



Full wwPDB NMR Structure Validation Report ⓘ

Jun 23, 2024 – 06:31 AM EDT

PDB ID : 6PSI
BMRB ID : 30638
Title : Structural Basis for Client Recognition and Activity of Hsp40 Chaperones
Authors : Jiang, Y.; Rossi, P.; Kalodimos, C.G.
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 ⓘ 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 ⓘ](#)) 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) : 2.37.1

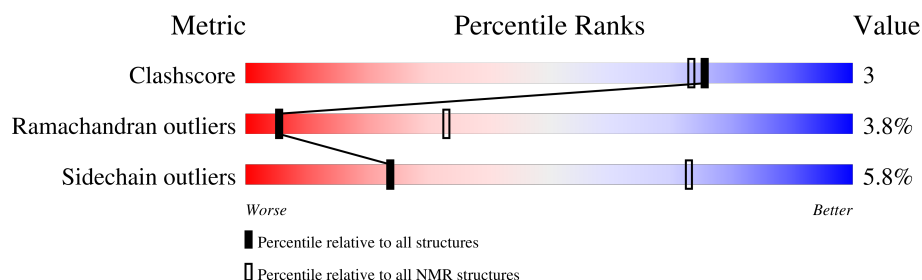
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 23%.

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	280	88% 9% .
1	C	280	86% 9% .
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)	2.80	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 [i](#)

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.

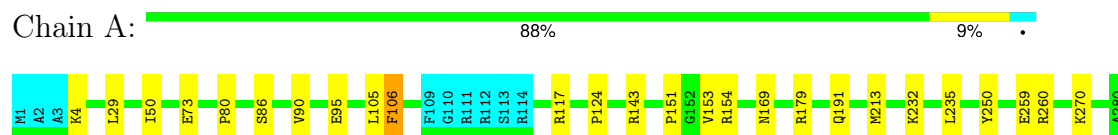
Mol	Chain	Residues	Atoms						Trace
2	B	471	Total	C	H	N	O	S	0
			6931	2154	3459	609	696	13	

4 Residue-property plots

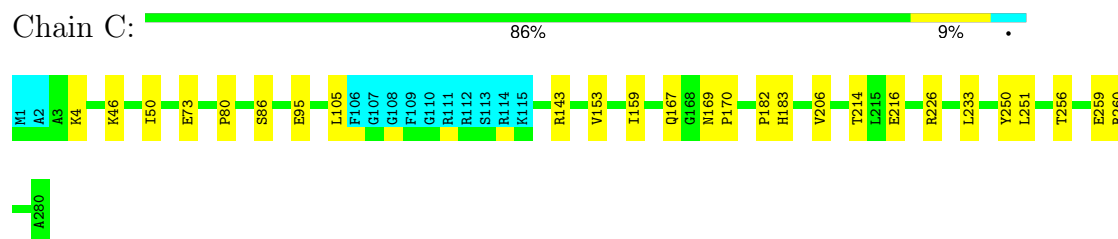
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, 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.

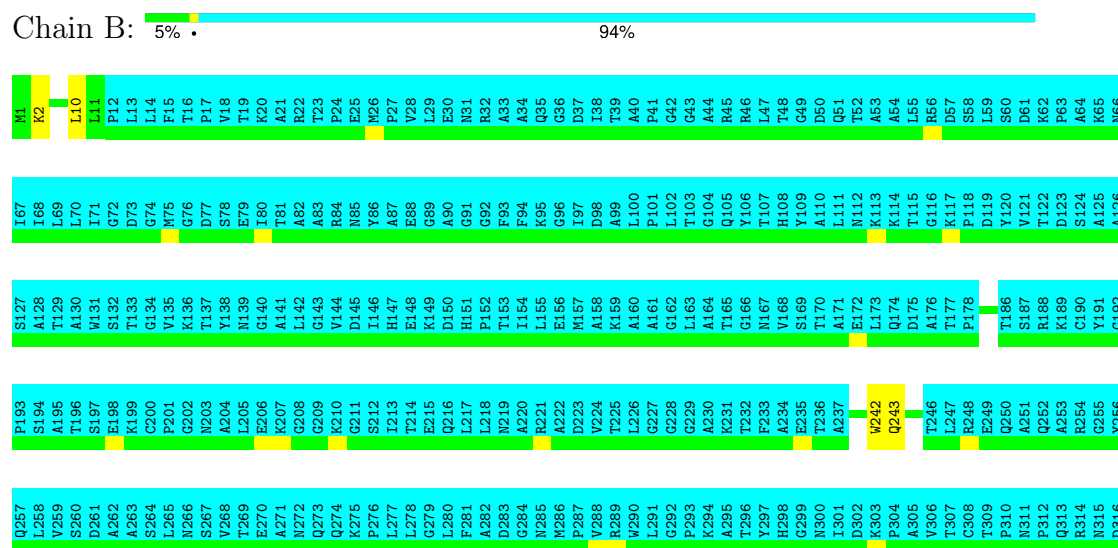
- Molecule 1: Chaperone protein DnaJ 2

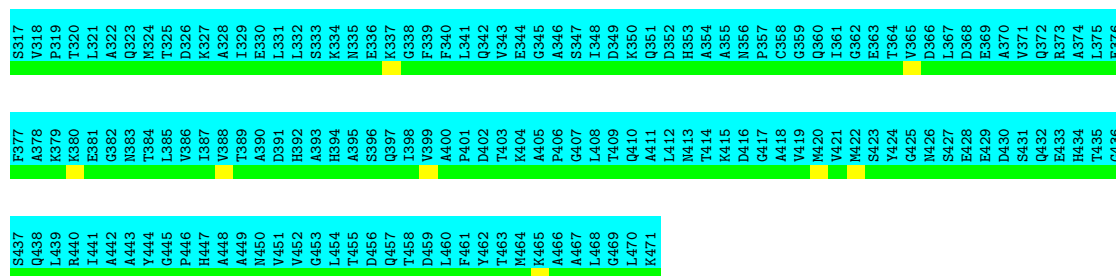


- Molecule 1: Chaperone protein DnaJ 2



- Molecule 2: Alkaline phosphatase



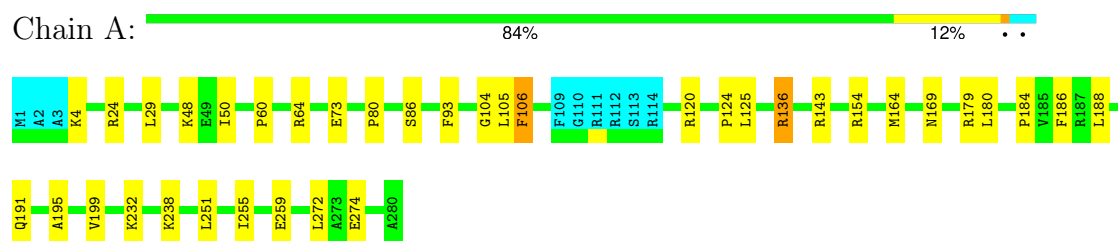


4.2 Scores per residue for each member of the ensemble

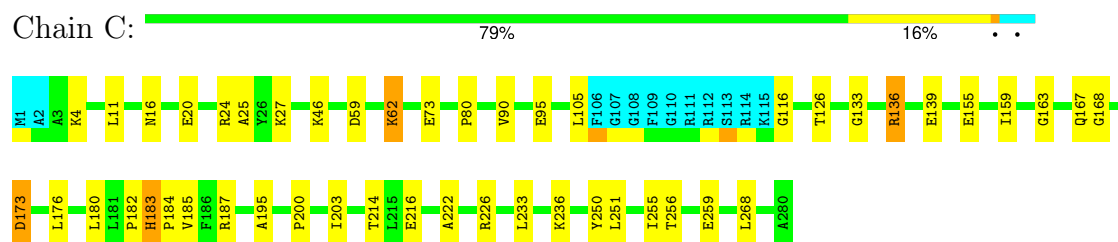
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

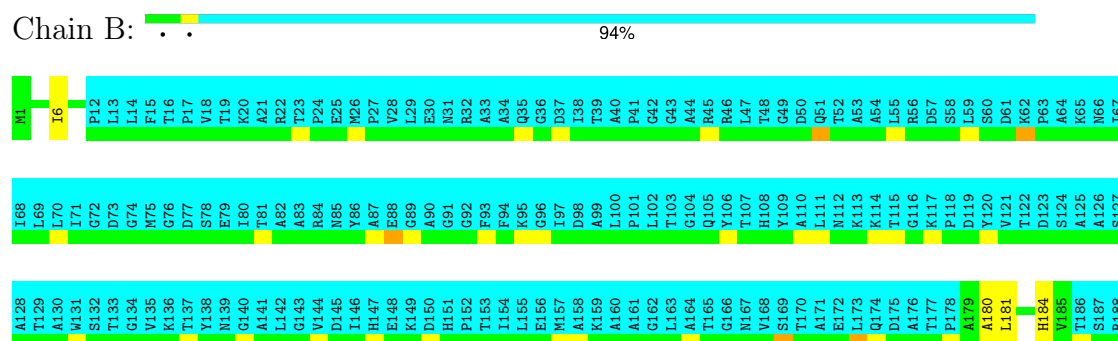
- Molecule 1: Chaperone protein DnaJ 2

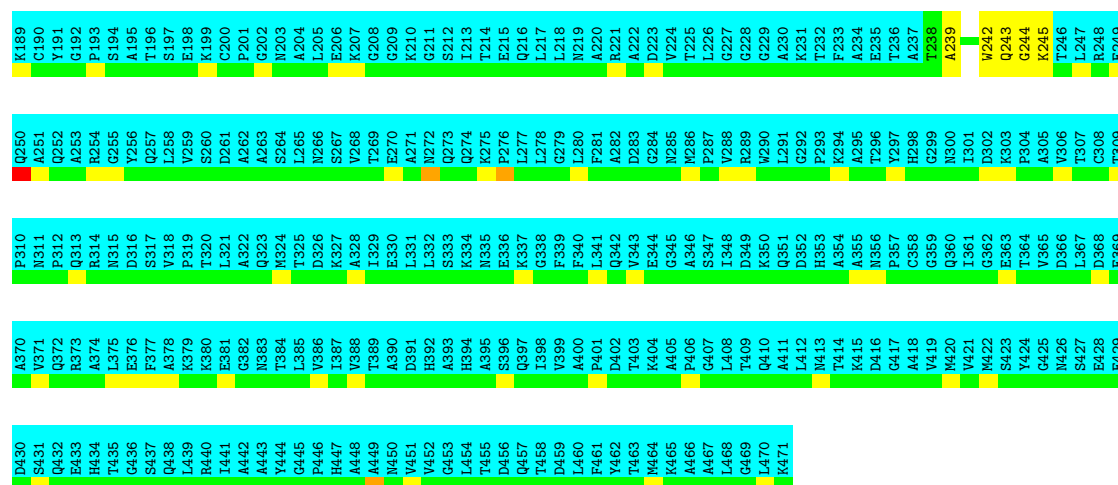


- Molecule 1: Chaperone protein DnaJ 2



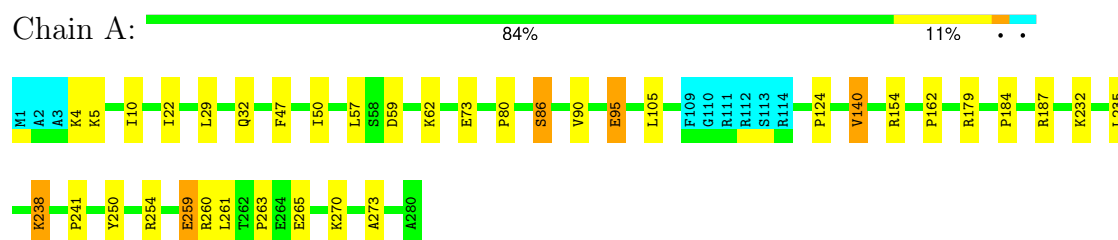
- Molecule 2: Alkaline phosphatase





4.2.2 Score per residue for model 2

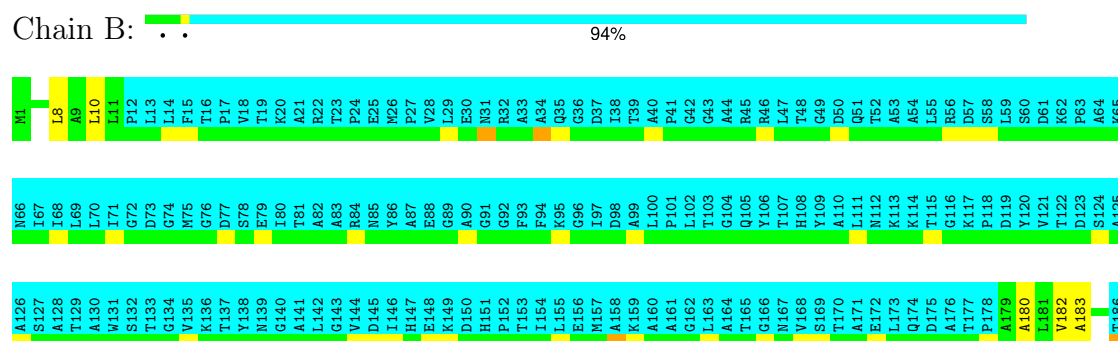
- Molecule 1: Chaperone protein DnaJ 2

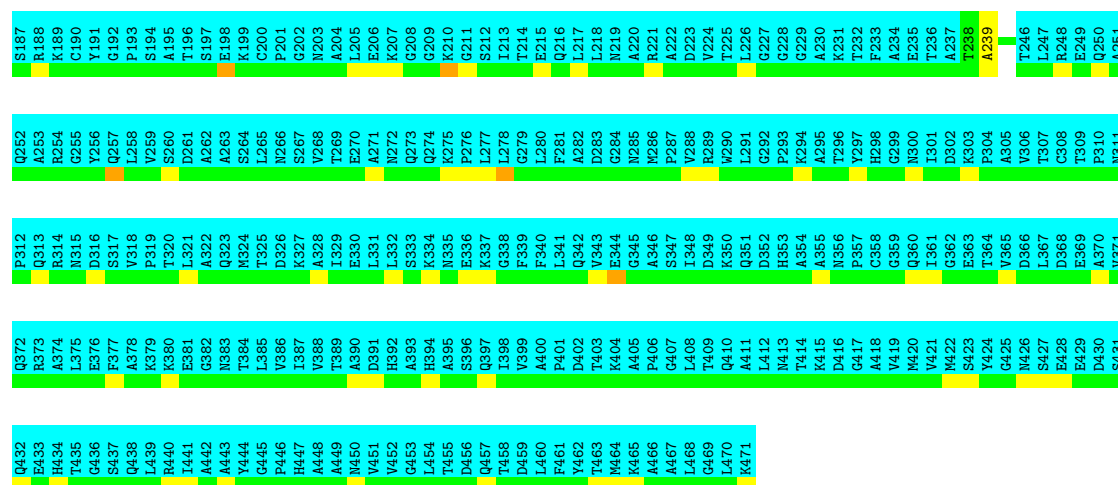


- Molecule 1: Chaperone protein DnaJ 2



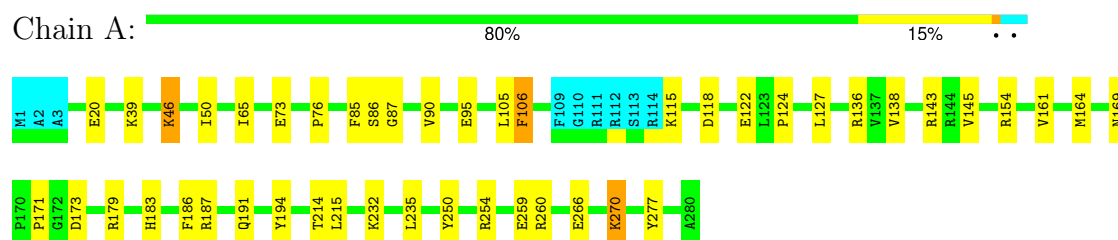
- Molecule 2: Alkaline phosphatase



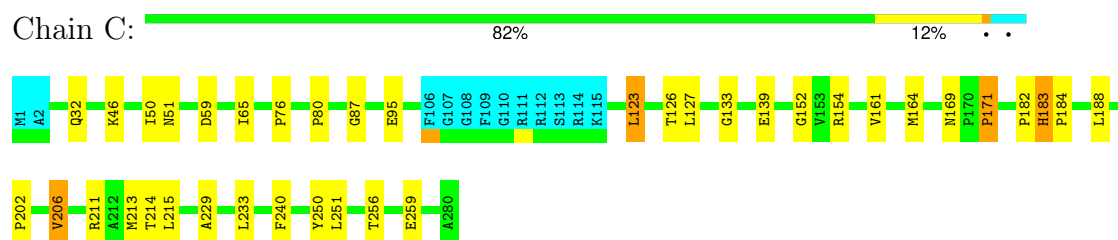


4.2.3 Score per residue for model 3

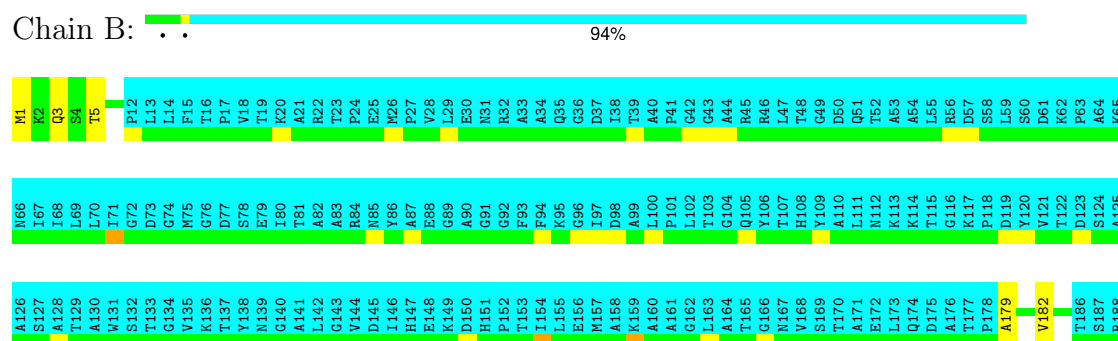
- Molecule 1: Chaperone protein DnaJ 2

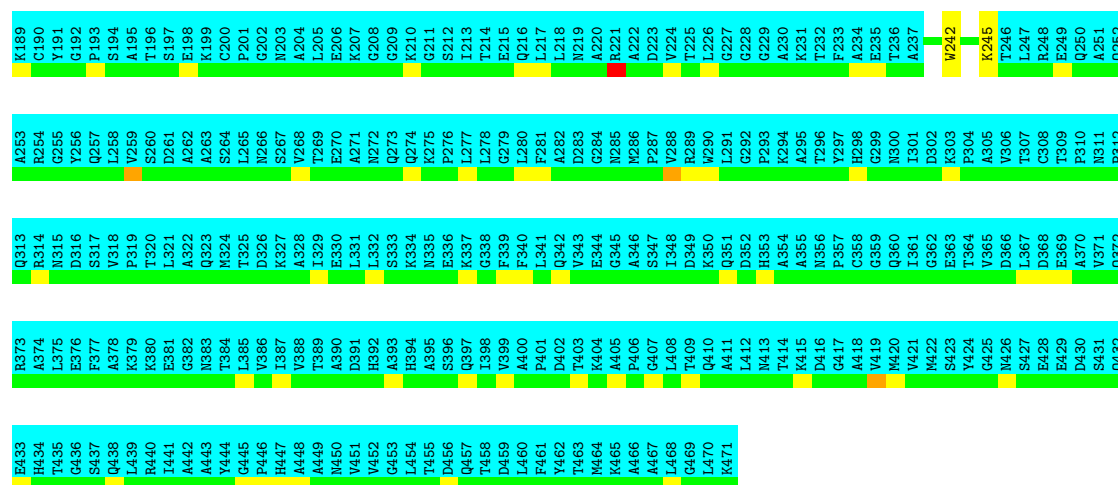


- Molecule 1: Chaperone protein DnaJ 2



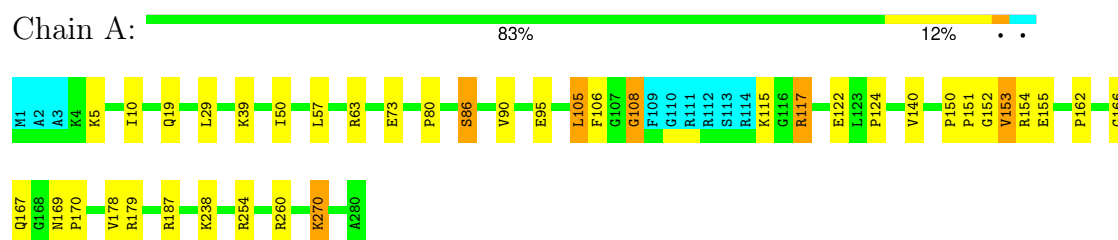
- Molecule 2: Alkaline phosphatase



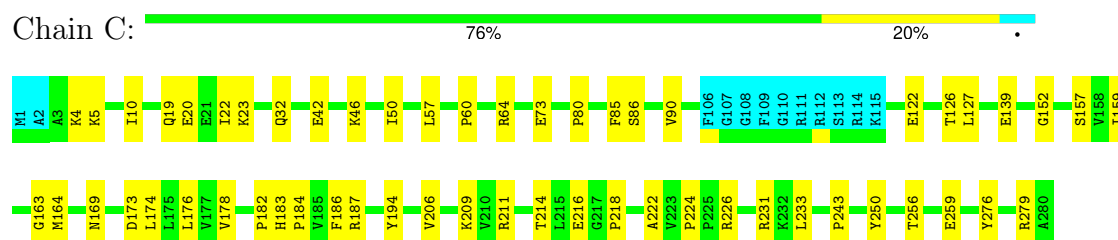


4.2.4 Score per residue for model 4 (medoid)

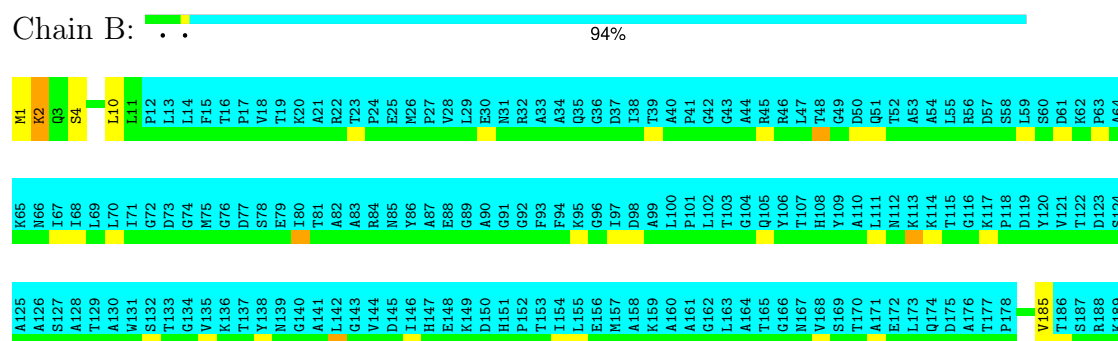
- Molecule 1: Chaparone protein DnaJ 2

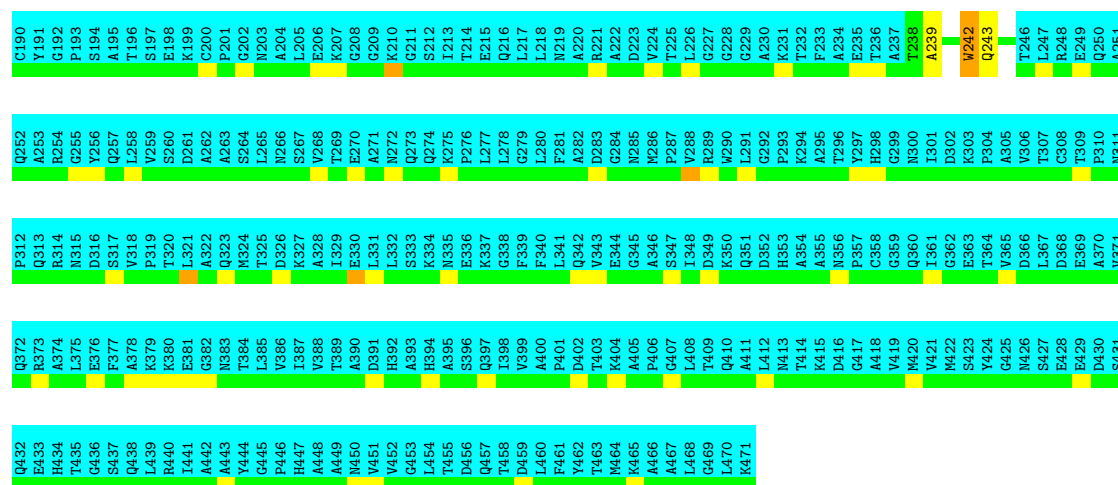


- Molecule 1: Chaparone protein DnaJ 2



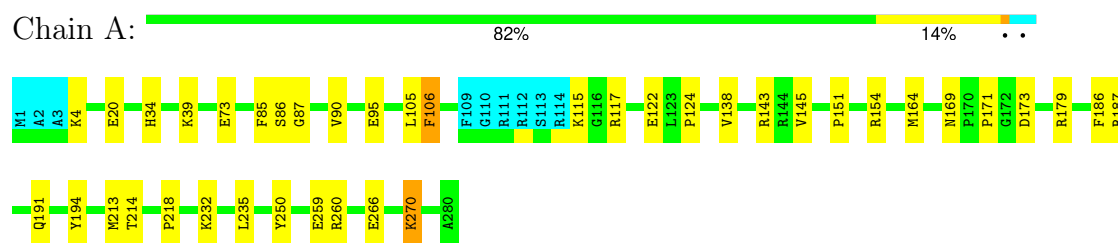
- Molecule 2: Alkaline phosphatase



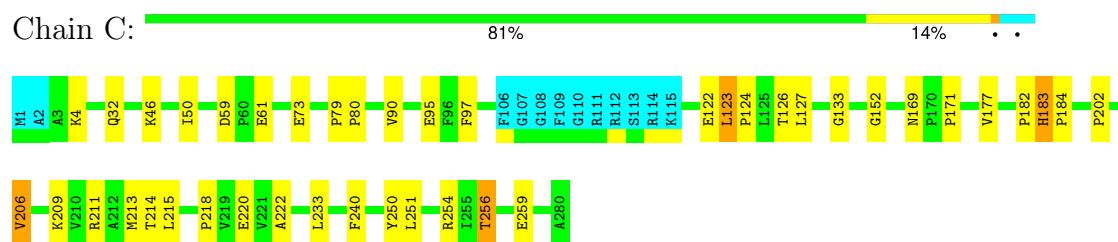


4.2.5 Score per residue for model 5

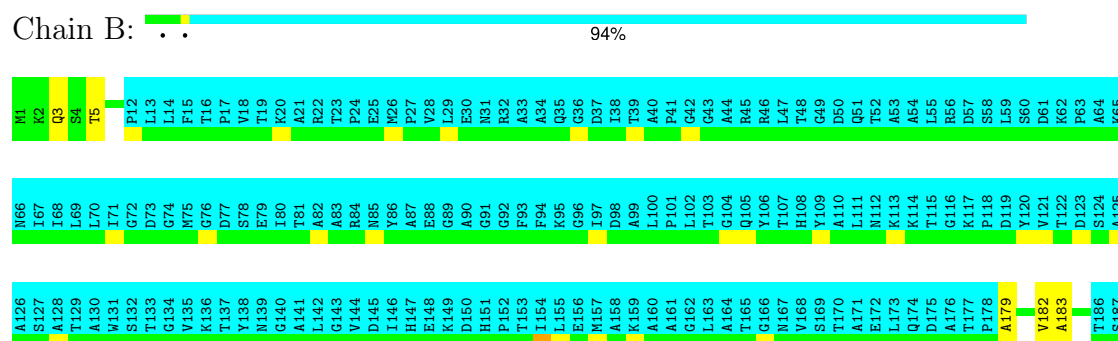
- Molecule 1: Chaperone protein DnaJ 2

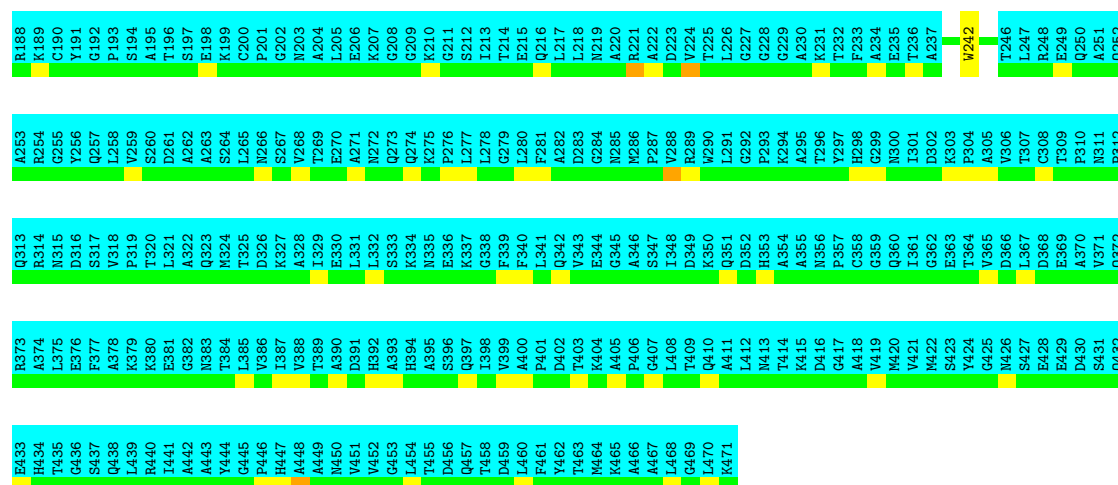


- Molecule 1: Chaperone protein DnaJ 2



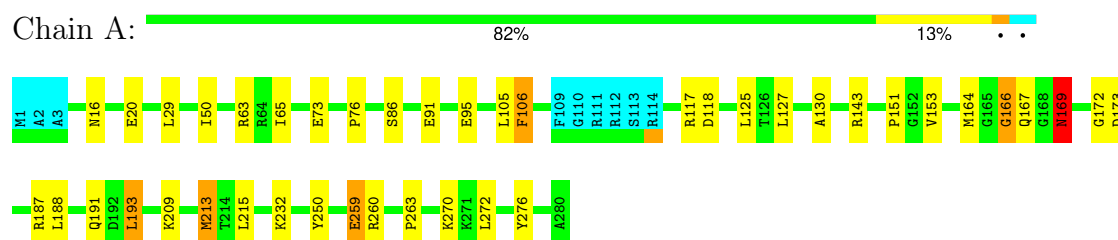
- Molecule 2: Alkaline phosphatase



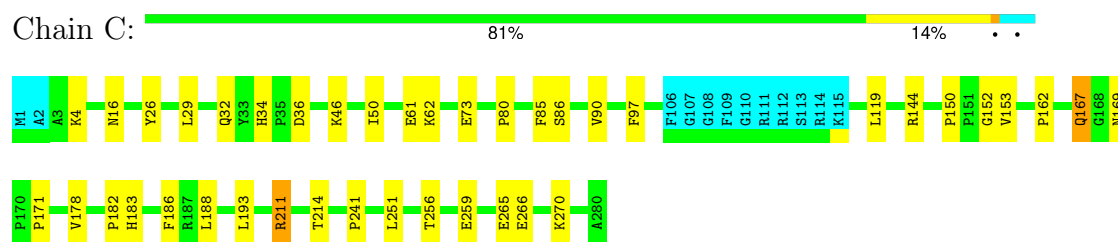


4.2.6 Score per residue for model 6

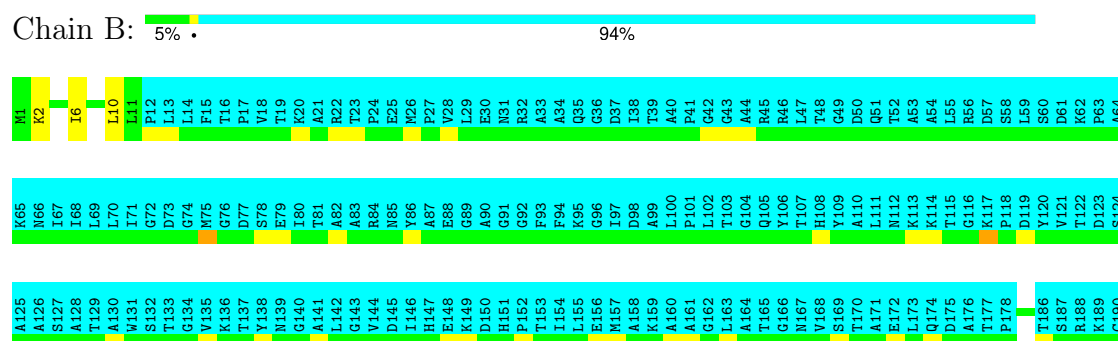
- Molecule 1: Chaperone protein DnaJ 2

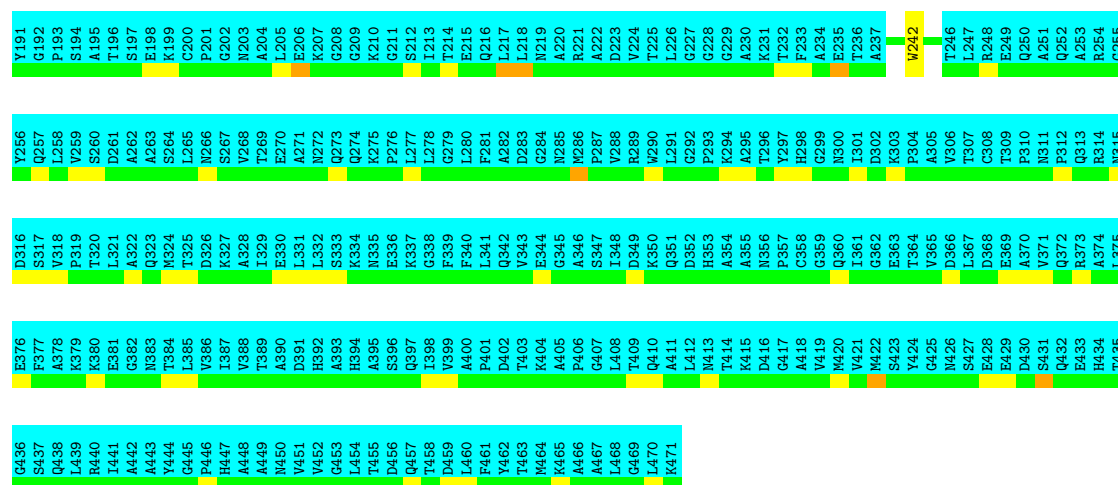


- Molecule 1: Chaperone protein DnaJ 2



- Molecule 2: Alkaline phosphatase

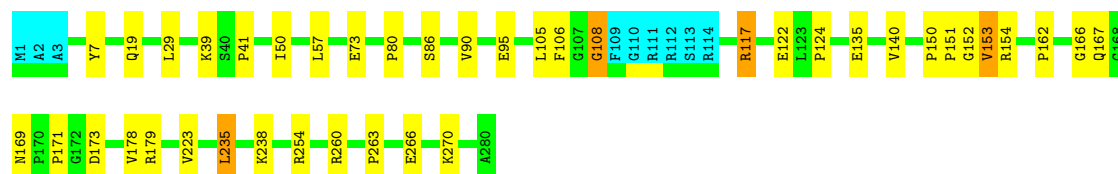




4.2.7 Score per residue for model 7

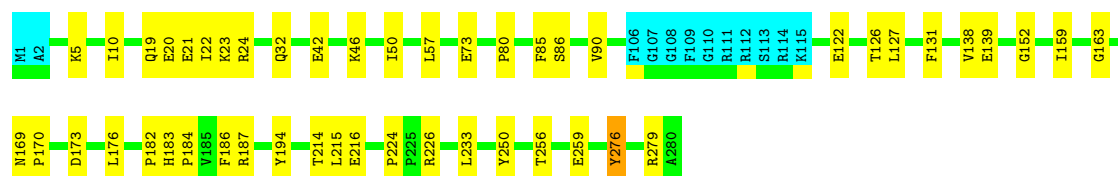
- Molecule 1: Chaperone protein DnaJ 2

Chain A: 82% 13% ..



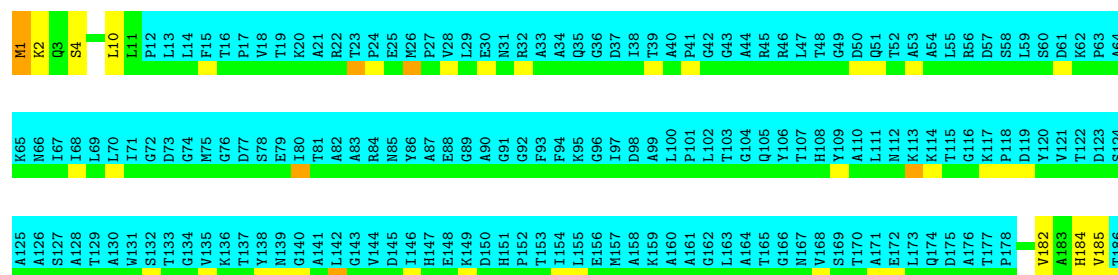
- Molecule 1: Chaperone protein DnaJ 2

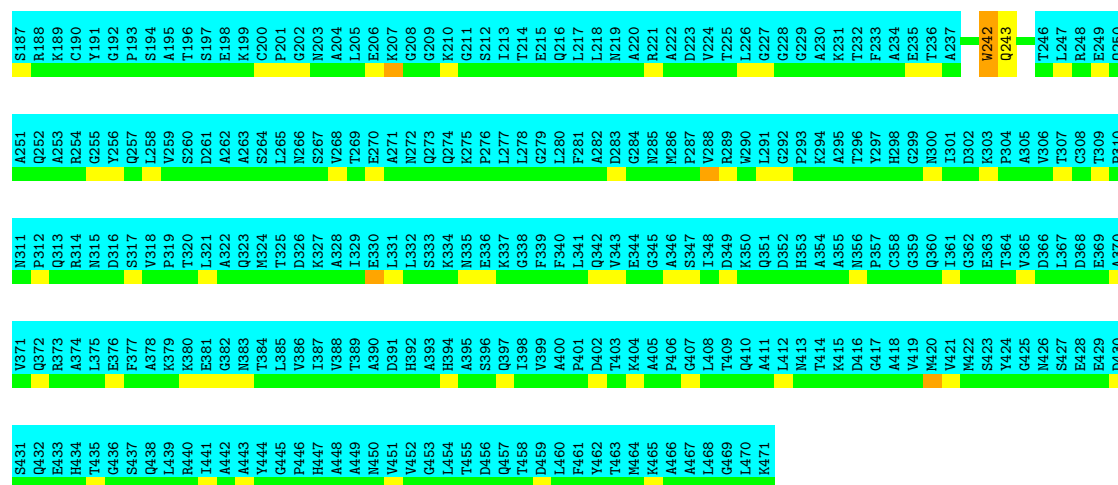
Chain C: 79% 17% .



- Molecule 2: Alkaline phosphatase

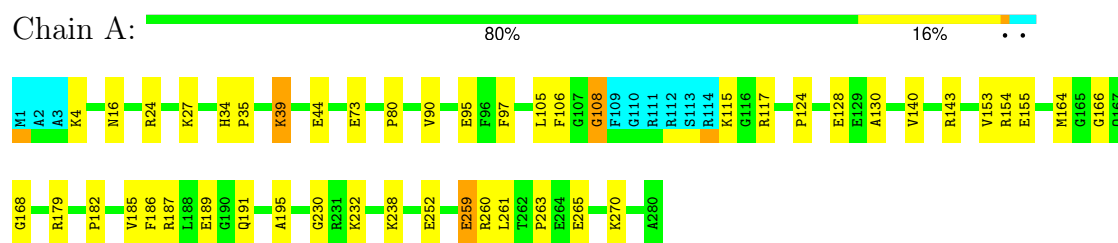
Chain B: 94%



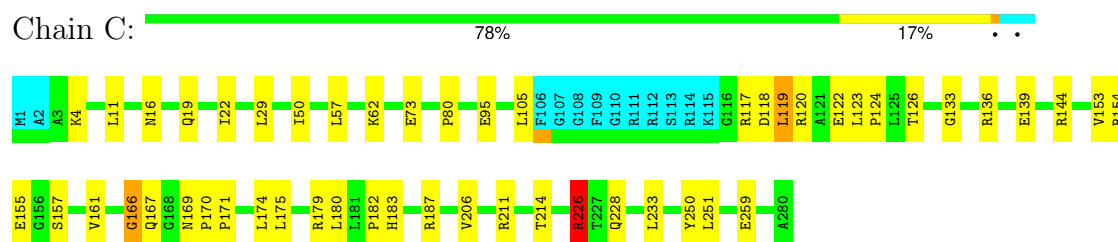


4.2.8 Score per residue for model 8

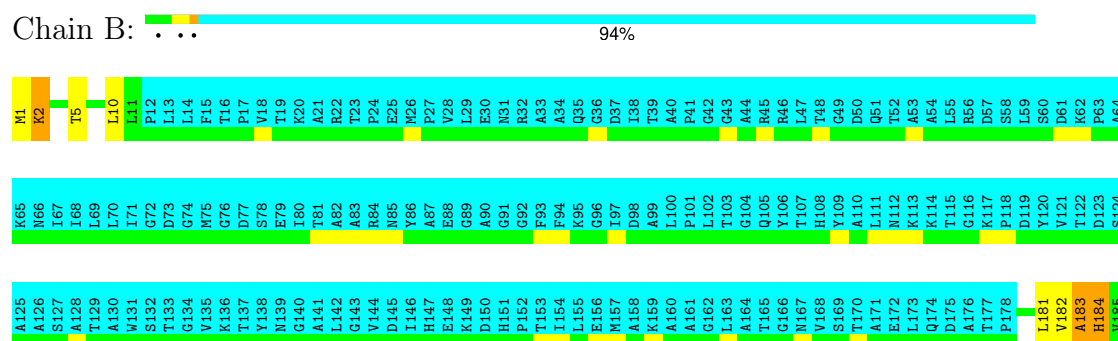
- Molecule 1: Chaperone protein DnaJ 2

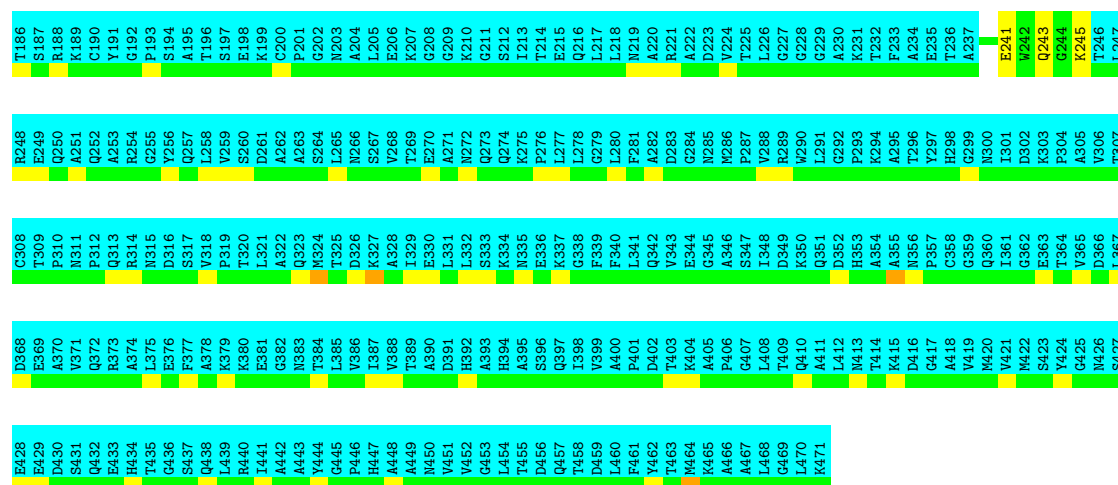


- Molecule 1: Chaperone protein DnaJ 2



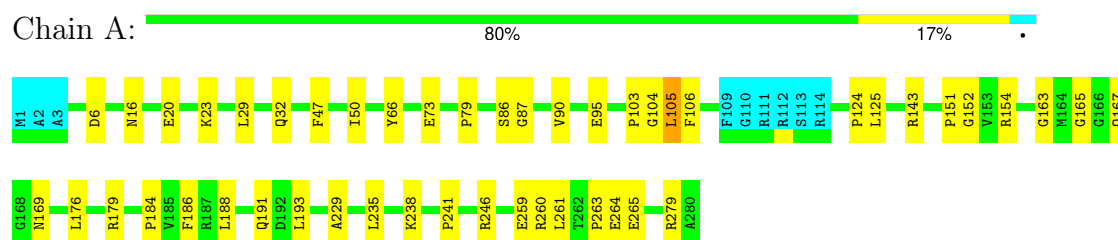
- Molecule 2: Alkaline phosphatase



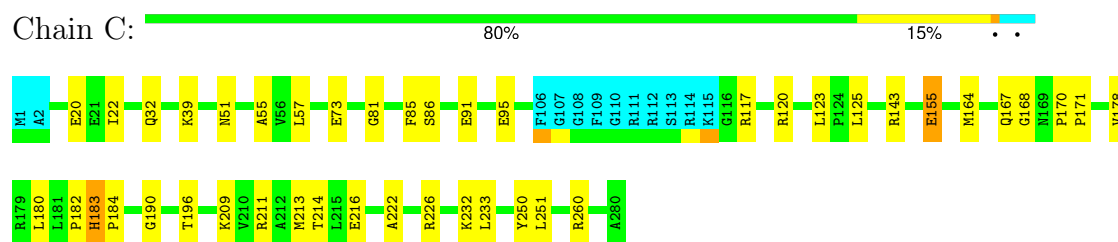


4.2.9 Score per residue for model 9

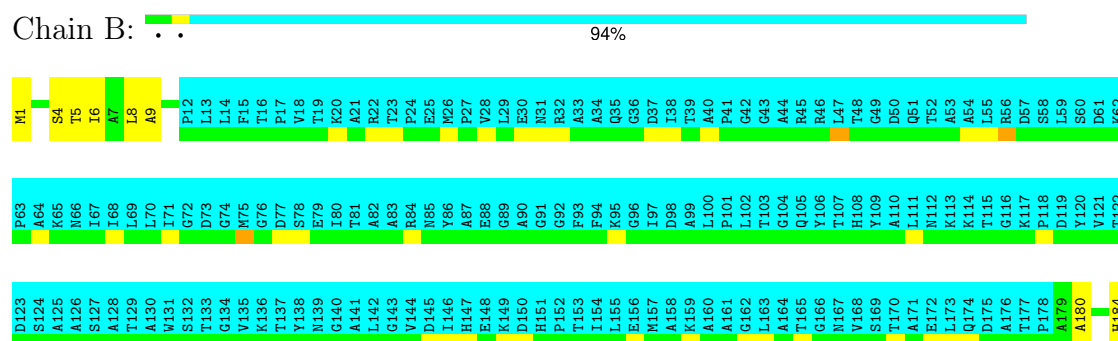
- Molecule 1: Chaperone protein DnaJ 2

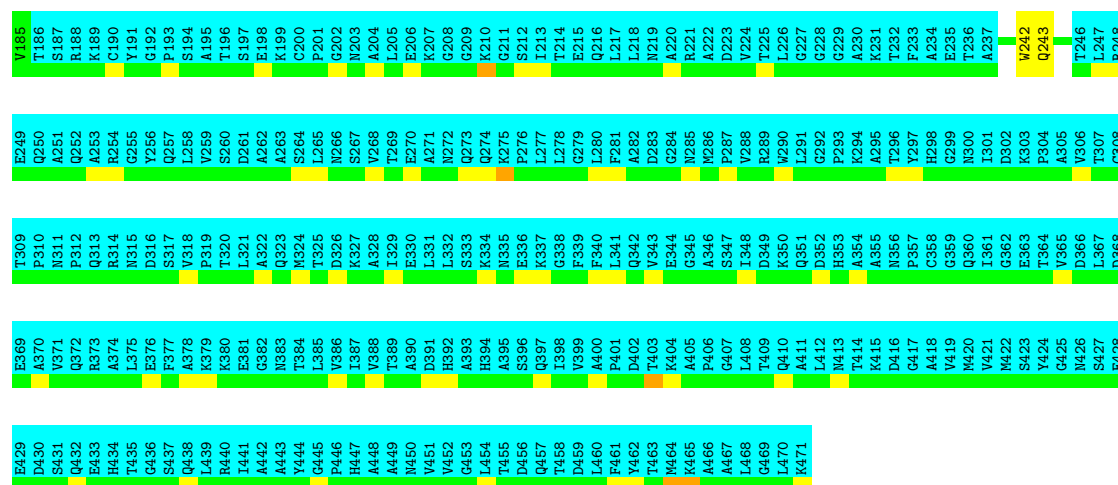


- Molecule 1: Chaperone protein DnaJ 2



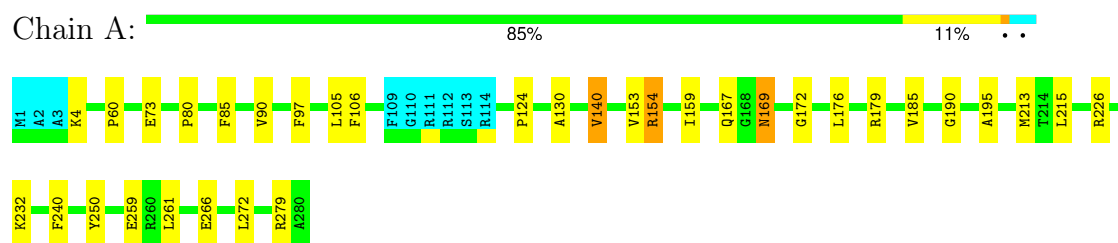
- Molecule 2: Alkaline phosphatase



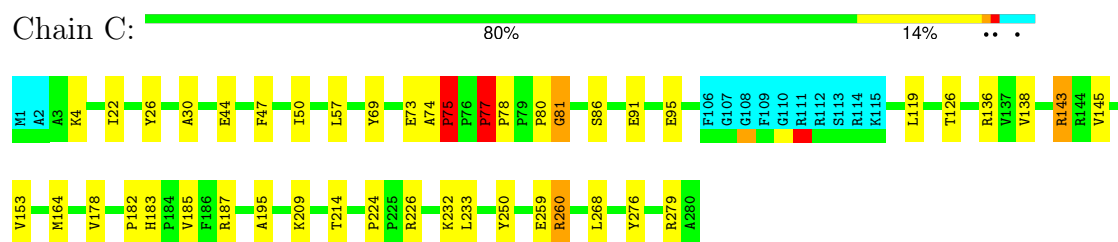


4.2.10 Score per residue for model 10

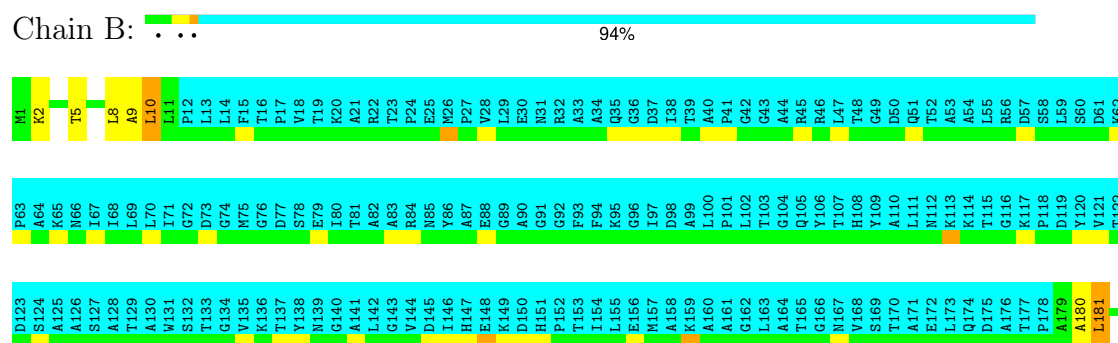
- Molecule 1: Chaperone protein DnaJ 2

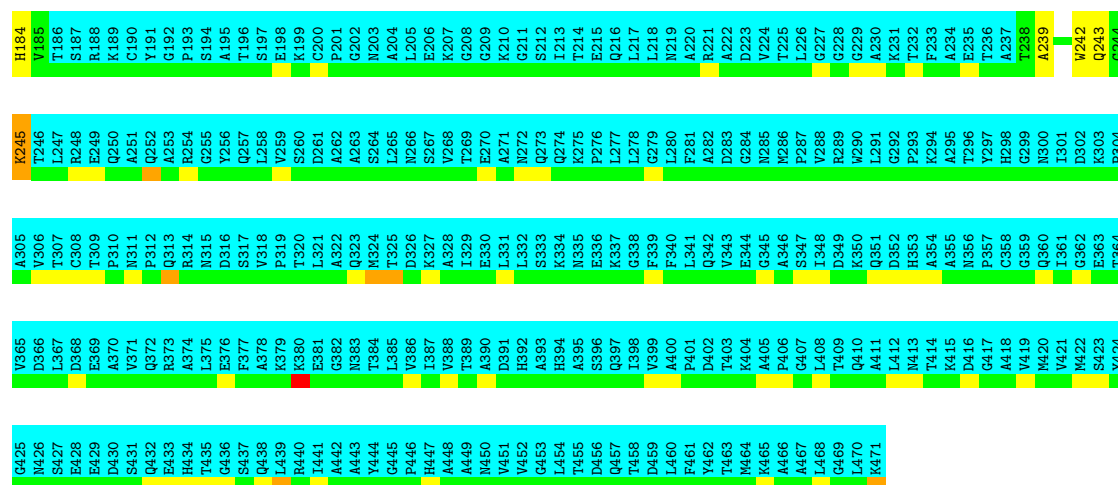


- Molecule 1: Chaperone protein DnaJ 2



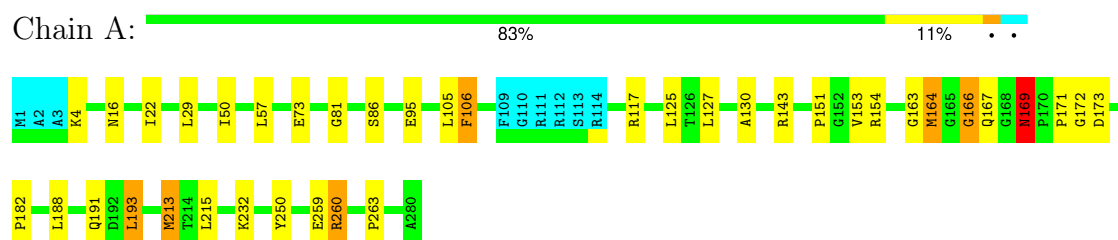
- Molecule 2: Alkaline phosphatase



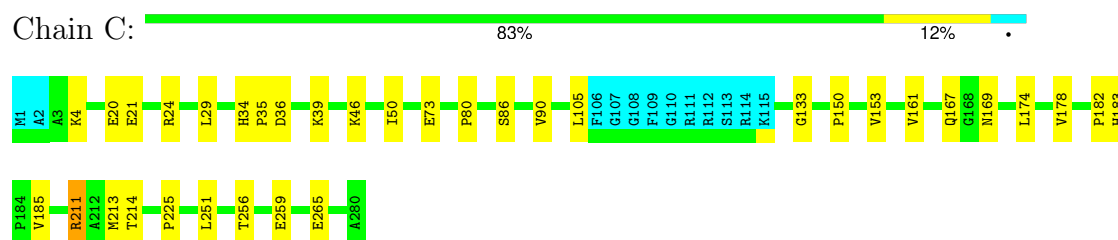


4.2.11 Score per residue for model 11

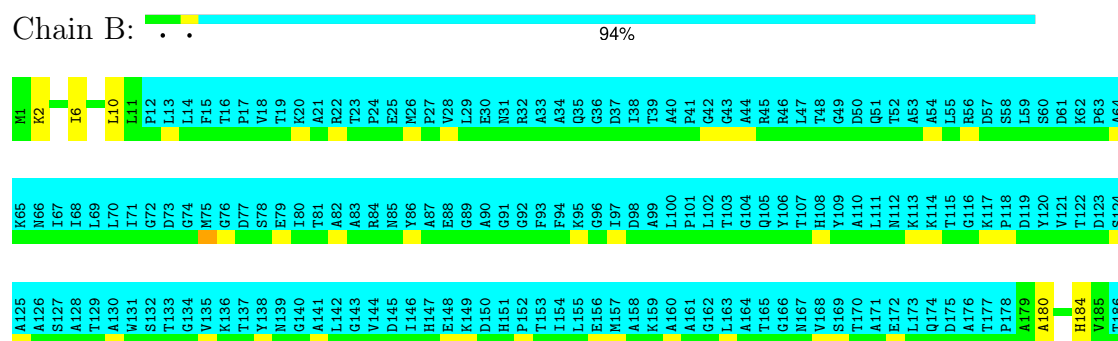
- Molecule 1: Chaperone protein DnaJ 2

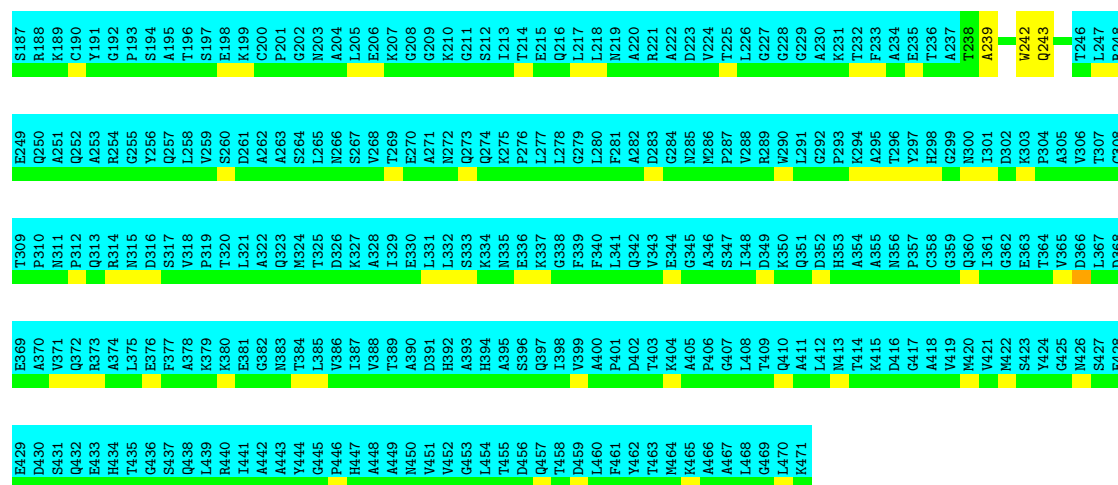


- Molecule 1: Chaperone protein DnaJ 2



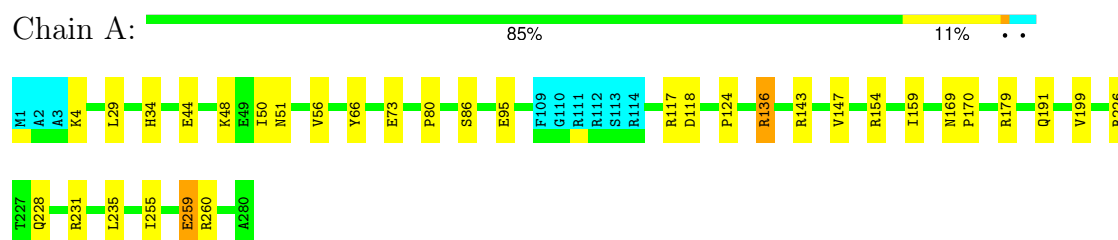
- Molecule 2: Alkaline phosphatase



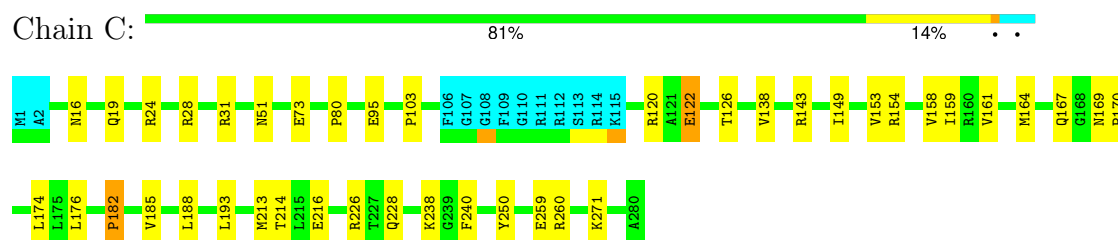


4.2.12 Score per residue for model 12

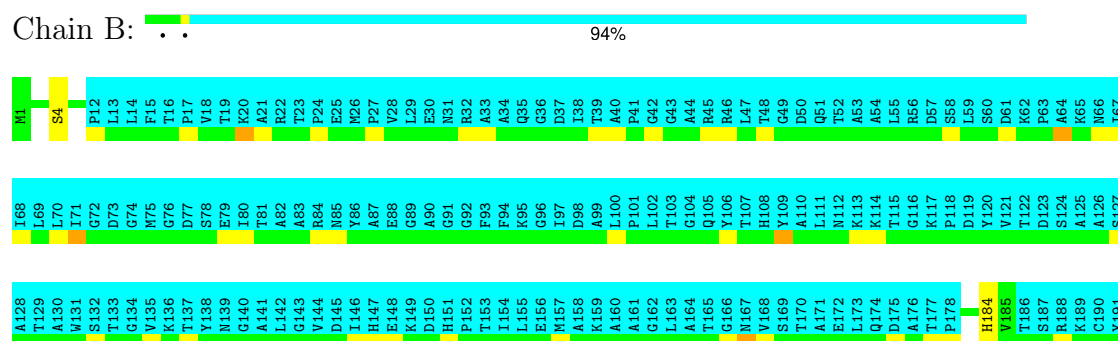
- Molecule 1: Chaperone protein DnaJ 2

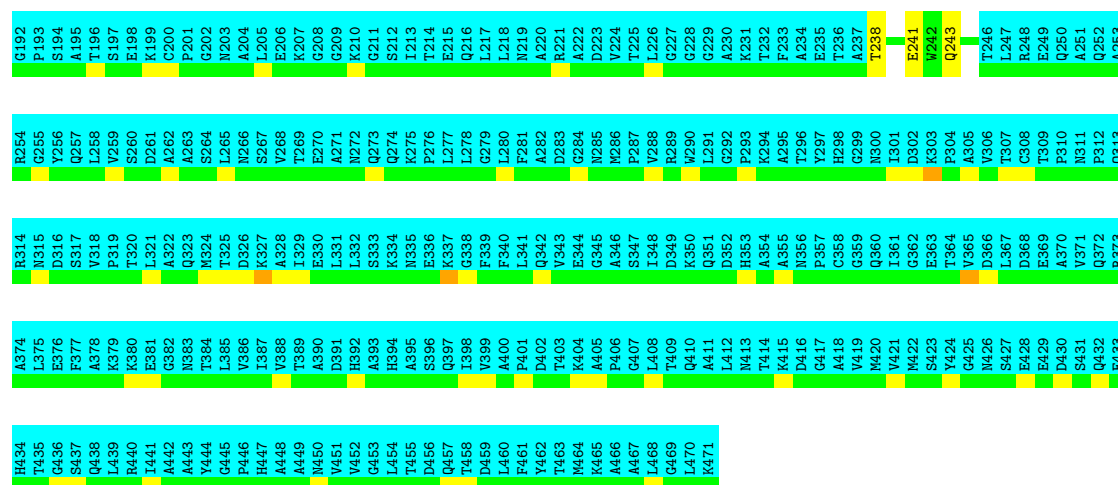


- Molecule 1: Chaperone protein DnaJ 2



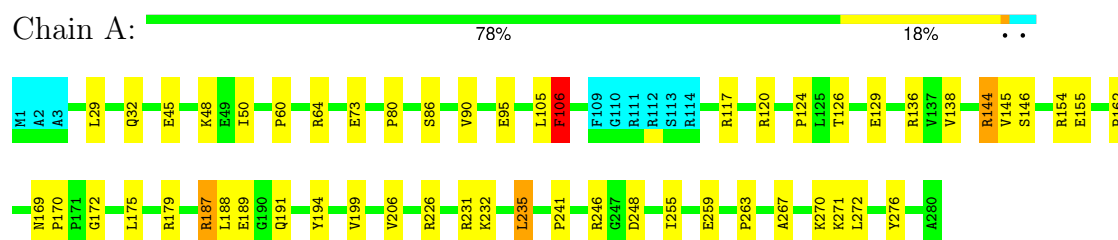
- Molecule 2: Alkaline phosphatase



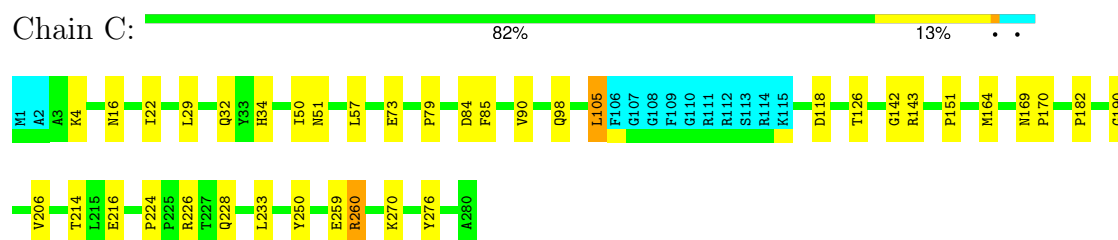


4.2.13 Score per residue for model 13

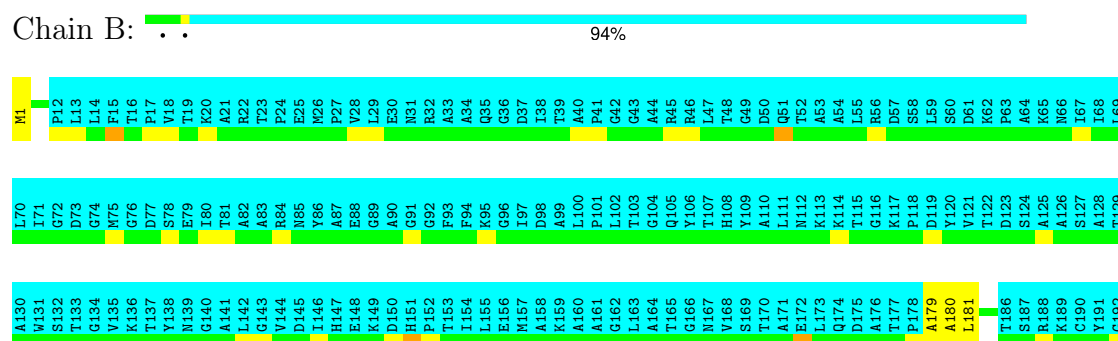
- Molecule 1: Chaperone protein DnaJ 2

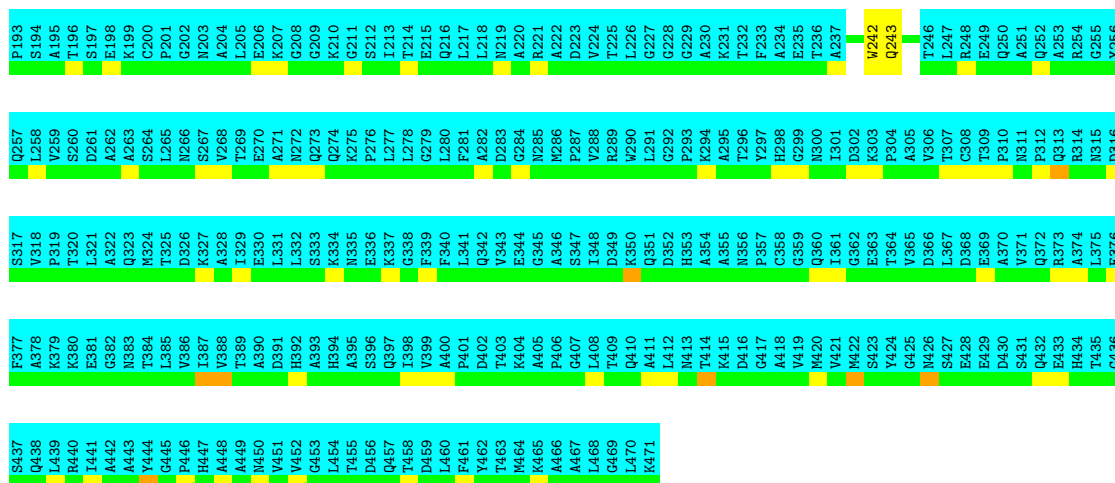


- Molecule 1: Chaperone protein DnaJ 2



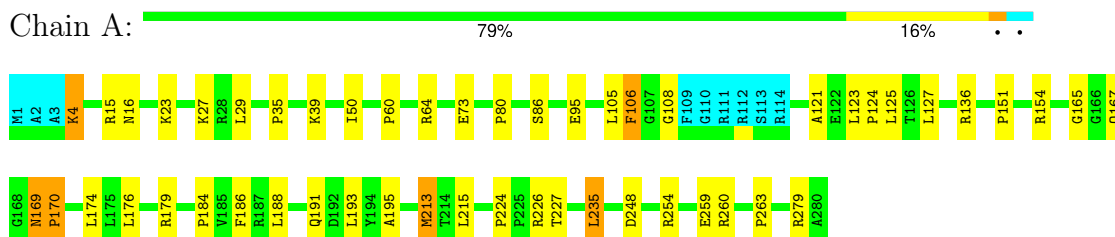
- Molecule 2: Alkaline phosphatase



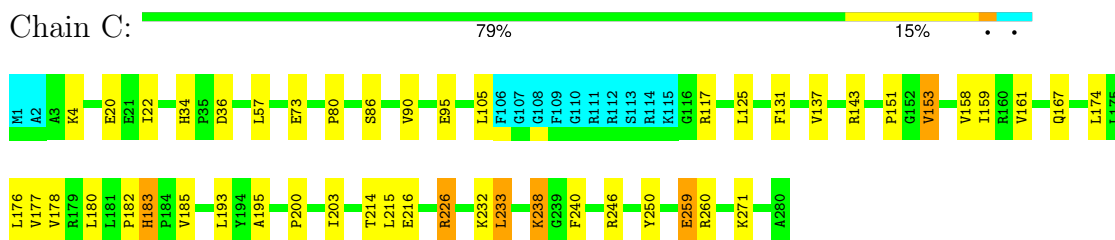


4.2.14 Score per residue for model 14

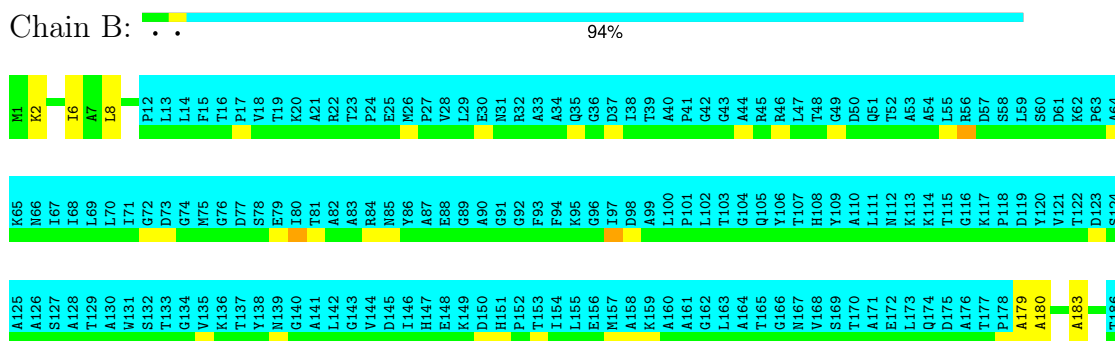
- Molecule 1: Chaparone protein DnaJ 2

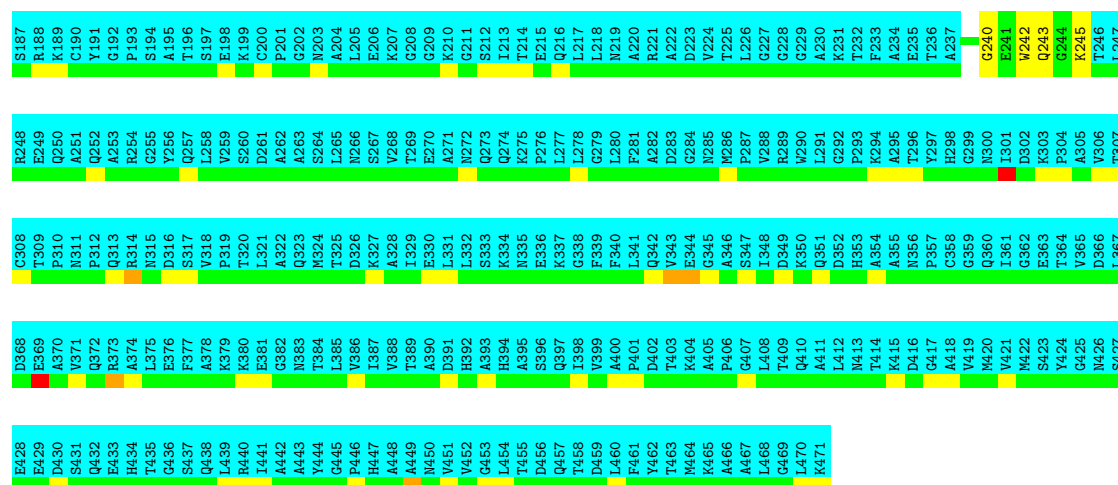


- Molecule 1: Chaparone protein DnaJ 2



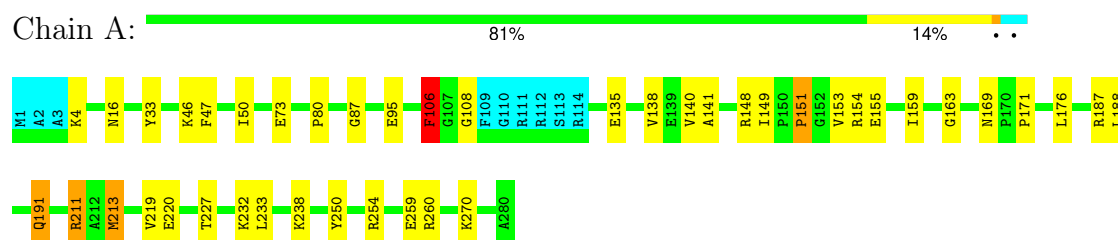
- Molecule 2: Alkaline phosphatase



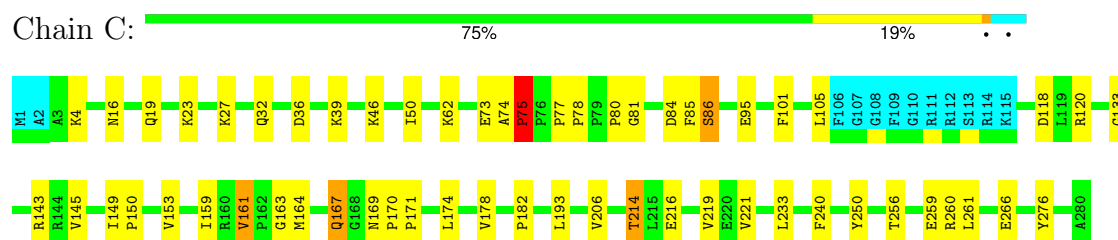


4.2.15 Score per residue for model 15

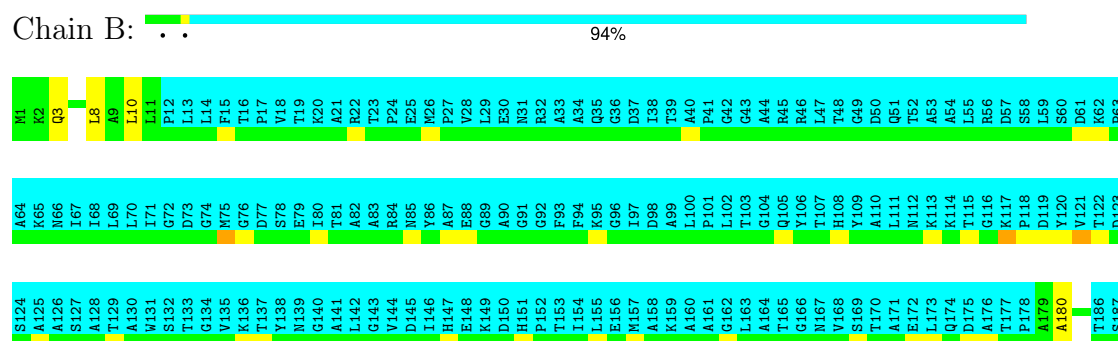
- Molecule 1: Chaperone protein DnaJ 2

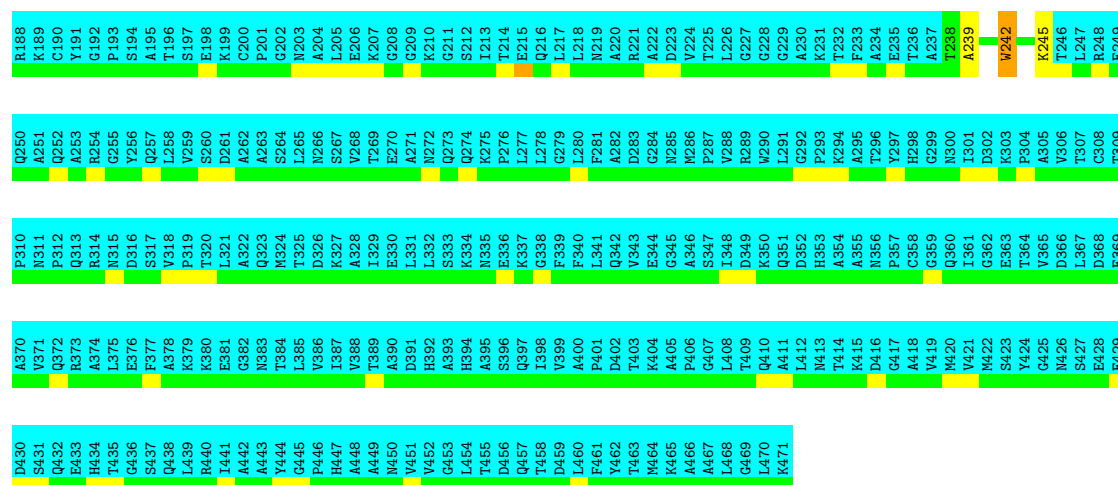


- Molecule 1: Chaperone protein DnaJ 2



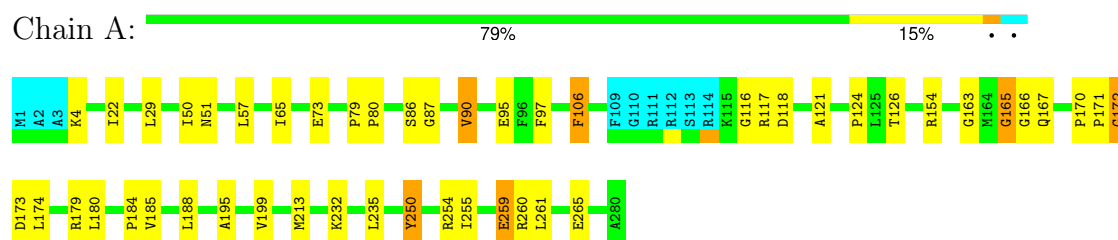
- Molecule 2: Alkaline phosphatase



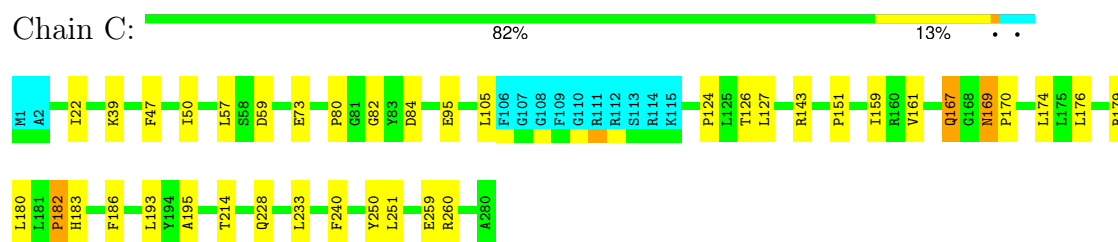


4.2.16 Score per residue for model 16

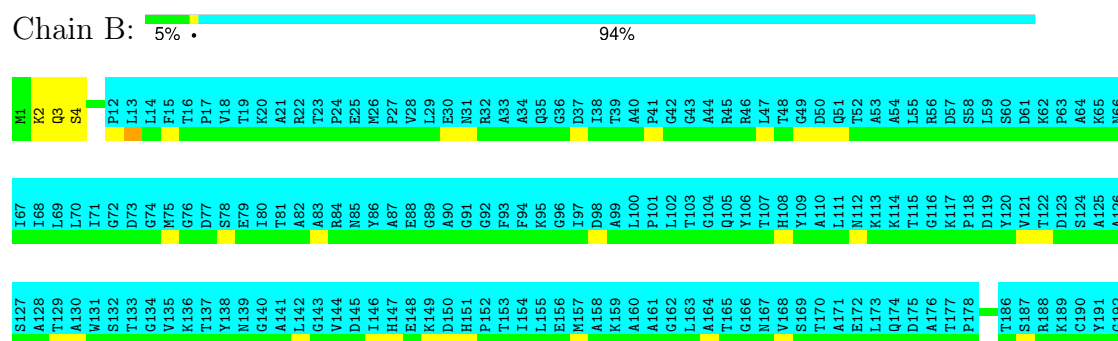
- Molecule 1: Chaperone protein DnaJ 2

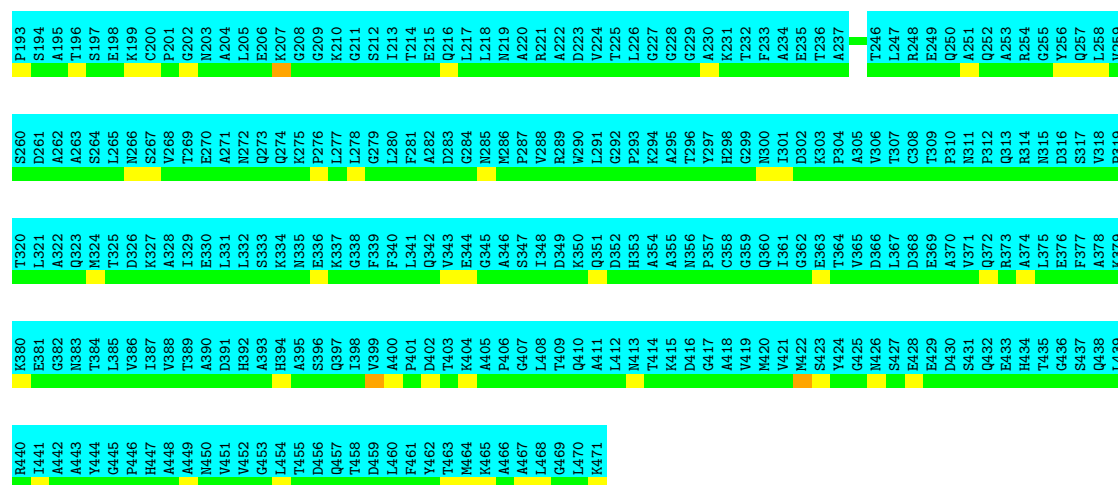


- Molecule 1: Chaperone protein DnaJ 2



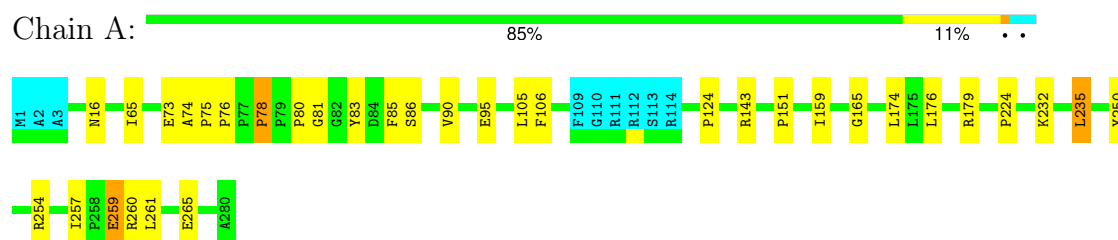
- Molecule 2: Alkaline phosphatase



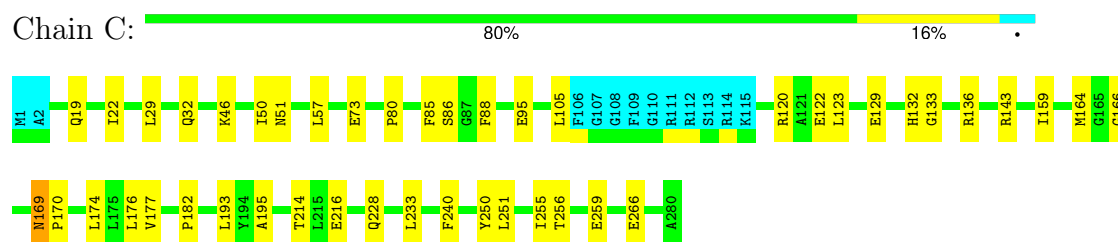


4.2.17 Score per residue for model 17

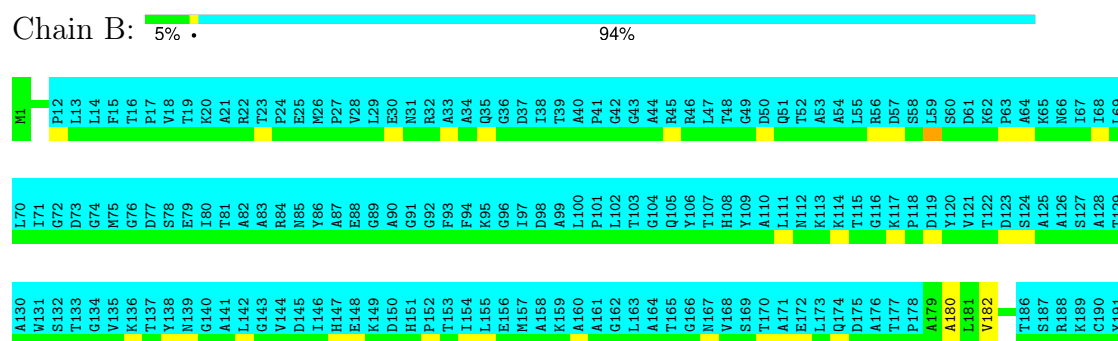
- Molecule 1: Chaparone protein DnaJ 2

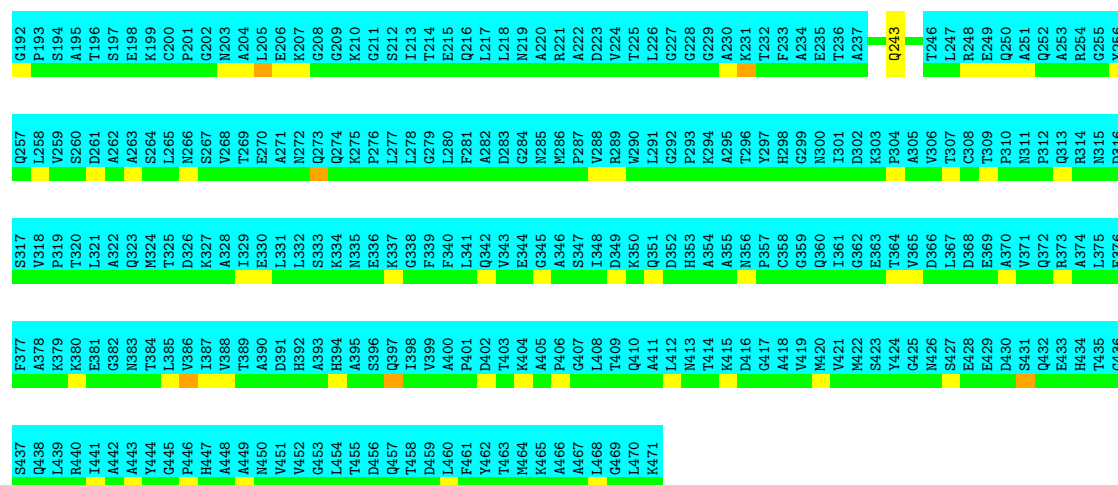


- Molecule 1: Chaparone protein DnaJ 2



- Molecule 2: Alkaline phosphatase

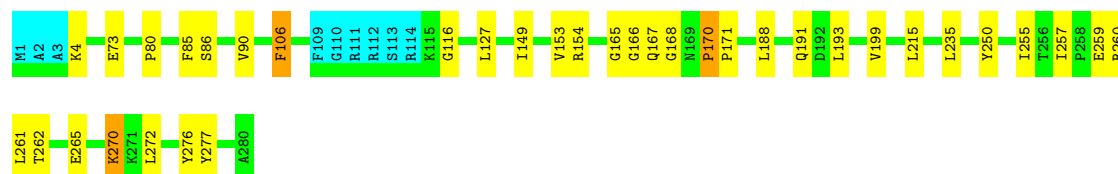




4.2.18 Score per residue for model 18

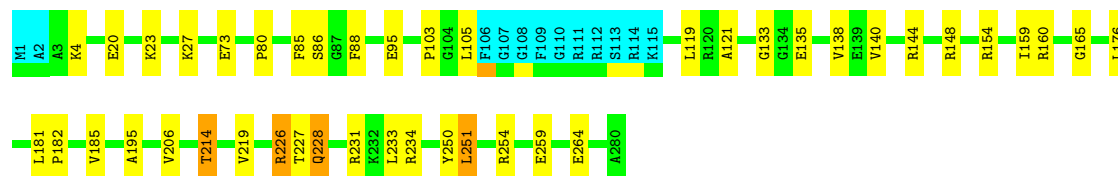
- Molecule 1: Chaperone protein DnaJ 2

Chain A: 84% 12% . .



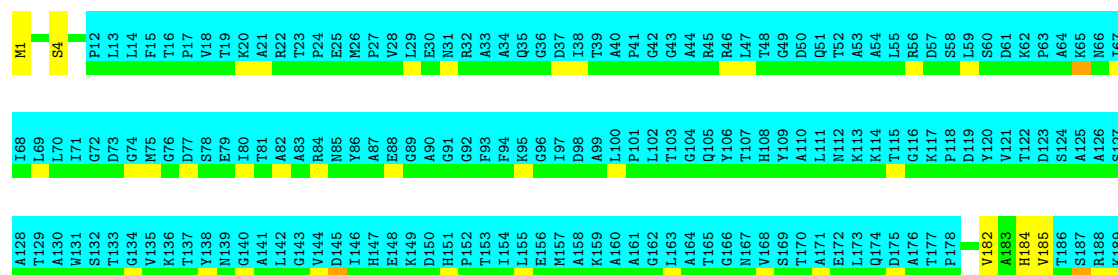
- Molecule 1: Chaperone protein DnaJ 2

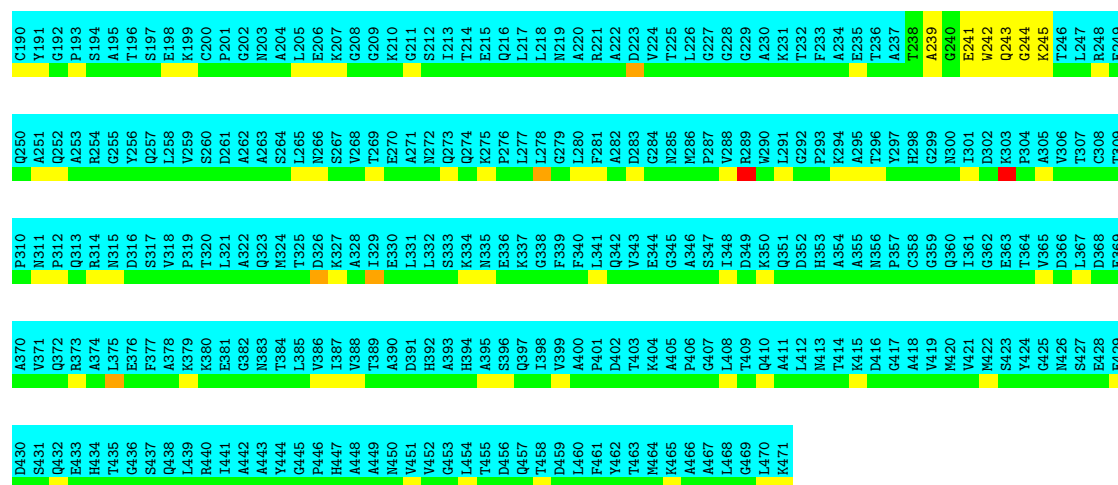
Chain C: 80% 14% . .



- Molecule 2: Alkaline phosphatase

Chain B: 94%

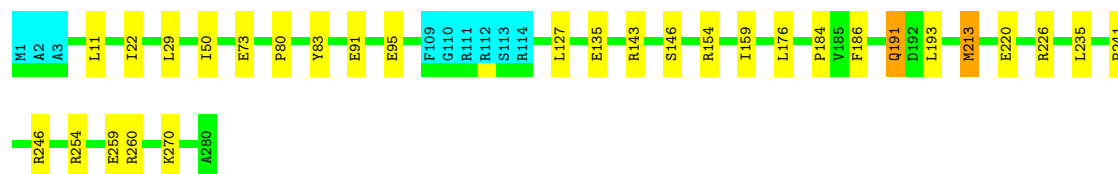




4.2.19 Score per residue for model 19

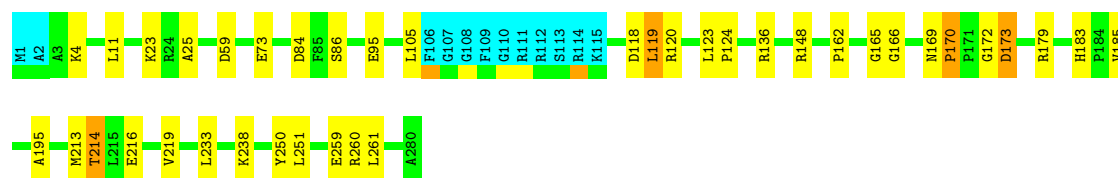
- Molecule 1: Chaperone protein DnaJ 2

Chain A: 86% 10% . .



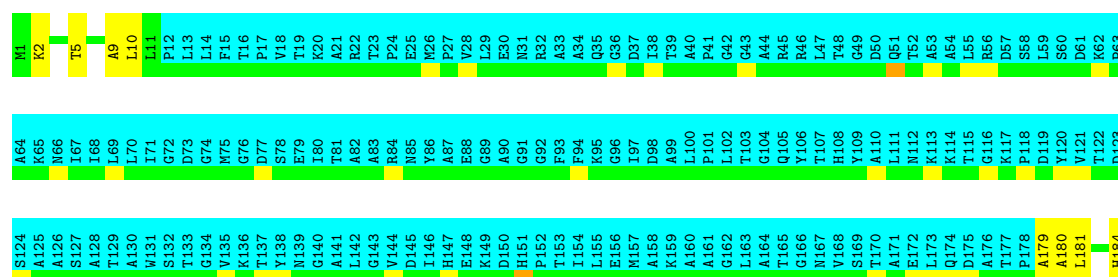
- Molecule 1: Chaperone protein DnaJ 2

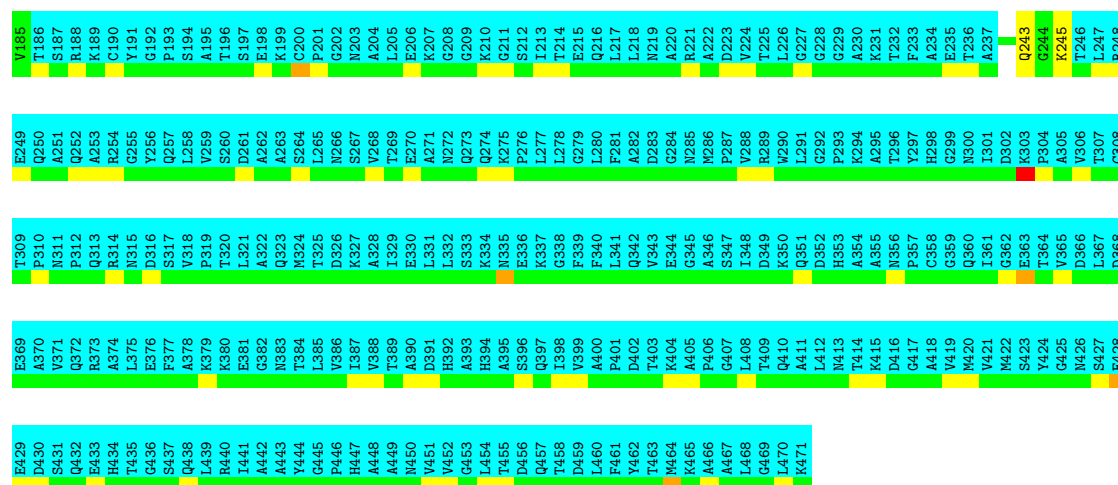
Chain C: 82% 12% . .



- Molecule 2: Alkaline phosphatase

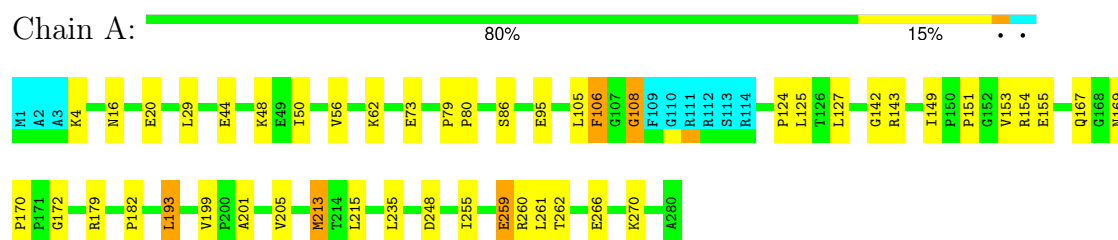
Chain B: 94%



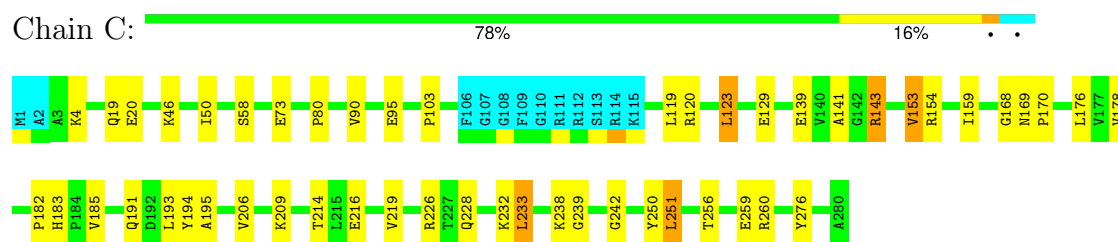


4.2.20 Score per residue for model 20

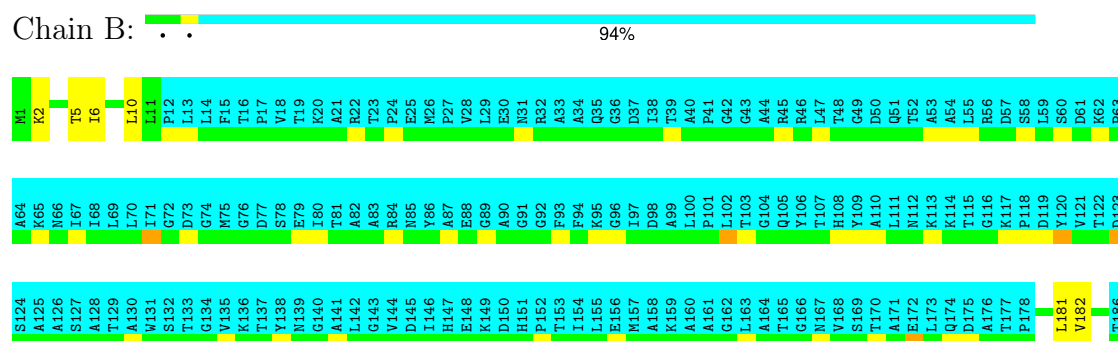
- Molecule 1: Chaperone protein DnaJ 2



- Molecule 1: Chaperone protein DnaJ 2



- Molecule 2: Alkaline phosphatase



D430	A370	P310	Q250	S187
S431	V371	N311	A251	R186
Q432	Q372	P312	A252	K189
E433	R373	Q313	A253	C190
H434	A374	R314	R254	Y191
T435	L375	N315	G255	G192
G436	E376	D316	Y256	P193
S437	F377	S317	Q257	S194
Q438	A378	V318	L258	A195
L439	K379	P319	V259	T196
R440	K380	T320	S260	S197
I441	E381	L321	D261	E198
A442	G382	A322	A262	K199
A443	N383	Q323	A263	C200
Y444	T384	M324	S264	P201
G445	L385	T325	L265	G202
P446	V386	D326	N266	M203
H447	I387	K327	S267	A204
A448	V388	A328	V268	L205
A449	T389	T329	T269	E206
M450	A390	E330	E270	K207
V451	D391	L331	A271	G208
V452	H392	L332	N272	G209
G453	A393	S333	Q273	K210
L454	H394	K334	Q274	G211
T455	A395	N335	K275	S212
D456	S396	E336	P276	L213
Q457	Q397	K337	L277	T214
T458	I398	G338	L278	E215
D459	V399	F339	Q279	Q216
L460	A400	F340	L280	L217
F461	P401	L341	F281	L218
T462	D402	Q342	A282	N219
T463	T403	V343	D283	A220
M464	K404	E344	G284	R221
K465	A405	G345	N285	A222
A466	P406	A346	M286	D223
A467	G407	S347	P287	V224
L468	L408	T348	V288	T225
G469	T409	D349	R289	L226
L470	Q410	K350	W290	G227
K471	A411	Q351	L291	G228
	L412	D352	G292	G229
	N413	H353	P293	A230
	T414	A354	K294	K231
	K415	A355	A295	T232
	D416	N356	T296	F233
	G417	P357	Y297	A234
	A418	C358	H298	E235
	V419	G359	G299	T236
	M420	Q360	N300	A237
	V421	L361	I301	
	M422	G362	D302	W242
	S423	E363	K303	Q243
	Y424	T364	P304	G244
	G425	V365	A305	K245
	N426	D366	V306	T246
	S427	L367	T307	L247
	E428	D368	C308	R248
	E429	E369	T309	E249

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 7 of this report.

Chemical shift file(s)	working_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)	23%

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	0.91±0.01	0±0/2175 (0.0± 0.0%)	0.69±0.02	0±0/2949 (0.0± 0.0%)
1	C	0.92±0.02	0±0/2151 (0.0± 0.0%)	0.69±0.01	0±0/2919 (0.0± 0.0%)
2	B	0.92±0.04	0±0/192 (0.0± 0.0%)	0.73±0.05	0±0/262 (0.0± 0.0%)
All	All	0.92	0/90360 (0.0%)	0.69	4/122600 (0.0%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	144	ARG	NE-CZ-NH2	-5.51	117.54	120.30	6	1
1	C	226	ARG	NE-CZ-NH2	-5.38	117.61	120.30	2	1
1	C	75	PRO	CA-N-CD	-5.29	104.09	111.50	10	2

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	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
2:B:245:LYS:HE2	1:C:222:ALA:HB1	0.55	1.77	1	1
1:A:117:ARG:H	1:A:166:GLY:HA3	0.55	1.62	4	2
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:180:LEU:HD12	1:A:188:LEU:HB3	0.52	1.81	1	1
1:A:87:GLY:H	1:A:163:GLY:HA3	0.52	1.65	9	2
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:N	1:A:213:MET:SD	0.51	2.83	14	8
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: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:A:125:LEU:HA	2:B:6:ILE:HG21	0.50	1.84	14	6
1:C:276:TYR:HA	1:C:279:ARG:HD3	0.50	1.82	10	3
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
1:A:35:PRO:HB3	1:A:44:GLU:HG2	0.48	1.85	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:A:136:ARG:NE	1:A:136:ARG:HA	0.47	2.24	1	1
1:C:145:VAL:HG21	1:C:164:MET:SD	0.47	2.48	10	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:C:183:HIS:H	1:C:184:PRO:HD3	0.47	1.70	1	1
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: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
1:C:195:ALA:HB3	1:C:251:LEU:HG	0.46	1.88	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
1:A:226:ARG:HD2	1:C:259:GLU:O	0.45	2.12	14	1
2:B:180:ALA:HB1	1:C:137:VAL:HG23	0.45	1.87	14	1
1:C:46:LYS:O	1:C:50:ILE:HG12	0.45	2.11	2	9
1:C:167:GLN:HE21	1:C:167:GLN:HA	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:163:GLY:H	1:C:173:ASP:HB3	0.45	1.71	1	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: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:60:PRO:O	1:A:64:ARG:HG3	0.44	2.11	13	1
1:A:206:VAL:HG21	1:C:270:LYS:HA	0.44	1.88	13	1
1:A:272:LEU:HD21	1:C:268:LEU:HB2	0.44	1.88	1	2
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:121:ALA:HB1	2:B:8:LEU:HD11	0.44	1.88	14	1
1:A:22:ILE:HD13	1:A:57:LEU:HD13	0.44	1.88	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	2
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:A:272:LEU:O	1:A:276:TYR:HB2	0.43	2.12	13	3
1:C:152:GLY:HA3	1:C:188:LEU:HD23	0.43	1.89	6	1
1:A:144:ARG:NH1	1:A:146:SER:HB2	0.43	2.28	13	1
1:A:186:PHE:CD1	1:A:195:ALA:HB2	0.43	2.48	1	2
1:C:200:PRO:HG2	1:C:203:ILE:HD12	0.43	1.91	14	2
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: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:C:24:ARG:HA	1:C:27:LYS:HE3	0.43	1.90	1	1
1:A:126:THR:HB	1:A:129:GLU:HG2	0.43	1.90	13	1
1:A:255:ILE:HB	1:C:255:ILE:O	0.43	2.14	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:C:85:PHE:O	1:C:171:PRO:HG3	0.43	2.14	6	1
2:B:181:LEU:HB2	1:C:136:ARG:HB3	0.43	1.90	1	3
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
1:C:59:ASP:HB2	1:C:62:LYS:HD3	0.43	1.90	1	1
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:HA	1:C:238:LYS:NZ	0.43	2.29	14	1
1:C:213:MET:SD	1:C:214:THR:N	0.43	2.91	19	1
1:C:116:GLY:HA2	1:C:168:GLY:HA3	0.42	1.91	1	1
1:C:123:LEU:HD23	1:C:123:LEU:H	0.42	1.74	19	2
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:143:ARG:NH1	1:C:164:MET:SD	0.42	2.92	15	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:195:ALA:HB3	1:A:251:LEU:HD23	0.42	1.92	1	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: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:HE3	2:B:2:LYS:HA	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
1:A:115:LYS:HD2	1:A:170:PRO:HB2	0.42	1.91	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:C:185:VAL:HG12	1:C:195:ALA:HB1	0.42	1.92	1	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:A:60:PRO:O	1:A:64:ARG:HG2	0.41	2.15	14	2
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:C:254:ARG:NH2	1:C:256:THR:HB	0.41	2.30	5	1
2:B:242:TRP:CD2	1:C:233:LEU:HG	0.41	2.49	1	1
1:C:11:LEU:O	1:C:25:ALA:HB1	0.41	2.15	1	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:131:PHE:HB2	1:C:215:LEU:HD13	0.41	1.92	14	2
1:A:149:ILE:HB	1:A:153:VAL:HG11	0.41	1.91	20	3
1:C:86:SER:OG	1:C:163:GLY:HA2	0.41	2.15	15	1
1:C:233:LEU:HD22	1:C:251:LEU:HD12	0.41	1.92	1	1
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:A:48:LYS:HB3	1:A:93:PHE:CE1	0.41	2.50	1	1
1:C:155:GLU:HB2	1:C:180:LEU:HD12	0.41	1.93	8	2
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: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
1:C:191:GLN:NE2	1:C:242:GLY:HA3	0.41	2.31	20	1
1:A:235:LEU:HB3	1:A:238:LYS:HG3	0.41	1.92	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:195:ALA:HB3	1:C:251:LEU:HD23	0.40	1.93	16	2
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: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

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	8±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	A	86	SER	16
1	C	80	PRO	16
1	A	80	PRO	15
1	C	4	LYS	14
1	A	105	LEU	13
1	A	4	LYS	12
1	C	183	HIS	10
2	B	10	LEU	10
1	A	151	PRO	10
2	B	180	ALA	9
2	B	243	GLN	9
1	C	133	GLY	9
1	C	169	ASN	9
1	C	86	SER	9
1	C	105	LEU	8
1	A	106	PHE	8
1	A	16	ASN	8
1	A	263	PRO	7
1	A	184	PRO	6
2	B	184	HIS	6
2	B	239	ALA	5
1	C	16	ASN	5
2	B	179	ALA	5
2	B	4	SER	5
1	A	140	VAL	4
1	C	103	PRO	4
1	A	173	ASP	4

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Mol	Chain	Res	Type	Models (Total)
1	A	108	GLY	4
2	B	242	TRP	4
1	A	191	GLN	4
2	B	2	LYS	4
1	C	170	PRO	4
1	A	172	GLY	4
2	B	183	ALA	3
1	A	90	VAL	3
2	B	5	THR	3
1	C	171	PRO	3
1	A	169	ASN	3
1	C	34	HIS	3
1	C	150	PRO	3
1	A	182	PRO	3
1	A	165	GLY	3
1	C	81	GLY	3
2	B	181	LEU	3
1	C	151	PRO	3
1	A	170	PRO	3
2	B	244	GLY	2
1	C	173	ASP	2
1	A	118	ASP	2
2	B	3	GLN	2
1	A	150	PRO	2
1	A	152	GLY	2
1	A	153	VAL	2
2	B	185	VAL	2
1	C	152	GLY	2
1	C	184	PRO	2
1	A	166	GLY	2
1	C	167	GLN	2
2	B	182	VAL	2
1	C	226	ARG	2
2	B	9	ALA	2
1	C	74	ALA	2
1	C	75	PRO	2
1	C	77	PRO	2
1	A	81	GLY	2
1	A	241	PRO	1
1	C	140	VAL	1
1	C	246	ARG	1
1	C	247	GLY	1

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

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/224 (97%)	206±3 (95±1%)	12±3 (5±1%)	26	75
1	C	216/224 (96%)	204±3 (94±2%)	12±3 (6±2%)	24	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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	A	73	GLU	20
1	C	214	THR	20
1	C	73	GLU	19
1	A	95	GLU	17
1	A	260	ARG	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	126	THR	10
1	A	154	ARG	10
1	C	32	GLN	10
1	C	260	ARG	10
1	A	235	LEU	10
1	A	254	ARG	8
1	C	120	ARG	8
1	A	270	LYS	8
1	A	238	LYS	7
2	B	245	LYS	7
1	C	19	GLN	7
1	A	143	ARG	7
1	A	191	GLN	7
1	C	20	GLU	6
2	B	1	MET	6
2	B	2	LYS	6
1	A	213	MET	6
1	C	139	GLU	5
1	C	51	ASN	5
1	C	119	LEU	5
1	C	143	ARG	5
1	A	20	GLU	5
1	A	39	LYS	5
1	A	85	PHE	5

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Mol	Chain	Res	Type	Models (Total)
1	A	169	ASN	5
1	A	117	ARG	5
1	C	183	HIS	5
1	A	167	GLN	5
1	A	136	ARG	4
1	C	62	LYS	4
1	A	187	ARG	4
1	A	122	GLU	4
1	C	59	ASP	4
1	C	90	VAL	4
1	A	193	LEU	4
1	C	211	ARG	4
1	C	251	LEU	4
1	C	276	TYR	4
2	B	5	THR	4
1	C	153	VAL	4
1	C	167	GLN	4
1	A	232	LYS	3
1	A	32	GLN	3
1	C	123	LEU	3
1	C	85	PHE	3
1	A	90	VAL	3
1	A	279	ARG	3
1	C	39	LYS	3
1	A	248	ASP	3
1	A	120	ARG	2
1	C	46	LYS	2
1	C	136	ARG	2
1	C	187	ARG	2
1	A	115	LYS	2
1	A	277	TYR	2
1	C	206	VAL	2
1	A	19	GLN	2
1	C	42	GLU	2
1	C	265	GLU	2
1	A	34	HIS	2
1	A	189	GLU	2
2	B	184	HIS	2
2	B	241	GLU	2
1	C	118	ASP	2
1	C	91	GLU	2
1	C	117	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	C	75	PRO	2
1	A	51	ASN	2
1	A	226	ARG	2
1	C	271	LYS	2
1	C	228	GLN	2
1	C	233	LEU	2
2	B	3	GLN	2
1	A	250	TYR	2
1	A	262	THR	2
1	A	24	ARG	1
1	C	97	PHE	1
1	C	103	PRO	1
1	A	46	LYS	1
1	A	183	HIS	1
1	A	63	ARG	1
1	A	259	GLU	1
1	A	135	GLU	1
1	A	97	PHE	1
1	A	140	VAL	1
1	A	252	GLU	1
1	C	178	VAL	1
1	C	44	GLU	1
1	C	69	TYR	1
1	C	77	PRO	1
1	A	164	MET	1
2	B	243	GLN	1
1	A	147	VAL	1
2	B	238	THR	1
1	C	122	GLU	1
1	C	182	PRO	1
1	C	250	TYR	1
1	A	144	ARG	1
1	A	4	LYS	1
1	A	15	ARG	1
1	C	238	LYS	1
1	C	246	ARG	1
1	A	138	VAL	1
1	A	211	ARG	1
1	C	36	ASP	1
1	C	161	VAL	1
1	C	169	ASN	1
1	A	78	PRO	1

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Mol	Chain	Res	Type	Models (Total)
1	A	188	LEU	1
1	C	154	ARG	1
1	C	254	ARG	1
1	C	264	GLU	1
1	A	91	GLU	1
1	C	84	ASP	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

The completeness of assignment taking into account all chemical shift lists is 23% for the well-defined parts and 20% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping

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

Total number of shifts	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)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	225	-0.11 ± 0.05	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	194	0.21 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	86	-0.16 ± 0.11	None needed (< 0.5 ppm)
^{15}N	218	-0.00 ± 0.21	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 20%, i.e. 1586 atoms were assigned a chemical shift out of a possible 7766. 0 out of 102 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	810/2773 (29%)	295/1134 (26%)	301/1130 (27%)	214/509 (42%)
Sidechain	776/4475 (17%)	432/2907 (15%)	344/1371 (25%)	0/197 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	0/518 (0%)	0/247 (0%)	0/254 (0%)	0/17 (0%)
Overall	1586/7766 (20%)	727/4288 (17%)	645/2755 (23%)	214/723 (30%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 12%, i.e. 1621 atoms were assigned a chemical shift out of a possible 13715. 0 out of 164 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	830/5104 (16%)	301/2090 (14%)	311/2062 (15%)	218/952 (23%)
Sidechain	791/7778 (10%)	440/5059 (9%)	351/2392 (15%)	0/327 (0%)
Aromatic	0/833 (0%)	0/399 (0%)	0/397 (0%)	0/37 (0%)
Overall	1621/13715 (12%)	741/7548 (10%)	662/4851 (14%)	218/1316 (17%)

7.1.4 Statistically unusual chemical shifts ⓘ

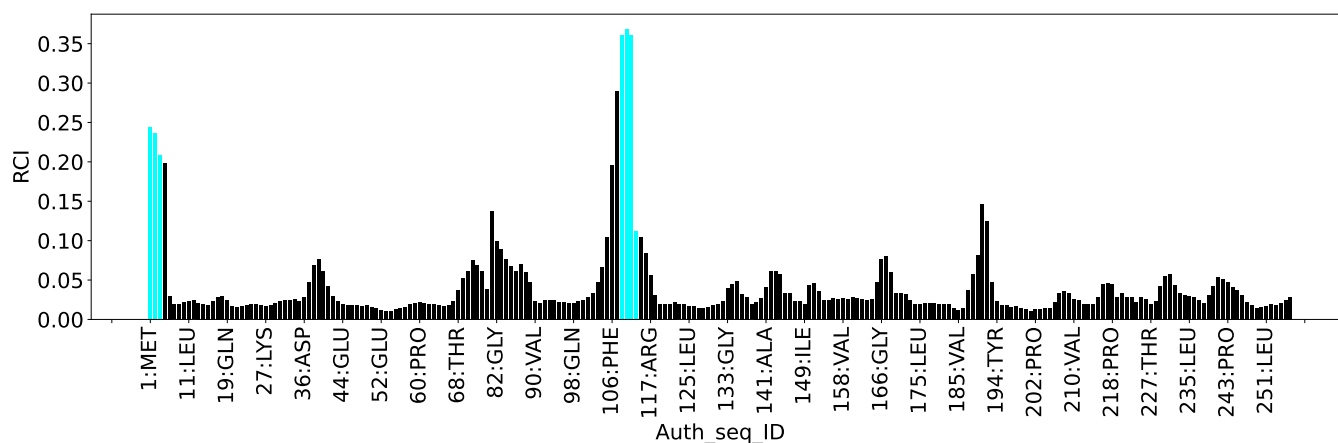
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	52	GLU	HA	2.21	2.24 – 6.23	-5.1
1	A	58	SER	HB2	2.59	2.61 – 5.13	-5.1

7.1.5 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. 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_shifts_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	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

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	31	-0.19 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	32	0.16 ± 0.26	None needed (< 0.5 ppm)
$^{13}\text{C}'$	23	—	None (insufficient data)
^{15}N	379	-0.80 ± 0.14	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 3%, i.e. 230 atoms were assigned a chemical shift out of a possible 7766. 0 out of 102 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	82/2773 (3%)	36/1134 (3%)	26/1130 (2%)	20/509 (4%)
Sidechain	136/4475 (3%)	95/2907 (3%)	40/1371 (3%)	1/197 (1%)
Aromatic	12/518 (2%)	6/247 (2%)	5/254 (2%)	1/17 (6%)
Overall	230/7766 (3%)	137/4288 (3%)	71/2755 (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. 1105 atoms were assigned a chemical shift out of a possible 13715. 0 out of 164 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	844/5104 (17%)	411/2090 (20%)	54/2062 (3%)	379/952 (40%)
Sidechain	241/7778 (3%)	166/5059 (3%)	74/2392 (3%)	1/327 (0%)
Aromatic	20/833 (2%)	10/399 (3%)	9/397 (2%)	1/37 (3%)
Overall	1105/13715 (8%)	587/7548 (8%)	137/4851 (3%)	381/1316 (29%)

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 B:

