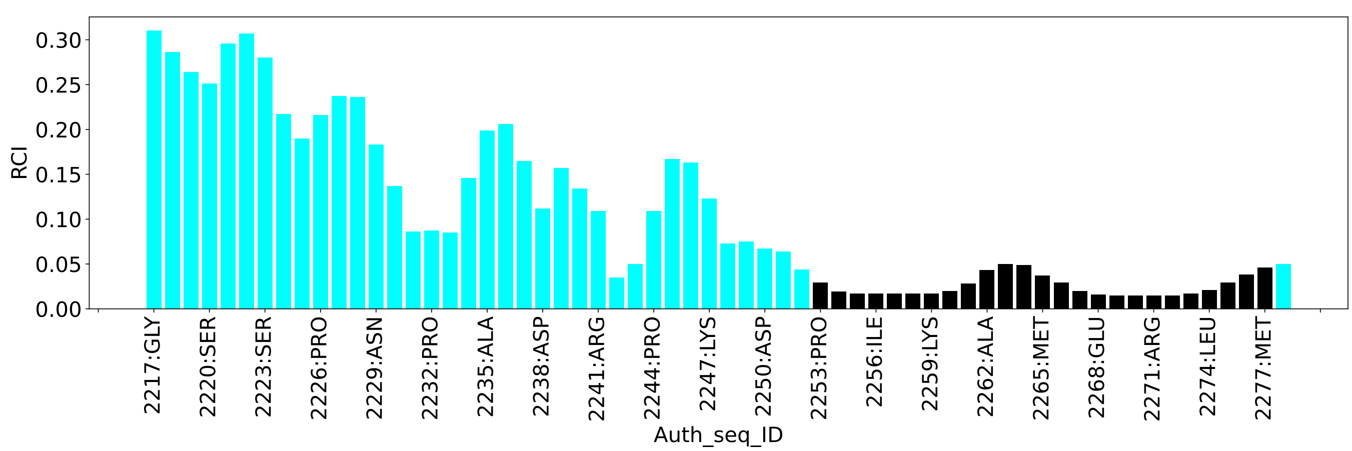
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

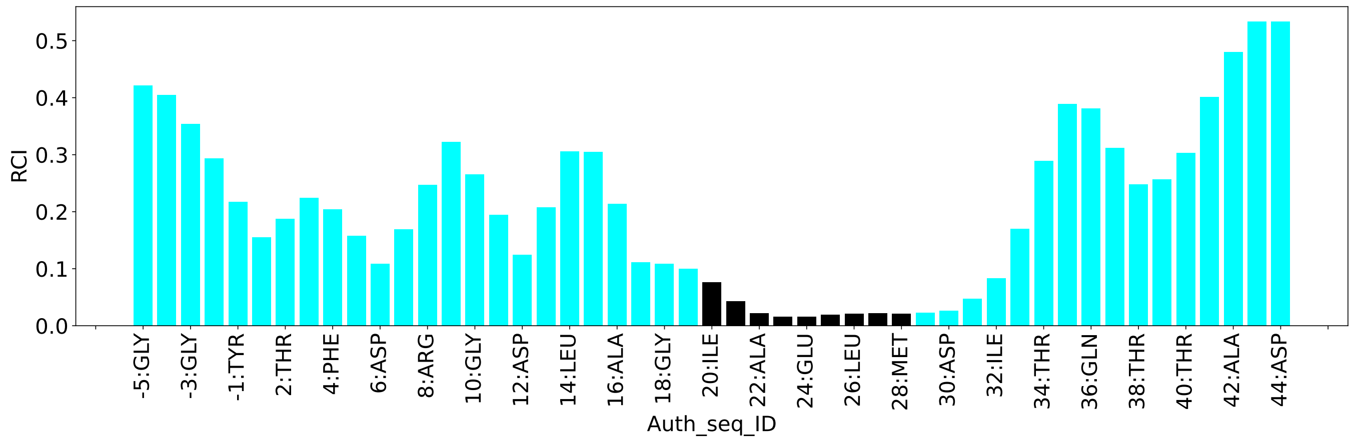
7.1.5 Random Coil Index (RCI) plots (i)

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:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
-5:GLY
-3:GLY
-1:TYR
2:THR
4:PHE
6:ASP
8:ARG
10:GLY
12:ASP
14:LEU
16:ALA
18:GLY
20:ILE
22:ALA
24:GLU
26:LEU
28:MET
30:ASP
32:ILE
34:THR
36:GLN
38:THR
40:THR
42:ALA
44:ASP
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	1257
Intra-residue (|i-j|=0)	347
Sequential (|i-j|=1)	392
Medium range (|i-j|>1 and |i-j|<5)	241
Long range (|i-j|≥5)	114
Inter-chain	163
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	68
Number of unmapped restraints	0
Number of restraints per residue	11.9
Number of long range restraints per residue[1]	1.0

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

8.2 Residual restraint violations (i)

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 (i)

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)	0.1	0.13
0.2-0.5 (Medium)	None	None
>0.5 (Large)	None	None

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	0.1	1.3
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

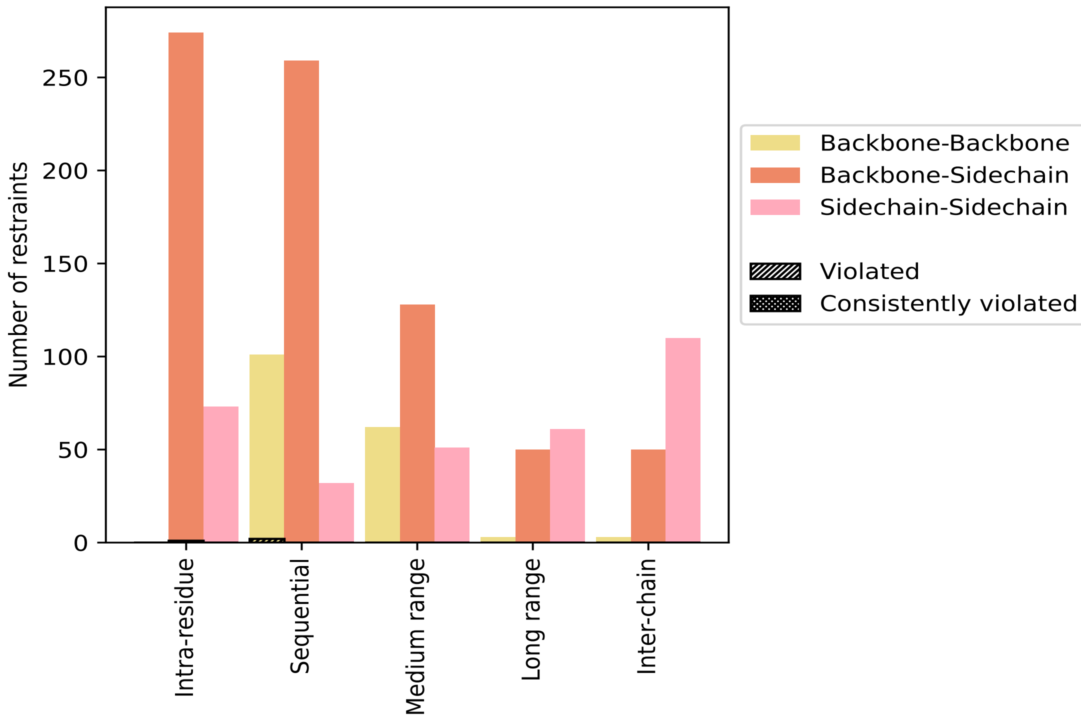
9.1 Summary of distance violations (i)

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)	347	27.6	1	0.3	0.1	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	274	21.8	1	0.4	0.1	0	0.0	0.0
Sidechain-Sidechain	73	5.8	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	392	31.2	2	0.5	0.2	0	0.0	0.0
Backbone-Backbone	101	8.0	2	2.0	0.2	0	0.0	0.0
Backbone-Sidechain	259	20.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	32	2.5	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	241	19.2	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	62	4.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	128	10.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	51	4.1	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	114	9.1	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	3	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	50	4.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	61	4.9	0	0.0	0.0	0	0.0	0.0
Inter-chain	163	13.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	3	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	50	4.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	110	8.8	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	1257	100.0	3	0.2	0.2	0	0.0	0.0
Backbone-Backbone	169	13.4	2	1.2	0.2	0	0.0	0.0
Backbone-Sidechain	761	60.5	1	0.1	0.1	0	0.0	0.0
Sidechain-Sidechain	327	26.0	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 disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	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	0	0	0	0	0	0	0.0	0.0	0.0	0.0
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	0	0	0	0	0	0	0.0	0.0	0.0	0.0

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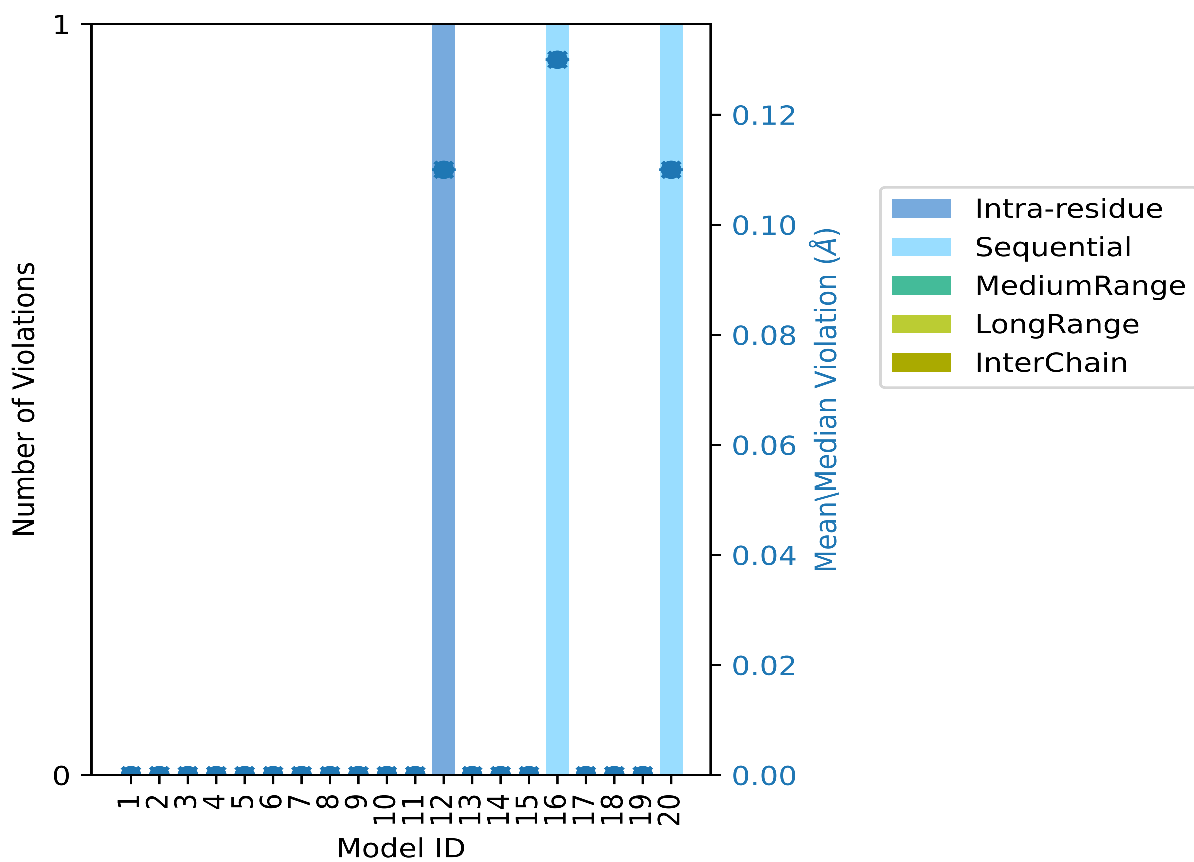
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	0	0	0	0	0	0	0.0	0.0	0.0	0.0
12	1	0	0	0	0	1	0.11	0.11	0.0	0.11
13	0	0	0	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0	0	0	0.0	0.0	0.0	0.0
16	0	1	0	0	0	1	0.13	0.13	0.0	0.13
17	0	0	0	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0	0	0	0.0	0.0	0.0	0.0
20	0	1	0	0	0	1	0.11	0.11	0.0	0.11

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard 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

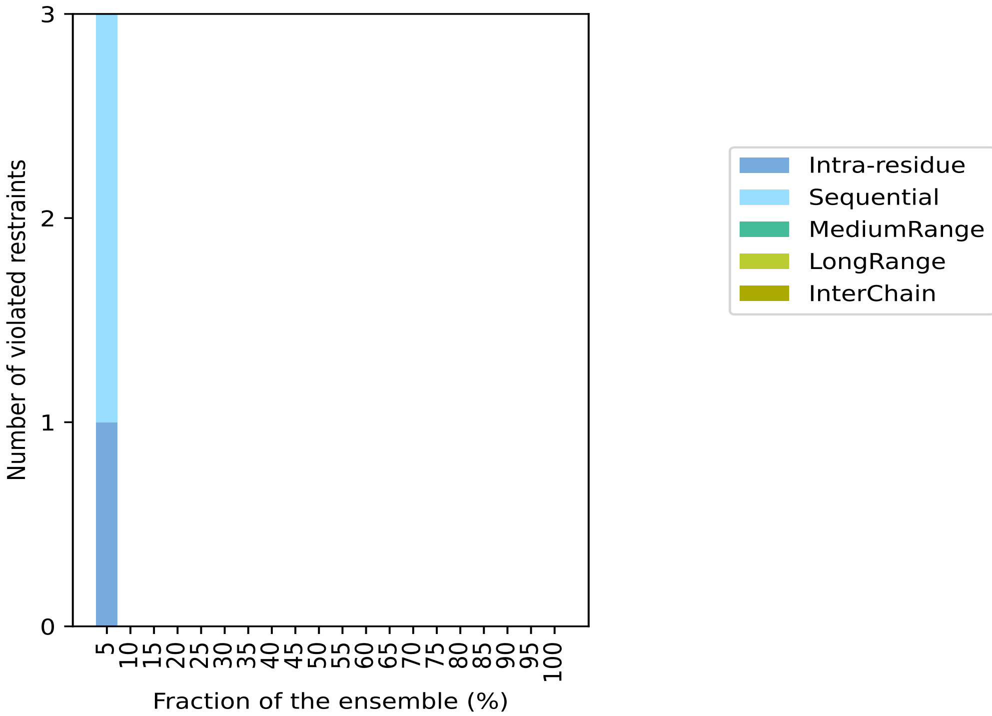
9.3 Distance violation statistics for the ensemble (i)

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, 1254(IR:346, SQ:390, MR:241, LR:114, IC:163) 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]	%
1	2	0	0	0	3	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-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)

No violations found

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.
Data insufficient to plot histogram

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)
(3,62)	1:2234:A:LYS:HA	1:2235:A:ALA:H	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,70)	1:2236:A:VAL:H	1:2236:A:VAL:HB	12	0.11
(1,69)	2:14:B:LEU:HA	2:15:B:ALA:H	20	0.11

10 Dihedral-angle violation analysis (i)

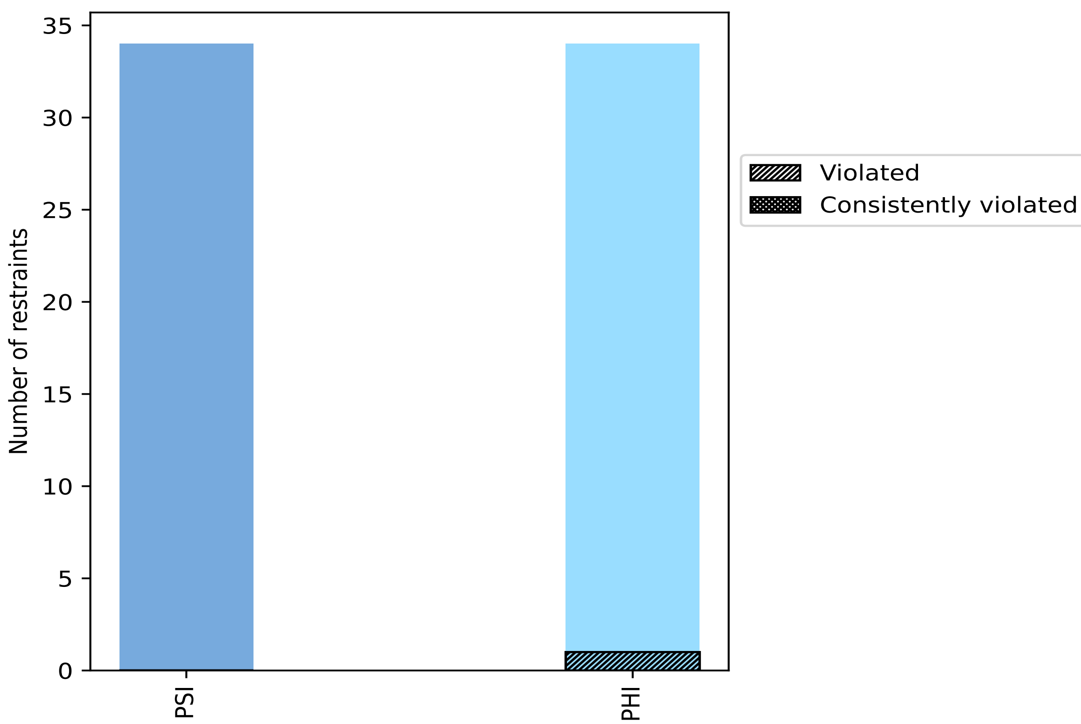
10.1 Summary of dihedral-angle violations (i)

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	34	50.0	0	0.0	0.0	0	0.0	0.0
PHI	34	50.0	1	2.9	1.5	0	0.0	0.0
Total	68	100.0	1	1.5	1.5	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 (i)



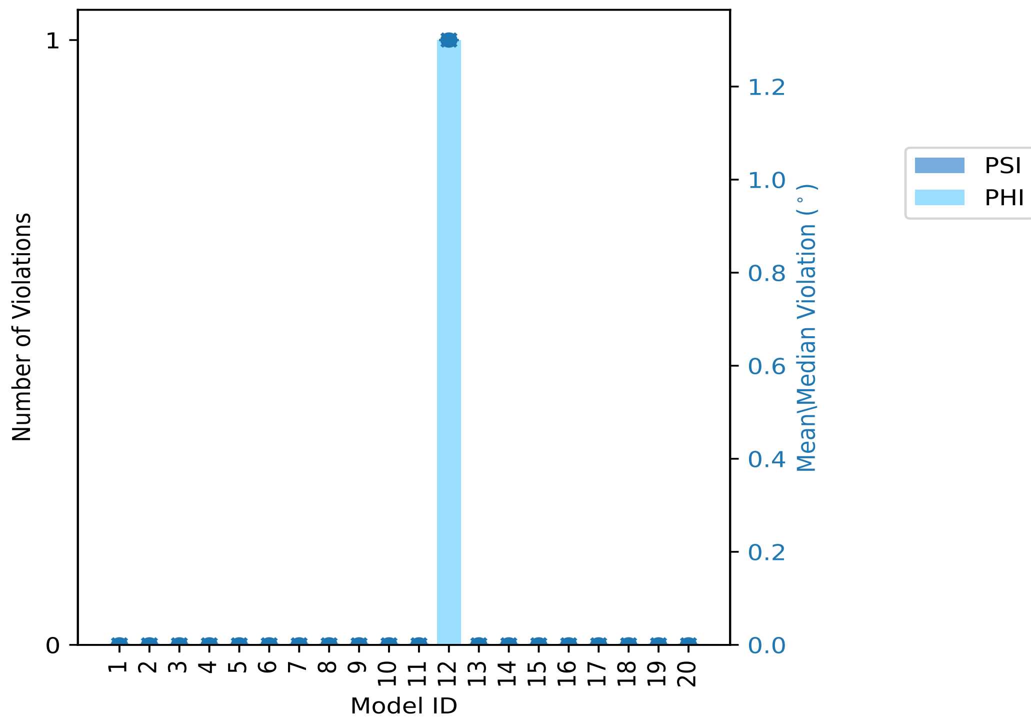
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0.0	0.0	0.0	0.0
11	0	0	0	0.0	0.0	0.0	0.0
12	0	1	1	1.3	1.3	0.0	1.3
13	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	0.0	0.0	0.0	0.0

10.2.1 Bar graph : Dihedral 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

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

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

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

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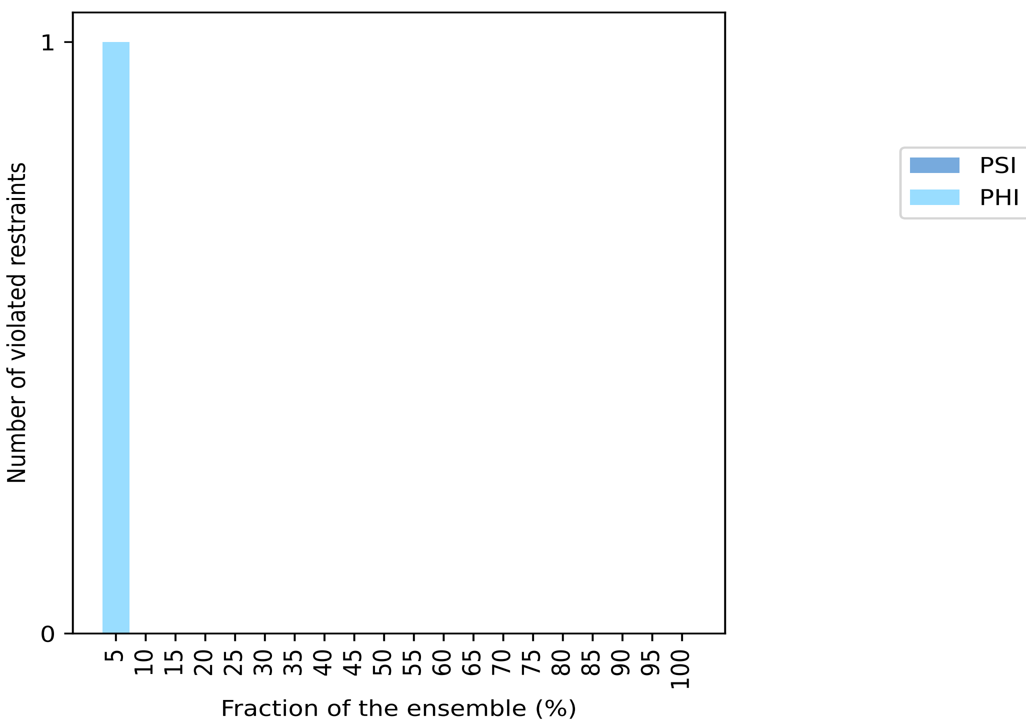
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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



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

No violations found

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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

10.5.2 Table: All violated dihedral-angle restraints (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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,59)	2:26:B:LEU:C	2:27:B:SER:N	2:27:B:SER:CA	2:27:B:SER:C	12	1.3