Full wwPDB NMR Structure Validation Report (i)

Jun 15, 2024 – 02:59 PM EDT

PDB ID	:	2BJC
BMRB ID	:	7354
Title	:	NMR structure of a protein-DNA complex of an altered specificity mutant of the lac repressor headpiece that mimics the gal repressor
Authors	:	Salinas, R.K.; Folkers, G.E.; Bonvin, A.M.J.J.; Das, D.; Boelens, R.; Kaptein, R.
Deposited on	:	2005-02-01

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:

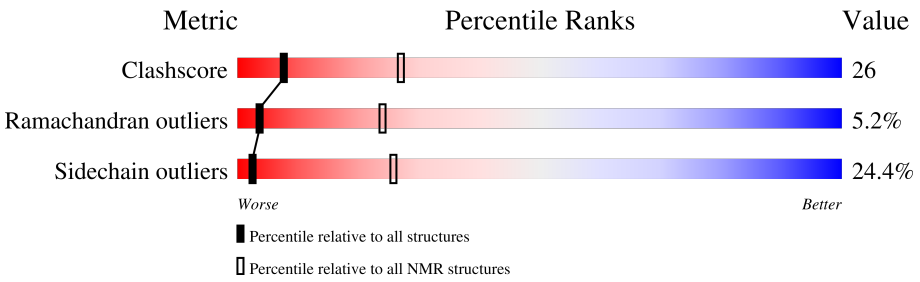
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 69%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	62	58% 32% • 8%
1	B	62	61% 29% • 8%
2	C	22	18% 82%
2	D	22	14% 86%

2 Ensemble composition and analysis (i)

This entry contains 16 models. Model 1 is the overall representative, medoid model (most similar to other models). The authors have identified model 3 as representative.

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:3-A:59, B:103-B:159 (114)	0.45	1

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3088 atoms, of which 1256 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called LACTOSE OPERON REPRESSOR.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	62	845	290	377	84	91	3	0
1	B	62	845	290	377	84	91	3	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	VAL	TYR	engineered mutation	UNP P03023
A	18	ALA	GLN	engineered mutation	UNP P03023
A	52	CYS	VAL	engineered mutation	UNP P03023
B	117	VAL	TYR	engineered mutation	UNP P03023
B	118	ALA	GLN	engineered mutation	UNP P03023
B	152	CYS	VAL	engineered mutation	UNP P03023

- Molecule 2 is a DNA chain called 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	C	22	699	216	251	81	130	21	0
2	D	22	699	216	251	81	130	21	0

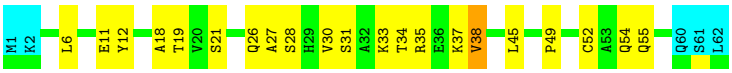
4 Residue-property plots (i)

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: LACTOSE OPERON REPRESSOR

Chain A: 58% 32% • 8%



• Molecule 1: LACTOSE OPERON REPRESSOR

Chain B: 61% 29% • 8%

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain C: 18% 82%

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain D: 14% 86%

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 (medoid)

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain A: 56% 32% • 8%

M1 K2 L6 E11 Y12 A13 T19 A27 S28 H29 V30 S31 A32 K33 T34 R35 E36 K37 V38 E39 L45 I48 P49 N50 R51 C52 A53 Q54 Q55 Q60 S61 L62

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain B: 56% 32% • 8%

M101 K102 L106 Y112 V115 T119 V120 S121 A127 S128 H129 V130 S131 A132 K133 T134 R135 E136 K137 V138 E139 L145 N146 Y147 I148 P149 N150 R151 Q154 Q155 Q160 S161 L162

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain C: 14% 86%

G1 A2 A3 T4 T5 G6 T7 A8 A9 G10 C11 G12 C13 T14 T15 A16 C17 A18 A19 T20 T21 C22

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain D: 9% 91%

G101 A102 A103 T104 T105 G106 T107 A108 A109 G110 C111 G112 C113 T114 T115 A116 C117 A118 A119 T120 T121 C122

4.2.2 Score per residue for model 2

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain A: 63% 26% • 8%

M1 K2 L6 Y12 T19 V20 S21 A27 S28 H29 V30 S31 A32 K33 T34 R35 E36 K37 V38 L45 P49 C52 A53 Q54 Q55 Q60 S61 L62

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain B: 68% 21% • 8%

M101 K102 L106 Y112 T119 V120 S121 A127 S128 H129 V130 S131 A132 K133 T134 R135 E136 K137 V138 P149 Q155 Q160 S161 L162

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain C: 23% 77%

G1 A2 A3 T4 T7 A8 A9 G10 C11 G12 C13 T14 T15 A16 C17 A18 A19 T20 T21 C22

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain D: 32% 68%

G101 A102 A103 T104 T107 A108 A109 G112 C113 T114 T115 A116 C117 T120 T121 C122

4.2.3 Score per residue for model 3

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain A: 63% 24% 5% 8%

M1 K2 P3 V4 T5 L6 V15 T19 V20 S21 R22 V23 A27 V30 S31 A32 K33 T34 R35 E36 K37 V38 L45 P49 Q54 Q55 Q60 S61 L62

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain B: 65% 24% • 8%

M101 K102 P103 V104 T105 L106 Y112 T119 V123 A127 V130 S131 A132 K133 T134 R135 E136 K137 V138 L145 P149 Q154 Q155 Q160 S161 L162

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain C: 14% 86%

G1 A2 A3 T4 T7 A8 A9 G10 C11 G12 C13 T14 T15 A16 C17 A18 A19 T20 T21 C22

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain D: 9% 91%

G101 A102 A103 T104 T107 A108 A109 G110 C111 G112 C113 T114 T115 A116 C117 A118 A119 T120 T121 C122

4.2.4 Score per residue for model 4

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain A: 60% 27% 5% 8%

M1 K2 L6 Y12 T19 V20 S21 V24 A27 S28 H29 V30 K33 T34 R35 E36 K37 V38 M42 P49 C52 A53 Q54 Q55 L56 K59 Q60 S61 L62

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain B: 58% 26% 6% • 8%

M101 K102 L106 E111 Y112 A113 T119 V120 S121 Q126 A127 S128 H129 V130 S131 A132 K133 T134 R135 E136 K137 V138 L145 P149 Q155 L156 K159 Q160 S161 L162

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain C: 9% 91%

G1 A2 A3 T4 T7 A8 A9 G10 C11 G12 C13 T14 T15 A16 C17 A18 A19 T20 T21 C22

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain D: 5% 95%

G101 A102 A103 T104 T105 G106 T107 A108 A109 G110 C111 G112 C113 T114 T115 A116 C117 A118 A119 T120 T121 C122

4.2.5 Score per residue for model 5

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain A: 60% 24% 8% 8%

M1 K2 L6 E11 Y12 A13 A18 T19 Q26 A27 V30 S31 A32 K33 T34 R35 E36 K37 V38 L45 N46 P49 C52 Q55 Q60 S61 L62

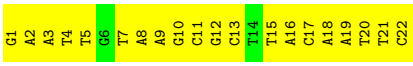
• Molecule 1: LACTOSE OPERON REPRESSOR

Chain B: 55% 29% 8% 8%

M101 K102 P103 V104 T105 L106 E111 Y112 A113 A118 T119 Q126 A127 S128 H129 V130 S131 A132 K133 T134 R135 E136 K137 V138 M142 L145 N146 Y147 I148 P149 C152 Q155 Q160 S161 L162

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain C: 9% 91%



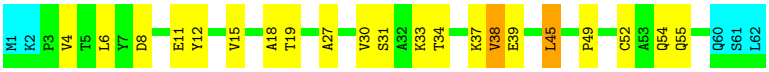
• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain D:

4.2.6 Score per residue for model 6

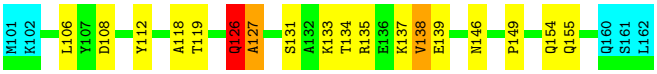
• Molecule 1: LACTOSE OPERON REPRESSOR

Chain A:



• Molecule 1: LACTOSE OPERON REPRESSOR

Chain B:



• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain C:

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain D:

4.2.7 Score per residue for model 7

• Molecule 1: LACTOSE OPERON REPRESSOR

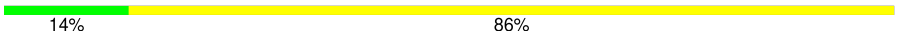
Chain A:

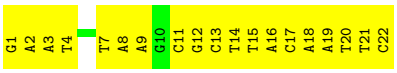
• Molecule 1: LACTOSE OPERON REPRESSOR

Chain B:

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

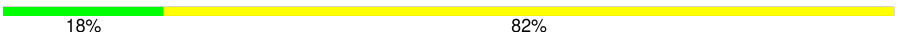
Chain C:

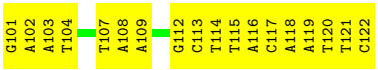




• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain D:





4.2.8 Score per residue for model 8

• Molecule 1: LACTOSE OPERON REPRESSOR

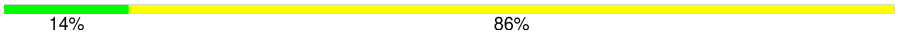
Chain A:

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain B:

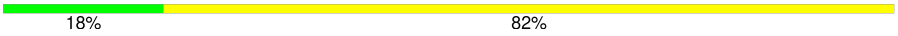
• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

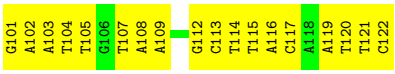
Chain C:



• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain D:

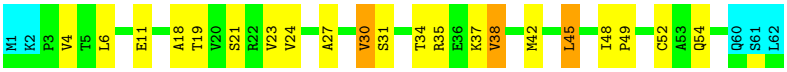




4.2.9 Score per residue for model 9

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain A:

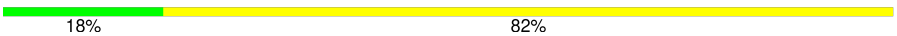


• Molecule 1: LACTOSE OPERON REPRESSOR

Chain B:

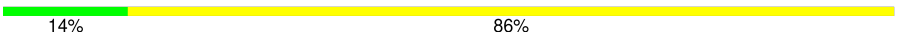
• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

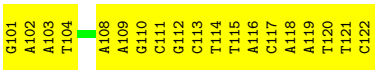
Chain C:



• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain D:





4.2.10 Score per residue for model 10

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain A:

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain B: 58% 27% 6% 8%

M101 K102 P103 V104 T105 L106 E111 Y112 A118 T119 Q126 A127 S128 S131 A132 K133 T134 R135 E136 K137 V138 E139 L145 N146 P149 N150 R151 Q154 Q160 S161 L162

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain C: 27% 73%

G1 A2 A3 T4 T7 A8 A9 G10 C11 G12 C13 A16 C17 A18 A19 T20 T21 C22

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain D: 32% 68%

G101 A102 A103 T104 T107 A108 A109 G110 C111 G112 C113 A119 T120 T121 C122

4.2.11 Score per residue for model 11

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain A: 53% 34% 5% 8%

M1 K2 P3 V4 T5 L6 E11 Y12 A18 T19 V20 S21 R22 A27 S28 H29 V30 S31 A32 K33 T34 R35 E36 K37 V38 E44 L45 N46 P49 N50 R51 Q54 Q55 Q60 S61 L62

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain B: 58% 29% 5% 8%

M101 K102 P103 V104 T105 L106 E111 A118 T119 A127 S128 H129 V130 S131 A132 K133 T134 R135 E136 K137 V138 L145 N146 P149 N150 R151 C152 A153 Q154 Q155 Q160 S161 L162

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain C: 14% 86%

G1 A2 A3 T4 T5 G6 T7 A8 A9 G10 C11 G12 C13 T14 T15 A16 C17 A18 A19 T20 T21 C22

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain D: 9% 91%

G101 A102 A103 T104 T105 G106 T107 A108 A109 G110 C111 G112 C113 T114 T115 A116 C117 A118 A119 T120 T121 C122

4.2.12 Score per residue for model 12

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain A: 56% 34% • 8%

M1 K2 P3 V4 T5 L6 E11 Y12 V15 A18 T19 A27 S28 H29 V30 S31 A32 K33 T34 R35 E36 K37 V38 A41 L45 P49 N50 R51 C52 Q60 S61 L62

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain B: 58% 32% • 8%

M101 K102 P103 L106 E111 Y112 A113 A118 T119 A127 S128 H129 V130 S131 A132 K133 T134 R135 E136 K137 V138 P149 N150 R151 C152 A153 Q154 Q155 Q160 S161 L162

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain C: 18% 82%

G1 A2 A3 T4 T7 A8 A9 G10 C11 G12 C13 T14 T15 A16 C17 A18 A19 T20 T21 C22

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain D: 18% 82%

G101 A102 A103 T104 T107 A108 A109 G110 C111 G112 C113 T114 T115 A116 C117 A118 A119 T120 T121 C122

4.2.13 Score per residue for model 13

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain A: 53% 35% • • 8%

M1 K2 L6 E11 Y12 A13 A18 T19 V20 S21 V24 N25 Q26 A27 S28 H29 V30 S31 A32 K33 T34 R35 E36 K37 V38 M42 L45 P49 C52 A53 Q54 Q55 Q60 S61 L62

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain B: 55% 32% • • 8%

M101 K102 L106 E111 Y112 T119 V120 S121 R122 V123 V124 N125 Q126 A127 S128 H129 V130 S131 A132 K133 T134 R135 V138 E139 M142 L145 I148 P149 Q154 Q155 Q160 S161 L162

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain C: 5% 95%

G1 A2 A3 T4 T5 G6 T7 A8 A9 G10 C11 G12 C13 T14 T15 A16 C17 A18 A19 T20 T21 C22

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain D: 9% 91%

G101 A102 A103 T104 T105 G106 T107 A108 A109 G110 C111 G112 C113 T114 T115 A116 C117 A118 A119 T120 T121 C122

4.2.14 Score per residue for model 14

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain A: 63% 23% 6% 8%

M1 K2 L6 E11 Y12 A18 T19 V23 A27 S28 H29 V30 S31 T34 R35 E36 K37 V38 Y47 I48 C52 A53 Q54 Q60 S61 L62

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain B: 60% 26% 6% 8%

M101 K102 L106 Y112 A113 G114 V115 T119 V123 A127 S128 H129 V130 S131 T134 R135 E136 K137 V138 E139 A140 E144 Y147 I148 Q154 Q155 Q160 S161 L162

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain C: 14% 86%

G1 A2 A3 T4 T5 G6 T7 A8 A9 G10 C11 G12 C13 T14 T15 A16 C17 A18 A19 T20 T21 C22

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain D: 14% 86%

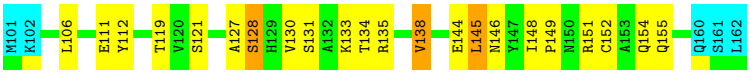
4.2.15 Score per residue for model 15

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain A:

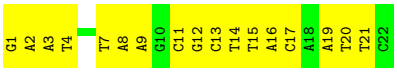
• Molecule 1: LACTOSE OPERON REPRESSOR

Chain B:



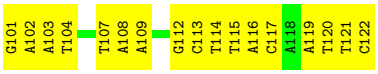
• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain C:



• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain D:



4.2.16 Score per residue for model 16

• Molecule 1: LACTOSE OPERON REPRESSOR

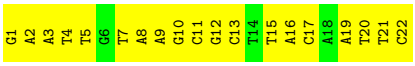
Chain A:

• Molecule 1: LACTOSE OPERON REPRESSOR

Chain B:

• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain C: 14% 86%



• Molecule 2: 5'-D(*GP*AP*AP*TP*TP*GP*TP*AP*AP*GP *CP*GP*CP*TP*TP*AP*CP*AP*AP*TP*TP*C)-3'

Chain D: 9% 91%

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *HADDOCK*.

Of the 50 calculated structures, 16 were deposited, based on the following criterion: *RMSD TO AVERAGE STRUCTURE AND LOWEST ENERGY*.

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

Software name	Classification	Version
CNS	refinement	
CNS	structure solution	

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	1752
Number of shifts mapped to atoms	1540
Number of unparsed shifts	0
Number of shifts with mapping errors	212
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	69%

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	427	337	374	10±2
1	B	427	337	374	9±3
2	C	448	251	251	29±5
2	D	448	251	251	31±5
All	All	28000	18816	20000	1229

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 26.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:115:DT:H2"	2:D:116:DA:O5'	0.83	1.74	11	6
2:C:15:DT:H2"	2:C:16:DA:O5'	0.79	1.76	11	6
2:C:15:DT:H2"	2:C:16:DA:N7	0.77	1.95	4	3
2:D:115:DT:H1'	2:D:116:DA:N7	0.76	1.96	14	3
2:C:15:DT:H1'	2:C:16:DA:N7	0.74	1.98	14	3
2:D:115:DT:H2"	2:D:116:DA:N7	0.73	1.99	4	3
2:C:12:DG:H1'	2:C:13:DC:O4'	0.73	1.83	3	14
2:D:112:DG:H1'	2:D:113:DC:O4'	0.71	1.85	13	15
2:C:7:DT:H1'	2:C:8:DA:O5'	0.70	1.85	10	3
1:A:27:ALA:HB1	1:A:30:VAL:HB	0.69	1.65	5	2
2:D:107:DT:H1'	2:D:108:DA:O5'	0.69	1.88	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:GLN:NE2	1:A:55:GLN:HA	0.67	2.03	5	2
1:B:155:GLN:NE2	1:B:155:GLN:HA	0.67	2.05	5	2
1:A:49:PRO:HA	2:D:113:DC:OP1	0.66	1.90	1	14
2:D:108:DA:H4'	2:D:109:DA:O5'	0.65	1.91	1	4
2:D:107:DT:H1'	2:D:108:DA:C8	0.65	2.27	13	8
1:A:30:VAL:HG13	1:A:34:THR:HB	0.64	1.67	2	9
2:D:114:DT:H2"	2:D:115:DT:O5'	0.64	1.93	4	1
2:C:8:DA:H4'	2:C:9:DA:O5'	0.63	1.92	1	4
2:C:7:DT:H1'	2:C:8:DA:C8	0.63	2.29	13	9
2:C:14:DT:H2"	2:C:15:DT:O5'	0.63	1.94	4	1
2:C:15:DT:H2"	2:C:16:DA:C8	0.63	2.29	1	9
2:D:115:DT:C2'	2:D:116:DA:C8	0.62	2.82	1	6
1:B:149:PRO:HA	2:C:13:DC:OP1	0.62	1.94	15	13
2:D:115:DT:H2"	2:D:116:DA:C8	0.61	2.29	1	9
2:D:107:DT:H2"	2:D:108:DA:C8	0.61	2.29	4	7
1:B:130:VAL:HG13	1:B:134:THR:HB	0.61	1.71	2	7
2:D:115:DT:H2'	2:D:116:DA:N7	0.60	2.11	2	5
2:C:15:DT:C2'	2:C:16:DA:C8	0.60	2.85	5	6
2:D:120:DT:C2'	2:D:121:DT:H71	0.59	2.28	13	15
2:C:8:DA:H2"	2:C:9:DA:O5'	0.59	1.98	16	7
2:C:20:DT:C2'	2:C:21:DT:H71	0.59	2.27	5	15
2:D:104:DT:H2"	2:D:105:DT:H71	0.59	1.74	5	7
2:C:1:DG:H2"	2:C:2:DA:C8	0.59	2.31	16	16
2:C:20:DT:C2'	2:C:21:DT:H72	0.58	2.28	16	1
2:D:111:DC:C2'	2:D:112:DG:H5"	0.58	2.27	3	9
2:C:20:DT:H2'	2:C:21:DT:H72	0.58	1.74	16	1
2:D:108:DA:H2"	2:D:109:DA:O5'	0.58	1.98	8	9
2:C:7:DT:C1'	2:C:8:DA:O5'	0.58	2.52	14	4
2:D:101:DG:H2"	2:D:102:DA:C8	0.58	2.34	8	16
2:D:110:DG:N3	2:D:111:DC:C4	0.58	2.72	9	10
2:D:109:DA:H1'	2:D:110:DG:O5'	0.57	2.00	4	2
2:D:120:DT:H2'	2:D:121:DT:H72	0.57	1.76	5	1
2:D:116:DA:H2"	2:D:117:DC:C5	0.57	2.34	3	15
2:C:15:DT:H2'	2:C:16:DA:N7	0.57	2.14	2	5
2:C:15:DT:H4'	2:C:16:DA:O5'	0.57	2.00	9	2
2:D:120:DT:H2"	2:D:121:DT:H71	0.56	1.76	13	15
2:C:16:DA:H2"	2:C:17:DC:C5	0.56	2.34	3	16
1:B:147:TYR:O	1:B:148:ILE:HB	0.56	1.99	14	4
1:B:156:LEU:O	1:B:159:LYS:HB2	0.56	2.00	4	1
1:B:147:TYR:CG	1:B:148:ILE:N	0.56	2.73	16	4
2:C:11:DC:C2'	2:C:12:DG:H5"	0.56	2.31	3	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:120:DT:C2'	2:D:121:DT:H72	0.56	2.31	5	1
2:D:107:DT:C1'	2:D:108:DA:O5'	0.56	2.54	1	4
2:C:20:DT:H2"	2:C:21:DT:H71	0.55	1.76	13	15
2:D:108:DA:H1'	2:D:109:DA:C8	0.55	2.37	10	3
2:C:15:DT:C2'	2:C:16:DA:O5'	0.55	2.54	1	6
1:A:34:THR:O	1:A:37:LYS:HB3	0.55	2.02	2	15
1:A:47:TYR:O	1:A:48:ILE:HB	0.54	2.01	14	1
2:C:4:DT:H2"	2:C:5:DT:H71	0.54	1.77	8	7
2:D:108:DA:C6	2:D:109:DA:C6	0.54	2.96	4	9
2:C:16:DA:C8	2:C:17:DC:N4	0.54	2.75	13	7
2:D:115:DT:H4'	2:D:116:DA:O5'	0.54	2.01	9	2
2:C:8:DA:H1'	2:C:9:DA:C8	0.54	2.38	10	3
2:C:8:DA:C6	2:C:9:DA:C6	0.54	2.96	6	10
2:D:116:DA:C8	2:D:117:DC:N4	0.53	2.76	5	7
1:A:56:LEU:O	1:A:59:LYS:HB2	0.53	2.02	4	1
1:A:34:THR:O	1:A:38:VAL:HG13	0.53	2.03	3	16
1:B:134:THR:O	1:B:137:LYS:HB3	0.53	2.03	2	13
1:A:23:VAL:HG22	1:A:30:VAL:HG11	0.53	1.79	9	4
2:D:103:DA:H2"	2:D:104:DT:H71	0.53	1.81	7	13
2:C:8:DA:C2'	2:C:9:DA:O5'	0.53	2.57	16	9
1:B:134:THR:O	1:B:138:VAL:HG13	0.53	2.04	9	16
2:D:110:DG:H1'	2:D:111:DC:C5	0.53	2.39	9	10
2:C:11:DC:N4	2:C:12:DG:O6	0.52	2.42	5	16
2:C:10:DG:N3	2:C:11:DC:C4	0.52	2.78	9	6
2:C:9:DA:H1'	2:C:10:DG:O5'	0.52	2.03	4	2
1:A:18:ALA:HA	2:D:115:DT:H72	0.52	1.80	6	2
2:D:115:DT:C2'	2:D:116:DA:O5'	0.52	2.57	1	6
2:D:119:DA:H2"	2:D:120:DT:H71	0.52	1.81	10	14
2:D:119:DA:C2'	2:D:120:DT:H71	0.51	2.35	13	11
2:D:108:DA:C1'	2:D:109:DA:O5'	0.51	2.59	9	1
2:C:19:DA:H2"	2:C:20:DT:H71	0.51	1.82	13	15
2:D:108:DA:C2'	2:D:109:DA:O5'	0.51	2.59	6	10
2:C:3:DA:H2"	2:C:4:DT:H71	0.51	1.82	7	11
2:D:116:DA:H2"	2:D:117:DC:C6	0.51	2.40	14	10
1:B:123:VAL:HG22	1:B:130:VAL:HG11	0.51	1.81	14	4
2:C:19:DA:C2'	2:C:20:DT:H71	0.50	2.36	13	11
1:B:118:ALA:HA	2:C:15:DT:H72	0.50	1.83	6	1
2:C:7:DT:H2"	2:C:8:DA:C8	0.50	2.41	7	4
2:C:21:DT:C5	2:C:22:DC:N4	0.50	2.80	4	15
2:C:1:DG:H2"	2:C:2:DA:N7	0.50	2.21	16	4
2:C:16:DA:H2"	2:C:17:DC:C6	0.49	2.42	14	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:101:DG:C5	2:D:102:DA:N6	0.49	2.80	4	10
2:C:2:DA:H2"	2:C:3:DA:C8	0.49	2.42	1	16
2:D:121:DT:C5	2:D:122:DC:N4	0.49	2.81	1	14
2:C:8:DA:C1'	2:C:9:DA:O5'	0.49	2.60	9	1
2:C:10:DG:H1'	2:C:11:DC:C5	0.49	2.43	9	5
2:C:21:DT:H2"	2:C:22:DC:C6	0.49	2.43	2	8
2:D:108:DA:C2'	2:D:109:DA:C8	0.49	2.96	8	2
1:B:121:SER:OG	2:C:14:DT:H71	0.49	2.08	7	4
2:C:4:DT:H2"	2:C:5:DT:C7	0.48	2.38	1	3
1:A:55:GLN:HA	1:A:55:GLN:HE21	0.48	1.67	5	1
2:C:3:DA:H2"	2:C:4:DT:C6	0.48	2.44	3	6
1:A:47:TYR:CG	1:A:48:ILE:N	0.48	2.82	14	1
2:C:1:DG:C5	2:C:2:DA:N6	0.48	2.82	9	11
2:C:12:DG:H2"	2:C:13:DC:O5'	0.48	2.08	9	5
2:D:104:DT:H2"	2:D:105:DT:C7	0.48	2.39	5	4
1:B:127:ALA:HB1	1:B:130:VAL:HB	0.47	1.86	2	1
2:C:17:DC:C4	2:C:18:DA:N6	0.47	2.81	4	5
1:B:138:VAL:O	1:B:142:MET:HG3	0.47	2.09	13	1
2:D:103:DA:H2"	2:D:104:DT:C6	0.47	2.44	4	10
2:D:102:DA:H2"	2:D:103:DA:C8	0.47	2.45	12	15
1:B:145:LEU:HD22	1:B:145:LEU:H	0.47	1.70	5	2
2:C:7:DT:C4	2:C:8:DA:C6	0.47	3.03	8	1
2:C:20:DT:H2"	2:C:21:DT:C6	0.47	2.45	2	14
2:D:107:DT:H1'	2:D:108:DA:C4	0.47	2.44	2	2
2:D:111:DC:N4	2:D:112:DG:O6	0.47	2.48	5	10
2:D:107:DT:H2"	2:D:108:DA:N7	0.47	2.24	4	2
1:A:38:VAL:HG23	1:A:42:MET:HE3	0.47	1.87	7	1
2:C:17:DC:H2"	2:C:18:DA:C8	0.47	2.44	14	7
2:D:117:DC:H2"	2:D:118:DA:C8	0.47	2.45	14	7
2:D:121:DT:H2"	2:D:122:DC:C6	0.47	2.45	15	10
1:B:155:GLN:HA	1:B:155:GLN:HE21	0.47	1.69	5	1
2:C:4:DT:C2'	2:C:5:DT:H71	0.47	2.40	8	1
1:A:4:VAL:HG21	1:A:45:LEU:O	0.47	2.10	3	5
2:D:104:DT:C2'	2:D:105:DT:H71	0.47	2.40	4	3
2:D:112:DG:H2"	2:D:113:DC:O5'	0.46	2.10	9	3
2:C:12:DG:C5	2:C:13:DC:C4	0.46	3.04	5	1
2:D:115:DT:C2	2:D:116:DA:C6	0.46	3.04	9	1
2:D:108:DA:C5	2:D:109:DA:C6	0.46	3.04	8	3
1:A:21:SER:OG	2:D:114:DT:H71	0.46	2.11	7	5
2:D:120:DT:H2"	2:D:121:DT:C6	0.46	2.45	2	15
2:D:109:DA:C1'	2:D:110:DG:O5'	0.46	2.64	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:101:DG:H2"	2:D:102:DA:N7	0.46	2.26	1	5
2:D:103:DA:C2'	2:D:104:DT:H71	0.46	2.41	7	1
1:B:140:ALA:O	1:B:144:GLU:HG3	0.46	2.11	14	1
2:D:102:DA:C5	2:D:103:DA:N6	0.46	2.84	11	7
2:C:9:DA:C2'	2:C:10:DG:O5'	0.46	2.64	4	3
1:B:145:LEU:HD22	1:B:145:LEU:N	0.45	2.26	5	3
2:C:4:DT:H2"	2:C:5:DT:C5	0.45	2.46	1	1
2:C:2:DA:C5	2:C:3:DA:N6	0.45	2.83	5	8
2:C:2:DA:C6	2:C:3:DA:N6	0.45	2.85	16	3
2:C:20:DT:C2'	2:C:21:DT:C7	0.45	2.95	5	13
2:C:8:DA:C4'	2:C:9:DA:O5'	0.45	2.63	1	3
2:D:108:DA:C4'	2:D:109:DA:O5'	0.45	2.62	1	3
2:D:117:DC:C4	2:D:118:DA:N6	0.45	2.84	6	6
1:B:113:ALA:O	1:B:137:LYS:HD3	0.45	2.11	9	7
2:D:103:DA:H2"	2:D:104:DT:C5	0.45	2.47	4	11
2:C:7:DT:H1'	2:C:8:DA:C4	0.45	2.47	2	2
1:B:142:MET:HA	1:B:145:LEU:HD21	0.45	1.89	7	2
2:C:19:DA:H2"	2:C:20:DT:C6	0.45	2.47	16	6
2:C:16:DA:C8	2:C:17:DC:C4	0.45	3.05	2	3
2:D:115:DT:H2'	2:D:116:DA:C8	0.45	2.47	2	2
2:D:120:DT:C2'	2:D:121:DT:C7	0.45	2.95	16	12
2:D:107:DT:C4	2:D:108:DA:C6	0.44	3.06	8	3
2:C:15:DT:H2'	2:C:16:DA:C8	0.44	2.47	5	1
2:C:7:DT:H4'	2:C:8:DA:OP1	0.44	2.13	8	7
1:B:124:VAL:HG23	1:B:142:MET:HE2	0.44	1.88	13	1
2:D:111:DC:C2'	2:D:112:DG:C5'	0.44	2.95	14	1
2:D:109:DA:C2'	2:D:110:DG:O5'	0.44	2.66	4	3
2:C:3:DA:C2'	2:C:4:DT:H71	0.44	2.43	7	2
2:D:103:DA:H2"	2:D:104:DT:C7	0.44	2.42	14	5
2:D:116:DA:C8	2:D:117:DC:C4	0.44	3.05	11	3
2:C:9:DA:C1'	2:C:10:DG:O5'	0.44	2.65	4	2
2:C:3:DA:H2"	2:C:4:DT:C5	0.44	2.48	4	7
2:D:107:DT:H4'	2:D:108:DA:OP1	0.44	2.12	8	6
2:D:114:DT:H2"	2:D:115:DT:C6	0.44	2.47	8	1
1:A:13:ALA:O	1:A:37:LYS:HD3	0.44	2.13	10	5
1:A:21:SER:OG	2:D:115:DT:C7	0.44	2.66	9	1
1:A:55:GLN:NE2	1:A:55:GLN:CA	0.43	2.79	5	1
2:C:8:DA:C8	2:C:8:DA:H5'	0.43	2.48	9	1
1:A:27:ALA:HB3	1:A:30:VAL:HB	0.43	1.89	16	1
1:B:121:SER:HB3	2:C:15:DT:C7	0.43	2.43	8	1
1:B:124:VAL:HG23	1:B:142:MET:CE	0.43	2.43	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:LEU:HD22	1:A:45:LEU:N	0.43	2.28	5	3
1:A:45:LEU:HD22	1:A:45:LEU:H	0.43	1.73	7	3
2:C:3:DA:H2"	2:C:4:DT:C7	0.43	2.43	16	5
2:D:104:DT:H2"	2:D:105:DT:C5	0.43	2.48	1	2
2:D:107:DT:C2	2:D:108:DA:C4	0.43	3.07	3	1
1:A:24:VAL:HG23	1:A:42:MET:HE1	0.43	1.91	4	1
2:C:8:DA:C4	2:C:9:DA:C5	0.43	3.07	14	1
1:A:21:SER:HB3	2:D:115:DT:C7	0.43	2.44	8	1
1:A:18:ALA:HA	2:D:115:DT:C7	0.43	2.44	6	1
2:D:119:DA:H2"	2:D:120:DT:C6	0.43	2.49	13	4
1:B:104:VAL:HG21	1:B:145:LEU:O	0.43	2.13	3	3
2:D:111:DC:C3'	2:D:112:DG:C5'	0.43	2.96	3	1
2:C:15:DT:H1'	2:C:16:DA:C8	0.43	2.49	8	1
1:A:4:VAL:HG11	1:A:45:LEU:HB2	0.43	1.91	11	1
2:D:107:DT:H1'	2:D:108:DA:C5	0.42	2.49	2	1
2:D:111:DC:C3'	2:D:112:DG:H5"	0.42	2.43	3	1
2:D:118:DA:H2"	2:D:119:DA:C8	0.42	2.49	7	2
2:D:114:DT:C5	2:D:115:DT:H73	0.42	2.48	9	1
1:B:104:VAL:HG11	1:B:145:LEU:HB2	0.42	1.91	10	1
2:D:108:DA:C8	2:D:108:DA:H5'	0.42	2.49	9	1
2:C:14:DT:H2"	2:C:15:DT:C6	0.42	2.50	8	1
2:C:14:DT:C2'	2:C:15:DT:H71	0.42	2.45	7	1
1:B:124:VAL:HG23	1:B:142:MET:HE1	0.42	1.91	16	1
2:C:11:DC:N4	2:C:12:DG:C6	0.42	2.88	7	1
2:C:8:DA:C5	2:C:9:DA:C6	0.42	3.08	14	1
2:D:102:DA:C6	2:D:103:DA:N6	0.42	2.87	16	1
2:C:18:DA:H2"	2:C:19:DA:C8	0.42	2.50	7	2
2:D:115:DT:H1'	2:D:116:DA:C8	0.42	2.50	8	1
2:C:8:DA:C2'	2:C:9:DA:C8	0.42	3.03	8	1
2:D:104:DT:C2'	2:D:105:DT:C7	0.41	2.97	4	2
2:D:112:DG:C5	2:D:113:DC:C4	0.41	3.09	5	1
1:A:42:MET:HA	1:A:45:LEU:HD21	0.41	1.92	7	1
1:B:127:ALA:HB3	1:B:130:VAL:HB	0.41	1.92	16	1
2:D:109:DA:C4	2:D:110:DG:C8	0.41	3.09	5	1
2:D:110:DG:H4'	2:D:111:DC:OP1	0.41	2.16	1	1
1:B:138:VAL:HG23	1:B:142:MET:HE3	0.41	1.90	7	1
1:B:147:TYR:O	1:B:148:ILE:CB	0.41	2.69	16	2
2:C:19:DA:C2'	2:C:20:DT:C7	0.41	2.99	13	1
2:D:107:DT:H1'	2:D:108:DA:N9	0.41	2.31	16	1
1:B:126:GLN:O	1:B:127:ALA:HB3	0.41	2.16	13	3
1:A:24:VAL:HG23	1:A:42:MET:CE	0.41	2.46	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:119:DA:C2'	2:D:120:DT:C7	0.41	2.98	13	1
2:C:4:DT:C2'	2:C:5:DT:C7	0.41	2.99	1	2
2:D:114:DT:H2"	2:D:115:DT:H71	0.41	1.93	7	1
1:A:26:GLN:O	1:A:27:ALA:HB3	0.41	2.16	8	3
1:B:121:SER:OG	2:C:15:DT:C7	0.41	2.69	9	1
2:D:109:DA:C6	2:D:110:DG:C6	0.41	3.09	14	1
2:D:108:DA:C4	2:D:109:DA:C5	0.41	3.09	15	1
2:C:15:DT:C2	2:C:16:DA:C6	0.40	3.09	9	1
2:D:109:DA:C8	2:D:110:DG:N7	0.40	2.90	9	1
1:A:12:TYR:CD2	1:A:41:ALA:HA	0.40	2.51	12	1
2:D:103:DA:C2'	2:D:104:DT:C7	0.40	2.99	7	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	63/62 (102%)	55±1 (88±2%)	5±1 (8±2%)	3±1 (5±2%)	4	27
1	B	63/62 (102%)	55±1 (87±2%)	4±2 (7±3%)	4±1 (6±2%)	3	22
All	All	2016/1984 (102%)	1766 (88%)	146 (7%)	104 (5%)	4	24

All 20 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	27	ALA	15
1	B	127	ALA	14
1	B	128	SER	11
1	A	28	SER	10
1	B	146[1]	ASN	6
1	B	146[2]	ASN	6
1	B	126	GLN	6
1	A	15	VAL	4
1	A	26	GLN	4
1	A	46[1]	ASN	4

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Mol	Chain	Res	Type	Models (Total)
1	A	46[2]	ASN	4
1	B	147	TYR	4
1	B	148	ILE	4
1	B	115	VAL	2
1	A	31	SER	2
1	B	131	SER	2
1	A	3	PRO	2
1	B	103	PRO	2
1	A	47	TYR	1
1	A	48	ILE	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	51/50 (102%)	38±2 (75±4%)	12±2 (25±4%)	2 25
1	B	51/50 (102%)	39±2 (76±5%)	12±2 (24±5%)	2 26
All	All	1632/1600 (102%)	1233 (76%)	399 (24%)	2 26

All 46 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	6	LEU	16
1	A	19	THR	16
1	B	106	LEU	16
1	B	119	THR	16
1	B	135[1]	ARG	16
1	B	135[2]	ARG	16
1	B	138	VAL	16
1	A	35[1]	ARG	15
1	A	35[2]	ARG	15
1	A	38	VAL	15
1	B	112	TYR	15
1	A	33	LYS	14
1	B	133	LYS	14
1	A	12	TYR	13

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Mol	Chain	Res	Type	Models (Total)
1	A	31	SER	13
1	B	131	SER	13
1	A	30	VAL	12
1	A	45	LEU	12
1	B	155	GLN	12
1	A	52	CYS	11
1	B	130	VAL	11
1	B	111	GLU	11
1	A	11	GLU	10
1	B	145	LEU	9
1	A	55	GLN	9
1	A	51[1]	ARG	7
1	A	51[2]	ARG	7
1	B	151[1]	ARG	7
1	B	151[2]	ARG	7
1	B	148	ILE	4
1	B	152	CYS	4
1	A	44	GLU	4
1	A	48	ILE	3
1	B	126	GLN	3
1	A	28	SER	3
1	B	128	SER	3
1	B	144	GLU	2
1	A	59	LYS	1
1	B	159	LYS	1
1	A	8	ASP	1
1	B	108	ASP	1
1	A	22[1]	ARG	1
1	A	22[2]	ARG	1
1	A	26	GLN	1
1	B	122[1]	ARG	1
1	B	122[2]	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 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 69% for the well-defined parts and 68% 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	1752
Number of shifts mapped to atoms	1540
Number of unparsed shifts	0
Number of shifts with mapping errors	212
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

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

- No matching atom found in the structure. All 212 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	VAL	HG11	1.147	.	2
1	B	104	VAL	HG11	1.147	.	2
1	A	4	VAL	HG12	1.147	.	2
1	B	104	VAL	HG12	1.147	.	2
1	A	4	VAL	HG13	1.147	.	2
1	B	104	VAL	HG13	1.147	.	2
1	A	4	VAL	HG21	1.228	.	2
1	B	104	VAL	HG21	1.228	.	2
1	A	4	VAL	HG22	1.228	.	2
1	B	104	VAL	HG22	1.228	.	2
1	A	4	VAL	HG23	1.228	.	2
1	B	104	VAL	HG23	1.228	.	2
1	A	5	THR	HG21	1.635	.	1
1	B	105	THR	HG21	1.635	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	THR	HG22	1.635	.	1
1	B	105	THR	HG22	1.635	.	1
1	A	5	THR	HG23	1.635	.	1
1	B	105	THR	HG23	1.635	.	1
1	A	6	LEU	HD11	0.719	.	2
1	B	106	LEU	HD11	0.719	.	2
1	A	6	LEU	HD12	0.719	.	2
1	B	106	LEU	HD12	0.719	.	2
1	A	6	LEU	HD13	0.719	.	2
1	B	106	LEU	HD13	0.719	.	2
1	A	6	LEU	HD21	0.691	.	2
1	B	106	LEU	HD21	0.691	.	2
1	A	6	LEU	HD22	0.691	.	2
1	B	106	LEU	HD22	0.691	.	2
1	A	6	LEU	HD23	0.691	.	2
1	B	106	LEU	HD23	0.691	.	2
1	A	9	VAL	HG11	0.389	.	2
1	B	109	VAL	HG11	0.389	.	2
1	A	9	VAL	HG12	0.389	.	2
1	B	109	VAL	HG12	0.389	.	2
1	A	9	VAL	HG13	0.389	.	2
1	B	109	VAL	HG13	0.389	.	2
1	A	9	VAL	HG21	0.722	.	2
1	B	109	VAL	HG21	0.722	.	2
1	A	9	VAL	HG22	0.722	.	2
1	B	109	VAL	HG22	0.722	.	2
1	A	9	VAL	HG23	0.722	.	2
1	B	109	VAL	HG23	0.722	.	2
1	A	15	VAL	HG11	0.746	.	2
1	B	115	VAL	HG11	0.746	.	2
1	A	15	VAL	HG12	0.746	.	2
1	B	115	VAL	HG12	0.746	.	2
1	A	15	VAL	HG13	0.746	.	2
1	B	115	VAL	HG13	0.746	.	2
1	A	15	VAL	HG21	0.926	.	2
1	B	115	VAL	HG21	0.926	.	2
1	A	15	VAL	HG22	0.926	.	2
1	B	115	VAL	HG22	0.926	.	2
1	A	15	VAL	HG23	0.926	.	2
1	B	115	VAL	HG23	0.926	.	2
1	A	17	VAL	HG11	0.79	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	117	VAL	HG11	0.79	.	2
1	A	17	VAL	HG12	0.79	.	2
1	B	117	VAL	HG12	0.79	.	2
1	A	17	VAL	HG13	0.79	.	2
1	B	117	VAL	HG13	0.79	.	2
1	A	17	VAL	HG21	0.924	.	2
1	B	117	VAL	HG21	0.924	.	2
1	A	17	VAL	HG22	0.924	.	2
1	B	117	VAL	HG22	0.924	.	2
1	A	17	VAL	HG23	0.924	.	2
1	B	117	VAL	HG23	0.924	.	2
1	A	19	THR	HG21	1.135	.	1
1	B	119	THR	HG21	1.135	.	1
1	A	19	THR	HG22	1.135	.	1
1	B	119	THR	HG22	1.135	.	1
1	A	19	THR	HG23	1.135	.	1
1	B	119	THR	HG23	1.135	.	1
1	A	20	VAL	HG11	0.774	.	2
1	B	120	VAL	HG11	0.774	.	2
1	A	20	VAL	HG12	0.774	.	2
1	B	120	VAL	HG12	0.774	.	2
1	A	20	VAL	HG13	0.774	.	2
1	B	120	VAL	HG13	0.774	.	2
1	A	20	VAL	HG21	0.818	.	2
1	B	120	VAL	HG21	0.818	.	2
1	A	20	VAL	HG22	0.818	.	2
1	B	120	VAL	HG22	0.818	.	2
1	A	20	VAL	HG23	0.818	.	2
1	B	120	VAL	HG23	0.818	.	2
1	A	23	VAL	HG11	1.069	.	2
1	B	123	VAL	HG11	1.069	.	2
1	A	23	VAL	HG12	1.069	.	2
1	B	123	VAL	HG12	1.069	.	2
1	A	23	VAL	HG13	1.069	.	2
1	B	123	VAL	HG13	1.069	.	2
1	A	23	VAL	HG21	1.147	.	2
1	B	123	VAL	HG21	1.147	.	2
1	A	23	VAL	HG22	1.147	.	2
1	B	123	VAL	HG22	1.147	.	2
1	A	23	VAL	HG23	1.147	.	2
1	B	123	VAL	HG23	1.147	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	24	VAL	HG11	0.962	.	2
1	B	124	VAL	HG11	0.962	.	2
1	A	24	VAL	HG12	0.962	.	2
1	B	124	VAL	HG12	0.962	.	2
1	A	24	VAL	HG13	0.962	.	2
1	B	124	VAL	HG13	0.962	.	2
1	A	24	VAL	HG21	1.212	.	2
1	B	124	VAL	HG21	1.212	.	2
1	A	24	VAL	HG22	1.212	.	2
1	B	124	VAL	HG22	1.212	.	2
1	A	24	VAL	HG23	1.212	.	2
1	B	124	VAL	HG23	1.212	.	2
1	A	25	ASN	HD22	8.059	.	2
1	B	125	ASN	HD22	8.059	.	2
1	A	26	GLN	HE21	6.784	.	2
1	B	126	GLN	HE21	6.784	.	2
1	A	26	GLN	HE22	7.484	.	2
1	B	126	GLN	HE22	7.484	.	2
1	A	30	VAL	HG11	1.044	.	2
1	B	130	VAL	HG11	1.044	.	2
1	A	30	VAL	HG12	1.044	.	2
1	B	130	VAL	HG12	1.044	.	2
1	A	30	VAL	HG13	1.044	.	2
1	B	130	VAL	HG13	1.044	.	2
1	A	30	VAL	HG21	0.839	.	2
1	B	130	VAL	HG21	0.839	.	2
1	A	30	VAL	HG22	0.839	.	2
1	B	130	VAL	HG22	0.839	.	2
1	A	30	VAL	HG23	0.839	.	2
1	B	130	VAL	HG23	0.839	.	2
1	A	34	THR	HG21	1.125	.	1
1	B	134	THR	HG21	1.125	.	1
1	A	34	THR	HG22	1.125	.	1
1	B	134	THR	HG22	1.125	.	1
1	A	34	THR	HG23	1.125	.	1
1	B	134	THR	HG23	1.125	.	1
1	A	38	VAL	HG11	0.971	.	2
1	B	138	VAL	HG11	0.971	.	2
1	A	38	VAL	HG12	0.971	.	2
1	B	138	VAL	HG12	0.971	.	2
1	A	38	VAL	HG13	0.971	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	138	VAL	HG13	0.971	.	2
1	A	38	VAL	HG21	0.966	.	2
1	B	138	VAL	HG21	0.966	.	2
1	A	38	VAL	HG22	0.966	.	2
1	B	138	VAL	HG22	0.966	.	2
1	A	38	VAL	HG23	0.966	.	2
1	B	138	VAL	HG23	0.966	.	2
1	A	45	LEU	HD11	0.458	.	2
1	B	145	LEU	HD11	0.458	.	2
1	A	45	LEU	HD12	0.458	.	2
1	B	145	LEU	HD12	0.458	.	2
1	A	45	LEU	HD13	0.458	.	2
1	B	145	LEU	HD13	0.458	.	2
1	A	45	LEU	HD21	0.585	.	2
1	B	145	LEU	HD21	0.585	.	2
1	A	45	LEU	HD22	0.585	.	2
1	B	145	LEU	HD22	0.585	.	2
1	A	45	LEU	HD23	0.585	.	2
1	B	145	LEU	HD23	0.585	.	2
1	A	46	ASN	HD22	7.392	.	2
1	B	146	ASN	HD22	7.392	.	2
1	A	48	ILE	HD11	0.798	.	1
1	B	148	ILE	HD11	0.798	.	1
1	A	48	ILE	HD12	0.798	.	1
1	B	148	ILE	HD12	0.798	.	1
1	A	48	ILE	HD13	0.798	.	1
1	B	148	ILE	HD13	0.798	.	1
1	A	48	ILE	HG12	1.397	.	1
1	B	148	ILE	HG12	1.397	.	1
1	A	48	ILE	HG13	0.953	.	1
1	B	148	ILE	HG13	0.953	.	1
1	A	48	ILE	HG21	0.789	.	2
1	B	148	ILE	HG21	0.789	.	2
1	A	48	ILE	HG22	0.789	.	2
1	B	148	ILE	HG22	0.789	.	2
1	A	48	ILE	HG23	0.789	.	2
1	B	148	ILE	HG23	0.789	.	2
1	A	50	ASN	HD22	8.043	.	2
1	B	150	ASN	HD22	8.043	.	2
1	A	54	GLN	HE21	6.59	.	2
1	B	154	GLN	HE21	6.59	.	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	54	GLN	HE22	8.358	.	2
1	B	154	GLN	HE22	8.358	.	2
1	A	55	GLN	HE21	7.32	.	2
1	B	155	GLN	HE21	7.32	.	2
1	A	55	GLN	HE22	6.728	.	2
1	B	155	GLN	HE22	6.728	.	2
1	A	56	LEU	HD11	0.588	.	2
1	B	156	LEU	HD11	0.588	.	2
1	A	56	LEU	HD12	0.588	.	2
1	B	156	LEU	HD12	0.588	.	2
1	A	56	LEU	HD13	0.588	.	2
1	B	156	LEU	HD13	0.588	.	2
1	A	56	LEU	HD21	0.21	.	2
1	B	156	LEU	HD21	0.21	.	2
1	A	56	LEU	HD22	0.21	.	2
1	B	156	LEU	HD22	0.21	.	2
1	A	56	LEU	HD23	0.21	.	2
1	B	156	LEU	HD23	0.21	.	2
1	A	60	GLN	HE21	7.533	.	2
1	B	160	GLN	HE21	7.533	.	2
1	A	60	GLN	HE22	6.822	.	2
1	B	160	GLN	HE22	6.822	.	2
1	A	62	LEU	HD11	0.919	.	2
1	B	162	LEU	HD11	0.919	.	2
1	A	62	LEU	HD12	0.919	.	2
1	B	162	LEU	HD12	0.919	.	2
1	A	62	LEU	HD13	0.919	.	2
1	B	162	LEU	HD13	0.919	.	2
1	A	62	LEU	HD21	0.88	.	2
1	B	162	LEU	HD21	0.88	.	2
1	A	62	LEU	HD22	0.88	.	2
1	B	162	LEU	HD22	0.88	.	2
1	A	62	LEU	HD23	0.88	.	2
1	B	162	LEU	HD23	0.88	.	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	120	-0.47 ± 0.18	None needed (< 0.5 ppm)

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Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\beta}$	116	-0.07 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	114	-0.28 ± 0.08	None needed (< 0.5 ppm)
^{15}N	118	0.60 ± 0.21	Should be applied

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 69%, i.e. 1626 atoms were assigned a chemical shift out of a possible 2358. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	560/566 (99%)	226/228 (99%)	224/228 (98%)	110/110 (100%)
Sidechain	780/862 (90%)	530/566 (94%)	230/260 (88%)	20/36 (56%)
Aromatic	32/70 (46%)	16/32 (50%)	16/34 (47%)	0/4 (0%)
Sugar	182/528 (34%)	182/308 (59%)	0/220 (0%)	0/0 (—%)
Base	72/332 (22%)	72/200 (36%)	0/80 (0%)	0/52 (0%)
Overall	1626/2358 (69%)	1026/1334 (77%)	470/822 (57%)	130/202 (64%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 68%, i.e. 1706 atoms were assigned a chemical shift out of a possible 2506. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	592/616 (96%)	240/248 (97%)	234/248 (94%)	118/120 (98%)
Sidechain	828/960 (86%)	562/630 (89%)	244/290 (84%)	22/40 (55%)
Aromatic	32/70 (46%)	16/32 (50%)	16/34 (47%)	0/4 (0%)
Sugar	182/528 (34%)	182/308 (59%)	0/220 (0%)	0/0 (—%)
Base	72/332 (22%)	72/200 (36%)	0/80 (0%)	0/52 (0%)
Overall	1706/2506 (68%)	1072/1418 (76%)	494/872 (57%)	140/216 (65%)

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	12	TYR	CG	175.12	112.42 – 146.96	13.2
1	B	112	TYR	CG	175.12	112.42 – 146.96	13.2
1	A	35	ARG	NH1	113.70	49.05 – 99.42	7.8

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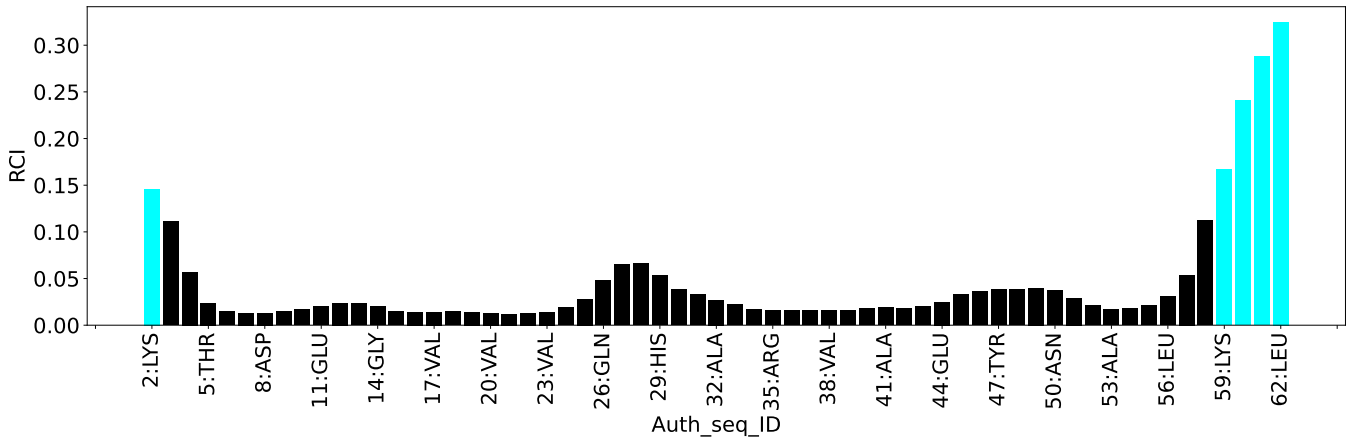
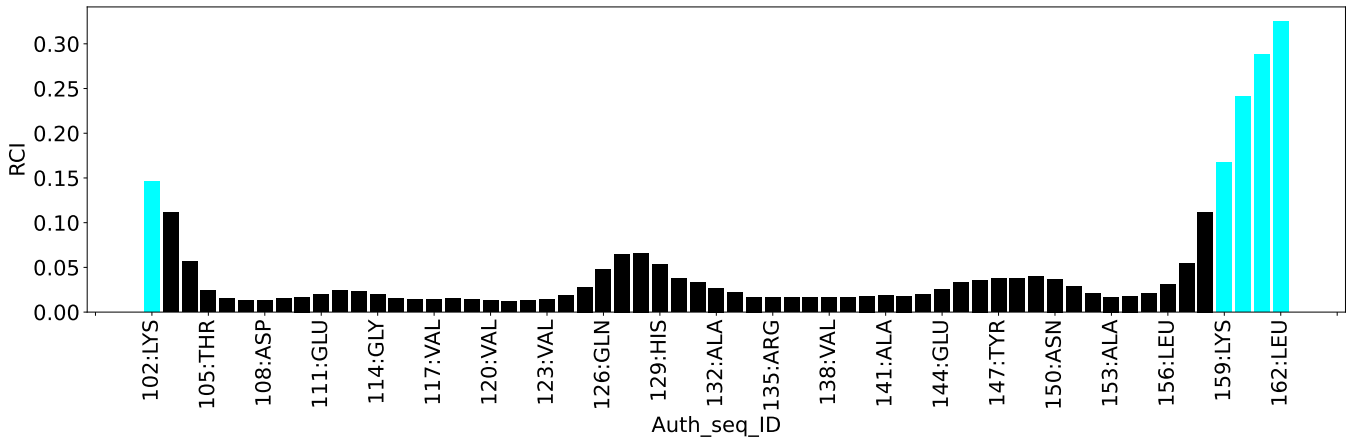
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	B	135	ARG	NH1	113.70	49.05 – 99.42	7.8
1	A	22	ARG	CB	40.08	21.74 – 39.52	5.3
1	B	122	ARG	CB	40.08	21.74 – 39.52	5.3

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: