



# Full wwPDB NMR Structure Validation Report ⓘ

Sep 13, 2016 – 06:56 PM EDT

PDB ID : 5JTQ  
Title : The structure of chaperone SecB in complex with unstructured MBP binding site d  
Authors : Huang, C.; Saio, T.; Rossi, P.; Kalodimos, C.G.  
Deposited on : 2016-05-09

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027939  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

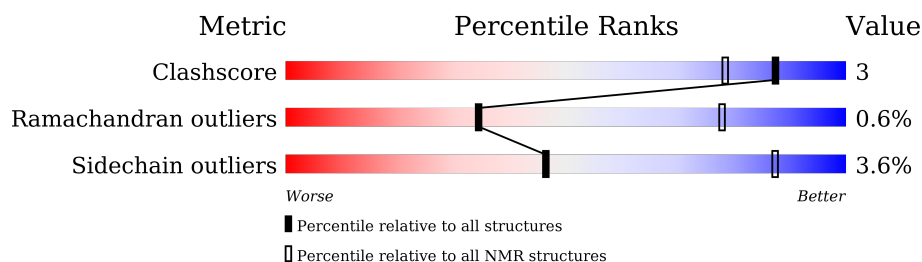
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 13%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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  $\geq 3$ , 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	155	 75% 6% 19%
1	B	155	 77% 6% 17%
1	C	155	 79% • 19%
1	D	155	 77% • 19%
2	E	42	 100%
2	F	42	 100%

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 9 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:10-A:134, B:9-B:136, C:9-C:134, D:9-D:133 (504)	0.56	9

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 4 single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10864 atoms, of which 5322 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein-export protein SecB.

Mol	Chain	Residues	Atoms						Trace
1	A	155	Total	C	H	N	O	S	0
			2367	762	1155	198	243	9	
1	B	155	Total	C	H	N	O	S	0
			2367	762	1155	198	243	9	
1	C	155	Total	C	H	N	O	S	0
			2367	762	1155	198	243	9	
1	D	155	Total	C	H	N	O	S	0
			2367	762	1155	198	243	9	

- Molecule 2 is a protein called Maltose-binding periplasmic protein.

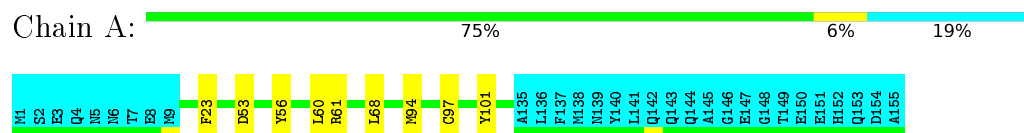
Mol	Chain	Residues	Atoms					Trace
2	E	42	Total	C	H	N	O	0
			698	232	351	53	62	
2	F	42	Total	C	H	N	O	0
			698	232	351	53	62	

## 4 Residue-property plots [i](#)

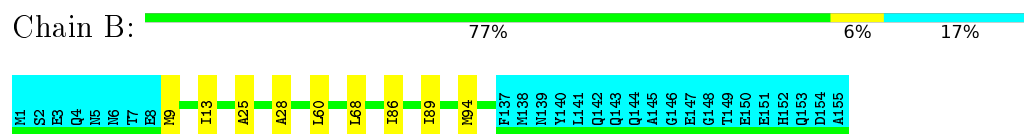
### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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.

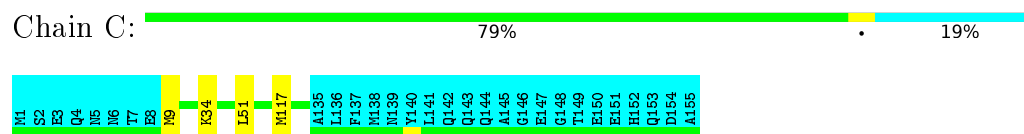
- Molecule 1: Protein-export protein SecB



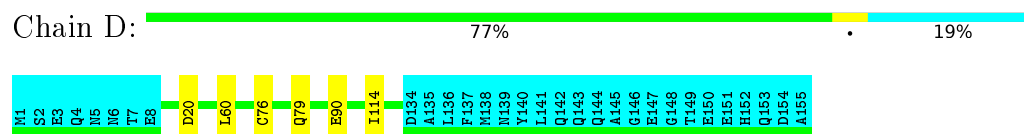
- Molecule 1: Protein-export protein SecB



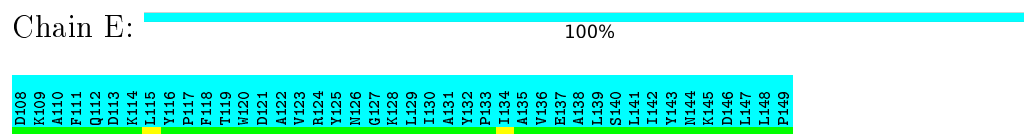
- Molecule 1: Protein-export protein SecB



- Molecule 1: Protein-export protein SecB



- Molecule 2: Maltose-binding periplasmic protein



- Molecule 2: Maltose-binding periplasmic protein

Chain F:  100%

D108 K109 A110 F111 Q112 D113 K114 L115 Y116 P117 F118 T119 H120 D121 A122 V123 R124 Y125 N126 G127 K128 L129 I130 A131 Y132 P133 I134 A135 V136 E137 A138 L139 S140 L141 I142 Y143 N144 K145 D146 L147 L148 P149

## 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: Protein-export protein SecB

Chain A:  70% 8% 19%

M1 S2 E3 Q4 N5 N6 T7 T8 E8 M9 F23 K34 V40 D43 L44 D45 D53 Y56 L60 R61 V62 T63 L68 E71 I86 L98 C113 M117 A135 L136 F137 M138 M139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

- Molecule 1: Protein-export protein SecB

Chain B:  74% 8% 17%

M1 S2 E3 Q4 N5 N6 T7 T8 E8 M9 Q12 I13 K34 T46 L68 A73 S85 I86 I89 Q93 M104 R120 Q125 F137 M138 M139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

- Molecule 1: Protein-export protein SecB

Chain C:  74% 8% 19%

M1 S2 E3 Q4 N5 N6 T7 T8 E8 M9 D20 K34 L44 D45 R61 A73 Q79 C113 M117 P124 Q125 L126 A135 L136 F137 M138 M139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

- Molecule 1: Protein-export protein SecB

Chain D:  71% 10% 19%

M1 S2 E3 Q4 N5 N6 T7 T8 E8 M9 D20 F23 D43 L60 T63 V64 E70 C76 Q79 E90 M94 I114 R120 L126 D134 A135 L136 F137 M138 M139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

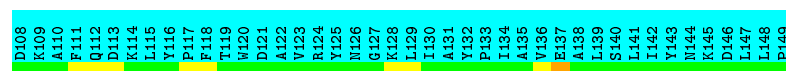
- Molecule 2: Maltose-binding periplasmic protein

Chain E:  100%

D108 K109 A110 F111 Q112 D113 K114 L115 Y116 P117 F118 T119 H120 D121 A122 V123 R124 Y125 N126 G127 K128 L129 I130 A131 Y132 P133 I134 A135 V136 E137 A138 L139 S140 L141 I142 Y143 N144 K145 D146 L147 L148 P149

- Molecule 2: Maltose-binding periplasmic protein

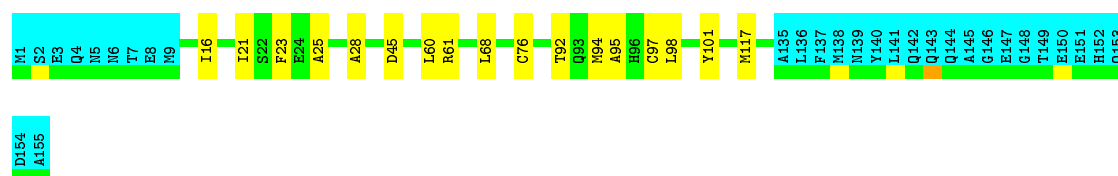
Chain F:  100%




#### 4.2.2 Score per residue for model 2

- Molecule 1: Protein-export protein SecB

Chain A:  70% 11% 19%



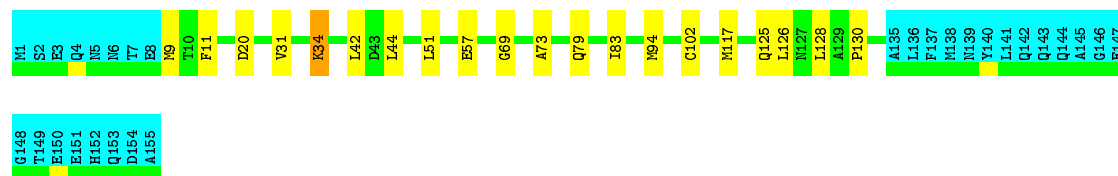
- Molecule 1: Protein-export protein SecB

Chain B:  77% 6% 17%



- Molecule 1: Protein-export protein SecB

Chain C:  68% 12% 19%



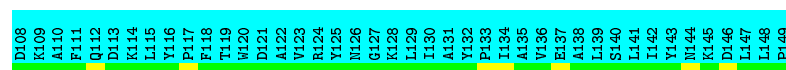
- Molecule 1: Protein-export protein SecB

Chain D:  73% 8% 19%

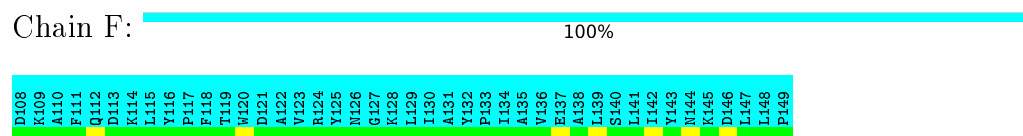


- Molecule 2: Maltose-binding periplasmic protein

Chain E:  100%

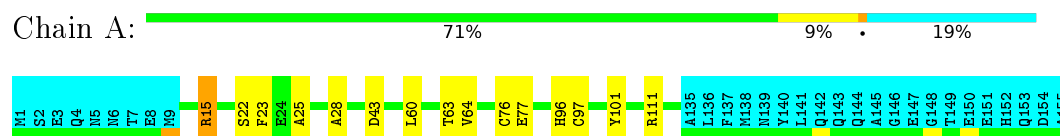


- Molecule 2: Maltose-binding periplasmic protein

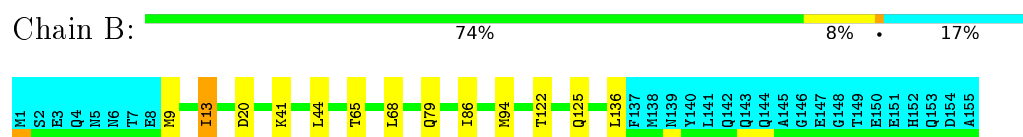


#### 4.2.3 Score per residue for model 3

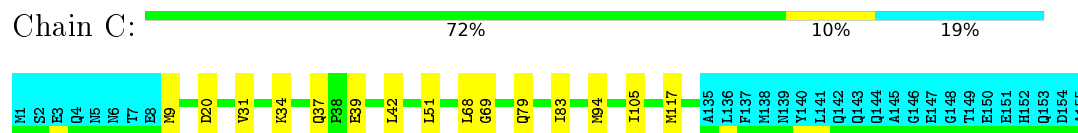
- Molecule 1: Protein-export protein SecB



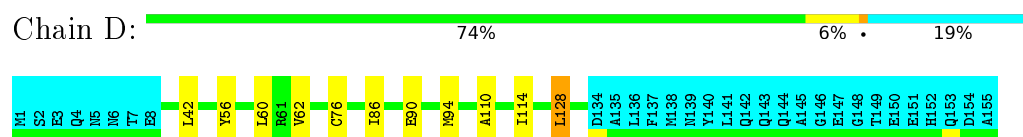
- Molecule 1: Protein-export protein SecB



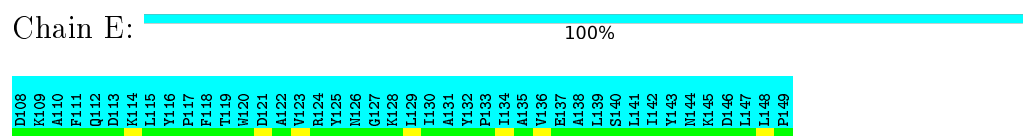
- Molecule 1: Protein-export protein SecB



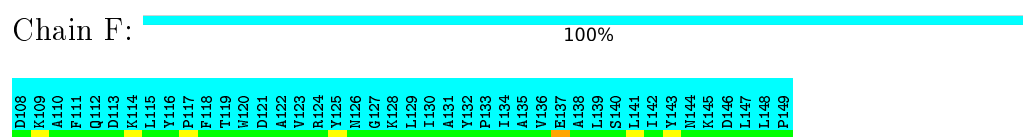
- Molecule 1: Protein-export protein SecB



- Molecule 2: Maltose-binding periplasmic protein



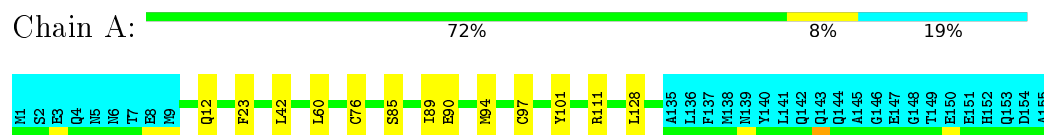
- Molecule 2: Maltose-binding periplasmic protein



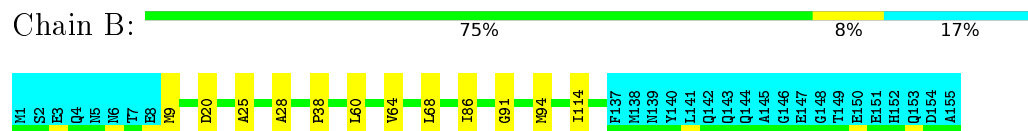


#### 4.2.4 Score per residue for model 4

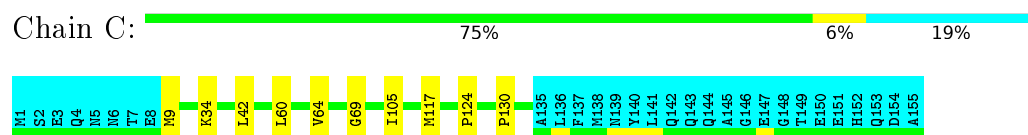
- Molecule 1: Protein-export protein SecB



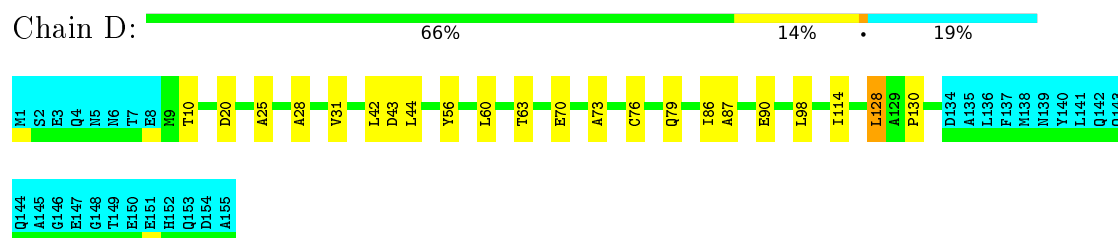
- Molecule 1: Protein-export protein SecB



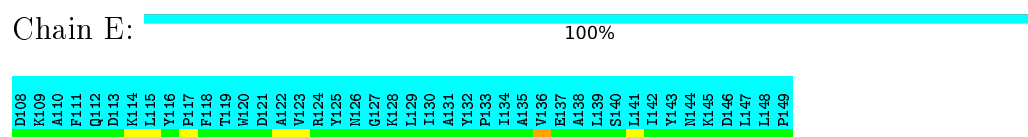
- Molecule 1: Protein-export protein SecB



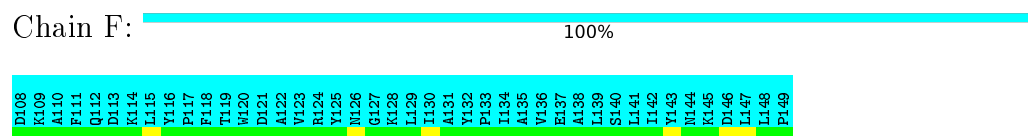
- Molecule 1: Protein-export protein SecB



- Molecule 2: Maltose-binding periplasmic protein




- Molecule 2: Maltose-binding periplasmic protein



#### 4.2.5 Score per residue for model 5

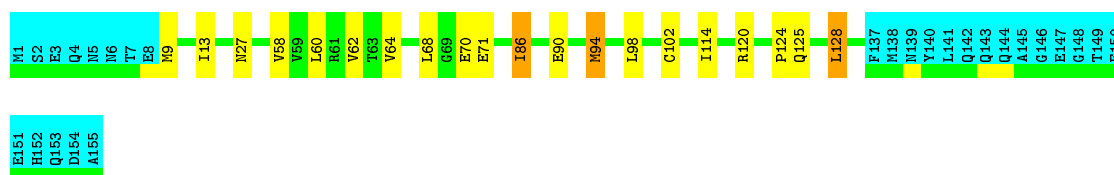
- Molecule 1: Protein-export protein SecB

Chain A:  75% 6% 19%



- Molecule 1: Protein-export protein SecB

Chain B:  70% 11% 17%



- Molecule 1: Protein-export protein SecB

Chain C:  72% 8% 19%



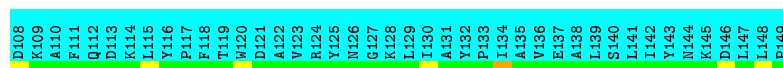
- Molecule 1: Protein-export protein SecB

Chain D:  72% 9% 19%



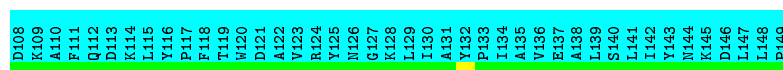
- Molecule 2: Maltose-binding periplasmic protein

Chain E:  100%



- Molecule 2: Maltose-binding periplasmic protein

Chain F:  100%



#### 4.2.6 Score per residue for model 6

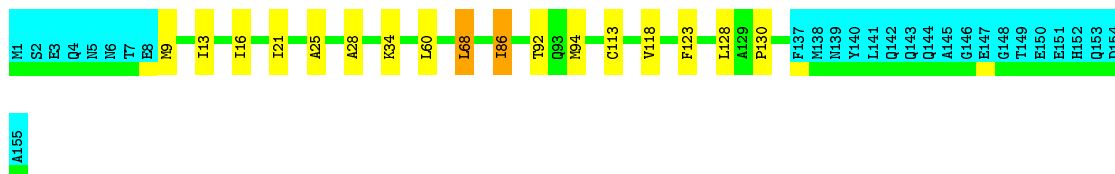
- Molecule 1: Protein-export protein SecB

Chain A:  75% 5% 19%



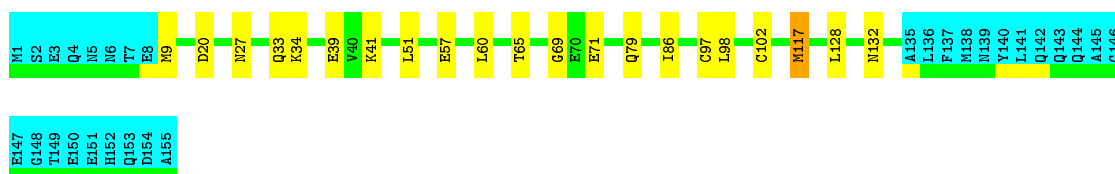
- Molecule 1: Protein-export protein SecB

Chain B: 72% 10% 17%



- Molecule 1: Protein-export protein SecB

Chain C: 68% 13% 19%



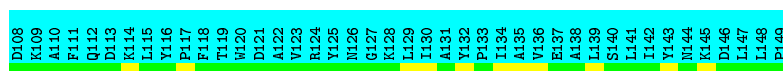
- Molecule 1: Protein-export protein SecB

Chain D: 72% 8% 19%



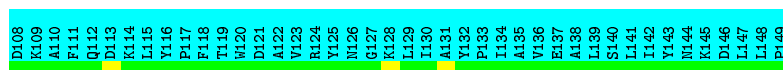
- Molecule 2: Maltose-binding periplasmic protein

Chain E: 100%



- Molecule 2: Maltose-binding periplasmic protein

Chain F: 100%



#### 4.2.7 Score per residue for model 7

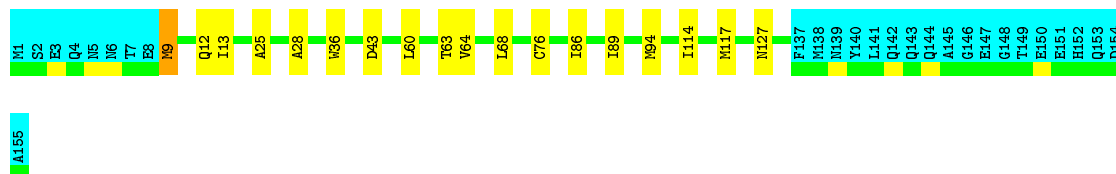
- Molecule 1: Protein-export protein SecB

Chain A: 71% 9% 19%



- Molecule 1: Protein-export protein SecB

Chain B: 71% 11% 17%



- Molecule 1: Protein-export protein SecB

Chain C: 72% 10% 19%



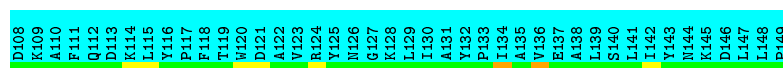
- Molecule 1: Protein-export protein SecB

Chain D: 76% 5% 19%



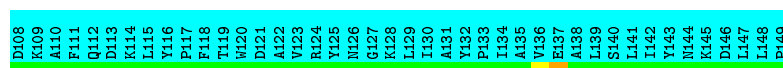
- Molecule 2: Maltose-binding periplasmic protein

Chain E: 100%



- Molecule 2: Maltose-binding periplasmic protein

Chain F: 100%



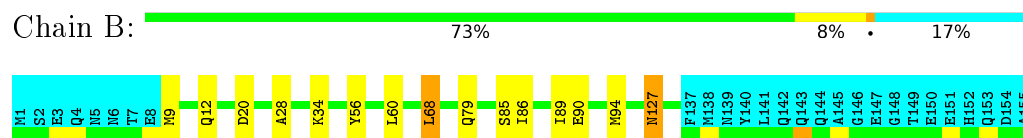
#### 4.2.8 Score per residue for model 8

- Molecule 1: Protein-export protein SecB

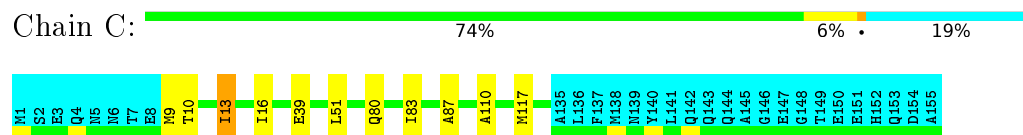
Chain A: 71% 9% 19%



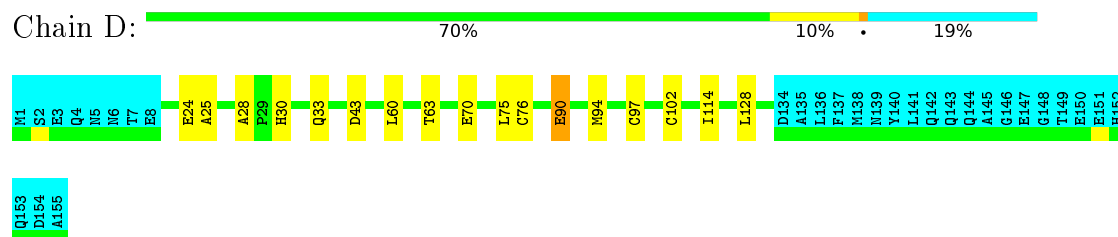
- Molecule 1: Protein-export protein SecB



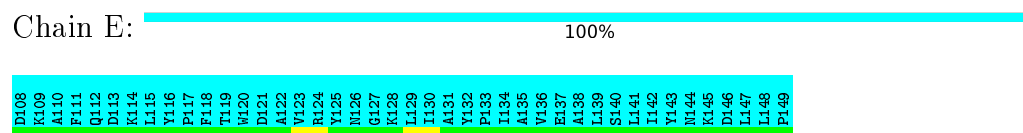
- Molecule 1: Protein-export protein SecB



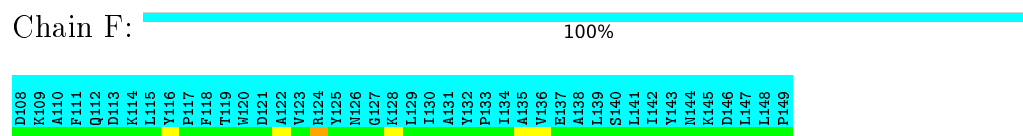
- Molecule 1: Protein-export protein SecB



- Molecule 2: Maltose-binding periplasmic protein

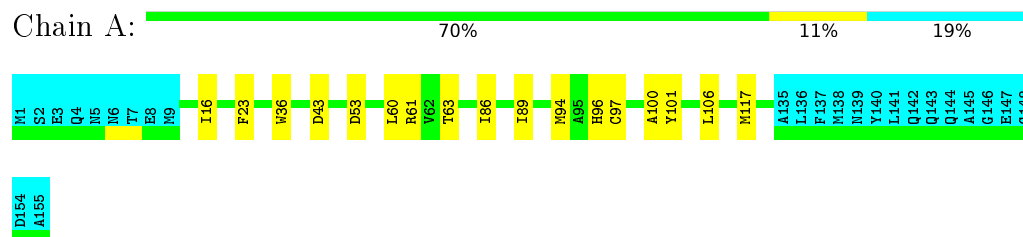


- Molecule 2: Maltose-binding periplasmic protein

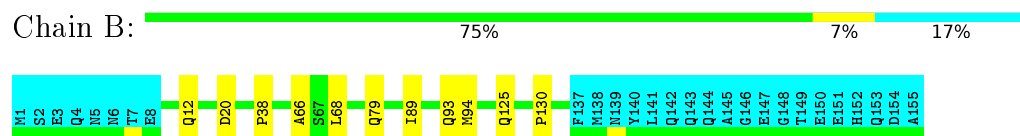


#### 4.2.9 Score per residue for model 9 (medoid)

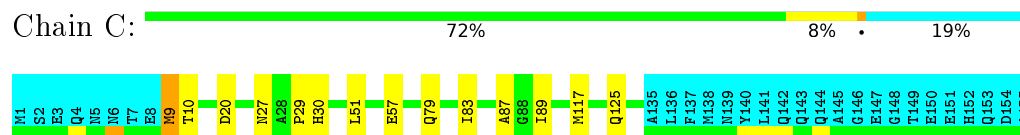
- Molecule 1: Protein-export protein SecB



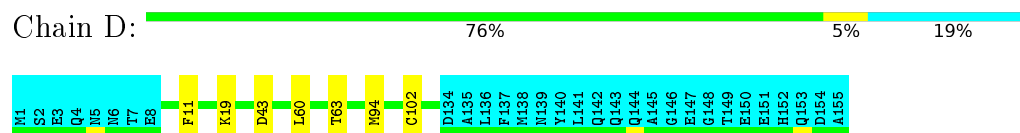
- Molecule 1: Protein-export protein SecB



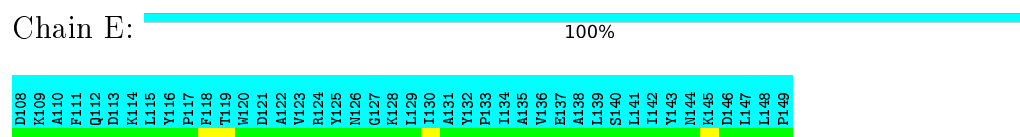
- Molecule 1: Protein-export protein SecB



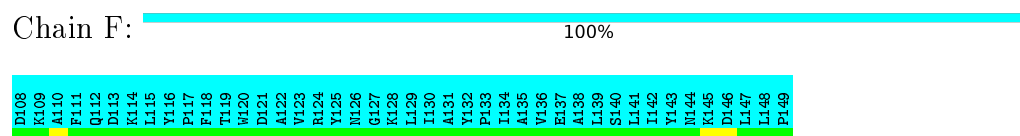
- Molecule 1: Protein-export protein SecB



- Molecule 2: Maltose-binding periplasmic protein

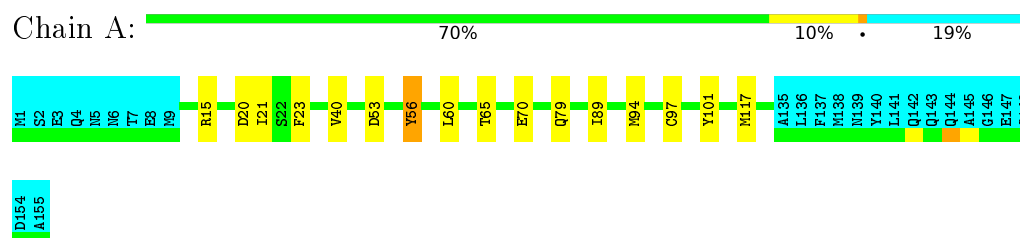


- Molecule 2: Maltose-binding periplasmic protein

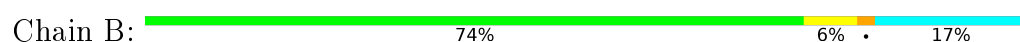


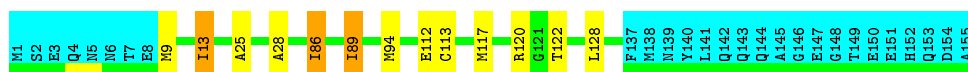
#### 4.2.10 Score per residue for model 10

- Molecule 1: Protein-export protein SecB



- Molecule 1: Protein-export protein SecB





- Molecule 1: Protein-export protein SecB

Chain C: 75% 6% 19%



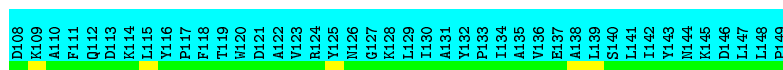
- Molecule 1: Protein-export protein SecB

Chain D: 72% 8% 19%



- Molecule 2: Maltose-binding periplasmic protein

Chain E: 100%



- Molecule 2: Maltose-binding periplasmic protein

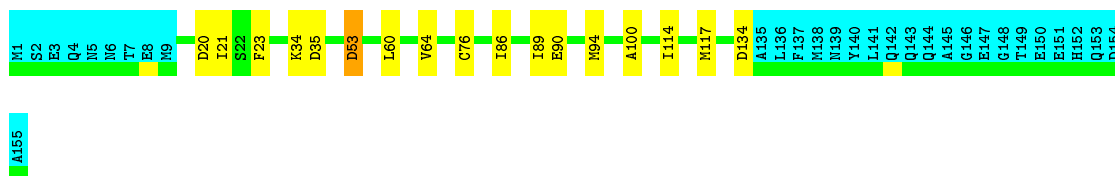
Chain F: 100%



#### 4.2.11 Score per residue for model 11

- Molecule 1: Protein-export protein SecB

Chain A: 70% 10% 19%



- Molecule 1: Protein-export protein SecB

Chain B: 71% 11% 17%



- Molecule 1: Protein-export protein SecB

Chain C:  71% 10% 19%



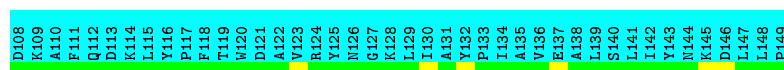
- Molecule 1: Protein-export protein SecB

Chain D:  74% 7% 19%



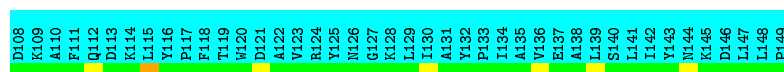
- Molecule 2: Maltose-binding periplasmic protein

Chain E:  100%



- Molecule 2: Maltose-binding periplasmic protein

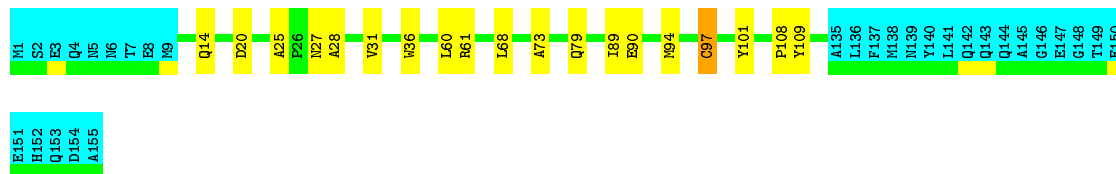
Chain F:  100%




#### 4.2.12 Score per residue for model 12

- Molecule 1: Protein-export protein SecB

Chain A:  68% 12% 19%



- Molecule 1: Protein-export protein SecB

Chain B:  75% 7% 17%



- Molecule 1: Protein-export protein SecB

Chain C:  75% 5% 19%





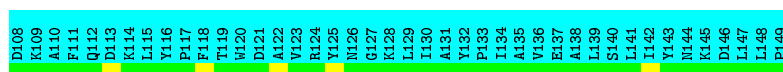
- Molecule 1: Protein-export protein SecB

Chain D: 74% 7% 19%



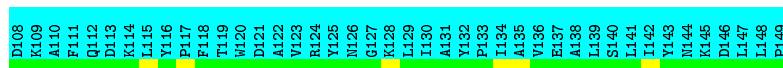
- Molecule 2: Maltose-binding periplasmic protein

Chain E: 100%



- Molecule 2: Maltose-binding periplasmic protein

Chain F: 100%



#### 4.2.13 Score per residue for model 13

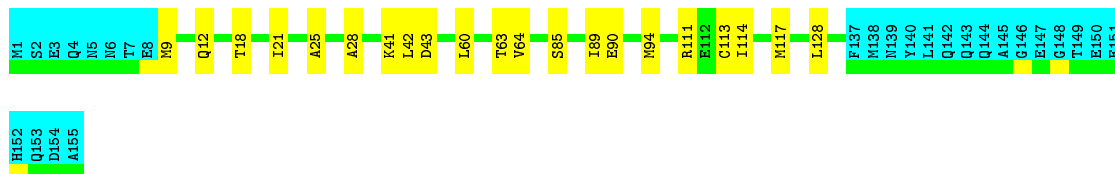
- Molecule 1: Protein-export protein SecB

Chain A: 74% 6% 19%



- Molecule 1: Protein-export protein SecB

Chain B: 69% 14% 17%




- Molecule 1: Protein-export protein SecB

Chain C: 76% 5% 19%



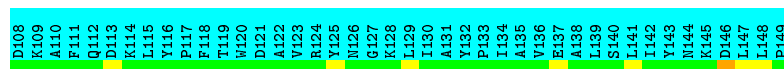
- Molecule 1: Protein-export protein SecB

Chain D:  78% 19%



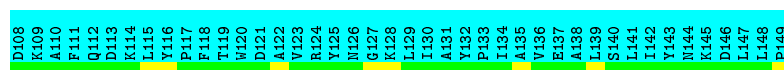
- Molecule 2: Maltose-binding periplasmic protein

Chain E:  100%



- Molecule 2: Maltose-binding periplasmic protein

Chain F:  100%



#### 4.2.14 Score per residue for model 14

- Molecule 1: Protein-export protein SecB

Chain A:  68% 11% 19%



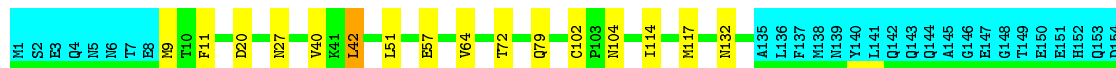
- Molecule 1: Protein-export protein SecB

Chain B:  70% 13% 17%




- Molecule 1: Protein-export protein SecB

Chain C:  71% 10% 19%



A155

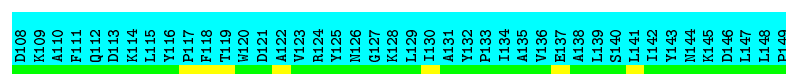
- Molecule 1: Protein-export protein SecB

Chain D:  75% 5% 19%



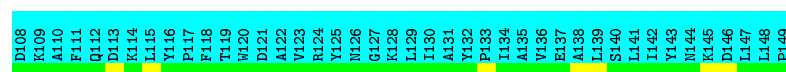
- Molecule 2: Maltose-binding periplasmic protein

Chain E:  100%



- Molecule 2: Maltose-binding periplasmic protein

Chain F:  100%



#### 4.2.15 Score per residue for model 15

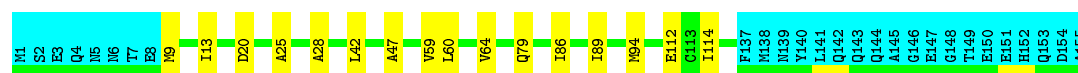
- Molecule 1: Protein-export protein SecB

Chain A:  70% 10% 19%


D154  
A155

- Molecule 1: Protein-export protein SecB

Chain B:  72% 10% 17%

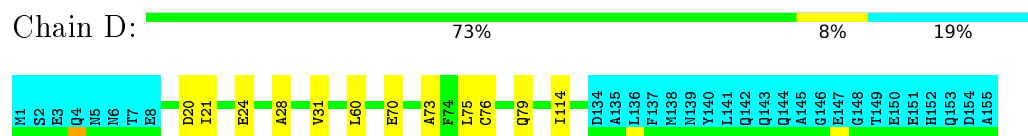


- Molecule 1: Protein-export protein SecB

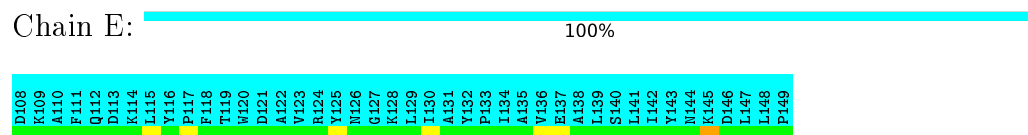
Chain C:  75% 6% 19%



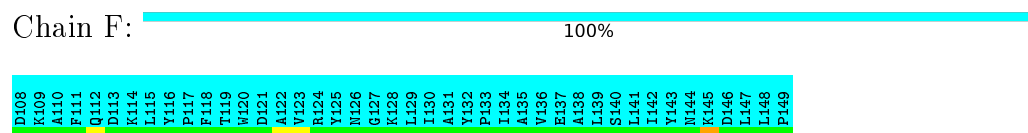
- Molecule 1: Protein-export protein SecB



- Molecule 2: Maltose-binding periplasmic protein

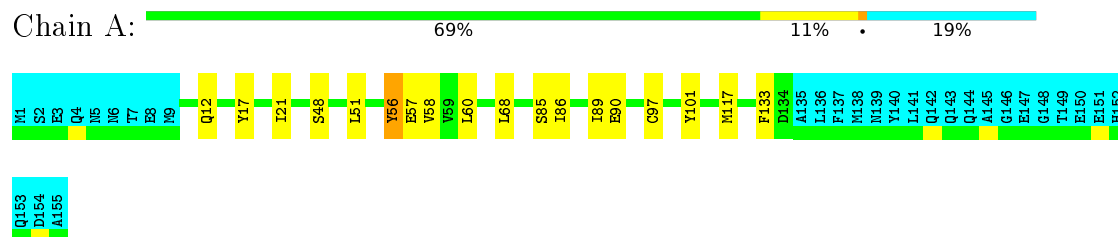


- Molecule 2: Maltose-binding periplasmic protein

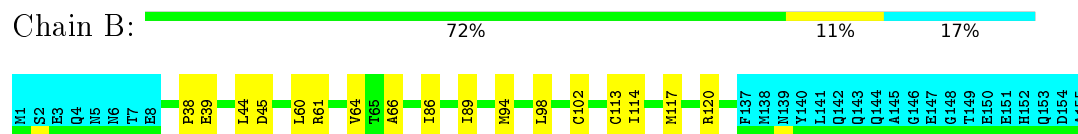


#### 4.2.16 Score per residue for model 16

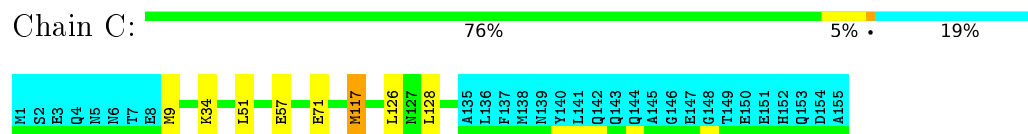
- Molecule 1: Protein-export protein SecB



- Molecule 1: Protein-export protein SecB



- Molecule 1: Protein-export protein SecB



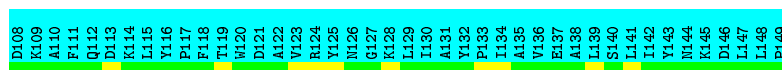
- Molecule 1: Protein-export protein SecB





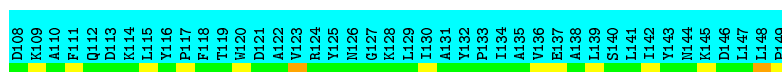
- Molecule 2: Maltose-binding periplasmic protein

Chain E: 100%



- Molecule 2: Maltose-binding periplasmic protein

Chain F: 100%



#### 4.2.17 Score per residue for model 17

- Molecule 1: Protein-export protein SecB

Chain A: 77% 19%



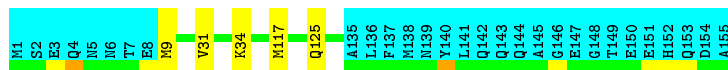
- Molecule 1: Protein-export protein SecB

Chain B: 72% 11% 17%



- Molecule 1: Protein-export protein SecB

Chain C: 78% 19%



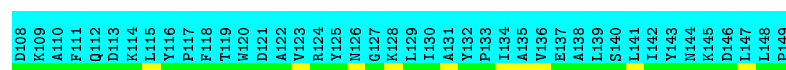
- Molecule 1: Protein-export protein SecB

Chain D: 75% 5% 19%



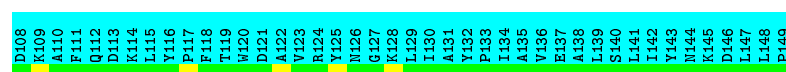
- Molecule 2: Maltose-binding periplasmic protein

Chain E:  100%



- Molecule 2: Maltose-binding periplasmic protein

Chain F:  100%



#### 4.2.18 Score per residue for model 18

- Molecule 1: Protein-export protein SecB

Chain A:  74% 6% 19%




- Molecule 1: Protein-export protein SecB

Chain B:  74% 8% 17%



- Molecule 1: Protein-export protein SecB

Chain C:  75% 6% 19%



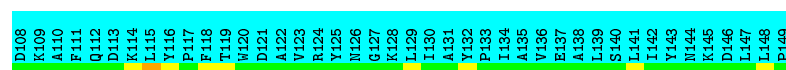
- Molecule 1: Protein-export protein SecB

Chain D:  74% 7% 19%



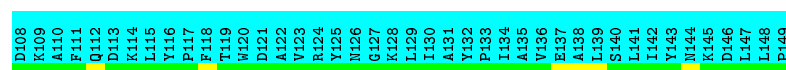
- Molecule 2: Maltose-binding periplasmic protein

Chain E:  100%



- Molecule 2: Maltose-binding periplasmic protein

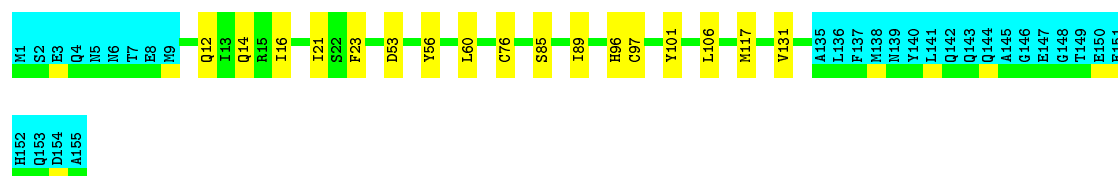
Chain F:  100%



#### 4.2.19 Score per residue for model 19

- Molecule 1: Protein-export protein SecB

Chain A:  70% 11% 19%




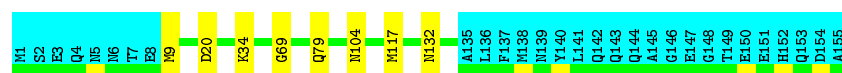
- Molecule 1: Protein-export protein SecB

Chain B:  73% 10% 17%



- Molecule 1: Protein-export protein SecB

Chain C:  76% 5% 19%



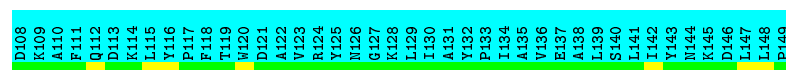
- Molecule 1: Protein-export protein SecB

Chain D:  72% 8% 19%



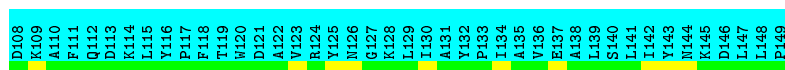
- Molecule 2: Maltose-binding periplasmic protein

Chain E:  100%



- Molecule 2: Maltose-binding periplasmic protein

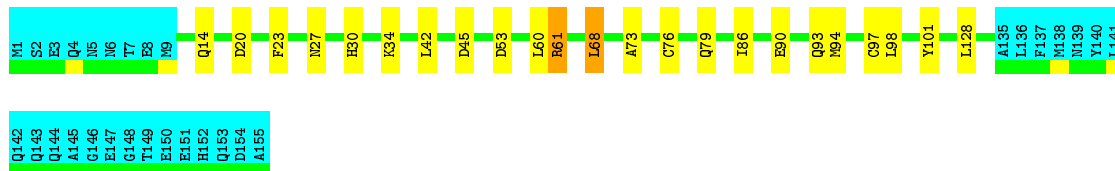
Chain F:  100%



#### 4.2.20 Score per residue for model 20

- Molecule 1: Protein-export protein SecB

Chain A: 66% 14% 19%



- Molecule 1: Protein-export protein SecB

Chain B: 75% 8% 17%



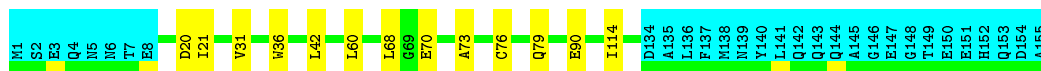
- Molecule 1: Protein-export protein SecB

Chain C: 74% 6% 19%



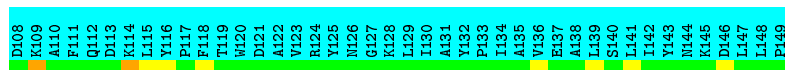
- Molecule 1: Protein-export protein SecB

Chain D: 72% 8% 19%



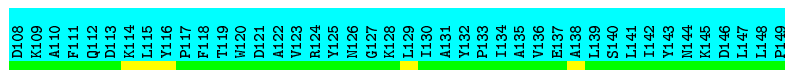
- Molecule 2: Maltose-binding periplasmic protein

Chain E: 100%



- Molecule 2: Maltose-binding periplasmic protein

Chain F: 100%





## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	5jtg_cs.cif
Number of chemical shift lists	6
Total number of shifts	4726
Number of shifts mapped to atoms	4726
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	13%

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 6.1 Standard geometry

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	0.85±0.01	0±0/996 (0.0±0.0%)	0.64±0.02	0±1/1359 (0.0±0.0%)
1	B	0.85±0.01	0±0/1017 (0.0±0.0%)	0.62±0.01	0±0/1387 (0.0±0.0%)
1	C	0.85±0.01	0±0/1004 (0.0±0.0%)	0.62±0.01	0±0/1369 (0.0±0.0%)
1	D	0.84±0.02	0±0/996 (0.0±0.0%)	0.61±0.01	0±0/1358 (0.0±0.0%)
All	All	0.85	0/80260 (0.0%)	0.62	8/109460 (0.0%)

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	56	TYR	CB-CG-CD1	5.63	124.38	121.00	16	6
1	A	61	ARG	NE-CZ-NH2	-5.52	117.54	120.30	6	1
1	A	56	TYR	CB-CG-CD2	-5.02	117.99	121.00	16	1

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	973	946	944	6±2
1	B	994	971	969	6±2
1	C	981	955	953	5±2
1	D	973	951	949	5±2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
2	E	0	0	0	0±0
2	F	0	0	0	0±0
All	All	78420	76460	76300	390

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:25:ALA:HB1	1:B:28:ALA:HB2	0.78	1.54	18	7
1:D:76:CYS:SG	1:D:114:ILE:HG12	0.67	2.30	10	12
1:D:25:ALA:HB1	1:D:28:ALA:HB2	0.63	1.70	2	4
1:A:20:ASP:HB2	1:A:79:GLN:HB2	0.62	1.72	10	2
1:B:25:ALA:CB	1:B:28:ALA:HB2	0.61	2.26	6	9
1:B:43:ASP:HB2	1:B:63:THR:HB	0.59	1.74	11	3
1:A:23:PHE:HB2	1:A:117:MET:SD	0.59	2.37	5	7
1:B:36:TRP:HB2	1:B:68:LEU:HD21	0.59	1.74	20	2
1:A:23:PHE:HD1	1:A:76:CYS:HG	0.58	1.41	4	6
1:A:97:CYS:HA	1:A:101:TYR:HB3	0.58	1.74	4	16
1:B:64:VAL:HG21	1:B:114:ILE:HG21	0.58	1.75	18	9
1:A:51:LEU:HD11	1:A:57:GLU:HB2	0.58	1.74	14	3
1:D:43:ASP:HB2	1:D:63:THR:HB	0.58	1.76	4	4
1:B:89:ILE:HD13	1:B:94:MET:SD	0.58	2.39	15	2
1:C:9:MET:SD	1:C:11:PHE:HB2	0.57	2.39	10	1
1:A:43:ASP:HB2	1:A:63:THR:HB	0.57	1.74	3	5
1:A:100:ALA:HB1	1:A:134:ASP:HA	0.57	1.75	18	3
1:D:11:PHE:HZ	1:D:102:CYS:HG	0.56	1.43	19	1
1:A:15:ARG:HD2	1:B:122:THR:HG21	0.56	1.76	10	1
1:B:40:VAL:HG11	1:B:126:LEU:HD21	0.55	1.77	14	1
1:D:20:ASP:HB3	1:D:79:GLN:HB2	0.55	1.77	5	12
1:C:20:ASP:HB3	1:C:79:GLN:HB2	0.54	1.79	19	8
1:B:97:CYS:SG	1:B:102:CYS:SG	0.54	3.05	14	1
1:B:86:ILE:HB	1:B:89:ILE:HD11	0.54	1.79	1	3
1:D:31:VAL:HG21	1:D:73:ALA:HA	0.53	1.80	15	4
1:B:98:LEU:HA	1:B:102:CYS:SG	0.53	2.43	5	1
1:A:68:LEU:HD23	1:A:68:LEU:H	0.53	1.62	12	2
1:A:86:ILE:HG12	1:A:98:LEU:HD11	0.53	1.80	1	1
1:D:97:CYS:SG	1:D:102:CYS:SG	0.53	3.06	8	1
1:C:64:VAL:HG23	1:C:114:ILE:HD13	0.53	1.81	14	4
1:B:111:ARG:HG3	1:B:128:LEU:HB2	0.53	1.81	13	2
1:B:89:ILE:HD11	1:B:93:GLN:HB2	0.52	1.82	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:125:GLN:HB3	1:C:124:PRO:HA	0.52	1.81	5	1
1:B:25:ALA:HB3	1:B:28:ALA:HB2	0.52	1.82	10	1
1:B:42:LEU:HD12	1:B:64:VAL:HG22	0.52	1.80	18	1
1:B:45:ASP:HB3	1:B:61:ARG:HB3	0.52	1.82	11	3
1:A:20:ASP:HB3	1:A:79:GLN:HB2	0.52	1.81	12	3
1:A:25:ALA:HB1	1:A:28:ALA:HB2	0.51	1.82	12	5
1:C:34:LYS:HE3	1:C:73:ALA:HA	0.51	1.82	2	2
1:C:51:LEU:HD11	1:C:57:GLU:HB2	0.51	1.82	11	8
1:B:62:VAL:HG11	1:B:128:LEU:HD11	0.51	1.82	5	1
1:C:31:VAL:HA	1:C:34:LYS:HE2	0.50	1.82	18	3
1:A:45:ASP:HB3	1:A:61:ARG:HB2	0.50	1.83	20	4
1:D:42:LEU:HD11	1:D:128:LEU:HD21	0.50	1.83	4	1
1:C:37:GLN:HB3	1:C:68:LEU:HD13	0.50	1.81	3	1
1:C:41:LYS:HB2	1:C:65:THR:HB	0.49	1.84	6	2
1:B:36:TRP:HB3	1:B:68:LEU:HD21	0.49	1.84	12	2
1:C:61:ARG:HG2	1:C:79:GLN:HG2	0.49	1.83	1	1
1:B:9:MET:HB3	1:B:89:ILE:HG23	0.49	1.84	7	1
1:B:125:GLN:HB3	1:C:125:GLN:HE21	0.49	1.68	9	1
1:B:31:VAL:HG21	1:B:73:ALA:HA	0.49	1.85	17	1
1:D:42:LEU:HD22	1:D:128:LEU:HD11	0.49	1.84	17	1
1:C:51:LEU:HD11	1:C:83:ILE:HD12	0.49	1.83	7	6
1:C:60:LEU:H	1:C:60:LEU:HD23	0.49	1.68	13	1
1:A:21:ILE:HD13	1:B:117:MET:SD	0.48	2.48	10	2
1:C:10:THR:HB	1:C:87:ALA:HB3	0.48	1.83	9	2
1:A:34:LYS:HD3	1:A:68:LEU:HD21	0.48	1.85	1	1
1:C:31:VAL:HA	1:C:34:LYS:HE3	0.48	1.84	3	2
1:C:97:CYS:SG	1:C:102:CYS:SG	0.48	3.10	7	2
1:A:16:ILE:HG23	1:A:106:LEU:HD23	0.48	1.86	9	4
1:C:13:ILE:HD11	1:C:16:ILE:HG13	0.48	1.84	8	4
1:A:15:ARG:HH11	1:A:83:ILE:HD12	0.48	1.67	14	1
1:C:27:ASN:HB3	1:C:30:HIS:HB2	0.47	1.86	11	1
1:D:10:THR:HB	1:D:87:ALA:HB3	0.47	1.85	11	2
1:C:9:MET:HG2	1:C:89:ILE:HB	0.47	1.86	9	1
1:C:42:LEU:HD23	1:C:42:LEU:H	0.47	1.69	3	1
1:D:76:CYS:SG	1:D:114:ILE:HG23	0.47	2.49	2	3
1:D:56:TYR:HB2	1:D:86:ILE:HD13	0.47	1.86	4	2
1:B:47:ALA:HB3	1:B:59:VAL:HB	0.47	1.87	15	1
1:A:34:LYS:NZ	1:A:71:GLU:HG3	0.47	2.25	1	1
1:B:13:ILE:H	1:B:13:ILE:HD13	0.47	1.70	1	2
1:B:34:LYS:HB3	1:B:68:LEU:HD22	0.47	1.87	6	1
1:B:86:ILE:HG21	1:B:94:MET:SD	0.47	2.50	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:39:GLU:O	1:B:66:ALA:HA	0.46	2.09	16	3
1:B:20:ASP:HB3	1:B:79:GLN:HB2	0.46	1.86	8	5
1:A:94:MET:SD	1:A:98:LEU:HG	0.46	2.50	2	1
1:D:86:ILE:HG21	1:D:94:MET:HG2	0.46	1.86	3	1
1:B:12:GLN:HB3	1:B:85:SER:HB2	0.46	1.86	13	3
1:D:90:GLU:HA	1:D:94:MET:HB2	0.46	1.87	8	2
1:B:13:ILE:HD13	1:B:13:ILE:H	0.46	1.70	11	2
1:B:130:PRO:HG3	1:D:16:ILE:HD13	0.46	1.86	19	1
1:A:128:LEU:HD23	1:A:128:LEU:H	0.46	1.71	7	1
1:D:42:LEU:H	1:D:42:LEU:HD23	0.46	1.71	11	1
1:D:36:TRP:HB3	1:D:68:LEU:HD11	0.46	1.86	18	4
1:A:64:VAL:HB	1:A:76:CYS:HB2	0.46	1.86	3	2
1:A:13:ILE:HD12	1:A:13:ILE:H	0.46	1.71	15	1
1:A:114:ILE:O	1:A:118:VAL:HG23	0.46	2.11	14	1
1:C:17:TYR:HE2	1:D:28:ALA:HB1	0.45	1.71	12	2
1:C:117:MET:HE3	1:D:21:ILE:HD13	0.45	1.88	16	3
1:A:108:PRO:HB2	1:C:108:PRO:HG2	0.45	1.88	12	1
1:B:118:VAL:HG22	1:B:123:PHE:HB2	0.45	1.87	6	1
1:B:38:PRO:HB2	1:B:66:ALA:HB1	0.45	1.88	16	2
1:B:18:THR:HG21	1:B:21:ILE:HD11	0.45	1.88	13	1
1:A:115:THR:HG23	1:A:125:GLN:HB2	0.45	1.88	14	1
1:A:12:GLN:HB3	1:A:85:SER:HB3	0.45	1.87	19	2
1:D:62:VAL:HG21	1:D:110:ALA:HB1	0.45	1.89	3	1
1:A:21:ILE:HG23	1:A:117:MET:SD	0.45	2.52	19	1
1:D:11:PHE:CE2	1:D:102:CYS:SG	0.45	3.09	5	1
1:C:86:ILE:HG13	1:C:98:LEU:HD21	0.45	1.89	6	1
1:A:17:TYR:HE2	1:B:28:ALA:HB1	0.45	1.72	8	1
1:B:68:LEU:HD12	1:B:73:ALA:HB2	0.44	1.89	1	1
1:B:90:GLU:HA	1:B:94:MET:SD	0.44	2.51	8	1
1:C:14:GLN:HB2	1:C:83:ILE:HB	0.44	1.89	18	1
1:A:27:ASN:HB3	1:A:30:HIS:HB2	0.44	1.87	20	3
1:A:64:VAL:HG21	1:A:114:ILE:HG21	0.44	1.88	11	1
1:A:113:CYS:SG	1:B:120:ARG:HD3	0.44	2.53	5	2
1:D:11:PHE:HA	1:D:85:SER:O	0.44	2.12	2	1
1:D:42:LEU:HD13	1:D:128:LEU:HD21	0.44	1.88	3	1
1:A:89:ILE:HB	1:A:94:MET:SD	0.44	2.53	11	1
1:B:21:ILE:HD11	1:B:113:CYS:SG	0.44	2.52	13	2
1:D:42:LEU:HG	1:D:128:LEU:HD21	0.44	1.89	10	1
1:A:31:VAL:HG11	1:A:73:ALA:HA	0.44	1.90	12	1
1:C:27:ASN:HB2	1:C:72:THR:O	0.44	2.13	14	1
1:D:64:VAL:HG11	1:D:126:LEU:HD11	0.44	1.90	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:42:LEU:HD23	1:C:64:VAL:HG22	0.44	1.90	4	1
1:D:16:ILE:N	1:D:16:ILE:HD12	0.44	2.27	7	3
1:D:34:LYS:HB3	1:D:68:LEU:HD23	0.44	1.89	12	1
1:C:28:ALA:HB3	1:C:29:PRO:HD3	0.44	1.90	20	1
1:C:113:CYS:SG	1:D:120:ARG:HD3	0.44	2.53	1	1
1:A:21:ILE:CG2	1:A:117:MET:SD	0.44	3.06	16	2
1:B:13:ILE:HG21	1:B:16:ILE:HG13	0.44	1.90	6	1
1:A:122:THR:HG22	1:B:17:TYR:HB3	0.44	1.89	17	1
1:B:68:LEU:HB2	1:B:73:ALA:HB2	0.44	1.90	19	1
1:C:45:ASP:HB3	1:C:61:ARG:HB2	0.44	1.90	1	1
1:C:29:PRO:HD3	1:D:19:LYS:HZ1	0.44	1.73	9	1
1:D:24:GLU:HB2	1:D:75:LEU:HB2	0.43	1.90	11	4
1:C:27:ASN:ND2	1:C:71:GLU:HG3	0.43	2.28	6	1
1:A:16:ILE:HD13	1:C:130:PRO:HG3	0.43	1.89	2	1
1:B:34:LYS:HD2	1:B:68:LEU:HB3	0.43	1.88	8	1
1:B:58:VAL:HG21	1:B:98:LEU:HB3	0.43	1.89	5	1
1:C:125:GLN:NE2	1:C:127:ASN:HD21	0.43	2.12	11	1
1:B:34:LYS:HA	1:B:34:LYS:HE2	0.43	1.90	19	1
1:A:34:LYS:HD3	1:A:35:ASP:H	0.43	1.73	11	1
1:C:42:LEU:HD13	1:C:42:LEU:H	0.43	1.72	14	1
1:B:113:CYS:O	1:B:117:MET:HG2	0.43	2.14	14	7
1:C:11:PHE:HE1	1:C:102:CYS:SG	0.43	2.37	2	1
1:B:117:MET:HA	1:B:120:ARG:HD2	0.43	1.91	10	1
1:A:12:GLN:HB2	1:A:85:SER:HB3	0.43	1.90	16	1
1:B:98:LEU:HD12	1:B:102:CYS:SG	0.43	2.54	16	1
1:A:100:ALA:HB2	1:A:133:PHE:HD2	0.42	1.73	8	1
1:A:96:HIS:O	1:A:100:ALA:HB3	0.42	2.14	9	1
1:C:27:ASN:HB3	1:C:30:HIS:HB3	0.42	1.90	9	1
1:B:94:MET:SD	1:B:98:LEU:HD11	0.42	2.54	12	1
1:B:11:PHE:HE1	1:B:97:CYS:SG	0.42	2.38	14	1
1:C:20:ASP:HA	1:D:23:PHE:O	0.42	2.14	13	2
1:A:21:ILE:HB	1:B:23:PHE:HB3	0.42	1.89	18	2
1:B:86:ILE:HG12	1:B:98:LEU:HD13	0.42	1.91	16	1
1:B:27:ASN:ND2	1:B:71:GLU:HB2	0.42	2.30	5	1
1:A:11:PHE:HZ	1:A:102:CYS:HG	0.42	1.57	14	1
1:B:86:ILE:HG21	1:B:98:LEU:HD11	0.42	1.91	5	1
1:C:61:ARG:HG3	1:C:79:GLN:HG2	0.42	1.91	20	1
1:A:34:LYS:HB3	1:A:68:LEU:HD11	0.42	1.92	17	1
1:B:41:LYS:HB3	1:B:65:THR:HB	0.42	1.91	3	1
1:B:76:CYS:SG	1:B:117:MET:HB2	0.42	2.55	7	1
1:C:42:LEU:HD13	1:C:128:LEU:HD11	0.41	1.90	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:9:MET:SD	1:C:89:ILE:HD12	0.41	2.55	9	1
1:A:17:TYR:HB3	1:B:120:ARG:O	0.41	2.15	16	1
1:A:92:THR:HA	1:A:95:ALA:HB3	0.41	1.93	2	1
1:D:44:LEU:H	1:D:44:LEU:HD23	0.41	1.75	5	1
1:D:45:ASP:HB3	1:D:61:ARG:HB3	0.41	1.91	6	1
1:D:21:ILE:CG2	1:D:117:MET:SD	0.41	3.08	12	1
1:D:25:ALA:CB	1:D:28:ALA:HB2	0.41	2.45	6	1
1:D:11:PHE:HE2	1:D:102:CYS:HG	0.41	1.52	9	1
1:A:109:TYR:CE1	1:C:108:PRO:HA	0.41	2.51	12	1
1:A:74:PHE:HE1	1:A:76:CYS:HG	0.41	1.53	14	1
1:A:42:LEU:HD23	1:A:42:LEU:H	0.41	1.75	4	1
1:A:74:PHE:CE1	1:A:76:CYS:SG	0.41	3.12	14	1
1:C:34:LYS:HE3	1:C:71:GLU:HG3	0.41	1.92	16	1
1:D:51:LEU:HD11	1:D:57:GLU:HB2	0.41	1.91	19	1
1:B:61:ARG:HB2	1:B:79:GLN:HG2	0.41	1.93	20	1
1:A:15:ARG:HD3	1:B:122:THR:HG21	0.41	1.92	3	1
1:A:111:ARG:NH1	1:C:105:ILE:HD12	0.41	2.31	3	2
1:D:30:HIS:HA	1:D:33:GLN:NE2	0.41	2.30	8	1
1:A:19:LYS:HE3	1:B:28:ALA:HB3	0.41	1.93	13	1
1:C:104:ASN:ND2	1:C:132:ASN:HD22	0.41	2.13	19	1
1:B:34:LYS:HD2	1:B:68:LEU:HB2	0.41	1.93	1	1
1:D:64:VAL:HG21	1:D:114:ILE:HG21	0.41	1.92	5	1
1:C:11:PHE:CE1	1:C:102:CYS:SG	0.41	3.11	14	1
1:B:44:LEU:HD21	1:B:131:VAL:HG11	0.41	1.92	17	1
1:C:11:PHE:HE1	1:C:102:CYS:HG	0.41	1.57	2	1
1:D:86:ILE:HG12	1:D:98:LEU:HD21	0.41	1.92	4	1
1:C:80:GLN:HB2	1:C:110:ALA:HB2	0.41	1.92	10	3
1:A:25:ALA:CB	1:A:28:ALA:HB2	0.41	2.46	8	1
1:A:40:VAL:HA	1:A:65:THR:O	0.41	2.16	10	1
1:A:20:ASP:HA	1:B:23:PHE:O	0.41	2.16	11	1
1:A:22:SER:HB3	1:A:77:GLU:HB2	0.41	1.92	3	1
1:C:122:THR:HG23	1:D:17:TYR:HB3	0.41	1.93	12	1
1:C:17:TYR:CE2	1:D:28:ALA:HB1	0.41	2.51	15	1
1:B:9:MET:SD	1:B:89:ILE:HD12	0.41	2.55	18	1
1:D:47:ALA:HB3	1:D:59:VAL:HB	0.41	1.93	19	1
1:A:48:SER:HB3	1:A:58:VAL:HG22	0.40	1.93	16	1
1:A:23:PHE:O	1:B:20:ASP:HA	0.40	2.17	4	1
1:B:89:ILE:H	1:B:89:ILE:HD13	0.40	1.75	10	1
1:B:125:GLN:OE1	1:C:124:PRO:HA	0.40	2.17	1	1
1:B:86:ILE:H	1:B:86:ILE:HD13	0.40	1.76	6	1
1:B:43:ASP:HB3	1:B:63:THR:HB	0.40	1.94	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:LEU:HB2	1:A:73:ALA:HB2	0.40	1.94	20	1
1:B:21:ILE:CD1	1:B:113:CYS:SG	0.40	3.10	14	1
1:C:104:ASN:HD21	1:C:132:ASN:ND2	0.40	2.15	14	1
1:D:90:GLU:HA	1:D:94:MET:SD	0.40	2.57	14	1
1:C:117:MET:HE2	1:D:21:ILE:HG21	0.40	1.93	20	1

## 6.3 Torsion angles

### 6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	125/155 (81%)	120±2 (96±1%)	5±1 (4±1%)	0±0 (0±0%)	43	81
1	B	128/155 (83%)	121±1 (94±1%)	6±1 (5±1%)	1±1 (1±0%)	31	76
1	C	126/155 (81%)	116±2 (92±2%)	8±2 (6±2%)	2±1 (1±0%)	21	68
1	D	125/155 (81%)	120±2 (96±1%)	5±2 (4±2%)	0±0 (0±0%)	56	85
2	E	0	-	-	-	-	-
2	F	0	-	-	-	-	-
All	All	10080/14080 (72%)	9525 (94%)	493 (5%)	62 (1%)	34	78

All 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	9	MET	20
1	B	9	MET	14
1	C	69	GLY	8
1	A	53	ASP	8
1	D	9	MET	4
1	B	130	PRO	3
1	C	130	PRO	2
1	B	38	PRO	1
1	A	36	TRP	1
1	B	124	PRO	1



### 6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	107/132 (81%)	103±2 (96±2%)	4±2 (4±2%)	42	84
1	B	109/132 (83%)	105±2 (96±1%)	4±2 (4±1%)	42	85
1	C	108/132 (82%)	105±2 (97±2%)	3±2 (3±2%)	51	90
1	D	107/132 (81%)	104±1 (97±1%)	3±1 (3±1%)	50	89
2	E	0	-	-	-	-
2	F	0	-	-	-	-
All	All	8620/12000 (72%)	8309 (96%)	311 (4%)	46	87

All 84 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	C	117	MET	20
1	A	60	LEU	20
1	D	60	LEU	20
1	B	60	LEU	16
1	D	90	GLU	15
1	B	86	ILE	10
1	B	13	ILE	9
1	A	68	LEU	8
1	C	34	LYS	8
1	D	70	GLU	8
1	A	89	ILE	7
1	B	68	LEU	7
1	A	61	ARG	6
1	D	128	LEU	6
1	B	94	MET	5
1	A	56	TYR	5
1	A	90	GLU	5
1	C	128	LEU	5
1	C	125	GLN	4
1	A	86	ILE	4
1	B	112	GLU	4
1	B	128	LEU	4
1	B	90	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	C	44	LEU	4
1	D	94	MET	4
1	B	89	ILE	4
1	A	94	MET	4
1	A	14	GLN	4
1	C	94	MET	4
1	C	39	GLU	4
1	C	60	LEU	4
1	C	42	LEU	3
1	B	42	LEU	3
1	B	127	ASN	3
1	B	125	GLN	3
1	A	15	ARG	3
1	D	42	LEU	3
1	B	104	ASN	2
1	A	128	LEU	2
1	A	44	LEU	2
1	C	104	ASN	2
1	B	70	GLU	2
1	A	98	LEU	2
1	C	13	ILE	2
1	B	56	TYR	2
1	B	36	TRP	2
1	A	96	HIS	2
1	D	44	LEU	2
1	A	13	ILE	2
1	C	126	LEU	2
1	D	36	TRP	2
1	C	70	GLU	1
1	B	93	GLN	1
1	C	93	GLN	1
1	B	12	GLN	1
1	A	101	TYR	1
1	B	98	LEU	1
1	C	86	ILE	1
1	B	33	GLN	1
1	A	93	GLN	1
1	C	132	ASN	1
1	A	34	LYS	1
1	A	70	GLU	1
1	A	53	ASP	1
1	A	42	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	C	33	GLN	1
1	D	125	GLN	1
1	A	74	PHE	1
1	D	40	VAL	1
1	B	41	LYS	1
1	D	9	MET	1
1	A	97	CYS	1
1	B	92	THR	1
1	D	54	ASP	1
1	A	27	ASN	1
1	A	30	HIS	1
1	D	13	ILE	1
1	D	14	GLN	1
1	B	136	LEU	1
1	D	93	GLN	1
1	A	39	GLU	1
1	B	46	THR	1
1	A	133	PHE	1
1	D	53	ASP	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 6.7 Other polymers ⓘ

There are no such molecules in this entry.

## 6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 13% for the well-defined parts and 13% for the entire structure.

### 7.1 Chemical shift list 1

File name: 5jtq\_cs.cif

Chemical shift list name: *assigned\_chemical\_shift\_5*

#### 7.1.1 Bookkeeping

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

Total number of shifts	270
Number of shifts mapped to atoms	270
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	40	$-0.51 \pm 0.07$	Should be applied
$^{13}\text{C}_\beta$	39	$0.54 \pm 0.20$	Should be applied
$^{13}\text{C}'$	35	$-0.45 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	34	$-1.17 \pm 0.30$	Should be applied

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 6 atoms were assigned a chemical shift out of a possible 6023. 0 out of 81 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	4/2464 (0%)	1/980 (0%)	2/1008 (0%)	1/476 (0%)
Sidechain	2/3031 (0%)	1/1767 (0%)	1/1152 (0%)	0/112 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	0/528 (0%)	0/280 (0%)	0/228 (0%)	0/20 (0%)
Overall	6/6023 (0%)	2/3027 (0%)	3/2388 (0%)	1/608 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 3%, i.e. 223 atoms were assigned a chemical shift out of a possible 8466. 0 out of 104 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	143/3452 (4%)	34/1374 (2%)	75/1408 (5%)	34/670 (5%)
Sidechain	80/4262 (2%)	23/2486 (1%)	57/1612 (4%)	0/164 (0%)
Aromatic	0/752 (0%)	0/396 (0%)	0/326 (0%)	0/30 (0%)
Overall	223/8466 (3%)	57/4256 (1%)	132/3346 (4%)	34/864 (4%)

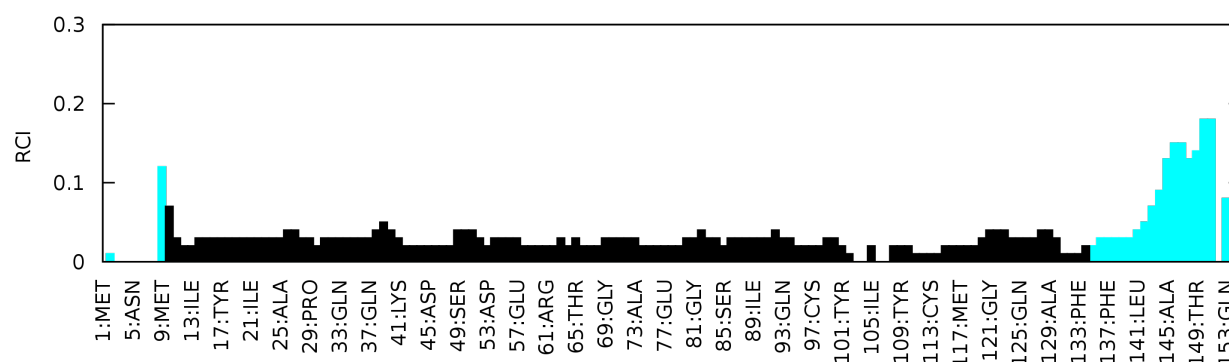
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

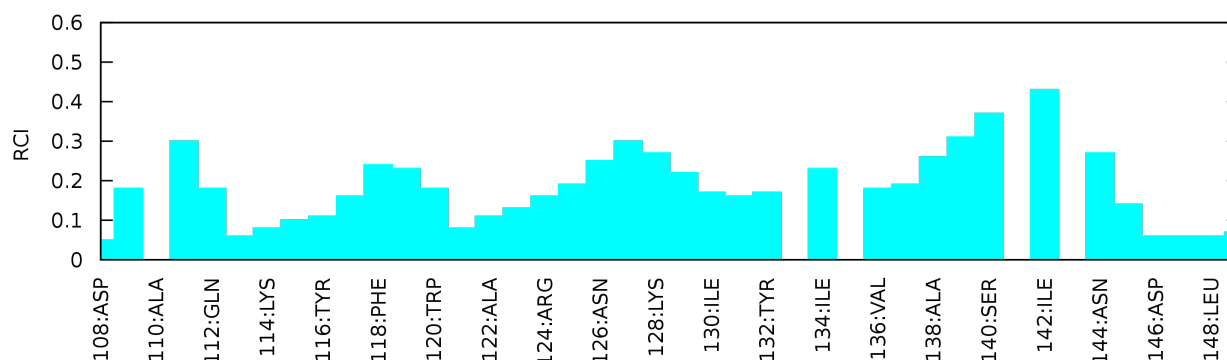
#### 7.1.5 Random Coil Index (RCI) plots [i](#)

The images below report *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.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain E:



## 7.2 Chemical shift list 2

File name: 5jtq\_cs.cif

Chemical shift list name: *assigned\_chemical\_shift\_6*

### 7.2.1 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	270
Number of shifts mapped to atoms	270
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

### 7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	40	$-0.50 \pm 0.18$	Should be applied
$^{13}\text{C}_\beta$	39	$0.52 \pm 0.38$	None needed (imprecise)
$^{13}\text{C}'$	35	$-0.43 \pm 0.24$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	34	$-1.16 \pm 0.37$	Should be applied

### 7.2.3 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 0%, i.e. 6 atoms were assigned a chemical shift out of a possible 6023. 0 out of 81 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	4/2464 (0%)	1/980 (0%)	2/1008 (0%)	1/476 (0%)
Sidechain	2/3031 (0%)	1/1767 (0%)	1/1152 (0%)	0/112 (0%)
Aromatic	0/528 (0%)	0/280 (0%)	0/228 (0%)	0/20 (0%)
Overall	6/6023 (0%)	2/3027 (0%)	3/2388 (0%)	1/608 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 3%, i.e. 223 atoms were assigned a chemical shift out of a possible 8466. 0 out of 104 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	143/3452 (4%)	34/1374 (2%)	75/1408 (5%)	34/670 (5%)
Sidechain	80/4262 (2%)	23/2486 (1%)	57/1612 (4%)	0/164 (0%)
Aromatic	0/752 (0%)	0/396 (0%)	0/326 (0%)	0/30 (0%)
Overall	223/8466 (3%)	57/4256 (1%)	132/3346 (4%)	34/864 (4%)

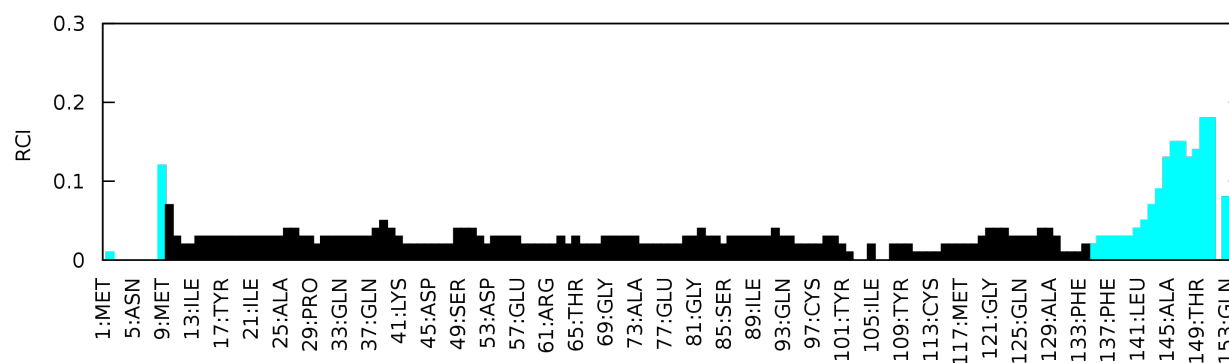
#### 7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

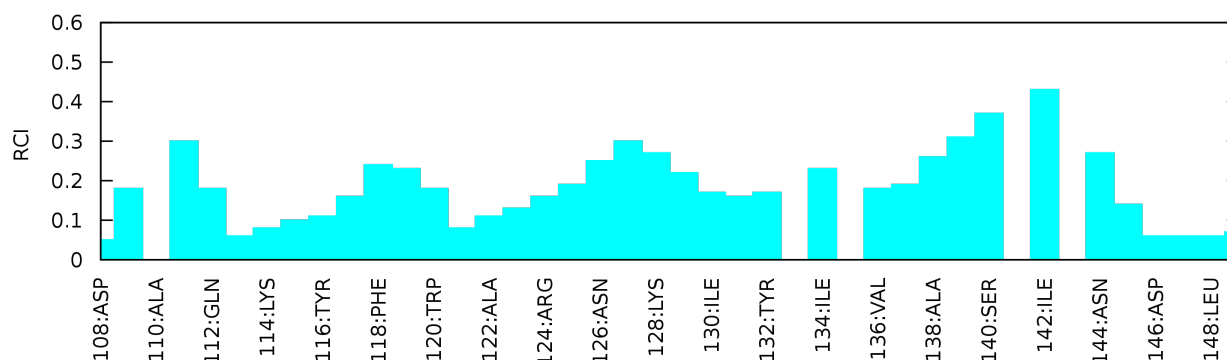
The images below report *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted 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.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain E:





### 7.3 Chemical shift list 3

File name: 5jtq\_cs.cif

Chemical shift list name: *assigned\_chemical\_shift\_list\_1*

#### 7.3.1 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	1049
Number of shifts mapped to atoms	1049
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

#### 7.3.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	139	$0.25 \pm 0.10$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	128	$0.85 \pm 0.18$	Should be applied
$^{13}\text{C}'$	137	$0.29 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	133	$-1.14 \pm 0.32$	Should be applied

#### 7.3.3 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 13%, i.e. 790 atoms were assigned a chemical shift out of a possible 6023. 0 out of 81 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	459/2464 (19%)	112/980 (11%)	235/1008 (23%)	112/476 (24%)
Sidechain	218/3031 (7%)	60/1767 (3%)	158/1152 (14%)	0/112 (0%)
Aromatic	113/528 (21%)	57/280 (20%)	55/228 (24%)	1/20 (5%)
Overall	790/6023 (13%)	229/3027 (8%)	448/2388 (19%)	113/608 (19%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 11%, i.e. 930 atoms were assigned a chemical shift out of a possible 8466. 0 out of 104 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	542/3452 (16%)	133/1374 (10%)	276/1408 (20%)	133/670 (20%)
Sidechain	255/4262 (6%)	70/2486 (3%)	185/1612 (11%)	0/164 (0%)
Aromatic	133/752 (18%)	67/396 (17%)	65/326 (20%)	1/30 (3%)
Overall	930/8466 (11%)	270/4256 (6%)	526/3346 (16%)	134/864 (16%)

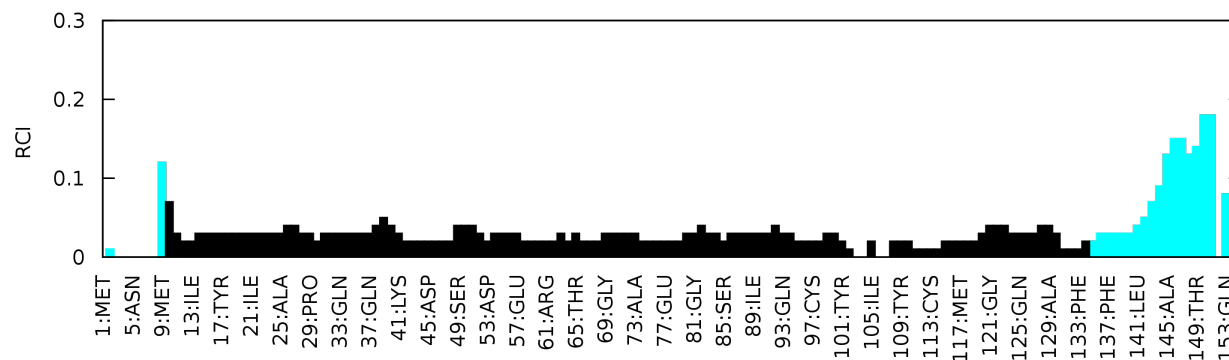
### 7.3.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

### 7.3.5 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.

Random coil index (RCI) for chain A:



## 7.4 Chemical shift list 4

File name: 5jtq\_cs.cif

Chemical shift list name: *assigned\_chemical\_shift\_list\_2*

### 7.4.1 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	1044
Number of shifts mapped to atoms	1044
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

### 7.4.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	140	$0.27 \pm 0.10$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	126	$0.79 \pm 0.13$	Should be applied
$^{13}\text{C}'$	135	$0.26 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	132	$-1.08 \pm 0.37$	Should be applied

### 7.4.3 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 13%, i.e. 785 atoms were assigned a chemical shift out of a possible 6023. 0 out of 81 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	456/2464 (19%)	111/980 (11%)	234/1008 (23%)	111/476 (23%)
Sidechain	216/3031 (7%)	60/1767 (3%)	156/1152 (14%)	0/112 (0%)
Aromatic	113/528 (21%)	57/280 (20%)	55/228 (24%)	1/20 (5%)
Overall	785/6023 (13%)	228/3027 (8%)	445/2388 (19%)	112/608 (18%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 11%, i.e. 925 atoms were assigned a chemical shift out of a possible 8466. 0 out of 104 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	539/3452 (16%)	132/1374 (10%)	275/1408 (20%)	132/670 (20%)
Sidechain	253/4262 (6%)	70/2486 (3%)	183/1612 (11%)	0/164 (0%)
Aromatic	133/752 (18%)	67/396 (17%)	65/326 (20%)	1/30 (3%)
Overall	925/8466 (11%)	269/4256 (6%)	523/3346 (16%)	133/864 (15%)

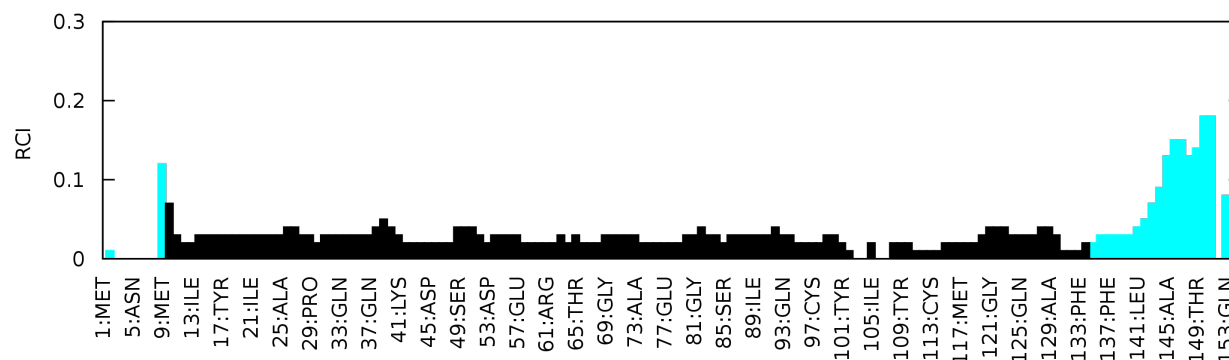
#### 7.4.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 7.4.5 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.

Random coil index (RCI) for chain A:



### 7.5 Chemical shift list 5

File name: 5jtq\_cs.cif

Chemical shift list name: *assigned\_chemical\_shift\_list\_3*

#### 7.5.1 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	1044
Number of shifts mapped to atoms	1044

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

### 7.5.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	140	$0.28 \pm 0.05$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	126	$0.79 \pm 0.16$	Should be applied
$^{13}\text{C}'$	135	$0.26 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	132	$-1.09 \pm 0.20$	Should be applied

### 7.5.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 13%, i.e. 785 atoms were assigned a chemical shift out of a possible 6023. 0 out of 81 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	456/2464 (19%)	111/980 (11%)	234/1008 (23%)	111/476 (23%)
Sidechain	216/3031 (7%)	60/1767 (3%)	156/1152 (14%)	0/112 (0%)
Aromatic	113/528 (21%)	57/280 (20%)	55/228 (24%)	1/20 (5%)
Overall	785/6023 (13%)	228/3027 (8%)	445/2388 (19%)	112/608 (18%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 11%, i.e. 925 atoms were assigned a chemical shift out of a possible 8466. 0 out of 104 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	539/3452 (16%)	132/1374 (10%)	275/1408 (20%)	132/670 (20%)
Sidechain	253/4262 (6%)	70/2486 (3%)	183/1612 (11%)	0/164 (0%)
Aromatic	133/752 (18%)	67/396 (17%)	65/326 (20%)	1/30 (3%)
Overall	925/8466 (11%)	269/4256 (6%)	523/3346 (16%)	133/864 (15%)

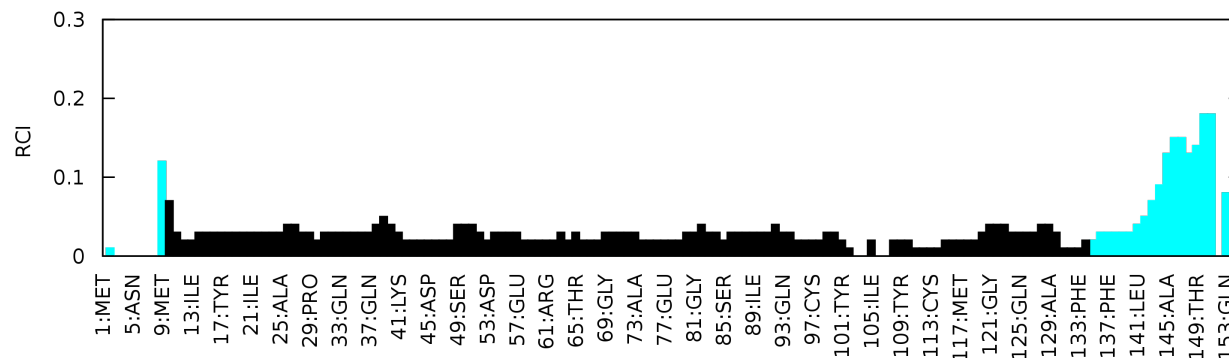
### 7.5.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

### 7.5.5 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.

Random coil index (RCI) for chain A:



## 7.6 Chemical shift list 6

File name: 5jttq\_cs.cif

Chemical shift list name: *assigned\_chemical\_shift\_list\_4*

### 7.6.1 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	1049
Number of shifts mapped to atoms	1049
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

### 7.6.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

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Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	139	$0.26 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	128	$0.85 \pm 0.17$	Should be applied
$^{13}\text{C}'$	137	$0.29 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	133	$-1.15 \pm 0.37$	Should be applied

### 7.6.3 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 13%, i.e. 790 atoms were assigned a chemical shift out of a possible 6023. 0 out of 81 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	459/2464 (19%)	112/980 (11%)	235/1008 (23%)	112/476 (24%)
Sidechain	218/3031 (7%)	60/1767 (3%)	158/1152 (14%)	0/112 (0%)
Aromatic	113/528 (21%)	57/280 (20%)	55/228 (24%)	1/20 (5%)
Overall	790/6023 (13%)	229/3027 (8%)	448/2388 (19%)	113/608 (19%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 11%, i.e. 930 atoms were assigned a chemical shift out of a possible 8466. 0 out of 104 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	542/3452 (16%)	133/1374 (10%)	276/1408 (20%)	133/670 (20%)
Sidechain	255/4262 (6%)	70/2486 (3%)	185/1612 (11%)	0/164 (0%)
Aromatic	133/752 (18%)	67/396 (17%)	65/326 (20%)	1/30 (3%)
Overall	930/8466 (11%)	270/4256 (6%)	526/3346 (16%)	134/864 (16%)

### 7.6.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

### 7.6.5 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.

Random coil index (RCI) for chain A:

