Full wwPDB NMR Structure Validation Report (i)

Apr 20, 2024 – 08:29 AM EDT

PDB ID	:	5JTN
BMRB ID	:	30082
Title	:	The structure of chaperone SecB in complex with unstructured proPhoA binding site c
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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

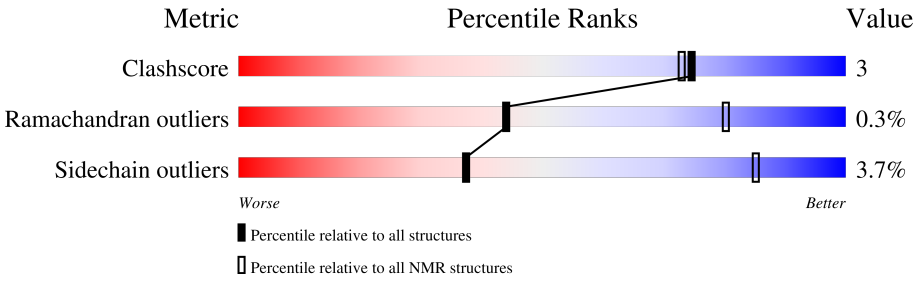
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 14%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	155	79% · 17%
1	B	155	74% 6% 20%
1	C	155	77% 5% 18%
1	D	155	69% 8% 23%
2	E	55	100%
2	F	55	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:10-A:137, B:9-B:132, C:11-C:137, D:10-D:48, D:54-D:133 (498)	0.73	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 2 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11068 atoms, of which 5408 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	55	Total	C	H	N	O	0
			800	259	394	66	81	
2	F	55	Total	C	H	N	O	0
			800	259	394	66	81	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

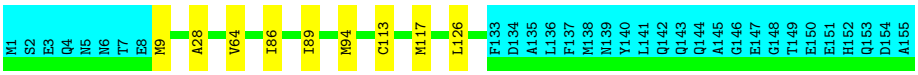
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for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

• Molecule 1: Protein-export protein SecB

Chain A:

• Molecule 1: Protein-export protein SecB

Chain B:

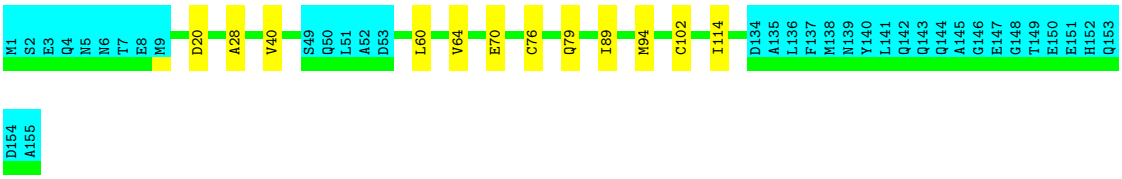


• Molecule 1: Protein-export protein SecB

Chain C:

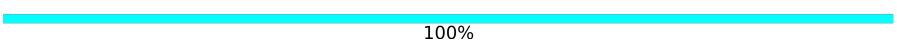
• Molecule 1: Protein-export protein SecB

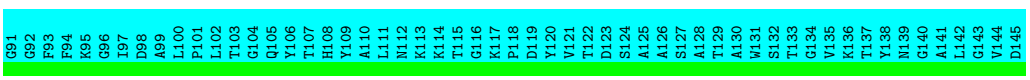
Chain D:



• Molecule 2: Alkaline phosphatase

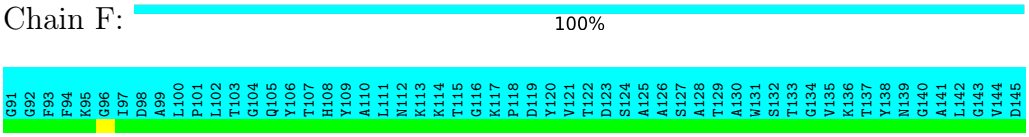
Chain E:





• Molecule 2: Alkaline phosphatase

Chain F:



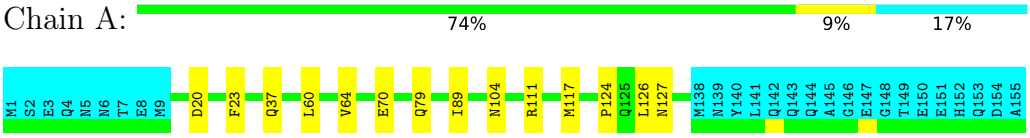
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

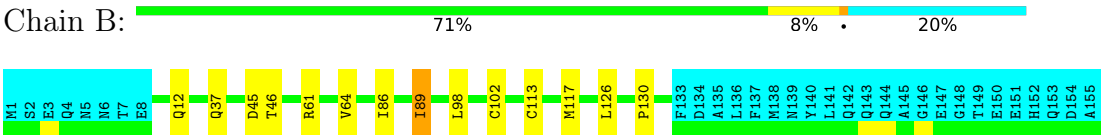
• Molecule 1: Protein-export protein SecB

Chain A:



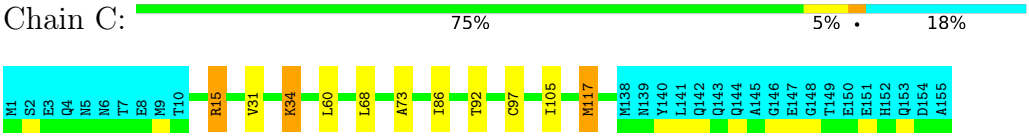
• Molecule 1: Protein-export protein SecB

Chain B:



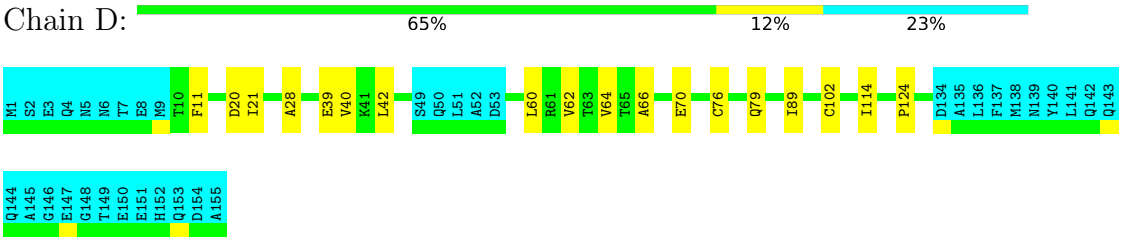
• Molecule 1: Protein-export protein SecB

Chain C:



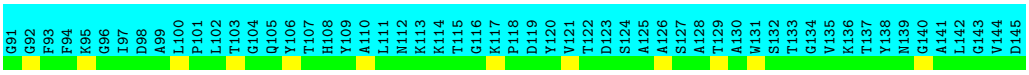
• Molecule 1: Protein-export protein SecB

Chain D:



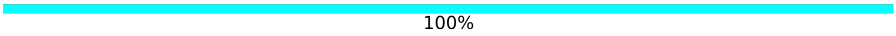
• Molecule 2: Alkaline phosphatase

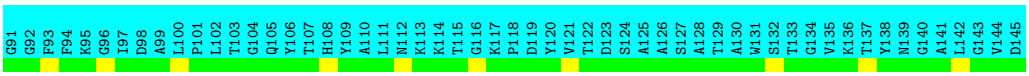
Chain E:



• Molecule 2: Alkaline phosphatase

Chain F:





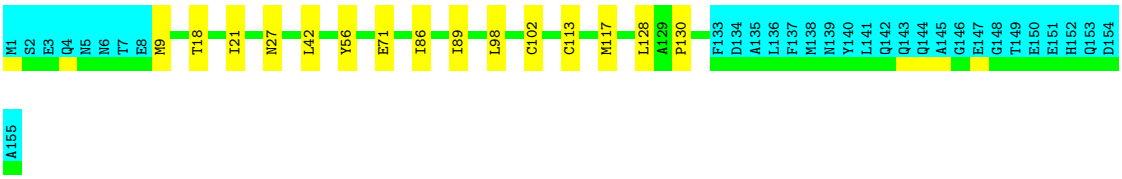
4.2.2 Score per residue for model 2

• Molecule 1: Protein-export protein SecB

Chain A:

• Molecule 1: Protein-export protein SecB

Chain B:

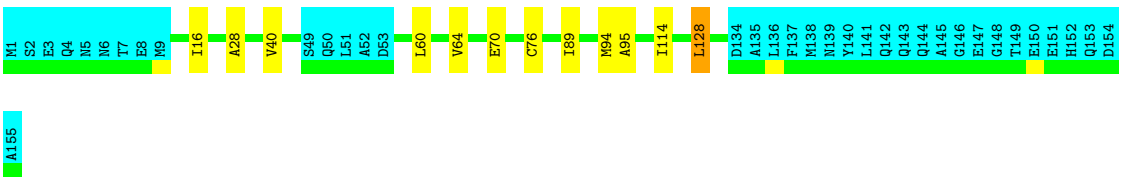


• Molecule 1: Protein-export protein SecB

Chain C:

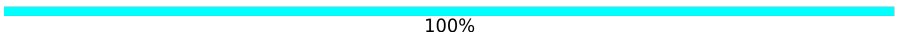
• Molecule 1: Protein-export protein SecB

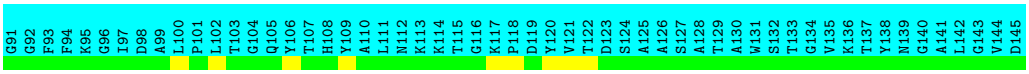
Chain D:



• Molecule 2: Alkaline phosphatase

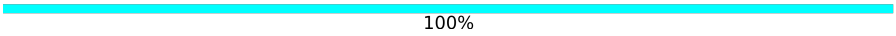
Chain E:

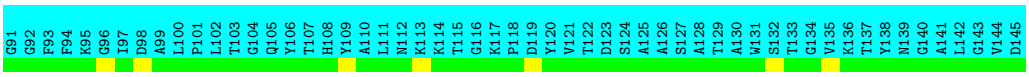




• Molecule 2: Alkaline phosphatase

Chain F:





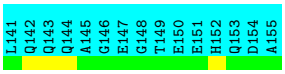
4.2.3 Score per residue for model 3

• Molecule 1: Protein-export protein SecB

Chain A:

• Molecule 1: Protein-export protein SecB

Chain B:

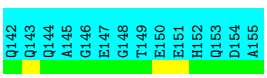


• Molecule 1: Protein-export protein SecB

Chain C:

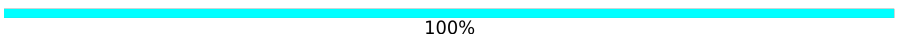
• Molecule 1: Protein-export protein SecB

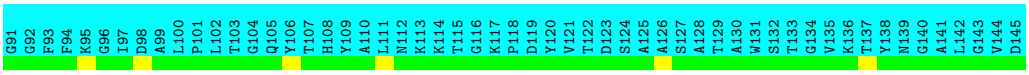
Chain D:



• Molecule 2: Alkaline phosphatase

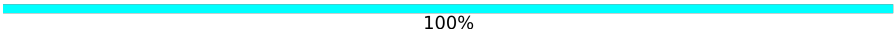
Chain E:

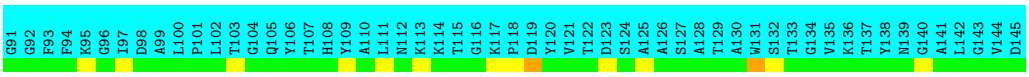




• Molecule 2: Alkaline phosphatase

Chain F:

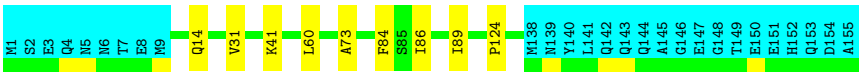




4.2.4 Score per residue for model 4

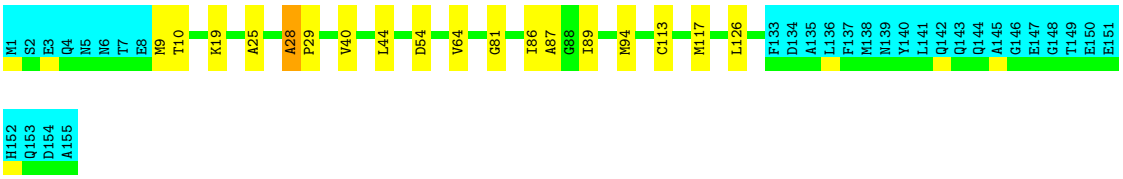
• Molecule 1: Protein-export protein SecB

Chain A:



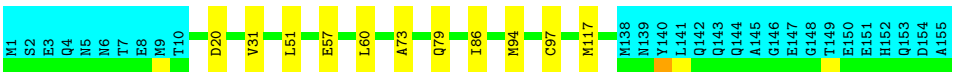
• Molecule 1: Protein-export protein SecB

Chain B:



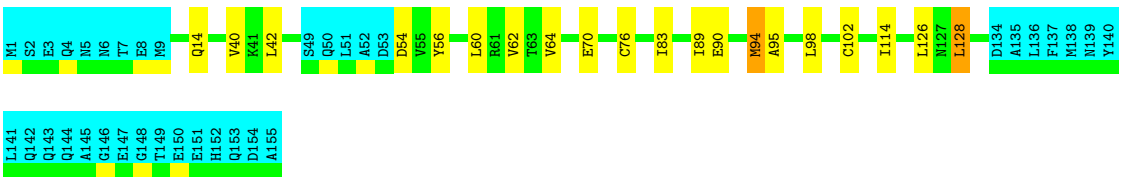
• Molecule 1: Protein-export protein SecB

Chain C:



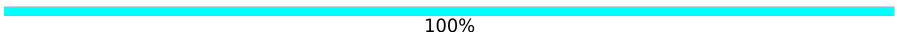
• Molecule 1: Protein-export protein SecB

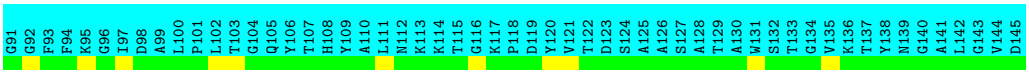
Chain D:



• Molecule 2: Alkaline phosphatase

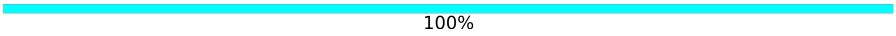
Chain E:

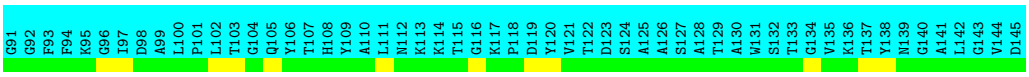




• Molecule 2: Alkaline phosphatase

Chain F:





4.2.5 Score per residue for model 5

• Molecule 1: Protein-export protein SecB

Chain A:

• Molecule 1: Protein-export protein SecB

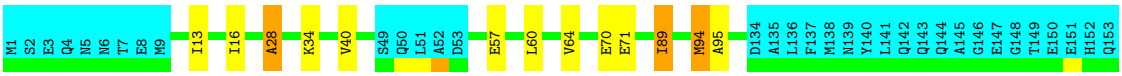
Chain B:

• Molecule 1: Protein-export protein SecB

Chain C:

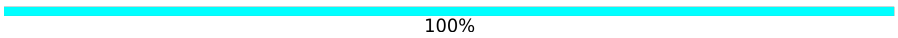
• Molecule 1: Protein-export protein SecB

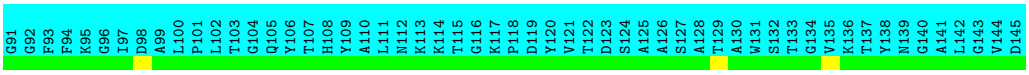
Chain D:



• Molecule 2: Alkaline phosphatase

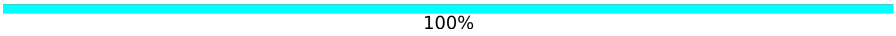
Chain E:

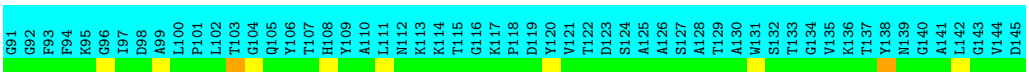




• Molecule 2: Alkaline phosphatase

Chain F:





4.2.6 Score per residue for model 6

• Molecule 1: Protein-export protein SecB

Chain A:

• Molecule 1: Protein-export protein SecB

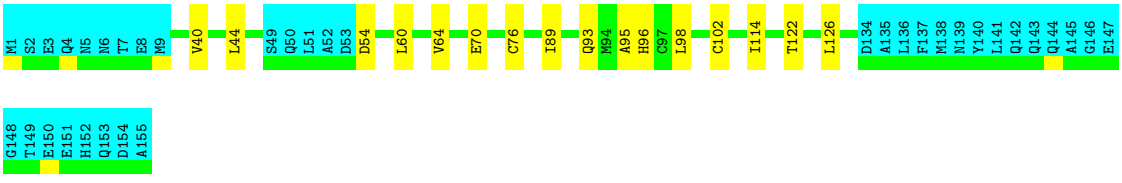
Chain B:

• Molecule 1: Protein-export protein SecB

Chain C:

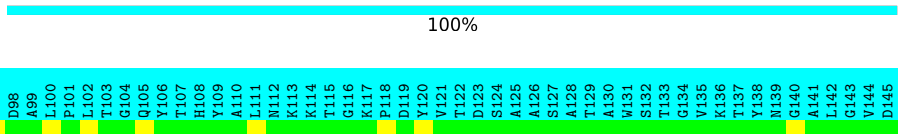
• Molecule 1: Protein-export protein SecB

Chain D:



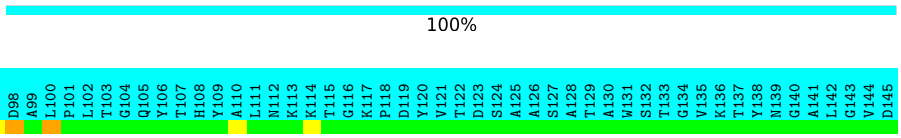
• Molecule 2: Alkaline phosphatase

Chain E:



• Molecule 2: Alkaline phosphatase

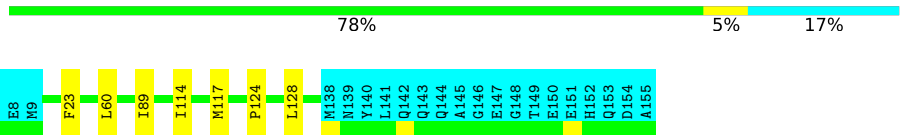
Chain F:



4.2.7 Score per residue for model 7

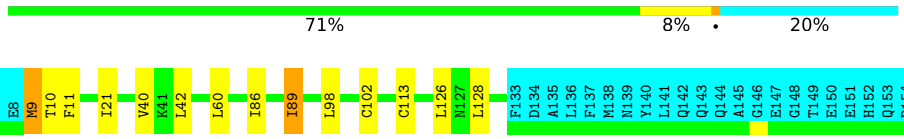
• Molecule 1: Protein-export protein SecB

Chain A:



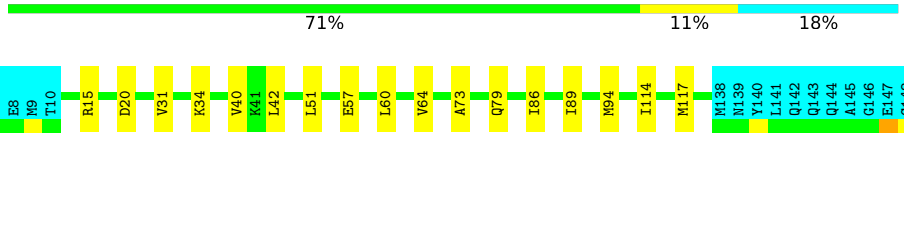
• Molecule 1: Protein-export protein SecB

Chain B:



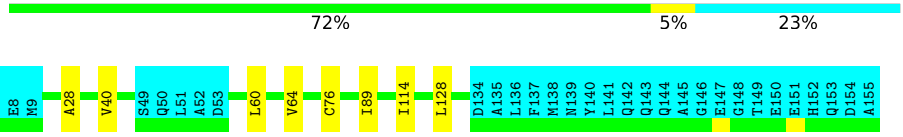
• Molecule 1: Protein-export protein SecB

Chain C:



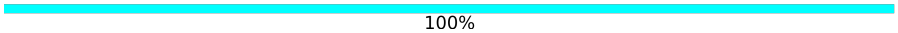
• Molecule 1: Protein-export protein SecB

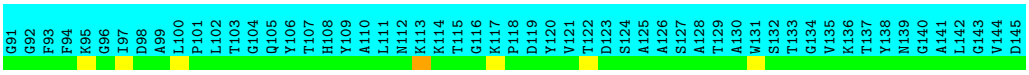
Chain D:



• Molecule 2: Alkaline phosphatase

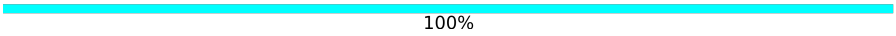
Chain E:

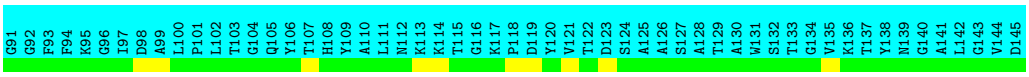




• Molecule 2: Alkaline phosphatase

Chain F:





4.2.8 Score per residue for model 8

• Molecule 1: Protein-export protein SecB

Chain A:

• Molecule 1: Protein-export protein SecB

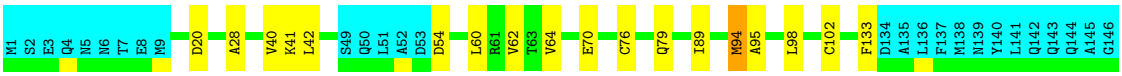
Chain B:

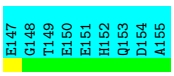
• Molecule 1: Protein-export protein SecB

Chain C:

• Molecule 1: Protein-export protein SecB

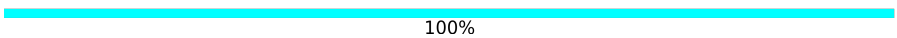
Chain D:

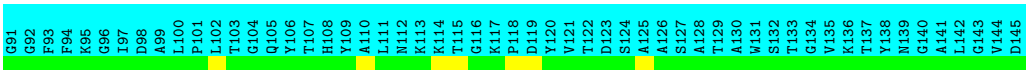




• Molecule 2: Alkaline phosphatase

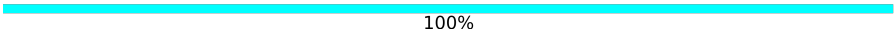
Chain E:

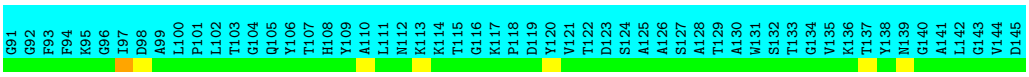




• Molecule 2: Alkaline phosphatase

Chain F:

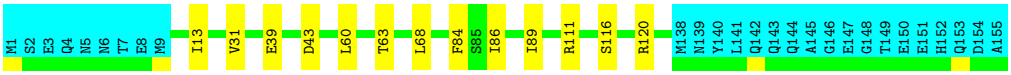




4.2.9 Score per residue for model 9

• Molecule 1: Protein-export protein SecB

Chain A:

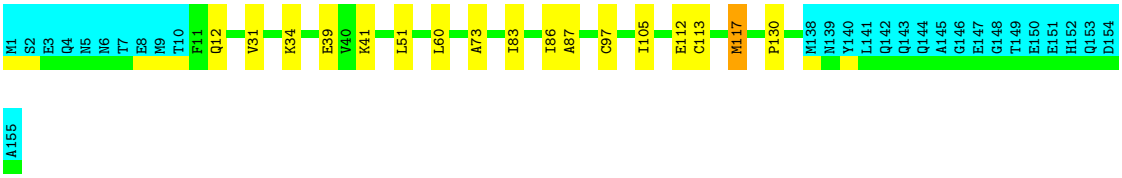


• Molecule 1: Protein-export protein SecB

Chain B:

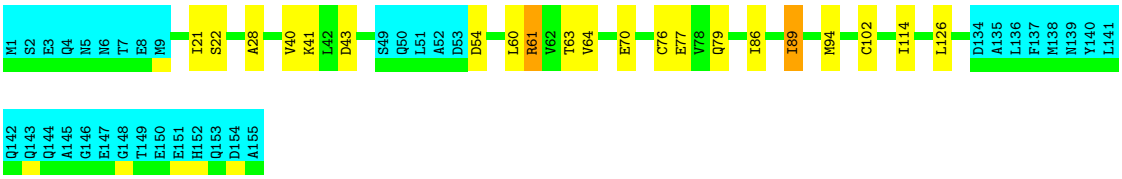
• Molecule 1: Protein-export protein SecB

Chain C:



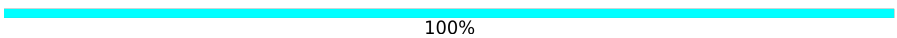
• Molecule 1: Protein-export protein SecB

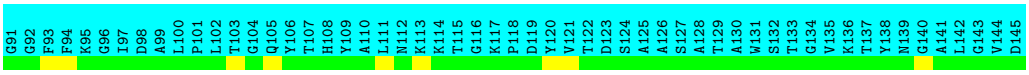
Chain D:



• Molecule 2: Alkaline phosphatase

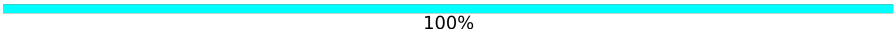
Chain E:

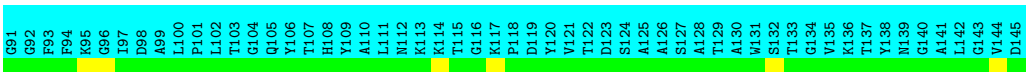




• Molecule 2: Alkaline phosphatase

Chain F:

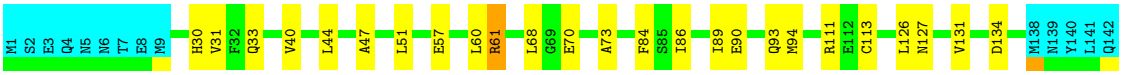


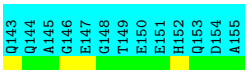


4.2.10 Score per residue for model 10

• Molecule 1: Protein-export protein SecB

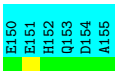
Chain A:





• Molecule 1: Protein-export protein SecB

Chain B:



• Molecule 1: Protein-export protein SecB

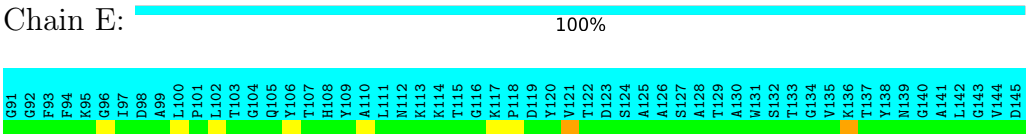
Chain C:

• Molecule 1: Protein-export protein SecB

Chain D:

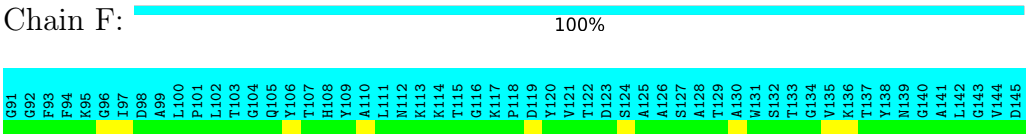
• Molecule 2: Alkaline phosphatase

Chain E:



• Molecule 2: Alkaline phosphatase

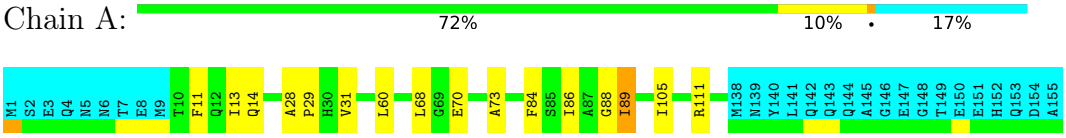
Chain F:



4.2.11 Score per residue for model 11

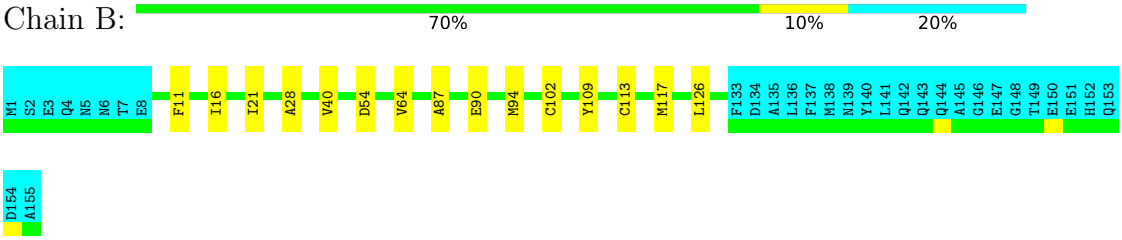
• Molecule 1: Protein-export protein SecB

Chain A:



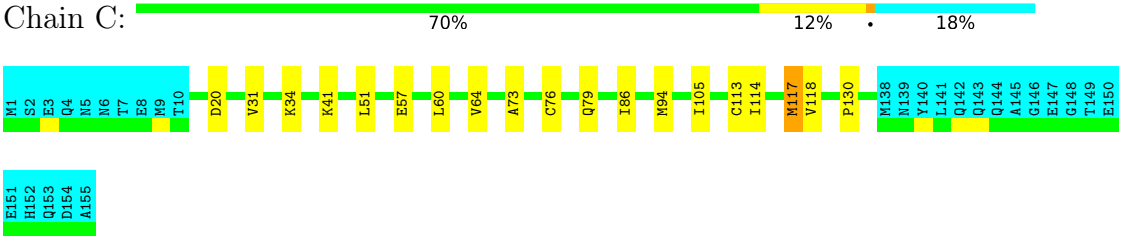
• Molecule 1: Protein-export protein SecB

Chain B:



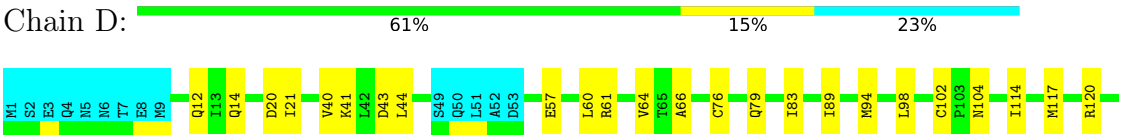
• Molecule 1: Protein-export protein SecB

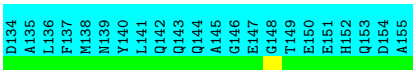
Chain C:



• Molecule 1: Protein-export protein SecB

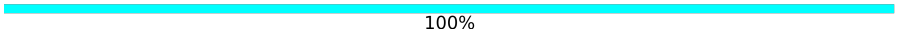
Chain D:

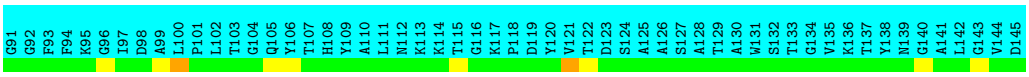




• Molecule 2: Alkaline phosphatase

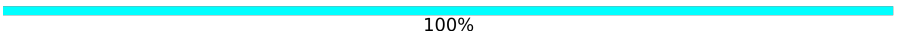
Chain E:

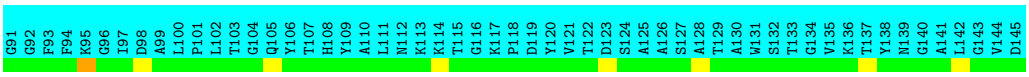




• Molecule 2: Alkaline phosphatase

Chain F:

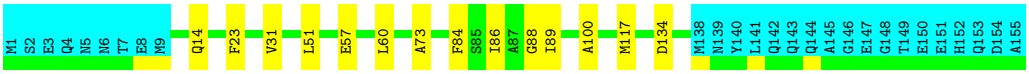




4.2.12 Score per residue for model 12

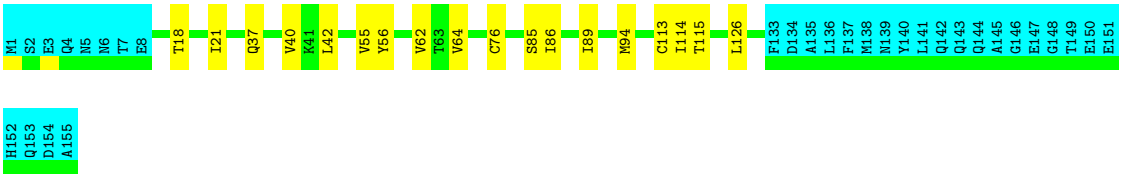
• Molecule 1: Protein-export protein SecB

Chain A:



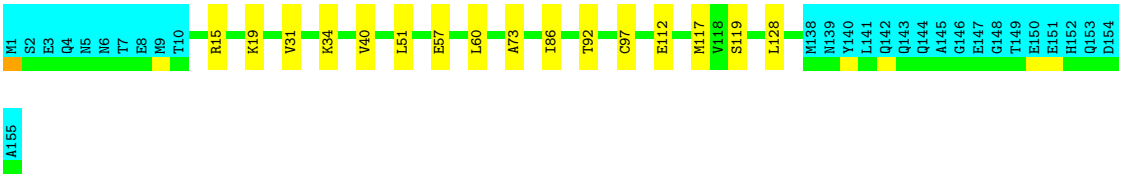
• Molecule 1: Protein-export protein SecB

Chain B:



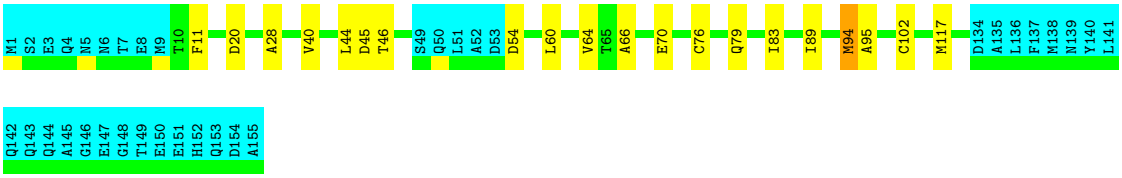
• Molecule 1: Protein-export protein SecB

Chain C:



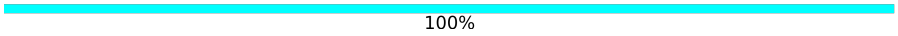
• Molecule 1: Protein-export protein SecB

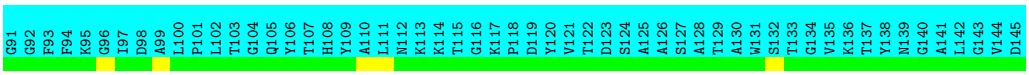
Chain D:



• Molecule 2: Alkaline phosphatase

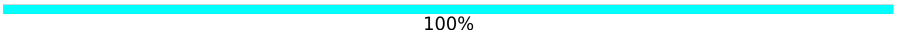
Chain E:

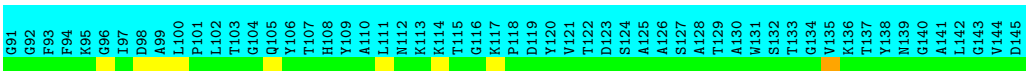




• Molecule 2: Alkaline phosphatase

Chain F:





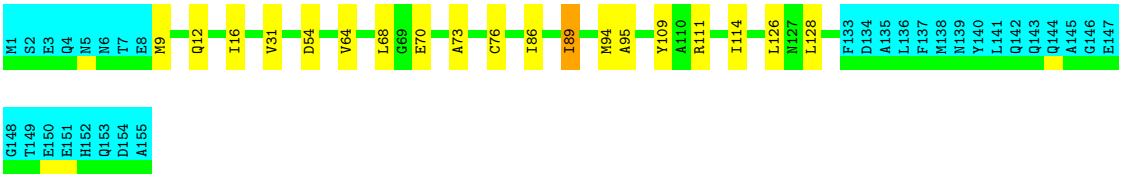
4.2.13 Score per residue for model 13

• Molecule 1: Protein-export protein SecB

Chain A:

• Molecule 1: Protein-export protein SecB

Chain B:

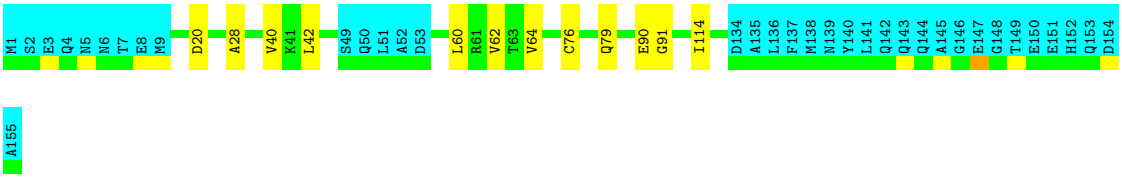


• Molecule 1: Protein-export protein SecB

Chain C:

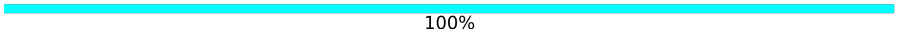
• Molecule 1: Protein-export protein SecB

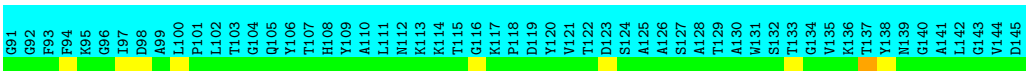
Chain D:



• Molecule 2: Alkaline phosphatase

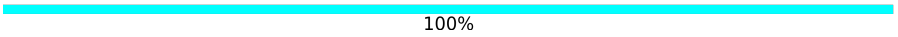
Chain E:

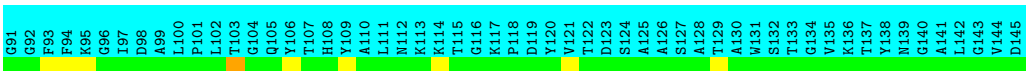




• Molecule 2: Alkaline phosphatase

Chain F:

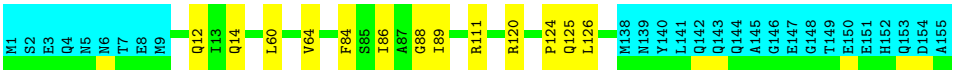




4.2.14 Score per residue for model 14

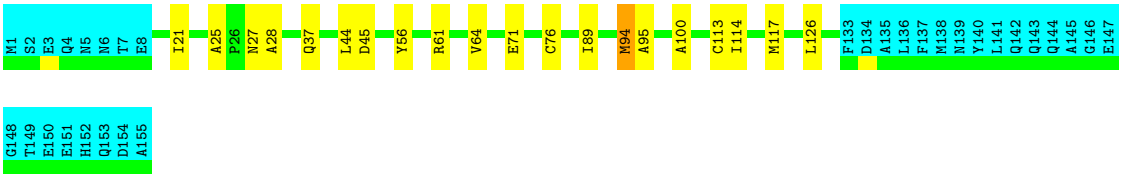
• Molecule 1: Protein-export protein SecB

Chain A:



• Molecule 1: Protein-export protein SecB

Chain B:



• Molecule 1: Protein-export protein SecB

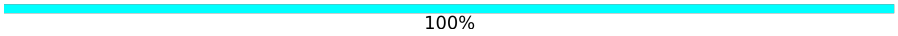
Chain C:

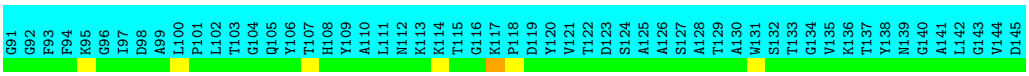
• Molecule 1: Protein-export protein SecB

Chain D:

• Molecule 2: Alkaline phosphatase

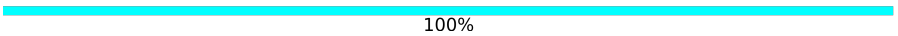
Chain E:

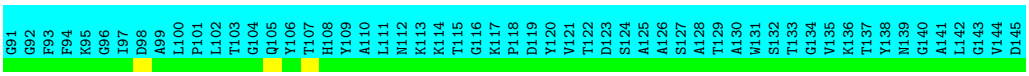




• Molecule 2: Alkaline phosphatase

Chain F:





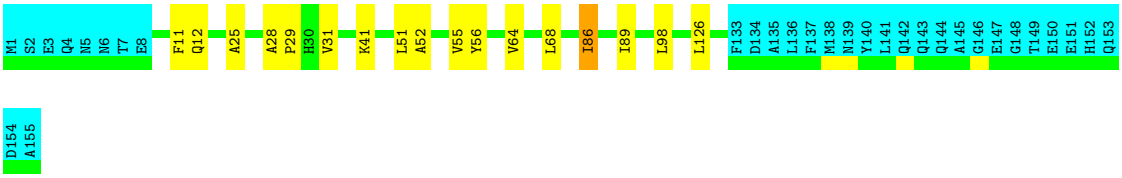
4.2.15 Score per residue for model 15

• Molecule 1: Protein-export protein SecB

Chain A:

• Molecule 1: Protein-export protein SecB

Chain B:

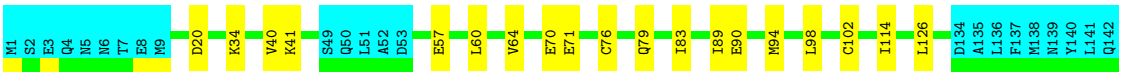


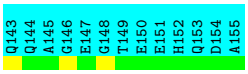
• Molecule 1: Protein-export protein SecB

Chain C:

• Molecule 1: Protein-export protein SecB

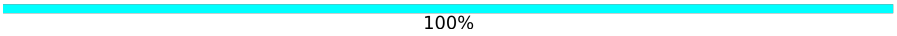
Chain D:

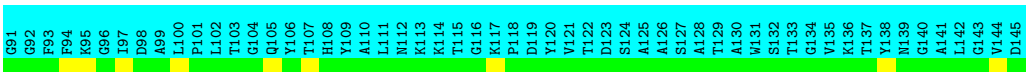




• Molecule 2: Alkaline phosphatase

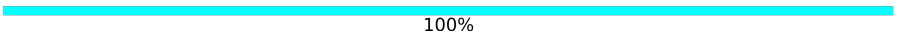
Chain E:

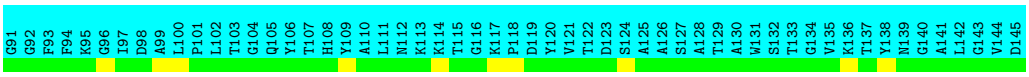




• Molecule 2: Alkaline phosphatase

Chain F:

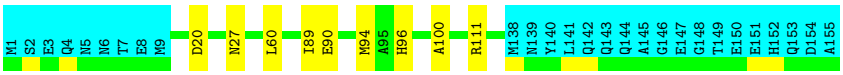




4.2.16 Score per residue for model 16

• Molecule 1: Protein-export protein SecB

Chain A:

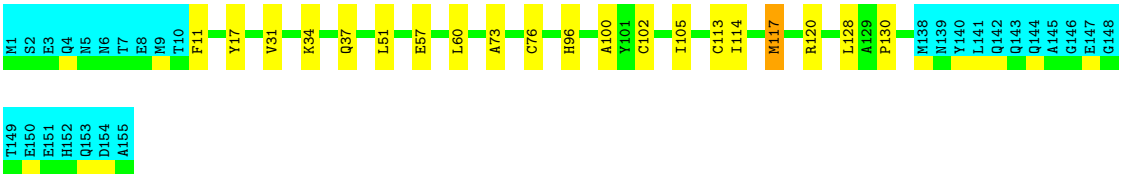


• Molecule 1: Protein-export protein SecB

Chain B:

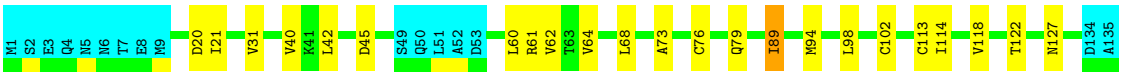
• Molecule 1: Protein-export protein SecB

Chain C:



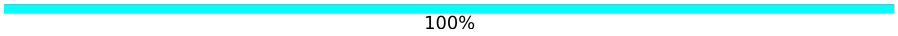
• Molecule 1: Protein-export protein SecB

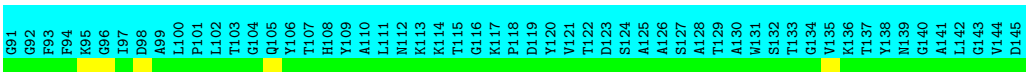
Chain D:



• Molecule 2: Alkaline phosphatase

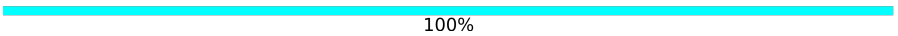
Chain E:

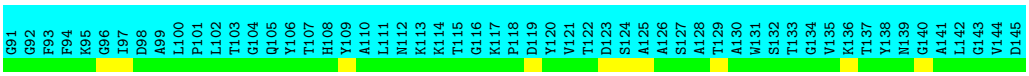




• Molecule 2: Alkaline phosphatase

Chain F:





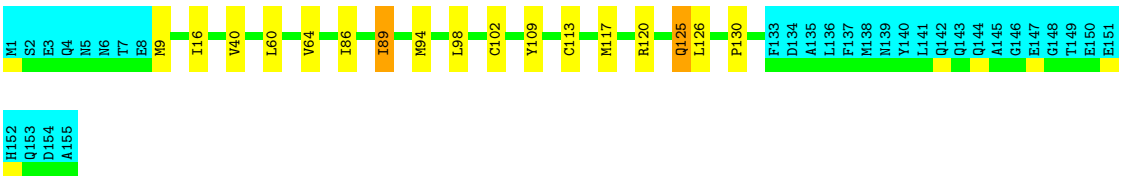
4.2.17 Score per residue for model 17

• Molecule 1: Protein-export protein SecB

Chain A:

• Molecule 1: Protein-export protein SecB

Chain B:

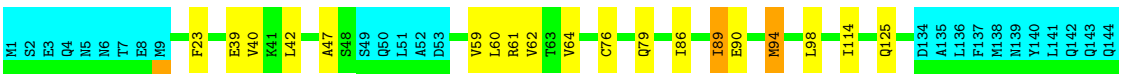


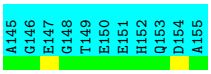
• Molecule 1: Protein-export protein SecB

Chain C:

• Molecule 1: Protein-export protein SecB

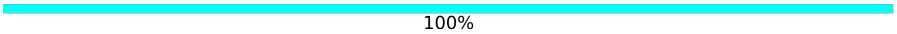
Chain D:

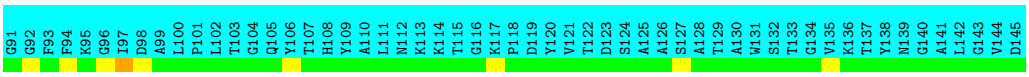




• Molecule 2: Alkaline phosphatase

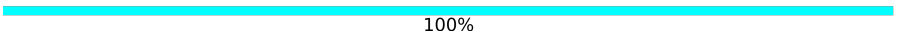
Chain E:

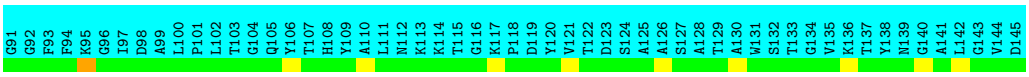




• Molecule 2: Alkaline phosphatase

Chain F:

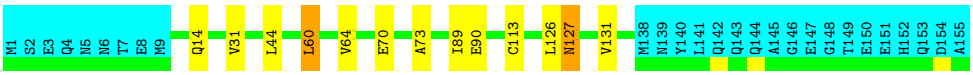




4.2.18 Score per residue for model 18

• Molecule 1: Protein-export protein SecB

Chain A:

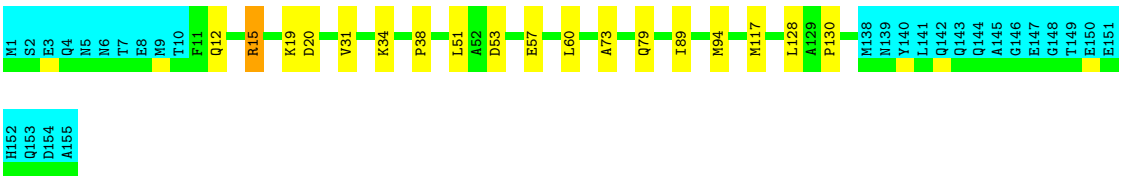


• Molecule 1: Protein-export protein SecB

Chain B:

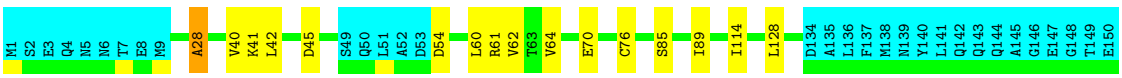
• Molecule 1: Protein-export protein SecB

Chain C:



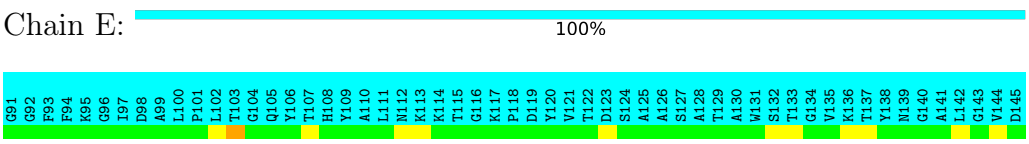
• Molecule 1: Protein-export protein SecB

Chain D:



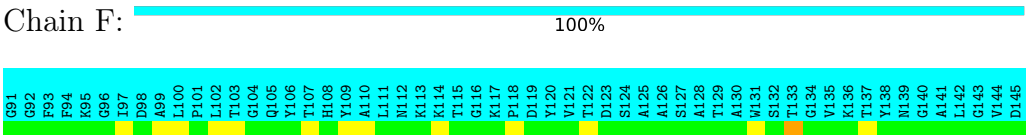
• Molecule 2: Alkaline phosphatase

Chain E:



• Molecule 2: Alkaline phosphatase

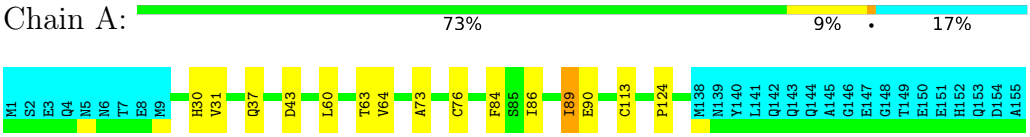
Chain F:



4.2.19 Score per residue for model 19

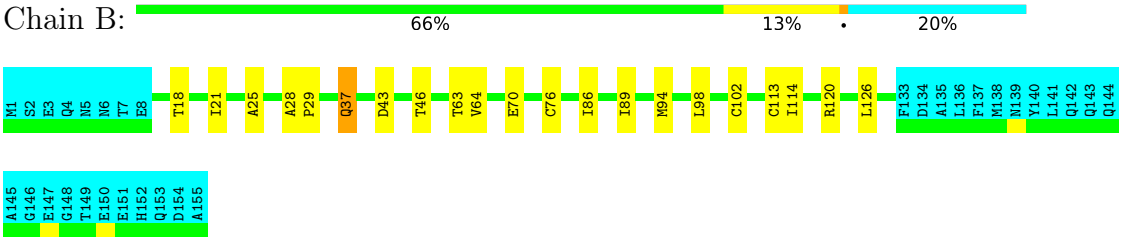
• Molecule 1: Protein-export protein SecB

Chain A:



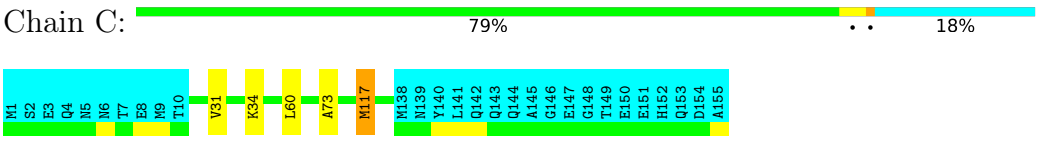
• Molecule 1: Protein-export protein SecB

Chain B:



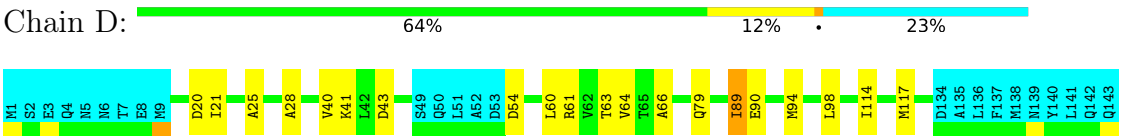
• Molecule 1: Protein-export protein SecB

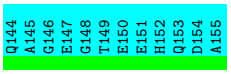
Chain C:



• Molecule 1: Protein-export protein SecB

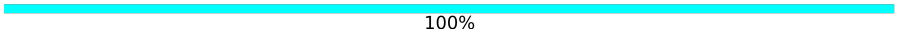
Chain D:

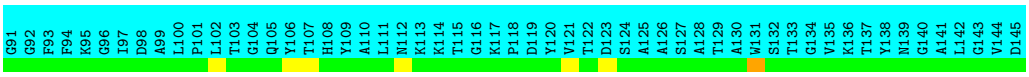




• Molecule 2: Alkaline phosphatase

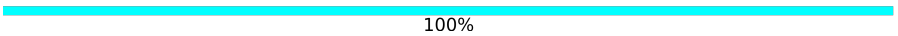
Chain E:

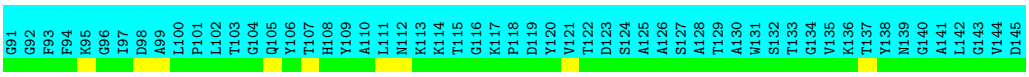




• Molecule 2: Alkaline phosphatase

Chain F:

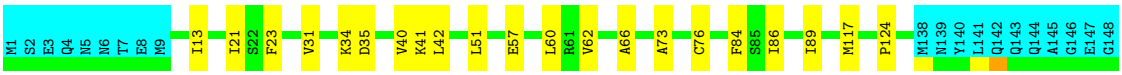




4.2.20 Score per residue for model 20 (medoid)

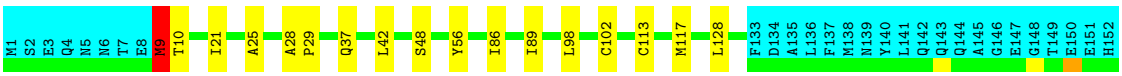
• Molecule 1: Protein-export protein SecB

Chain A:



• Molecule 1: Protein-export protein SecB

Chain B:

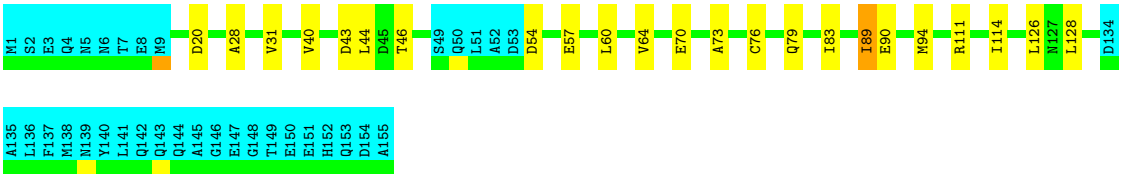


• Molecule 1: Protein-export protein SecB

Chain C:

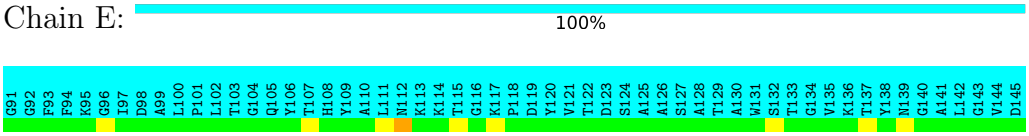
• Molecule 1: Protein-export protein SecB

Chain D:



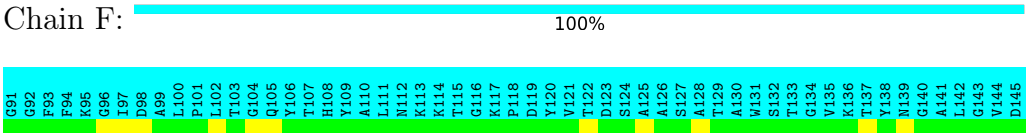
- Molecule 2: Alkaline phosphatase

Chain E:



- Molecule 2: Alkaline phosphatase

Chain F:



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	
CYANA	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	6
Total number of shifts	4940
Number of shifts mapped to atoms	4940
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	14%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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	997	971	969	6±3
1	B	962	942	940	8±2
1	C	990	964	962	6±2
1	D	929	909	907	7±2
2	E	0	0	0	0±0
2	F	0	0	0	0±0
All	All	77560	75720	75560	493

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:A:31:VAL:HG21	1:A:73:ALA:HA	0.73	1.60	5	13
1:D:40:VAL:HG13	1:D:64:VAL:HG13	0.72	1.61	12	18
1:C:31:VAL:HG21	1:C:73:ALA:HA	0.71	1.63	12	19
1:B:64:VAL:HG11	1:B:126:LEU:HD21	0.69	1.65	16	16
1:C:117:MET:HE2	1:D:21:ILE:HG21	0.69	1.62	16	3
1:A:84:PHE:HB3	1:A:86:ILE:HD11	0.66	1.66	4	16
1:B:21:ILE:HD11	1:B:113:CYS:SG	0.64	2.33	3	8
1:D:76:CYS:SG	1:D:114:ILE:HG12	0.63	2.34	18	10
1:C:11:PHE:HE1	1:C:102:CYS:HG	0.61	1.36	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:PHE:HB2	1:A:117:MET:SD	0.60	2.36	1	6
1:B:98:LEU:HA	1:B:102:CYS:SG	0.59	2.37	20	7
1:C:34:LYS:HG2	1:C:68:LEU:HD13	0.59	1.74	1	4
1:B:45:ASP:HB3	1:B:61:ARG:HD2	0.59	1.74	1	1
1:C:43:ASP:HB2	1:C:63:THR:HB	0.58	1.75	13	1
1:D:42:LEU:HD22	1:D:128:LEU:HD11	0.58	1.75	4	1
1:D:98:LEU:HA	1:D:102:CYS:SG	0.57	2.40	3	6
1:A:31:VAL:HG22	1:A:68:LEU:HD12	0.57	1.77	11	5
1:D:43:ASP:HB2	1:D:63:THR:HB	0.56	1.77	9	2
1:B:25:ALA:CB	1:B:28:ALA:HB2	0.56	2.30	19	8
1:C:117:MET:HE3	1:D:21:ILE:HD13	0.56	1.78	11	2
1:D:11:PHE:HE2	1:D:102:CYS:HG	0.55	1.44	12	3
1:B:18:THR:HG21	1:B:21:ILE:HD11	0.55	1.78	2	3
1:B:42:LEU:HD13	1:B:128:LEU:HD22	0.55	1.78	20	4
1:D:20:ASP:HB3	1:D:79:GLN:HB2	0.54	1.79	8	11
1:B:9:MET:HB3	1:B:89:ILE:HG23	0.54	1.80	3	2
1:C:20:ASP:HB3	1:C:79:GLN:HB2	0.54	1.80	7	10
1:D:42:LEU:HD11	1:D:62:VAL:HG13	0.54	1.80	17	7
1:B:125:GLN:HB2	1:C:124:PRO:HA	0.54	1.79	6	2
1:A:44:LEU:HD11	1:A:131:VAL:HG21	0.54	1.79	18	3
1:B:94:MET:SD	1:B:95:ALA:N	0.53	2.81	13	2
1:B:52:ALA:HB3	1:B:55:VAL:HB	0.53	1.80	15	2
1:D:31:VAL:HG21	1:D:73:ALA:HA	0.53	1.81	20	2
1:A:127:ASN:ND2	1:C:15:ARG:HA	0.53	2.19	18	4
1:D:114:ILE:HA	1:D:117:MET:HE1	0.53	1.79	19	1
1:D:98:LEU:HD23	1:D:102:CYS:SG	0.53	2.44	4	1
1:B:86:ILE:HG22	1:B:89:ILE:HD11	0.52	1.81	17	5
1:D:76:CYS:SG	1:D:114:ILE:HG23	0.52	2.44	6	5
1:C:113:CYS:SG	1:D:120:ARG:HD3	0.52	2.45	11	1
1:C:86:ILE:HD13	1:C:97:CYS:SG	0.52	2.44	9	7
1:D:93:GLN:HA	1:D:96:HIS:HB3	0.52	1.81	6	1
1:C:19:LYS:HE3	1:D:28:ALA:HB3	0.52	1.79	5	3
1:D:45:ASP:HB3	1:D:61:ARG:HB3	0.52	1.81	16	2
1:D:40:VAL:HG21	1:D:126:LEU:HD13	0.52	1.82	20	5
1:D:94:MET:SD	1:D:95:ALA:N	0.51	2.83	10	8
1:B:25:ALA:HB3	1:B:28:ALA:HB2	0.51	1.83	5	2
1:C:86:ILE:HG21	1:C:94:MET:HE1	0.51	1.82	15	4
1:A:113:CYS:SG	1:B:120:ARG:HD3	0.50	2.46	19	6
1:A:23:PHE:HD1	1:A:76:CYS:HG	0.50	1.48	20	1
1:B:9:MET:SD	1:B:10:THR:N	0.50	2.85	20	4
1:B:40:VAL:HG11	1:B:126:LEU:HD11	0.50	1.83	8	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:31:VAL:HG22	1:B:68:LEU:HD12	0.50	1.83	6	4
1:C:76:CYS:SG	1:C:114:ILE:HG23	0.50	2.47	16	3
1:D:89:ILE:HD12	1:D:94:MET:HA	0.50	1.83	16	1
1:A:20:ASP:HB3	1:A:79:GLN:HB2	0.50	1.83	1	1
1:A:21:ILE:HD13	1:B:117:MET:SD	0.50	2.46	20	2
1:B:11:PHE:HE1	1:B:102:CYS:HG	0.50	1.50	10	2
1:C:51:LEU:HD11	1:C:57:GLU:HB2	0.49	1.85	11	10
1:D:61:ARG:HG2	1:D:79:GLN:HG2	0.49	1.85	9	2
1:C:113:CYS:O	1:C:117:MET:SD	0.49	2.71	16	3
1:D:40:VAL:HG22	1:D:66:ALA:HB2	0.49	1.84	11	4
1:A:13:ILE:HG21	1:C:130:PRO:HG2	0.49	1.85	20	3
1:C:11:PHE:HE1	1:C:102:CYS:SG	0.48	2.31	16	1
1:B:25:ALA:HB1	1:B:28:ALA:HB2	0.48	1.84	19	2
1:D:57:GLU:HG2	1:D:83:ILE:HG13	0.48	1.85	20	2
1:A:100:ALA:HB1	1:A:134:ASP:HA	0.48	1.85	13	3
1:A:47:ALA:HB2	1:A:61:ARG:HH22	0.48	1.67	10	1
1:C:51:LEU:HD11	1:C:83:ILE:HD12	0.48	1.86	2	3
1:B:55:VAL:HG22	1:B:85:SER:HA	0.48	1.85	8	2
1:B:113:CYS:O	1:B:117:MET:HG2	0.47	2.09	11	10
1:C:64:VAL:HG21	1:C:114:ILE:HG21	0.47	1.87	14	3
1:A:40:VAL:HG22	1:A:66:ALA:HB2	0.47	1.86	20	1
1:D:14:GLN:HB2	1:D:83:ILE:HG23	0.47	1.86	4	2
1:A:64:VAL:HG11	1:A:126:LEU:HD21	0.47	1.86	1	6
1:B:16:ILE:HG21	1:B:109:TYR:CD1	0.47	2.45	11	6
1:B:54:ASP:HB3	1:B:87:ALA:HB2	0.47	1.87	11	1
1:A:42:LEU:HD21	1:A:62:VAL:HG13	0.47	1.85	20	1
1:D:76:CYS:SG	1:D:117:MET:HE3	0.47	2.49	11	2
1:A:89:ILE:H	1:A:89:ILE:HD13	0.47	1.69	11	1
1:C:42:LEU:H	1:C:42:LEU:HD23	0.46	1.71	2	1
1:C:17:TYR:HB3	1:D:122:THR:HG23	0.46	1.87	6	3
1:A:51:LEU:HD11	1:A:57:GLU:HB2	0.46	1.87	12	4
1:B:48:SER:HB3	1:B:56:TYR:HE1	0.46	1.71	20	2
1:A:40:VAL:HG11	1:A:126:LEU:HD11	0.46	1.86	5	2
1:C:64:VAL:HG23	1:C:114:ILE:HD13	0.46	1.87	7	2
1:B:40:VAL:HG13	1:B:64:VAL:HG13	0.46	1.88	18	1
1:D:86:ILE:HG12	1:D:98:LEU:HD21	0.46	1.88	17	1
1:A:44:LEU:HD22	1:A:60:LEU:HD21	0.45	1.87	18	2
1:D:13:ILE:HD13	1:D:105:ILE:HG21	0.45	1.88	3	1
1:D:40:VAL:CG1	1:D:64:VAL:HG13	0.45	2.41	7	2
1:A:31:VAL:CG2	1:A:68:LEU:HD12	0.45	2.40	11	2
1:A:111:ARG:HH12	1:C:105:ILE:HD12	0.45	1.71	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:9:MET:HG2	1:B:89:ILE:HG23	0.45	1.88	20	1
1:A:120:ARG:HD3	1:B:113:CYS:SG	0.45	2.52	6	2
1:B:130:PRO:HG3	1:D:16:ILE:HD11	0.45	1.88	2	1
1:D:64:VAL:HB	1:D:76:CYS:HB2	0.45	1.87	8	1
1:B:45:ASP:HB2	1:B:61:ARG:HB3	0.45	1.88	14	1
1:B:43:ASP:HB2	1:B:63:THR:HB	0.45	1.88	3	1
1:D:54:ASP:O	1:D:85:SER:HA	0.45	2.11	18	1
1:B:76:CYS:SG	1:B:114:ILE:HA	0.45	2.52	12	5
1:C:44:LEU:HD11	1:C:131:VAL:HG11	0.45	1.89	5	1
1:D:89:ILE:HD13	1:D:94:MET:HA	0.45	1.88	20	2
1:A:43:ASP:HB2	1:A:63:THR:HB	0.44	1.87	19	3
1:A:114:ILE:HD13	1:A:128:LEU:HD11	0.44	1.89	7	1
1:A:90:GLU:HA	1:A:94:MET:HB2	0.44	1.89	10	2
1:C:89:ILE:HD11	1:C:94:MET:HE3	0.44	1.89	18	2
1:A:45:ASP:HB2	1:A:61:ARG:HB3	0.44	1.89	13	1
1:B:27:ASN:ND2	1:B:71:GLU:HB2	0.44	2.26	18	3
1:C:84:PHE:CZ	1:C:106:LEU:HD11	0.44	2.47	8	1
1:B:16:ILE:HB	1:D:127:ASN:ND2	0.44	2.28	16	1
1:C:120:ARG:HD3	1:D:113:CYS:SG	0.44	2.53	16	1
1:A:64:VAL:HB	1:A:76:CYS:HB2	0.44	1.88	19	1
1:A:111:ARG:NH1	1:C:105:ILE:HD12	0.44	2.27	5	6
1:A:61:ARG:HG3	1:A:79:GLN:HG2	0.44	1.88	13	1
1:C:20:ASP:HA	1:D:23:PHE:O	0.44	2.13	17	1
1:D:128:LEU:H	1:D:128:LEU:HD23	0.44	1.73	2	1
1:A:30:HIS:HA	1:A:33:GLN:NE2	0.44	2.27	6	2
1:B:21:ILE:CD1	1:B:113:CYS:SG	0.44	3.05	14	1
1:B:86:ILE:HB	1:B:89:ILE:HD11	0.44	1.89	4	2
1:D:98:LEU:HD12	1:D:102:CYS:SG	0.44	2.53	11	1
1:B:76:CYS:SG	1:B:117:MET:HB2	0.43	2.52	6	1
1:D:31:VAL:HG22	1:D:68:LEU:HD12	0.43	1.90	3	2
1:A:21:ILE:HG21	1:B:117:MET:SD	0.43	2.53	5	1
1:D:34:LYS:NZ	1:D:71:GLU:HB3	0.43	2.29	15	1
1:B:31:VAL:HG21	1:B:73:ALA:HA	0.43	1.90	13	2
1:B:111:ARG:HG3	1:B:128:LEU:HB2	0.43	1.89	13	1
1:B:9:MET:SD	1:B:89:ILE:HG23	0.43	2.54	2	1
1:C:34:LYS:HZ3	1:C:71:GLU:HG2	0.43	1.73	10	1
1:D:34:LYS:HZ1	1:D:71:GLU:HB3	0.43	1.73	15	1
1:A:42:LEU:HD11	1:A:128:LEU:HD13	0.43	1.91	3	1
1:B:28:ALA:HB3	1:B:29:PRO:HD3	0.43	1.91	15	4
1:D:13:ILE:HG21	1:D:16:ILE:HD11	0.43	1.91	5	1
1:A:11:PHE:CD1	1:A:86:ILE:HD12	0.43	2.48	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:47:ALA:HB3	1:D:59:VAL:HB	0.43	1.89	17	2
1:D:25:ALA:HB1	1:D:28:ALA:HB2	0.43	1.89	19	1
1:C:86:ILE:HG21	1:C:94:MET:HE3	0.43	1.90	3	1
1:B:19:LYS:HD2	1:B:81:GLY:HA3	0.43	1.90	4	1
1:C:94:MET:HE3	1:C:94:MET:HA	0.43	1.91	4	1
1:C:96:HIS:O	1:C:100:ALA:HB3	0.43	2.14	16	1
1:D:22:SER:HB3	1:D:77:GLU:HB2	0.43	1.91	9	1
1:A:40:VAL:HG21	1:A:126:LEU:HD13	0.42	1.90	6	1
1:A:36:TRP:CE3	1:A:68:LEU:HD21	0.42	2.49	8	1
1:B:115:THR:HG21	1:C:119:SER:OG	0.42	2.14	12	1
1:C:43:ASP:HB3	1:C:63:THR:HB	0.42	1.89	10	1
1:A:13:ILE:CD1	1:A:105:ILE:HG21	0.42	2.44	5	2
1:A:23:PHE:HB3	1:B:21:ILE:HB	0.42	1.90	8	1
1:B:86:ILE:H	1:B:86:ILE:HD13	0.42	1.74	9	1
1:B:42:LEU:HD11	1:B:62:VAL:CG1	0.42	2.44	12	1
1:A:64:VAL:O	1:A:75:LEU:HD12	0.42	2.15	15	1
1:D:111:ARG:HD3	1:D:128:LEU:O	0.42	2.14	20	1
1:B:9:MET:HG3	1:B:89:ILE:HG23	0.42	1.92	4	1
1:A:28:ALA:HB3	1:A:29:PRO:HD3	0.42	1.91	11	1
1:A:20:ASP:HA	1:B:23:PHE:O	0.42	2.14	16	1
1:B:89:ILE:HB	1:B:94:MET:HA	0.42	1.92	5	2
1:B:11:PHE:CE1	1:B:102:CYS:SG	0.42	3.13	7	1
1:A:96:HIS:O	1:A:100:ALA:HB3	0.42	2.14	16	2
1:A:34:LYS:HD3	1:A:35:ASP:N	0.42	2.29	20	1
1:B:21:ILE:HD12	1:B:113:CYS:SG	0.42	2.55	14	1
1:B:40:VAL:CG1	1:B:64:VAL:HG13	0.42	2.45	18	1
1:D:89:ILE:HD13	1:D:94:MET:HB2	0.41	1.92	5	1
1:B:89:ILE:HD12	1:B:94:MET:HA	0.41	1.91	9	1
1:D:34:LYS:NZ	1:D:71:GLU:HG2	0.41	2.31	5	1
1:A:116:SER:O	1:A:120:ARG:HB2	0.41	2.15	9	1
1:A:30:HIS:O	1:A:33:GLN:HG2	0.41	2.15	15	1
1:A:21:ILE:HG23	1:A:117:MET:SD	0.41	2.55	20	1
1:D:24:GLU:HB2	1:D:75:LEU:HB2	0.41	1.90	14	1
1:B:48:SER:HB2	1:B:56:TYR:CE2	0.41	2.50	3	1
1:D:16:ILE:HD12	1:D:16:ILE:N	0.41	2.31	5	1
1:D:86:ILE:HG22	1:D:89:ILE:HD11	0.41	1.91	10	1
1:C:128:LEU:HD23	1:C:128:LEU:H	0.41	1.76	12	1
1:C:31:VAL:HA	1:C:34:LYS:HZ2	0.41	1.76	10	1
1:B:64:VAL:HG23	1:B:114:ILE:HD13	0.40	1.92	12	1
1:D:86:ILE:HD11	1:D:102:CYS:SG	0.40	2.57	9	1
1:A:130:PRO:HB3	1:C:101:TYR:OH	0.40	2.16	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:56:TYR:HE1	1:B:86:ILE:HD12	0.40	1.75	15	1
1:D:114:ILE:O	1:D:118:VAL:HG23	0.40	2.17	16	1
1:B:20:ASP:HB3	1:B:79:GLN:HB2	0.40	1.93	3	1
1:C:122:THR:HG21	1:D:16:ILE:O	0.40	2.15	5	1
1:C:114:ILE:O	1:C:118:VAL:HG23	0.40	2.17	11	1
1:B:37:GLN:NE2	1:B:37:GLN:H	0.40	2.15	19	1
1:B:43:ASP:HB3	1:B:63:THR:HB	0.40	1.94	19	1
1:B:64:VAL:HG11	1:B:126:LEU:CD2	0.40	2.42	6	1
1:C:89:ILE:HD12	1:C:94:MET:HA	0.40	1.93	7	1
1:C:102:CYS:HB2	1:C:103:PRO:HD3	0.40	1.92	8	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	128/155 (83%)	123±1 (96±1%)	5±1 (4±1%)	0±0 (0±0%)	100	100
1	B	124/155 (80%)	116±1 (93±1%)	8±1 (6±1%)	1±1 (1±1%)	32	76
1	C	127/155 (82%)	120±1 (95±1%)	7±1 (5±1%)	0±0 (0±0%)	54	85
1	D	119/155 (77%)	113±2 (95±1%)	5±2 (4±2%)	1±0 (0±0%)	32	76
2	E	0	-	-	-	-	
2	F	0	-	-	-	-	
All	All	9960/14600 (68%)	9449 (95%)	484 (5%)	27 (0%)	44	80

All 6 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	11
1	B	9	MET	7
1	B	130	PRO	3
1	C	130	PRO	3
1	B	28	ALA	2
1	B	53	ASP	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	109/132 (83%)	105±1 (97±1%)	4±1 (3±1%)	41 87
1	B	106/132 (80%)	103±1 (97±1%)	3±1 (3±1%)	45 89
1	C	108/132 (82%)	104±1 (96±1%)	4±1 (4±1%)	33 82
1	D	102/132 (77%)	97±2 (95±2%)	5±2 (5±2%)	31 79
2	E	0	-	-	-
2	F	0	-	-	-
All	All	8500/12160 (70%)	8184 (96%)	316 (4%)	37 85

All 74 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	60	LEU	20
1	A	89	ILE	20
1	C	60	LEU	20
1	C	117	MET	20
1	D	60	LEU	20
1	D	89	ILE	19
1	C	34	LYS	13
1	D	70	GLU	13
1	B	89	ILE	11
1	C	15	ARG	9
1	D	94	MET	9
1	B	86	ILE	7
1	A	70	GLU	6
1	B	37	GLN	6
1	A	14	GLN	6
1	D	41	LYS	6
1	B	56	TYR	5
1	B	54	ASP	5
1	D	54	ASP	5
1	D	90	GLU	5
1	C	112	GLU	5
1	A	37	GLN	4
1	D	128	LEU	4

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Mol	Chain	Res	Type	Models (Total)
1	C	41	LYS	4
1	C	128	LEU	4
1	B	94	MET	4
1	B	12	GLN	3
1	B	9	MET	3
1	D	61	ARG	3
1	B	70	GLU	3
1	A	104	ASN	2
1	B	46	THR	2
1	D	39	GLU	2
1	C	53	ASP	2
1	A	41	LYS	2
1	D	57	GLU	2
1	B	60	LEU	2
1	B	44	LEU	2
1	C	37	GLN	2
1	A	90	GLU	2
1	C	70	GLU	1
1	A	122	THR	1
1	C	61	ARG	1
1	A	54	ASP	1
1	B	96	HIS	1
1	C	130	PRO	1
1	C	42	LEU	1
1	B	127	ASN	1
1	A	39	GLU	1
1	B	112	GLU	1
1	C	39	GLU	1
1	A	61	ARG	1
1	A	93	GLN	1
1	B	90	GLU	1
1	D	12	GLN	1
1	D	43	ASP	1
1	D	104	ASN	1
1	C	19	LYS	1
1	C	92	THR	1
1	D	83	ILE	1
1	A	12	GLN	1
1	C	94	MET	1
1	B	11	PHE	1
1	B	41	LYS	1
1	B	51	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	27	ASN	1
1	B	125	GLN	1
1	C	104	ASN	1
1	C	126	LEU	1
1	A	127	ASN	1
1	B	98	LEU	1
1	A	30	HIS	1
1	C	54	ASP	1
1	D	46	THR	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 monosaccharides 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 14% for the well-defined parts and 15% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shift_list_1*

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	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

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	139	0.25 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	128	0.84 ± 0.15	Should be checked
$^{13}C'$	137	0.29 ± 0.12	None needed (< 0.5 ppm)
^{15}N	133	-1.15 ± 0.28	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 14%, i.e. 923 atoms were assigned a chemical shift out of a possible 6671. 0 out of 81 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	471/2462 (19%)	115/996 (12%)	241/996 (24%)	115/470 (24%)
Sidechain	383/3623 (11%)	213/2375 (9%)	170/1137 (15%)	0/111 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	69/586 (12%)	35/285 (12%)	33/281 (12%)	1/20 (5%)
Overall	923/6671 (14%)	363/3656 (10%)	444/2414 (18%)	116/601 (19%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 11%, i.e. 1049 atoms were assigned a chemical shift out of a possible 9548. 0 out of 102 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	542/3638 (15%)	133/1480 (9%)	276/1460 (19%)	133/698 (19%)
Sidechain	430/5074 (8%)	237/3306 (7%)	193/1608 (12%)	0/160 (0%)
Aromatic	77/836 (9%)	39/404 (10%)	37/398 (9%)	1/34 (3%)
Overall	1049/9548 (11%)	409/5190 (8%)	506/3466 (15%)	134/892 (15%)

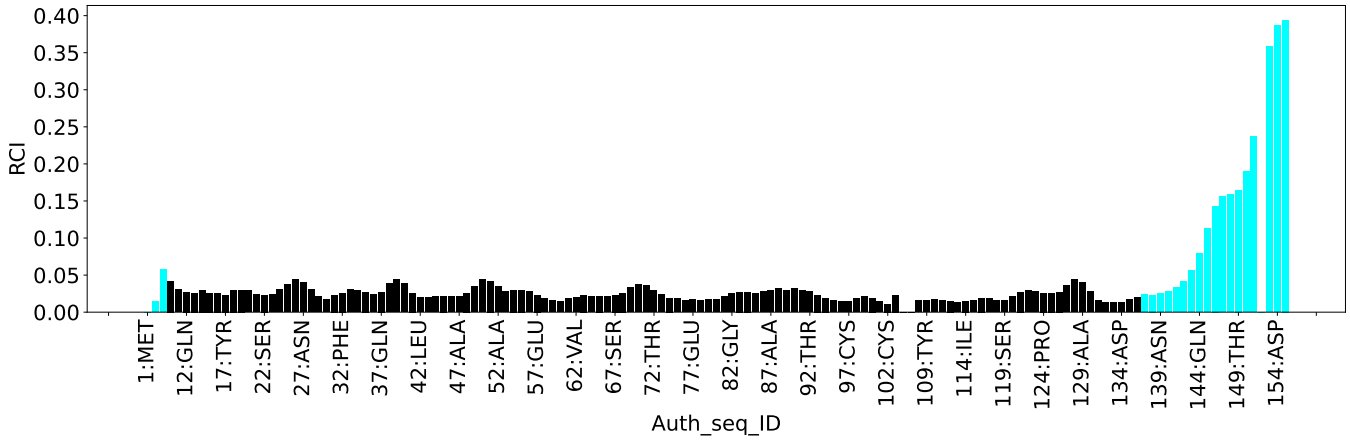
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shift_list_2*

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	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

7.2.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	140	0.28 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	126	0.79 ± 0.19	Should be checked
$^{13}C'$	135	0.26 ± 0.08	None needed (< 0.5 ppm)
^{15}N	132	-1.09 ± 0.24	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 14%, i.e. 918 atoms were assigned a chemical shift out of a possible 6671. 0 out of 81 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	468/2462 (19%)	114/996 (11%)	240/996 (24%)	114/470 (24%)
Sidechain	381/3623 (11%)	213/2375 (9%)	168/1137 (15%)	0/111 (0%)
Aromatic	69/586 (12%)	35/285 (12%)	33/281 (12%)	1/20 (5%)
Overall	918/6671 (14%)	362/3656 (10%)	441/2414 (18%)	115/601 (19%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 11%, i.e. 1044 atoms were assigned a chemical shift out of a possible 9548. 0 out of 102 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	539/3638 (15%)	132/1480 (9%)	275/1460 (19%)	132/698 (19%)
Sidechain	428/5074 (8%)	237/3306 (7%)	191/1608 (12%)	0/160 (0%)
Aromatic	77/836 (9%)	39/404 (10%)	37/398 (9%)	1/34 (3%)
Overall	1044/9548 (11%)	408/5190 (8%)	503/3466 (15%)	133/892 (15%)

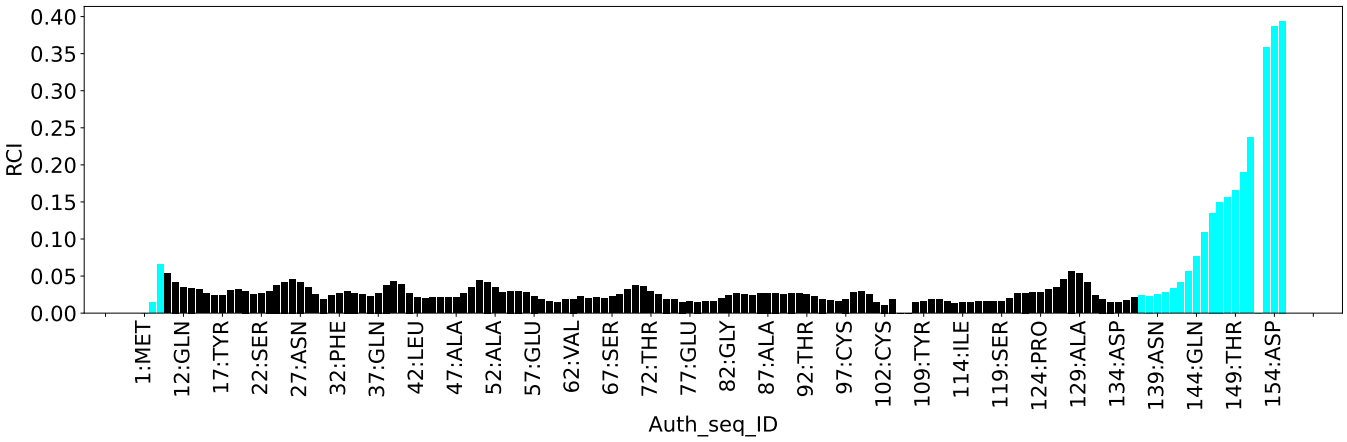
7.2.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.2.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



7.3 Chemical shift list 3

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shift_list_3*

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	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

7.3.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	140	0.28 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	126	0.78 ± 0.10	Should be checked
$^{13}C'$	135	0.26 ± 0.09	None needed (< 0.5 ppm)
^{15}N	132	-1.09 ± 0.33	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 14%, i.e. 918 atoms were assigned a chemical shift out of a possible 6671. 0 out of 81 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	468/2462 (19%)	114/996 (11%)	240/996 (24%)	114/470 (24%)
Sidechain	381/3623 (11%)	213/2375 (9%)	168/1137 (15%)	0/111 (0%)
Aromatic	69/586 (12%)	35/285 (12%)	33/281 (12%)	1/20 (5%)
Overall	918/6671 (14%)	362/3656 (10%)	441/2414 (18%)	115/601 (19%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 11%, i.e. 1044 atoms were assigned a chemical shift out of a possible 9548. 0 out of 102 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	539/3638 (15%)	132/1480 (9%)	275/1460 (19%)	132/698 (19%)
Sidechain	428/5074 (8%)	237/3306 (7%)	191/1608 (12%)	0/160 (0%)
Aromatic	77/836 (9%)	39/404 (10%)	37/398 (9%)	1/34 (3%)
Overall	1044/9548 (11%)	408/5190 (8%)	503/3466 (15%)	133/892 (15%)

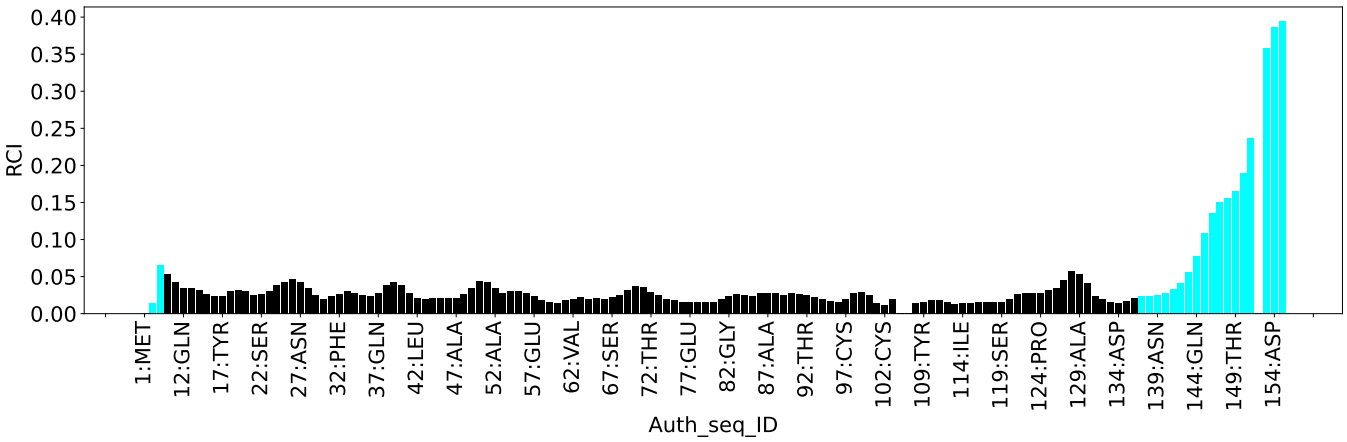
7.3.4 Statistically unusual chemical shifts (i)

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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



7.4 Chemical shift list 4

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shift_list_4*

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	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

7.4.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	139	0.25 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	128	0.85 ± 0.17	Should be checked
$^{13}C'$	137	0.28 ± 0.08	None needed (< 0.5 ppm)
^{15}N	133	-1.16 ± 0.32	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 14%, i.e. 923 atoms were assigned a chemical shift out of a possible 6671. 0 out of 81 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	471/2462 (19%)	115/996 (12%)	241/996 (24%)	115/470 (24%)
Sidechain	383/3623 (11%)	213/2375 (9%)	170/1137 (15%)	0/111 (0%)
Aromatic	69/586 (12%)	35/285 (12%)	33/281 (12%)	1/20 (5%)
Overall	923/6671 (14%)	363/3656 (10%)	444/2414 (18%)	116/601 (19%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 11%, i.e. 1049 atoms were assigned a chemical shift out of a possible 9548. 0 out of 102 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	542/3638 (15%)	133/1480 (9%)	276/1460 (19%)	133/698 (19%)
Sidechain	430/5074 (8%)	237/3306 (7%)	193/1608 (12%)	0/160 (0%)
Aromatic	77/836 (9%)	39/404 (10%)	37/398 (9%)	1/34 (3%)
Overall	1049/9548 (11%)	409/5190 (8%)	506/3466 (15%)	134/892 (15%)

7.4.4 Statistically unusual chemical shifts (i)

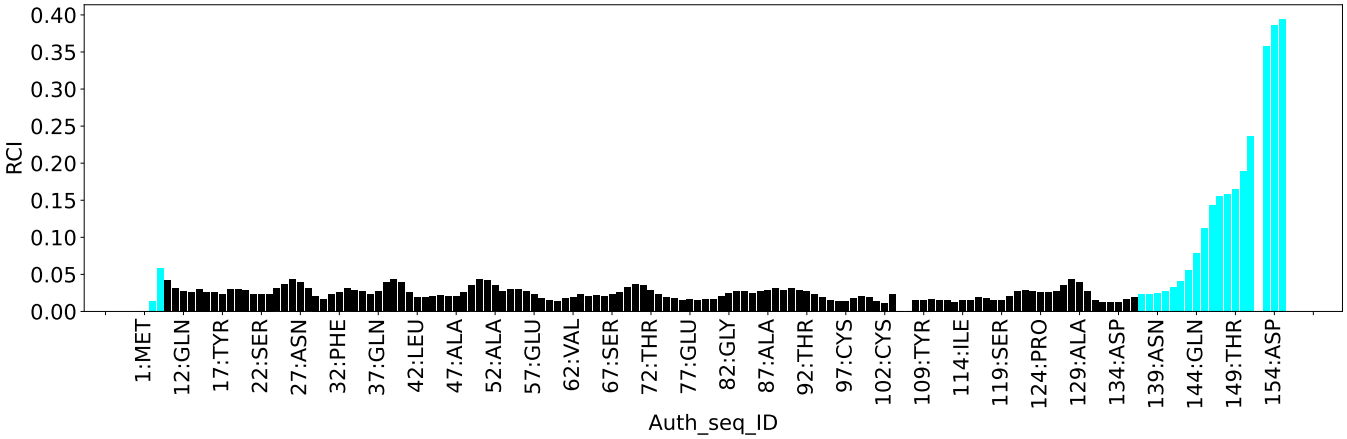
There are no statistically unusual chemical shifts.

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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



7.5 Chemical shift list 5

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shift_5*

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	377
Number of shifts mapped to atoms	377
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 ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	45	-0.19 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	37	0.15 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)

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Nucleus	# values	Correction ± precision, *ppm*	Suggested action
^{15}N	52	-0.99 ± 0.30	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 1%, i.e. 37 atoms were assigned a chemical shift out of a possible 6671. 0 out of 81 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	19/2462 (1%)	9/996 (1%)	5/996 (1%)	5/470 (1%)
Sidechain	14/3623 (0%)	8/2375 (0%)	6/1137 (1%)	0/111 (0%)
Aromatic	4/586 (1%)	2/285 (1%)	2/281 (1%)	0/20 (0%)
Overall	37/6671 (1%)	19/3656 (1%)	13/2414 (1%)	5/601 (1%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 4%, i.e. 377 atoms were assigned a chemical shift out of a possible 9548. 0 out of 102 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	183/3638 (5%)	86/1480 (6%)	45/1460 (3%)	52/698 (7%)
Sidechain	162/5074 (3%)	93/3306 (3%)	69/1608 (4%)	0/160 (0%)
Aromatic	32/836 (4%)	16/404 (4%)	15/398 (4%)	1/34 (3%)
Overall	377/9548 (4%)	195/5190 (4%)	129/3466 (4%)	53/892 (6%)

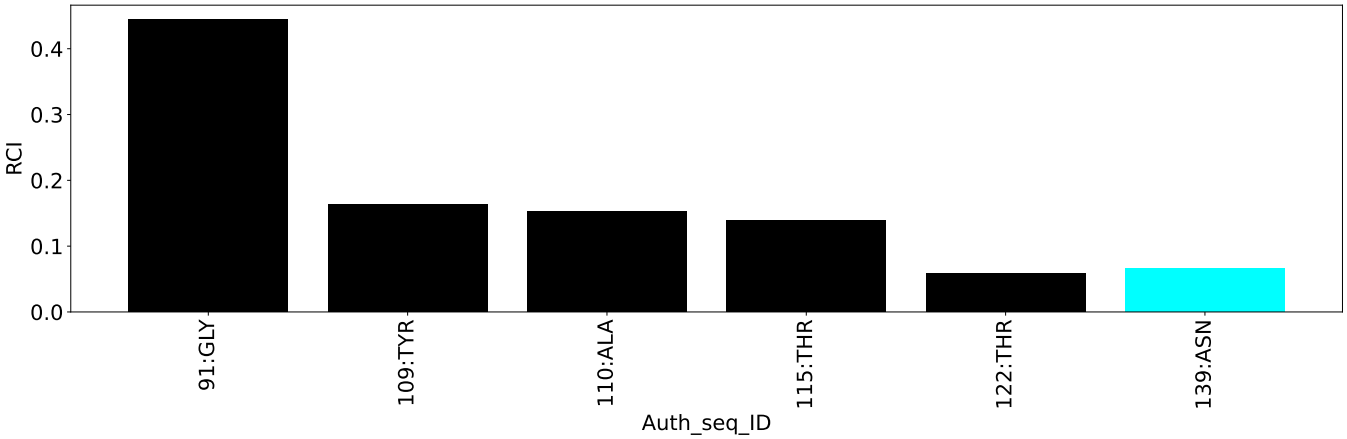
7.5.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

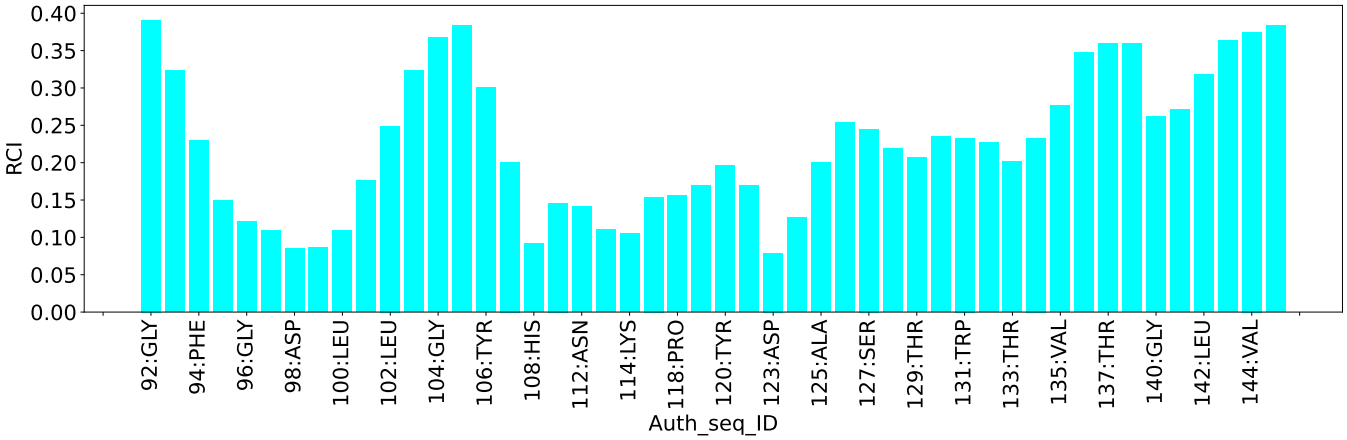
7.5.5 Random Coil Index (RCI) plots

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain E:



7.6 Chemical shift list 6

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shift_6*

7.6.1 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	377
Number of shifts mapped to atoms	377
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 ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	45	-0.20 ± 0.07	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	37	0.15 ± 0.07	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	52	-0.98 ± 0.25	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 1%, i.e. 37 atoms were assigned a chemical shift out of a possible 6671. 0 out of 81 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	19/2462 (1%)	9/996 (1%)	5/996 (1%)	5/470 (1%)
Sidechain	14/3623 (0%)	8/2375 (0%)	6/1137 (1%)	0/111 (0%)
Aromatic	4/586 (1%)	2/285 (1%)	2/281 (1%)	0/20 (0%)
Overall	37/6671 (1%)	19/3656 (1%)	13/2414 (1%)	5/601 (1%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 4%, i.e. 377 atoms were assigned a chemical shift out of a possible 9548. 0 out of 102 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	183/3638 (5%)	86/1480 (6%)	45/1460 (3%)	52/698 (7%)
Sidechain	162/5074 (3%)	93/3306 (3%)	69/1608 (4%)	0/160 (0%)
Aromatic	32/836 (4%)	16/404 (4%)	15/398 (4%)	1/34 (3%)
Overall	377/9548 (4%)	195/5190 (4%)	129/3466 (4%)	53/892 (6%)

7.6.4 Statistically unusual chemical shifts (i)

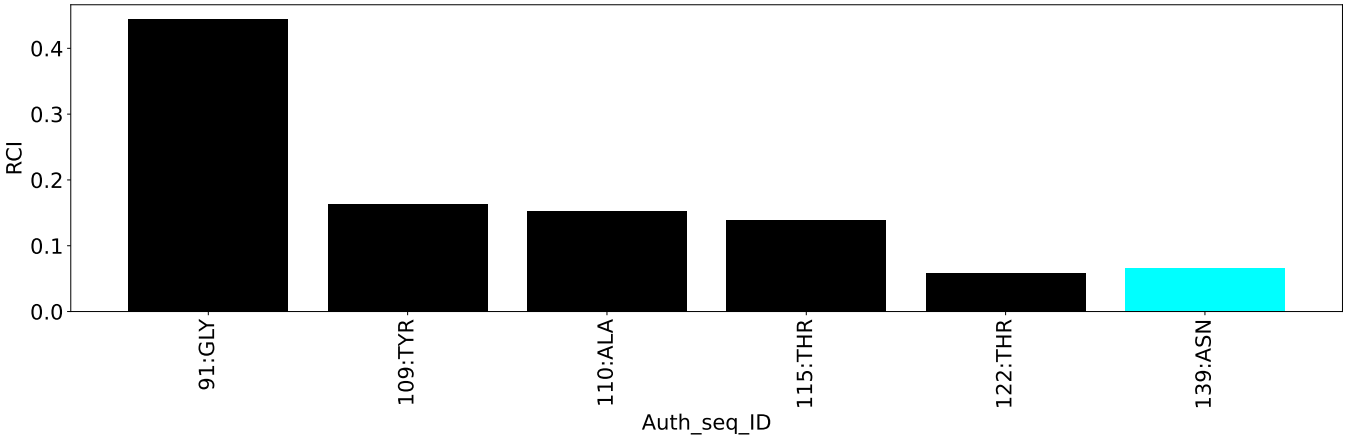
There are no statistically unusual chemical shifts.

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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain E: