Full wwPDB NMR Structure Validation Report (i)

Apr 20, 2024 – 09:11 AM EDT

PDB ID	:	5JTL
BMRB ID	:	30080
Title	:	The structure of chaperone SecB in complex with unstructured proPhoA
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:

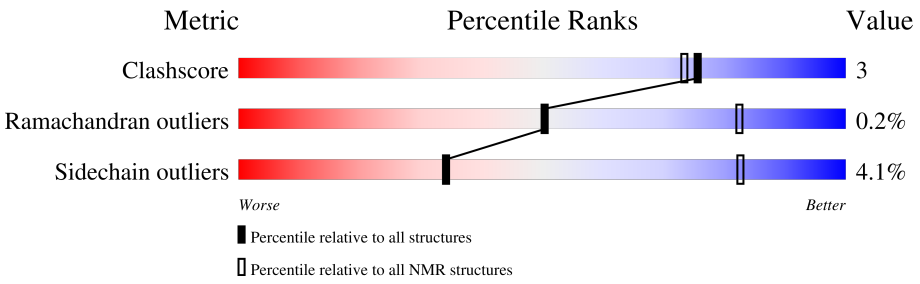
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 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	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	68% • 30%
1	B	155	73% 6% 21%
1	C	155	69% • 27%
1	D	155	75% 5% 19%
2	E	471	• 99%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 13 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:12-A:85, A:98-A:131, B:11-B:132, C:11-C:86, C:97-C:133, D:10-D:134, E:290-E:292 (471)	1.75	13

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16399 atoms, of which 8079 are hydrogens and 0 are deuteriums.

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

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

- Molecule 2 is a protein called Alkaline phosphatase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	E	471	6931	2154	3459	609	696	13	0

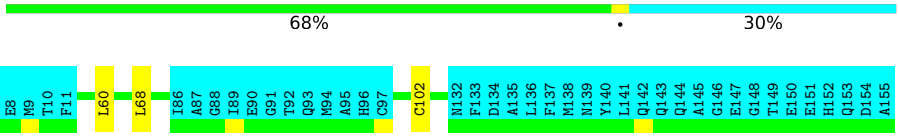
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

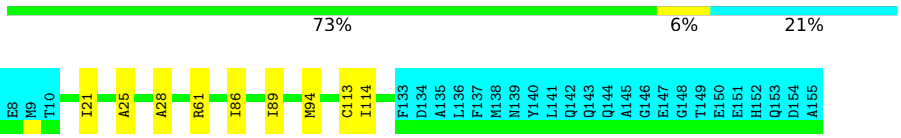
• Molecule 1: Protein-export protein SecB

Chain A:



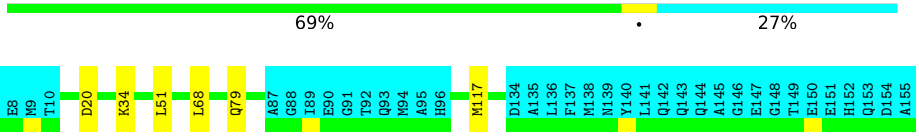
• Molecule 1: Protein-export protein SecB

Chain B:



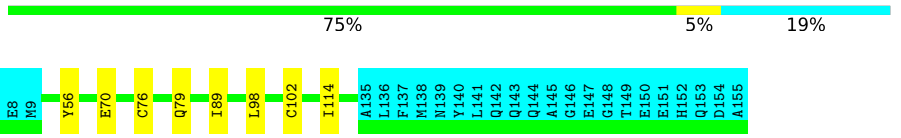
• Molecule 1: Protein-export protein SecB

Chain C:



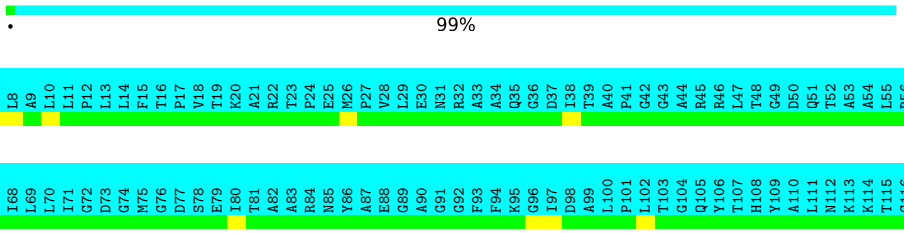
• Molecule 1: Protein-export protein SecB

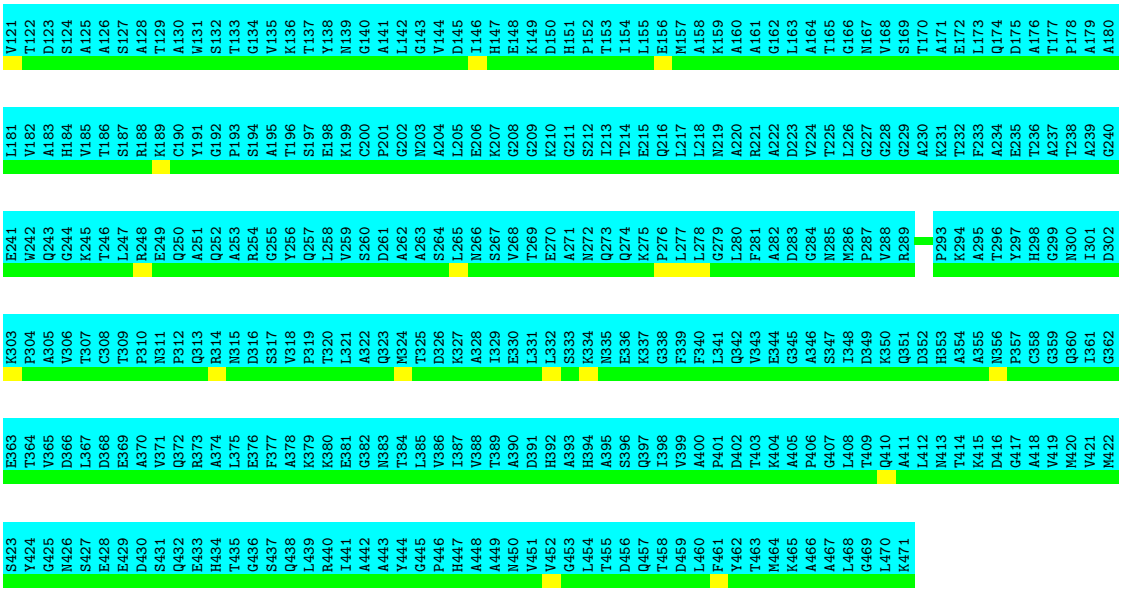
Chain D:



• Molecule 2: Alkaline phosphatase

Chain E:





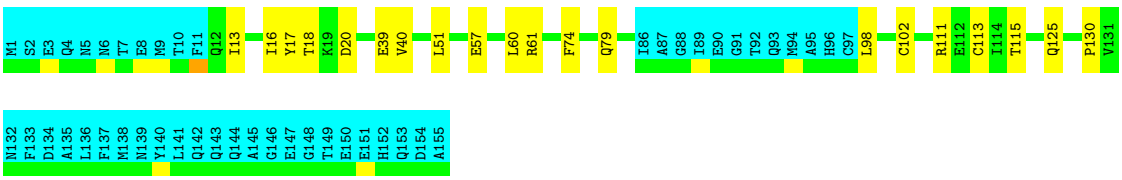
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Protein-export protein SecB

Chain A: 57% 13% 30%

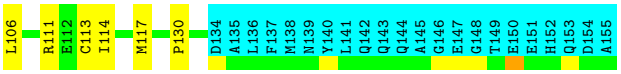


- Molecule 1: Protein-export protein SecB

Chain B: 72% 6% 21%

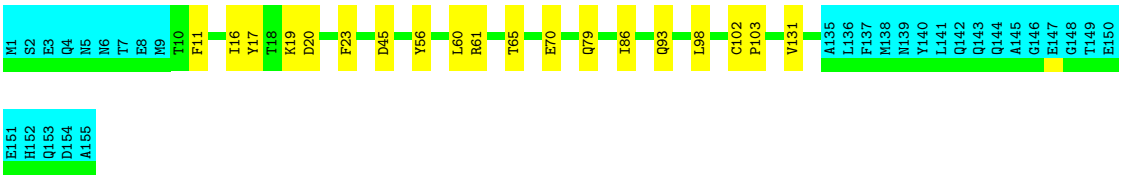
- Molecule 1: Protein-export protein SecB

Chain C: 55% 17% 27%



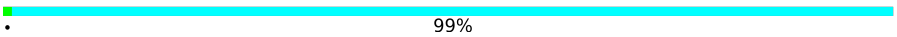
• Molecule 1: Protein-export protein SecB

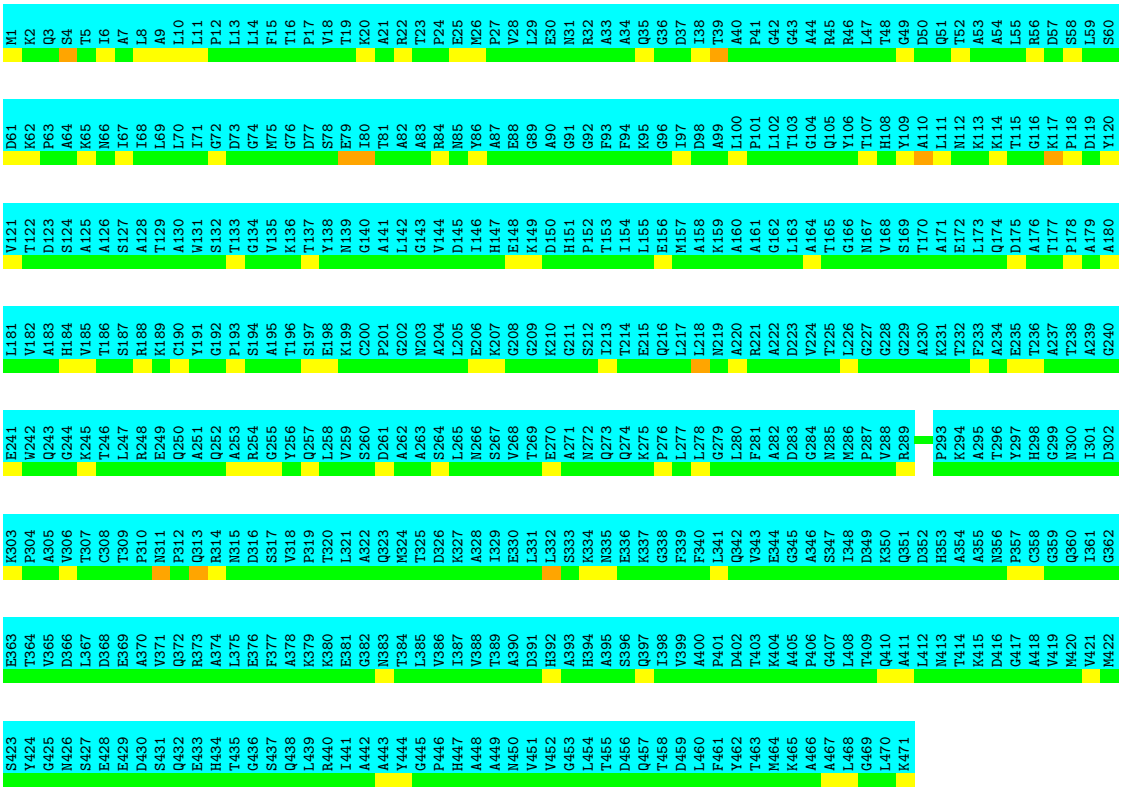
Chain D:



• Molecule 2: Alkaline phosphatase

Chain E:

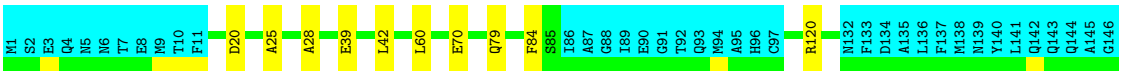




4.2.2 Score per residue for model 2

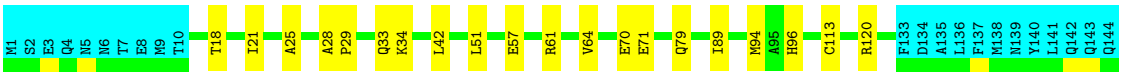
• Molecule 1: Protein-export protein SecB

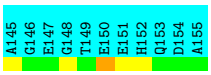
Chain A:



• Molecule 1: Protein-export protein SecB

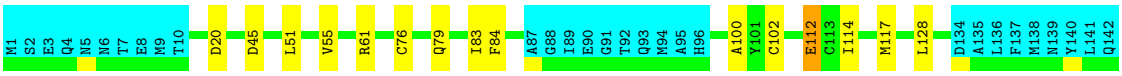
Chain B:

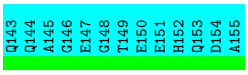




• Molecule 1: Protein-export protein SecB

Chain C:



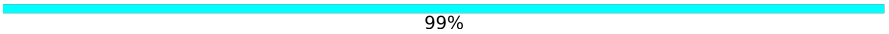


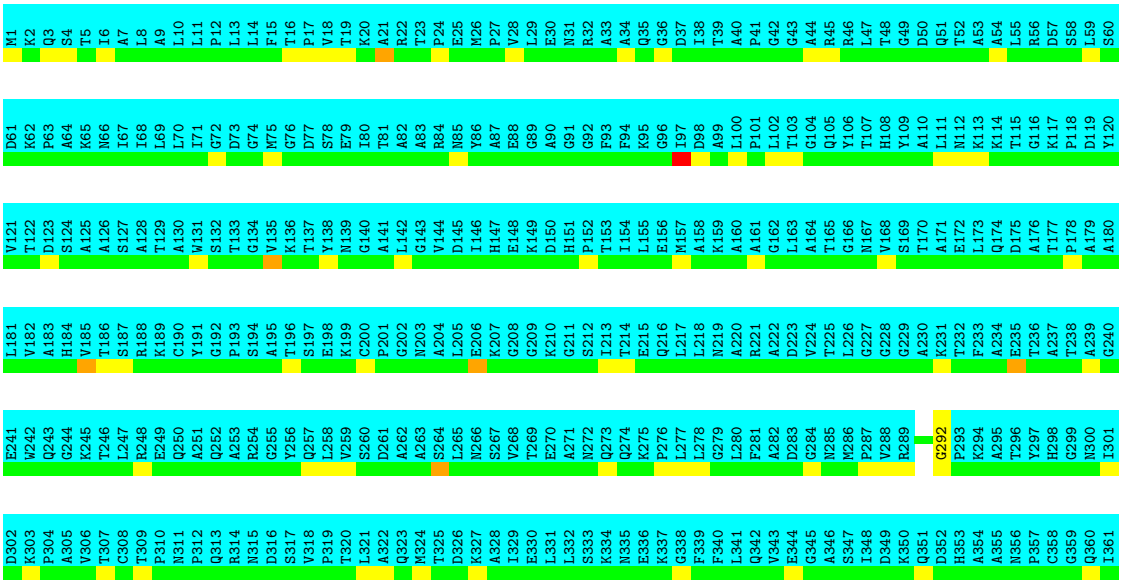
• Molecule 1: Protein-export protein SecB

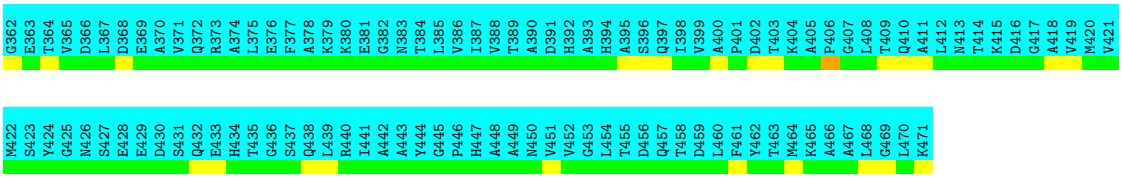
Chain D:

• Molecule 2: Alkaline phosphatase

Chain E:



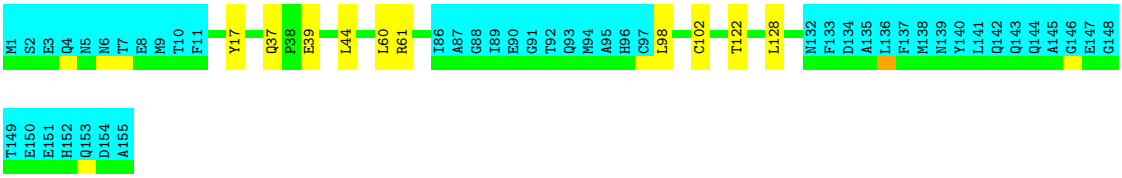




4.2.3 Score per residue for model 3

- Molecule 1: Protein-export protein SecB

Chain A:

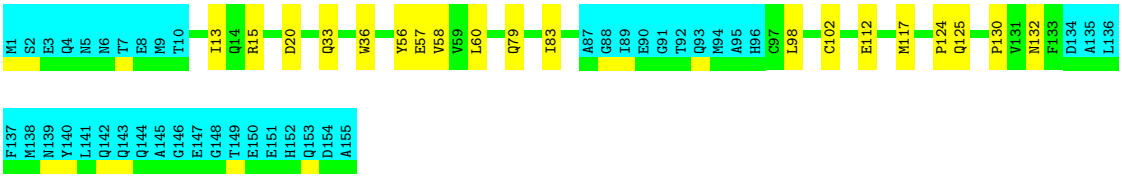


- Molecule 1: Protein-export protein SecB

Chain B:

- Molecule 1: Protein-export protein SecB

Chain C:

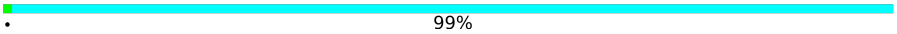


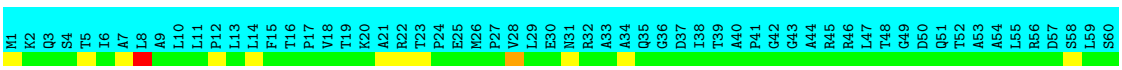
- Molecule 1: Protein-export protein SecB

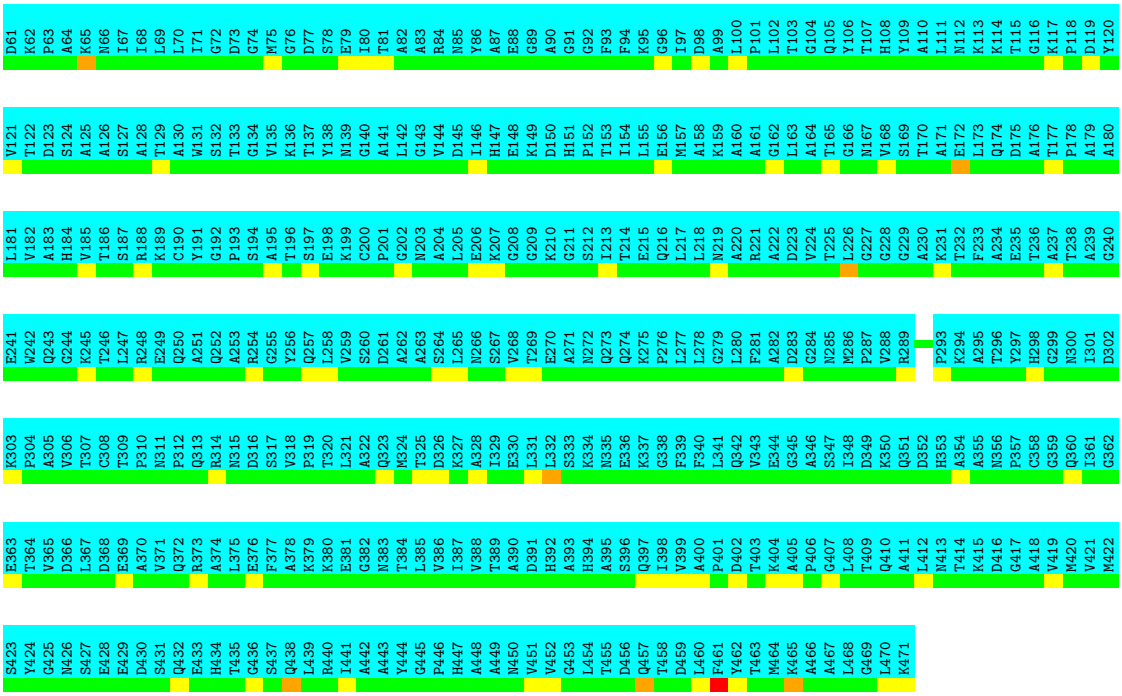
Chain D:

- Molecule 2: Alkaline phosphatase

Chain E:



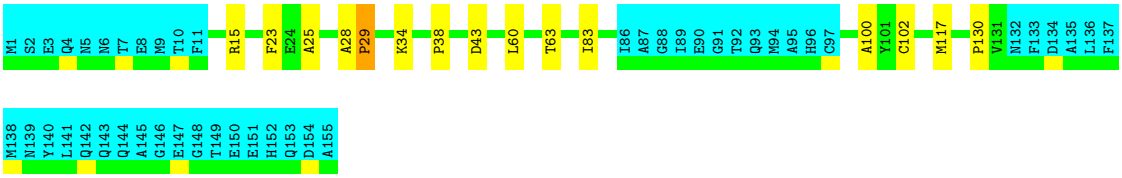




4.2.4 Score per residue for model 4

- Molecule 1: Protein-export protein SecB

Chain A:

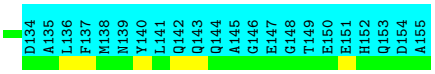


- Molecule 1: Protein-export protein SecB

Chain B:

- Molecule 1: Protein-export protein SecB

Chain C:

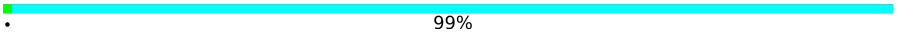


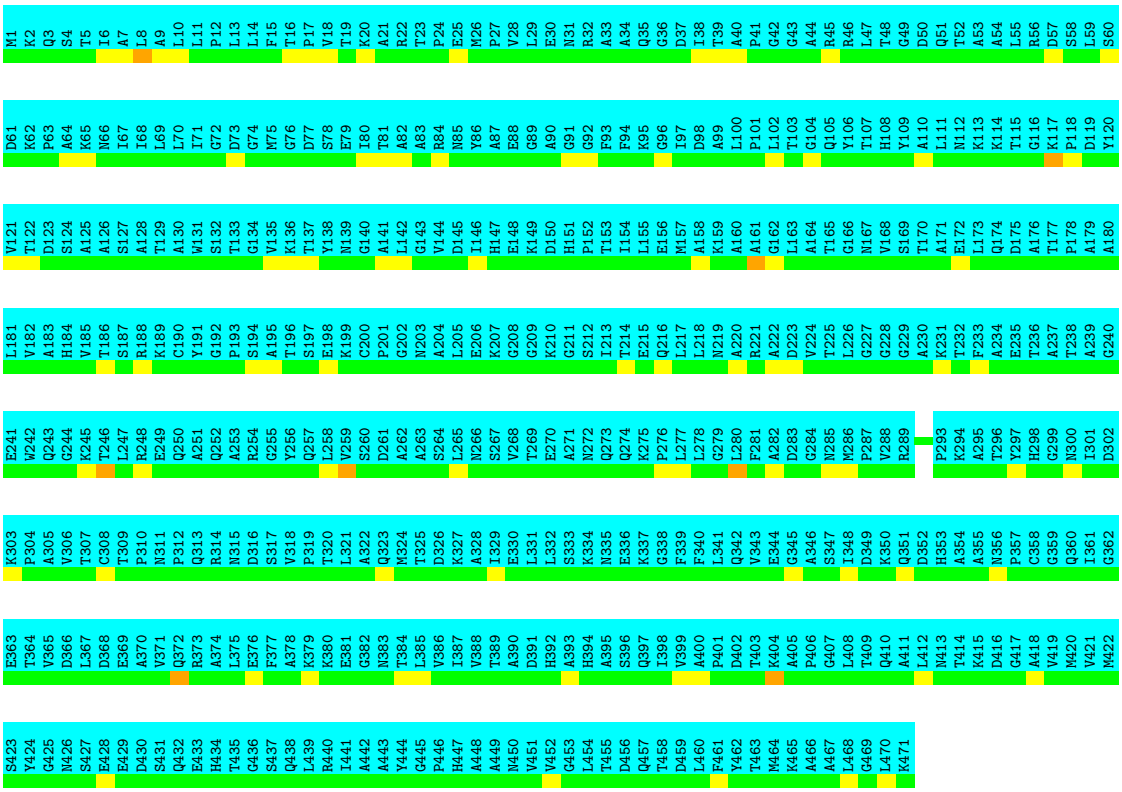
• Molecule 1: Protein-export protein SecB

Chain D:

• Molecule 2: Alkaline phosphatase

Chain E:





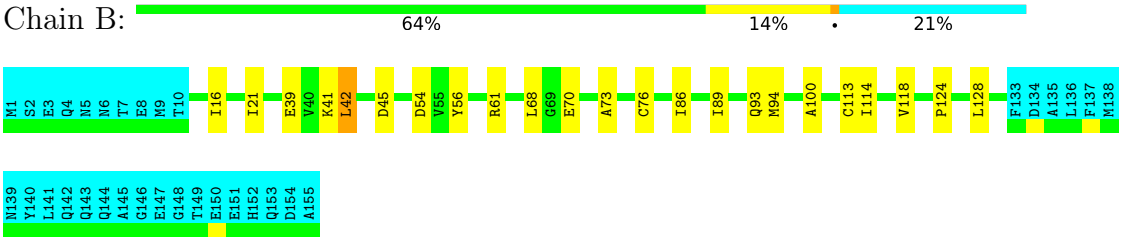
4.2.5 Score per residue for model 5

• Molecule 1: Protein-export protein SecB

Chain A:

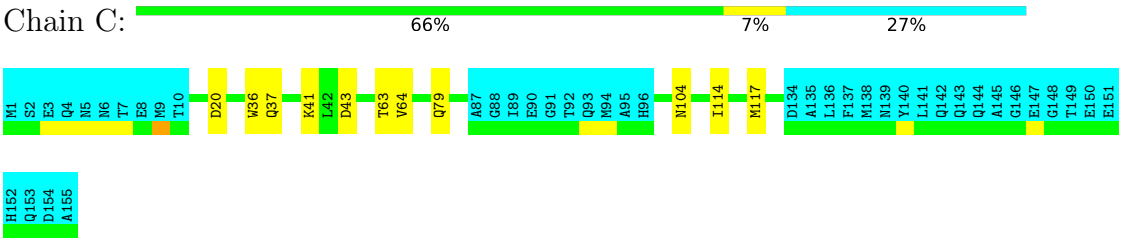
• Molecule 1: Protein-export protein SecB

Chain B:



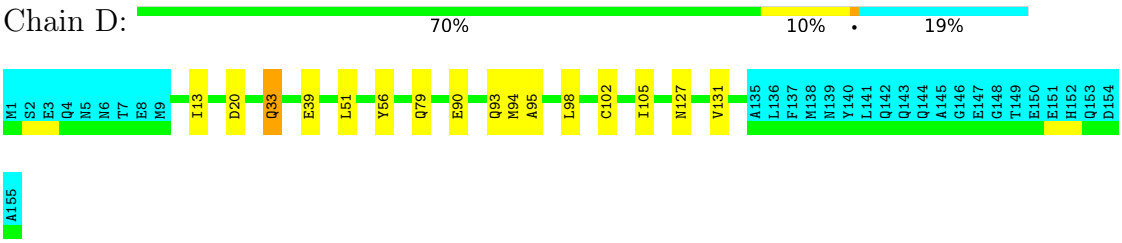
• Molecule 1: Protein-export protein SecB

Chain C:



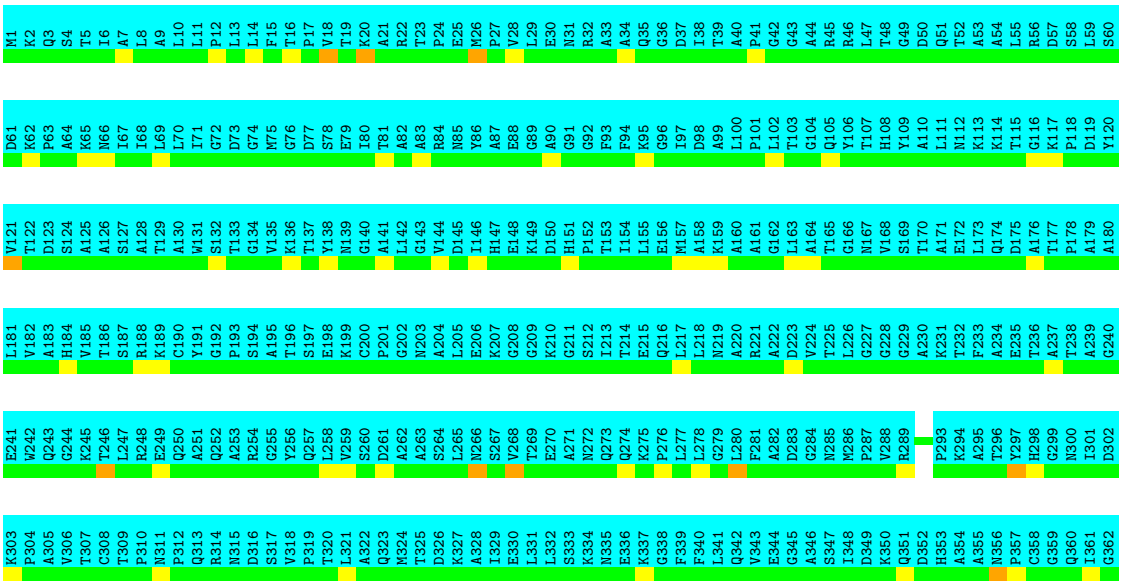
• Molecule 1: Protein-export protein SecB

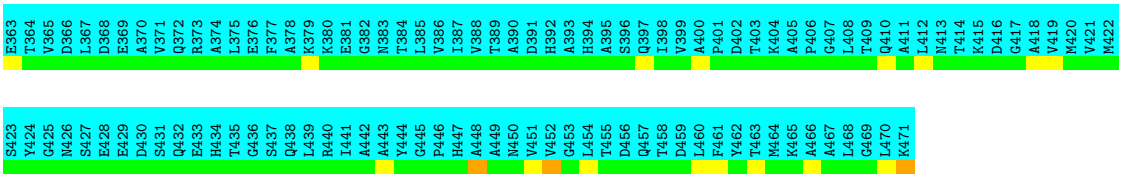
Chain D:



• Molecule 2: Alkaline phosphatase

Chain E:

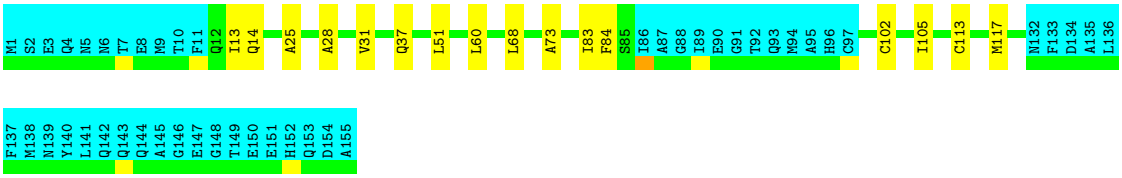




4.2.6 Score per residue for model 6

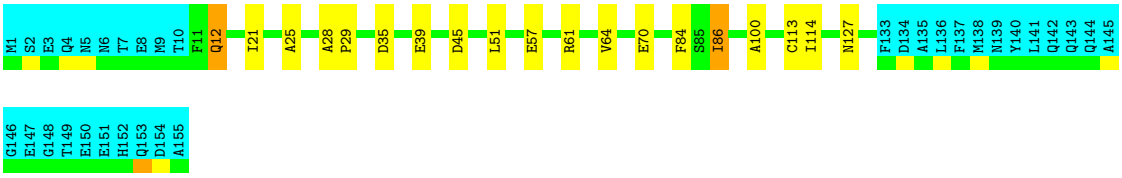
- Molecule 1: Protein-export protein SecB

Chain A:



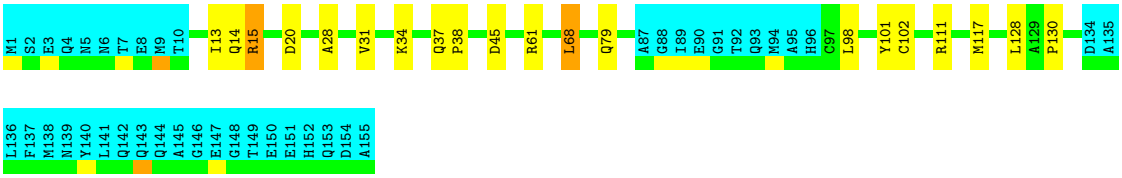
- Molecule 1: Protein-export protein SecB

Chain B:



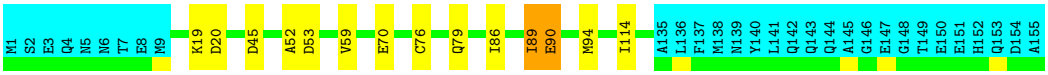
- Molecule 1: Protein-export protein SecB

Chain C:



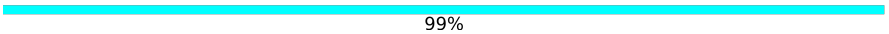
- Molecule 1: Protein-export protein SecB

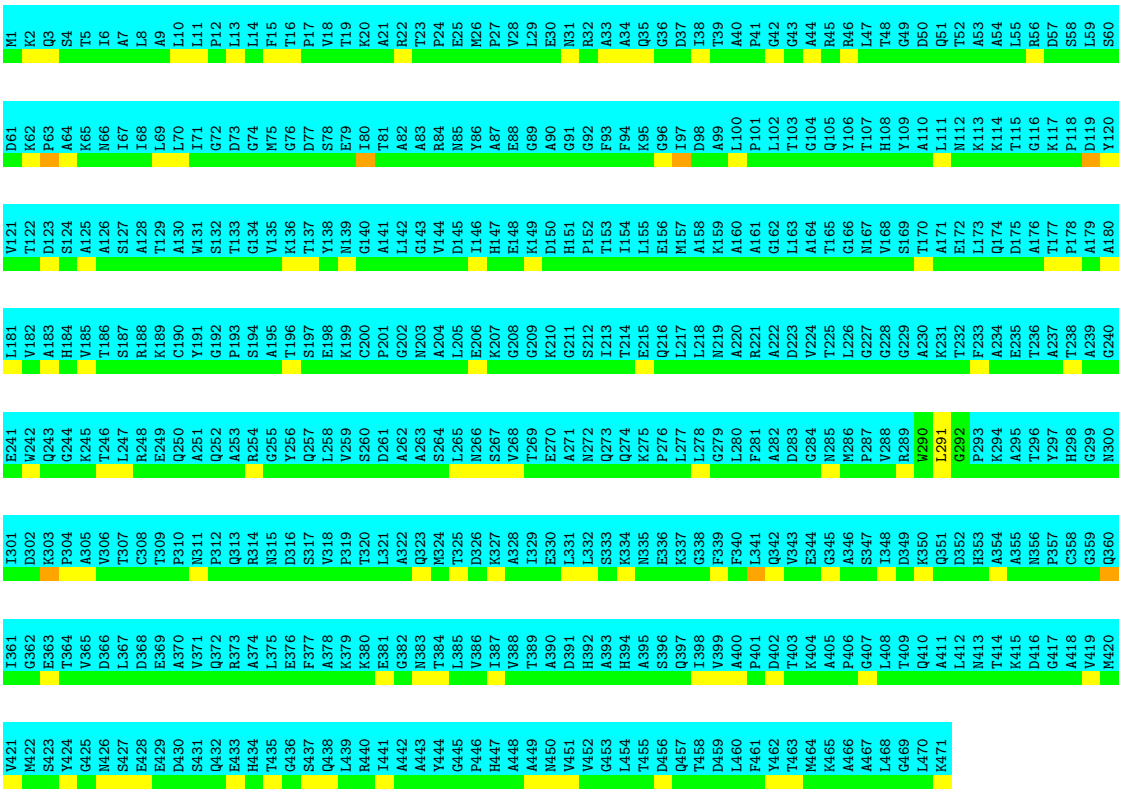
Chain D:



- Molecule 2: Alkaline phosphatase

Chain E:

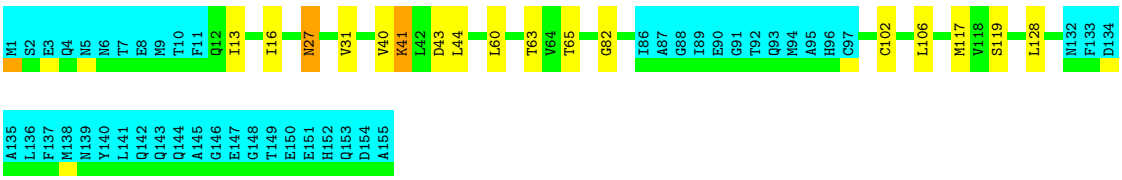




4.2.7 Score per residue for model 7

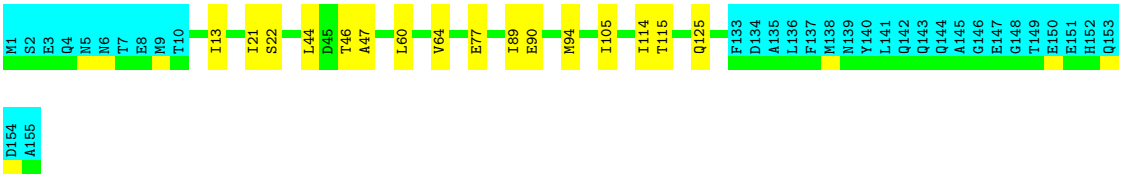
- Molecule 1: Protein-export protein SecB

Chain A:



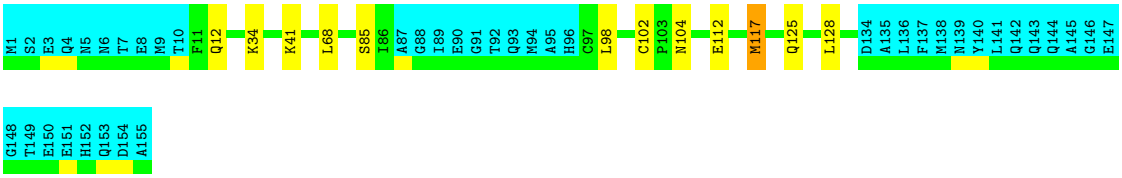
- Molecule 1: Protein-export protein SecB

Chain B:



- Molecule 1: Protein-export protein SecB

Chain C:

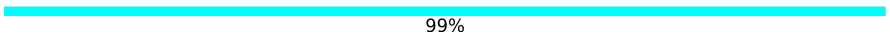


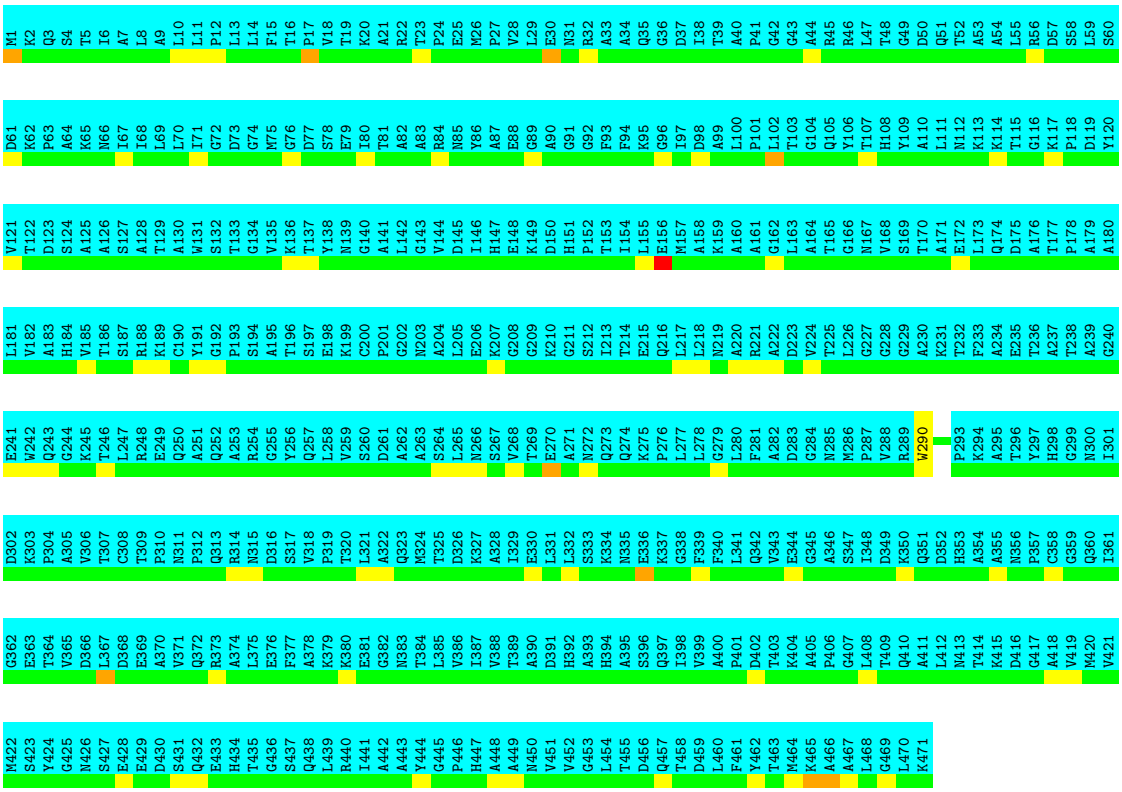
• Molecule 1: Protein-export protein SecB

Chain D:

• Molecule 2: Alkaline phosphatase

Chain E:

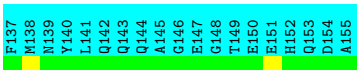




4.2.8 Score per residue for model 8

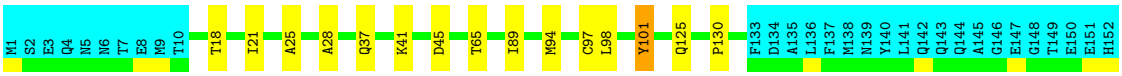
• Molecule 1: Protein-export protein SecB

Chain A:



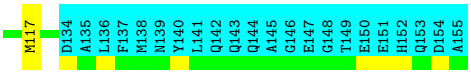
• Molecule 1: Protein-export protein SecB

Chain B:



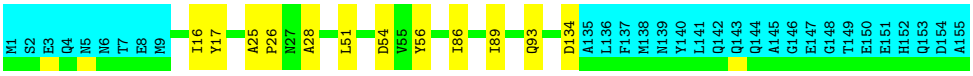
• Molecule 1: Protein-export protein SecB

Chain C:



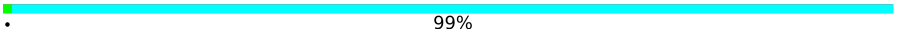
• Molecule 1: Protein-export protein SecB

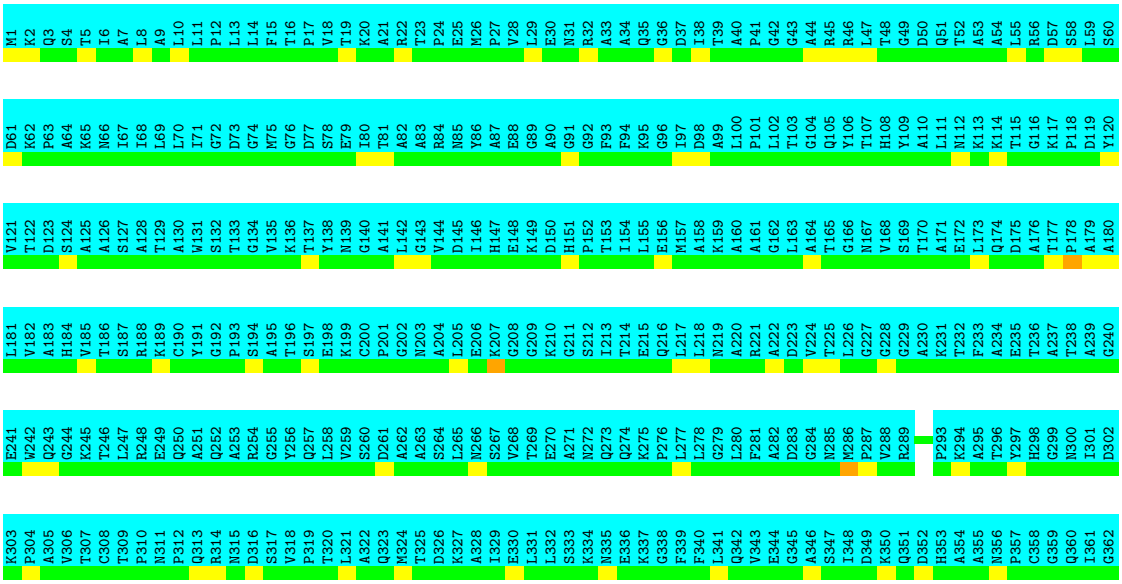
Chain D:



• Molecule 2: Alkaline phosphatase

Chain E:





E363 T364 V365 D366 L367 D368 E369 A370 V371 Q372 R373 A374 L375 E376 F377 A378 K379 K380 E381 G382 N383 T384 L385 V386 I387 V388 T389 A390 D391 H392 A393 H394 A395 S396 Q397 I398 V399 A400 P401 D402 T403 K404 A405 P406 G407 L408 T409 Q410 A411 L412 N413 T414 K415 D416 G417 A418 V419 M420 V421 M422

S423 Y424 G425 N426 S427 E428 E429 D430 S431 Q432 E433 H434 T435 G436 S437 Q438 L439 R440 I441 A442 A443 Y444 G445 P446 H447 A448 A449 M450 V451 V452 G453 L454 T455 D456 Q457 T458 D459 L460 F461 Y462 T463 M464 K465 A466 A467 L468 G469 L470 K471

4.2.9 Score per residue for model 9

- Molecule 1: Protein-export protein SecB

Chain A: 56% 14% 30%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 T10 F11 Q14 D20 E24 P38 D43 L44 D45 L60 R61 V62 T63 V64 E70 F74 L75 C76 Q79 I86 A87 G88 I89 E90 G91 T92 Q93 M94 A95 H96 C97 L98 C102 R111 M117 P124

L128 A129 P130 V131 N132 F133 D134 A135 L136 F137 M138 N139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

- Molecule 1: Protein-export protein SecB

Chain B: 61% 17% 21%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 T10 F11 I21 A25 P26 N27 A28 P29 E39 D43 L44 D45 V58 R61 V62 T63 E71 C76 Q79 I89 E90 Q93 M94 A95 H96 C97 L98 C102 C113 I114 Q125 L128 F133 D134 A135

L136 F137 M138 N139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

- Molecule 1: Protein-export protein SecB

Chain C: 59% 13% • 27%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 T10 R15 D20 A28 V31 K34 D43 L51 T63 L68 A73 C76 Q79 I83 I86 A87 G88 I89 E90 G91 T92 Q93 M94 A95 H96 R111 I114 T115 S116 M117 Q125 L126 N127 L128

D134 A135 L136 F137 M138 N139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

- Molecule 1: Protein-export protein SecB

Chain D: 68% 12% • 19%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 Y17 F23 E24 A25 A28 L44 Y56 R61 E70 C76 Q79 F84 I89 Q93 L98 G99 A100 Y101 C102 I105 I114 F133 D134 A135 L136 F137 M138 N139 Y140 L141 Q142 Q143 Q144 A145 G146

E147 G148 T149 E150 E151 H152 Q153 D154 A155

- Molecule 2: Alkaline phosphatase

Chain E: 99%

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 M26 P27 V28 L29 E30 N31 R32 A33 A34 Q35 G36 D37 I38 T39 A40 P41 G42 G43 A44 R45 R46 L47 T48 G49 D50 Q51 T52 A53 A54 L55 R56 D57 S58 L59 S60

D61 K62 P63 A64 K65 N66 I67 I68 L69 L70 I71 G72 D73 G74 M75 G76 D77 S78 E79 I80 T81 A82 A83 R84 N85 Y86 A87 E88 G89 A90 G91 G92 F93 F94 K95 Q96 I97 D98 A99 L100 P101 L102 T103 G104 Q105 Y106 T107 H108 Y109 A110 L111 N112 K113 K114 T115 G116 K117 P118 D119 Y120

V121 T122 D123 S124 A125 A126 S127 A128 T129 A130 W131 S132 T133 G134 V135 K136 T137 Y138 N139 G140 A141 L142 G143 V144 D145 I146 H147 E148 K149 D150 H151 P152 T153 I154 L155 E156 M157 A158 K159 A160 A161 G162 L163 A164 T165 G166 N167 V168 S169 T170 A171 E172 L173 Q174 D175 A176 T177 P178 A179 A180

L181 V182 A183 H184 V185 T186 S187 R188 K189 C190 Y191 G192 P193 S194 A195 T196 S197 E198 K199 C200 P201 G202 N203 A204 L205 E206 K207 G208 G209 K210 G211 S212 I213 T214 E215 Q216 L217 L218 N219 A220 R221 A222 D223 V224 T225 L226 G227 G228 G229 A230 K231 T232 F233 A234 E235 T236 A237 T238 A239 G240

E241 W242 Q243 G244 K245 T246 L247 R248 E249 Q250 A251 Q252 A253 R254 G255 Y256 Q257 L258 V259 S260 D261 A262 A263 S264 L265 N266 S267 V268 T269 E270 A271 N272 Q273 Q274 K275 P276 L277 L278 G279 L280 F281 A282 D283 G284 N285 M286 P287 V288 R289 P293 K294 A295 T296 Y297 H298 G299 N300 I301 D302

K303 P304 A305 V306 T307 C308 T309 P310 N311 P312 Q313 R314 N315 D316 S317 V318 P319 T320 L321 A322 Q323 M324 T325 D326 K327 A328 I329 E330 L331 L332 S333 K334 N335 E336 K337 G338 F339 F340 L341 Q342 V343 E344 G345 A346 S347 I348 D349 K350 Q351 D352 H353 A354 A355 N356 P357 C358 G359 Q360 I361 G362

E363 T364 V365 D366 L367 D368 E369 A370 V371 Q372 R373 A374 L375 E376 F377 A378 K379 K380 E381 G382 N383 T384 L385 V386 I387 V388 T389 A390 D391 H392 A393 H394 A395 S396 Q397 I398 V399 A400 P401 D402 T403 K404 A405 P406 G407 L408 T409 Q410 A411 L412 N413 T414 K415 D416 C417 A418 V419 M420 V421 M422

S423 Y424 G425 N426 S427 E428 E429 D430 S431 Q432 E433 H434 T435 G436 S437 Q438 L439 R440 I441 A442 A443 Y444 G445 P446 H447 A448 A449 N450 V451 V452 G453 L454 T455 D456 Q457 T458 D459 L460 F461 Y462 T463 M464 K465 A466 A467 L468 G469 L470 K471

4.2.10 Score per residue for model 10

- Molecule 1: Protein-export protein SecB

Chain A: 61% 6% 30%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 T10 F11 D20 N27 A28 P29 H30 V31 L44 V58 V59 L60 L68 F74 Q79 I86 A87 G88 I89 E90 G91 T92 Q93 M94 A95 H96 C97 C102 R111 L128 N132 F133 D134 A135 L136 F137 M138 N139 Y140

L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

- Molecule 1: Protein-export protein SecB

Chain B: 65% 14% 21%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 T10 F11 A25 A28 Q33 K34 D43 L44 D45 L51 E57 R61 L68 C76 E90 L98 C102 P103 N104 I114 M117 Q125 L126 N127 N132 F133 D134 A135 L136 F137 M138 N139 Y140 L141 Q142

Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

- Molecule 1: Protein-export protein SecB

Chain C: 60% 13% 27%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 T10 Q14 I21 Q33 K34 Q37 K41 L42 D43 L51 T63 L68 I83 I86 A87 G88 I89 E90 G91 T92 Q93 M94 A95 H96 C97 N104 I105 M117 P124 P130 V131 N132 F133 D134 A135 L136 F137

M138 N139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

- Molecule 1: Protein-export protein SecB

Chain D: 70% 11% 19%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 I13 I16 F23 L51 C76 G88 I89 E90 L98 G99 A100 Y101 C102 I105 R111 I114 P124 L128 N132 F133 D134 A135 L136 F137 M138 N139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151

H152 Q153 D154 A155

- Molecule 2: Alkaline phosphatase

Chain E: 99%

M1 K2 Q3 S4 T5 T6 A7 L8 A9 L10 L11 P12 L13 L14 F15 T16 P17 V18 T19 K20 A21 R22 T23 P24 E25 M26 P27 V28 L29 E30 N31 R32 A33 A34 Q35 G36 D37 I38 T39 A40 P41 G42 G43 A44 R45 R46 L47 T48 G49 D50 Q51 T52 A53 A54 L55 R56 D57 S58 L59 S60

D61 K62 P63 A64 K65 N66 I67 I68 L69 L70 I71 G72 D73 G74 M75 G76 D77 S78 E79 I80 T81 A82 A83 R84 N85 Y86 A87 E88 G89 A90 G91 G92 F93 F94 K95 G96 I97 D98 A99 L100 P101 L102 T103 G104 Q105 Y106 T107 H108 Y109 A110 L111 N112 K113 K114 T115 G116 K117 P118 D119 Y120

V121 T122 D123 S124 A125 A126 S127 A128 T129 A130 W131 S132 T133 G134 V135 K136 T137 Y138 N139 G140 A141 L142 G143 V144 D145 I146 H147 E148 K149 D150 H151 P152 T153 I154 L155 E156 M157 A158 K159 A160 A161 G162 L163 A164 T165 G166 N167 V168 S169 T170 A171 E172 L173 Q174 D175 A176 T177 P178 A179 A180

L181 V182 A183 H184 V185 T186 S187 R188 K189 C190 Y191 G192 P193 S194 A195 T196 S197 E198 K199 C200 P201 G202 N203 A204 L205 E206 K207 G208 G209 K210 G211 S212 I213 T214 E215 Q216 L217 L218 N219 A220 R221 A222 D223 V224 T225 L226 G227 G228 G229 A230 K231 T232 F233 A234 E235 T236 A237 T238 A239 G240

E241 W242 Q243 G244 K245 T246 L247 R248 E249 Q250 A251 Q252 A253 R254 G255 Y256 Q257 L258 V259 S260 D261 A262 A263 S264 L265 N266 S267 V268 T269 E270 A271 N272 Q273 Q274 K275 P276 L277 L278 G279 L280 F281 A282 D283 G284 N285 M286 P287 V288 R289 W290 L291 G292 P293 K294 A295 T296 Y297 H298 G299 N300

I301 D302 K303 P304 A305 V306 T307 C308 T309 P310 N311 P312 Q313 R314 N315 D316 S317 V318 P319 T320 L321 A322 Q323 M324 T325 D326 K327 A328 I329 E330 L331 L332 S333 K334 N335 E336 K337 G338 F339 F340 L341 Q342 V343 E344 G345 A346 S347 I348 D349 K350 Q351 D352 H353 A354 A355 N356 P357 C358 G359 Q360

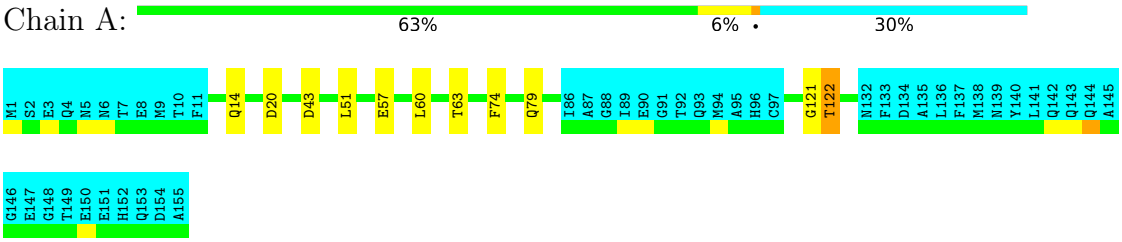
I361 G362 E363 T364 V365 D366 L367 D368 E369 A370 V371 Q372 R373 A374 L375 E376 F377 A378 K379 K380 E381 G382 N383 T384 L385 V386 I387 V388 T389 A390 D391 H392 A393 H394 A395 S396 Q397 I398 V399 A400 P401 D402 T403 K404 A405 P406 G407 L408 T409 Q410 A411 L412 N413 T414 K415 D416 G417 A418 V419 M420

V421 M422 S423 Y424 G425 N426 S427 E428 E429 D430 S431 Q432 E433 H434 T435 G436 S437 Q438 L439 R440 I441 A442 A443 Y444 G445 P446 H447 A448 A449 N450 V451 V452 G453 L454 T455 D456 Q457 T458 D459 L460 F461 Y462 T463 M464 K465 A466 A467 L468 G469 L470 K471

4.2.11 Score per residue for model 11

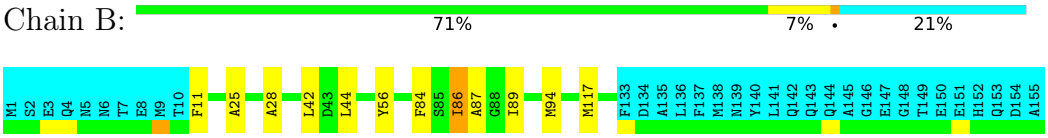
- Molecule 1: Protein-export protein SecB

Chain A:



• Molecule 1: Protein-export protein SecB

Chain B:

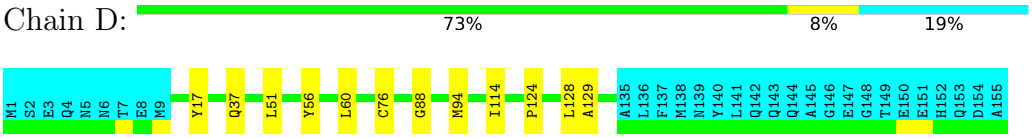


• Molecule 1: Protein-export protein SecB

Chain C:

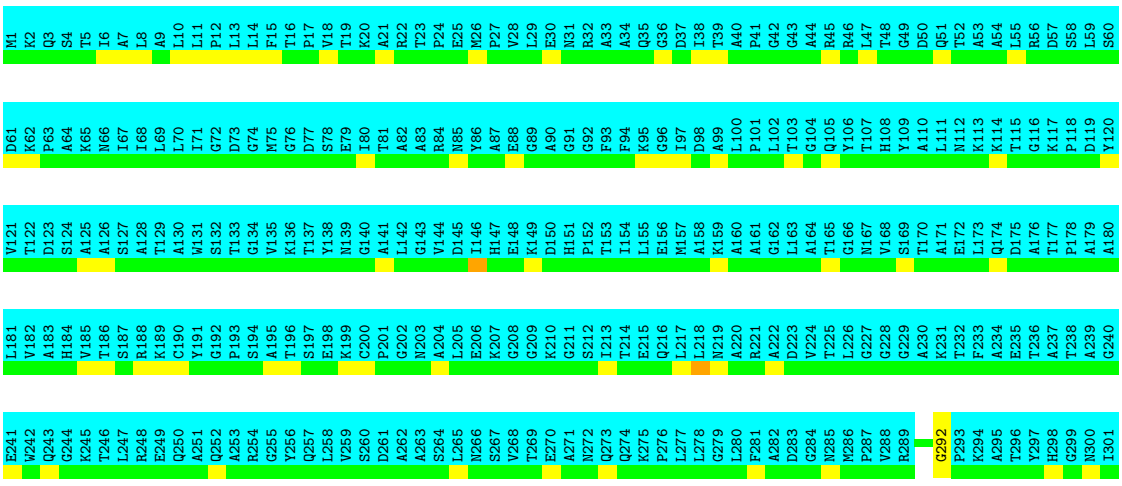
• Molecule 1: Protein-export protein SecB

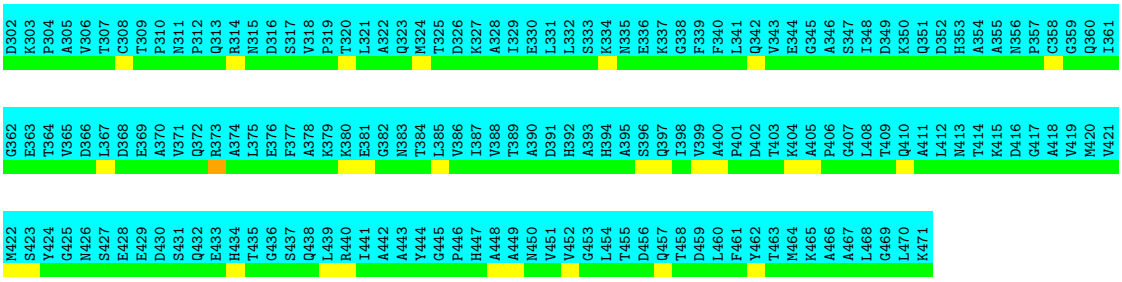
Chain D:



• Molecule 2: Alkaline phosphatase

Chain E:

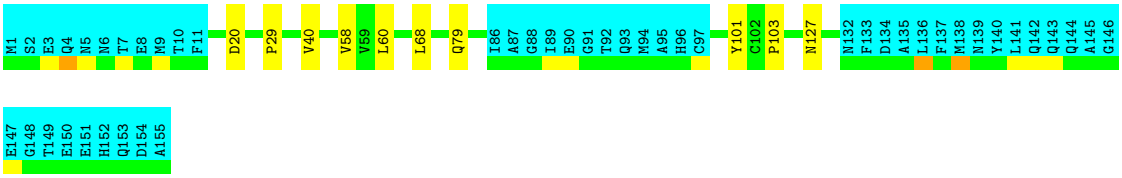




4.2.12 Score per residue for model 12

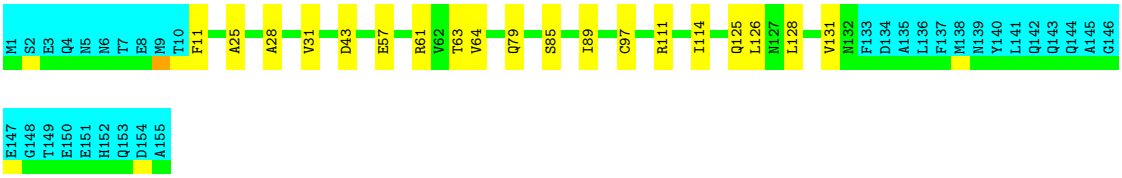
- Molecule 1: Protein-export protein SecB

Chain A:



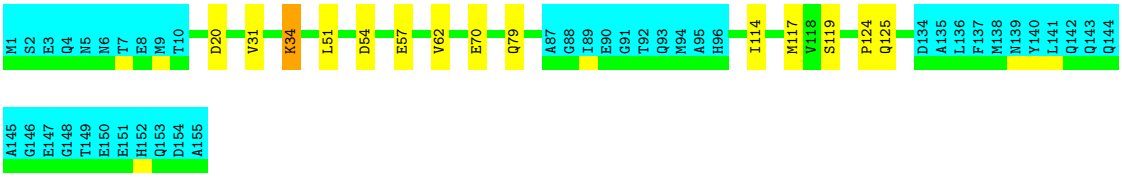
- Molecule 1: Protein-export protein SecB

Chain B:



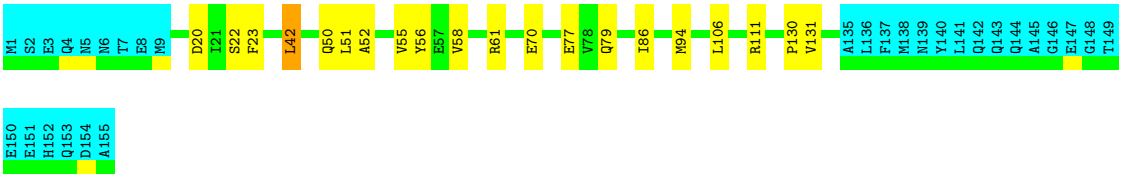
- Molecule 1: Protein-export protein SecB

Chain C:



- Molecule 1: Protein-export protein SecB

Chain D:



• Molecule 2: Alkaline phosphatase

Chain E: 99%

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 M26 P27 V28 E30 N31 R32 A33 A34 Q35 G36 D37 I38 T39 A40 P41 G42 G43 A44 R45 R46 L47 T48 G49 D50 Q51 T52 A53 A54 L55 R56 D57 S58 L59 S60

D61 K62 P63 A64 K65 N66 I67 I68 L69 L70 I71 G72 D73 G74 M75 G76 D77 S78 E79 I80 T81 A82 A83 R84 N85 Y86 A87 E88 G89 A90 G91 G92 F93 F94 K95 G96 I97 D98 A99 L100 P101 L102 T103 G104 Q105 Y106 T107 H108 Y109 A110 L111 N112 K113 K114 T115 G116 K117 P118 D119 Y120

V121 T122 D123 S124 A125 A126 S127 A128 T129 A130 W131 S132 T133 G134 V135 K136 T137 Y138 N139 G140 A141 L142 G143 V144 D145 L146 H147 E148 K149 D150 H151 P152 T153 I154 L155 E156 M157 A158 K159 A160 A161 G162 L163 A164 T165 G166 N167 V168 S169 T170 A171 E172 L173 Q174 D175 A176 T177 P178 A179 A180

L181 V182 A183 H184 V185 T186 S187 R188 K189 C190 Y191 G192 P193 S194 A195 T196 S197 E198 K199 C200 P201 G202 N203 A204 L205 E206 K207 G208 G209 K210 G211 S212 T213 T214 E215 Q216 L217 L218 N219 A220 R221 A222 D223 V224 T225 L226 G227 G228 G229 A230 K231 T232 F233 A234 E235 T236 A237 T238 A239 G240

E241 W242 Q243 G244 K245 T246 L247 R248 E249 Q250 A251 Q252 A253 R254 G255 Y256 Q257 L258 V259 S260 D261 A262 A263 S264 L265 N266 S267 V268 T269 E270 A271 N272 Q273 Q274 K275 P276 L277 L278 G279 L280 F281 A282 D283 G284 N285 M286 P287 V288 R289 P293 K294 A295 T296 Y297 H298 G299 N300 I301 D302

K303 P304 A305 V306 T307 C308 T309 P310 N311 P312 Q313 R314 N315 D316 S317 V318 P319 T320 L321 A322 Q323 M324 T325 D326 K327 A328 I329 E330 L331 L332 S333 K334 N335 E336 K337 G338 F339 F340 L341 Q342 V343 E344 G345 A346 S347 I348 D349 K350 Q351 D352 H353 A354 A355 N356 P357 C358 G359 Q360 I361 G362

E363 T364 V365 D366 L367 D368 E369 A370 V371 Q372 R373 A374 L375 E376 F377 A378 K379 K380 E381 G382 N383 T384 L385 V386 I387 V388 T389 A390 D391 H392 A393 H394 A395 S396 Q397 I398 V399 A400 P401 D402 T403 K404 A405 P406 G407 L408 T409 Q410 A411 L412 N413 T414 K415 D416 G417 A418 V419 M420 V421 M422

S423 Y424 G425 N426 S427 E428 E429 D430 S431 Q432 E433 H434 T435 G436 S437 Q438 L439 R440 I441 A442 A443 Y444 G445 P446 H447 A448 A449 N450 V451 V452 G453 L454 T455 D456 Q457 T458 D459 L460 F461 Y462 T463 M464 K465 A466 A467 L468 G469 L470 K471

4.2.13 Score per residue for model 13 (medoid)

• Molecule 1: Protein-export protein SecB

Chain A: 59% 10% 30%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 T10 F11 V31 W36 L42 D43 A47 L51 D54 E57 V58 V59 L60 T63 L68 I86 A87 G88 I89 E90 G91 T92 D93 M94 A95 H96 C97 C102 P103 L128 N132 F133 D134 A135 L136 F137 M138 N139

Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

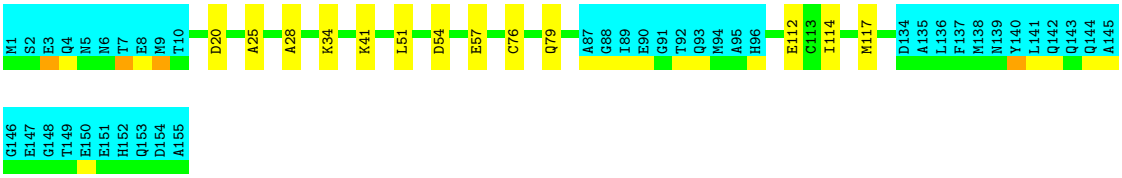
• Molecule 1: Protein-export protein SecB

Chain B: 72% 7% 21%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 T10 A25 A28 V31 F32 Q33 K34 D45 R61 M94 E112 F123 L126 F133 D134 A135 L136 F137 M138 N139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

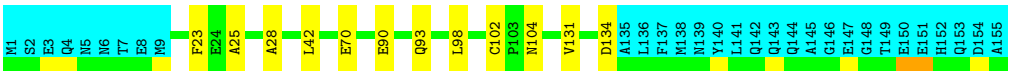
• Molecule 1: Protein-export protein SecB

Chain C: 65% 8% 27%



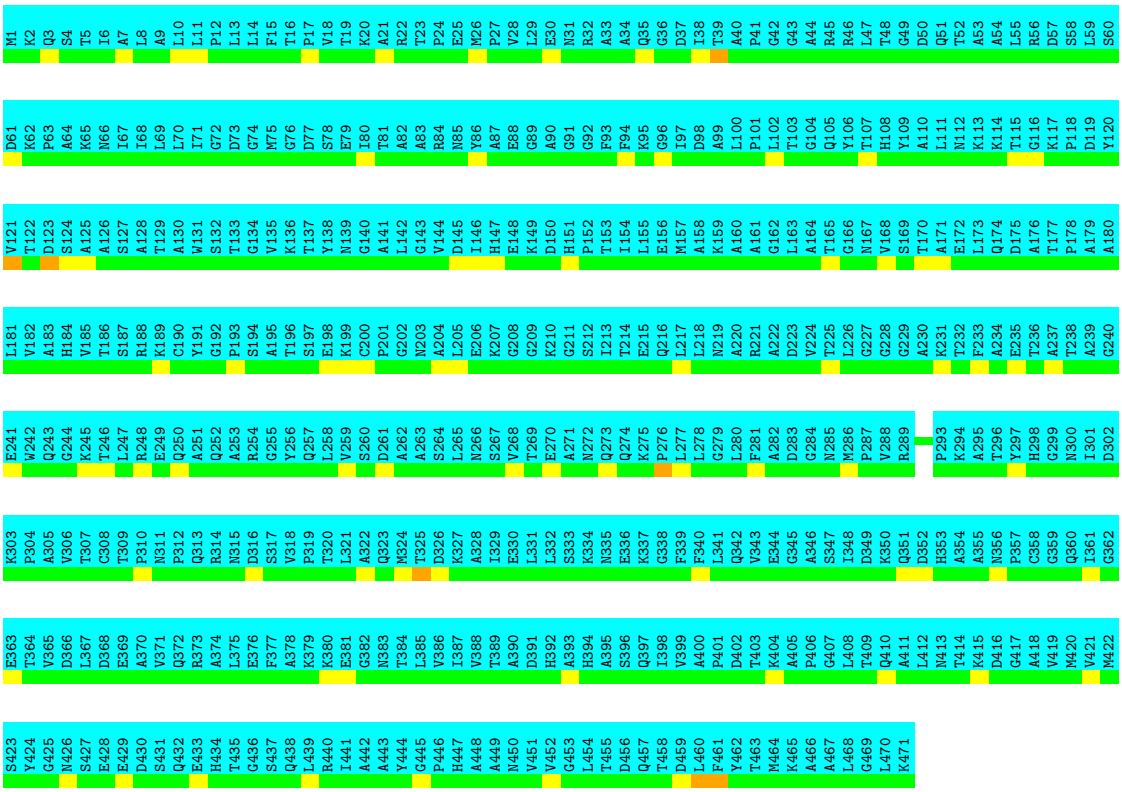
• Molecule 1: Protein-export protein SecB

Chain D: 73% 8% 19%



• Molecule 2: Alkaline phosphatase

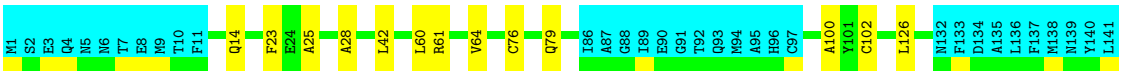
Chain E: 99%

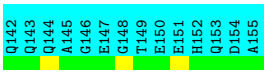


4.2.14 Score per residue for model 14

• Molecule 1: Protein-export protein SecB

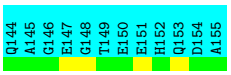
Chain A: 61% 8% 30%





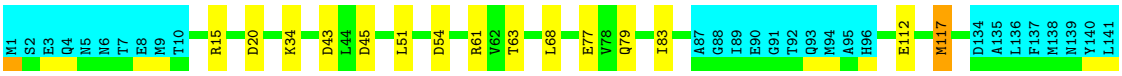
• Molecule 1: Protein-export protein SecB

Chain B:



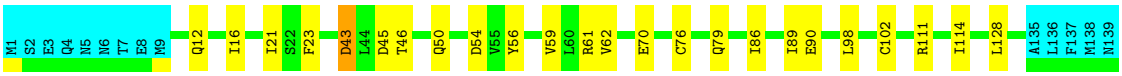
• Molecule 1: Protein-export protein SecB

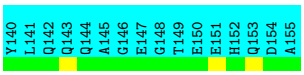
Chain C:



• Molecule 1: Protein-export protein SecB

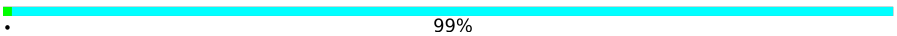
Chain D:

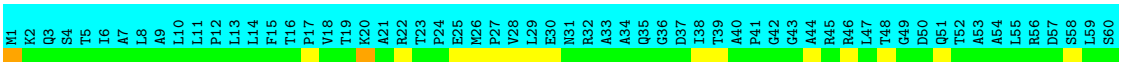


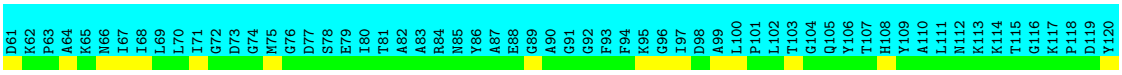


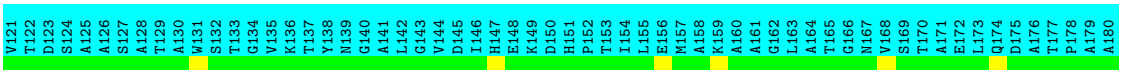
• Molecule 2: Alkaline phosphatase

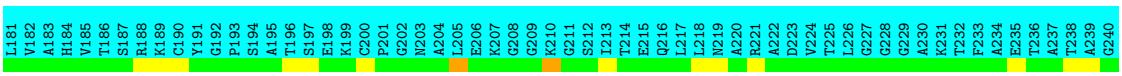
Chain E:

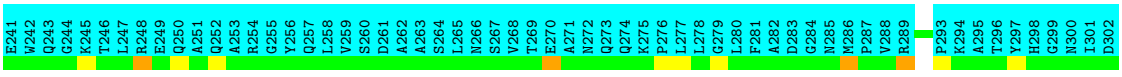












K303 P304 A305 V306 T307 C308 T309 P310 N311 P312 Q313 R314 N315 D316 S317 V318 P319 T320 L321 A322 Q323 M324 T325 D326 K327 A328 I329 E330 L331 L332 S333 K334 N335 E336 K337 G338 F339 F340 L341 Q342 V343 E344 G345 A346 S347 I348 D349 K350 Q351 D352 H353 A354 A355 N356 P357 C358 G359 Q360 I361 G362

E363 T364 V365 D366 L367 D368 E369 A370 V371 Q372 R373 A374 L375 E376 F377 A378 K379 K380 E381 G382 N383 T384 L385 V386 I387 V388 T389 A390 D391 H392 A393 H394 A395 S396 Q397 I398 V399 A400 P401 D402 T403 K404 A405 P406 G407 L408 T409 Q410 A411 L412 N413 T414 K415 D416 G417 A418 V419 M420 V421 M422

S423 Y424 G425 M426 S427 E428 E429 D430 S431 Q432 E433 H434 T435 G436 S437 Q438 L439 R440 I441 A442 A443 Y444 G445 P446 H447 A448 A449 N450 V451 V452 G453 L454 T455 D456 Q457 T458 D459 L460 F461 Y462 T463 M464 K465 A466 A467 L468 G469 L470 K471

4.2.15 Score per residue for model 15

- Molecule 1: Protein-export protein SecB

Chain A: 57% 12% • 30%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 T10 F11 D20 A28 V31 K34 E39 L44 D54 V55 Y56 L60 A66 C76 Q79 I86 A87 G88 I89 E90 G91 T92 Q93 M94 A95 H96 C97 L98 G99 A100 R111 V118 L126 P130 V131

N132 F133 D134 A135 L136 F137 M138 N139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

- Molecule 1: Protein-export protein SecB

Chain B: 67% 10% • 21%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 T10 I13 I21 S22 F23 H30 V31 Q37 L42 D45 R61 E70 A73 C76 I89 E90 C97 L98 C113 I114 F133 D134 A135 L136 F137 M138 N139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149

E150 E151 H152 Q153 D154 A155

- Molecule 1: Protein-export protein SecB

Chain C: 64% 8% • 27%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 T10 F11 Q12 R15 K34 L51 E57 L60 L68 Q80 S85 I86 A87 G88 I89 E90 G91 T92 Q93 M94 A95 H96 C97 L98 C102 A110 M117 D134 A135 L136 F137 M138 N139 Y140 L141 Q142 Q143 Q144 A145

G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

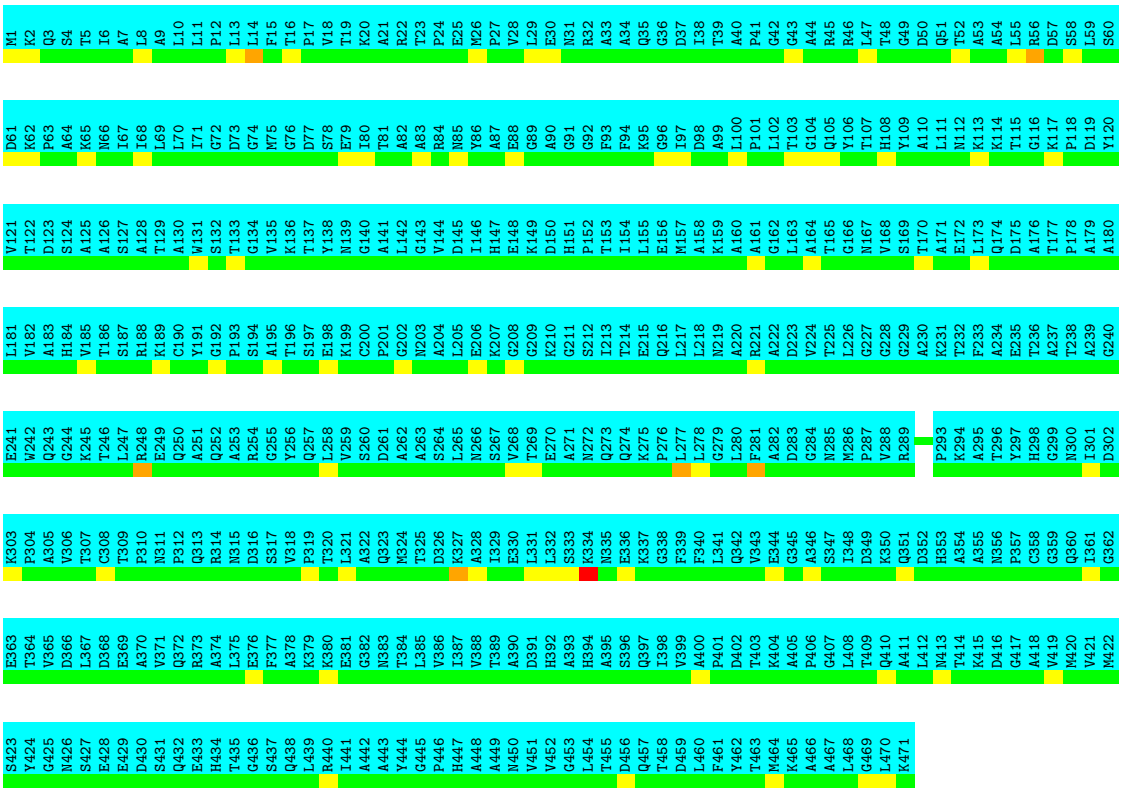
- Molecule 1: Protein-export protein SecB

Chain D: 70% 10% 19%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 T10 F11 D20 A25 A28 E39 E70 C76 Q79 A87 E90 L98 Y101 C102 I114 T122 A135 L136 F137 M138 N139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

- Molecule 2: Alkaline phosphatase

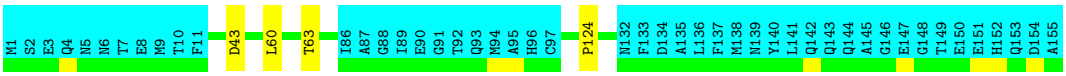
Chain E: 99%



4.2.16 Score per residue for model 16

- Molecule 1: Protein-export protein SecB

Chain A: 67% 30%



- Molecule 1: Protein-export protein SecB

Chain B: 66% 12% 21%

- Molecule 1: Protein-export protein SecB

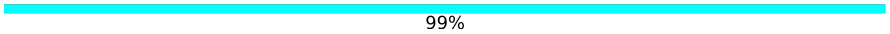
Chain C: 61% 10% 27%

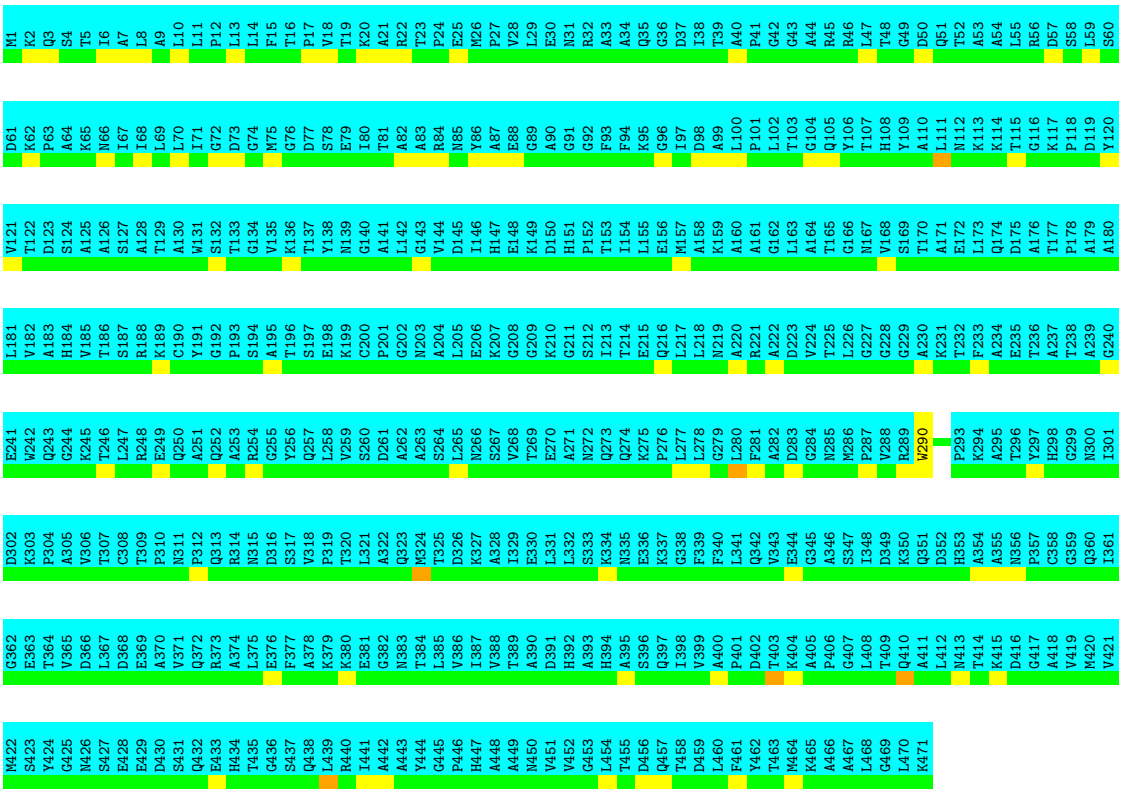
• Molecule 1: Protein-export protein SecB

Chain D:

• Molecule 2: Alkaline phosphatase

Chain E:

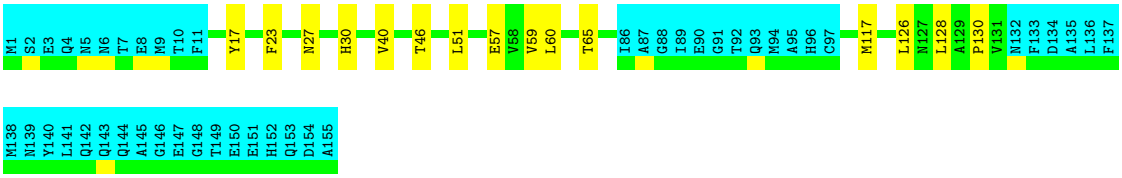




4.2.17 Score per residue for model 17

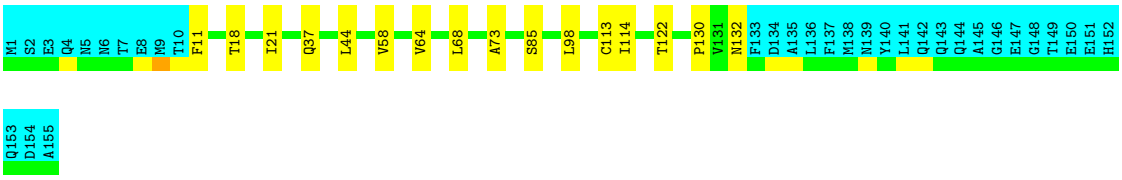
• Molecule 1: Protein-export protein SecB

Chain A:



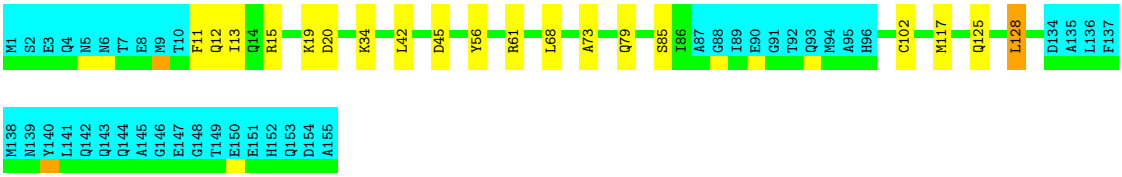
• Molecule 1: Protein-export protein SecB

Chain B:



• Molecule 1: Protein-export protein SecB

Chain C:

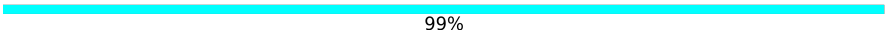


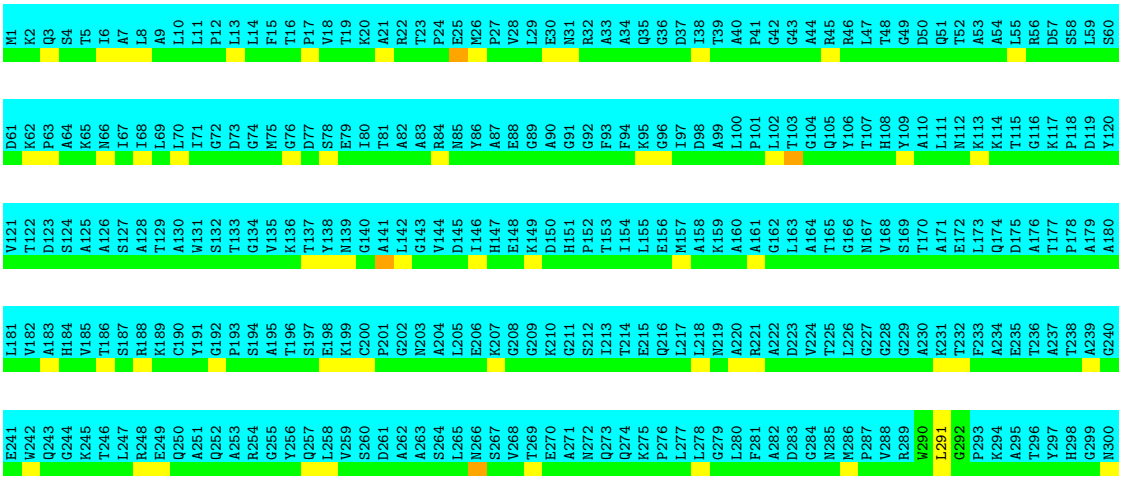
• Molecule 1: Protein-export protein SecB

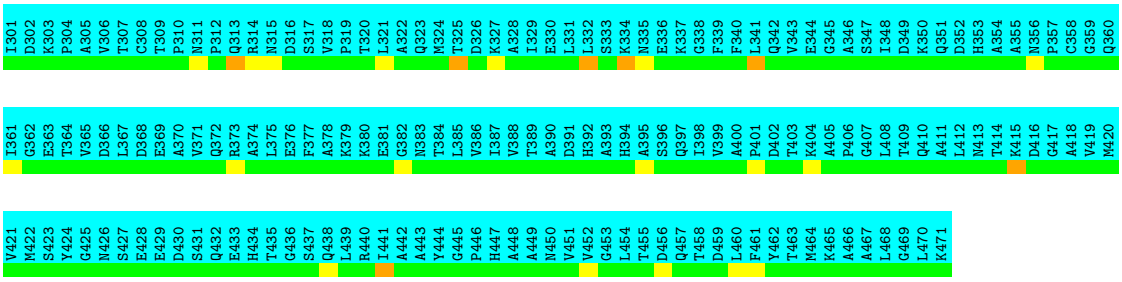
Chain D:

• Molecule 2: Alkaline phosphatase

Chain E:







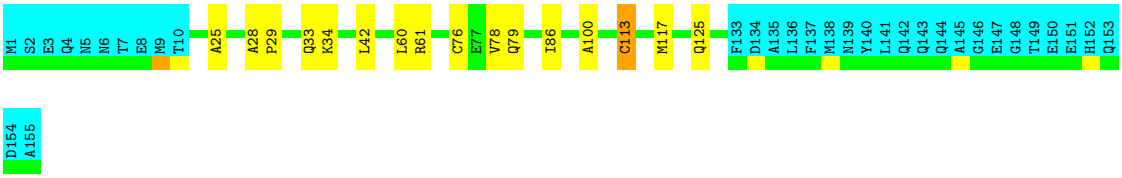
4.2.18 Score per residue for model 18

- Molecule 1: Protein-export protein SecB

Chain A:

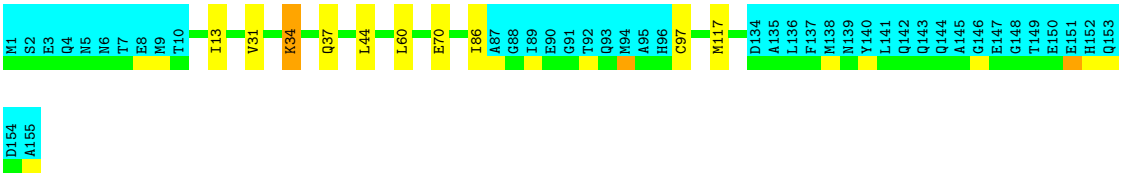
- Molecule 1: Protein-export protein SecB

Chain B:



- Molecule 1: Protein-export protein SecB

Chain C:

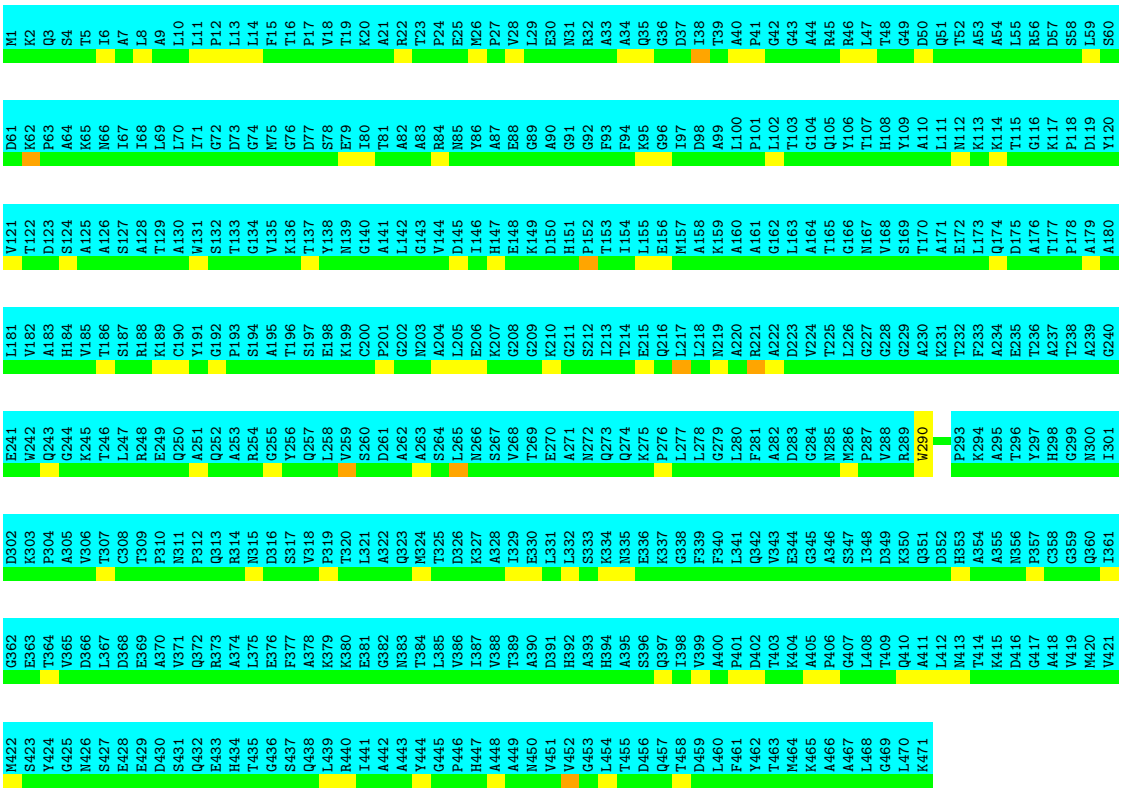


- Molecule 1: Protein-export protein SecB

Chain D:

- Molecule 2: Alkaline phosphatase

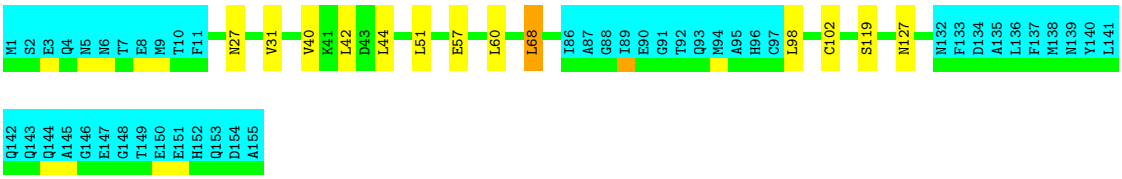
Chain E: 99%



4.2.19 Score per residue for model 19

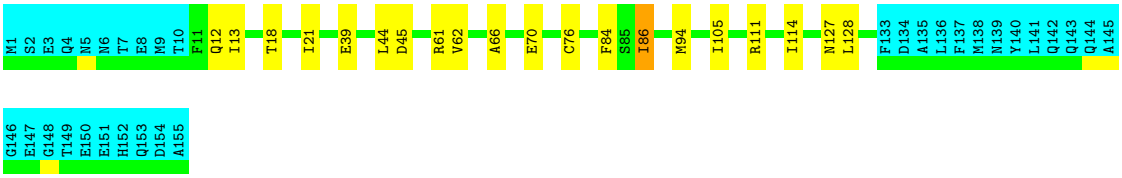
- Molecule 1: Protein-export protein SecB

Chain A: 61% 8% • 30%



- Molecule 1: Protein-export protein SecB

Chain B: 66% 12% • 21%



- Molecule 1: Protein-export protein SecB

Chain C: 68% 5% 27%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 T10 T18 K19 D20 W36 Q79 Q80 A87 G88 I89 E90 G91 T92 Q93 M94 A95 H96 E112 M117 D134 A135 L136 F137 M138 N139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

- Molecule 1: Protein-export protein SecB

Chain D: 72% 8% • 19%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 T10 F11 K34 K41 E70 E71 I86 I89 M94 N104 R111 S119 R120 P130 A135 L136 F137 M138 N139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

- Molecule 2: Alkaline phosphatase

Chain E: 99%

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 M26 P27 V28 L29 E30 N31 R32 A33 A34 Q35 G36 D37 I38 T39 A40 P41 G42 G43 A44 R45 R46 L47 T48 G49 D50 Q51 T52 A53 A54 L55 R56 D57 S58 L59 S60

D61 K62 P63 A64 K65 N66 I67 I68 L69 L70 I71 G72 D73 G74 M75 G76 D77 S78 E79 I80 T81 A82 A83 R84 N85 Y86 A87 E88 G89 A90 G91 G92 F93 F94 K95 G96 I97 D98 A99 L100 P101 L102 T103 G104 Q105 Y106 T107 H108 Y109 A110 L111 N112 K113 K114 T115 G116 K117 P118 D119 Y120

V121 T122 D123 S124 A125 A126 S127 A128 T129 A130 W131 S132 T133 G134 V135 K136 T137 Y138 N139 G140 A141 L142 G143 V144 D145 I146 H147 E148 K149 D150 H151 P152 T153 I154 L155 E156 M157 A158 K159 A160 A161 G162 L163 A164 T165 G166 N167 V168 S169 T170 A171 E172 L173 Q174 D175 A176 T177 P178 A179 A180

L181 V182 A183 H184 V185 T186 S187 R188 K189 C190 Y191 G192 P193 S194 A195 T196 S197 E198 K199 C200 P201 G202 N203 A204 L205 E206 K207 G208 G209 K210 G211 S212 I213 T214 E215 Q216 L217 L218 N219 A220 R221 A222 D223 V224 T225 L226 G227 G228 G229 A230 K231 T232 F233 A234 E235 T236 A237 T238 A239 G240

E241 W242 Q243 G244 K245 T246 L247 R248 E249 Q250 A251 Q252 A253 R254 G255 Y256 Q257 L258 V259 S260 D261 A262 A263 S264 L265 N266 S267 V268 T269 E270 A271 N272 Q273 Q274 K275 P276 L277 L278 G279 L280 F281 A282 D283 G284 N285 M286 P287 V288 R289 W290 L291 G292 P293 K294 A295 T296 Y297 H298 G299 N300

I301 D302 K303 P304 A305 V306 T307 C308 T309 P310 N311 P312 Q313 R314 N315 D316 S317 V318 P319 T320 L321 A322 Q323 M324 T325 D326 K327 A328 I329 E330 L331 L332 S333 K334 N335 E336 K337 G338 F339 F340 L341 Q342 V343 E344 G345 A346 S347 I348 D349 K350 Q351 D352 H353 A354 A355 N356 P357 C358 G359 Q360

I361 G362 E363 T364 V365 D366 L367 D368 E369 A370 V371 Q372 R373 A374 L375 E376 F377 A378 K379 K380 E381 G382 N383 T384 L385 V386 I387 V388 T389 A390 D391 H392 A393 H394 A395 S396 Q397 I398 V399 A400 P401 D402 T403 K404 A405 P406 G407 L408 T409 Q410 A411 L412 N413 T414 K415 D416 G417 A418 V419 M420

V421 M422 S423 Y424 G425 N426 S427 E428 E429 D430 S431 Q432 E433 H434 T435 G436 S437 Q438 L439 R440 I441 A442 A443 Y444 G445 P446 H447 A448 A449 N450 V451 V452 G453 L454 T455 D456 Q457 T458 D459 L460 F461 Y462 T463 M464 K465 A466 A467 L468 G469 L470 K471

4.2.20 Score per residue for model 20

- Molecule 1: Protein-export protein SecB

Chain A: 64% 5% • 30%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 T10 F11 Y17 K34 L60 L68 F84 S85 I86 A87 G88 I89 E90 G91 T92 Q93 M94 A95 H96 C97 Y101 R120 L128 V131 N132 F133 D134 A135 L136 F137 M138 N139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149

E150 E151 H152 Q153 D154 A155

- Molecule 1: Protein-export protein SecB

Chain B: 72% 7% 21%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 T10 A25 A28 P29 L42 C76 I89 Q93 E112 M117 Q125 L128 F133 D134 A135 L136 F137 M138 N139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

- Molecule 1: Protein-export protein SecB

Chain C: 60% 13% 27%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 T10 D20 W36 V40 K41 L42 D43 L44 L51 Y56 E57 V58 V59 L60 L68 E71 Q79 I83 I86 A87 G88 I89 E90 G91 T92 Q93 M94 A95 H96 C97 L98 C102 E112 M117 P124 Q125

D134 A135 L136 F137 M138 N139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

- Molecule 1: Protein-export protein SecB

Chain D: 73% 8% 19%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 D20 A25 A28 E39 A66 E70 C76 Q79 I89 M94 I114 A129 A135 L136 F137 M138 N139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

- Molecule 2: Alkaline phosphatase

Chain E: 99%

M1 K2 Q3 S4 T5 T6 A7 L8 A9 L10 L11 P12 L13 L14 F15 T16 P17 V18 T19 K20 A21 R22 T23 P24 E25 M26 P27 V28 L29 E30 N31 R32 A33 A34 Q35 G36 D37 I38 T39 A40 P41 G42 G43 A44 R45 R46 L47 T48 G49 D50 Q51 T52 A53 A54 L55 R56 D57 S58 L59 S60

D61 K62 P63 A64 K65 N66 I67 I68 L69 L70 I71 G72 D73 G74 M75 G76 D77 S78 E79 I80 T81 A82 A83 R84 N85 Y86 A87 E88 G89 A90 G91 G92 F93 F94 K95 G96 I97 D98 A99 L100 P101 L102 T103 G104 Q105 Y106 T107 H108 Y109 A110 L111 N112 K113 K114 T115 G116 K117 P118 D119 Y120

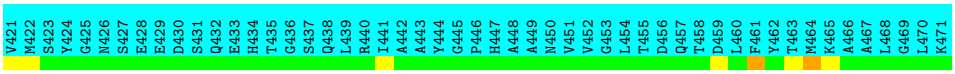
V121 T122 D123 S124 A125 A126 S127 A128 T129 A130 W131 S132 T133 G134 V135 K136 T137 Y138 N139 G140 A141 L142 G143 V144 D145 I146 H147 E148 K149 D150 H151 P152 T153 I154 L155 E156 M157 A158 K159 A160 A161 G162 L163 A164 T165 G166 N167 V168 S169 T170 A171 E172 L173 Q174 D175 A176 T177 P178 A179 A180

L181 V182 A183 H184 V185 T186 S187 R188 K189 C190 Y191 G192 P193 S194 A195 T196 S197 E198 K199 C200 P201 G202 N203 A204 L205 E206 K207 G208 G209 K210 G211 S212 T213 T214 E215 Q216 L217 L218 N219 A220 R221 A222 D223 V224 T225 L226 G227 G228 G229 A230 K231 T232 F233 A234 E235 T236 A237 T238 A239 G240

E241 W242 Q243 G244 K245 T246 L247 R248 E249 Q250 A251 Q252 A253 R254 G255 Y256 Q257 L258 V259 S260 D261 A262 A263 S264 L265 N266 S267 V268 T269 E270 A271 N272 Q273 Q274 K275 P276 L277 L278 G279 L280 F281 A282 D283 G284 N285 M286 P287 V288 R289 W290 L291 G292 P293 K294 A295 T296 Y297 H298 G299 N300

I301 D302 K303 P304 A305 V306 T307 C308 T309 P310 N311 P312 Q313 R314 N315 D316 S317 V318 P319 T320 L321 A322 Q323 N383 M324 T325 D326 K327 A328 T329 E330 L331 L332 S333 K334 N335 E336 K337 G338 F339 F340 L341 Q342 V343 E344 G345 A346 S347 I348 D349 K350 Q351 D352 H353 A354 A355 N356 P357 C358 G359 Q360

I361 G362 E363 T364 V365 D366 L367 D368 E369 A370 V371 Q372 R373 A374 L375 E376 F377 A378 K379 K380 E381 G382 N383 T384 L385 V386 I387 V388 T389 A390 D391 H392 A393 H394 A395 S396 Q397 I398 V399 A400 P401 D402 T403 K404 A405 P406 G407 L408 T409 Q410 A411 L412 N413 T414 K415 D416 G417 A418 V419 M420


V421
M422
S423
Y424
G425
N426
S427
E428
E429
D430
S431
Q432
E433
H434
T435
G436
S437
Q438
L439
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Y444
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V451
V452
G453
L454
T455
D456
Q457
T458
D459
L460
F461
Y462
T463
M464
K465
A466
A467
L468
G469
L470
K471

5 Refinement protocol and experimental data overview (i)

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	5
Total number of shifts	6416
Number of shifts mapped to atoms	6416
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%

6 Model quality (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.87±0.01	0±0/865 (0.0± 0.0%)	0.64±0.01	0±0/1182 (0.0± 0.0%)
1	B	0.88±0.02	0±0/969 (0.0± 0.0%)	0.63±0.02	0±0/1322 (0.0± 0.0%)
1	C	0.88±0.02	0±0/911 (0.0± 0.0%)	0.64±0.02	0±0/1244 (0.0± 0.0%)
1	D	0.87±0.02	0±0/996 (0.0± 0.0%)	0.63±0.02	0±0/1359 (0.0± 0.0%)
2	E	0.91±0.08	0±0/28 (0.0± 0.0%)	0.65±0.14	0±0/40 (0.0± 0.0%)
All	All	0.87	0/75380 (0.0%)	0.64	2/102940 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	111	ARG	NE-CZ-NH2	-5.55	117.52	120.30	15	1
1	B	101	TYR	CA-CB-CG	5.37	123.60	113.40	8	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	845	830	829	5±3
1	B	947	926	924	8±2
1	C	889	870	869	6±3
1	D	973	946	944	6±2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
2	E	26	24	24	0±0
All	All	73600	71920	71800	457

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:25:ALA:HB1	1:B:28:ALA:HB2	0.78	1.53	12	6
1:B:89:ILE:HG21	1:B:97:CYS:SG	0.67	2.29	15	1
1:A:20:ASP:HB3	1:A:79:GLN:HB2	0.66	1.66	5	7
1:A:98:LEU:HA	1:A:102:CYS:SG	0.66	2.31	1	3
1:A:16:ILE:HB	1:C:111:ARG:HH12	0.65	1.51	1	1
1:D:76:CYS:SG	1:D:114:ILE:HG12	0.65	2.31	16	8
1:B:25:ALA:CB	1:B:28:ALA:HB2	0.65	2.21	12	12
1:D:25:ALA:HB1	1:D:28:ALA:HB2	0.63	1.70	20	6
1:A:43:ASP:HB2	1:A:63:THR:HB	0.62	1.72	7	4
1:B:61:ARG:HD3	1:B:79:GLN:HG3	0.61	1.72	2	1
1:C:20:ASP:HB2	1:C:79:GLN:HB2	0.61	1.71	12	2
1:D:76:CYS:SG	1:D:114:ILE:HG23	0.61	2.35	20	4
1:D:98:LEU:HA	1:D:102:CYS:SG	0.60	2.36	13	11
1:B:58:VAL:HG11	1:B:98:LEU:HB2	0.60	1.73	9	1
1:C:20:ASP:HB3	1:C:79:GLN:HB2	0.60	1.72	3	12
1:A:45:ASP:HB2	1:A:61:ARG:HB3	0.59	1.75	9	1
1:C:45:ASP:HB3	1:C:61:ARG:HB3	0.59	1.75	17	5
1:B:18:THR:HG21	1:B:21:ILE:HD11	0.59	1.74	2	6
1:D:61:ARG:HG2	1:D:79:GLN:HG2	0.58	1.76	1	1
1:A:119:SER:HB2	1:D:119:SER:HB2	0.58	1.76	7	2
1:B:76:CYS:SG	1:B:114:ILE:HG23	0.57	2.39	5	3
1:B:43:ASP:HB2	1:B:63:THR:HB	0.57	1.76	14	4
1:C:98:LEU:HA	1:C:102:CYS:SG	0.57	2.39	20	4
1:D:89:ILE:HD13	1:D:94:MET:HB2	0.57	1.76	19	3
1:A:36:TRP:HA	1:A:68:LEU:HD11	0.57	1.75	8	2
1:B:76:CYS:SG	1:B:114:ILE:HA	0.56	2.41	10	5
1:B:78:VAL:HG21	1:B:113:CYS:HB3	0.56	1.78	18	2
1:D:100:ALA:HB1	1:D:134:ASP:HA	0.56	1.76	10	2
1:D:20:ASP:HB3	1:D:79:GLN:HB2	0.55	1.78	12	9
1:A:58:VAL:HG11	1:A:103:PRO:HD3	0.55	1.77	13	2
1:A:31:VAL:HG13	1:A:68:LEU:HD22	0.55	1.79	13	1
1:A:120:ARG:HD3	1:B:113:CYS:SG	0.55	2.42	2	2
1:B:64:VAL:HG21	1:B:114:ILE:HG21	0.55	1.79	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:MET:SD	1:B:21:ILE:HG21	0.55	2.41	7	1
1:A:36:TRP:HA	1:A:68:LEU:HD23	0.54	1.78	5	1
1:D:84:PHE:HB2	1:D:98:LEU:HD21	0.54	1.78	9	1
1:D:31:VAL:HG21	1:D:73:ALA:HA	0.54	1.78	3	1
1:B:41:LYS:HB2	1:B:65:THR:HB	0.54	1.79	14	2
1:D:10:THR:HB	1:D:12:GLN:HE22	0.54	1.63	7	1
1:B:45:ASP:HB3	1:B:61:ARG:HB3	0.54	1.80	6	7
1:B:111:ARG:HG3	1:B:128:LEU:HB3	0.54	1.78	12	1
1:B:98:LEU:HA	1:B:102:CYS:SG	0.54	2.42	10	3
1:C:34:LYS:HE2	1:C:73:ALA:HA	0.54	1.80	9	2
1:B:31:VAL:HG21	1:B:73:ALA:HA	0.54	1.80	15	1
1:B:13:ILE:HD13	1:B:105:ILE:HD13	0.54	1.79	19	1
1:B:61:ARG:HB2	1:B:79:GLN:HG2	0.53	1.79	9	4
1:C:117:MET:HE2	1:D:21:ILE:HG21	0.53	1.80	14	2
1:C:34:LYS:HB2	1:C:34:LYS:HZ2	0.53	1.64	8	1
1:B:16:ILE:HD12	1:D:127:ASN:HD21	0.53	1.63	5	1
1:A:25:ALA:HB1	1:A:28:ALA:HB2	0.53	1.79	6	4
1:C:86:ILE:HD12	1:C:97:CYS:SG	0.53	2.43	8	1
1:C:43:ASP:HB2	1:C:63:THR:HB	0.53	1.79	14	2
1:C:115:THR:HG22	1:C:125:GLN:HE21	0.53	1.64	9	1
1:C:34:LYS:HE3	1:C:71:GLU:HG3	0.53	1.80	11	2
1:A:27:ASN:HA	1:A:31:VAL:HB	0.52	1.79	10	1
1:A:51:LEU:HD11	1:A:57:GLU:HB2	0.52	1.80	17	6
1:B:89:ILE:HB	1:B:94:MET:SD	0.52	2.45	5	1
1:A:41:LYS:HB2	1:A:65:THR:HB	0.52	1.82	7	1
1:C:56:TYR:HB2	1:C:86:ILE:HD12	0.52	1.81	20	1
1:A:76:CYS:SG	1:A:118:VAL:HG12	0.52	2.45	15	1
1:D:58:VAL:HG22	1:D:98:LEU:HD12	0.52	1.80	17	1
1:C:51:LEU:HD11	1:C:83:ILE:HD12	0.52	1.80	20	6
1:B:84:PHE:HB2	1:B:86:ILE:HD12	0.52	1.81	6	2
1:C:12:GLN:HB3	1:C:85:SER:HB2	0.52	1.79	17	4
1:A:111:ARG:HH22	1:A:130:PRO:HG3	0.52	1.65	15	1
1:B:44:LEU:HD23	1:B:60:LEU:HD21	0.51	1.81	7	1
1:A:27:ASN:HB2	1:A:30:HIS:HB2	0.51	1.83	17	1
1:C:14:GLN:HB3	1:C:15:ARG:HH11	0.51	1.66	6	1
1:D:43:ASP:HB3	1:D:62:VAL:HG13	0.51	1.81	14	1
1:B:62:VAL:HG11	1:B:128:LEU:HD21	0.51	1.82	19	1
1:A:18:THR:HG21	1:A:113:CYS:SG	0.51	2.46	1	1
1:B:98:LEU:HD23	1:B:102:CYS:SG	0.51	2.46	3	1
1:C:51:LEU:HD11	1:C:57:GLU:HB2	0.51	1.83	13	6
1:A:31:VAL:HG21	1:A:73:ALA:HA	0.51	1.83	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:111:ARG:HG3	1:C:128:LEU:HB3	0.51	1.82	9	1
1:D:86:ILE:HG12	1:D:89:ILE:HD11	0.50	1.82	6	1
1:B:13:ILE:HG12	1:B:105:ILE:HG21	0.50	1.82	7	1
1:B:97:CYS:SG	1:B:98:LEU:N	0.50	2.85	15	2
1:D:45:ASP:HB3	1:D:61:ARG:HB3	0.50	1.84	14	1
1:C:20:ASP:HA	1:D:23:PHE:O	0.50	2.06	9	6
1:B:11:PHE:HA	1:B:85:SER:O	0.50	2.05	12	4
1:D:13:ILE:HD13	1:D:105:ILE:HG21	0.50	1.83	5	4
1:C:111:ARG:HG3	1:C:128:LEU:HB2	0.50	1.82	6	1
1:B:21:ILE:HD11	1:B:113:CYS:SG	0.50	2.47	15	6
1:C:42:LEU:HD13	1:C:128:LEU:HD11	0.50	1.82	17	1
1:B:68:LEU:HG	1:B:73:ALA:HB2	0.50	1.82	16	4
1:D:86:ILE:HB	1:D:89:ILE:HD11	0.50	1.84	18	1
1:B:34:LYS:HB3	1:B:68:LEU:HB3	0.49	1.84	10	1
1:D:59:VAL:HG13	1:D:79:GLN:HG3	0.49	1.83	14	1
1:A:43:ASP:HB3	1:A:63:THR:HB	0.49	1.83	4	2
1:C:18:THR:HG21	1:C:113:CYS:SG	0.49	2.47	1	1
1:C:31:VAL:HA	1:C:34:LYS:HE2	0.49	1.83	4	3
1:A:120:ARG:HH12	1:B:112:GLU:HG3	0.49	1.67	20	1
1:C:119:SER:HB3	1:C:125:GLN:HE22	0.49	1.68	12	1
1:C:112:GLU:HG3	1:D:120:ARG:HH12	0.49	1.68	19	1
1:B:76:CYS:SG	1:B:117:MET:HB2	0.49	2.48	3	4
1:A:58:VAL:HG21	1:A:102:CYS:HB3	0.49	1.85	10	1
1:B:89:ILE:HD12	1:B:94:MET:SD	0.49	2.48	8	1
1:D:21:ILE:HG23	1:D:78:VAL:HG22	0.49	1.84	16	1
1:D:90:GLU:HA	1:D:94:MET:SD	0.48	2.49	6	1
1:A:115:THR:HG23	1:A:125:GLN:HG3	0.48	1.86	1	1
1:A:64:VAL:HB	1:A:76:CYS:HB2	0.48	1.85	8	3
1:A:44:LEU:HD23	1:A:60:LEU:HD21	0.48	1.83	10	1
1:D:43:ASP:HB2	1:D:63:THR:HB	0.48	1.85	17	1
1:B:51:LEU:HD11	1:B:57:GLU:HB2	0.48	1.85	6	3
1:B:89:ILE:HD11	1:B:97:CYS:SG	0.48	2.48	12	1
1:B:28:ALA:O	1:B:31:VAL:HG12	0.48	2.09	12	1
1:C:84:PHE:CE1	1:C:102:CYS:SG	0.48	3.07	1	2
1:B:89:ILE:HD12	1:B:94:MET:HA	0.48	1.85	11	2
1:A:23:PHE:HD1	1:A:76:CYS:HG	0.48	1.51	14	2
1:B:111:ARG:HB2	1:B:128:LEU:HB2	0.47	1.86	19	1
1:A:47:ALA:HB3	1:A:59:VAL:HB	0.47	1.86	13	1
1:B:86:ILE:H	1:B:86:ILE:HD13	0.47	1.70	11	1
1:B:33:GLN:HG3	1:B:34:LYS:HG3	0.47	1.87	2	3
1:D:43:ASP:HB3	1:D:63:THR:HB	0.47	1.85	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:PHE:HB3	1:B:21:ILE:HB	0.47	1.85	5	1
1:D:56:TYR:CE1	1:D:58:VAL:HB	0.47	2.44	12	1
1:C:76:CYS:SG	1:C:114:ILE:HA	0.47	2.50	13	6
1:D:42:LEU:HD21	1:D:62:VAL:HG13	0.47	1.86	7	2
1:C:64:VAL:HG21	1:C:114:ILE:HG21	0.47	1.85	5	2
1:A:130:PRO:HB3	1:C:105:ILE:HD11	0.46	1.87	1	1
1:A:130:PRO:HG3	1:C:105:ILE:HD11	0.46	1.87	4	1
1:B:89:ILE:HD12	1:B:97:CYS:SG	0.46	2.49	8	1
1:B:27:ASN:ND2	1:B:71:GLU:HB2	0.46	2.26	9	1
1:C:115:THR:HG21	1:C:127:ASN:HD22	0.46	1.70	9	1
1:C:34:LYS:HG2	1:C:68:LEU:HD13	0.46	1.86	15	1
1:C:34:LYS:HE3	1:C:73:ALA:HA	0.46	1.85	17	1
1:C:43:ASP:HB3	1:C:63:THR:HB	0.46	1.86	10	2
1:D:111:ARG:HH12	1:D:130:PRO:HB3	0.46	1.71	12	2
1:B:89:ILE:HD13	1:B:97:CYS:SG	0.45	2.51	15	1
1:B:54:ASP:HA	1:B:56:TYR:CE1	0.45	2.46	5	1
1:C:28:ALA:HB1	1:D:17:TYR:HE2	0.45	1.70	9	3
1:D:22:SER:HB3	1:D:77:GLU:HB2	0.45	1.89	12	1
1:D:61:ARG:HB2	1:D:79:GLN:HG2	0.45	1.89	9	1
1:C:28:ALA:HB3	1:D:19:LYS:HE3	0.45	1.89	6	2
1:A:44:LEU:H	1:A:44:LEU:HD23	0.45	1.71	7	1
1:A:61:ARG:HB2	1:A:79:GLN:HG2	0.45	1.89	1	1
1:A:20:ASP:HA	1:B:23:PHE:O	0.45	2.12	15	1
1:C:84:PHE:HE1	1:C:102:CYS:HG	0.44	1.54	1	1
1:A:29:PRO:HB3	1:B:57:GLU:HG3	0.44	1.88	12	2
1:C:62:VAL:HB	1:C:114:ILE:HD11	0.44	1.88	12	1
1:D:97:CYS:SG	1:D:102:CYS:SG	0.44	3.14	17	1
1:A:111:ARG:NH1	1:C:105:ILE:HD12	0.44	2.27	10	2
1:C:13:ILE:HD12	1:C:13:ILE:N	0.44	2.26	17	1
1:C:19:LYS:HE3	1:D:28:ALA:HB3	0.44	1.88	17	1
1:D:52:ALA:HB3	1:D:55:VAL:HB	0.44	1.88	12	1
1:C:20:ASP:HB3	1:C:79:GLN:HB3	0.44	1.89	16	1
1:C:14:GLN:HB2	1:C:83:ILE:HB	0.44	1.88	10	1
1:D:46:THR:HG22	1:D:60:LEU:HD22	0.44	1.89	16	1
1:A:40:VAL:HA	1:A:65:THR:O	0.44	2.13	17	1
1:A:17:TYR:HE2	1:B:28:ALA:HB1	0.44	1.73	8	4
1:B:125:GLN:HB3	1:C:124:PRO:HA	0.44	1.89	10	1
1:A:61:ARG:HD2	1:A:79:GLN:HG2	0.44	1.89	14	1
1:B:34:LYS:HZ1	1:B:71:GLU:HB3	0.44	1.73	2	1
1:A:111:ARG:NH2	1:A:130:PRO:HB3	0.44	2.28	9	1
1:B:13:ILE:H	1:B:13:ILE:HD13	0.44	1.72	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:11:PHE:HA	1:C:85:SER:O	0.44	2.13	11	1
1:C:45:ASP:HB2	1:C:61:ARG:HD2	0.44	1.89	14	1
1:B:25:ALA:HB3	1:B:28:ALA:HB2	0.44	1.90	16	1
1:A:17:TYR:HB3	1:B:122:THR:HG23	0.44	1.89	17	1
1:A:68:LEU:H	1:A:68:LEU:HD23	0.43	1.73	10	3
1:C:68:LEU:HD23	1:C:68:LEU:H	0.43	1.73	6	1
1:B:125:GLN:HB3	1:C:125:GLN:HG3	0.43	1.88	9	1
1:C:24:GLU:HB2	1:C:75:LEU:HB3	0.43	1.88	1	1
1:B:11:PHE:HZ	1:B:102:CYS:HG	0.43	1.56	3	1
1:A:15:ARG:HD3	1:A:83:ILE:HD12	0.43	1.90	4	1
1:C:68:LEU:HB2	1:C:71:GLU:HB3	0.43	1.89	20	1
1:A:20:ASP:HB2	1:A:79:GLN:HB2	0.43	1.89	1	1
1:B:119:SER:HA	1:C:125:GLN:HE22	0.43	1.74	3	1
1:A:23:PHE:HB2	1:A:117:MET:SD	0.43	2.54	4	2
1:D:34:LYS:HZ1	1:D:71:GLU:HB3	0.43	1.74	19	1
1:D:111:ARG:HD3	1:D:128:LEU:O	0.43	2.14	10	2
1:B:11:PHE:CE1	1:B:102:CYS:SG	0.43	3.10	4	2
1:D:40:VAL:HG13	1:D:64:VAL:HG13	0.43	1.90	16	2
1:D:19:LYS:HD3	1:D:59:VAL:HG12	0.43	1.90	6	1
1:B:11:PHE:HE1	1:B:102:CYS:SG	0.43	2.36	14	2
1:B:125:GLN:OE1	1:C:124:PRO:HA	0.43	2.14	12	1
1:B:21:ILE:CD1	1:B:113:CYS:SG	0.43	3.07	16	1
1:D:55:VAL:HG11	1:D:83:ILE:HG23	0.43	1.89	16	1
1:A:113:CYS:O	1:A:117:MET:HG2	0.43	2.14	6	1
1:A:68:LEU:HB2	1:A:73:ALA:HB2	0.43	1.91	8	1
1:A:121:GLY:O	1:A:122:THR:HG22	0.43	2.14	11	1
1:B:39:GLU:O	1:B:66:ALA:HA	0.42	2.14	4	2
1:A:34:LYS:HD3	1:A:68:LEU:HD11	0.42	1.91	20	1
1:B:114:ILE:O	1:B:118:VAL:HG23	0.42	2.15	5	1
1:C:11:PHE:CZ	1:C:102:CYS:SG	0.42	3.12	17	2
1:C:60:LEU:HD23	1:C:106:LEU:HD12	0.42	1.90	1	1
1:C:58:VAL:HG21	1:C:102:CYS:HB3	0.42	1.91	3	1
1:C:14:GLN:HE22	1:C:85:SER:H	0.42	1.57	16	1
1:C:44:LEU:HD11	1:C:60:LEU:HD23	0.42	1.91	18	1
1:D:51:LEU:H	1:D:51:LEU:HD23	0.42	1.73	12	1
1:A:51:LEU:HD13	1:B:29:PRO:HB3	0.42	1.92	6	1
1:A:13:ILE:HD13	1:A:16:ILE:HD11	0.42	1.92	7	1
1:C:44:LEU:HD21	1:C:60:LEU:HD11	0.42	1.91	8	1
1:A:111:ARG:HH12	1:C:105:ILE:HD12	0.42	1.75	10	1
1:B:130:PRO:HG3	1:D:16:ILE:HB	0.42	1.89	8	1
1:A:39:GLU:O	1:A:66:ALA:HA	0.42	2.14	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:60:LEU:HB2	1:D:103:PRO:HB3	0.42	1.90	1	1
1:D:94:MET:HG3	1:D:95:ALA:N	0.42	2.29	5	1
1:C:104:ASN:HD21	1:C:133:PHE:HB2	0.42	1.74	10	1
1:B:120:ARG:NH2	1:C:112:GLU:HG3	0.42	2.30	2	1
1:D:40:VAL:HG23	1:D:64:VAL:HG13	0.42	1.91	18	1
1:D:33:GLN:HE21	1:D:33:GLN:HA	0.41	1.75	5	1
1:A:14:GLN:NE2	1:A:83:ILE:HG21	0.41	2.29	6	1
1:D:114:ILE:HD12	1:D:128:LEU:HD11	0.41	1.91	11	2
1:B:33:GLN:HG3	1:B:34:LYS:HG2	0.41	1.92	10	1
1:D:113:CYS:O	1:D:117:MET:SD	0.41	2.77	18	1
1:C:18:THR:HG22	1:C:80:GLN:HE22	0.41	1.74	19	1
1:D:39:GLU:O	1:D:66:ALA:HA	0.41	2.15	20	1
1:C:25:ALA:HB1	1:C:28:ALA:HB2	0.41	1.93	13	1
1:B:115:THR:HG23	1:B:125:GLN:HB2	0.41	1.90	7	1
1:B:31:VAL:HG11	1:B:123:PHE:CE1	0.41	2.51	13	1
1:B:94:MET:SD	1:B:94:MET:C	0.41	2.99	13	1
1:D:11:PHE:HZ	1:D:102:CYS:HG	0.41	1.58	15	1
1:B:128:LEU:HD23	1:B:128:LEU:H	0.41	1.76	5	1
1:A:82:GLY:HA3	1:A:106:LEU:HD21	0.41	1.93	7	1
1:A:13:ILE:HG12	1:A:84:PHE:HD2	0.41	1.76	6	1
1:A:27:ASN:O	1:A:31:VAL:HG23	0.41	2.15	19	2
1:C:41:LYS:HB3	1:C:65:THR:HB	0.41	1.91	8	1
1:C:13:ILE:H	1:C:13:ILE:HD12	0.41	1.76	3	1
1:D:37:GLN:HE21	1:D:124:PRO:HG3	0.41	1.76	11	1
1:A:64:VAL:HG11	1:A:126:LEU:HD21	0.41	1.92	14	1
1:C:44:LEU:HD21	1:C:60:LEU:HD12	0.41	1.93	20	1
1:B:45:ASP:HB3	1:B:61:ARG:HD3	0.41	1.93	1	1
1:D:11:PHE:CE2	1:D:102:CYS:SG	0.41	3.13	1	1
1:B:28:ALA:HB3	1:B:29:PRO:HD3	0.41	1.93	20	3
1:B:56:TYR:HB2	1:B:86:ILE:HD11	0.41	1.92	11	1
1:D:58:VAL:HG13	1:D:106:LEU:HD11	0.41	1.91	12	1
1:A:35:ASP:O	1:A:68:LEU:HB3	0.41	2.15	5	1
1:A:41:LYS:HB3	1:A:65:THR:HB	0.41	1.92	5	1
1:A:17:TYR:CE2	1:B:28:ALA:HB1	0.41	2.51	8	1
1:C:21:ILE:HB	1:D:23:PHE:HB3	0.41	1.92	10	1
1:C:80:GLN:HB2	1:C:110:ALA:HB2	0.41	1.92	15	1
1:A:13:ILE:HD12	1:C:130:PRO:HG3	0.41	1.93	1	1
1:C:83:ILE:HD11	1:D:29:PRO:HB3	0.40	1.91	3	1
1:C:42:LEU:HD21	1:C:64:VAL:HG22	0.40	1.91	16	1
1:D:98:LEU:O	1:D:103:PRO:HD3	0.40	2.15	17	1
1:C:40:VAL:HA	1:C:65:THR:O	0.40	2.17	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:13:ILE:HG21	1:D:16:ILE:HG23	0.40	1.93	2	1
1:B:58:VAL:HG11	1:B:98:LEU:HD22	0.40	1.94	17	1
1:B:113:CYS:O	1:B:117:MET:HG2	0.40	2.16	1	1
1:D:114:ILE:O	1:D:118:VAL:HG23	0.40	2.16	4	1
1:B:22:SER:HB2	1:B:77:GLU:HB3	0.40	1.93	7	1
1:A:67:SER:HA	1:A:72:THR:HA	0.40	1.92	5	1
1:D:61:ARG:NH1	1:D:77:GLU:HB3	0.40	2.32	12	1
1:C:38:PRO:HA	1:C:68:LEU:HB3	0.40	1.94	6	1
1:B:104:ASN:HB2	1:B:132:ASN:HD21	0.40	1.76	10	1
1:A:28:ALA:O	1:A:31:VAL:HG22	0.40	2.16	15	1
1:B:111:ARG:HG3	1:B:128:LEU:HB2	0.40	1.93	16	1
1:A:46:THR:HA	1:A:59:VAL:O	0.40	2.16	17	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	108/155 (70%)	102±2 (94±1%)	6±2 (5±1%)	0±0 (0±0%)	54	85
1	B	122/155 (79%)	115±3 (94±2%)	7±3 (6±2%)	0±0 (0±0%)	54	85
1	C	113/155 (73%)	105±2 (93±2%)	8±2 (7±2%)	0±1 (0±1%)	44	80
1	D	125/155 (81%)	119±2 (95±2%)	6±2 (4±2%)	0±0 (0±0%)	54	85
2	E	3/471 (1%)	2±1 (72±24%)	1±1 (22±22%)	0±0 (7±13%)	2	18
All	All	9420/21820 (43%)	8856 (94%)	545 (6%)	19 (0%)	50	82

All 13 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	130	PRO	4
2	E	292	GLY	3
1	A	29	PRO	2
1	C	124	PRO	1
1	C	53	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	B	124	PRO	1
1	D	52	ALA	1
1	D	53	ASP	1
2	E	290	TRP	1
1	D	26	PRO	1
1	A	124	PRO	1
1	C	29	PRO	1
1	B	130	PRO	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	94/132 (71%)	90±2 (96±2%)	4±2 (4±2%)	35 83
1	B	104/132 (79%)	101±2 (97±2%)	3±2 (3±2%)	44 89
1	C	99/132 (75%)	94±2 (95±2%)	5±2 (5±2%)	26 75
1	D	107/132 (81%)	103±1 (96±1%)	4±1 (4±1%)	36 84
2	E	2/359 (1%)	2±0 (82±24%)	0±0 (18±24%)	4 39
All	All	8120/17740 (46%)	7791 (96%)	329 (4%)	34 82

All 104 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	C	117	MET	20
1	D	70	GLU	15
1	C	34	LYS	10
1	C	68	LEU	9
1	B	70	GLU	8
1	C	112	GLU	8
1	C	15	ARG	8
1	D	16	ILE	7
1	D	51	LEU	7
1	D	89	ILE	7
1	D	56	TYR	7

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Mol	Chain	Res	Type	Models (Total)
1	C	37	GLN	6
1	D	86	ILE	6
1	A	128	LEU	6
1	D	90	GLU	6
1	C	128	LEU	5
1	B	93	GLN	5
2	E	291	LEU	5
1	A	68	LEU	5
1	A	74	PHE	4
1	B	127	ASN	4
1	B	39	GLU	4
1	B	90	GLU	4
1	C	41	LYS	4
1	B	86	ILE	4
1	C	125	GLN	4
1	A	39	GLU	3
1	A	37	GLN	3
1	A	122	THR	3
1	B	126	LEU	3
1	A	42	LEU	3
1	A	126	LEU	3
1	C	104	ASN	3
1	D	42	LEU	3
1	B	37	GLN	3
1	B	125	GLN	3
1	D	93	GLN	3
1	A	14	GLN	3
1	C	54	ASP	3
1	D	17	TYR	2
1	A	61	ARG	2
1	B	44	LEU	2
1	C	56	TYR	2
1	C	60	LEU	2
1	C	132	ASN	2
1	A	34	LYS	2
1	A	98	LEU	2
1	B	42	LEU	2
1	B	12	GLN	2
1	C	31	VAL	2
1	A	27	ASN	2
1	D	39	GLU	2
1	D	54	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	D	134	ASP	2
1	A	70	GLU	2
1	B	117	MET	2
1	C	86	ILE	2
1	B	84	PHE	2
1	C	36	TRP	2
1	D	60	LEU	2
1	C	70	GLU	2
1	A	54	ASP	2
1	D	104	ASN	2
1	C	77	GLU	2
1	A	44	LEU	2
1	A	131	VAL	2
2	E	290	TRP	2
1	B	89	ILE	1
1	B	11	PHE	1
1	B	104	ASN	1
1	C	33	GLN	1
1	C	57	GLU	1
1	C	98	LEU	1
1	B	94	MET	1
1	B	98	LEU	1
1	C	42	LEU	1
1	B	41	LYS	1
1	D	33	GLN	1
1	C	101	TYR	1
1	A	41	LYS	1
1	B	45	ASP	1
1	B	101	TYR	1
1	A	24	GLU	1
1	A	117	MET	1
1	B	128	LEU	1
1	C	127	ASN	1
1	D	98	LEU	1
1	C	43	ASP	1
1	D	94	MET	1
1	B	112	GLU	1
1	D	12	GLN	1
1	D	43	ASP	1
1	A	56	TYR	1
1	B	13	ILE	1
1	B	30	HIS	1

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Mol	Chain	Res	Type	Models (Total)
1	C	14	GLN	1
1	B	29	PRO	1
1	B	113	CYS	1
1	D	44	LEU	1
1	A	40	VAL	1
1	A	127	ASN	1
1	D	11	PHE	1
1	D	41	LYS	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 13% for the well-defined parts and 23% 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 (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

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	139	0.25 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	128	0.85 ± 0.17	Should be checked
$^{13}C'$	137	0.29 ± 0.10	None needed (< 0.5 ppm)
^{15}N	133	-1.15 ± 0.27	Should be applied

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 12%, i.e. 777 atoms were assigned a chemical shift out of a possible 6330. 0 out of 81 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	396/2324 (17%)	97/939 (10%)	202/942 (21%)	97/443 (22%)
Sidechain	329/3464 (9%)	183/2268 (8%)	146/1087 (13%)	0/109 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	52/542 (10%)	26/263 (10%)	25/262 (10%)	1/17 (6%)
Overall	777/6330 (12%)	306/3470 (9%)	373/2291 (16%)	98/569 (17%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 7%, i.e. 1049 atoms were assigned a chemical shift out of a possible 14183. 0 out of 156 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	542/5434 (10%)	133/2212 (6%)	276/2182 (13%)	133/1040 (13%)
Sidechain	430/7760 (6%)	237/5059 (5%)	193/2442 (8%)	0/259 (0%)
Aromatic	77/989 (8%)	39/479 (8%)	37/459 (8%)	1/51 (2%)
Overall	1049/14183 (7%)	409/7750 (5%)	506/5083 (10%)	134/1350 (10%)

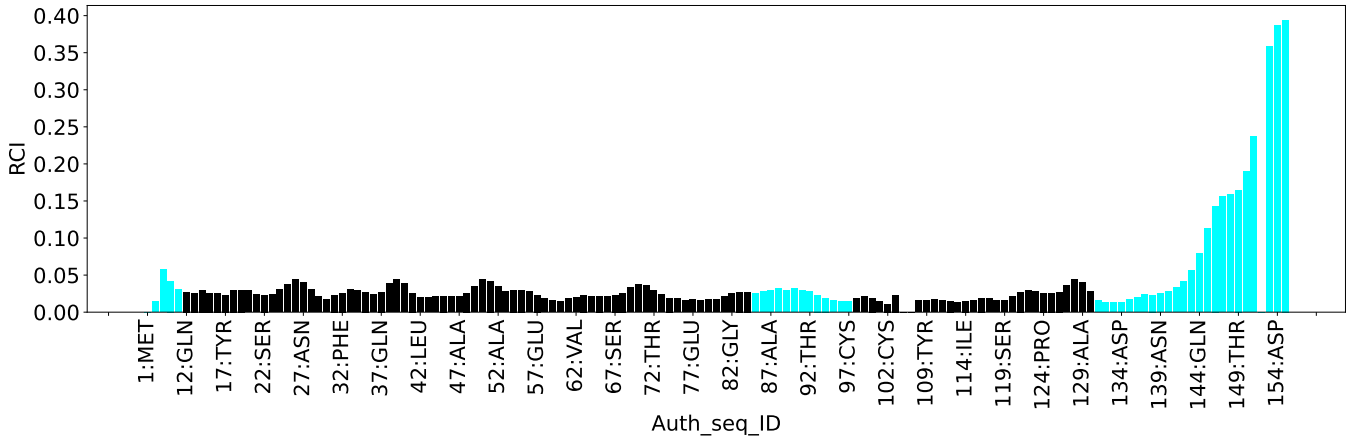
7.1.4 Statistically unusual chemical shifts (i)

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 (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

7.2.2 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 ± 0.06	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	126	0.79 ± 0.20	Should be checked
$^{13}C'$	135	0.26 ± 0.08	None needed (< 0.5 ppm)
^{15}N	132	-1.09 ± 0.25	Should be applied

7.2.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 12%, i.e. 774 atoms were assigned a chemical shift out of a possible 6330. 0 out of 81 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	393/2324 (17%)	96/939 (10%)	201/942 (21%)	96/443 (22%)
Sidechain	329/3464 (9%)	183/2268 (8%)	146/1087 (13%)	0/109 (0%)
Aromatic	52/542 (10%)	26/263 (10%)	25/262 (10%)	1/17 (6%)
Overall	774/6330 (12%)	305/3470 (9%)	372/2291 (16%)	97/569 (17%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 7%, i.e. 1044 atoms were assigned a chemical shift out of a possible 14183. 0 out of 156 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	539/5434 (10%)	132/2212 (6%)	275/2182 (13%)	132/1040 (13%)
Sidechain	428/7760 (6%)	237/5059 (5%)	191/2442 (8%)	0/259 (0%)
Aromatic	77/989 (8%)	39/479 (8%)	37/459 (8%)	1/51 (2%)
Overall	1044/14183 (7%)	408/7750 (5%)	503/5083 (10%)	133/1350 (10%)

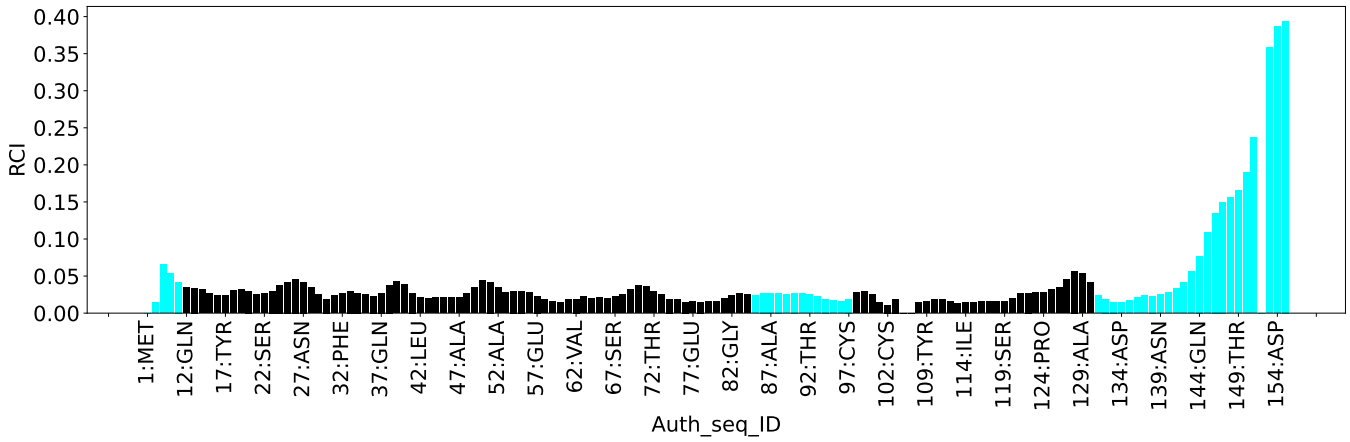
7.2.4 Statistically unusual chemical shifts (i)

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 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	126	0.77 ± 0.14	Should be checked
$^{13}C'$	135	0.26 ± 0.11	None needed (< 0.5 ppm)
^{15}N	132	-1.09 ± 0.28	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 12%, i.e. 774 atoms were assigned a chemical shift out of a possible 6330. 0 out of 81 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	393/2324 (17%)	96/939 (10%)	201/942 (21%)	96/443 (22%)
Sidechain	329/3464 (9%)	183/2268 (8%)	146/1087 (13%)	0/109 (0%)
Aromatic	52/542 (10%)	26/263 (10%)	25/262 (10%)	1/17 (6%)
Overall	774/6330 (12%)	305/3470 (9%)	372/2291 (16%)	97/569 (17%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 7%, i.e. 1044 atoms were assigned a chemical shift out of a possible 14183. 0 out of 156 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	539/5434 (10%)	132/2212 (6%)	275/2182 (13%)	132/1040 (13%)
Sidechain	428/7760 (6%)	237/5059 (5%)	191/2442 (8%)	0/259 (0%)
Aromatic	77/989 (8%)	39/479 (8%)	37/459 (8%)	1/51 (2%)
Overall	1044/14183 (7%)	408/7750 (5%)	503/5083 (10%)	133/1350 (10%)

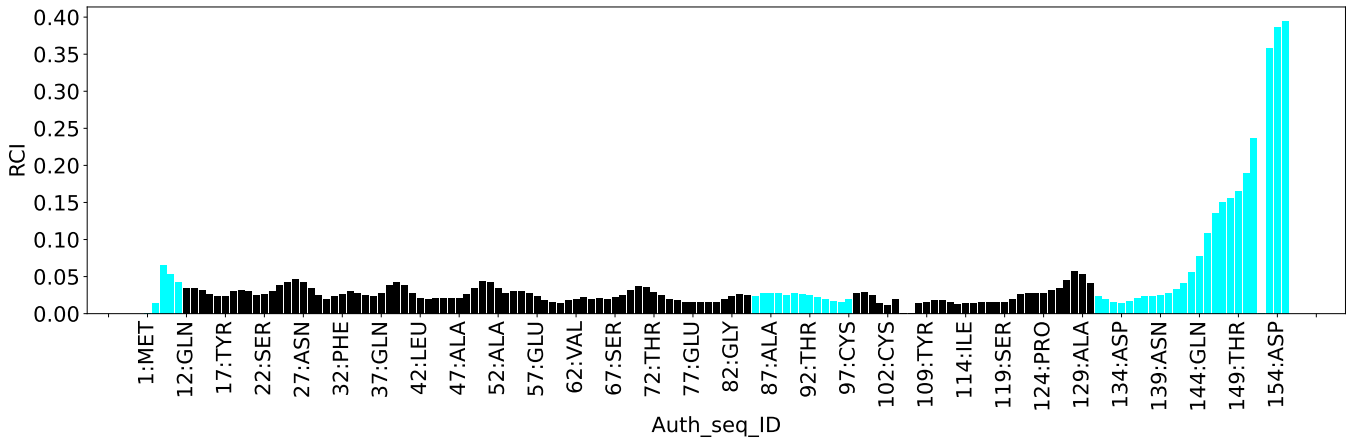
7.3.4 Statistically unusual chemical shifts (i)

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 ± 0.17	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	128	0.84 ± 0.11	Should be checked
$^{13}C'$	137	0.29 ± 0.17	None needed (< 0.5 ppm)
^{15}N	133	-1.15 ± 0.13	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 12%, i.e. 777 atoms were assigned a chemical shift out of a possible 6330. 0 out of 81 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	396/2324 (17%)	97/939 (10%)	202/942 (21%)	97/443 (22%)
Sidechain	329/3464 (9%)	183/2268 (8%)	146/1087 (13%)	0/109 (0%)
Aromatic	52/542 (10%)	26/263 (10%)	25/262 (10%)	1/17 (6%)
Overall	777/6330 (12%)	306/3470 (9%)	373/2291 (16%)	98/569 (17%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 7%, i.e. 1049 atoms were assigned a chemical shift out of a possible 14183. 0 out of 156 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	542/5434 (10%)	133/2212 (6%)	276/2182 (13%)	133/1040 (13%)
Sidechain	430/7760 (6%)	237/5059 (5%)	193/2442 (8%)	0/259 (0%)
Aromatic	77/989 (8%)	39/479 (8%)	37/459 (8%)	1/51 (2%)
Overall	1049/14183 (7%)	409/7750 (5%)	506/5083 (10%)	134/1350 (10%)

7.4.4 Statistically unusual chemical shifts (i)

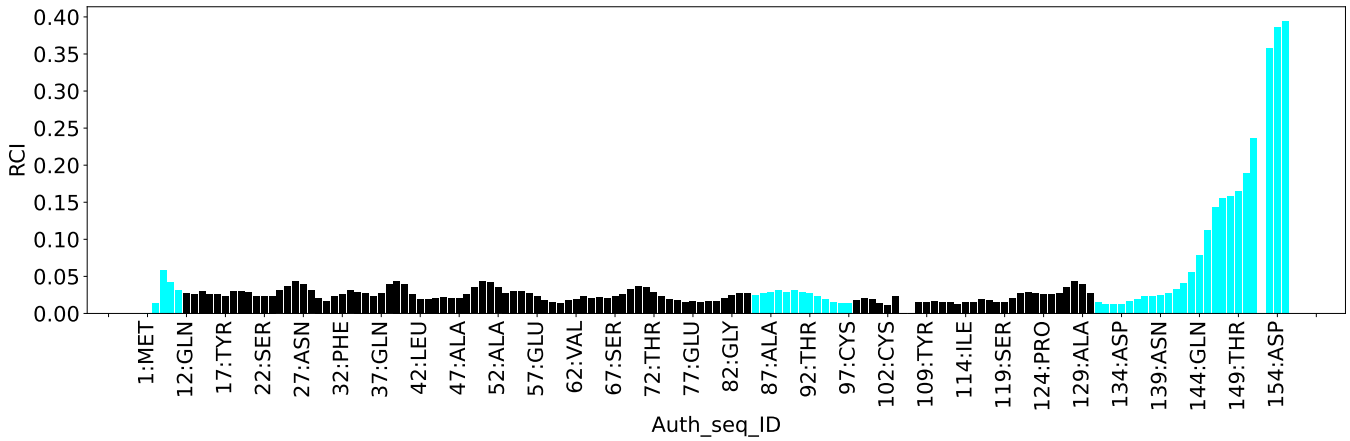
There are no statistically unusual chemical shifts.

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_list_5*

7.5.1 Bookkeeping (i)

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

Total number of shifts	2230
Number of shifts mapped to atoms	2230
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 (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	395	-0.41 ± 0.04	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	363	0.38 ± 0.03	None needed (< 0.5 ppm)
$^{13}C'$	90	-0.55 ± 0.05	Should be applied

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Nucleus	# values	Correction ± precision, *ppm*	Suggested action
^{15}N	390	-0.79 ± 0.09	Should be applied

7.5.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 26 atoms were assigned a chemical shift out of a possible 6330. 0 out of 81 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	9/2324 (0%)	3/939 (0%)	3/942 (0%)	3/443 (1%)
Sidechain	10/3464 (0%)	6/2268 (0%)	4/1087 (0%)	0/109 (0%)
Aromatic	7/542 (1%)	6/263 (2%)	0/262 (0%)	1/17 (6%)
Overall	26/6330 (0%)	15/3470 (0%)	7/2291 (0%)	4/569 (1%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 16%, i.e. 2229 atoms were assigned a chemical shift out of a possible 14183. 0 out of 156 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1341/5434 (25%)	466/2212 (21%)	485/2182 (22%)	390/1040 (38%)
Sidechain	831/7760 (11%)	343/5059 (7%)	488/2442 (20%)	0/259 (0%)
Aromatic	57/989 (6%)	35/479 (7%)	20/459 (4%)	2/51 (4%)
Overall	2229/14183 (16%)	844/7750 (11%)	993/5083 (20%)	392/1350 (29%)

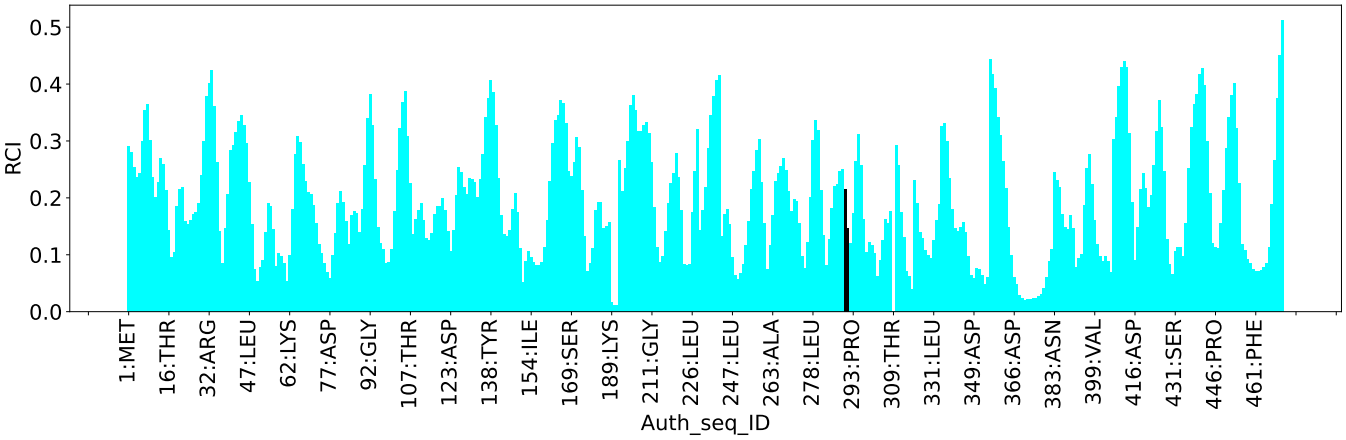
7.5.4 Statistically unusual chemical shifts (i)

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

Random coil index (RCI) for chain E:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
1:MET
16:THR
32:ARG
47:LEU
62:LYS
77:ASP
92:GLY
107:THR
123:ASP
138:TYR
154:ILE
169:SER
189:LYS
211:GLY
226:LEU
247:LEU
263:ALA
278:LEU
293:PRO
309:THR
331:LEU
349:ASP
366:ASP
383:ASN
399:VAL
416:ASP
431:SER
446:PRO
461:PHE
Auth_seq_ID