Full wwPDB NMR Structure Validation Report (i)

May 31, 2020 – 12:18 pm BST

PDB ID	:	6PSI
Title	:	Structural Basis for Client Recognition and Activity of Hsp40 Chaperones
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Deposited on	:	2019-07-12

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 following versions of software and data (see references (1)) were used in the production of this report:

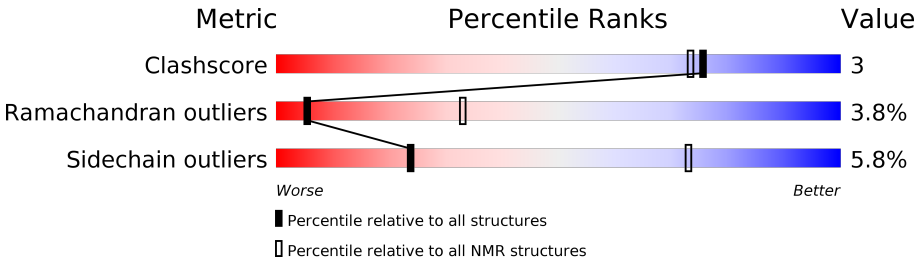
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 22%.

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	280	87% 10% •
1	C	280	86% 10% •
2	B	471	5% • 94%

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 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:4-A:108, A:115-A:280, B:1-B:11, B:179-B:185, B:238-B:245, C:3-C:105, C:116-C:280 (565)	1.61	4

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. No single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15729 atoms, of which 7873 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Chaperone protein DnaJ 2.

Mol	Chain	Residues	Atoms						Trace
1	A	280	Total	C	H	N	O	S	0
			4399	1398	2207	393	398	3	
1	C	280	Total	C	H	N	O	S	0
			4399	1398	2207	393	398	3	

- Molecule 2 is a protein called Alkaline phosphatase.

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

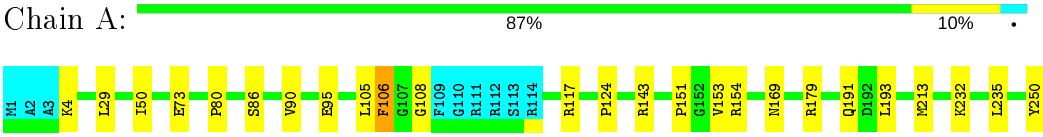
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

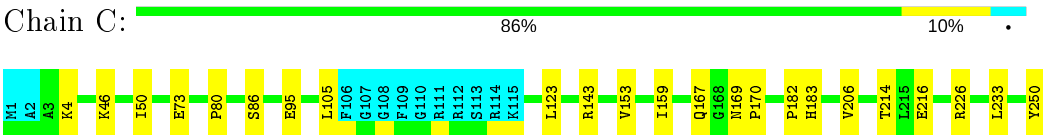
• Molecule 1: Chaperone protein DnaJ 2

Chain A:



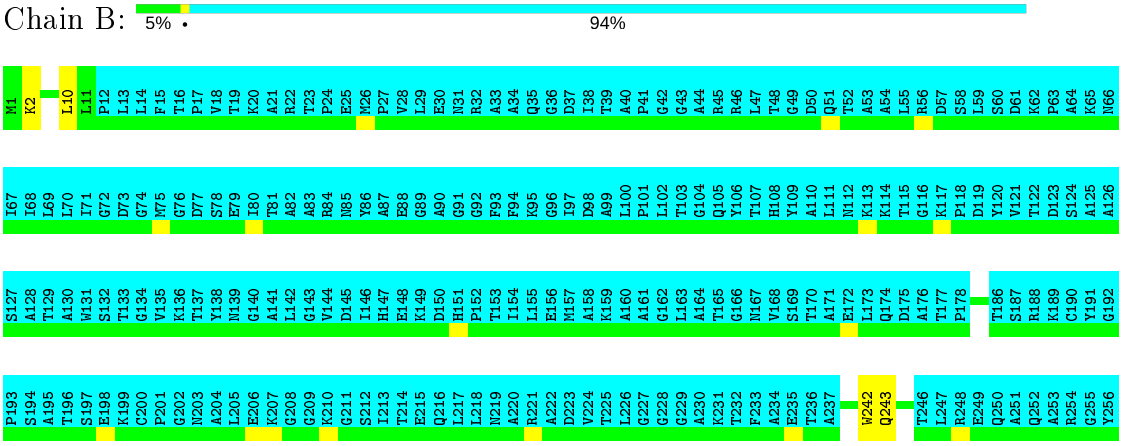
• Molecule 1: Chaperone protein DnaJ 2

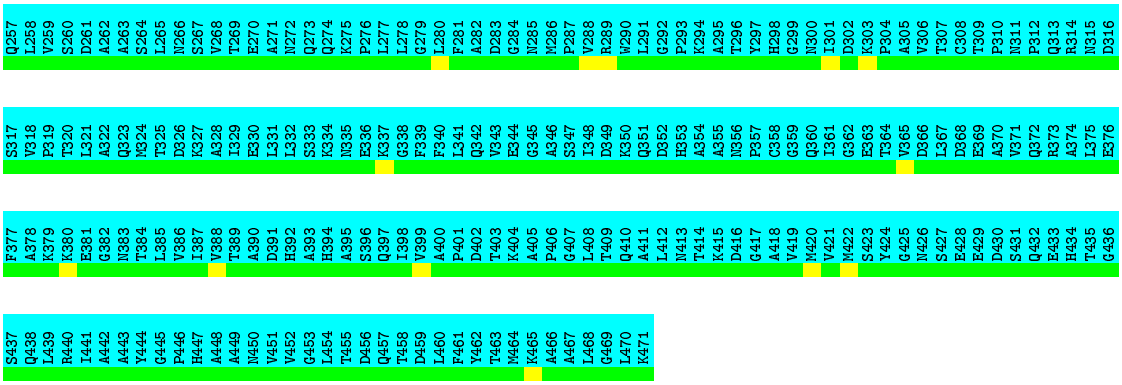
Chain C:



• Molecule 2: Alkaline phosphatase

Chain B:





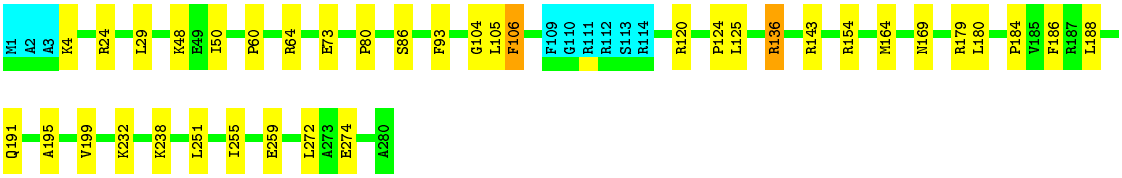
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

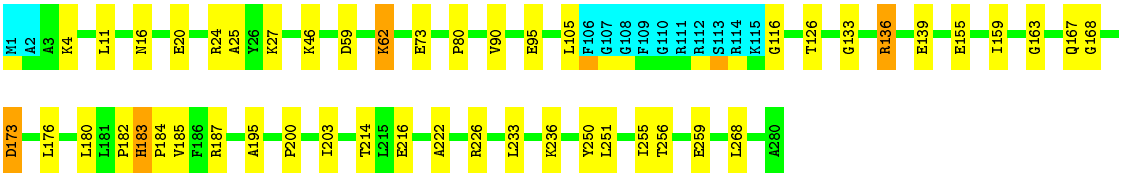
• Molecule 1: Chaperone protein DnaJ 2

Chain A:



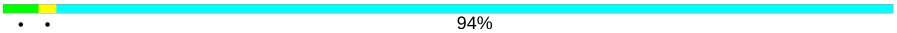
• Molecule 1: Chaperone protein DnaJ 2

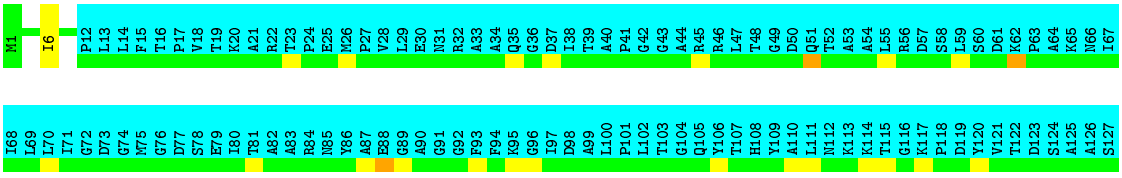
Chain C:

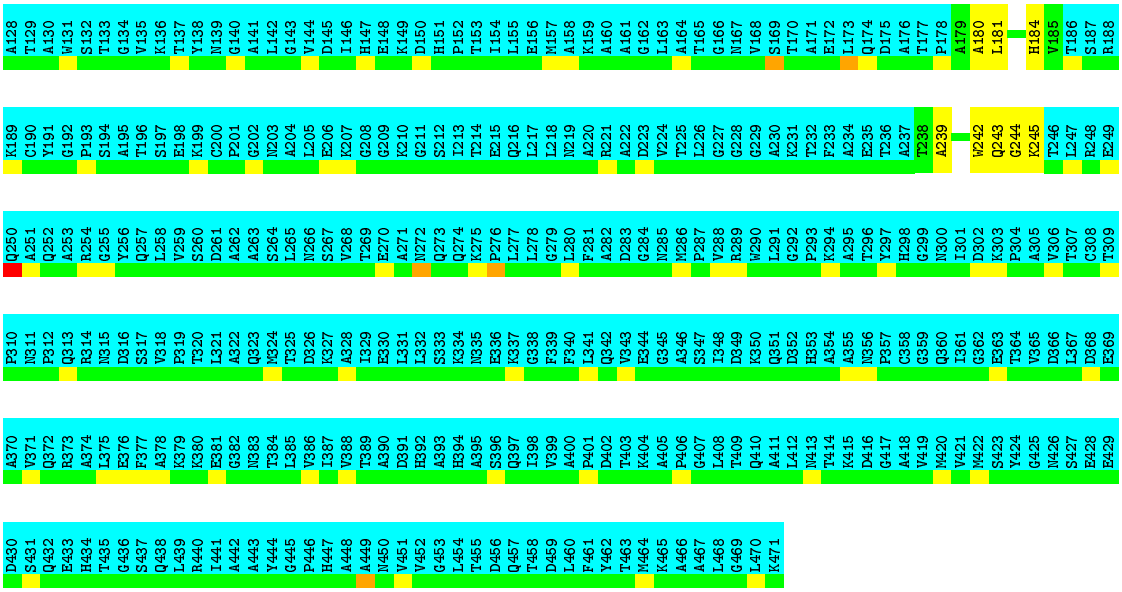


• Molecule 2: Alkaline phosphatase

Chain B:



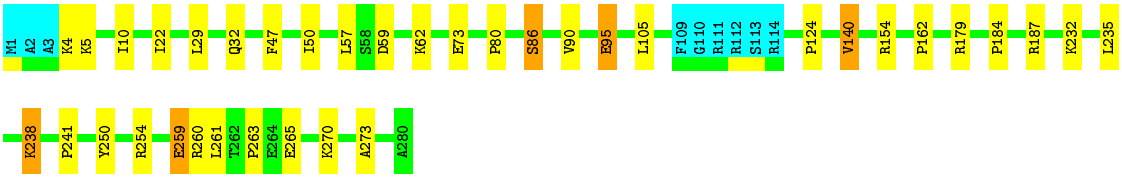




4.2.2 Score per residue for model 2

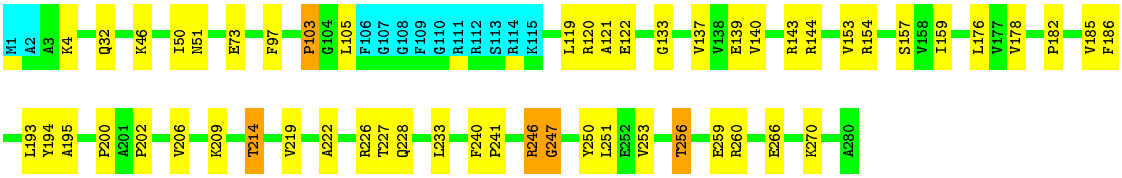
- Molecule 1: Chaperone protein DnaJ 2

Chain A:



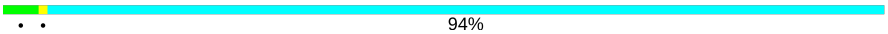
- Molecule 1: Chaperone protein DnaJ 2

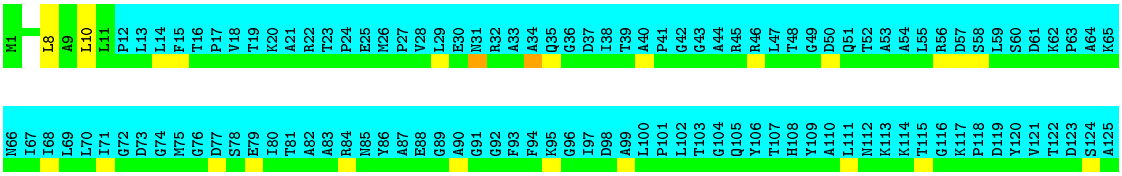
Chain C:

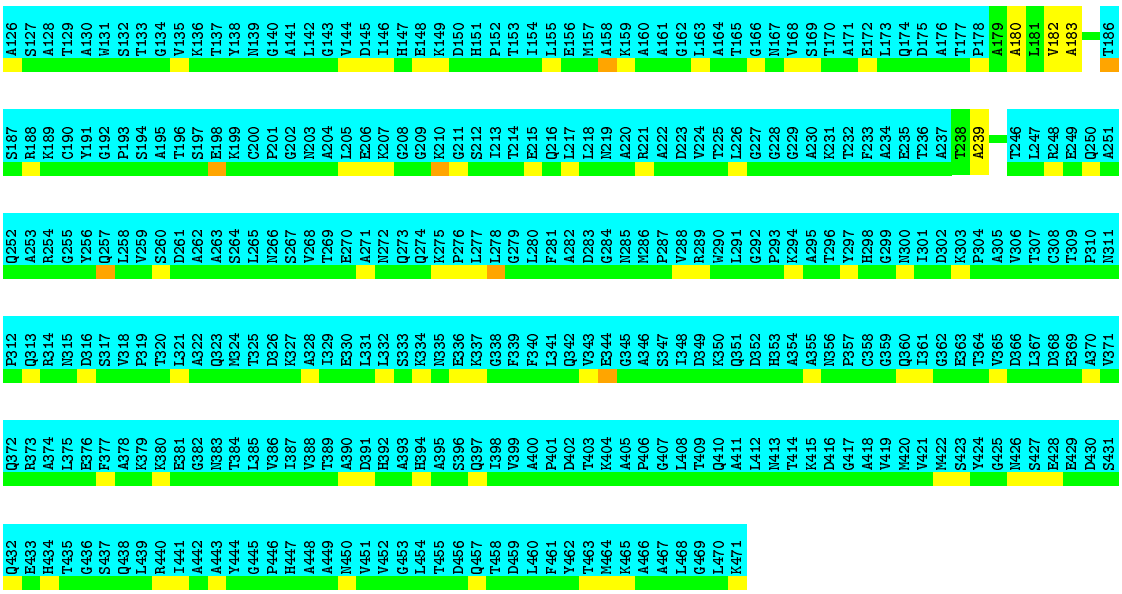


- Molecule 2: Alkaline phosphatase

Chain B:



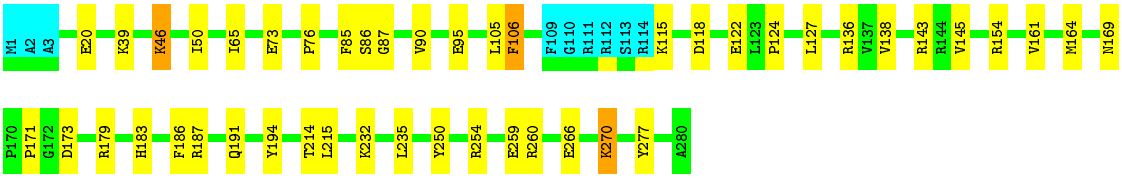




4.2.3 Score per residue for model 3

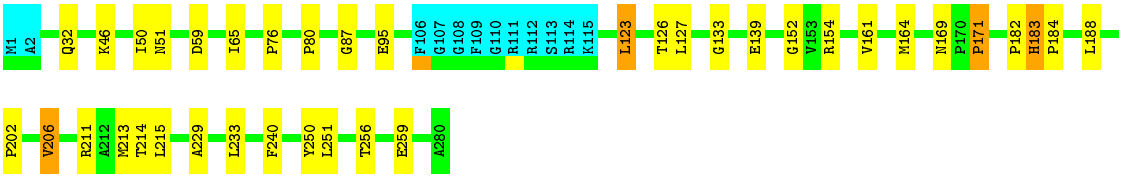
- Molecule 1: Chaperone protein DnaJ 2

Chain A:



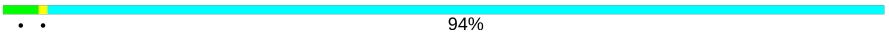
- Molecule 1: Chaperone protein DnaJ 2

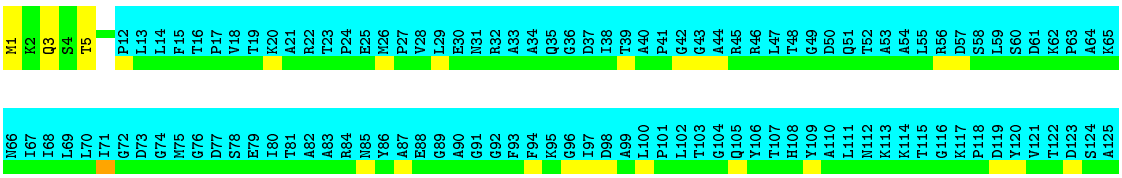
Chain C:

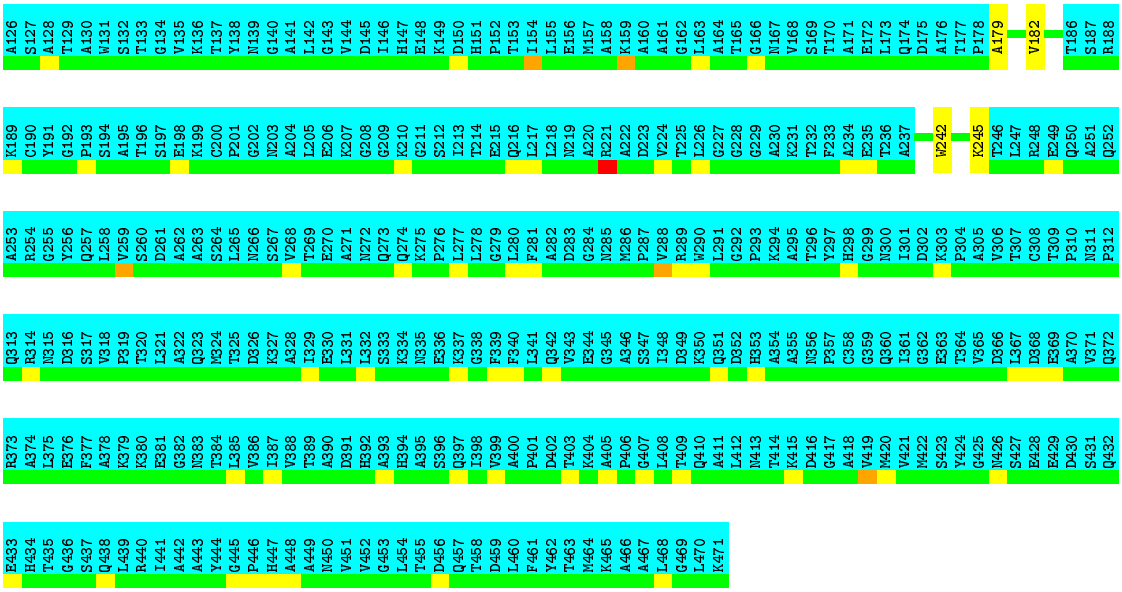


- Molecule 2: Alkaline phosphatase

Chain B:



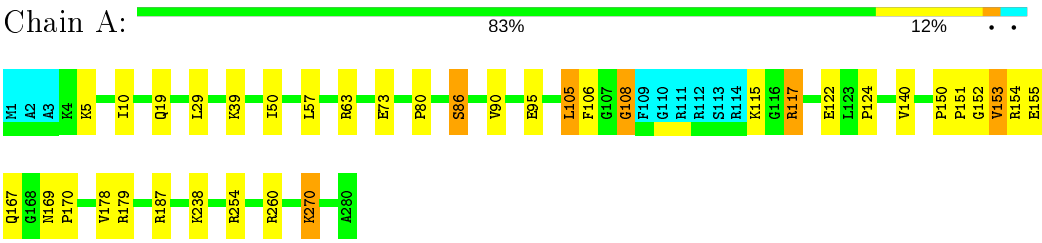




4.2.4 Score per residue for model 4 (medoid)

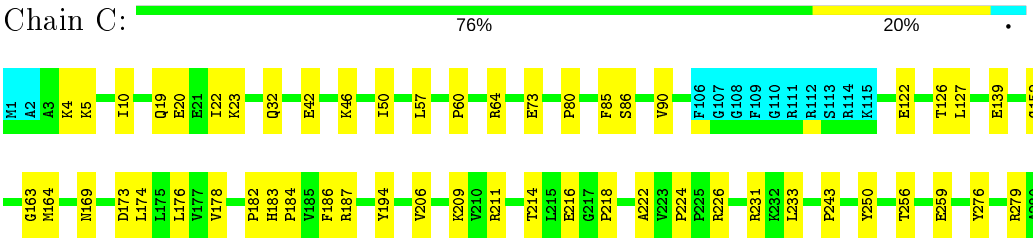
- Molecule 1: Chaperone protein DnaJ 2

Chain A:



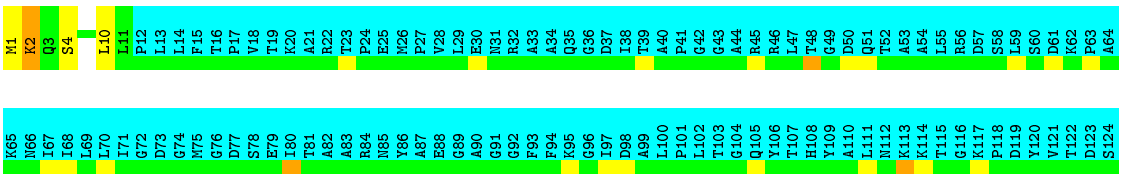
- Molecule 1: Chaperone protein DnaJ 2

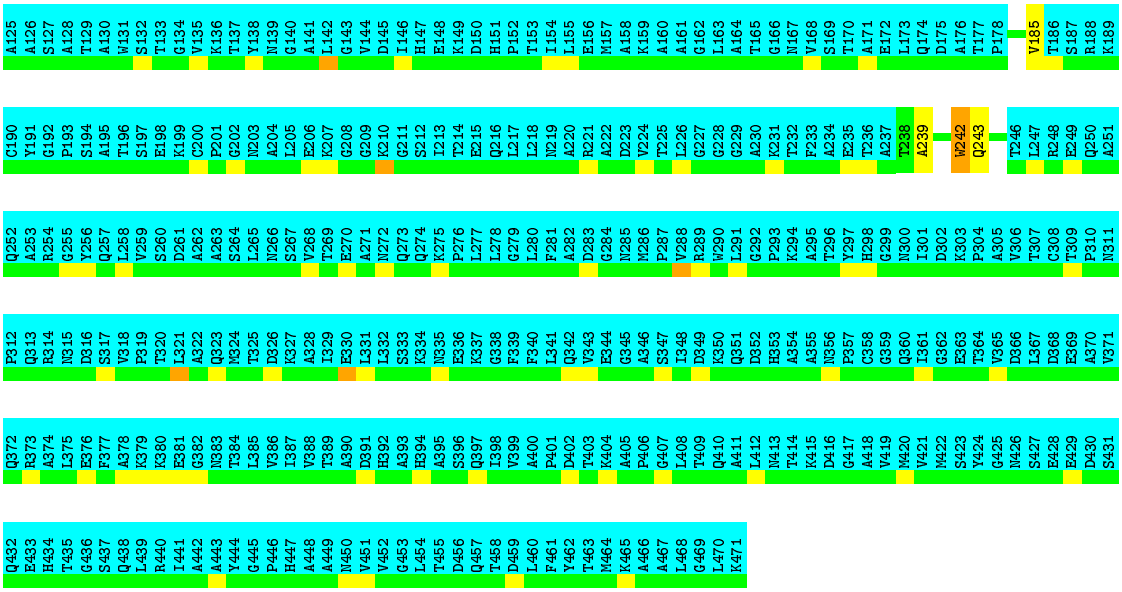
Chain C:



- Molecule 2: Alkaline phosphatase

Chain B:

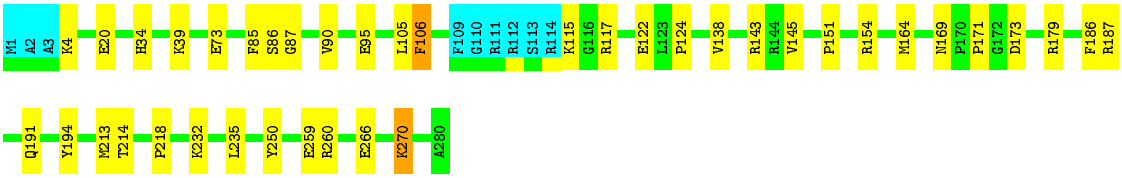




4.2.5 Score per residue for model 5

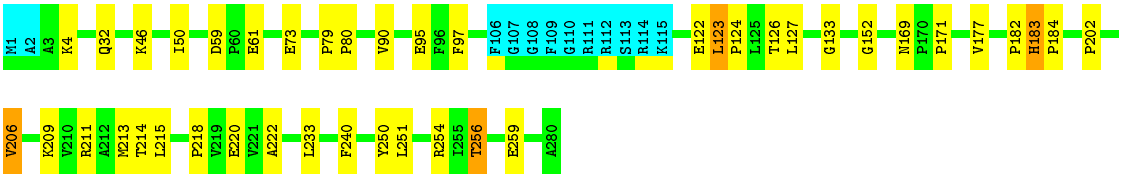
- Molecule 1: Chaperone protein DnaJ 2

Chain A:



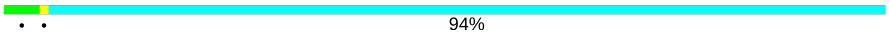
- Molecule 1: Chaperone protein DnaJ 2

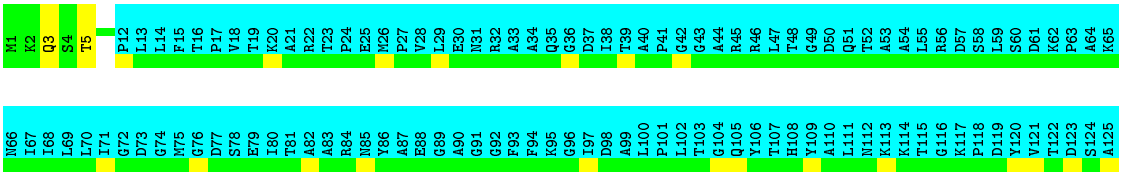
Chain C:

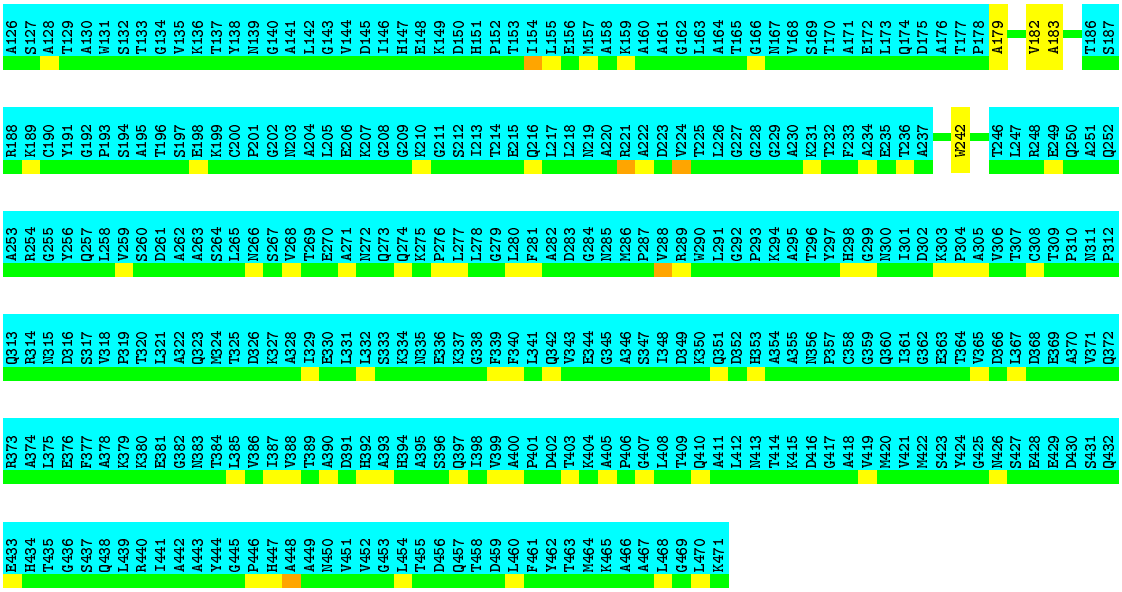


- Molecule 2: Alkaline phosphatase

Chain B:



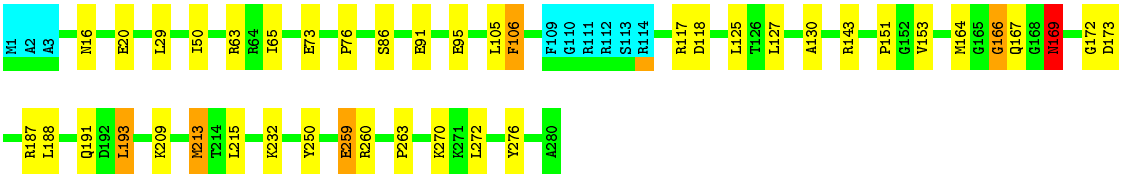




4.2.6 Score per residue for model 6

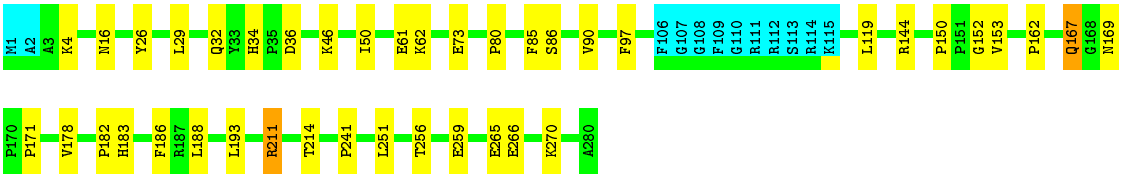
- Molecule 1: Chaperone protein DnaJ 2

Chain A:



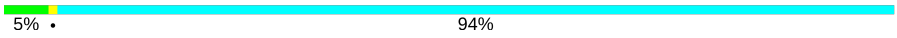
- Molecule 1: Chaperone protein DnaJ 2

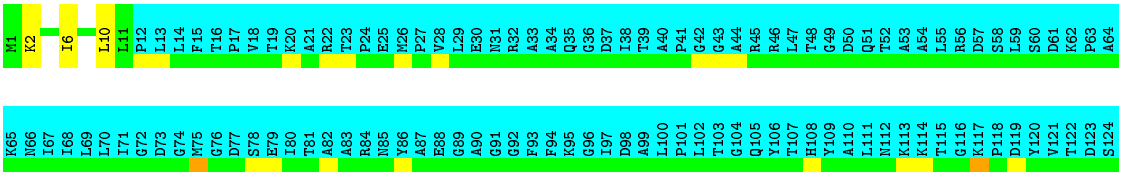
Chain C:

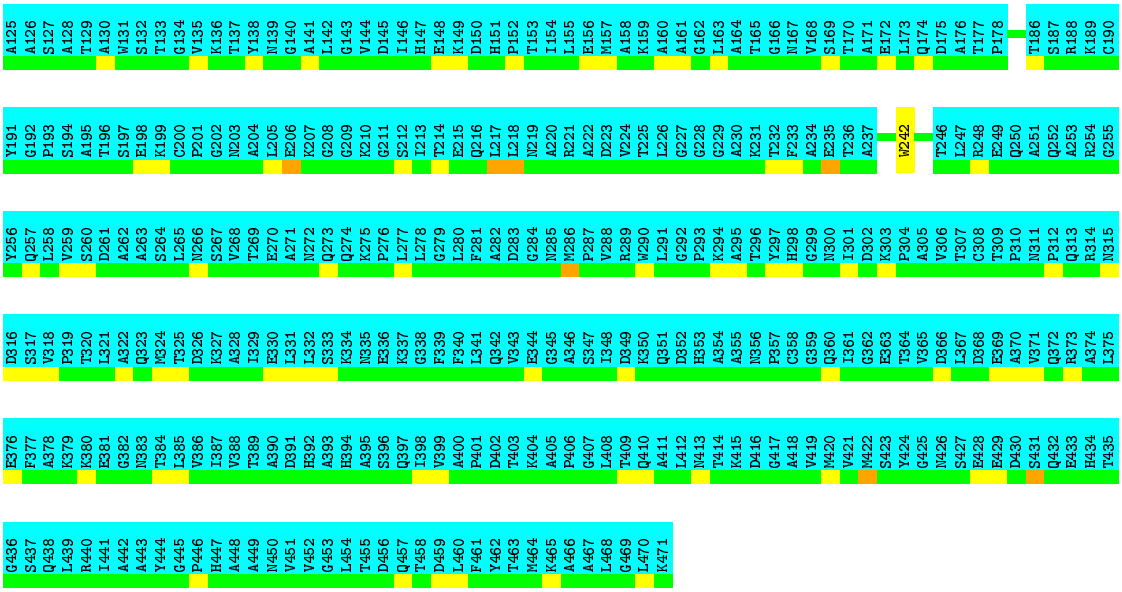


- Molecule 2: Alkaline phosphatase

Chain B:



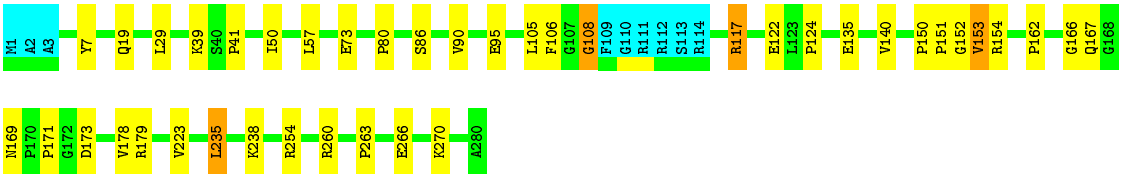




4.2.7 Score per residue for model 7

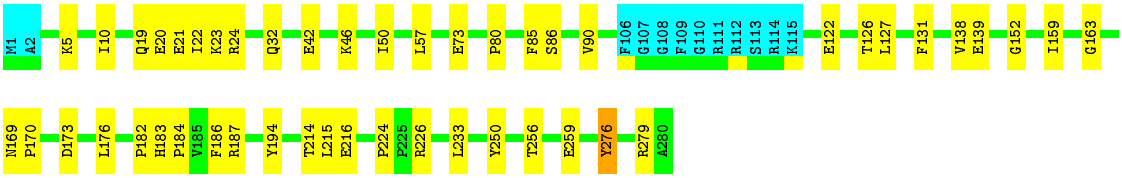
- Molecule 1: Chaperone protein DnaJ 2

Chain A:



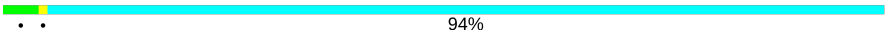
- Molecule 1: Chaperone protein DnaJ 2

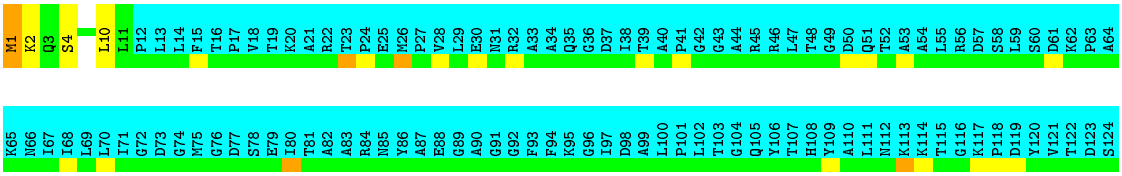
Chain C:

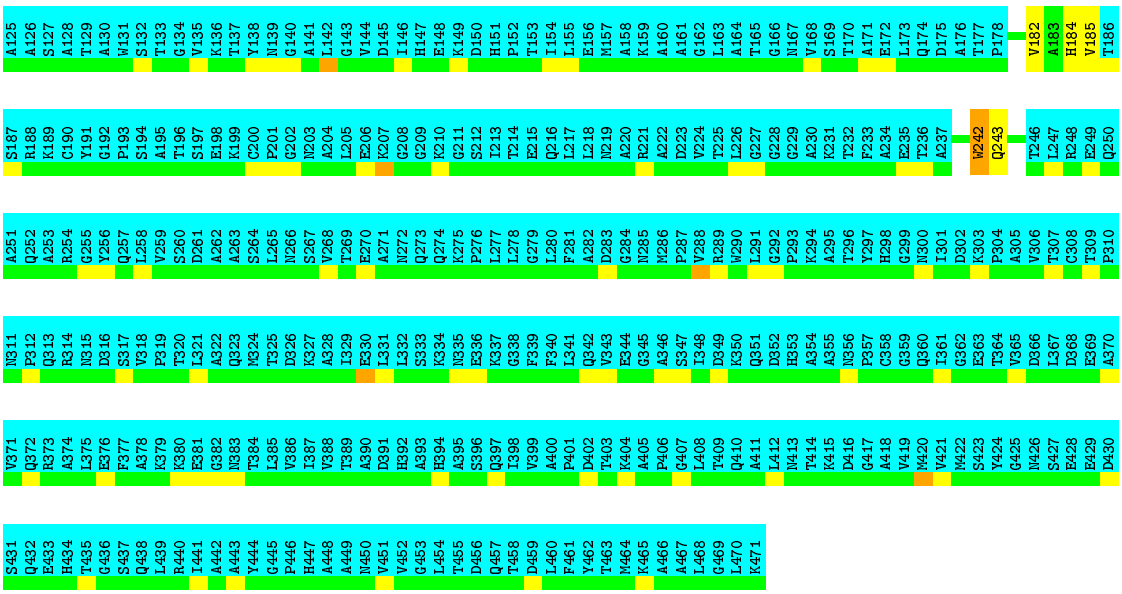


- Molecule 2: Alkaline phosphatase

Chain B:



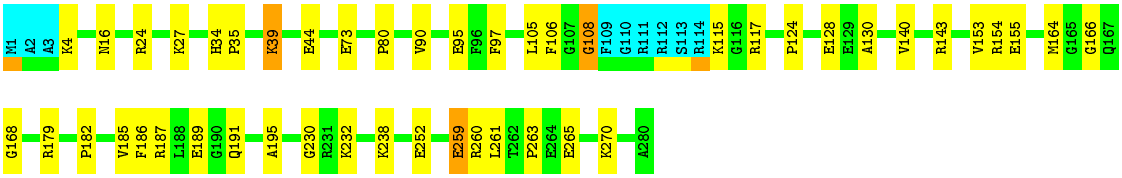




4.2.8 Score per residue for model 8

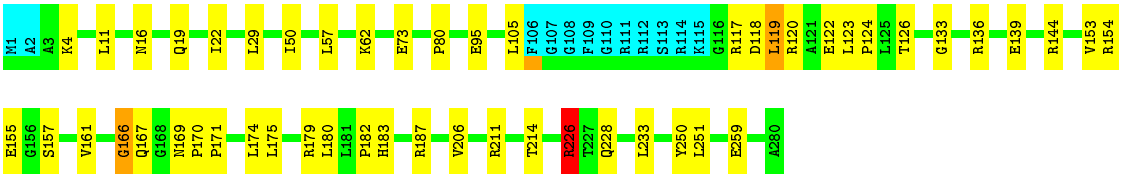
- Molecule 1: Chaperone protein DnaJ 2

Chain A:



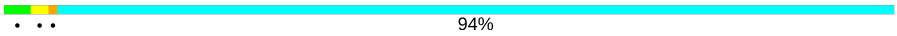
- Molecule 1: Chaperone protein DnaJ 2

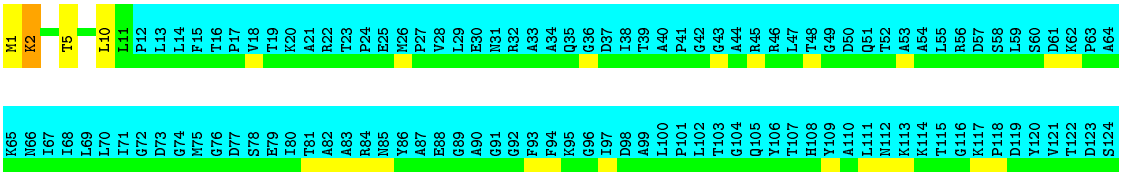
Chain C:

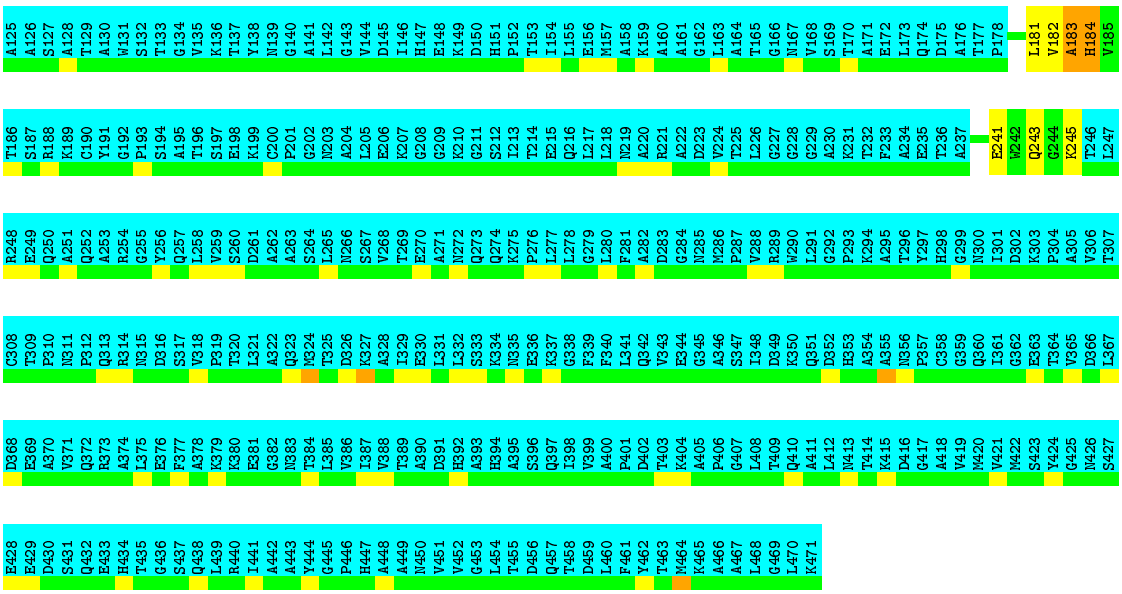


- Molecule 2: Alkaline phosphatase

Chain B:



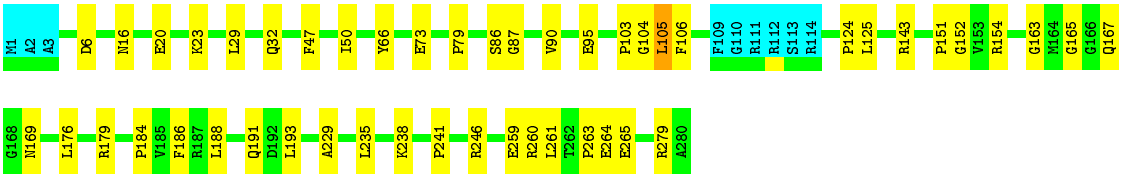




4.2.9 Score per residue for model 9

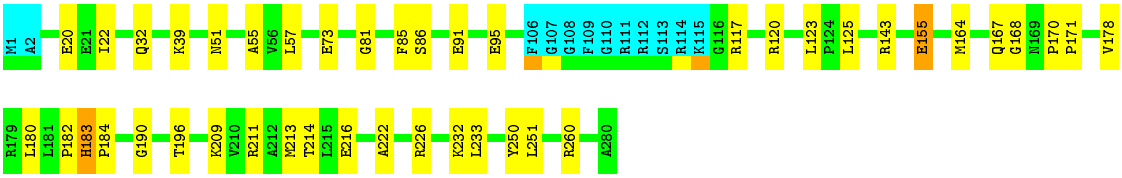
- Molecule 1: Chaperone protein DnaJ 2

Chain A:



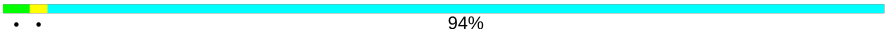
- Molecule 1: Chaperone protein DnaJ 2

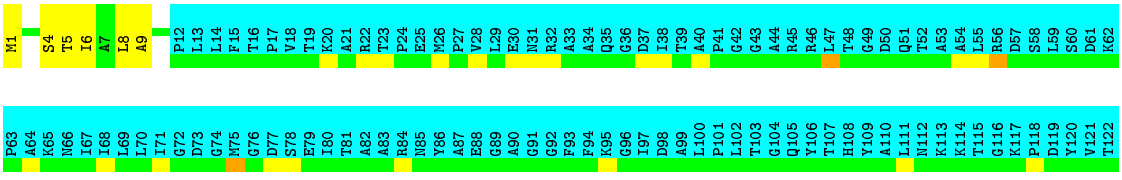
Chain C:

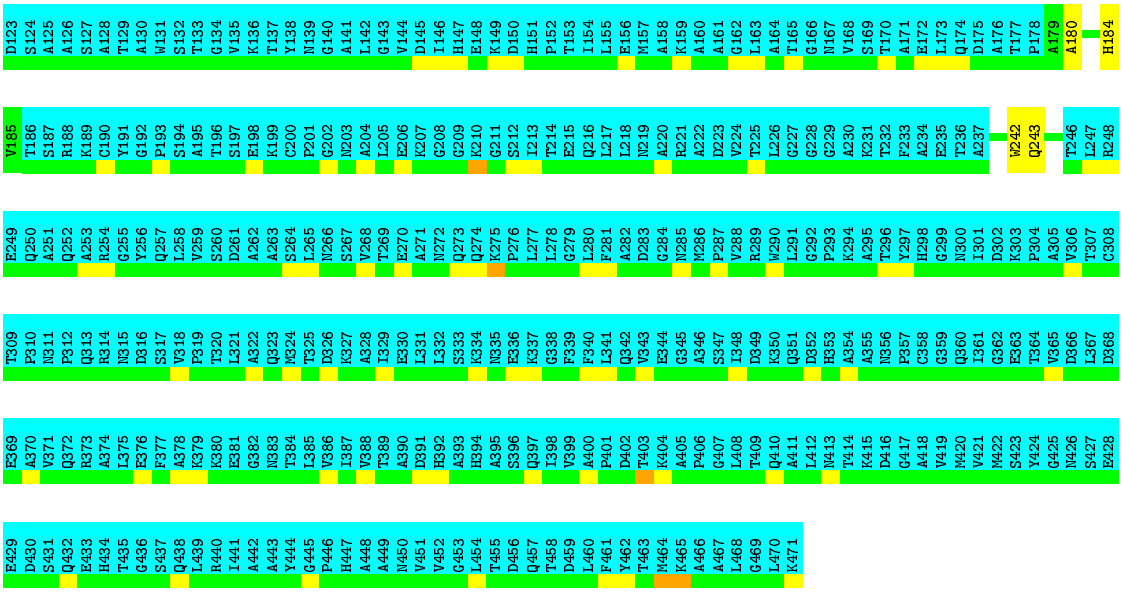


- Molecule 2: Alkaline phosphatase

Chain B:



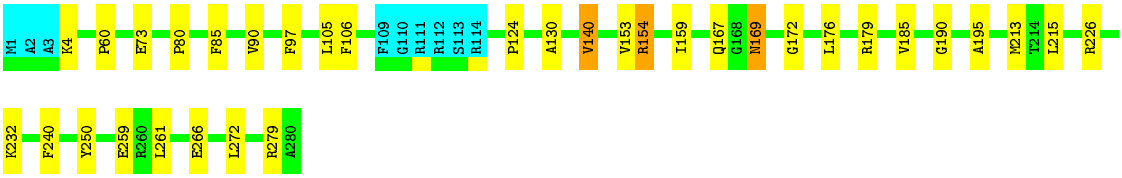




4.2.10 Score per residue for model 10

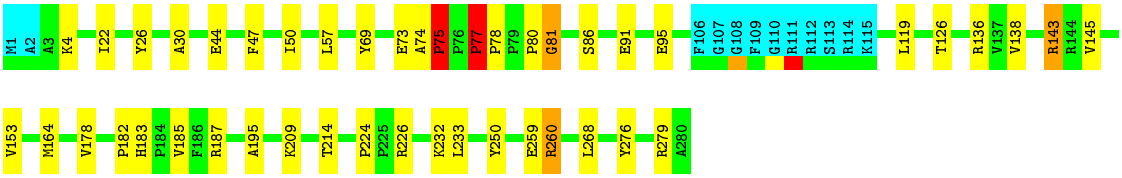
- Molecule 1: Chaperone protein DnaJ 2

Chain A:



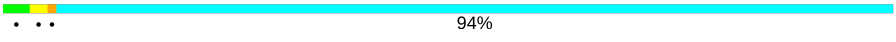
- Molecule 1: Chaperone protein DnaJ 2

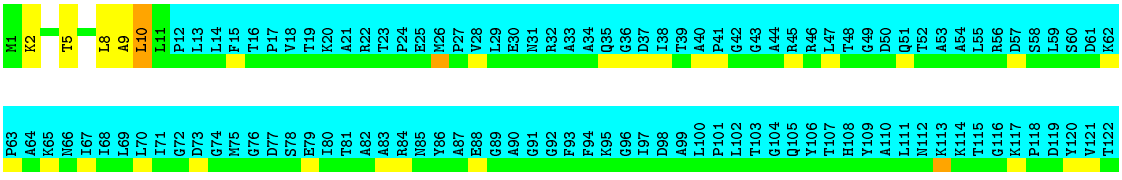
Chain C:

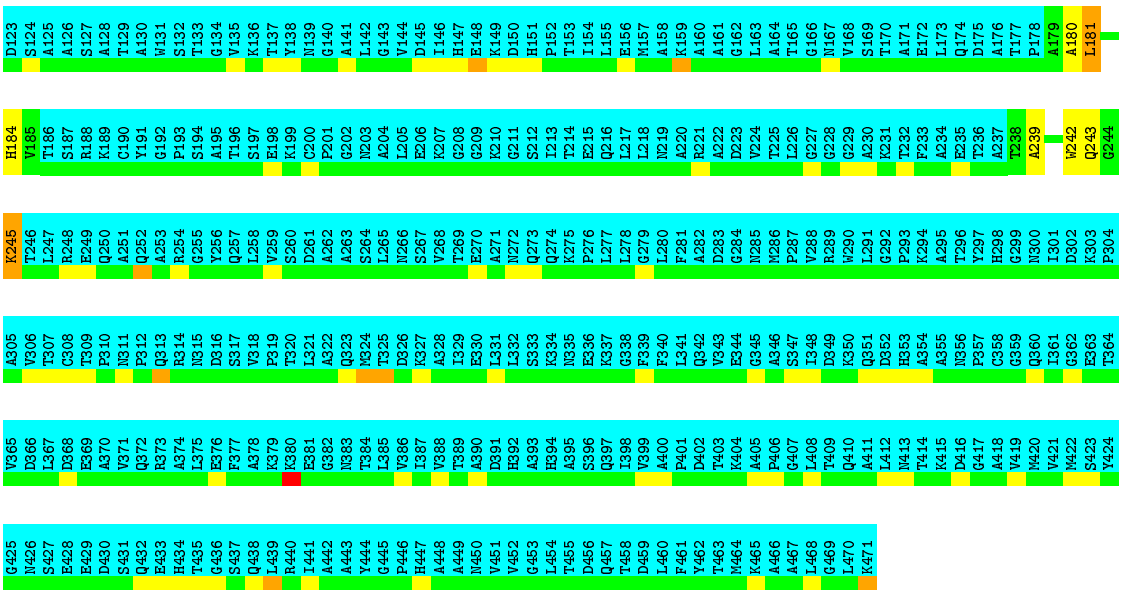


- Molecule 2: Alkaline phosphatase

Chain B:



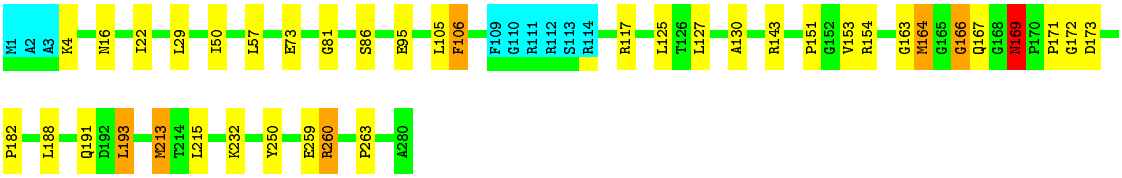




4.2.11 Score per residue for model 11

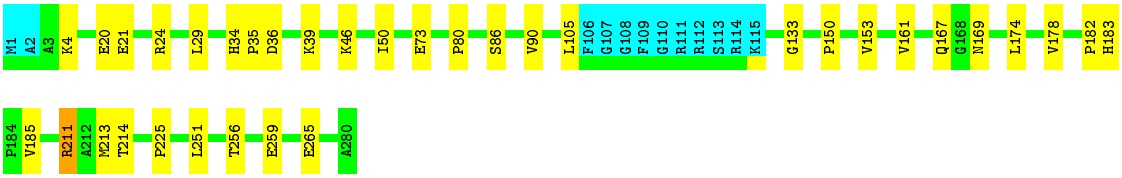
- Molecule 1: Chaperone protein DnaJ 2

Chain A:



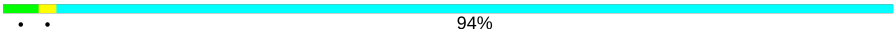
- Molecule 1: Chaperone protein DnaJ 2

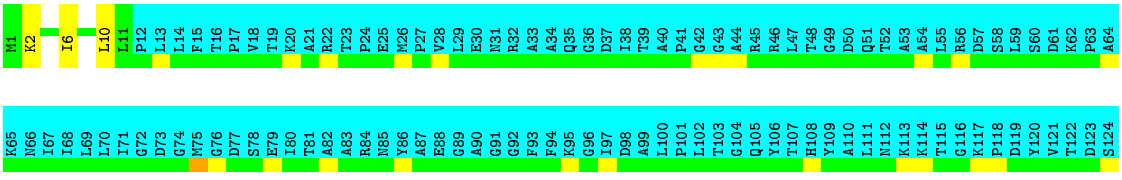
Chain C:

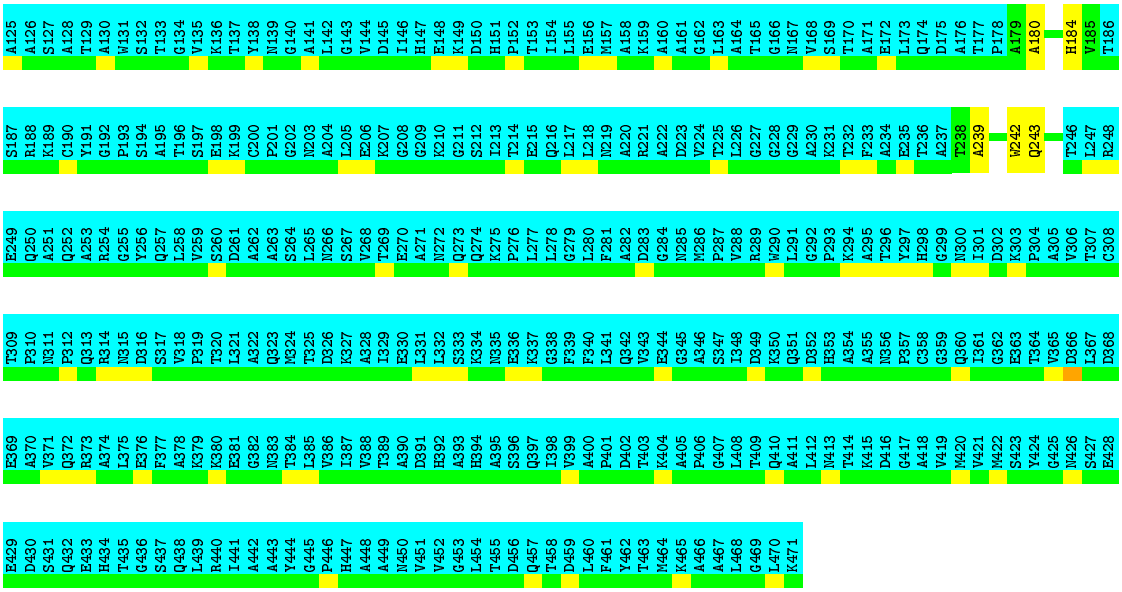


- Molecule 2: Alkaline phosphatase

Chain B:



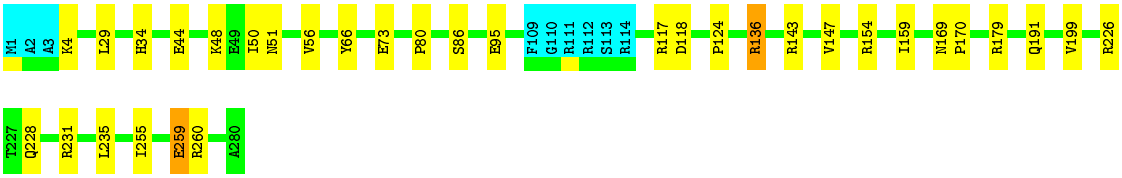




4.2.12 Score per residue for model 12

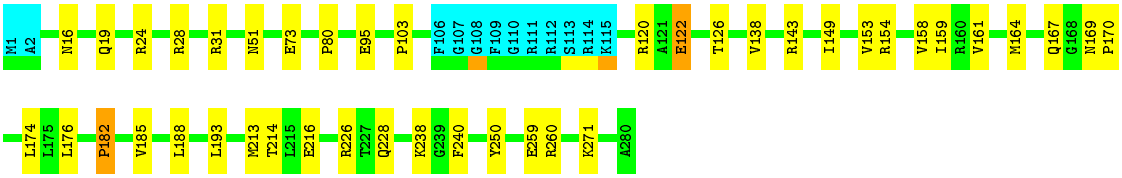
- Molecule 1: Chaperone protein DnaJ 2

Chain A:



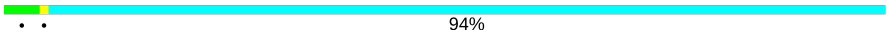
- Molecule 1: Chaperone protein DnaJ 2

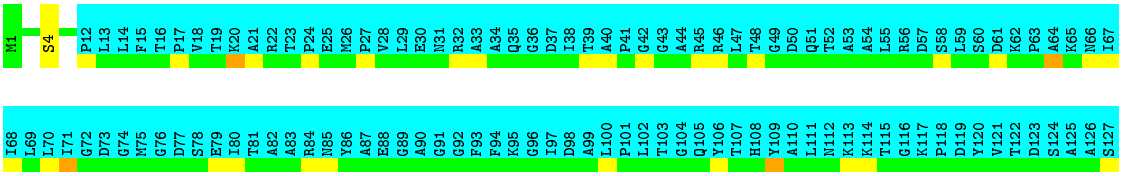
Chain C:

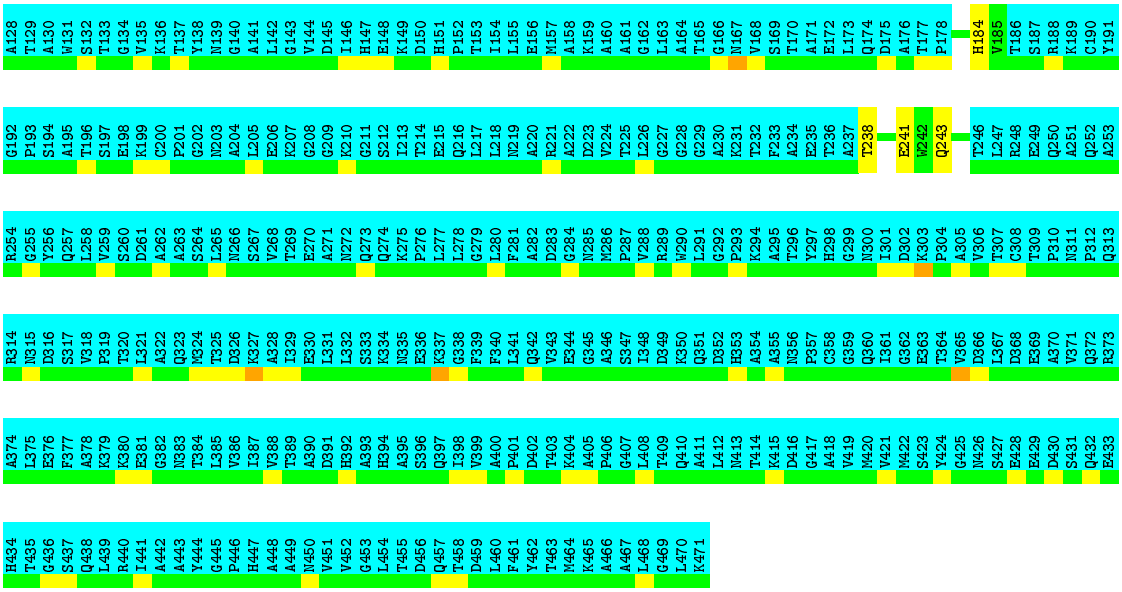


- Molecule 2: Alkaline phosphatase

Chain B:



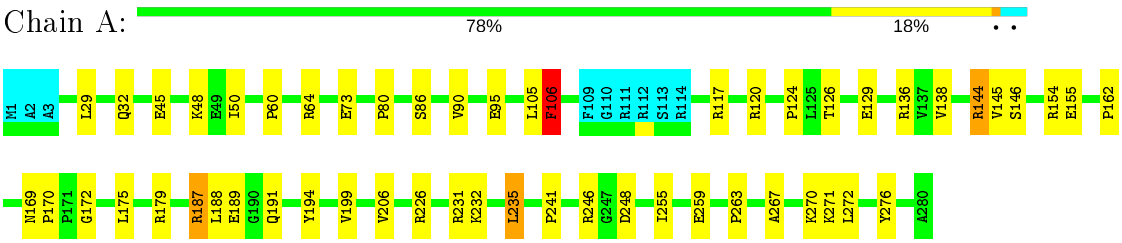




4.2.13 Score per residue for model 13

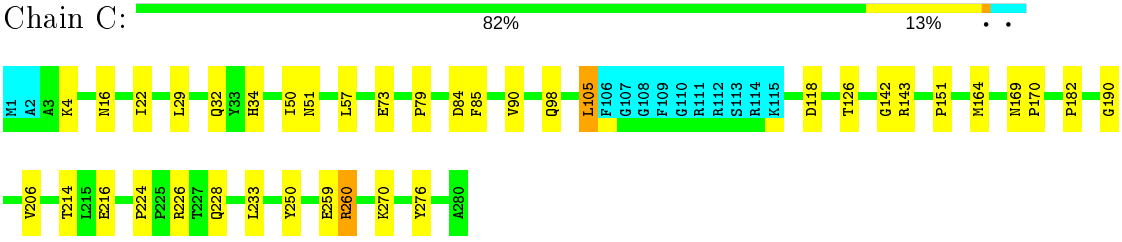
- Molecule 1: Chaperone protein DnaJ 2

Chain A:



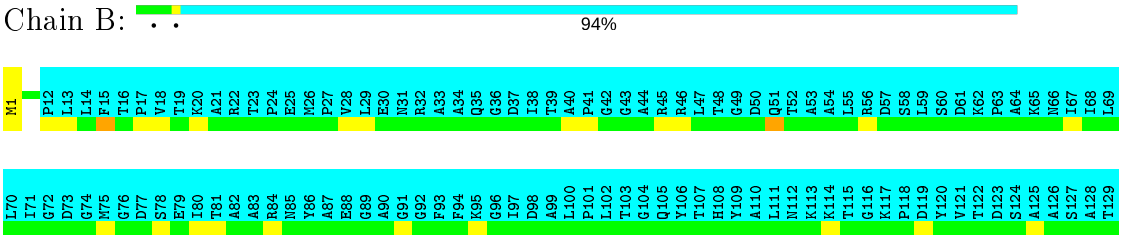
- Molecule 1: Chaperone protein DnaJ 2

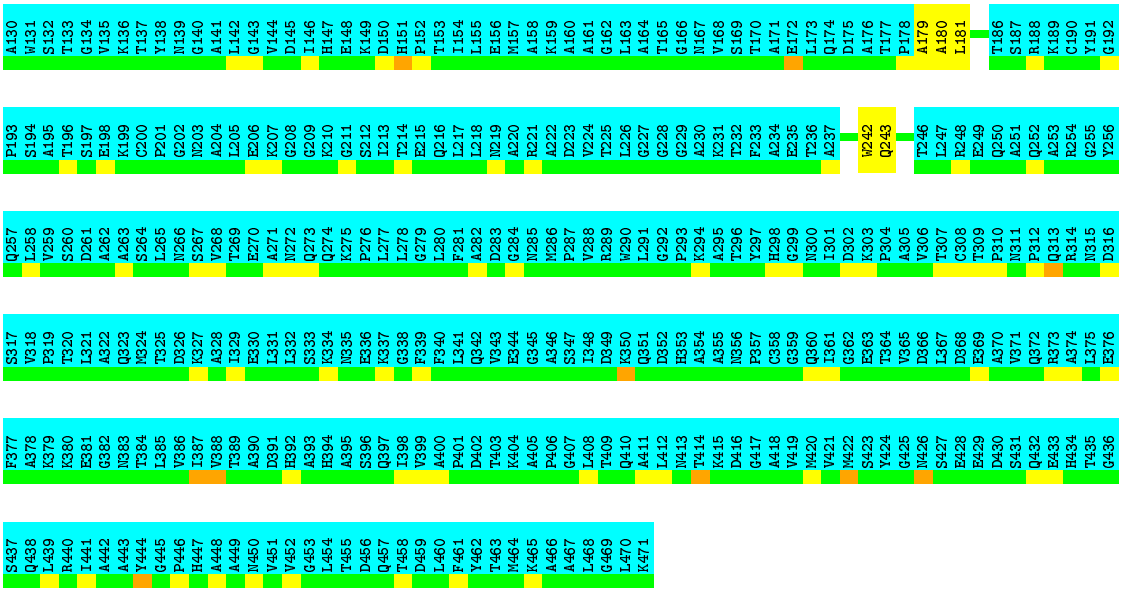
Chain C:



- Molecule 2: Alkaline phosphatase

Chain B:

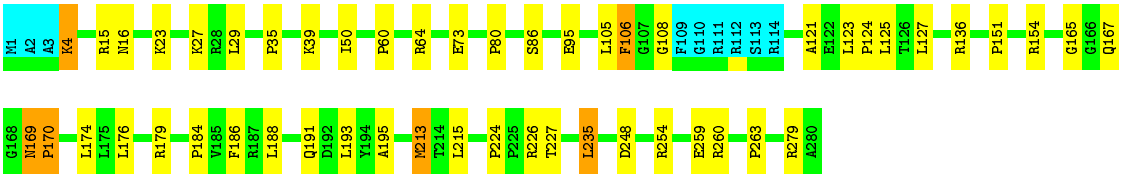




4.2.14 Score per residue for model 14

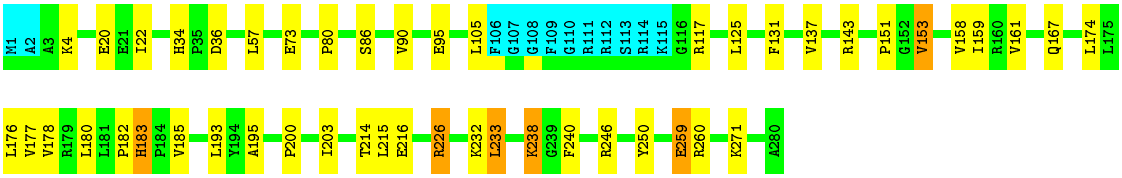
- Molecule 1: Chaperone protein DnaJ 2

Chain A:



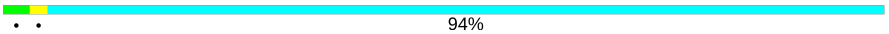
- Molecule 1: Chaperone protein DnaJ 2

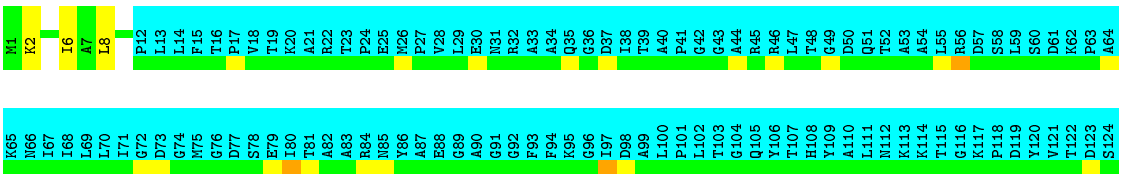
Chain C:

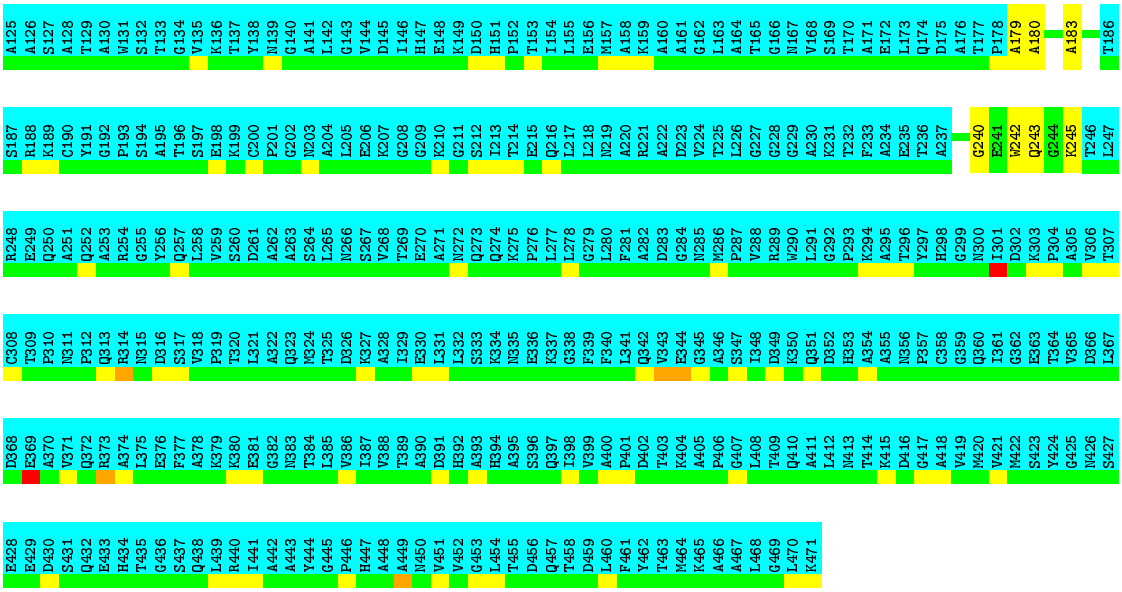


- Molecule 2: Alkaline phosphatase

Chain B:



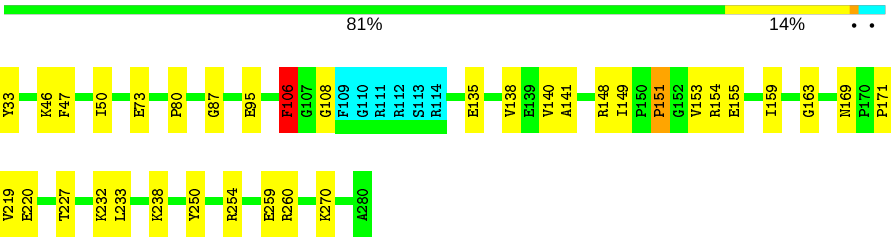




4.2.15 Score per residue for model 15

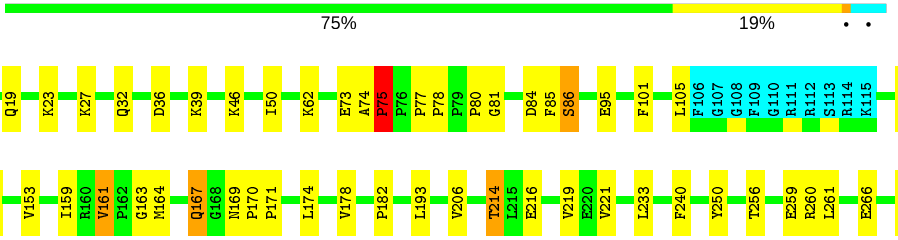
- Molecule 1: Chaperone protein DnaJ 2

Chain A:



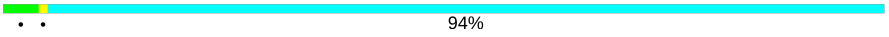
- Molecule 1: Chaperone protein DnaJ 2

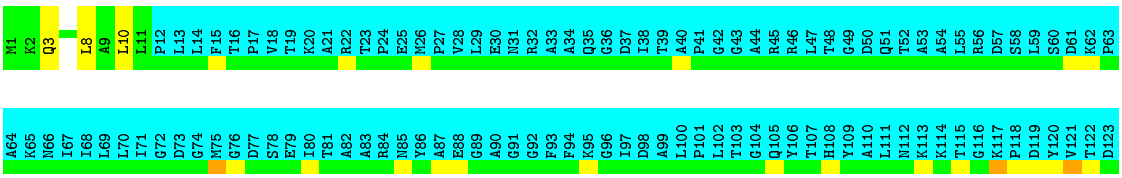
Chain C:

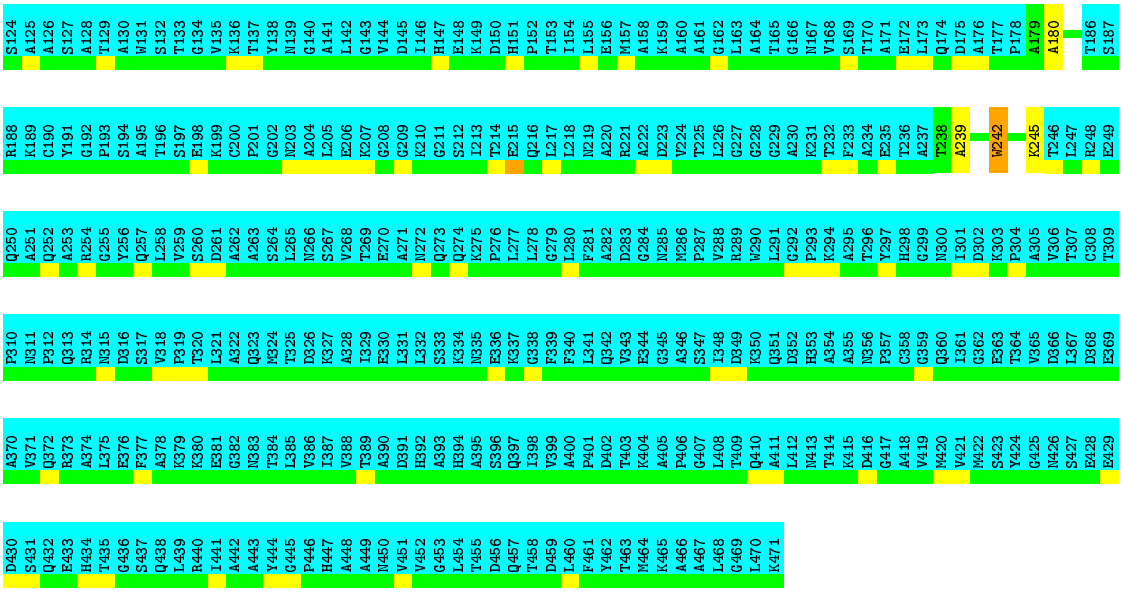


- Molecule 2: Alkaline phosphatase

Chain B:



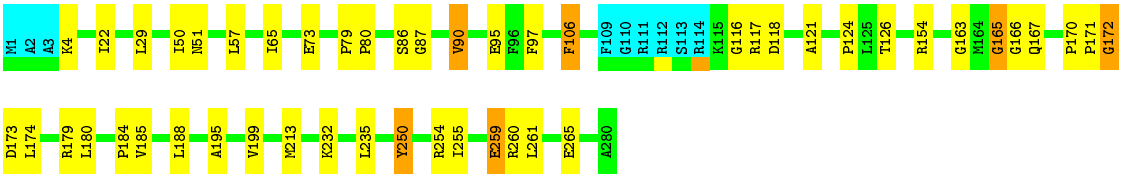




4.2.16 Score per residue for model 16

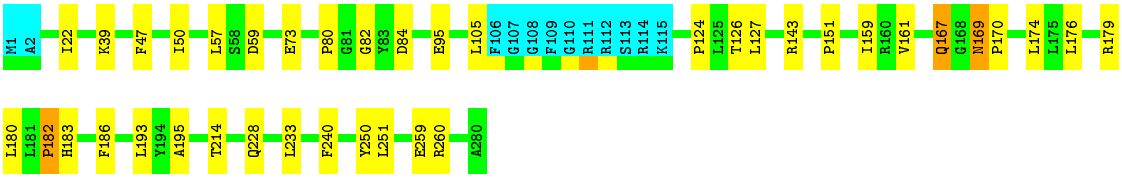
- Molecule 1: Chaperone protein DnaJ 2

Chain A:



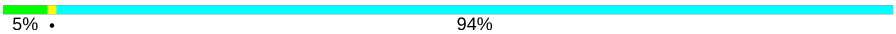
- Molecule 1: Chaperone protein DnaJ 2

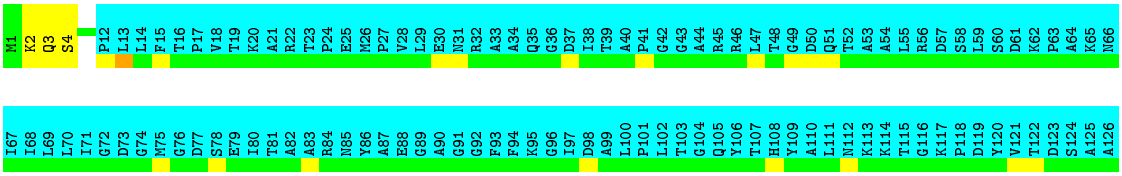
Chain C:

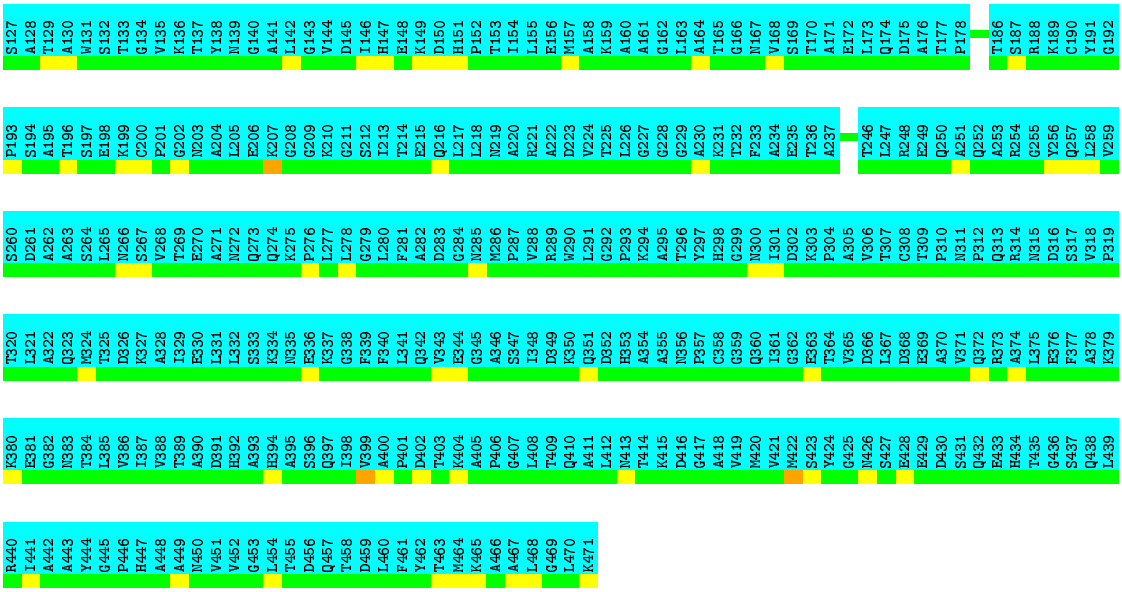


- Molecule 2: Alkaline phosphatase

Chain B:



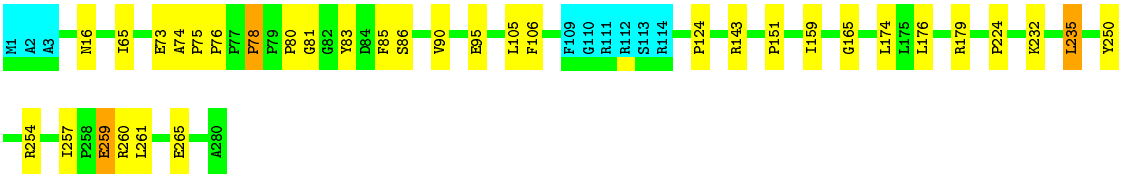




4.2.17 Score per residue for model 17

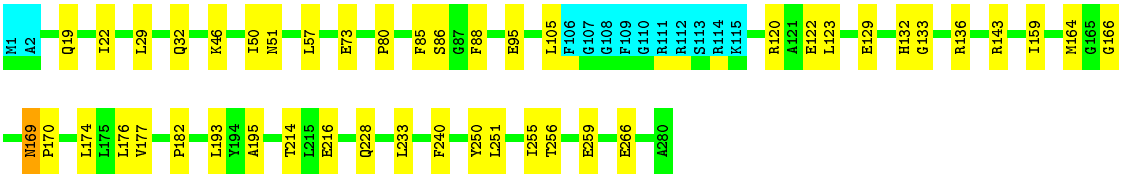
- Molecule 1: Chaperone protein DnaJ 2

Chain A:



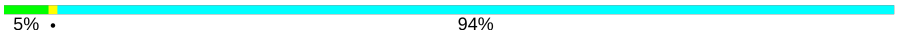
- Molecule 1: Chaperone protein DnaJ 2

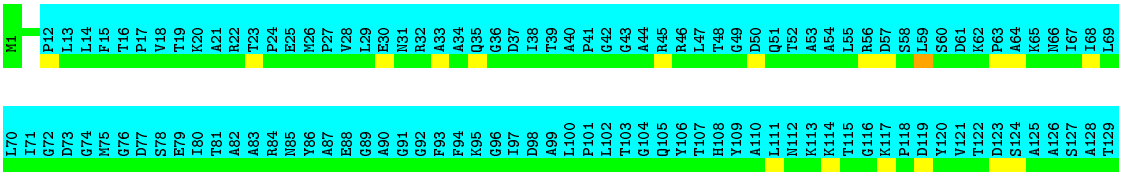
Chain C:

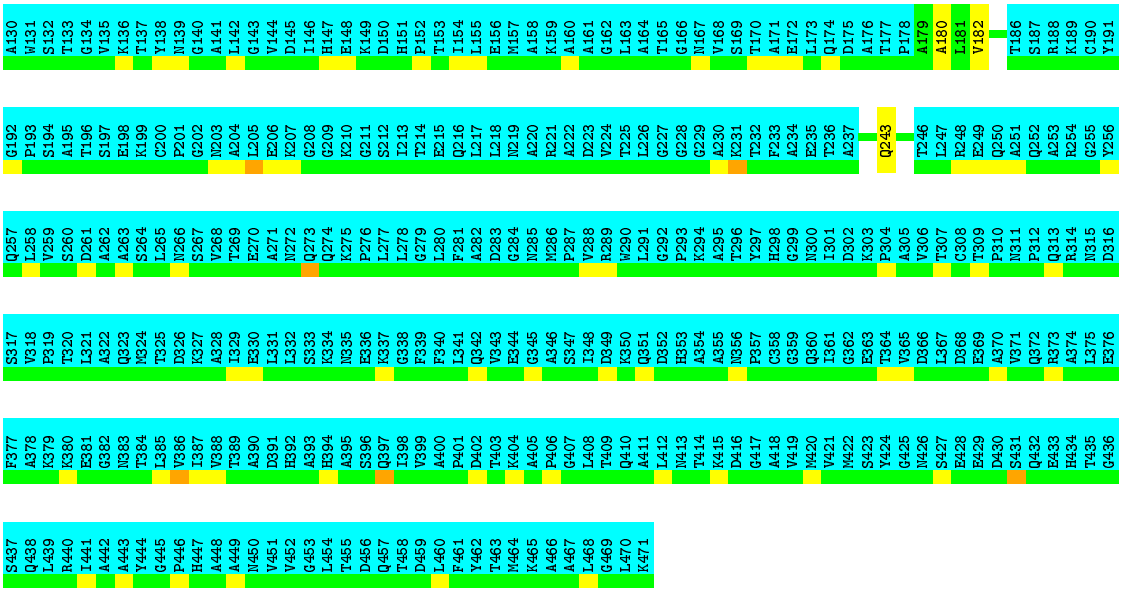


- Molecule 2: Alkaline phosphatase

Chain B:



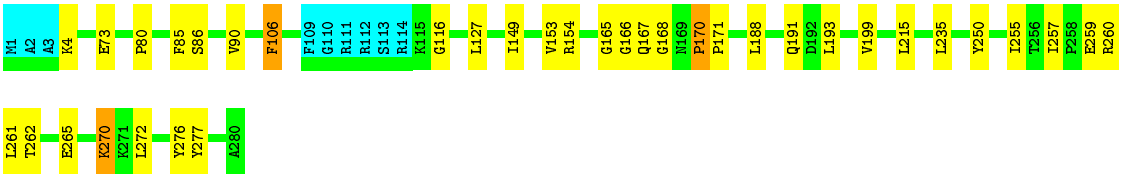




4.2.18 Score per residue for model 18

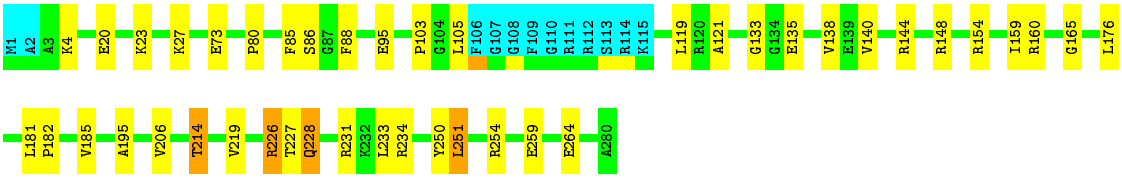
- Molecule 1: Chaperone protein DnaJ 2

Chain A:



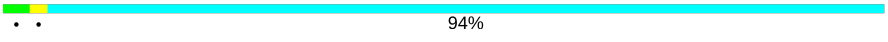
- Molecule 1: Chaperone protein DnaJ 2

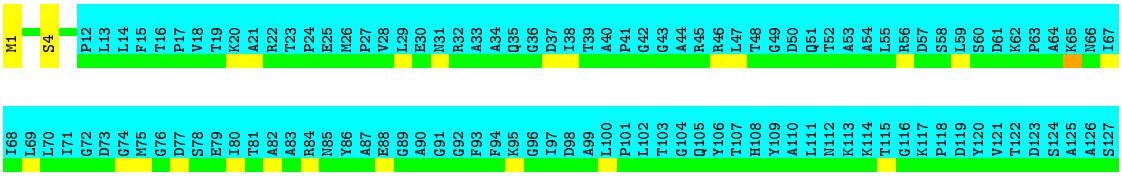
Chain C:

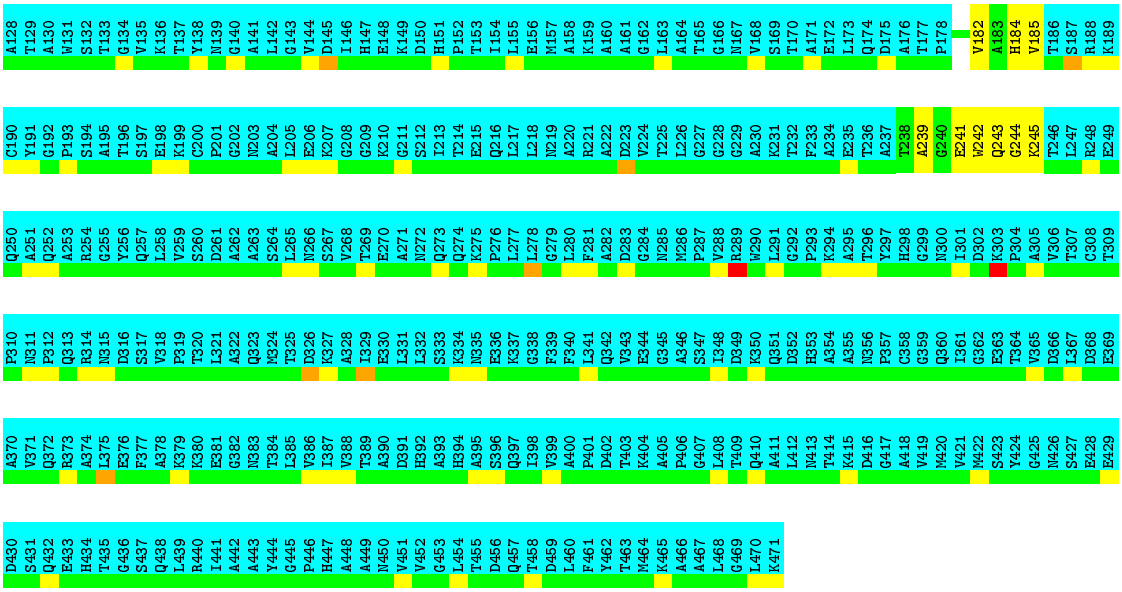


- Molecule 2: Alkaline phosphatase

Chain B:



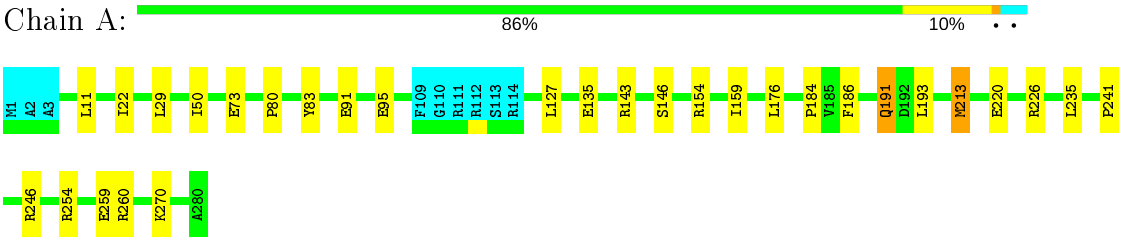




4.2.19 Score per residue for model 19

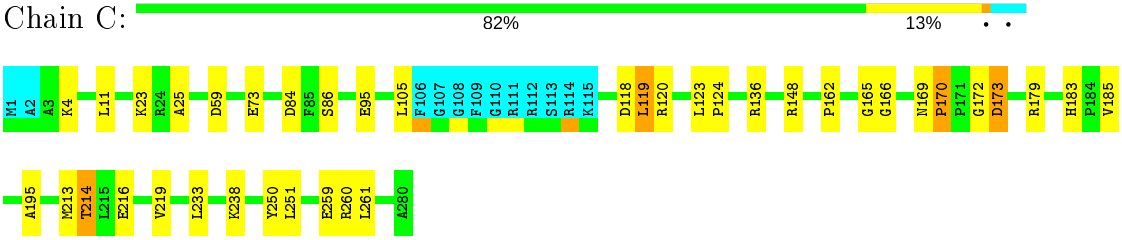
- Molecule 1: Chaperone protein DnaJ 2

Chain A:



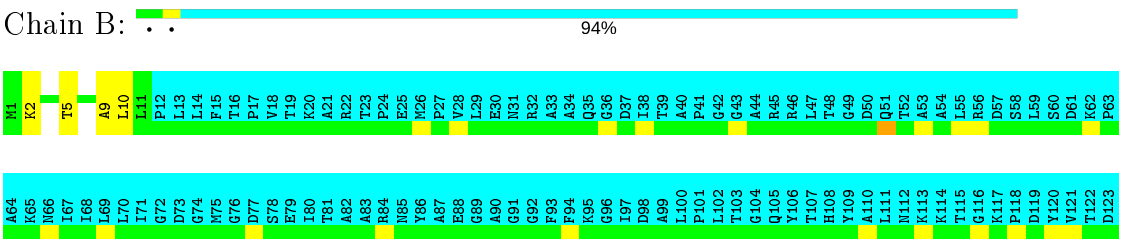
- Molecule 1: Chaperone protein DnaJ 2

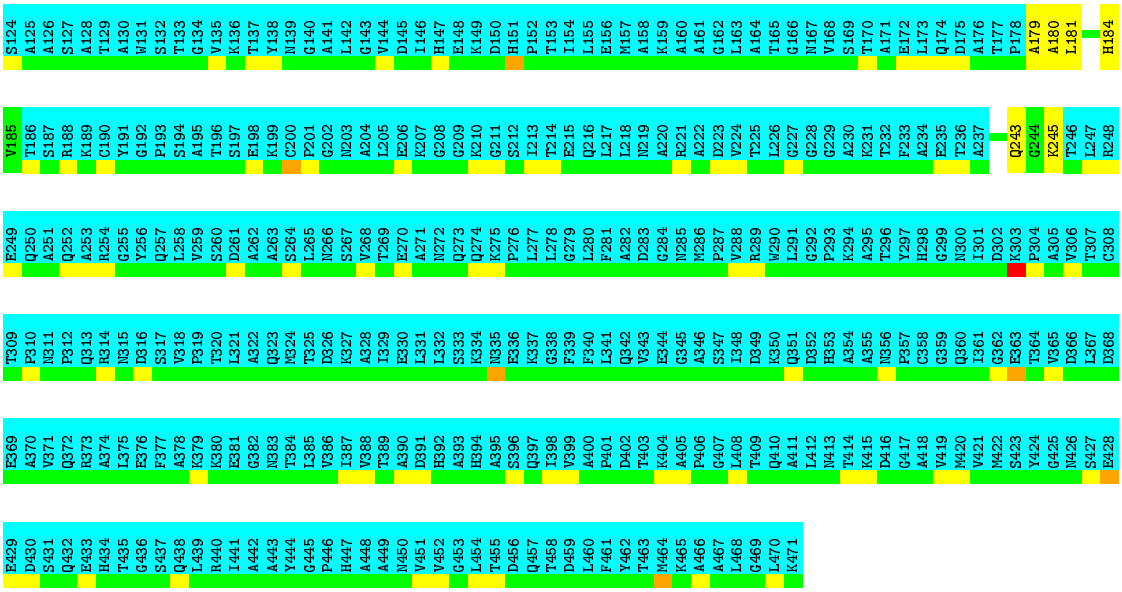
Chain C:



- Molecule 2: Alkaline phosphatase

Chain B:

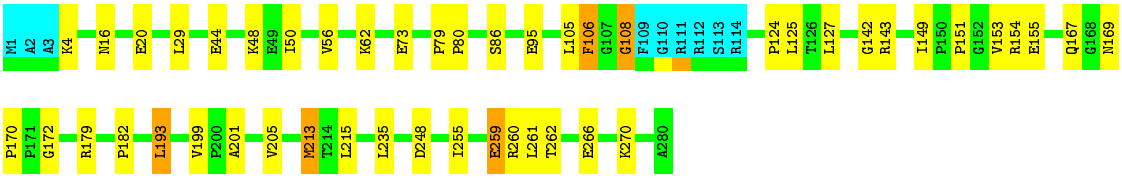




4.2.20 Score per residue for model 20

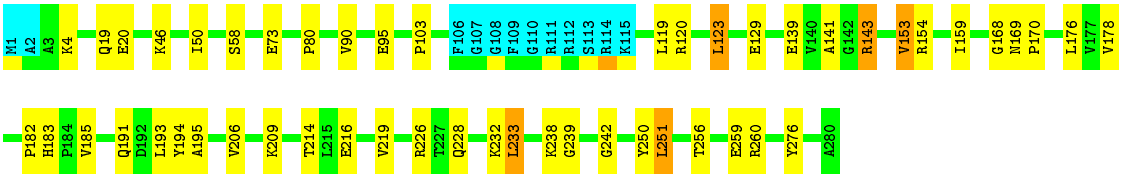
- Molecule 1: Chaperone protein DnaJ 2

Chain A:



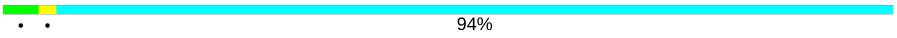
- Molecule 1: Chaperone protein DnaJ 2

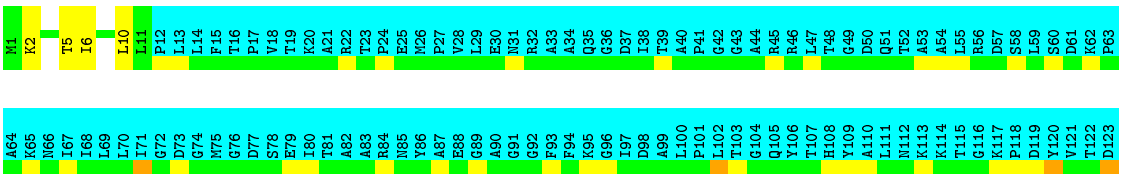
Chain C:

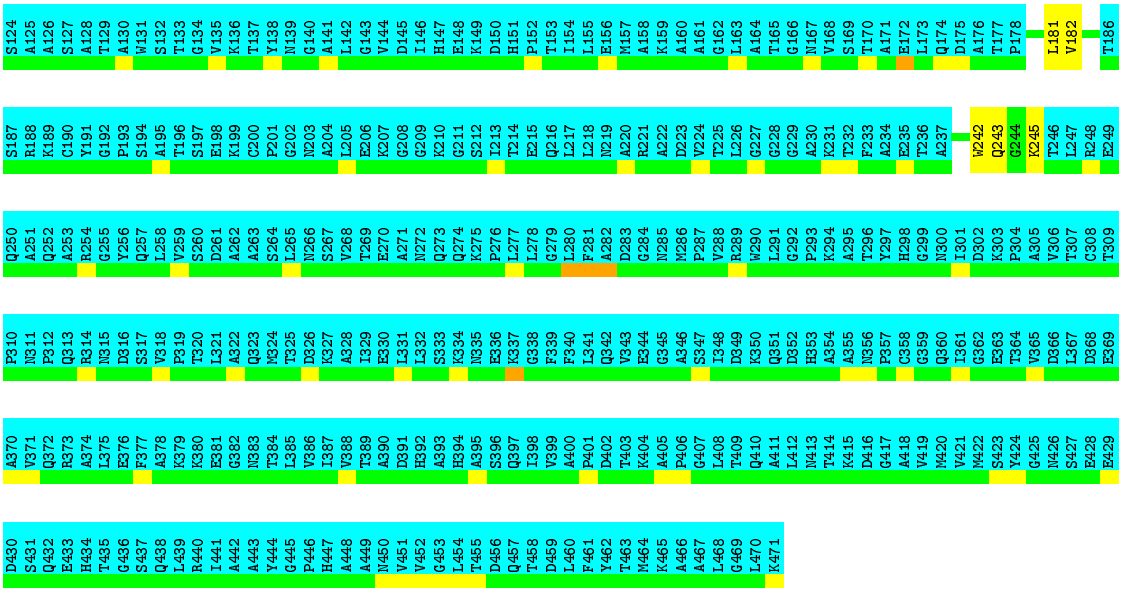


- Molecule 2: Alkaline phosphatase

Chain B:






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 L181 V182 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 P233 A234 E235 T236 A237 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 N324 T325 D326 K327 A328 I329 E330 L331 I332 S333 K334 N335 E336 K337 G338 F339 F340 I341 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 M413 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 T441 A442 A443 Y444 G445 P446 H447 A448 A449 N450 V451 V452 G453 L454 T455 D456 Q457 T458 D459 L460 F461 Y462 T463 N464 K465 A466 A467 L468 G469 L470 K471

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	
TALOS	geometry optimization	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	2
Total number of shifts	2726
Number of shifts mapped to atoms	2726
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	22%

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

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	2120	2130	2127	14±3
1	C	2097	2107	2104	15±4
2	B	189	205	204	2±1
All	All	88120	88840	88700	556

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:C:118:ASP:HA	1:C:166:GLY:HA2	0.70	1.62	19	1
1:A:127:LEU:HB3	1:A:215:LEU:HD22	0.68	1.64	18	6
1:C:22:ILE:HD13	1:C:57:LEU:HB3	0.68	1.64	8	7
1:A:166:GLY:HA3	1:A:172:GLY:HA3	0.63	1.69	6	2
1:A:108:GLY:HA3	1:A:167:GLN:HB3	0.62	1.71	20	4
1:A:90:VAL:HG21	1:A:105:LEU:HD22	0.61	1.70	2	3
1:A:154:ARG:HD2	1:A:191:GLN:HA	0.61	1.71	5	3
1:C:162:PRO:HA	1:C:173:ASP:HA	0.60	1.73	19	1
1:A:228:GLN:HB3	1:A:231:ARG:HD3	0.59	1.75	12	1
1:A:180:LEU:HD12	1:A:188:LEU:HG	0.59	1.74	16	1
1:A:47:PHE:HA	1:A:50:ILE:HD12	0.59	1.73	2	3
1:C:47:PHE:HA	1:C:50:ILE:HD12	0.58	1.75	16	2
2:B:243:GLN:HG3	1:C:224:PRO:HG2	0.58	1.76	7	2
1:A:259:GLU:HG2	1:C:228:GLN:HE21	0.57	1.59	20	4
1:A:123:LEU:HD23	1:A:176:LEU:HD22	0.57	1.76	14	1
1:A:143:ARG:NH1	1:A:164:MET:SD	0.57	2.77	1	1
1:A:232:LYS:HB3	1:A:250:TYR:HB3	0.56	1.77	2	9
1:C:169:ASN:HB2	1:C:170:PRO:HD3	0.55	1.79	13	1
1:C:159:ILE:HB	1:C:176:LEU:HB2	0.55	1.79	2	10
1:A:154:ARG:HD3	1:A:193:LEU:HD21	0.55	1.78	18	1
1:C:219:VAL:HB	1:C:238:LYS:HE3	0.55	1.77	20	2
1:A:117:ARG:H	1:A:166:GLY:HA3	0.55	1.62	4	2
2:B:245:LYS:HE2	1:C:222:ALA:HB1	0.55	1.77	1	1
1:A:29:LEU:HB3	1:A:50:ILE:HD13	0.55	1.78	12	13
1:A:124:PRO:HA	1:A:179:ARG:O	0.54	2.02	14	14
1:C:152:GLY:HA2	1:C:240:PHE:HB3	0.54	1.80	5	2
1:A:106:PHE:HB3	1:A:169:ASN:HA	0.54	1.79	13	5
1:C:233:LEU:O	1:C:250:TYR:HA	0.53	2.04	1	17
1:C:154:ARG:HG2	1:C:188:LEU:HD23	0.53	1.79	12	1
1:C:213:MET:HA	1:C:218:PRO:HA	0.52	1.81	5	1
1:A:257:ILE:HD11	1:C:228:GLN:HE21	0.52	1.64	18	1
1:A:44:GLU:O	1:A:48:LYS:HG2	0.52	2.05	20	2
1:A:87:GLY:H	1:A:163:GLY:HA3	0.52	1.65	9	2
1:A:180:LEU:HD12	1:A:188:LEU:HB3	0.52	1.81	1	1
1:C:90:VAL:HG21	1:C:105:LEU:HD22	0.52	1.81	14	1
1:C:161:VAL:HG11	1:C:164:MET:SD	0.52	2.45	3	1
1:C:163:GLY:H	1:C:173:ASP:HA	0.52	1.65	4	2
1:A:186:PHE:HE1	1:A:214:THR:HA	0.52	1.65	3	2
1:A:23:LYS:HG2	1:A:27:LYS:HE3	0.52	1.82	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:233:LEU:HD13	1:C:251:LEU:HB2	0.51	1.82	3	8
1:A:153:VAL:HG11	1:A:178:VAL:HG21	0.51	1.81	4	2
1:C:5:LYS:HD2	1:C:10:ILE:HD11	0.51	1.81	7	2
1:A:213:MET:SD	1:A:213:MET:N	0.51	2.83	14	5
1:A:226:ARG:HH11	1:C:260:ARG:HA	0.51	1.65	10	1
1:A:136:ARG:HH22	1:A:159:ILE:HD12	0.51	1.64	12	1
1:A:261:LEU:HD22	1:A:265:GLU:HB3	0.51	1.82	17	2
2:B:181:LEU:HD23	1:C:138:VAL:HB	0.51	1.83	10	1
1:C:185:VAL:HG11	1:C:213:MET:SD	0.51	2.45	12	1
1:C:90:VAL:HG21	1:C:169:ASN:HD21	0.51	1.65	6	2
1:C:164:MET:SD	1:C:174:LEU:HD23	0.51	2.45	17	2
1:A:213:MET:N	1:A:213:MET:SD	0.51	2.84	20	3
1:C:135:GLU:HG3	1:C:148:ARG:HB2	0.51	1.82	18	1
1:C:185:VAL:O	1:C:195:ALA:HA	0.51	2.06	18	6
1:C:55:ALA:HB1	1:C:85:PHE:HB3	0.51	1.82	9	1
1:C:143:ARG:HH12	1:C:164:MET:HA	0.51	1.66	15	1
1:A:106:PHE:CG	1:A:168:GLY:HA3	0.51	2.41	18	1
1:C:153:VAL:HG21	1:C:178:VAL:HG21	0.51	1.82	15	5
1:C:21:GLU:HG2	1:C:24:ARG:HH21	0.51	1.65	11	1
1:C:193:LEU:HD21	1:C:240:PHE:CD2	0.50	2.41	15	3
1:C:154:ARG:HB2	1:C:157:SER:HB2	0.50	1.81	2	2
2:B:183:ALA:HB3	1:C:124:PRO:HD2	0.50	1.82	5	1
1:A:241:PRO:HA	1:A:246:ARG:HA	0.50	1.83	13	3
1:A:65:ILE:HG23	1:A:76:PRO:HG3	0.50	1.83	3	1
1:C:276:TYR:HA	1:C:279:ARG:HD3	0.50	1.82	10	3
1:A:125:LEU:HA	2:B:6:ILE:HG21	0.50	1.84	14	6
1:C:29:LEU:HD13	1:C:50:ILE:HD12	0.50	1.84	11	3
2:B:183:ALA:HA	1:C:123:LEU:HB3	0.50	1.83	8	1
1:C:121:ALA:HB1	1:C:139:GLU:HG3	0.50	1.84	2	1
1:A:270:LYS:HG3	1:C:206:VAL:HG23	0.50	1.83	18	3
1:A:130:ALA:HB1	1:A:153:VAL:O	0.49	2.06	11	4
1:A:169:ASN:HB3	1:A:170:PRO:HD3	0.49	1.83	13	4
1:C:209:LYS:HG2	1:C:222:ALA:HA	0.49	1.84	5	3
1:A:165:GLY:HA2	1:A:174:LEU:HD13	0.49	1.85	16	3
1:C:183:HIS:N	1:C:184:PRO:HD3	0.49	2.22	1	4
1:A:154:ARG:HD3	1:A:186:PHE:HB3	0.49	1.83	8	1
1:A:166:GLY:O	1:A:171:PRO:HA	0.49	2.08	18	1
1:C:155:GLU:HB3	1:C:187:ARG:HG2	0.49	1.83	8	1
2:B:239:ALA:HB2	1:C:222:ALA:H	0.49	1.67	4	1
1:A:118:ASP:HA	1:A:173:ASP:O	0.49	2.07	16	1
1:A:164:MET:SD	1:A:164:MET:N	0.49	2.85	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:PRO:HB3	1:A:44:GLU:HG2	0.48	1.85	8	1
1:C:29:LEU:HB3	1:C:50:ILE:HD13	0.48	1.84	8	2
1:A:154:ARG:HA	1:A:188:LEU:HD21	0.48	1.84	9	1
1:C:232:LYS:HD3	1:C:250:TYR:HB3	0.48	1.84	14	2
1:A:155:GLU:HB3	1:A:188:LEU:O	0.48	2.08	15	2
1:A:270:LYS:HE2	1:C:206:VAL:HA	0.48	1.84	2	3
1:C:241:PRO:HA	1:C:246:ARG:H	0.48	1.67	2	1
1:C:187:ARG:HB3	1:C:194:TYR:HB3	0.48	1.85	4	2
1:C:143:ARG:NH2	1:C:164:MET:HA	0.48	2.24	9	1
1:A:121:ALA:HB3	1:A:174:LEU:HD11	0.48	1.85	16	1
1:A:135:GLU:HB3	1:A:146:SER:HB2	0.48	1.86	19	1
2:B:182:VAL:HG22	1:C:138:VAL:HA	0.48	1.85	7	1
2:B:182:VAL:HB	1:C:123:LEU:HB2	0.48	1.84	17	1
1:A:143:ARG:HD3	1:A:164:MET:SD	0.48	2.49	8	1
1:C:86:SER:HA	1:C:169:ASN:O	0.48	2.08	17	1
1:C:87:GLY:N	1:C:171:PRO:HA	0.47	2.23	3	1
1:C:145:VAL:HG21	1:C:164:MET:SD	0.47	2.48	10	1
1:A:136:ARG:HA	1:A:136:ARG:NE	0.47	2.24	1	1
2:B:241:GLU:HG3	1:C:234:ARG:HG3	0.47	1.85	18	1
1:A:199:VAL:O	1:A:255:ILE:HA	0.47	2.10	13	6
1:A:259:GLU:HG2	1:C:228:GLN:NE2	0.47	2.24	16	3
1:C:129:GLU:HA	1:C:132:HIS:HB2	0.47	1.86	17	1
1:C:183:HIS:H	1:C:184:PRO:HD3	0.47	1.70	1	1
1:A:57:LEU:HD22	1:A:63:ARG:HD2	0.47	1.85	4	1
1:A:116:GLY:H	1:A:172:GLY:HA3	0.47	1.68	16	1
2:B:182:VAL:HA	1:C:123:LEU:HB3	0.47	1.86	20	1
1:A:162:PRO:HA	1:A:173:ASP:HA	0.47	1.85	7	1
1:A:185:VAL:O	1:A:195:ALA:HA	0.47	2.10	10	3
1:C:22:ILE:HG12	1:C:57:LEU:HB3	0.47	1.86	10	2
1:A:105:LEU:HB3	1:A:169:ASN:ND2	0.47	2.25	7	3
1:C:61:GLU:HG2	1:C:79:PRO:HD3	0.47	1.87	5	1
1:C:90:VAL:HG23	1:C:97:PHE:HE2	0.47	1.70	6	1
1:A:166:GLY:HA3	1:A:171:PRO:HB2	0.46	1.84	16	1
1:C:137:VAL:HB	1:C:144:ARG:HG2	0.46	1.87	2	1
1:A:154:ARG:NH1	1:A:193:LEU:HD11	0.46	2.26	11	1
1:A:152:GLY:HA3	1:A:241:PRO:HD2	0.46	1.88	9	1
1:C:119:LEU:HB2	1:C:165:GLY:O	0.46	2.10	19	1
1:C:78:PRO:HG2	1:C:101:PHE:HA	0.46	1.88	15	1
1:C:193:LEU:HD21	1:C:240:PHE:CE2	0.46	2.46	14	3
1:C:60:PRO:O	1:C:64:ARG:HG2	0.46	2.10	4	1
1:C:117:ARG:HB2	1:C:167:GLN:HB2	0.46	1.88	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:195:ALA:HB3	1:C:251:LEU:HG	0.46	1.88	17	1
1:C:127:LEU:HB3	1:C:215:LEU:HD22	0.46	1.87	5	2
1:C:153:VAL:HG22	1:C:178:VAL:HG11	0.46	1.88	20	2
1:A:106:PHE:HB3	1:A:169:ASN:ND2	0.46	2.26	11	2
1:C:86:SER:HA	1:C:171:PRO:HG2	0.46	1.86	9	1
1:C:261:LEU:HD13	1:C:266:GLU:HA	0.46	1.87	15	1
1:A:155:GLU:HG2	1:A:187:ARG:NH1	0.46	2.26	4	1
1:C:161:VAL:HB	1:C:174:LEU:HB3	0.46	1.86	16	2
1:C:164:MET:HG3	1:C:174:LEU:HB2	0.46	1.87	15	1
2:B:182:VAL:HA	1:C:139:GLU:HB2	0.45	1.87	2	1
2:B:180:ALA:HB1	1:C:137:VAL:HG23	0.45	1.87	14	1
1:A:226:ARG:HD2	1:C:259:GLU:O	0.45	2.12	14	1
1:C:46:LYS:O	1:C:50:ILE:HG12	0.45	2.11	2	9
1:C:167:GLN:HA	1:C:167:GLN:HE21	0.45	1.71	16	2
1:A:187:ARG:HB3	1:A:194:TYR:HB2	0.45	1.87	13	3
2:B:182:VAL:HA	1:C:123:LEU:HB2	0.45	1.87	5	1
1:A:11:LEU:HD13	1:A:22:ILE:HG23	0.45	1.88	19	1
2:B:181:LEU:HD22	1:C:136:ARG:HB2	0.45	1.87	19	1
1:A:140:VAL:HG23	2:B:10:LEU:HB2	0.45	1.89	10	1
1:C:122:GLU:HA	1:C:177:VAL:O	0.45	2.11	5	2
1:A:261:LEU:HB3	1:A:266:GLU:HB2	0.45	1.89	10	1
1:C:163:GLY:H	1:C:173:ASP:HB3	0.45	1.71	1	1
1:A:90:VAL:HG21	1:A:169:ASN:ND2	0.45	2.26	10	2
2:B:245:LYS:HA	1:C:224:PRO:HB3	0.45	1.89	10	1
2:B:239:ALA:HB2	1:C:221:VAL:HA	0.45	1.87	15	1
1:C:169:ASN:HB3	1:C:170:PRO:HD3	0.45	1.87	17	3
1:C:214:THR:OG1	1:C:219:VAL:HG12	0.45	2.12	18	3
1:C:211:ARG:HH11	1:C:218:PRO:HB2	0.45	1.72	5	1
1:C:127:LEU:HD13	1:C:186:PHE:HD2	0.45	1.71	16	2
1:C:105:LEU:HB3	1:C:169:ASN:ND2	0.45	2.26	11	1
1:A:165:GLY:HA3	1:A:173:ASP:O	0.45	2.12	16	1
1:C:161:VAL:HG13	1:C:174:LEU:HB3	0.45	1.89	12	3
1:A:154:ARG:HD2	1:A:193:LEU:HD11	0.45	1.89	20	1
1:C:20:GLU:HA	1:C:23:LYS:HE3	0.44	1.89	7	2
1:A:206:VAL:HG21	1:C:270:LYS:HA	0.44	1.88	13	1
1:A:60:PRO:O	1:A:64:ARG:HG3	0.44	2.11	13	1
2:B:182:VAL:HG12	1:C:123:LEU:HD13	0.44	1.88	3	2
1:C:125:LEU:O	1:C:180:LEU:HA	0.44	2.12	9	2
1:C:232:LYS:HA	1:C:251:LEU:O	0.44	2.12	9	2
1:A:272:LEU:HD21	1:C:268:LEU:HB2	0.44	1.88	1	2
1:A:121:ALA:HB1	2:B:8:LEU:HD11	0.44	1.88	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:ILE:HD13	1:A:57:LEU:HD13	0.44	1.88	11	1
1:A:188:LEU:HD12	1:A:193:LEU:HA	0.44	1.89	11	2
1:C:124:PRO:HA	1:C:179:ARG:O	0.44	2.12	19	3
1:A:125:LEU:HD13	1:A:136:ARG:HH11	0.44	1.73	14	1
1:A:124:PRO:HA	1:A:179:ARG:HB2	0.44	1.89	10	1
1:A:159:ILE:HB	1:A:176:LEU:HB2	0.44	1.90	15	4
2:B:243:GLN:HB2	1:C:224:PRO:HG2	0.44	1.90	13	1
1:A:79:PRO:HG3	1:A:104:GLY:HA3	0.44	1.90	9	1
1:C:161:VAL:HG22	1:C:174:LEU:HB3	0.44	1.89	15	1
1:A:143:ARG:NH1	1:A:164:MET:HG2	0.44	2.28	5	2
2:B:1:MET:SD	2:B:1:MET:N	0.44	2.87	7	1
1:A:35:PRO:O	1:A:39:LYS:HG3	0.44	2.13	14	1
1:A:227:THR:HG23	1:A:233:LEU:HD21	0.44	1.90	15	1
1:A:90:VAL:HG12	1:A:171:PRO:HD3	0.43	1.89	7	1
1:C:166:GLY:HA3	1:C:173:ASP:N	0.43	2.27	19	1
1:C:266:GLU:O	1:C:270:LYS:HG2	0.43	2.13	6	2
1:C:202:PRO:O	1:C:206:VAL:HG13	0.43	2.13	3	2
1:A:154:ARG:HD2	1:A:215:LEU:HD12	0.43	1.90	10	1
1:C:26:TYR:O	1:C:30:ALA:HB3	0.43	2.13	10	1
1:A:22:ILE:HG12	1:A:57:LEU:HB3	0.43	1.88	16	1
1:C:227:THR:HA	1:C:231:ARG:NH1	0.43	2.29	18	1
1:A:138:VAL:HG13	1:A:145:VAL:HG13	0.43	1.89	3	2
1:C:127:LEU:HD13	1:C:186:PHE:CD2	0.43	2.48	4	2
1:C:152:GLY:HA3	1:C:188:LEU:HD23	0.43	1.89	6	1
1:A:272:LEU:O	1:A:276:TYR:HB2	0.43	2.12	13	3
1:A:144:ARG:NH1	1:A:146:SER:HB2	0.43	2.28	13	1
1:A:163:GLY:N	1:A:171:PRO:HB3	0.43	2.29	11	1
1:C:143:ARG:NH2	1:C:164:MET:SD	0.43	2.90	13	1
1:C:200:PRO:HG2	1:C:203:ILE:HD12	0.43	1.91	14	2
1:A:186:PHE:CD1	1:A:195:ALA:HB2	0.43	2.48	1	2
1:A:33:TYR:HD2	1:A:50:ILE:HD11	0.43	1.73	15	1
1:A:65:ILE:HD11	1:A:79:PRO:HG3	0.43	1.89	16	1
1:A:140:VAL:HB	2:B:8:LEU:HB3	0.43	1.89	2	1
1:C:186:PHE:HB3	1:C:193:LEU:HD22	0.43	1.89	6	2
1:A:143:ARG:HH12	1:A:164:MET:HG2	0.43	1.74	3	1
1:C:154:ARG:HA	1:C:188:LEU:HB3	0.43	1.91	3	1
1:A:126:THR:HB	1:A:129:GLU:HG2	0.43	1.90	13	1
1:C:24:ARG:HA	1:C:27:LYS:HE3	0.43	1.90	1	1
1:C:143:ARG:NH2	1:C:145:VAL:HG21	0.43	2.28	15	1
1:A:257:ILE:HG23	1:C:255:ILE:HG21	0.43	1.90	17	1
1:C:119:LEU:HD12	1:C:165:GLY:HA2	0.43	1.91	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:193:LEU:HG	1:C:239:GLY:HA2	0.43	1.91	20	1
1:A:255:ILE:HB	1:C:255:ILE:O	0.43	2.14	1	1
1:C:85:PHE:O	1:C:171:PRO:HG3	0.43	2.14	6	1
1:A:273:ALA:HA	1:C:202:PRO:HB2	0.43	1.90	2	1
1:A:117:ARG:N	1:A:166:GLY:HA3	0.43	2.28	8	1
2:B:181:LEU:HB2	1:C:136:ARG:HB3	0.43	1.90	1	3
1:C:65:ILE:HG23	1:C:76:PRO:HD2	0.43	1.91	3	1
1:C:153:VAL:HB	1:C:178:VAL:HG11	0.43	1.91	6	1
1:A:7:TYR:HB2	1:A:57:LEU:HD11	0.43	1.91	7	1
1:C:139:GLU:HG2	1:C:144:ARG:HG3	0.43	1.91	8	1
1:C:238:LYS:NZ	1:C:238:LYS:HA	0.43	2.29	14	1
1:C:213:MET:SD	1:C:214:THR:N	0.43	2.91	19	1
1:C:59:ASP:HB2	1:C:62:LYS:HD3	0.43	1.90	1	1
1:C:143:ARG:NH1	1:C:164:MET:SD	0.42	2.92	15	1
1:A:270:LYS:HE3	1:C:206:VAL:HG23	0.42	1.91	15	1
1:C:23:LYS:O	1:C:27:LYS:HG3	0.42	2.14	18	2
1:C:123:LEU:HD23	1:C:123:LEU:H	0.42	1.74	19	1
1:C:116:GLY:HA2	1:C:168:GLY:HA3	0.42	1.91	1	1
1:C:26:TYR:CD1	1:C:50:ILE:HG22	0.42	2.49	6	1
1:A:45:GLU:HA	1:A:48:LYS:HD3	0.42	1.89	13	1
1:C:85:PHE:CZ	1:C:105:LEU:HD22	0.42	2.49	15	1
1:C:127:LEU:HD21	1:C:180:LEU:HD13	0.42	1.89	16	1
2:B:185:VAL:HB	1:C:140:VAL:HG13	0.42	1.90	18	1
1:A:24:ARG:HA	1:A:27:LYS:HD3	0.42	1.90	8	1
1:A:267:ALA:O	1:A:271:LYS:HG3	0.42	2.14	13	1
1:A:116:GLY:HA2	1:A:170:PRO:HA	0.42	1.89	18	1
1:A:86:SER:HA	1:A:162:PRO:O	0.42	2.14	4	2
1:A:90:VAL:HG23	1:A:97:PHE:CZ	0.42	2.50	16	1
1:A:195:ALA:HB3	1:A:251:LEU:HD23	0.42	1.92	1	1
1:A:213:MET:HA	1:A:218:PRO:HA	0.42	1.91	5	1
1:C:119:LEU:HG	1:C:167:GLN:HG2	0.42	1.91	6	1
1:A:138:VAL:HB	1:A:145:VAL:HG13	0.42	1.90	13	1
1:A:126:THR:HG21	2:B:4:SER:HB2	0.42	1.92	16	1
1:C:23:LYS:HD3	1:C:148:ARG:NH2	0.42	2.30	19	1
1:A:261:LEU:HD22	1:A:265:GLU:HB2	0.42	1.90	9	4
1:A:87:GLY:HA2	1:A:171:PRO:HB3	0.42	1.90	3	2
1:A:176:LEU:HD22	2:B:8:LEU:HD11	0.42	1.89	9	1
1:A:22:ILE:HD13	1:A:57:LEU:HB3	0.42	1.91	2	1
2:B:2:LYS:HA	2:B:2:LYS:HE3	0.42	1.90	4	1
1:C:149:ILE:HD12	1:C:159:ILE:HG21	0.42	1.91	12	2
1:C:227:THR:HG22	1:C:253:VAL:HG11	0.42	1.91	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:LYS:HD2	1:A:170:PRO:HB2	0.42	1.91	4	1
1:C:143:ARG:NH2	1:C:164:MET:HB3	0.42	2.29	10	1
1:A:106:PHE:HD1	1:A:108:GLY:H	0.42	1.57	15	1
1:A:65:ILE:HD13	1:A:83:TYR:HE1	0.42	1.73	17	1
2:B:185:VAL:HG23	1:C:121:ALA:HA	0.42	1.91	18	1
1:A:261:LEU:HD13	1:A:266:GLU:HA	0.42	1.92	20	1
1:A:154:ARG:HH21	1:A:215:LEU:HD12	0.42	1.75	11	1
1:C:165:GLY:H	1:C:172:GLY:HA2	0.42	1.75	19	1
1:A:161:VAL:HG11	1:A:164:MET:SD	0.42	2.55	3	1
1:A:266:GLU:O	1:A:270:LYS:HG2	0.42	2.15	3	2
1:C:211:ARG:HD3	1:C:218:PRO:HB2	0.42	1.91	4	1
1:C:35:PRO:O	1:C:39:LYS:HG2	0.42	2.15	11	1
1:C:138:VAL:HG11	1:C:164:MET:SD	0.42	2.55	12	1
1:C:138:VAL:O	1:C:144:ARG:HA	0.42	2.14	18	1
1:C:185:VAL:HG12	1:C:195:ALA:HB1	0.42	1.92	1	1
1:A:186:PHE:HB3	1:A:193:LEU:HD22	0.41	1.92	9	1
1:C:98:GLN:HA	1:C:105:LEU:HD11	0.41	1.92	13	1
1:A:60:PRO:O	1:A:64:ARG:HG2	0.41	2.15	14	2
1:C:254:ARG:NH2	1:C:256:THR:HB	0.41	2.30	5	1
1:A:46:LYS:O	1:A:50:ILE:HG12	0.41	2.14	3	1
1:A:5:LYS:HD2	1:A:10:ILE:HD11	0.41	1.92	4	1
1:A:65:ILE:HA	1:A:76:PRO:HG2	0.41	1.93	6	1
1:C:143:ARG:NH1	1:C:164:MET:HA	0.41	2.30	15	1
1:A:168:GLY:C	1:A:171:PRO:HD3	0.41	2.36	18	1
1:A:56:VAL:O	1:A:62:LYS:HB2	0.41	2.16	20	1
1:C:141:ALA:HB3	1:C:143:ARG:HH21	0.41	1.75	20	1
1:C:11:LEU:O	1:C:25:ALA:HB1	0.41	2.15	1	1
2:B:242:TRP:CD2	1:C:233:LEU:HG	0.41	2.49	1	1
2:B:1:MET:N	2:B:1:MET:SD	0.41	2.89	3	1
1:C:131:PHE:HB2	1:C:215:LEU:HD13	0.41	1.92	14	2
1:C:86:SER:OG	1:C:163:GLY:HA2	0.41	2.15	15	1
1:A:149:ILE:HB	1:A:153:VAL:HG11	0.41	1.91	20	3
1:A:211:ARG:HH21	1:A:220:GLU:HA	0.41	1.75	15	1
1:C:11:LEU:HB3	1:C:25:ALA:HB1	0.41	1.92	19	1
1:C:233:LEU:HD22	1:C:251:LEU:HD12	0.41	1.92	1	1
1:A:5:LYS:HB3	1:A:10:ILE:HD11	0.41	1.93	2	1
1:C:194:TYR:HA	1:C:250:TYR:O	0.41	2.16	2	2
1:C:155:GLU:HB2	1:C:180:LEU:HD12	0.41	1.93	8	2
1:C:123:LEU:H	1:C:123:LEU:HD23	0.41	1.75	9	1
1:C:34:HIS:CD2	1:C:36:ASP:HB3	0.41	2.49	14	1
1:C:84:ASP:HB3	1:C:143:ARG:HG3	0.41	1.92	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:191:GLN:NE2	1:C:242:GLY:HA3	0.41	2.31	20	1
1:A:48:LYS:HB3	1:A:93:PHE:CE1	0.41	2.50	1	1
1:A:235:LEU:HB3	1:A:238:LYS:HG3	0.41	1.92	2	1
1:C:200:PRO:HA	1:C:256:THR:O	0.41	2.14	2	1
1:C:119:LEU:HD12	1:C:166:GLY:HA3	0.41	1.92	8	1
1:C:79:PRO:HB3	1:C:142:GLY:HA3	0.41	1.93	13	1
1:C:158:VAL:HG12	1:C:177:VAL:HG22	0.41	1.92	14	1
1:A:46:LYS:O	1:A:50:ILE:HG13	0.41	2.16	15	1
1:A:155:GLU:O	1:A:187:ARG:HG3	0.41	2.16	8	1
1:A:201:ALA:O	1:A:205:VAL:HG23	0.41	2.16	20	1
1:A:90:VAL:HG23	1:A:97:PHE:CE2	0.41	2.51	10	1
1:C:77:PRO:HA	1:C:78:PRO:HD3	0.41	1.82	10	1
1:C:85:PHE:O	1:C:171:PRO:HD2	0.41	2.16	15	1
1:A:116:GLY:HA3	1:A:170:PRO:C	0.41	2.36	18	1
1:A:127:LEU:HD13	1:A:186:PHE:HB2	0.41	1.93	19	1
1:A:79:PRO:HB2	1:A:142:GLY:HA3	0.41	1.93	20	1
2:B:243:GLN:HE22	1:C:231:ARG:NH1	0.40	2.14	4	1
1:A:263:PRO:O	1:A:266:GLU:HB3	0.40	2.15	7	1
1:A:226:ARG:HH12	1:C:261:LEU:HG	0.40	1.77	19	1
1:C:246:ARG:HG3	1:C:247:GLY:H	0.40	1.76	2	1
1:C:90:VAL:HG23	1:C:97:PHE:CZ	0.40	2.50	5	1
1:C:11:LEU:HD13	1:C:22:ILE:HG23	0.40	1.91	8	1
1:A:6:ASP:HA	1:A:66:TYR:OH	0.40	2.16	9	1
1:A:240:PHE:N	1:A:240:PHE:CD1	0.40	2.89	10	1
1:A:140:VAL:HG11	2:B:8:LEU:HD23	0.40	1.93	15	1
1:C:195:ALA:HB3	1:C:251:LEU:HD23	0.40	1.93	16	2
1:C:157:SER:O	1:C:178:VAL:HG12	0.40	2.17	4	1
1:A:128:GLU:HG2	2:B:2:LYS:HD3	0.40	1.92	8	1
1:C:28:ARG:HA	1:C:31:ARG:HH21	0.40	1.76	12	1
1:C:51:ASN:HB3	1:C:88:PHE:CD1	0.40	2.51	17	1
1:A:59:ASP:HB2	1:A:62:LYS:HD3	0.40	1.93	2	1
1:C:21:GLU:HG2	1:C:24:ARG:NH2	0.40	2.31	7	1
1:C:79:PRO:HG2	1:C:84:ASP:HB2	0.40	1.93	13	1
1:A:39:LYS:HE3	1:A:39:LYS:H	0.40	1.75	8	1
1:A:56:VAL:HG11	1:A:66:TYR:HB2	0.40	1.94	12	1
1:A:188:LEU:HB2	1:A:193:LEU:HD23	0.40	1.92	14	1
1:C:85:PHE:HA	1:C:88:PHE:CD2	0.40	2.52	18	1

5.2 Torsion angles (i)

5.2.1 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	270/280 (96%)	233±4 (86±2%)	29±4 (11±1%)	9±2 (3±1%)	6 37
1	C	267/280 (95%)	235±3 (88±1%)	24±3 (9±1%)	9±2 (3±1%)	7 38
2	B	25/471 (5%)	14±3 (56±11%)	7±3 (28±11%)	4±2 (16±7%)	0 4
All	All	11240/20620 (55%)	9630 (86%)	1183 (11%)	427 (4%)	5 33

All 102 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	182	PRO	19
1	C	259	GLU	19
1	A	259	GLU	18
1	C	80	PRO	16
1	A	86	SER	16
1	A	80	PRO	15
1	C	4	LYS	14
1	A	105	LEU	13
1	A	4	LYS	12
2	B	10	LEU	10
1	C	183	HIS	10
1	A	151	PRO	10
1	C	133	GLY	9
1	C	86	SER	9
2	B	243	GLN	9
2	B	180	ALA	9
1	C	169	ASN	9
1	C	105	LEU	8
1	A	16	ASN	8
1	A	106	PHE	8
1	A	263	PRO	7
1	A	184	PRO	6
2	B	184	HIS	6
2	B	239	ALA	5
2	B	4	SER	5

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Mol	Chain	Res	Type	Models (Total)
2	B	179	ALA	5
1	C	16	ASN	5
2	B	2	LYS	4
1	A	173	ASP	4
1	A	108	GLY	4
2	B	242	TRP	4
1	C	103	PRO	4
1	A	140	VAL	4
1	A	172	GLY	4
1	A	191	GLN	4
1	C	170	PRO	4
1	C	171	PRO	3
1	C	150	PRO	3
2	B	181	LEU	3
1	A	165	GLY	3
1	A	182	PRO	3
1	A	170	PRO	3
1	C	34	HIS	3
1	C	81	GLY	3
2	B	183	ALA	3
1	C	151	PRO	3
1	A	90	VAL	3
1	A	169	ASN	3
2	B	5	THR	3
2	B	3	GLN	2
1	C	77	PRO	2
1	A	166	GLY	2
1	A	152	GLY	2
1	A	81	GLY	2
1	A	118	ASP	2
1	C	152	GLY	2
1	C	173	ASP	2
1	C	167	GLN	2
2	B	244	GLY	2
2	B	182	VAL	2
1	C	74	ALA	2
1	A	150	PRO	2
1	C	75	PRO	2
1	C	184	PRO	2
1	C	226	ARG	2
1	A	153	VAL	2
2	B	185	VAL	2

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Mol	Chain	Res	Type	Models (Total)
2	B	9	ALA	2
1	A	41	PRO	1
1	C	241	PRO	1
1	A	155	GLU	1
1	A	115	LYS	1
1	A	76	PRO	1
1	C	190	GLY	1
1	C	85	PHE	1
1	A	171	PRO	1
1	C	118	ASP	1
1	A	74	ALA	1
1	A	75	PRO	1
1	A	78	PRO	1
1	C	155	GLU	1
1	A	34	HIS	1
1	A	227	THR	1
1	A	83	TYR	1
1	A	264	GLU	1
1	C	140	VAL	1
1	C	84	ASP	1
1	A	148	ARG	1
1	A	60	PRO	1
2	B	8	LEU	1
2	B	245	LYS	1
1	C	166	GLY	1
1	A	167	GLN	1
1	C	247	GLY	1
1	A	190	GLY	1
1	C	246	ARG	1
1	C	61	GLU	1
1	C	162	PRO	1
2	B	240	GLY	1
1	A	241	PRO	1
1	A	103	PRO	1
1	C	58	SER	1

5.2.2 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	218/224 (97%)	207±3 (95±1%)	12±3 (5±1%)	26 75
1	C	216/224 (96%)	204±3 (94±2%)	12±3 (6±2%)	24 73
2	B	18/359 (5%)	16±1 (88±7%)	2±1 (12±7%)	8 51
All	All	9040/16140 (56%)	8520 (94%)	520 (6%)	24 73

All 125 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	214	THR	20
1	A	73	GLU	20
1	C	73	GLU	19
1	A	260	ARG	17
1	A	95	GLU	17
1	C	95	GLU	14
1	A	106	PHE	13
2	B	242	TRP	12
1	C	216	GLU	11
1	C	226	ARG	11
1	C	256	THR	11
1	C	260	ARG	10
1	C	32	GLN	10
1	C	126	THR	10
1	A	235	LEU	10
1	A	154	ARG	10
1	A	270	LYS	8
1	C	120	ARG	8
1	A	254	ARG	8
1	C	19	GLN	7
1	A	238	LYS	7
2	B	245	LYS	7
1	A	191	GLN	7
1	A	143	ARG	7
1	A	213	MET	6
2	B	2	LYS	6
1	C	20	GLU	6
2	B	1	MET	6
1	C	51	ASN	5
1	A	39	LYS	5
1	A	20	GLU	5
1	C	139	GLU	5
1	C	143	ARG	5

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Mol	Chain	Res	Type	Models (Total)
1	A	85	PHE	5
1	C	183	HIS	5
1	A	167	GLN	5
1	A	169	ASN	5
1	A	117	ARG	5
1	C	119	LEU	5
1	A	136	ARG	4
1	A	187	ARG	4
1	C	211	ARG	4
1	A	122	GLU	4
1	A	193	LEU	4
1	C	153	VAL	4
1	C	251	LEU	4
1	C	276	TYR	4
1	C	167	GLN	4
1	C	62	LYS	4
1	C	90	VAL	4
2	B	5	THR	4
1	C	59	ASP	4
1	A	232	LYS	3
1	C	85	PHE	3
1	C	123	LEU	3
1	A	32	GLN	3
1	A	248	ASP	3
1	A	279	ARG	3
1	A	90	VAL	3
1	C	39	LYS	3
2	B	3	GLN	2
1	A	120	ARG	2
2	B	184	HIS	2
1	C	136	ARG	2
1	C	118	ASP	2
1	C	228	GLN	2
1	A	277	TYR	2
1	A	34	HIS	2
1	C	187	ARG	2
1	C	91	GLU	2
1	C	265	GLU	2
1	C	206	VAL	2
1	C	271	LYS	2
1	C	233	LEU	2
1	A	262	THR	2

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Mol	Chain	Res	Type	Models (Total)
1	C	117	ARG	2
1	C	75	PRO	2
1	A	115	LYS	2
2	B	241	GLU	2
1	C	46	LYS	2
1	A	51	ASN	2
1	A	226	ARG	2
1	A	19	GLN	2
1	A	250	TYR	2
1	A	189	GLU	2
1	C	42	GLU	2
1	C	69	TYR	1
1	C	264	GLU	1
1	A	144	ARG	1
1	C	77	PRO	1
1	A	97	PHE	1
1	C	182	PRO	1
1	C	161	VAL	1
1	A	24	ARG	1
1	A	78	PRO	1
1	A	46	LYS	1
1	C	254	ARG	1
1	A	259	GLU	1
1	A	135	GLU	1
1	A	4	LYS	1
1	A	147	VAL	1
1	A	211	ARG	1
1	C	154	ARG	1
1	A	252	GLU	1
1	C	103	PRO	1
1	C	36	ASP	1
1	A	91	GLU	1
1	A	138	VAL	1
1	A	15	ARG	1
1	A	188	LEU	1
1	C	97	PHE	1
2	B	243	GLN	1
1	A	140	VAL	1
1	C	84	ASP	1
2	B	238	THR	1
1	A	63	ARG	1
1	C	169	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	C	44	GLU	1
1	C	250	TYR	1
1	C	178	VAL	1
1	C	246	ARG	1
1	C	122	GLU	1
1	C	238	LYS	1
1	A	164	MET	1
1	A	183	HIS	1

5.2.3 RNA

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains

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

5.4 Carbohydrates

There are no carbohydrates in this entry.

5.5 Ligand geometry

There are no ligands in this entry.

5.6 Other polymers

There are no such molecules in this entry.

5.7 Polymer linkage issues

There are no chain breaks in this entry.

6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 22% for the well-defined parts and 19% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

6.1.1 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	1621
Number of shifts mapped to atoms	1621
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

6.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	225	-0.12 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	194	0.21 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	86	-0.16 ± 0.07	None needed (< 0.5 ppm)
^{15}N	218	0.01 ± 0.26	None needed (< 0.5 ppm)

6.1.3 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 19%, i.e. 1327 atoms were assigned a chemical shift out of a possible 7017. 0 out of 102 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	807/2713 (30%)	292/1074 (27%)	301/1130 (27%)	214/509 (42%)
Sidechain	520/3831 (14%)	181/2263 (8%)	339/1371 (25%)	0/197 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/473 (0%)	0/247 (0%)	0/209 (0%)	0/17 (0%)
Overall	1327/7017 (19%)	473/3584 (13%)	640/2710 (24%)	214/723 (30%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 11%, i.e. 1358 atoms were assigned a chemical shift out of a possible 12354. 0 out of 164 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	827/4997 (17%)	298/1983 (15%)	311/2062 (15%)	218/952 (23%)
Sidechain	531/6592 (8%)	185/3873 (5%)	346/2392 (14%)	0/327 (0%)
Aromatic	0/765 (0%)	0/399 (0%)	0/329 (0%)	0/37 (0%)
Overall	1358/12354 (11%)	483/6255 (8%)	657/4783 (14%)	218/1316 (17%)

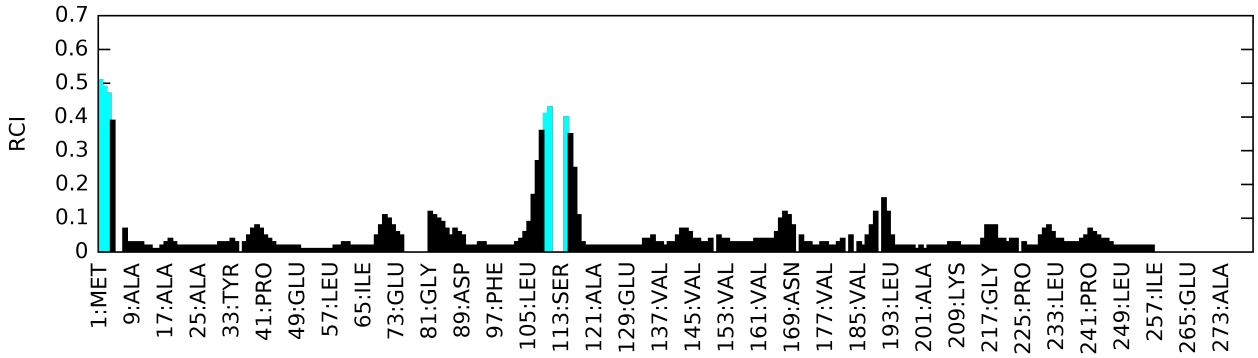
6.1.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

6.1.5 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.

Random coil index (RCI) for chain A:



6.2 Chemical shift list 2

File name: input_cs.cif

Chemical shift list name: *assigned_chemical_shifts_2*

6.2.1 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	1105
Number of shifts mapped to atoms	1105
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

6.2.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	31	-0.19 ± 0.16	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	32	0.18 ± 0.41	None needed (< 0.5 ppm)
$^{13}C'$	23	—	None (insufficient data)
^{15}N	379	-0.81 ± 0.14	Should be applied

6.2.3 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 3%, i.e. 187 atoms were assigned a chemical shift out of a possible 7017. 0 out of 102 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	81/2713 (3%)	35/1074 (3%)	26/1130 (2%)	20/509 (4%)
Sidechain	94/3831 (2%)	54/2263 (2%)	39/1371 (3%)	1/197 (1%)
Aromatic	12/473 (3%)	6/247 (2%)	5/209 (2%)	1/17 (6%)
Overall	187/7017 (3%)	95/3584 (3%)	70/2710 (3%)	22/723 (3%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 8%, i.e. 1040 atoms were assigned a chemical shift out of a possible 12354. 0 out of 164 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	843/4997 (17%)	410/1983 (21%)	54/2062 (3%)	379/952 (40%)

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	Total	^{1}H	^{13}C	^{15}N
Sidechain	177/6592 (3%)	105/3873 (3%)	71/2392 (3%)	1/327 (0%)
Aromatic	20/765 (3%)	10/399 (3%)	9/329 (3%)	1/37 (3%)
Overall	1040/12354 (8%)	525/6255 (8%)	134/4783 (3%)	381/1316 (29%)

6.2.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

6.2.5 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.

Random coil index (RCI) for chain B: