



Full wwPDB NMR Structure Validation Report ⓘ

Sep 13, 2016 – 04:47 PM EDT

PDB ID : 5JTM
Title : The structure of chaperone SecB in complex with unstructured PhoA binding site a
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

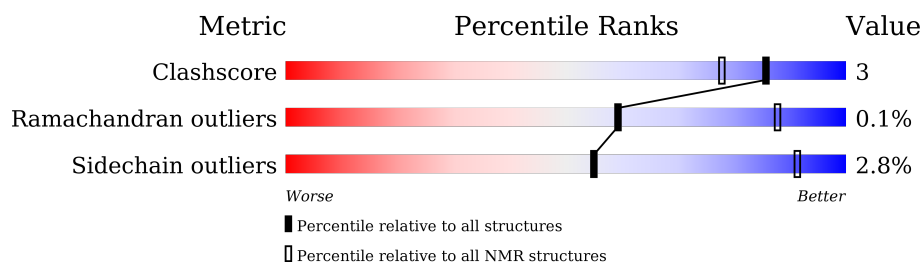
1 Overall quality at a glance

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 ≥ 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	71% 26%
1	B	155	77% 5% 19%
1	C	155	75% 20%
1	D	155	77% 21%
2	E	25	100%
2	F	25	100%
2	G	25	100%
2	H	25	100%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 20 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:11-A:86, A:95-A:133, B:9-B:134, C:11-C:134, D:10-D:131 (487)	0.44	20

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

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

The models can be grouped into 4 clusters and 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11104 atoms, of which 5488 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 Alkaline phosphatase.

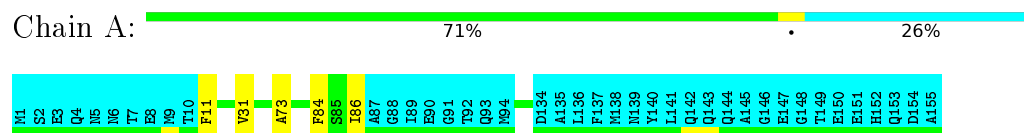
Mol	Chain	Residues	Atoms						Trace
2	E	25	Total	C	H	N	O	S	0
			409	126	217	31	34	1	
2	F	25	Total	C	H	N	O	S	0
			409	126	217	31	34	1	
2	G	25	Total	C	H	N	O	S	0
			409	126	217	31	34	1	
2	H	25	Total	C	H	N	O	S	0
			409	126	217	31	34	1	

4 Residue-property plots [i](#)

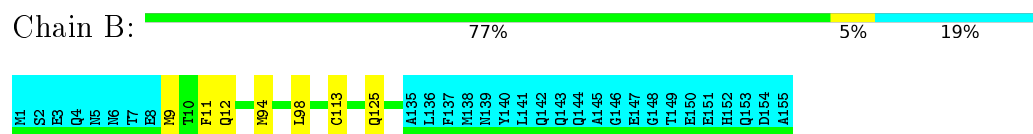
4.1 Average score per residue in the NMR ensemble

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.

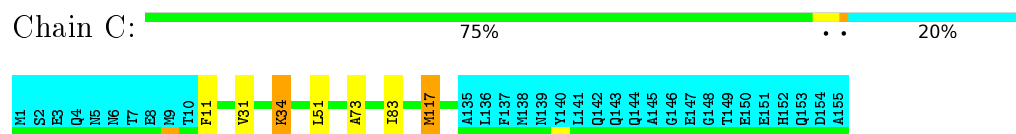
- Molecule 1: Protein-export protein SecB



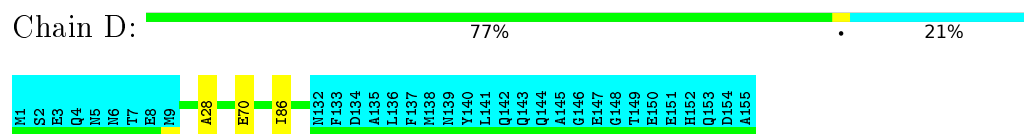
- Molecule 1: Protein-export protein SecB



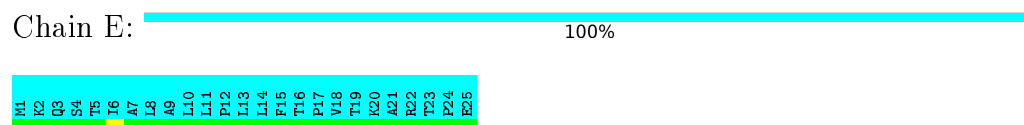
- Molecule 1: Protein-export protein SecB



- Molecule 1: Protein-export protein SecB

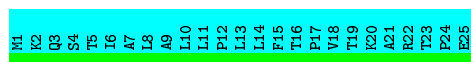


- Molecule 2: Alkaline phosphatase



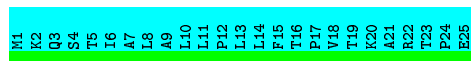
- Molecule 2: Alkaline phosphatase

Chain F:  100%



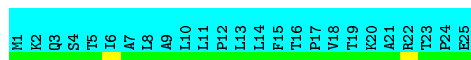
- Molecule 2: Alkaline phosphatase

Chain G:  100%



- Molecule 2: Alkaline phosphatase

Chain H:  100%



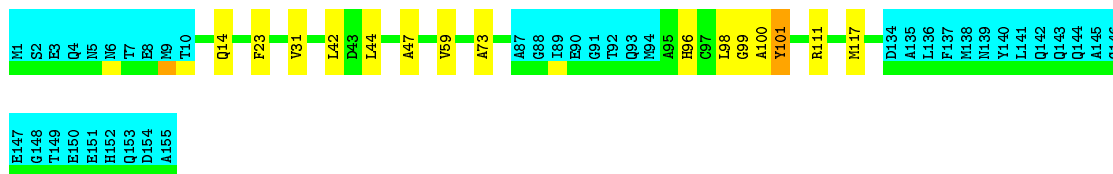
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.


4.2.1 Score per residue for model 1

- Molecule 1: Protein-export protein SecB

Chain A:  65% 9% 26%



- Molecule 1: Protein-export protein SecB

Chain B:  75% 19%



- Molecule 1: Protein-export protein SecB

Chain C:  67% 12% 20%



E147
G146
T149
E150
E151
H152
Q153
D154
A155

- Molecule 1: Protein-export protein SecB

Chain D:  71% 8% 21%

M1 S2 E3 Q4 N5 N6 N7 T7 E8 M9 F11 I21 A28 V31 V40 D45 R61 V64 E70 E90 C102 L126 M132 F133 D134 A135 L136 F137 M138 M139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

- Molecule 2: Alkaline phosphatase

Chain E:  100%

M1 K2 Q3 S4 T5 I6 A7 L8 A9 L10 L11 L12 L13 L14 F15 T16 P17 V18 T19 K20 A21 R22 T23 P24 E25

- Molecule 2: Alkaline phosphatase

Chain F:  100%

M1 K2 Q3 S4 T5 I6 A7 L8 A9 L10 L11 L12 L13 L14 F15 T16 P17 V18 T19 K20 A21 R22 T23 P24 E25

- Molecule 2: Alkaline phosphatase

Chain G:  100%

M1 K2 Q3 S4 T5 I6 A7 L8 A9 L10 L11 L12 L13 L14 F15 T16 P17 V18 T19 K20 A21 R22 T23 P24 E25

- Molecule 2: Alkaline phosphatase

Chain H:  100%

M1 K2 Q3 S4 T5 I6 A7 L8 A9 L10 L11 L12 L13 L14 F15 T16 P17 V18 T19 K20 A21 R22 T23 P24 E25

4.2.2 Score per residue for model 2

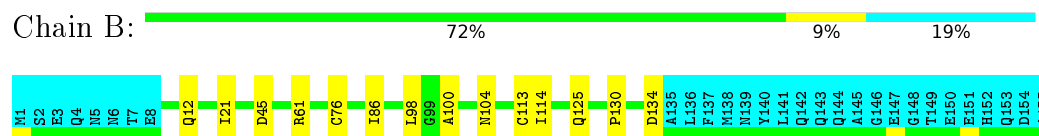
- Molecule 1: Protein-export protein SecB

Chain A:  65% 9% 26%

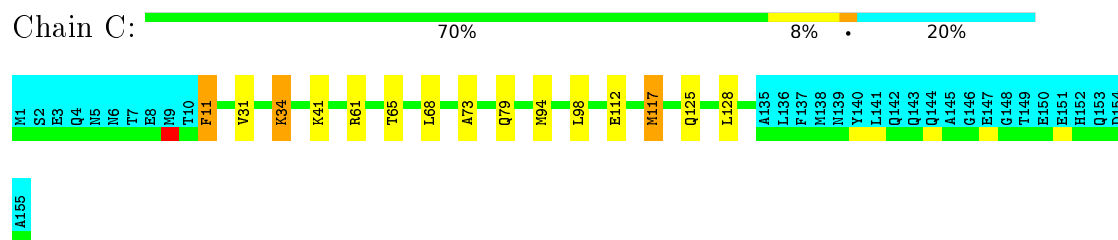
M1 S2 E3 Q4 N5 N6 N7 T7 E8 M9 F11 I21 S22 F23 L42 D45 L51 E57 R61 F84 S85 I86 A87 G88 I89 E90 G91 T92 Q93 M94 A95 H96 C97 Y101 M117 D134 A135 L136 F137 M138 M139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148

T149
E150
E151
H152
Q153
D154
A155

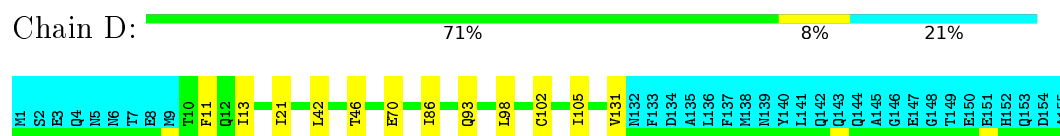
- Molecule 1: Protein-export protein SecB



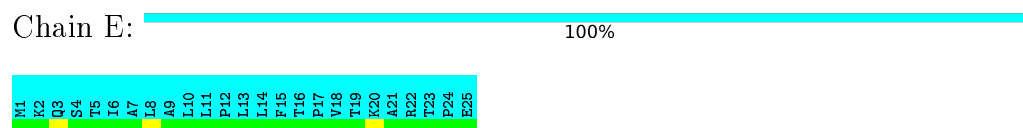
- Molecule 1: Protein-export protein SecB



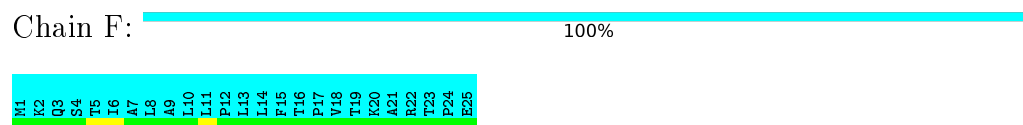
- Molecule 1: Protein-export protein SecB



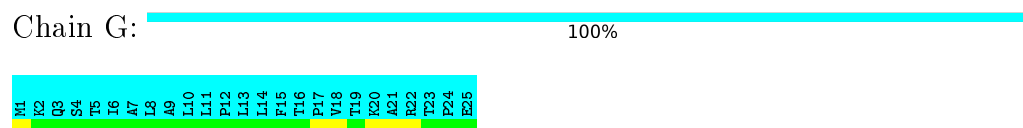
- Molecule 2: Alkaline phosphatase



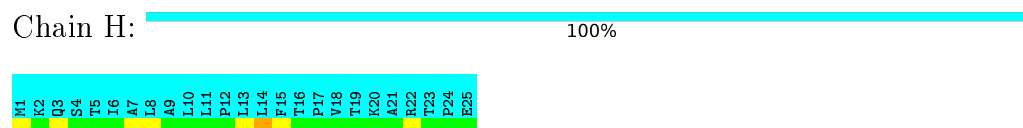
- Molecule 2: Alkaline phosphatase



- Molecule 2: Alkaline phosphatase

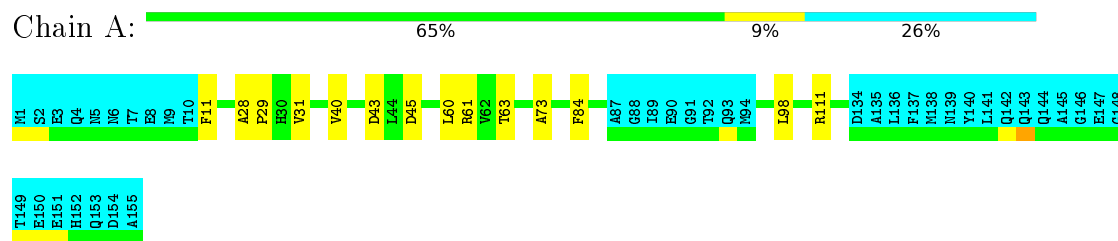


- Molecule 2: Alkaline phosphatase

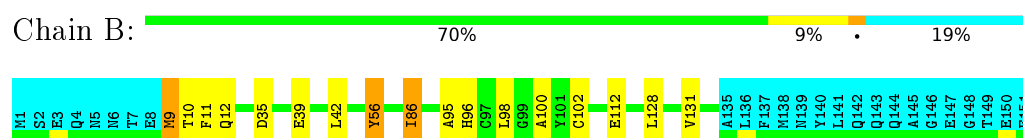


4.2.3 Score per residue for model 3

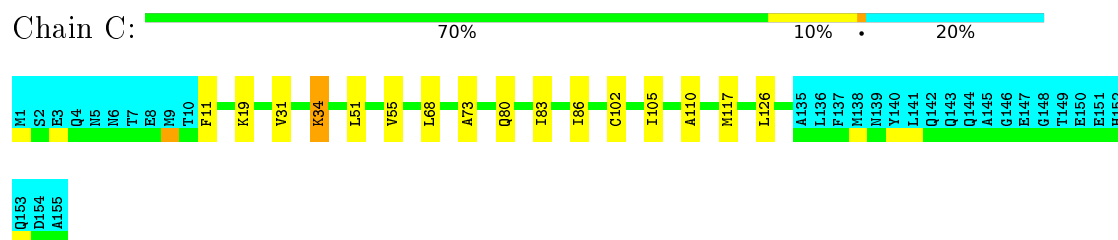
- Molecule 1: Protein-export protein SecB



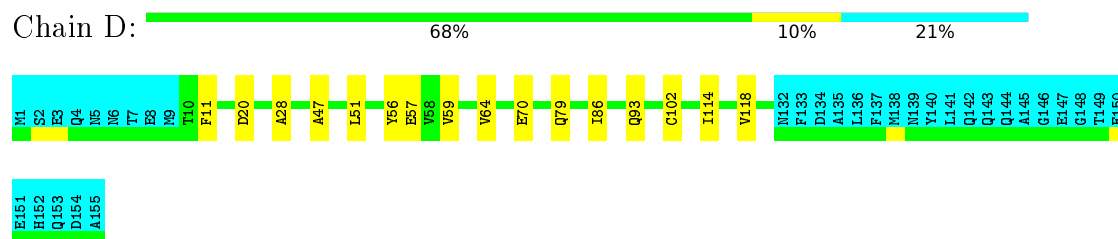
- Molecule 1: Protein-export protein SecB



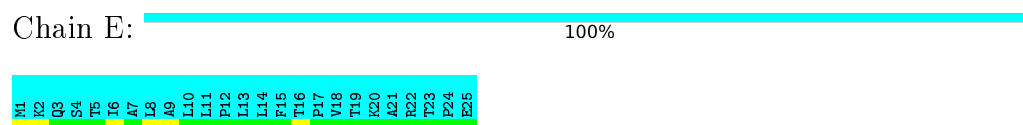
- Molecule 1: Protein-export protein SecB



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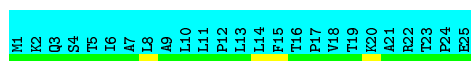


- Molecule 2: Alkaline phosphatase



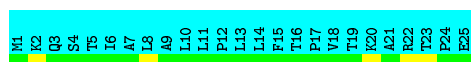
- Molecule 2: Alkaline phosphatase





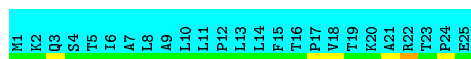
- Molecule 2: Alkaline phosphatase

Chain G: 100%



- Molecule 2: Alkaline phosphatase

Chain H: 100%



4.2.4 Score per residue for model 4

- Molecule 1: Protein-export protein SecB

Chain A: 65% 10% 26%



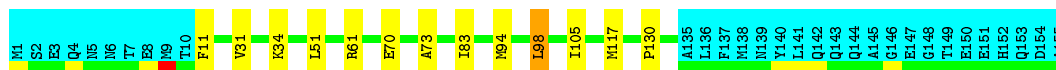
- Molecule 1: Protein-export protein SecB

Chain B: 72% 9% 19%



- Molecule 1: Protein-export protein SecB

Chain C: 72% 8% 20%



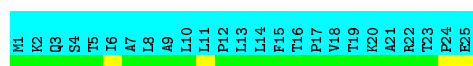
- Molecule 1: Protein-export protein SecB

Chain D: 73% 5% 21%



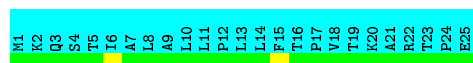
- Molecule 2: Alkaline phosphatase

Chain E:  100%



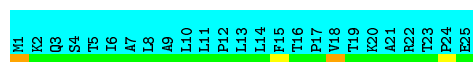
- Molecule 2: Alkaline phosphatase

Chain F:  100%



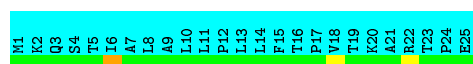
- Molecule 2: Alkaline phosphatase

Chain G:  100%



- Molecule 2: Alkaline phosphatase

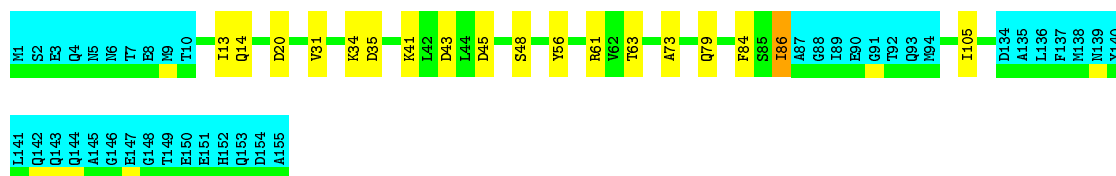
Chain H:  100%




4.2.5 Score per residue for model 5

- Molecule 1: Protein-export protein SecB

Chain A:  63% 11% 26%



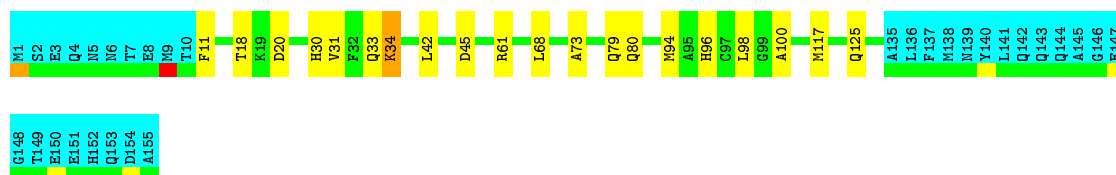
- Molecule 1: Protein-export protein SecB

Chain B:  77% 5% 19%



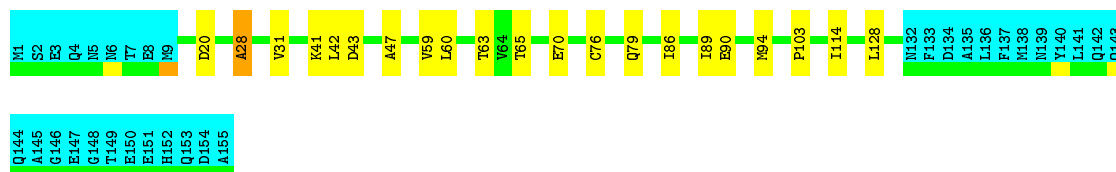
- Molecule 1: Protein-export protein SecB

Chain C:  67% 12% 20%



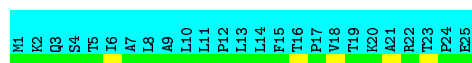
- Molecule 1: Protein-export protein SecB

Chain D: 65% 13% 21%



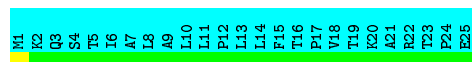
- Molecule 2: Alkaline phosphatase

Chain E: 100%



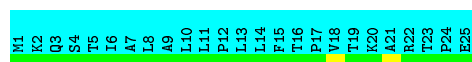
- Molecule 2: Alkaline phosphatase

Chain F: 100%



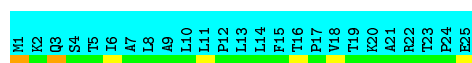
- Molecule 2: Alkaline phosphatase

Chain G: 100%



- Molecule 2: Alkaline phosphatase

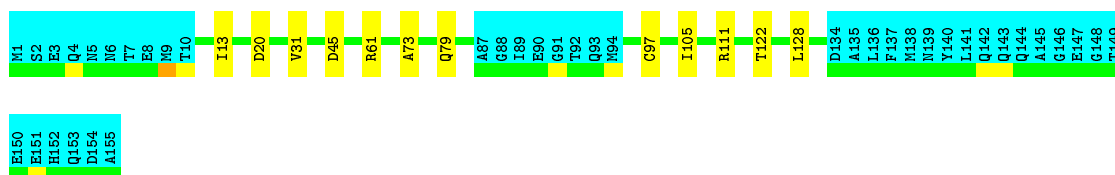
Chain H: 100%



4.2.6 Score per residue for model 6

- Molecule 1: Protein-export protein SecB

Chain A: 66% 8% 26%



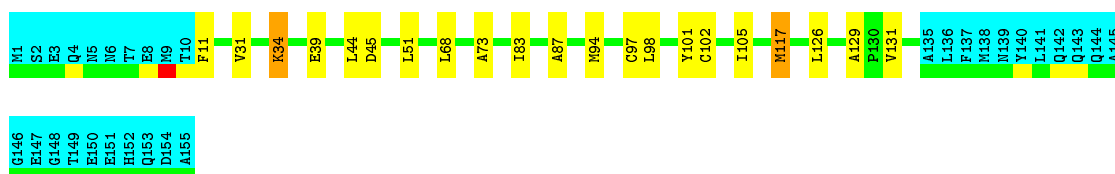
- Molecule 1: Protein-export protein SecB

Chain B: 75% 6% 19%



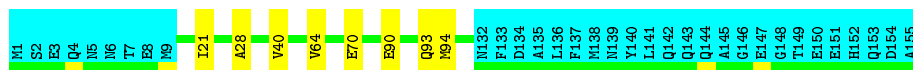
- Molecule 1: Protein-export protein SecB

Chain C: 66% 12% 20%



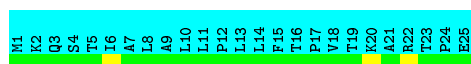
- Molecule 1: Protein-export protein SecB

Chain D: 74% 5% 21%



- Molecule 2: Alkaline phosphatase

Chain E: 100%



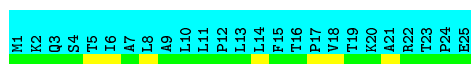
- Molecule 2: Alkaline phosphatase

Chain F: 100%



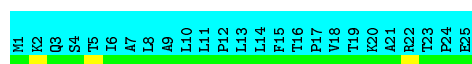
- Molecule 2: Alkaline phosphatase

Chain G: 100%



- Molecule 2: Alkaline phosphatase

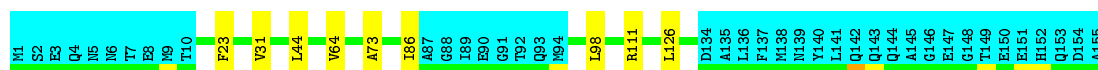
Chain H:  100%



4.2.7 Score per residue for model 7

- Molecule 1: Protein-export protein SecB

Chain A:  68% 6% 26%



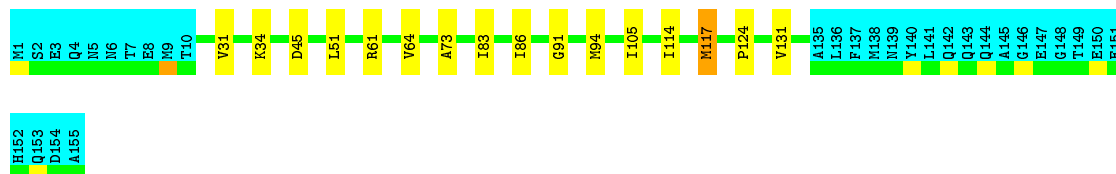
- Molecule 1: Protein-export protein SecB

Chain B:  75% 6% 19%



- Molecule 1: Protein-export protein SecB

Chain C:  70% 10% 20%



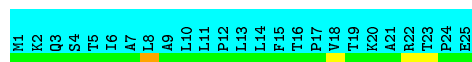
- Molecule 1: Protein-export protein SecB

Chain D:  74% 5% 21%



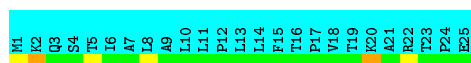
- Molecule 2: Alkaline phosphatase

Chain E:  100%



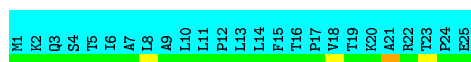
- Molecule 2: Alkaline phosphatase

Chain F:  100%



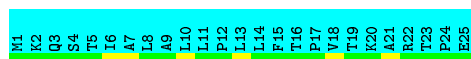
- Molecule 2: Alkaline phosphatase

Chain G: 100%



- Molecule 2: Alkaline phosphatase

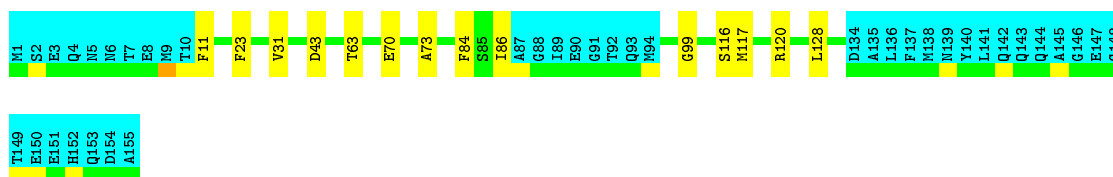
Chain H: 100%



4.2.8 Score per residue for model 8

- Molecule 1: Protein-export protein SecB

Chain A: 65% 9% 26%



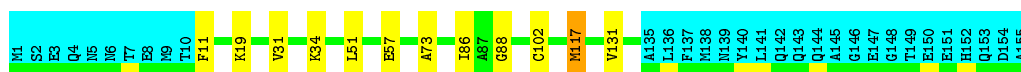
- Molecule 1: Protein-export protein SecB

Chain B: 75% 6% 19%



- Molecule 1: Protein-export protein SecB

Chain C: 72% 7% 20%



- Molecule 1: Protein-export protein SecB

Chain D: 74% 5% 21%



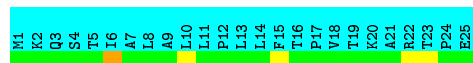
- Molecule 2: Alkaline phosphatase

Chain E:  100%



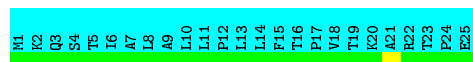
- Molecule 2: Alkaline phosphatase

Chain F:  100%



- Molecule 2: Alkaline phosphatase

Chain G:  100%



- Molecule 2: Alkaline phosphatase

Chain H:  100%



4.2.9 Score per residue for model 9

- Molecule 1: Protein-export protein SecB

Chain A:  66%  8%  26%



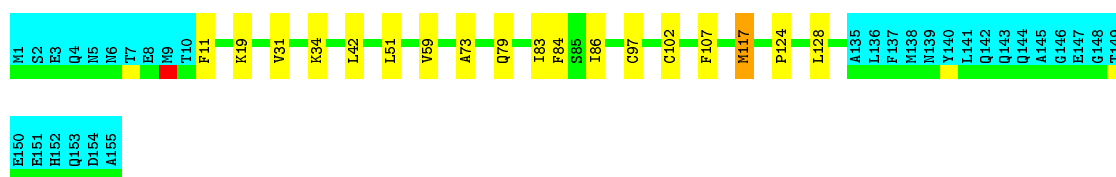
- Molecule 1: Protein-export protein SecB

Chain B:  73%  8%  19%



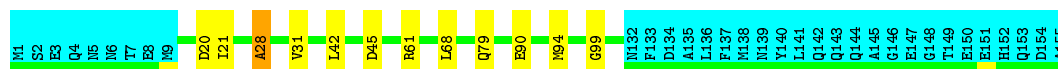
- Molecule 1: Protein-export protein SecB

Chain C:  68%  11%  20%



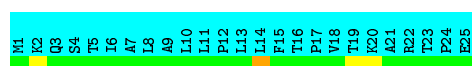
- Molecule 1: Protein-export protein SecB

Chain D: 71% 7% 21%



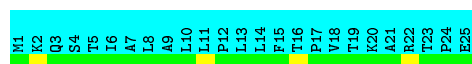
- Molecule 2: Alkaline phosphatase

Chain E: 100%



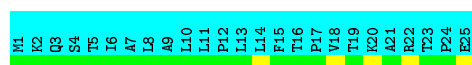
- Molecule 2: Alkaline phosphatase

Chain F: 100%



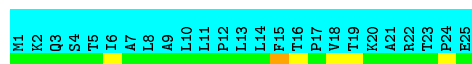
- Molecule 2: Alkaline phosphatase

Chain G: 100%



- Molecule 2: Alkaline phosphatase

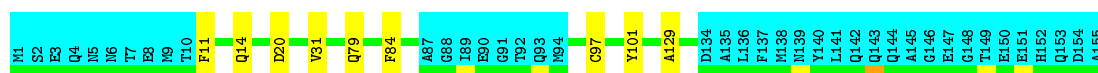
Chain H: 100%



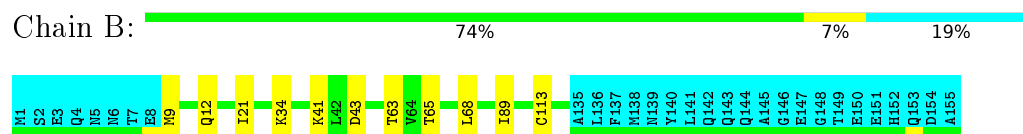
4.2.10 Score per residue for model 10

- Molecule 1: Protein-export protein SecB

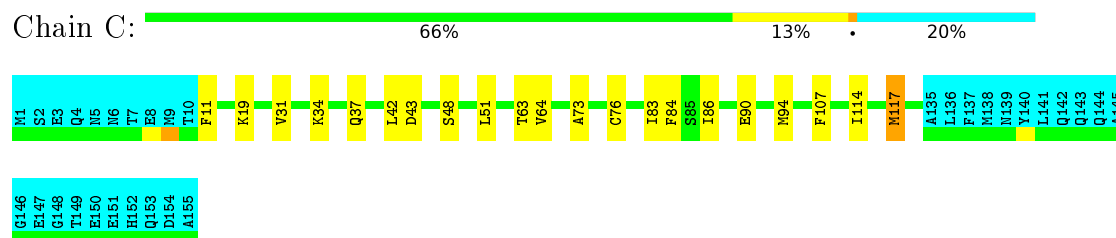
Chain A: 68% 6% 26%



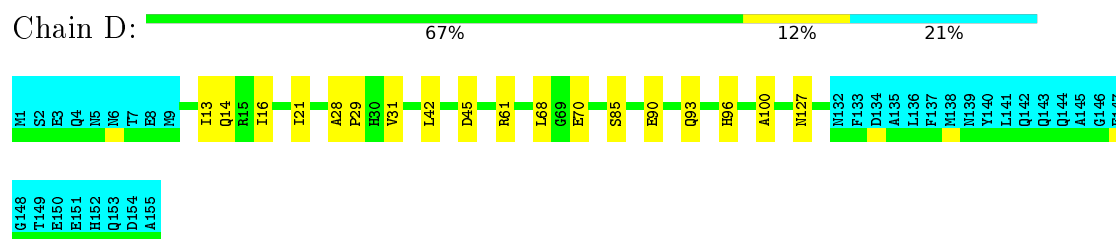
- Molecule 1: Protein-export protein SecB



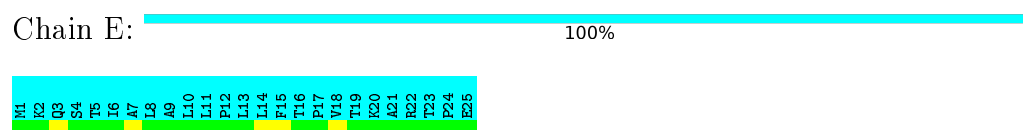
- Molecule 1: Protein-export protein SecB



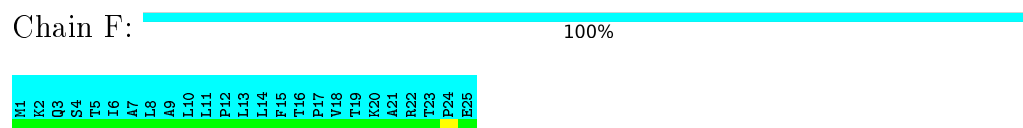
- Molecule 1: Protein-export protein SecB



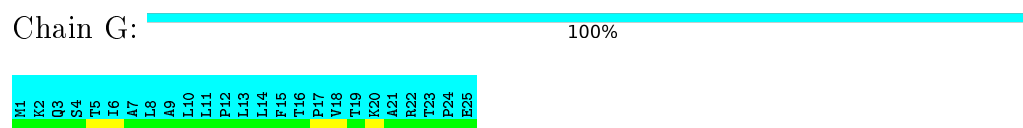
- Molecule 2: Alkaline phosphatase



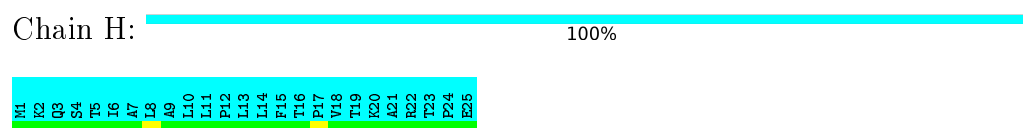
- Molecule 2: Alkaline phosphatase



- Molecule 2: Alkaline phosphatase

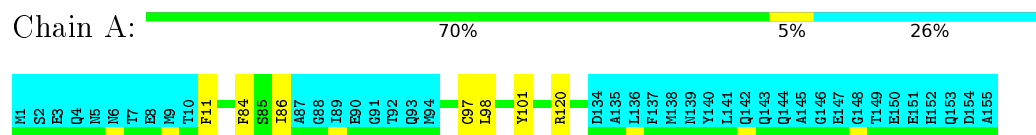


- Molecule 2: Alkaline phosphatase

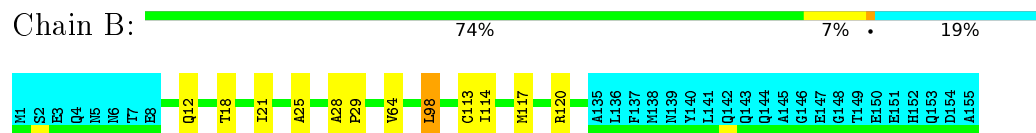


4.2.11 Score per residue for model 11

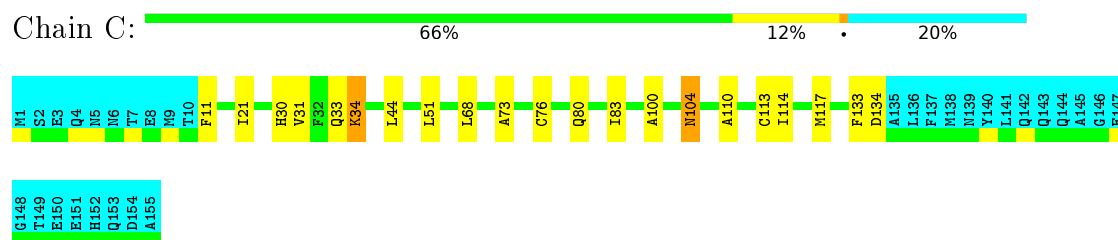
- Molecule 1: Protein-export protein SecB



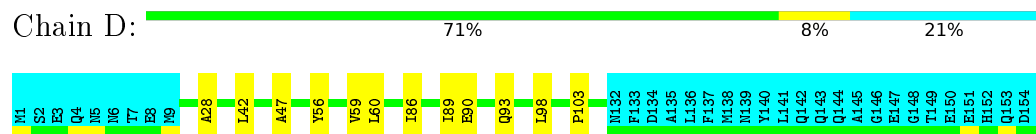
- Molecule 1: Protein-export protein SecB



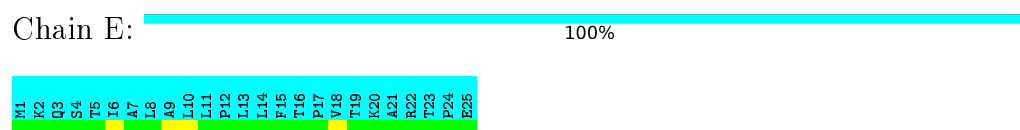
- Molecule 1: Protein-export protein SecB



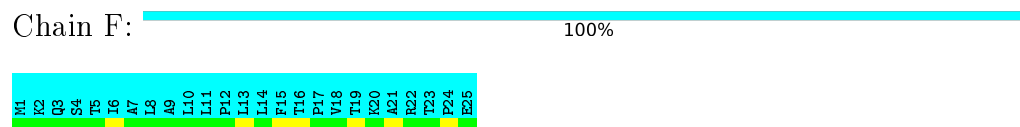
- Molecule 1: Protein-export protein SecB



- Molecule 2: Alkaline phosphatase

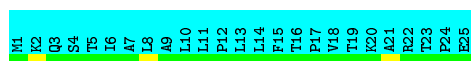


- Molecule 2: Alkaline phosphatase



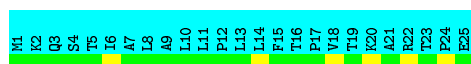
- Molecule 2: Alkaline phosphatase





- Molecule 2: Alkaline phosphatase

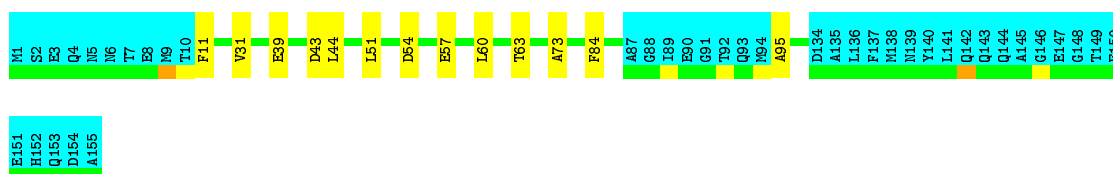
Chain H: 100%



4.2.12 Score per residue for model 12

- Molecule 1: Protein-export protein SecB

Chain A: 66% 8% 26%



- Molecule 1: Protein-export protein SecB

Chain B: 74% 6% 19%



- Molecule 1: Protein-export protein SecB

Chain C: 72% 6% 20%



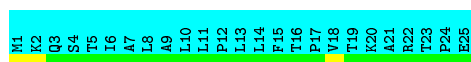
- Molecule 1: Protein-export protein SecB

Chain D: 71% 7% 21%



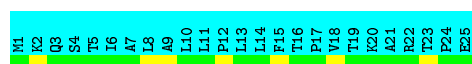
- Molecule 2: Alkaline phosphatase

Chain E: 100%



- Molecule 2: Alkaline phosphatase

Chain F:  100%



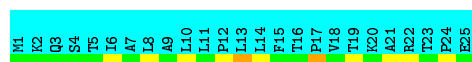
- Molecule 2: Alkaline phosphatase

Chain G:  100%



- Molecule 2: Alkaline phosphatase

Chain H:  100%



4.2.13 Score per residue for model 13

- Molecule 1: Protein-export protein SecB

Chain A:  67% 7% 26%



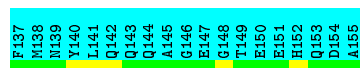
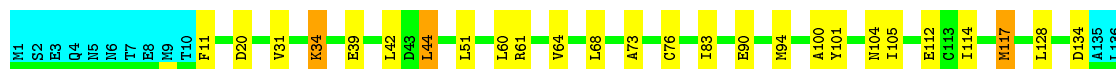
- Molecule 1: Protein-export protein SecB

Chain B:  71% 10% 19%

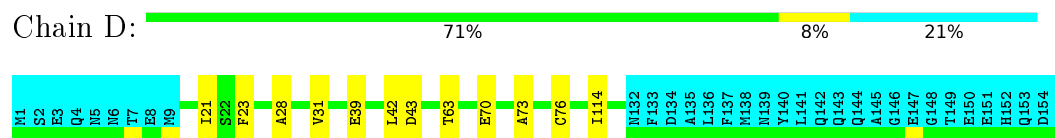


- Molecule 1: Protein-export protein SecB

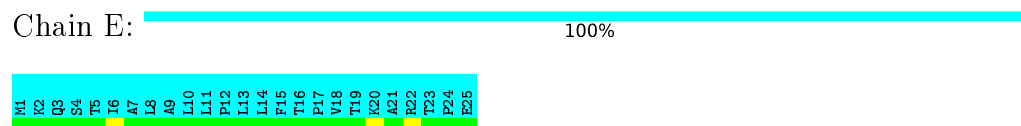
Chain C:  63% 15% 20%



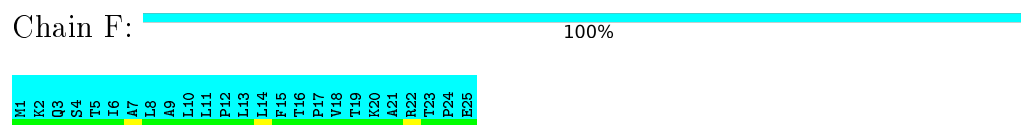
- Molecule 1: Protein-export protein SecB



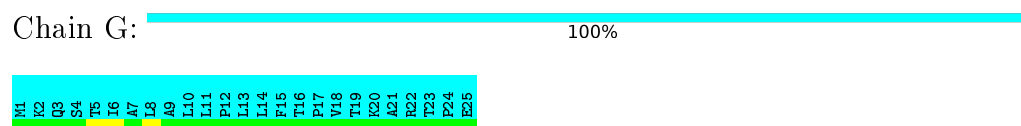
- Molecule 2: Alkaline phosphatase



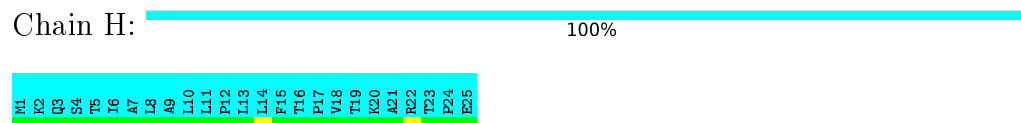
- Molecule 2: Alkaline phosphatase



- Molecule 2: Alkaline phosphatase

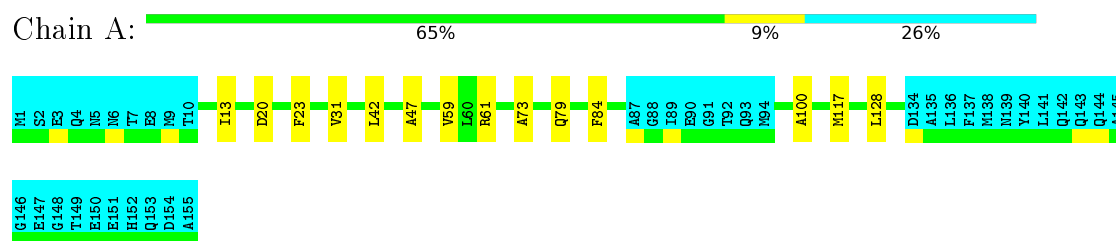


- Molecule 2: Alkaline phosphatase



4.2.14 Score per residue for model 14

- Molecule 1: Protein-export protein SecB

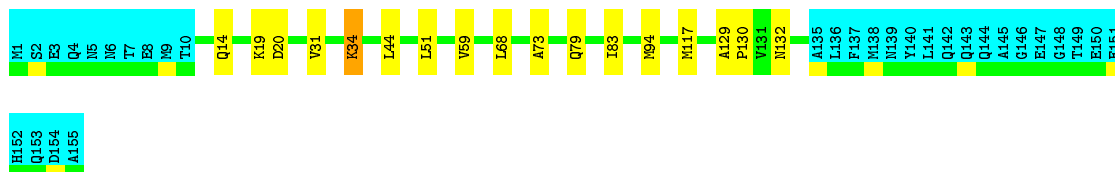


- Molecule 1: Protein-export protein SecB





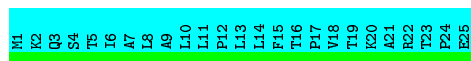
- Molecule 1: Protein-export protein SecB



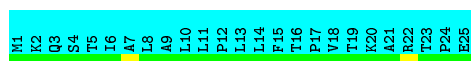
- Molecule 1: Protein-export protein SecB



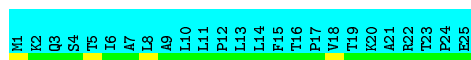
- Molecule 2: Alkaline phosphatase



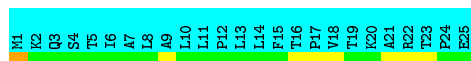
- Molecule 2: Alkaline phosphatase



- Molecule 2: Alkaline phosphatase

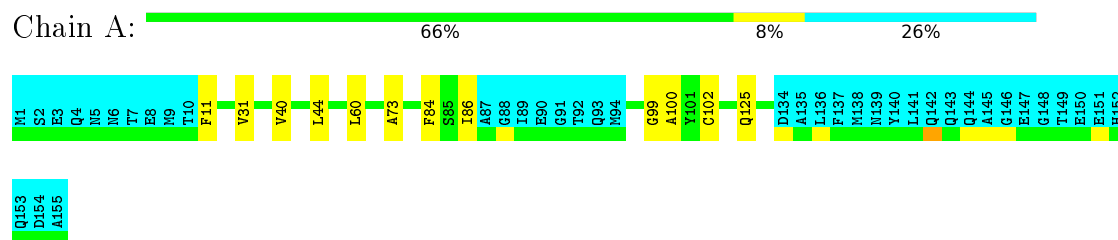


- Molecule 2: Alkaline phosphatase

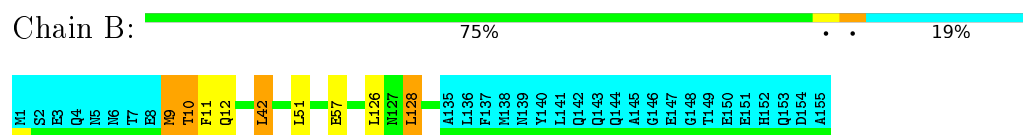


4.2.15 Score per residue for model 15

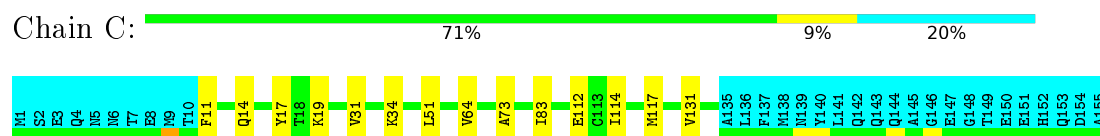
- Molecule 1: Protein-export protein SecB



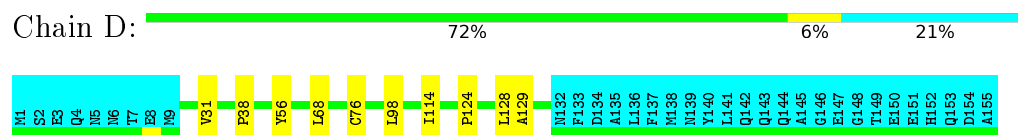
- Molecule 1: Protein-export protein SecB



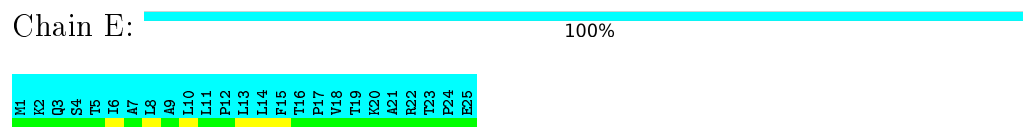
- Molecule 1: Protein-export protein SecB



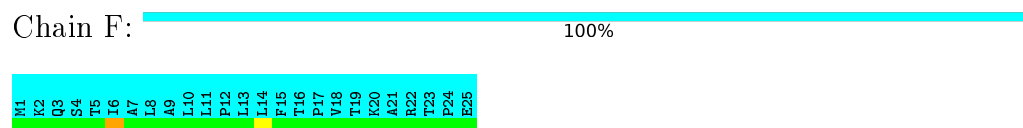
- Molecule 1: Protein-export protein SecB



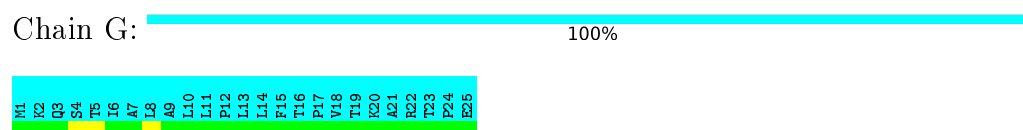
- Molecule 2: Alkaline phosphatase



- Molecule 2: Alkaline phosphatase



- Molecule 2: Alkaline phosphatase



- Molecule 2: Alkaline phosphatase

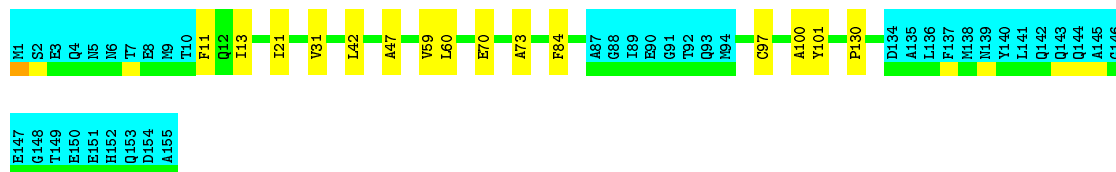
Chain H:  100%



4.2.16 Score per residue for model 16

- Molecule 1: Protein-export protein SecB

Chain A:  65% 10% 26%



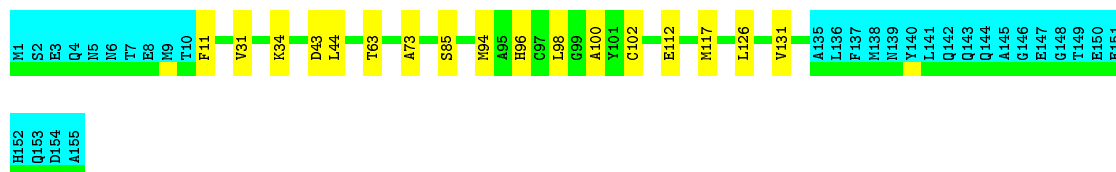
- Molecule 1: Protein-export protein SecB

Chain B:  70% 9% 19%



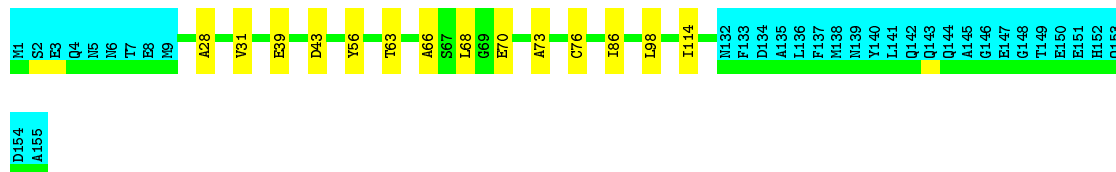
- Molecule 1: Protein-export protein SecB

Chain C:  69% 11% 20%



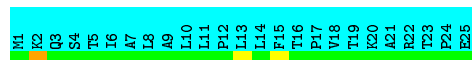
- Molecule 1: Protein-export protein SecB

Chain D:  70% 9% 21%

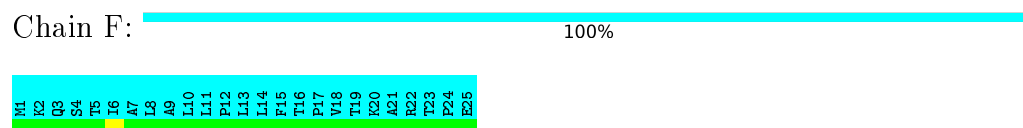


- Molecule 2: Alkaline phosphatase

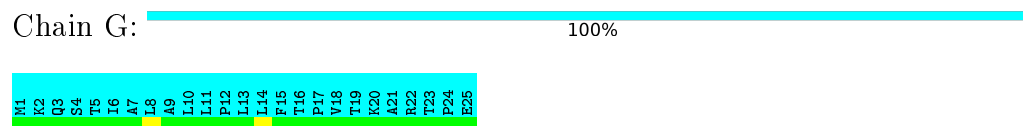
Chain E:  100%



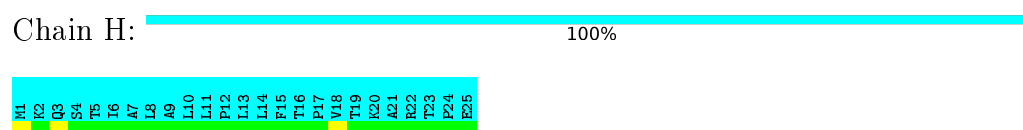
- Molecule 2: Alkaline phosphatase



- Molecule 2: Alkaline phosphatase

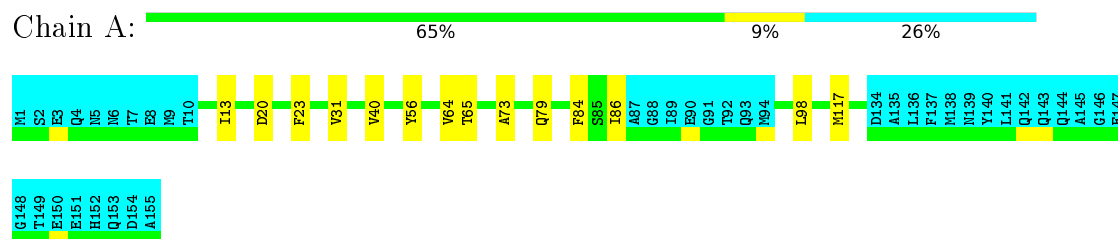


- Molecule 2: Alkaline phosphatase

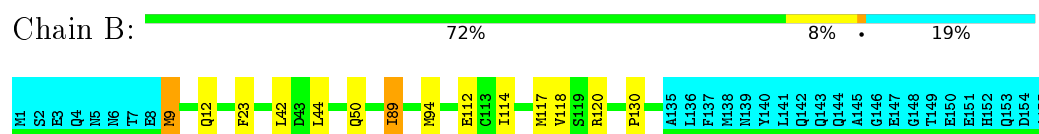


4.2.17 Score per residue for model 17

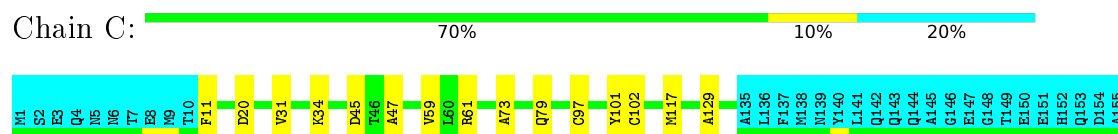
- Molecule 1: Protein-export protein SecB



- Molecule 1: Protein-export protein SecB

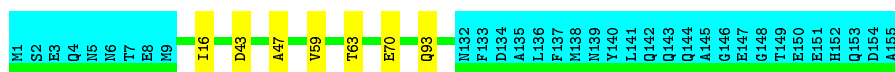


- Molecule 1: Protein-export protein SecB



- Molecule 1: Protein-export protein SecB





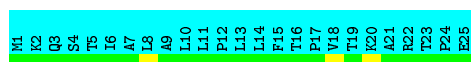
- Molecule 2: Alkaline phosphatase

Chain E: 100%



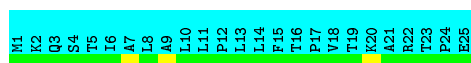
- Molecule 2: Alkaline phosphatase

Chain F: 100%



- Molecule 2: Alkaline phosphatase

Chain G: 100%



- Molecule 2: Alkaline phosphatase

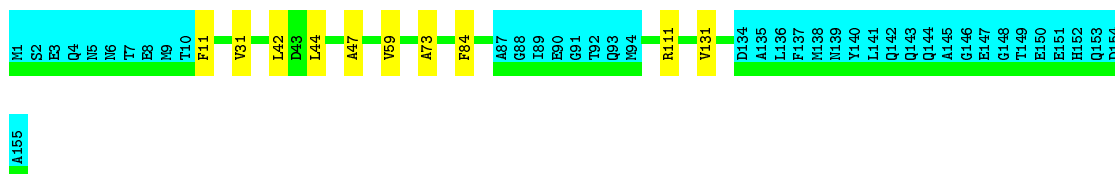
Chain H: 100%



4.2.18 Score per residue for model 18

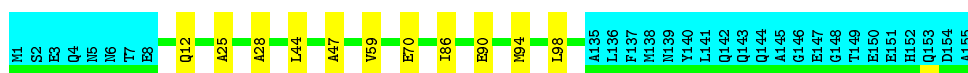
- Molecule 1: Protein-export protein SecB

Chain A: 68% 6% 26%

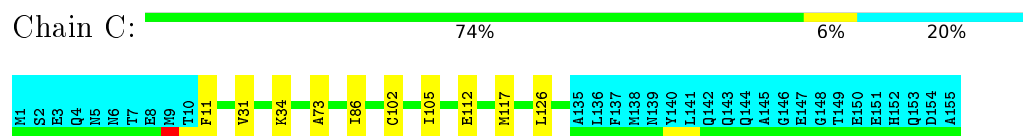


- Molecule 1: Protein-export protein SecB

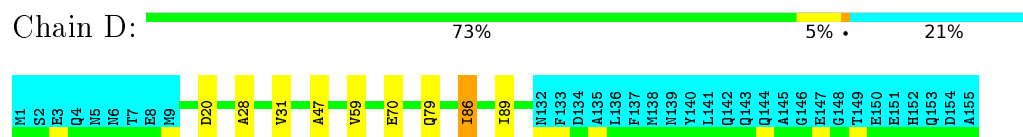
Chain B: 74% 7% 19%



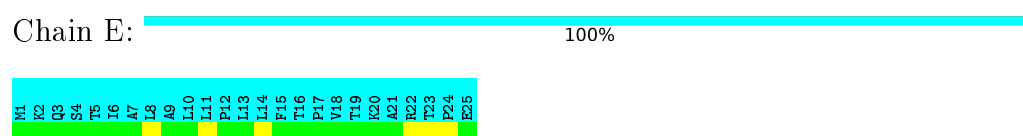
- Molecule 1: Protein-export protein SecB



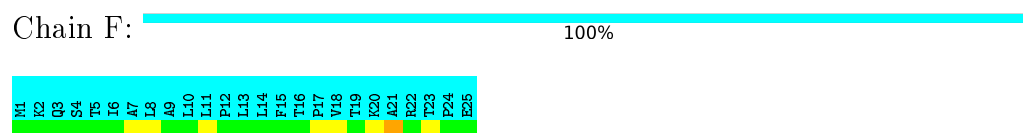
- Molecule 1: Protein-export protein SecB



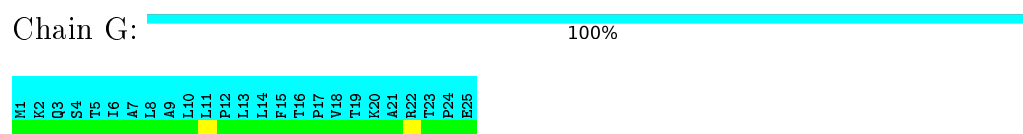
- Molecule 2: Alkaline phosphatase



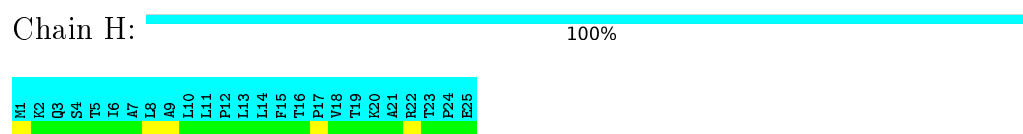
- Molecule 2: Alkaline phosphatase



- Molecule 2: Alkaline phosphatase

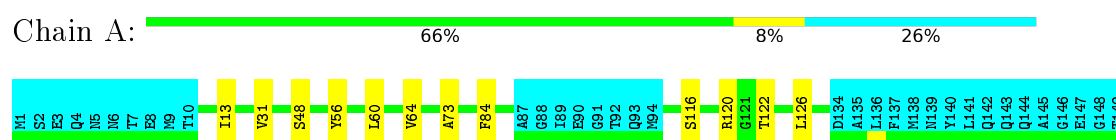


- Molecule 2: Alkaline phosphatase



4.2.19 Score per residue for model 19

- Molecule 1: Protein-export protein SecB



E150
E151
H152
Q153
D154
A155

- Molecule 1: Protein-export protein SecB

Chain B:  74% 8% 19%

M1 S2 E3 Q4 N5 N6 T7 E8 F11 Q12 T18 T21 L42 R61 Q79 A95 L98 F107 C113 Q125 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 C:  70% 9% 20%

M1 S2 E3 Q4 N5 N6 T7 E8 F11 Q12 Y17 V31 K34 K41 D45 L51 R61 T65 A73 L83 L98 M117 P130 V131 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:  69% 10% 21%

M1 S2 E3 Q4 N5 N6 T7 E8 F9 Q14 D20 I21 V40 K41 L42 D43 L60 T63 V64 T65 Q79 I83 I89 T122 M132 F133 D134 A135 L136 F137 M138 M139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

- Molecule 2: Alkaline phosphatase

Chain E:  100%

M1 K2 Q3 S4 T5 I6 A7 L8 A9 L10 L11 P12 L13 L14 F15 T16 P17 V18 T19 K20 A21 R22 T23 P24 E25

- Molecule 2: Alkaline phosphatase

Chain F:  100%

M1 K2 Q3 S4 T5 I6 A7 L8 A9 L10 L11 P12 L13 L14 F15 T16 P17 V18 T19 K20 A21 R22 T23 P24 E25

- Molecule 2: Alkaline phosphatase

Chain G:  100%

M1 K2 Q3 S4 T5 I6 A7 L8 A9 L10 L11 P12 L13 L14 F15 T16 P17 V18 T19 K20 A21 R22 T23 P24 E25

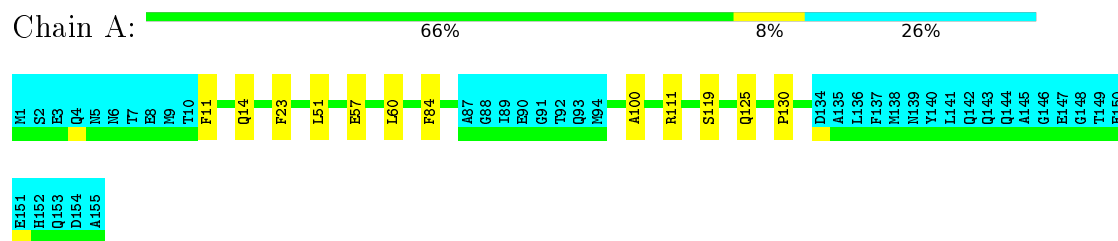
- Molecule 2: Alkaline phosphatase

Chain H:  100%

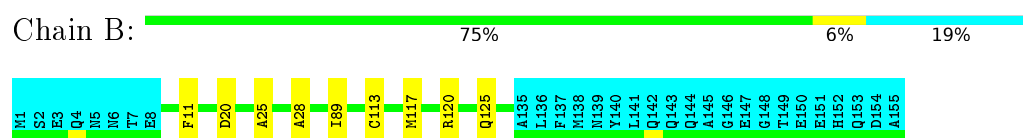
M1 K2 Q3 S4 T5 I6 A7 L8 A9 L10 L11 P12 L13 L14 F15 T16 P17 V18 T19 K20 A21 R22 T23 P24 E25

4.2.20 Score per residue for model 20 (medoid)

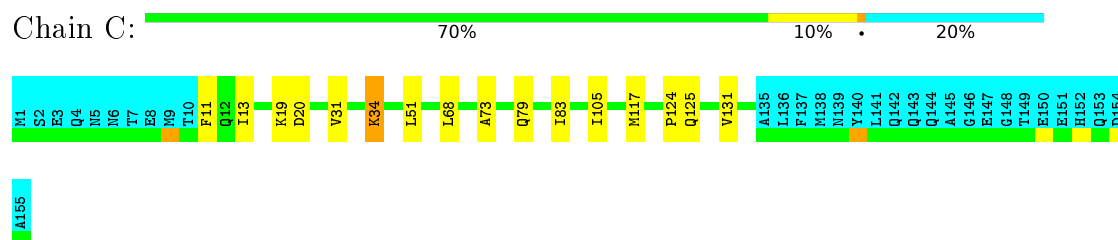
- Molecule 1: Protein-export protein SecB



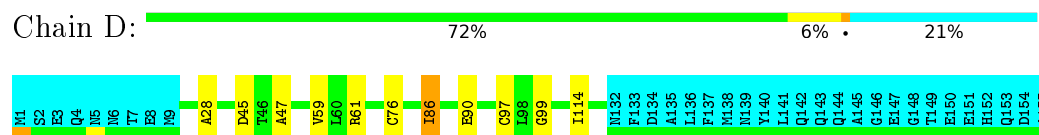
- Molecule 1: Protein-export protein SecB



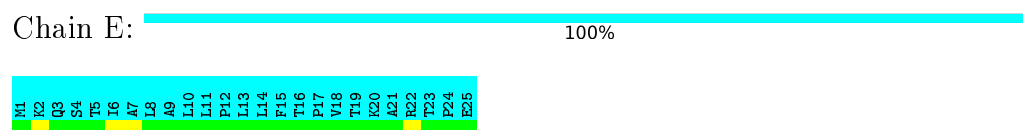
- Molecule 1: Protein-export protein SecB



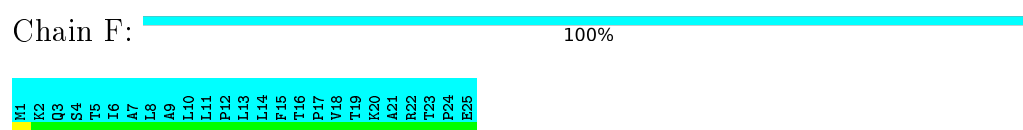
- Molecule 1: Protein-export protein SecB



- Molecule 2: Alkaline phosphatase

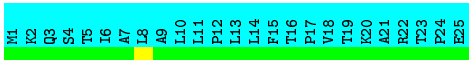


- Molecule 2: Alkaline phosphatase



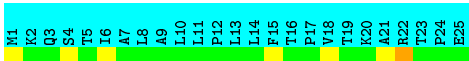
- Molecule 2: Alkaline phosphatase

Chain G:  100%



● Molecule 2: Alkaline phosphatase

Chain H:  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)	5jtm_cs.cif
Number of chemical shift lists	8
Total number of shifts	5090
Number of shifts mapped to atoms	5090
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	0.83±0.01	0±0/927 (0.0±0.0%)	0.62±0.02	0±0/1266 (0.0±0.0%)
1	B	0.85±0.02	0±0/1004 (0.0±0.0%)	0.63±0.01	0±0/1369 (0.0±0.0%)
1	C	0.84±0.02	0±0/989 (0.0±0.0%)	0.64±0.02	0±0/1349 (0.0±0.0%)
1	D	0.83±0.01	0±0/968 (0.0±0.0%)	0.62±0.01	0±0/1321 (0.0±0.0%)
All	All	0.84	0/77760 (0.0%)	0.63	2/106100 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	B	0.0±0.0	0.1±0.2
All	All	0	1

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	101	TYR	CB-CG-CD2	6.52	124.91	121.00	1	1
1	A	101	TYR	CA-CB-CG	5.75	124.31	113.40	1	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	B	10	THR	Peptide	1

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	904	883	881	5±1
1	B	981	955	953	6±2
1	C	966	939	937	7±2
1	D	946	927	925	5±2
2	E	0	0	0	0±0
2	F	0	0	0	0±0
2	G	0	0	0	0±0
2	H	0	0	0	0±0
All	All	75940	74080	73920	407

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	0.80	1.53	14	7
1:B:13:ILE:HD11	1:B:105:ILE:HD13	0.68	1.66	16	1
1:A:31:VAL:HG21	1:A:73:ALA:HA	0.64	1.67	5	16
1:B:25:ALA:CB	1:B:28:ALA:HB2	0.61	2.24	14	6
1:D:20:ASP:HB3	1:D:79:GLN:HB2	0.60	1.73	19	6
1:C:34:LYS:HG2	1:C:68:LEU:HD13	0.59	1.73	20	10
1:C:31:VAL:HG21	1:C:73:ALA:HA	0.58	1.75	17	20
1:C:11:PHE:HE1	1:C:102:CYS:HG	0.58	1.42	18	1
1:B:98:LEU:HA	1:B:102:CYS:SG	0.58	2.39	3	4
1:A:44:LEU:HD23	1:A:60:LEU:HD21	0.58	1.74	12	1
1:B:42:LEU:HD22	1:B:128:LEU:HD11	0.57	1.75	3	1
1:B:60:LEU:HD22	1:B:103:PRO:HB3	0.57	1.75	14	2
1:D:43:ASP:HB2	1:D:63:THR:HB	0.57	1.75	17	5
1:C:64:VAL:HG23	1:C:114:ILE:HD13	0.57	1.75	13	3
1:B:21:ILE:HD11	1:B:113:CYS:SG	0.57	2.40	14	6
1:B:41:LYS:HB2	1:B:65:THR:HB	0.56	1.76	10	1
1:A:43:ASP:HB2	1:A:63:THR:HB	0.56	1.77	3	4
1:D:86:ILE:HG12	1:D:89:ILE:HD13	0.55	1.77	5	2
1:C:45:ASP:HB3	1:C:61:ARG:HD2	0.55	1.76	19	2
1:A:86:ILE:HD11	1:A:102:CYS:SG	0.54	2.42	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:VAL:HG11	1:A:126:LEU:HD21	0.54	1.77	13	3
1:B:9:MET:SD	1:B:10:THR:N	0.54	2.80	15	4
1:D:40:VAL:HG13	1:D:64:VAL:HG13	0.54	1.79	4	5
1:C:41:LYS:HB2	1:C:65:THR:HB	0.54	1.80	19	2
1:B:43:ASP:HB2	1:B:63:THR:HB	0.54	1.79	7	2
1:C:117:MET:HE2	1:D:21:ILE:HG21	0.53	1.80	1	10
1:D:47:ALA:HB3	1:D:59:VAL:HB	0.53	1.80	8	7
1:B:11:PHE:CZ	1:B:13:ILE:HG13	0.53	2.38	16	1
1:A:23:PHE:HB2	1:A:117:MET:SD	0.53	2.43	2	5
1:D:90:GLU:HA	1:D:94:MET:HE3	0.53	1.80	6	1
1:A:111:ARG:NH1	1:C:105:ILE:HG23	0.53	2.18	20	2
1:A:20:ASP:HB3	1:A:79:GLN:HB2	0.52	1.81	5	5
1:C:60:LEU:HD22	1:C:103:PRO:HB2	0.52	1.80	1	1
1:C:20:ASP:HB3	1:C:79:GLN:HB2	0.52	1.82	17	5
1:C:51:LEU:HD11	1:C:83:ILE:HD12	0.52	1.82	9	14
1:A:51:LEU:HD11	1:A:57:GLU:HB2	0.52	1.82	2	4
1:D:76:CYS:SG	1:D:114:ILE:HG12	0.52	2.45	15	4
1:B:117:MET:SD	1:B:120:ARG:HD2	0.51	2.45	20	3
1:C:19:LYS:HE3	1:D:28:ALA:HB3	0.51	1.81	3	2
1:B:100:ALA:HB1	1:B:134:ASP:HA	0.51	1.83	2	2
1:C:97:CYS:SG	1:C:102:CYS:SG	0.51	3.08	17	3
1:B:64:VAL:HG21	1:B:114:ILE:HG21	0.51	1.83	8	4
1:A:61:ARG:HB2	1:A:79:GLN:HG2	0.51	1.83	14	1
1:D:38:PRO:HD3	1:D:124:PRO:HG2	0.51	1.83	15	1
1:A:47:ALA:HB3	1:A:59:VAL:HB	0.51	1.83	16	4
1:D:31:VAL:HG22	1:D:68:LEU:HD12	0.50	1.83	10	4
1:B:12:GLN:HE22	1:D:129:ALA:HB2	0.50	1.67	15	1
1:D:25:ALA:HB1	1:D:28:ALA:HB2	0.50	1.83	8	1
1:D:11:PHE:HE2	1:D:102:CYS:SG	0.50	2.29	2	2
1:A:45:ASP:HB3	1:A:61:ARG:HB3	0.49	1.84	2	5
1:D:40:VAL:HG21	1:D:126:LEU:HG	0.49	1.85	1	1
1:B:21:ILE:CD1	1:B:113:CYS:SG	0.49	3.00	19	5
1:C:19:LYS:HE2	1:D:29:PRO:HD3	0.49	1.84	8	2
1:C:100:ALA:HB1	1:C:134:ASP:HA	0.49	1.84	11	1
1:B:21:ILE:HD12	1:B:113:CYS:SG	0.49	2.47	19	2
1:D:54:ASP:HB3	1:D:86:ILE:O	0.49	2.08	14	1
1:C:100:ALA:HB1	1:C:134:ASP:HB2	0.48	1.84	13	1
1:A:130:PRO:HG3	1:C:11:PHE:HD2	0.48	1.68	16	1
1:B:31:VAL:HG22	1:B:68:LEU:HD12	0.48	1.84	13	2
1:B:76:CYS:SG	1:B:114:ILE:HA	0.48	2.49	2	1
1:B:89:ILE:HG22	1:B:94:MET:HB2	0.48	1.85	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:11:PHE:HE2	1:D:102:CYS:HG	0.48	1.52	1	1
1:A:11:PHE:HE2	1:A:84:PHE:HB3	0.47	1.69	2	11
1:B:86:ILE:HD13	1:B:98:LEU:HD21	0.47	1.86	2	1
1:B:9:MET:HB3	1:B:89:ILE:HG12	0.47	1.85	14	2
1:B:11:PHE:CE1	1:B:13:ILE:HG13	0.47	2.44	16	1
1:C:80:GLN:HB2	1:C:110:ALA:HB2	0.47	1.86	3	2
1:C:30:HIS:O	1:C:33:GLN:HG2	0.47	2.09	11	2
1:B:125:GLN:HB2	1:C:124:PRO:HA	0.46	1.85	7	3
1:D:86:ILE:HG13	1:D:97:CYS:SG	0.46	2.51	20	1
1:A:111:ARG:HH12	1:C:105:ILE:HD12	0.46	1.71	3	1
1:B:9:MET:HB2	1:B:89:ILE:HB	0.46	1.87	9	1
1:A:97:CYS:HA	1:A:101:TYR:HB3	0.46	1.88	16	4
1:D:31:VAL:HG21	1:D:73:ALA:HA	0.46	1.88	16	3
1:D:39:GLU:O	1:D:66:ALA:HA	0.46	2.11	16	1
1:B:40:VAL:HG13	1:B:64:VAL:HG13	0.46	1.88	12	1
1:A:13:ILE:HG12	1:A:84:PHE:HD2	0.45	1.71	14	7
1:B:56:TYR:HB2	1:B:86:ILE:HD11	0.45	1.89	7	2
1:B:22:SER:HB2	1:B:77:GLU:HB3	0.45	1.88	6	2
1:A:119:SER:HB2	1:A:125:GLN:HG3	0.45	1.89	20	1
1:B:10:THR:O	1:B:86:ILE:HA	0.45	2.12	1	1
1:C:94:MET:SD	1:C:98:LEU:HD12	0.45	2.51	1	1
1:C:11:PHE:HE1	1:C:102:CYS:SG	0.45	2.34	8	2
1:D:45:ASP:HB3	1:D:61:ARG:HB3	0.45	1.88	1	4
1:A:13:ILE:CD1	1:A:105:ILE:HG21	0.45	2.42	6	2
1:B:18:THR:HG21	1:B:21:ILE:HD11	0.45	1.88	11	2
1:B:130:PRO:HG3	1:D:16:ILE:HD13	0.45	1.87	17	1
1:A:111:ARG:NH1	1:C:105:ILE:HD12	0.45	2.27	1	5
1:B:9:MET:SD	1:B:89:ILE:HB	0.45	2.51	10	1
1:D:60:LEU:HD22	1:D:103:PRO:HB3	0.45	1.87	5	2
1:B:47:ALA:HB3	1:B:59:VAL:HB	0.45	1.88	6	2
1:B:113:CYS:O	1:B:117:MET:HG2	0.44	2.13	4	4
1:A:20:ASP:HA	1:B:23:PHE:O	0.44	2.12	17	3
1:D:76:CYS:SG	1:D:114:ILE:HA	0.44	2.52	16	1
1:A:28:ALA:HB3	1:A:29:PRO:HD3	0.44	1.88	3	2
1:B:61:ARG:HG3	1:B:79:GLN:HG2	0.44	1.90	19	1
1:D:90:GLU:HA	1:D:94:MET:SD	0.44	2.53	8	1
1:C:43:ASP:HB3	1:C:63:THR:HB	0.44	1.90	10	2
1:B:9:MET:HB3	1:B:89:ILE:HB	0.44	1.89	16	2
1:B:45:ASP:HB3	1:B:61:ARG:HB3	0.44	1.87	2	2
1:B:11:PHE:HE1	1:B:102:CYS:SG	0.44	2.36	3	2
1:B:9:MET:SD	1:B:89:ILE:HG22	0.44	2.53	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:HIS:O	1:A:100:ALA:HB3	0.44	2.13	1	1
1:D:41:LYS:HB2	1:D:65:THR:HB	0.44	1.90	19	1
1:C:96:HIS:O	1:C:100:ALA:HB3	0.43	2.12	5	2
1:C:19:LYS:HE2	1:D:28:ALA:HB3	0.43	1.88	9	2
1:D:13:ILE:HG21	1:D:16:ILE:HD11	0.43	1.89	10	1
1:D:16:ILE:N	1:D:16:ILE:HD12	0.43	2.27	10	1
1:C:11:PHE:HE2	1:C:84:PHE:HB3	0.43	1.73	1	3
1:C:90:GLU:HA	1:C:94:MET:HE3	0.43	1.90	13	1
1:B:9:MET:SD	1:B:11:PHE:HB2	0.43	2.54	4	1
1:C:51:LEU:HD11	1:C:57:GLU:HB2	0.43	1.90	8	1
1:A:120:ARG:HD3	1:B:113:CYS:SG	0.43	2.53	11	1
1:C:21:ILE:HG12	1:C:113:CYS:SG	0.43	2.53	11	1
1:C:64:VAL:HG21	1:C:114:ILE:HG21	0.43	1.89	15	1
1:A:43:ASP:HB3	1:A:63:THR:HB	0.43	1.90	5	1
1:B:11:PHE:HE1	1:B:102:CYS:HG	0.43	1.55	3	1
1:A:130:PRO:HD3	1:C:13:ILE:HG13	0.43	1.90	20	1
1:B:31:VAL:HG21	1:B:73:ALA:HA	0.42	1.91	13	1
1:A:98:LEU:HD12	1:A:99:GLY:N	0.42	2.29	1	1
1:C:76:CYS:SG	1:C:114:ILE:HG23	0.42	2.54	11	4
1:B:98:LEU:HD23	1:B:98:LEU:H	0.42	1.73	13	1
1:A:21:ILE:CG2	1:A:117:MET:SD	0.42	3.07	2	1
1:C:11:PHE:CE1	1:C:101:TYR:CE2	0.42	3.07	17	3
1:A:104:ASN:HD21	1:A:133:PHE:HB2	0.42	1.73	9	1
1:A:13:ILE:HG21	1:C:130:PRO:HG2	0.42	1.91	14	1
1:D:57:GLU:HB2	1:D:83:ILE:HG12	0.42	1.90	14	1
1:B:51:LEU:HD11	1:B:57:GLU:HB2	0.42	1.90	15	1
1:B:94:MET:SD	1:B:98:LEU:HD21	0.42	2.53	16	1
1:D:86:ILE:HB	1:D:89:ILE:HD12	0.42	1.92	18	1
1:B:61:ARG:HB2	1:B:79:GLN:HG2	0.42	1.91	9	1
1:C:59:VAL:HG12	1:C:79:GLN:HG2	0.42	1.91	9	1
1:D:28:ALA:O	1:D:31:VAL:HG12	0.42	2.15	5	3
1:A:40:VAL:HA	1:A:65:THR:O	0.42	2.15	17	1
1:D:86:ILE:HD13	1:D:98:LEU:HD21	0.42	1.91	2	1
1:B:96:HIS:O	1:B:100:ALA:HB3	0.42	2.14	3	1
1:D:64:VAL:CG2	1:D:114:ILE:HD13	0.42	2.45	3	1
1:D:51:LEU:HD11	1:D:57:GLU:HB2	0.42	1.92	3	1
1:C:45:ASP:HB3	1:C:61:ARG:HB3	0.42	1.92	17	3
1:A:52:ALA:HB3	1:A:55:VAL:HB	0.42	1.92	9	1
1:C:17:TYR:HB3	1:D:122:THR:HG23	0.42	1.92	19	1
1:B:56:TYR:HB3	1:B:86:ILE:HD13	0.41	1.90	12	1
1:A:116:SER:O	1:A:120:ARG:HB2	0.41	2.15	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:44:LEU:HA	1:C:61:ARG:O	0.41	2.14	13	1
1:C:20:ASP:HA	1:D:23:PHE:O	0.41	2.15	14	2
1:A:21:ILE:HD13	1:B:117:MET:SD	0.41	2.56	16	1
1:C:18:THR:HG22	1:C:80:GLN:HE22	0.41	1.74	5	1
1:C:47:ALA:HB3	1:C:59:VAL:HB	0.41	1.93	17	1
1:D:89:ILE:HG22	1:D:90:GLU:N	0.41	2.31	11	1
1:D:14:GLN:HE21	1:D:85:SER:HB2	0.41	1.76	10	1
1:D:56:TYR:HB3	1:D:86:ILE:HD13	0.41	1.91	11	2
1:B:42:LEU:HD13	1:B:128:LEU:HD21	0.41	1.91	15	1
1:D:41:LYS:HB3	1:D:65:THR:HB	0.41	1.92	12	2
1:A:23:PHE:O	1:B:20:ASP:HA	0.41	2.15	20	2
1:C:44:LEU:HD23	1:C:60:LEU:HD11	0.41	1.91	13	1
1:D:11:PHE:CE2	1:D:102:CYS:SG	0.41	3.13	2	1
1:A:34:LYS:HD3	1:A:35:ASP:N	0.40	2.31	5	1
1:B:76:CYS:SG	1:B:114:ILE:HG23	0.40	2.56	8	1
1:B:28:ALA:HB3	1:B:29:PRO:HD3	0.40	1.92	11	1
1:C:104:ASN:HD21	1:C:133:PHE:HB3	0.40	1.75	11	1
1:B:60:LEU:HD23	1:B:106:LEU:HD12	0.40	1.93	13	1
1:C:19:LYS:HE2	1:C:59:VAL:HG21	0.40	1.93	14	1
1:D:13:ILE:HD13	1:D:105:ILE:HG21	0.40	1.94	2	1
1:B:114:ILE:O	1:B:118:VAL:HG23	0.40	2.16	17	1
1:C:14:GLN:HB2	1:C:83:ILE:HB	0.40	1.93	1	2
1:C:61:ARG:HB2	1:C:79:GLN:HG2	0.40	1.94	2	1
1:C:44:LEU:HD23	1:C:45:ASP:N	0.40	2.31	6	1
1:B:34:LYS:HB2	1:B:68:LEU:HD13	0.40	1.93	10	1
1:C:98:LEU:HA	1:C:102:CYS:SG	0.40	2.57	16	1
1:C:94:MET:O	1:C:98:LEU:HG	0.40	2.16	16	1
1:D:14:GLN:HB2	1:D:83:ILE:HB	0.40	1.92	19	1
1:D:114:ILE:O	1:D:118:VAL:HG23	0.40	2.16	3	1
1:B:125:GLN:HA	1:B:125:GLN:HE21	0.40	1.77	9	1
1:C:17:TYR:CE2	1:C:19:LYS:HD3	0.40	2.51	15	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	115/155 (74%)	109±2 (95±1%)	6±2 (5±1%)	0±0 (0±0%)	100	100
1	B	126/155 (81%)	119±2 (94±2%)	7±2 (6±2%)	0±0 (0±0%)	56	85
1	C	124/155 (80%)	115±2 (93±2%)	9±2 (7±2%)	0±0 (0±0%)	59	88
1	D	122/155 (79%)	116±2 (95±1%)	5±2 (4±1%)	0±0 (0±0%)	56	85
2	E	0	-	-	-	-	-
2	F	0	-	-	-	-	-
2	G	0	-	-	-	-	-
2	H	0	-	-	-	-	-
All	All	9740/14400 (68%)	9171 (94%)	556 (6%)	13 (0%)	59	88

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	D	28	ALA	6
1	B	9	MET	3
1	C	130	PRO	2
1	B	130	PRO	2

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	100/132 (76%)	98±1 (98±1%)	2±1 (2±1%)	67	95
1	B	108/132 (82%)	105±2 (97±2%)	3±2 (3±2%)	51	90
1	C	106/132 (80%)	102±1 (96±1%)	4±1 (4±1%)	43	85
1	D	104/132 (79%)	102±1 (98±1%)	2±1 (2±1%)	66	94
2	E	0	-	-	-	-
2	F	0	-	-	-	-
2	G	0	-	-	-	-
2	H	0	-	-	-	-
All	All	8360/12320 (68%)	8130 (97%)	230 (3%)	55	91

All 70 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	34	LYS	20
1	C	117	MET	20
1	B	12	GLN	15
1	D	70	GLU	13
1	A	86	ILE	7
1	D	90	GLU	7
1	B	125	GLN	7
1	C	112	GLU	6
1	D	93	GLN	6
1	B	94	MET	6
1	B	11	PHE	6
1	A	60	LEU	5
1	A	42	LEU	5
1	B	9	MET	4
1	B	42	LEU	4
1	A	14	GLN	4
1	C	126	LEU	4
1	C	128	LEU	4
1	C	11	PHE	4
1	B	86	ILE	3
1	C	44	LEU	3
1	C	86	ILE	3
1	C	125	GLN	3
1	B	70	GLU	3
1	A	56	TYR	3
1	A	27	ASN	3
1	B	89	ILE	3
1	D	86	ILE	3
1	D	42	LEU	3
1	C	104	ASN	2
1	B	126	LEU	2
1	A	70	GLU	2
1	C	61	ARG	2
1	C	107	PHE	2
1	B	98	LEU	2
1	C	39	GLU	2
1	C	98	LEU	2
1	C	42	LEU	2
1	A	122	THR	2
1	B	112	GLU	2
1	B	132	ASN	2
1	D	98	LEU	1
1	B	107	PHE	1

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Mol	Chain	Res	Type	Models (Total)
1	D	127	ASN	1
1	B	60	LEU	1
1	B	39	GLU	1
1	B	93	GLN	1
1	A	125	GLN	1
1	D	39	GLU	1
1	C	14	GLN	1
1	A	98	LEU	1
1	D	104	ASN	1
1	D	41	LYS	1
1	B	128	LEU	1
1	A	54	ASP	1
1	D	56	TYR	1
1	B	56	TYR	1
1	D	60	LEU	1
1	C	70	GLU	1
1	A	31	VAL	1
1	D	94	MET	1
1	B	35	ASP	1
1	B	104	ASN	1
1	B	90	GLU	1
1	D	126	LEU	1
1	C	93	GLN	1
1	A	101	TYR	1
1	A	128	LEU	1
1	C	37	GLN	1
1	A	41	LYS	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: 5jtm_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	226
Number of shifts mapped to atoms	226
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
$^{13}\text{C}_\alpha$	19	-0.15 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	21	0.03 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
^{15}N	21	-2.47 ± 0.45	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. 0 atoms were assigned a chemical shift out of a possible 5840. 0 out of 80 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/2379 (0%)	0/946 (0%)	0/974 (0%)	0/459 (0%)
Sidechain	0/2942 (0%)	0/1716 (0%)	0/1116 (0%)	0/110 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/519 (0%)	0/275 (0%)	0/224 (0%)	0/20 (0%)
Overall	0/5840 (0%)	0/2937 (0%)	0/2314 (0%)	0/589 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 2%, i.e. 192 atoms were assigned a chemical shift out of a possible 8632. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	77/3520 (2%)	37/1400 (3%)	19/1440 (1%)	21/680 (3%)
Sidechain	106/4448 (2%)	53/2596 (2%)	53/1684 (3%)	0/168 (0%)
Aromatic	9/664 (1%)	5/352 (1%)	4/284 (1%)	0/28 (0%)
Overall	192/8632 (2%)	95/4348 (2%)	76/3408 (2%)	21/876 (2%)

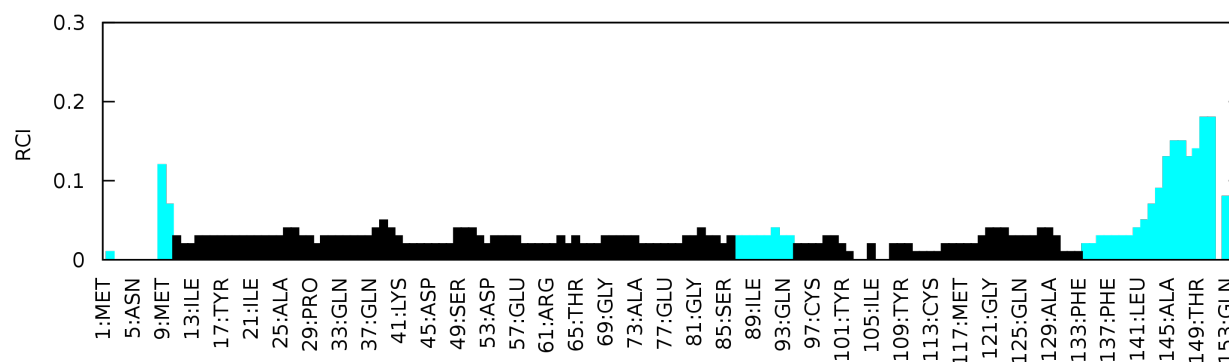
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

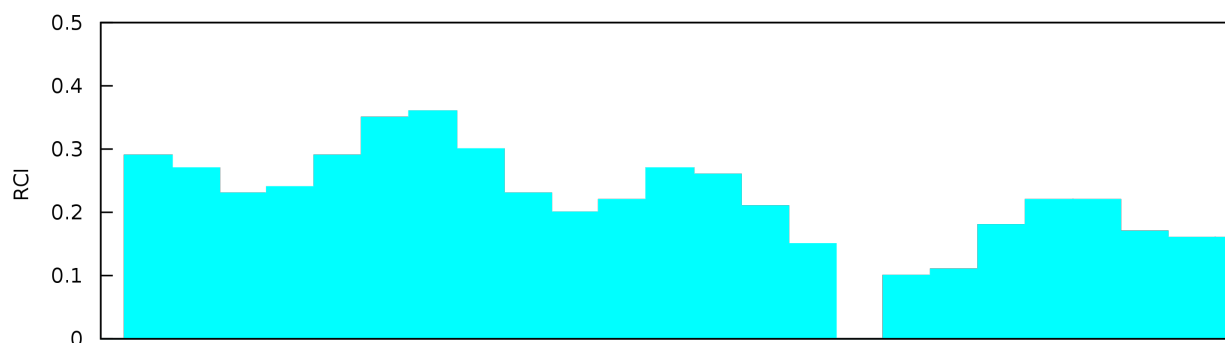
7.1.5 Random Coil Index (RCI) plots [i](#)

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: 5jtm_cs.cif

Chemical shift list name: *assigned_chemical_shift_6*

7.2.1 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	226
Number of shifts mapped to atoms	226
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 ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	19	-0.15 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	21	0.05 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
^{15}N	21	-2.48 ± 0.56	Should be applied

7.2.3 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. 0 atoms were assigned a chemical shift out of a possible 5840. 0 out of 80 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/2379 (0%)	0/946 (0%)	0/974 (0%)	0/459 (0%)
Sidechain	0/2942 (0%)	0/1716 (0%)	0/1116 (0%)	0/110 (0%)
Aromatic	0/519 (0%)	0/275 (0%)	0/224 (0%)	0/20 (0%)
Overall	0/5840 (0%)	0/2937 (0%)	0/2314 (0%)	0/589 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 2%, i.e. 192 atoms were assigned a chemical shift out of a possible 8632. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	77/3520 (2%)	37/1400 (3%)	19/1440 (1%)	21/680 (3%)
Sidechain	106/4448 (2%)	53/2596 (2%)	53/1684 (3%)	0/168 (0%)
Aromatic	9/664 (1%)	5/352 (1%)	4/284 (1%)	0/28 (0%)
Overall	192/8632 (2%)	95/4348 (2%)	76/3408 (2%)	21/876 (2%)

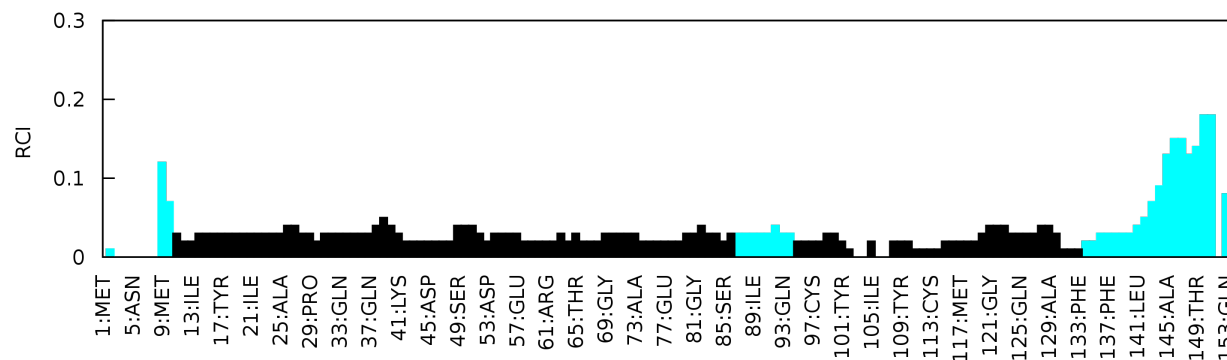
7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

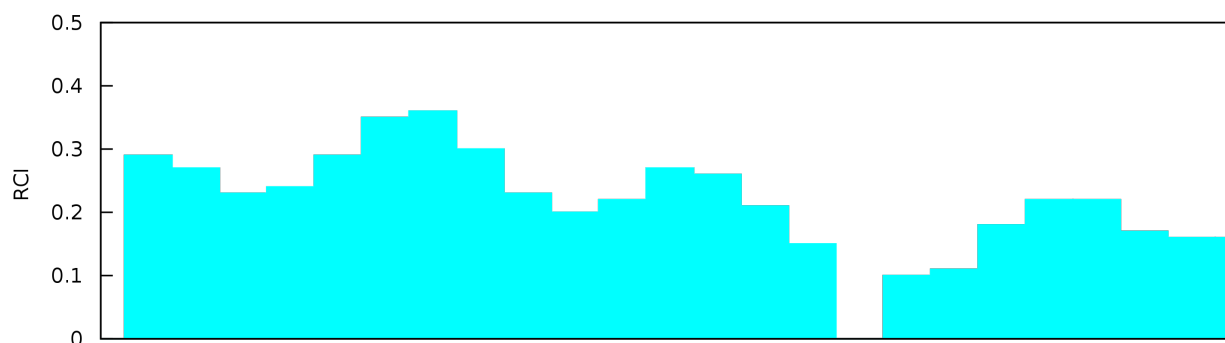
7.2.5 Random Coil Index (RCI) plots [i](#)

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: 5jtm_cs.cif

Chemical shift list name: *assigned_chemical_shift_7*

7.3.1 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	226
Number of shifts mapped to atoms	226
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 ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	19	-0.15 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	21	0.05 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
^{15}N	21	-2.47 ± 0.44	Should be applied

7.3.3 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. 0 atoms were assigned a chemical shift out of a possible 5840. 0 out of 80 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/2379 (0%)	0/946 (0%)	0/974 (0%)	0/459 (0%)
Sidechain	0/2942 (0%)	0/1716 (0%)	0/1116 (0%)	0/110 (0%)
Aromatic	0/519 (0%)	0/275 (0%)	0/224 (0%)	0/20 (0%)
Overall	0/5840 (0%)	0/2937 (0%)	0/2314 (0%)	0/589 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 2%, i.e. 192 atoms were assigned a chemical shift out of a possible 8632. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	77/3520 (2%)	37/1400 (3%)	19/1440 (1%)	21/680 (3%)
Sidechain	106/4448 (2%)	53/2596 (2%)	53/1684 (3%)	0/168 (0%)
Aromatic	9/664 (1%)	5/352 (1%)	4/284 (1%)	0/28 (0%)
Overall	192/8632 (2%)	95/4348 (2%)	76/3408 (2%)	21/876 (2%)

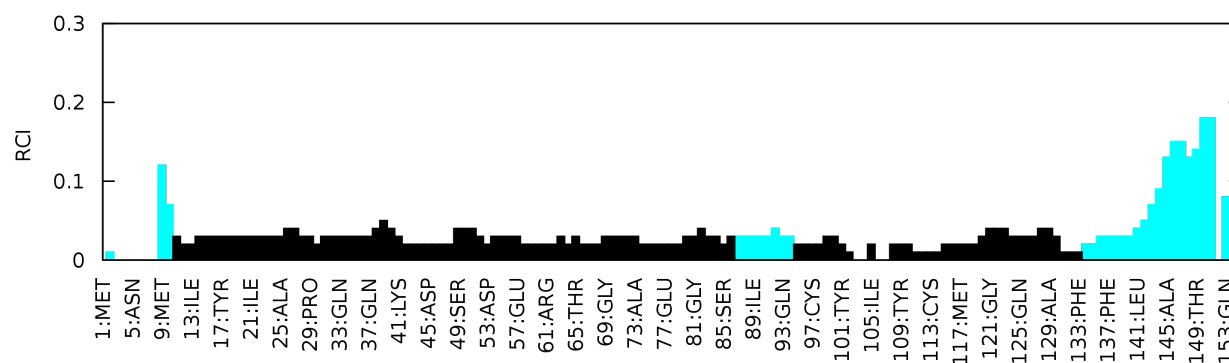
7.3.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

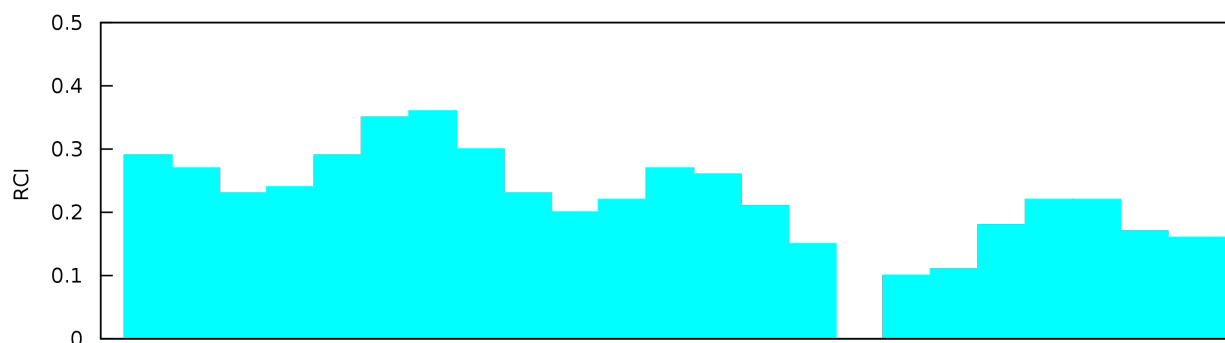
7.3.5 Random Coil Index (RCI) plots [i](#)

The 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:



7.4 Chemical shift list 4

File name: 5jtm_cs.cif

Chemical shift list name: *assigned_chemical_shift_8*

7.4.1 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	226
Number of shifts mapped to atoms	226
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 ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	19	-0.15 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	21	0.03 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
^{15}N	21	-2.48 ± 0.61	Should be applied

7.4.3 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. 0 atoms were assigned a chemical shift out of a possible 5840. 0 out of 80 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/2379 (0%)	0/946 (0%)	0/974 (0%)	0/459 (0%)
Sidechain	0/2942 (0%)	0/1716 (0%)	0/1116 (0%)	0/110 (0%)
Aromatic	0/519 (0%)	0/275 (0%)	0/224 (0%)	0/20 (0%)
Overall	0/5840 (0%)	0/2937 (0%)	0/2314 (0%)	0/589 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 2%, i.e. 192 atoms were assigned a chemical shift out of a possible 8632. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	77/3520 (2%)	37/1400 (3%)	19/1440 (1%)	21/680 (3%)
Sidechain	106/4448 (2%)	53/2596 (2%)	53/1684 (3%)	0/168 (0%)
Aromatic	9/664 (1%)	5/352 (1%)	4/284 (1%)	0/28 (0%)
Overall	192/8632 (2%)	95/4348 (2%)	76/3408 (2%)	21/876 (2%)

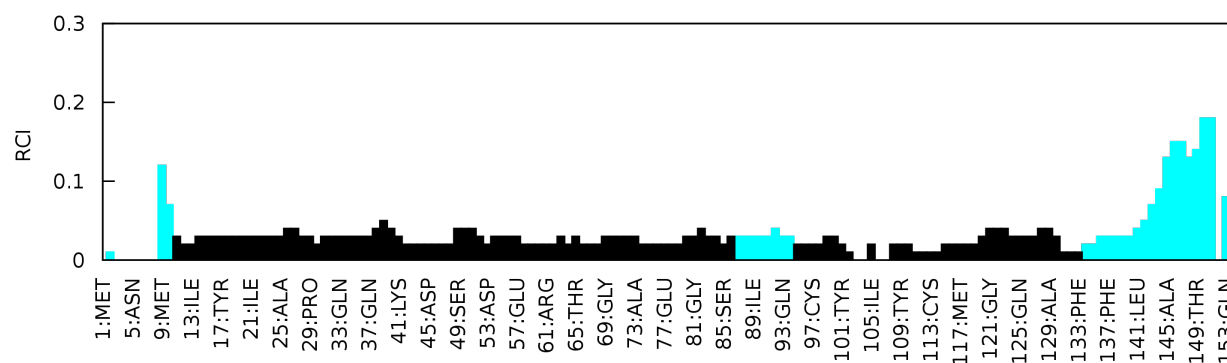
7.4.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

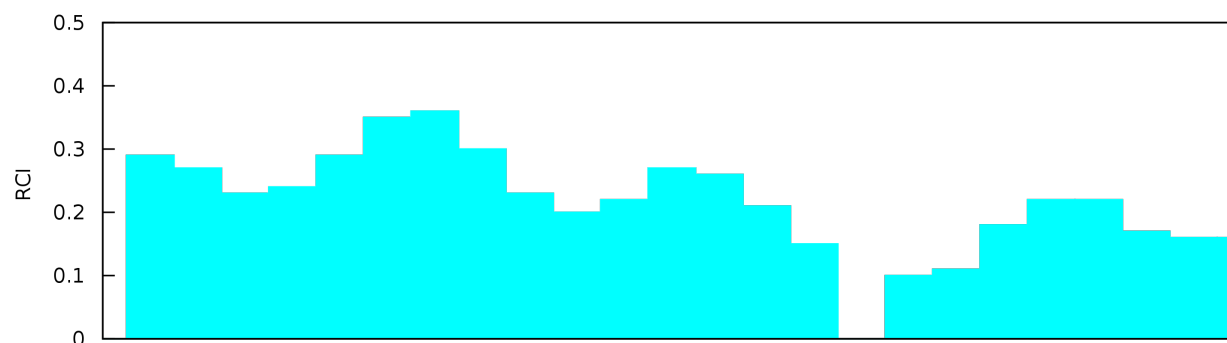
7.4.5 Random Coil Index (RCI) plots [i](#)

The 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:



7.5 Chemical shift list 5

File name: 5jtm_cs.cif

Chemical shift list name: *assigned_chemical_shift_list_1*

7.5.1 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	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

7.5.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	139	0.26 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	128	0.85 ± 0.21	Should be applied
$^{13}\text{C}'$	137	0.29 ± 0.07	None needed (< 0.5 ppm)
^{15}N	133	-1.16 ± 0.25	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. 740 atoms were assigned a chemical shift out of a possible 5840. 0 out of 80 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	422/2379 (18%)	103/946 (11%)	216/974 (22%)	103/459 (22%)
Sidechain	205/2942 (7%)	57/1716 (3%)	148/1116 (13%)	0/110 (0%)
Aromatic	113/519 (22%)	57/275 (21%)	55/224 (25%)	1/20 (5%)
Overall	740/5840 (13%)	217/2937 (7%)	419/2314 (18%)	104/589 (18%)

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 8632. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	542/3520 (15%)	133/1400 (10%)	276/1440 (19%)	133/680 (20%)
Sidechain	255/4448 (6%)	70/2596 (3%)	185/1684 (11%)	0/168 (0%)
Aromatic	133/664 (20%)	67/352 (19%)	65/284 (23%)	1/28 (4%)
Overall	930/8632 (11%)	270/4348 (6%)	526/3408 (15%)	134/876 (15%)

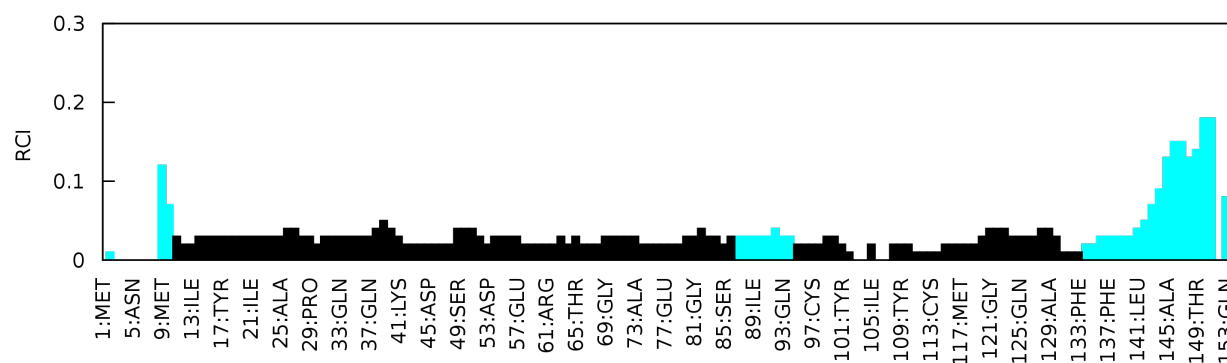
7.5.4 Statistically unusual chemical shifts [i](#)

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: 5jtm_cs.cif

Chemical shift list name: *assigned_chemical_shift_list_2*

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	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

7.6.2 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	0.28 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	126	0.79 ± 0.15	Should be applied
$^{13}\text{C}'$	135	0.26 ± 0.08	None needed (< 0.5 ppm)
^{15}N	132	-1.09 ± 0.20	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. 735 atoms were assigned a chemical shift out of a possible 5840. 0 out of 80 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	419/2379 (18%)	102/946 (11%)	215/974 (22%)	102/459 (22%)
Sidechain	203/2942 (7%)	57/1716 (3%)	146/1116 (13%)	0/110 (0%)
Aromatic	113/519 (22%)	57/275 (21%)	55/224 (25%)	1/20 (5%)
Overall	735/5840 (13%)	216/2937 (7%)	416/2314 (18%)	103/589 (17%)

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 8632. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	539/3520 (15%)	132/1400 (9%)	275/1440 (19%)	132/680 (19%)
Sidechain	253/4448 (6%)	70/2596 (3%)	183/1684 (11%)	0/168 (0%)
Aromatic	133/664 (20%)	67/352 (19%)	65/284 (23%)	1/28 (4%)
Overall	925/8632 (11%)	269/4348 (6%)	523/3408 (15%)	133/876 (15%)

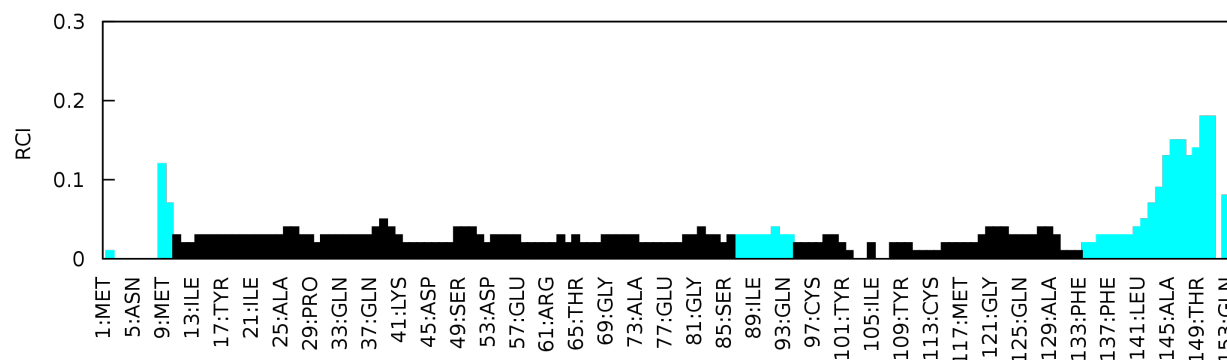
7.6.4 Statistically unusual chemical shifts [i](#)

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:



7.7 Chemical shift list 7

File name: 5jtm_cs.cif

Chemical shift list name: *assigned_chemical_shift_list_3*

7.7.1 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

7.7.2 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	0.27 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	126	0.78 ± 0.16	Should be applied
$^{13}\text{C}'$	135	0.26 ± 0.08	None needed (< 0.5 ppm)
^{15}N	132	-1.09 ± 0.31	Should be applied

7.7.3 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. 735 atoms were assigned a chemical shift out of a possible 5840. 0 out of 80 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	419/2379 (18%)	102/946 (11%)	215/974 (22%)	102/459 (22%)
Sidechain	203/2942 (7%)	57/1716 (3%)	146/1116 (13%)	0/110 (0%)
Aromatic	113/519 (22%)	57/275 (21%)	55/224 (25%)	1/20 (5%)
Overall	735/5840 (13%)	216/2937 (7%)	416/2314 (18%)	103/589 (17%)

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 8632. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	539/3520 (15%)	132/1400 (9%)	275/1440 (19%)	132/680 (19%)
Sidechain	253/4448 (6%)	70/2596 (3%)	183/1684 (11%)	0/168 (0%)
Aromatic	133/664 (20%)	67/352 (19%)	65/284 (23%)	1/28 (4%)
Overall	925/8632 (11%)	269/4348 (6%)	523/3408 (15%)	133/876 (15%)

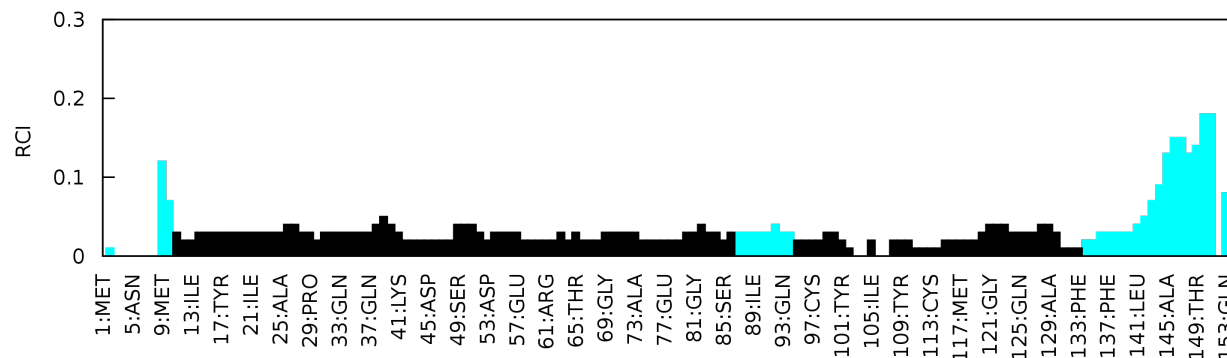
7.7.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.7.5 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:



7.8 Chemical shift list 8

File name: 5jtm_cs.cif

Chemical shift list name: *assigned_chemical_shift_list_4*

7.8.1 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

7.8.2 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	0.25 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	128	0.85 ± 0.11	Should be applied
$^{13}\text{C}'$	137	0.29 ± 0.11	None needed (< 0.5 ppm)
^{15}N	133	-1.16 ± 0.16	Should be applied

7.8.3 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. 740 atoms were assigned a chemical shift out of a possible 5840. 0 out of 80 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	422/2379 (18%)	103/946 (11%)	216/974 (22%)	103/459 (22%)
Sidechain	205/2942 (7%)	57/1716 (3%)	148/1116 (13%)	0/110 (0%)
Aromatic	113/519 (22%)	57/275 (21%)	55/224 (25%)	1/20 (5%)
Overall	740/5840 (13%)	217/2937 (7%)	419/2314 (18%)	104/589 (18%)

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 8632. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	542/3520 (15%)	133/1400 (10%)	276/1440 (19%)	133/680 (20%)
Sidechain	255/4448 (6%)	70/2596 (3%)	185/1684 (11%)	0/168 (0%)
Aromatic	133/664 (20%)	67/352 (19%)	65/284 (23%)	1/28 (4%)
Overall	930/8632 (11%)	270/4348 (6%)	526/3408 (15%)	134/876 (15%)

7.8.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.8.5 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:

