



## wwPDB EM Validation Summary Report ⓘ

Dec 19, 2022 – 04:30 am GMT

PDB ID : 7B5H  
EMDB ID : EMD-12029  
Title : Cryo-EM structure of the contractile injection system base plate from Anabaena PCC7120  
Authors : Eisenstein, F.; Weiss, G.L.; Pilhofer, M.  
Deposited on : 2020-12-03  
Resolution : 3.20 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

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:

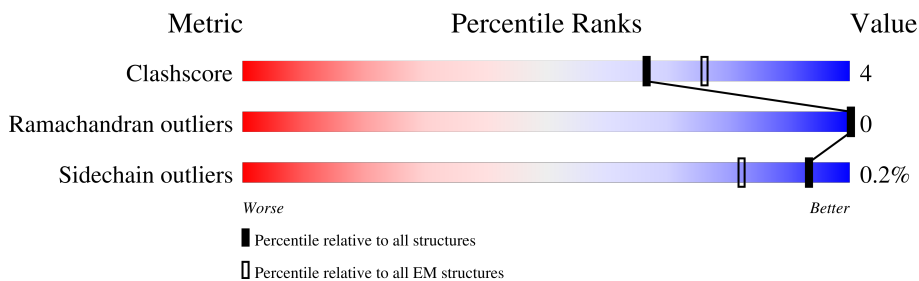
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1476	
1	AB	1476	
1	AC	1476	
1	BA	1476	
1	BB	1476	
1	BC	1476	
1	CA	1476	
1	CB	1476	

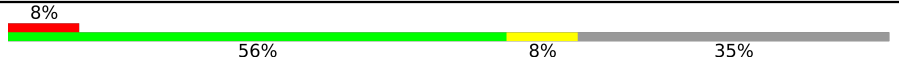

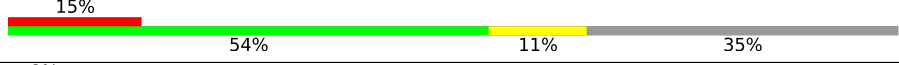

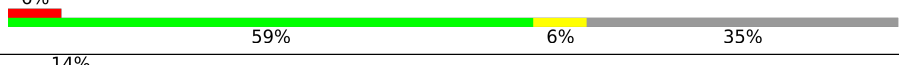
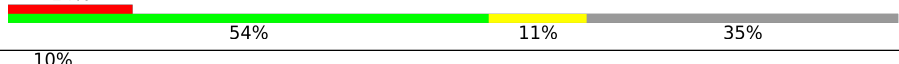
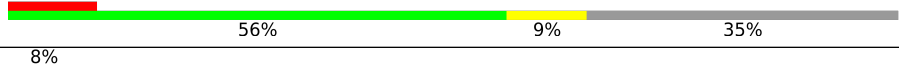

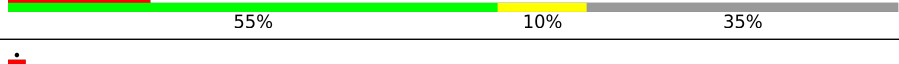
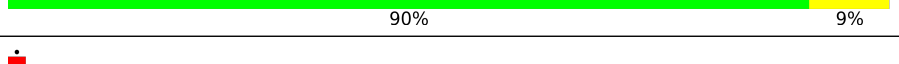
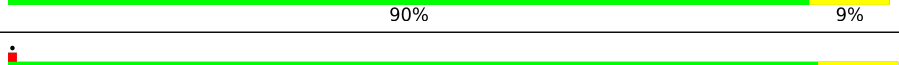
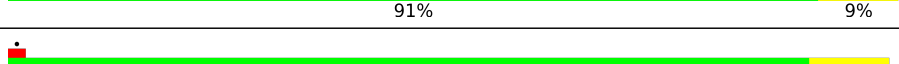
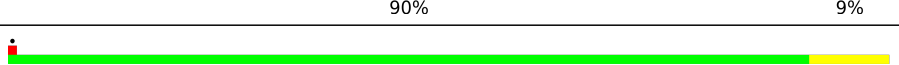
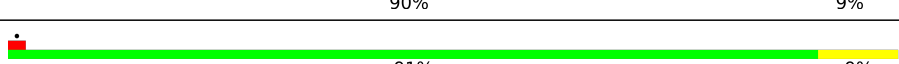
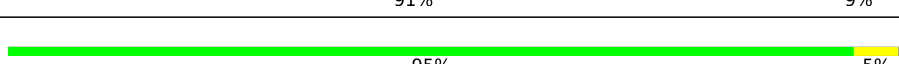
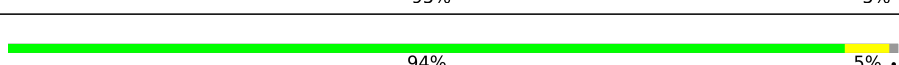
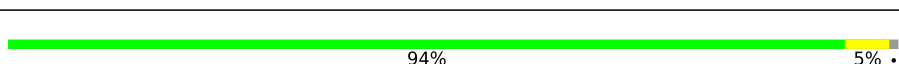
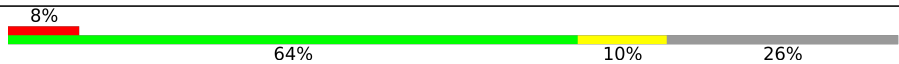
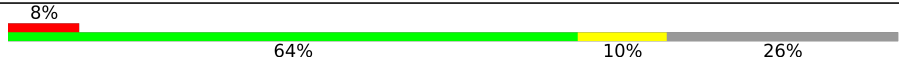


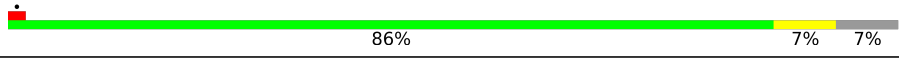
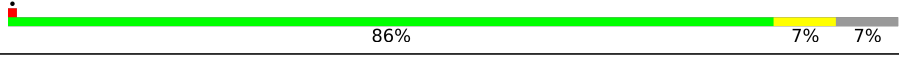


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	CC	1476	
1	DA	1476	
1	DB	1476	
1	DC	1476	
1	EA	1476	
1	EB	1476	
1	EC	1476	
1	FA	1476	
1	FB	1476	
1	FC	1476	
2	AD	1335	
2	BD	1335	
2	CD	1335	
2	DD	1335	
2	ED	1335	
2	FD	1335	
3	AE	154	
3	AF	154	
3	AG	154	
3	BE	154	
3	BF	154	
3	BG	154	
3	CE	154	
3	CF	154	
3	CG	154	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	DE	154	
3	DF	154	
3	DG	154	
3	EE	154	
3	EF	154	
3	EG	154	
3	FE	154	
3	FF	154	
3	FG	154	
4	AH	1231	
4	BH	1231	
4	CH	1231	
4	DH	1231	
4	EH	1231	
4	FH	1231	
5	AJ	589	
5	CJ	589	
5	EJ	589	
6	AL	50	
6	CL	50	
6	EL	50	
7	AI	149	
7	BI	149	
7	CI	149	
7	DI	149	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	EI	149	87% 6% 7%
7	FI	149	85% 7% 7%
8	AK	234	87% 12%
8	BK	234	88% 11%
8	CK	234	86% 13%
8	DK	234	88% 11%
8	EK	234	87% 12%
8	FK	234	87% 12%
9	AM	167	87% 5% 8%
9	BM	167	87% 5% 8%
9	CM	167	87% 5% 8%
9	DM	167	87% 5% 8%
9	EM	167	86% 6% 8%
9	FM	167	87% 5% 8%
10	AN	143	9% 77% 22%
10	BN	143	10% 76% 24%
10	CN	143	9% 78% 22%
10	DN	143	10% 77% 22%
10	EN	143	9% 77% 22%
10	FN	143	10% 76% 23%
11	AO	484	92% 6%
11	AP	484	93% 6%
11	AQ	484	53% 93% 6%
11	BO	484	92% 6%
11	BP	484	93% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
11	BQ	484	
11	CO	484	
11	CP	484	
11	CQ	484	
11	DO	484	
11	DP	484	
11	DQ	484	
11	EO	484	
11	EP	484	
11	EQ	484	
11	FO	484	
11	FP	484	
11	FQ	484	

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 346635 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called All3314 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AA	729	5899	3784	991	1111	13	0	0
1	AB	724	5886	3781	989	1103	13	0	0
1	AC	700	5690	3659	957	1063	11	0	0
1	BA	729	5899	3784	991	1111	13	0	0
1	BB	724	5886	3781	989	1103	13	0	0
1	BC	700	5690	3659	957	1063	11	0	0
1	CA	729	5899	3784	991	1111	13	0	0
1	CB	724	5886	3781	989	1103	13	0	0
1	CC	700	5690	3659	957	1063	11	0	0
1	DA	729	5899	3784	991	1111	13	0	0
1	DB	724	5886	3781	989	1103	13	0	0
1	DC	700	5690	3659	957	1063	11	0	0
1	EA	729	5899	3784	991	1111	13	0	0
1	EB	724	5886	3781	989	1103	13	0	0
1	EC	700	5690	3659	957	1063	11	0	0
1	FA	729	5899	3784	991	1111	13	0	0
1	FB	724	5886	3781	989	1103	13	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	FC	700	5690	3659	957	1063	11	0	0

- Molecule 2 is a protein called All3315 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AD	1109	9112	5798	1557	1744	13	0	0
2	BD	1109	9112	5798	1557	1744	13	0	0
2	CD	1109	9112	5798	1557	1744	13	0	0
2	DD	1109	9112	5798	1557	1744	13	0	0
2	ED	1109	9112	5798	1557	1744	13	0	0
2	FD	1109	9112	5798	1557	1744	13	0	0

- Molecule 3 is a protein called All3316 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AE	100	845	532	148	163	2	0	0
3	AF	100	845	532	148	163	2	0	0
3	AG	100	845	532	148	163	2	0	0
3	BE	100	845	532	148	163	2	0	0
3	BF	100	845	532	148	163	2	0	0
3	BG	100	845	532	148	163	2	0	0
3	CE	100	845	532	148	163	2	0	0
3	CF	100	845	532	148	163	2	0	0
3	CG	100	845	532	148	163	2	0	0
3	DE	100	845	532	148	163	2	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
3	DF	100	Total	C	N	O	S	0	0
			845	532	148	163	2		
3	DG	100	Total	C	N	O	S	0	0
			845	532	148	163	2		
3	EE	100	Total	C	N	O	S	0	0
			845	532	148	163	2		
3	EF	100	Total	C	N	O	S	0	0
			845	532	148	163	2		
3	EG	100	Total	C	N	O	S	0	0
			845	532	148	163	2		
3	FE	100	Total	C	N	O	S	0	0
			845	532	148	163	2		
3	FF	100	Total	C	N	O	S	0	0
			845	532	148	163	2		
3	FG	100	Total	C	N	O	S	0	0
			845	532	148	163	2		

- Molecule 4 is a protein called All3317 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AH	1227	Total	C	N	O	S	0	0
			9792	6278	1676	1825	13		
4	BH	1227	Total	C	N	O	S	0	0
			9792	6278	1676	1825	13		
4	CH	1227	Total	C	N	O	S	0	0
			9792	6278	1676	1825	13		
4	DH	1227	Total	C	N	O	S	0	0
			9792	6278	1676	1825	13		
4	EH	1227	Total	C	N	O	S	0	0
			9792	6278	1676	1825	13		
4	FH	1227	Total	C	N	O	S	0	0
			9792	6278	1676	1825	13		

- Molecule 5 is a protein called All3320 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AJ	585	Total	C	N	O	S	0	0
			4438	2782	775	870	11		
5	CJ	585	Total	C	N	O	S	0	0
			4438	2782	775	870	11		
5	EJ	585	Total	C	N	O	S	0	0
			4438	2782	775	870	11		

- Molecule 6 is a protein called Asl3322 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AL	37	Total	C	N	O	S	0	0
			285	179	49	56	1		
6	CL	37	Total	C	N	O	S	0	0
			285	179	49	56	1		
6	EL	37	Total	C	N	O	S	0	0
			285	179	49	56	1		

- Molecule 7 is a protein called All3318 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AI	138	Total	C	N	O	S	0	0
			1098	696	184	215	3		
7	BI	138	Total	C	N	O	S	0	0
			1098	696	184	215	3		
7	CI	138	Total	C	N	O	S	0	0
			1098	696	184	215	3		
7	DI	138	Total	C	N	O	S	0	0
			1098	696	184	215	3		
7	EI	138	Total	C	N	O	S	0	0
			1098	696	184	215	3		
7	FI	138	Total	C	N	O	S	0	0
			1098	696	184	215	3		

- Molecule 8 is a protein called All3321 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AK	232	Total	C	N	O	S	0	0
			1898	1210	328	357	3		
8	BK	232	Total	C	N	O	S	0	0
			1898	1210	328	357	3		
8	CK	232	Total	C	N	O	S	0	0
			1898	1210	328	357	3		
8	DK	232	Total	C	N	O	S	0	0
			1898	1210	328	357	3		
8	EK	232	Total	C	N	O	S	0	0
			1898	1210	328	357	3		
8	FK	232	Total	C	N	O	S	0	0
			1898	1210	328	357	3		

- Molecule 9 is a protein called All3323 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AM	153	Total	C	N	O	S	0	0
			1254	808	208	232	6		
9	BM	153	Total	C	N	O	S	0	0
			1254	808	208	232	6		
9	CM	153	Total	C	N	O	S	0	0
			1254	808	208	232	6		
9	DM	153	Total	C	N	O	S	0	0
			1254	808	208	232	6		
9	EM	153	Total	C	N	O	S	0	0
			1254	808	208	232	6		
9	FM	153	Total	C	N	O	S	0	0
			1254	808	208	232	6		

- Molecule 10 is a protein called All3324 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AN	142	Total	C	N	O	S	0	0
			1152	734	198	217	3		
10	BN	142	Total	C	N	O	S	0	0
			1152	734	198	217	3		
10	CN	142	Total	C	N	O	S	0	0
			1152	734	198	217	3		
10	DN	142	Total	C	N	O	S	0	0
			1152	734	198	217	3		
10	EN	142	Total	C	N	O	S	0	0
			1152	734	198	217	3		
10	FN	142	Total	C	N	O	S	0	0
			1152	734	198	217	3		

- Molecule 11 is a protein called All3325 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AO	473	Total	C	N	O	S	0	0
			3663	2328	616	705	14		
11	AP	480	Total	C	N	O	S	0	0
			3716	2365	624	713	14		
11	AQ	480	Total	C	N	O	S	0	0
			3716	2365	624	713	14		
11	BO	473	Total	C	N	O	S	0	0
			3663	2328	616	705	14		
11	BP	480	Total	C	N	O	S	0	0
			3716	2365	624	713	14		
11	BQ	480	Total	C	N	O	S	0	0
			3716	2365	624	713	14		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
11	CO	473	Total	C	N	O	S	0	0
			3663	2328	616	705	14		
11	CP	480	Total	C	N	O	S	0	0
			3716	2365	624	713	14		
11	CQ	480	Total	C	N	O	S	0	0
			3716	2365	624	713	14		
11	DO	473	Total	C	N	O	S	0	0
			3663	2328	616	705	14		
11	DP	480	Total	C	N	O	S	0	0
			3716	2365	624	713	14		
11	DQ	480	Total	C	N	O	S	0	0
			3716	2365	624	713	14		
11	EO	473	Total	C	N	O	S	0	0
			3663	2328	616	705	14		
11	EP	480	Total	C	N	O	S	0	0
			3716	2365	624	713	14		
11	EQ	480	Total	C	N	O	S	0	0
			3716	2365	624	713	14		
11	FO	473	Total	C	N	O	S	0	0
			3663	2328	616	705	14		
11	FP	480	Total	C	N	O	S	0	0
			3716	2365	624	713	14		
11	FQ	480	Total	C	N	O	S	0	0
			3716	2365	624	713	14		





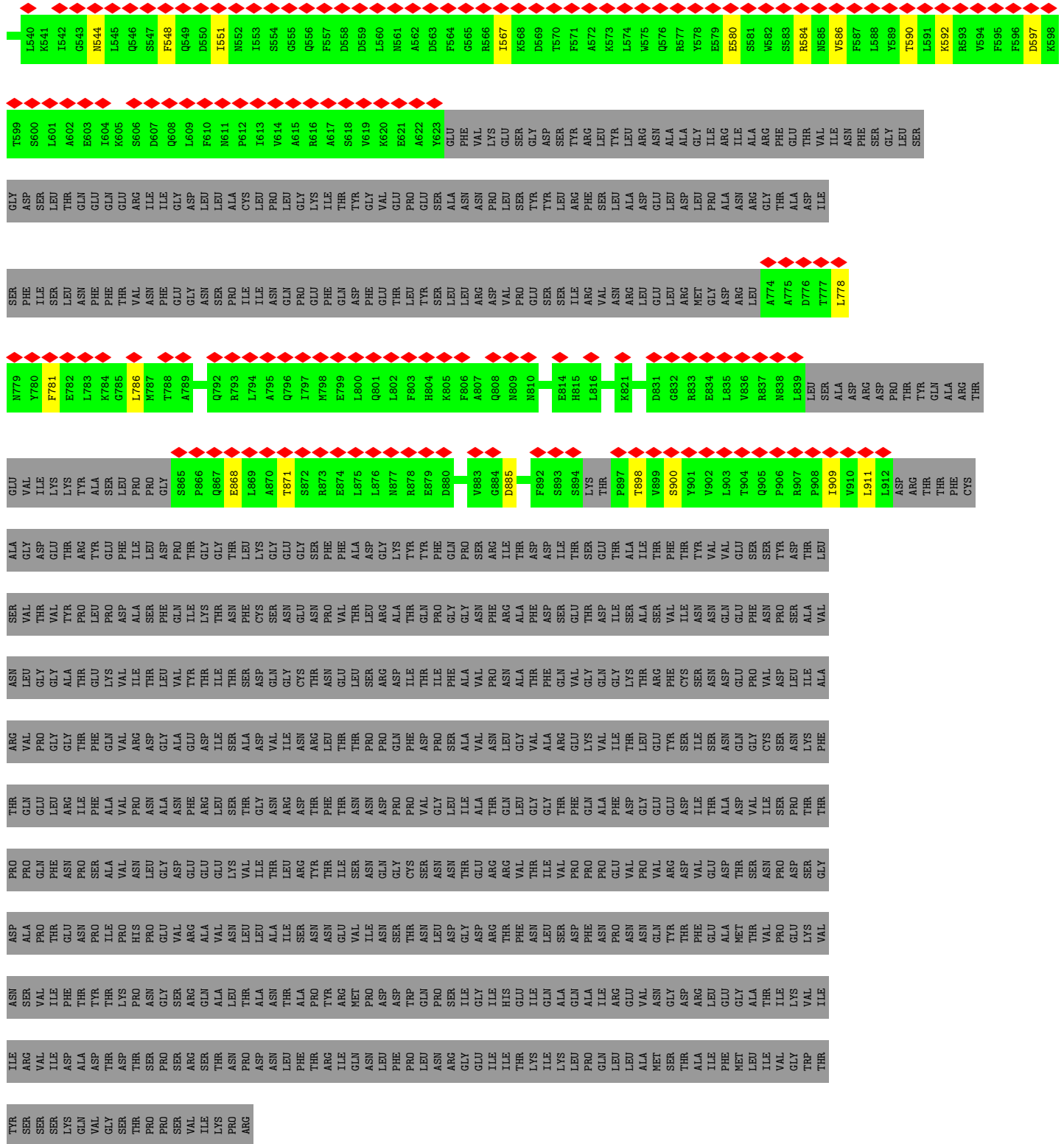




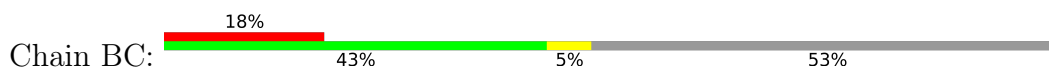






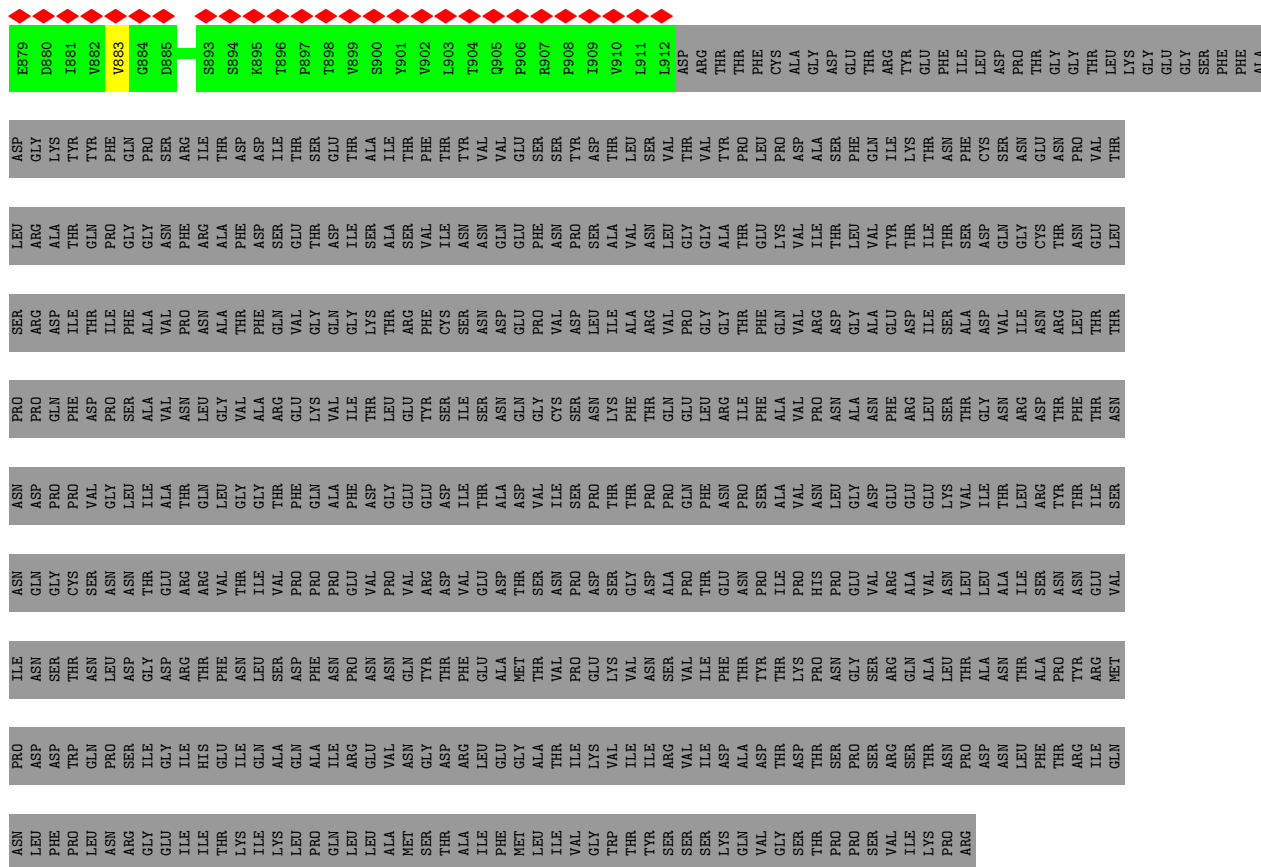


● Molecule 1: All3314 protein

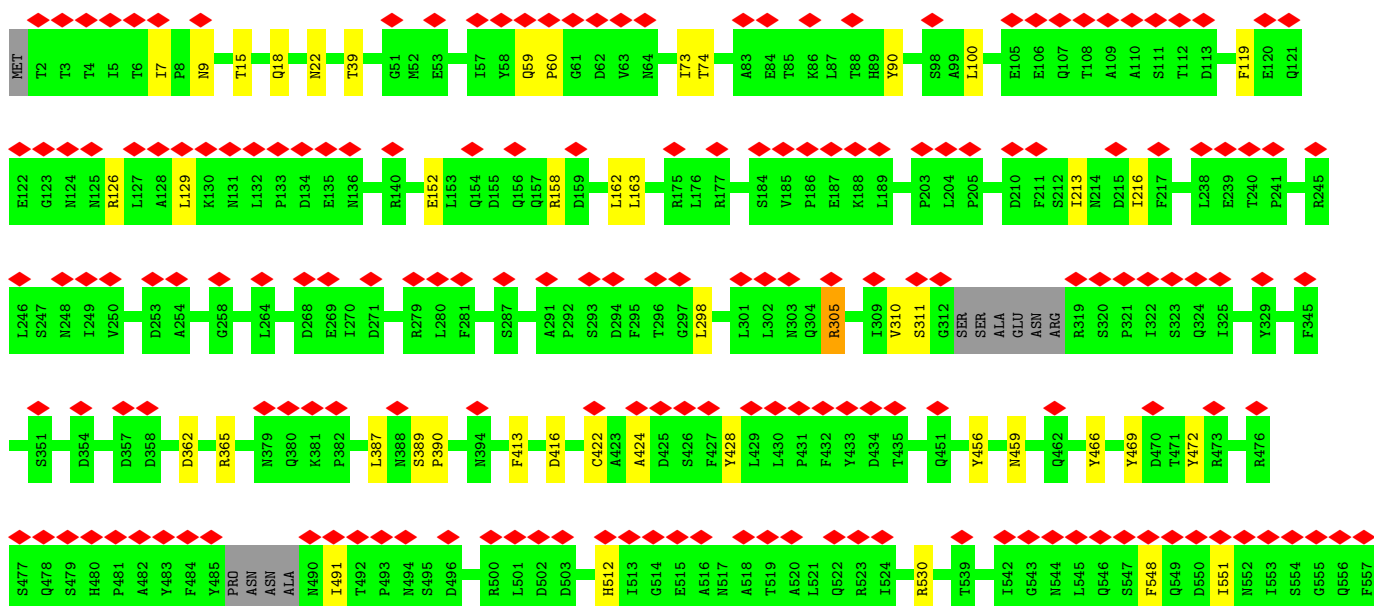








● Molecule 1: All3314 protein











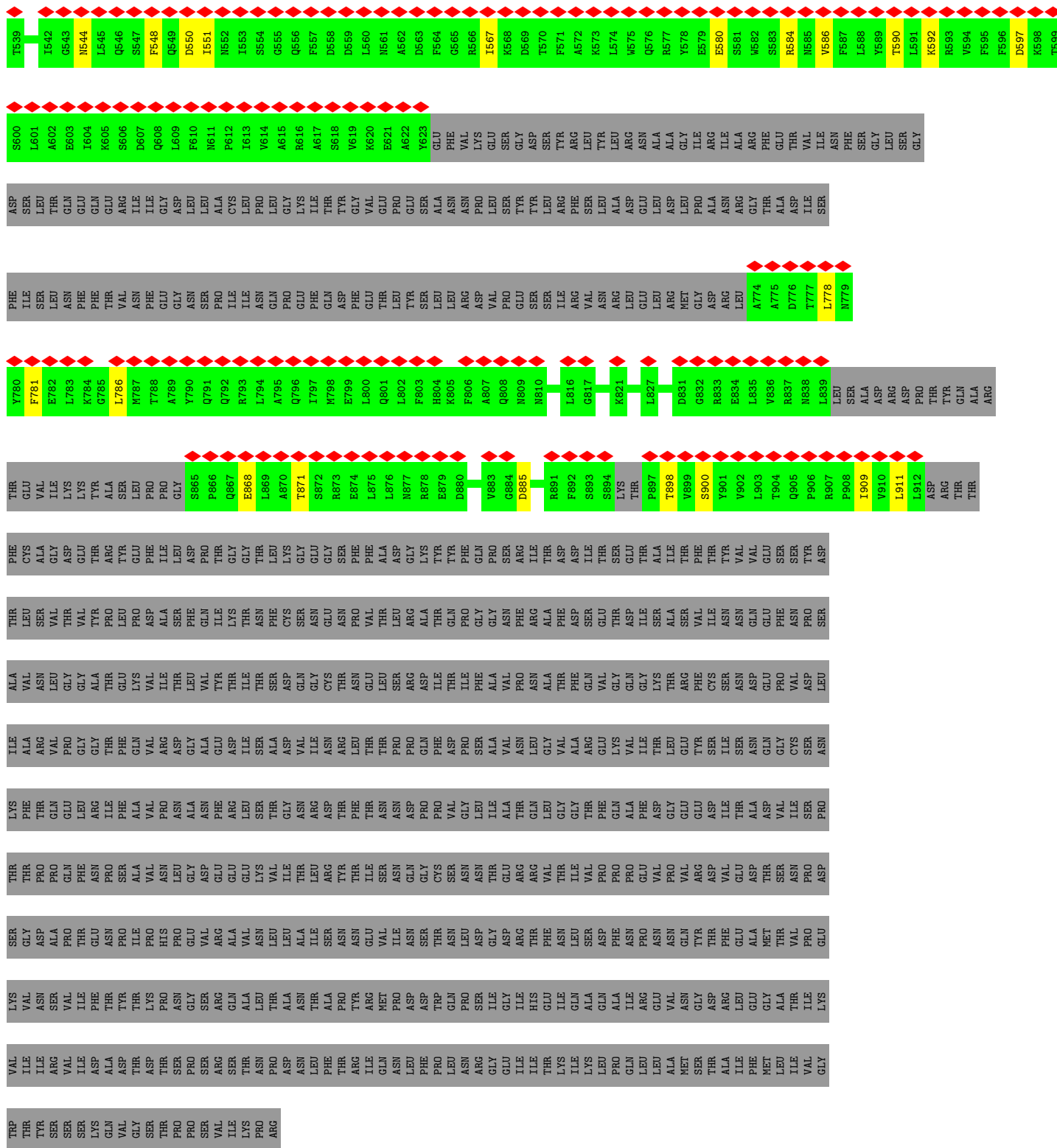












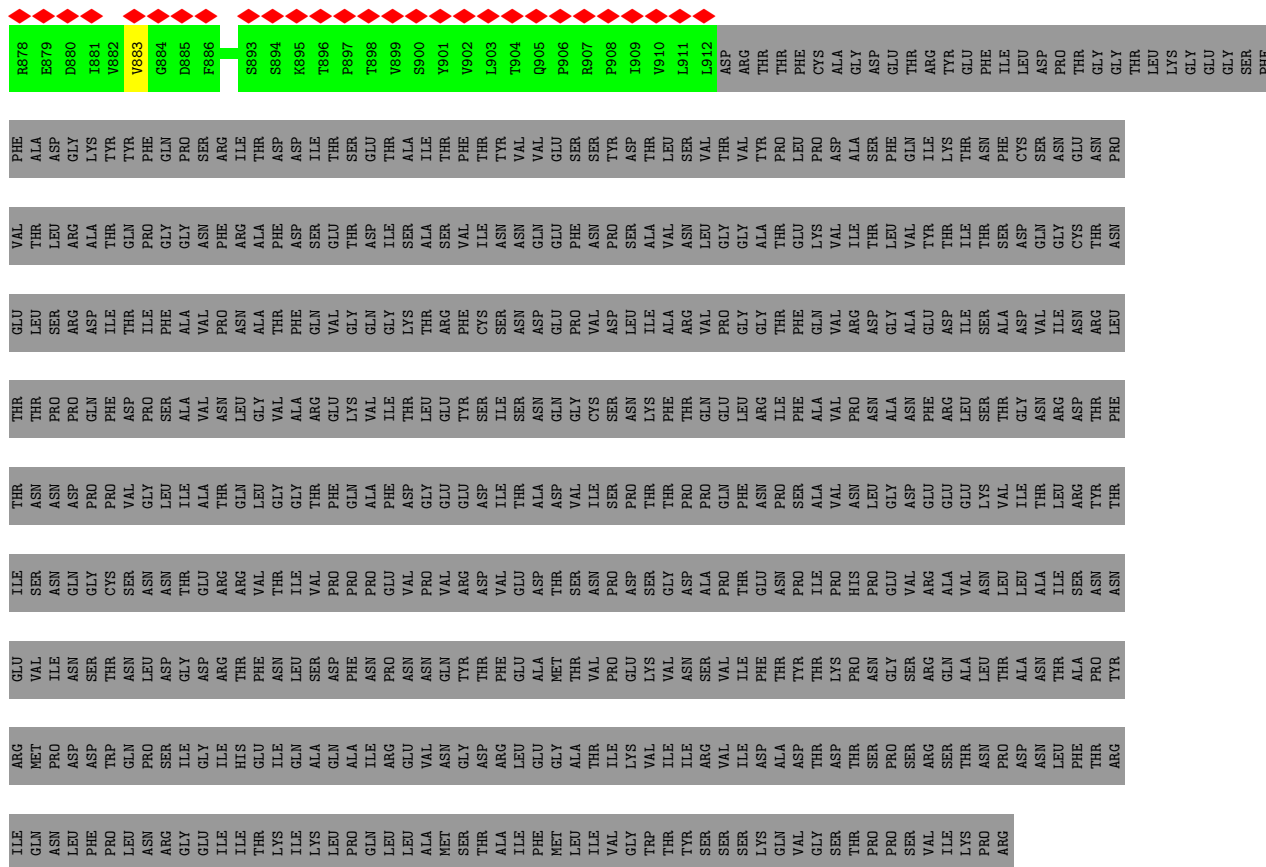
● Molecule 1: All3314 protein



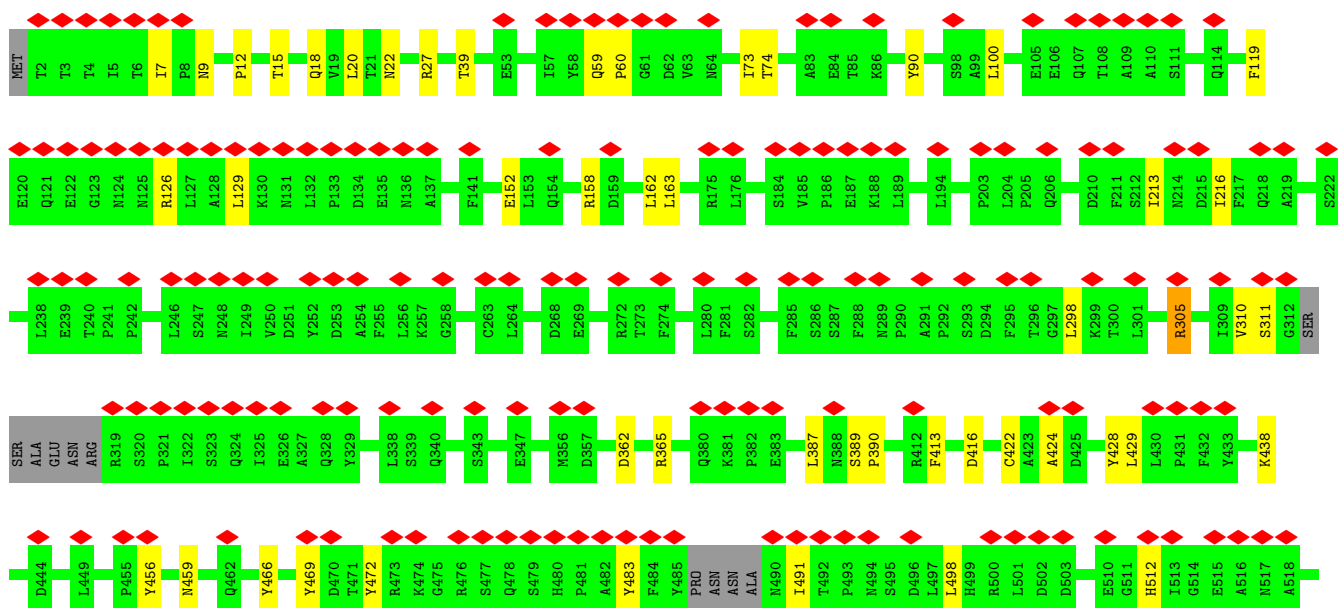


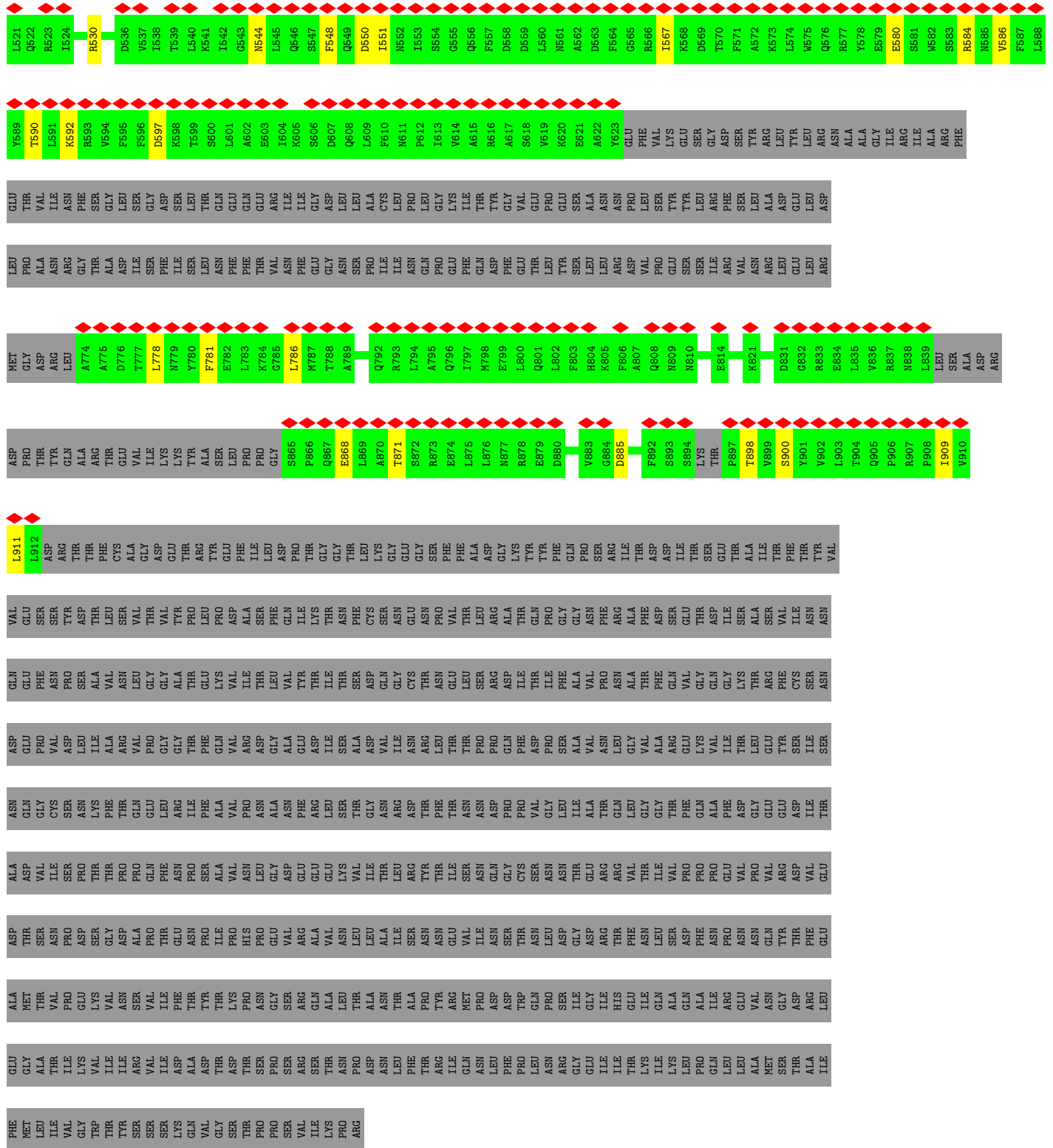






● Molecule 1: All3314 protein





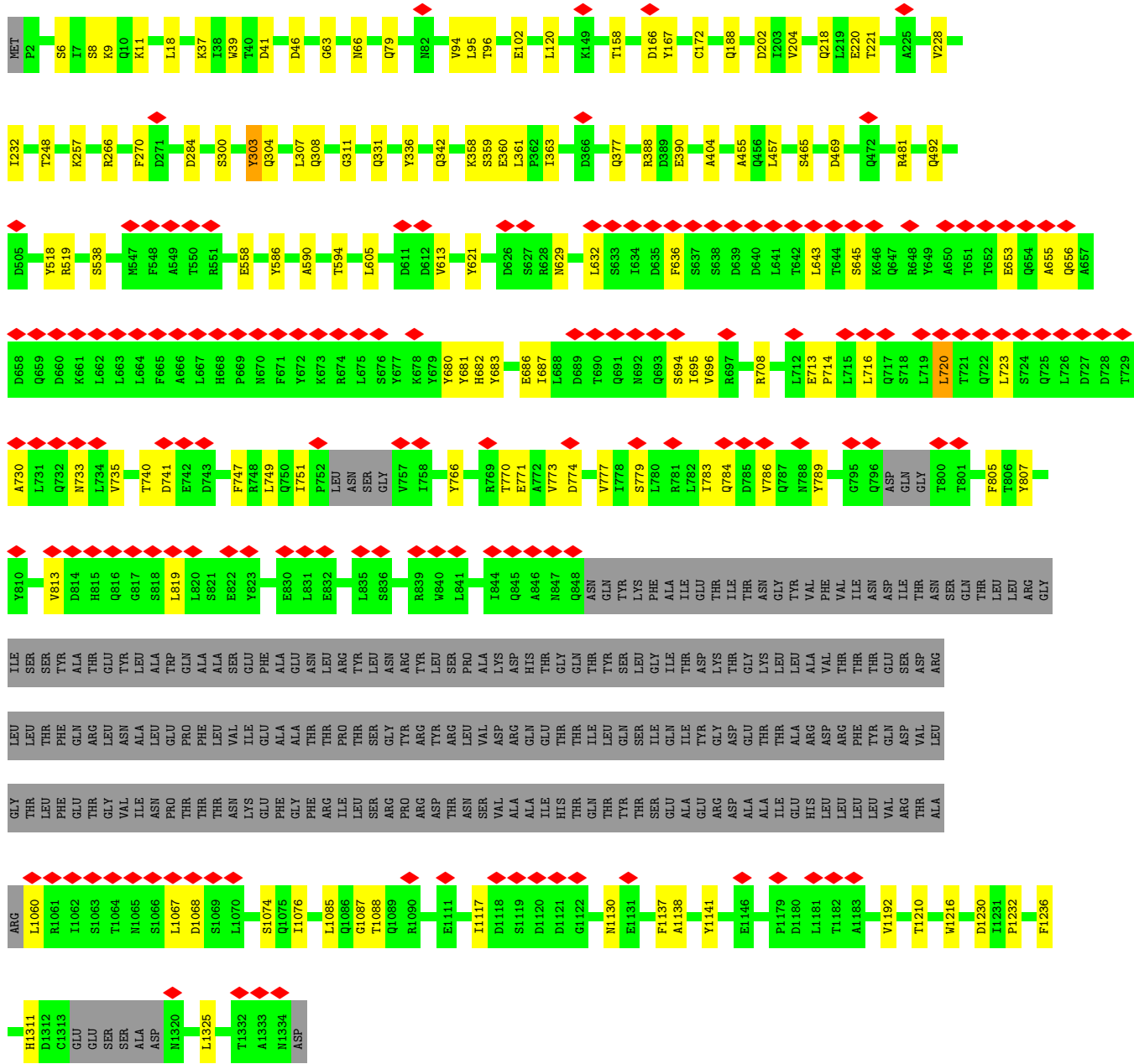
● Molecule 1: All3314 protein



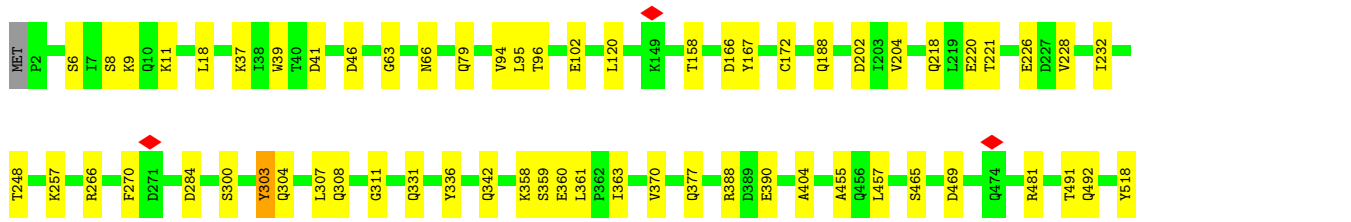
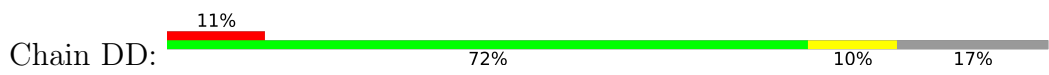


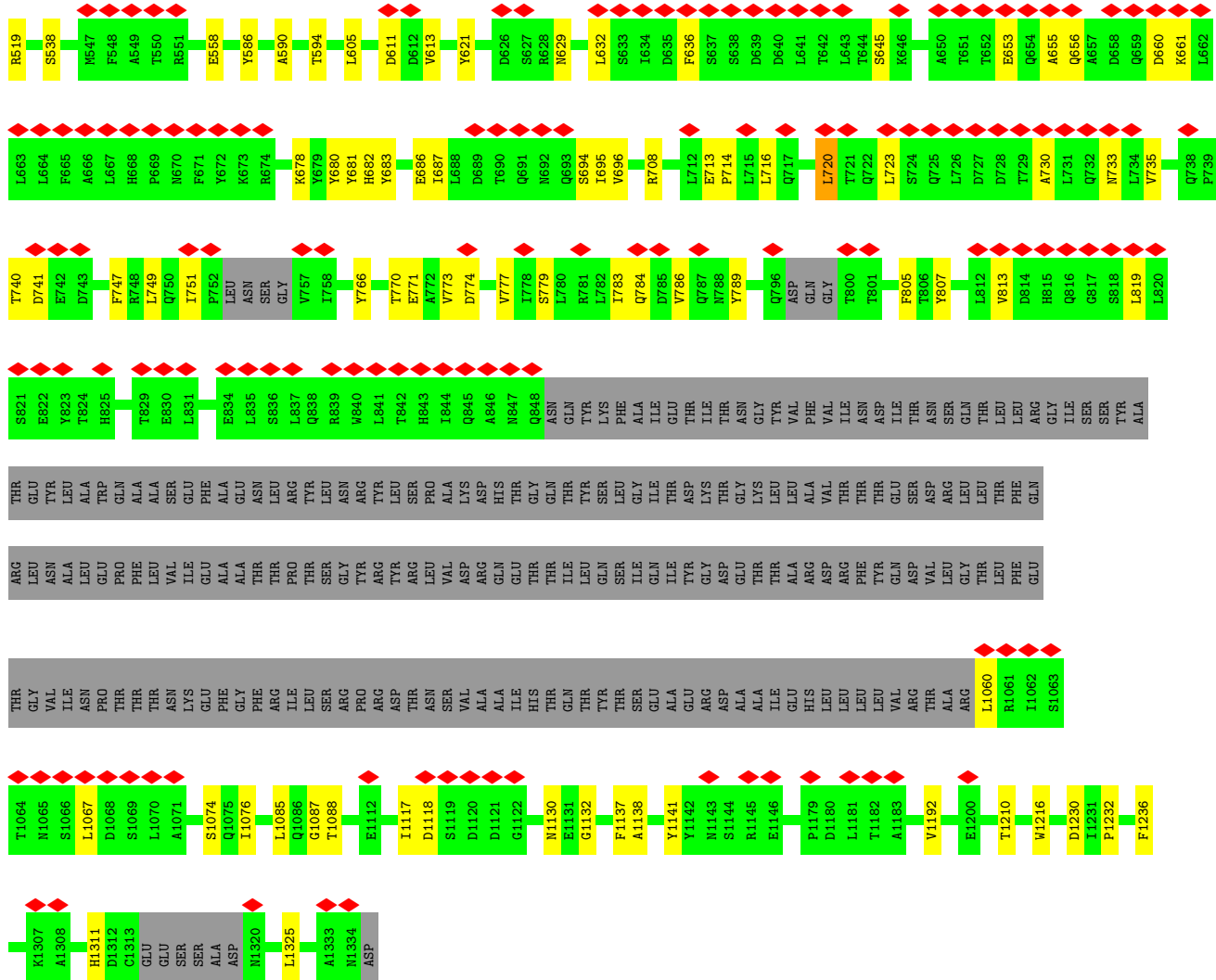




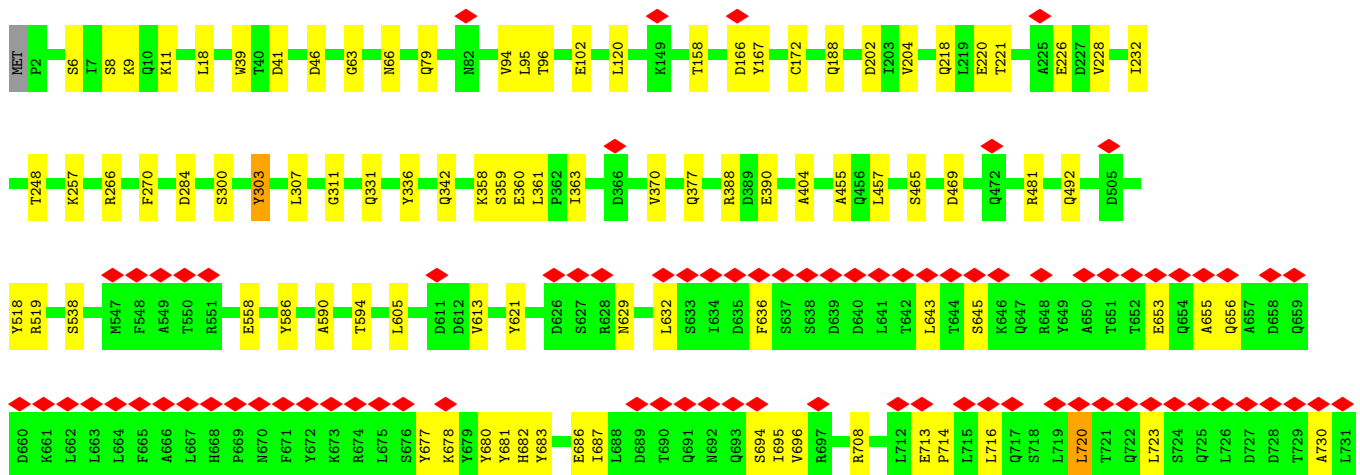
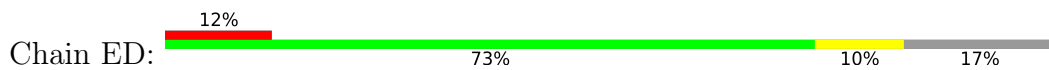


● Molecule 2: All3315 protein

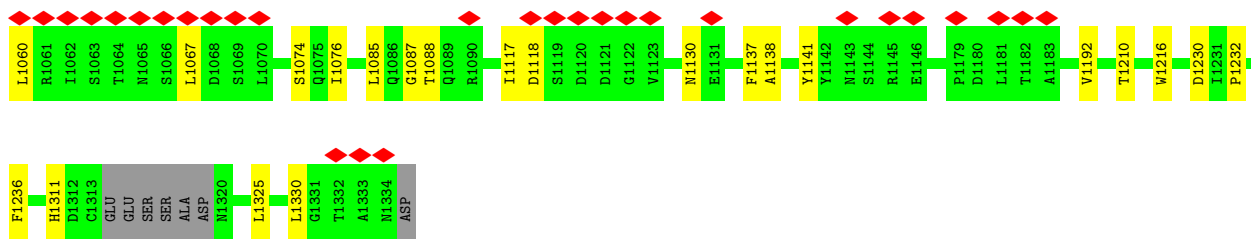
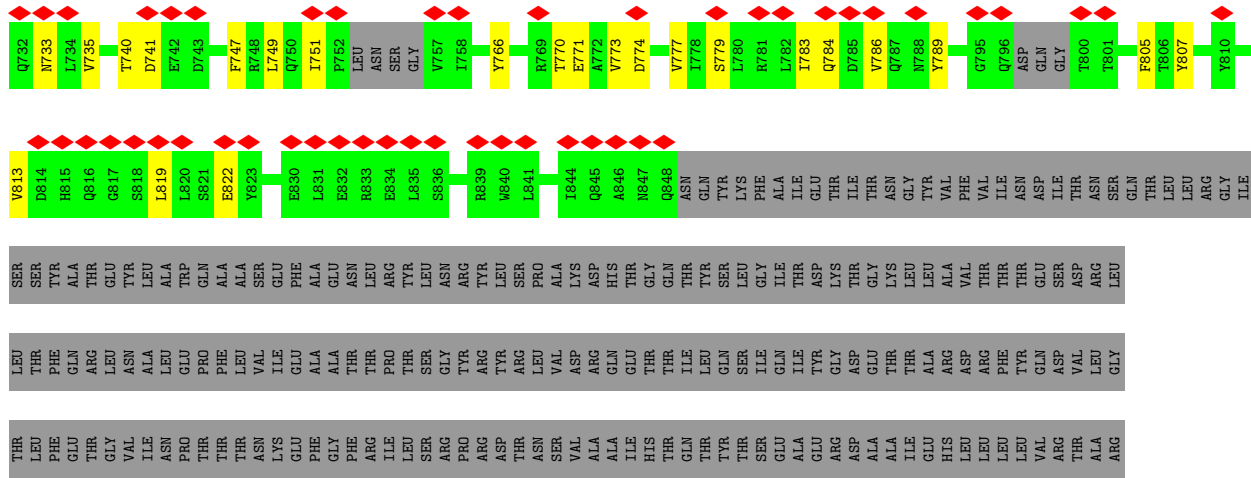




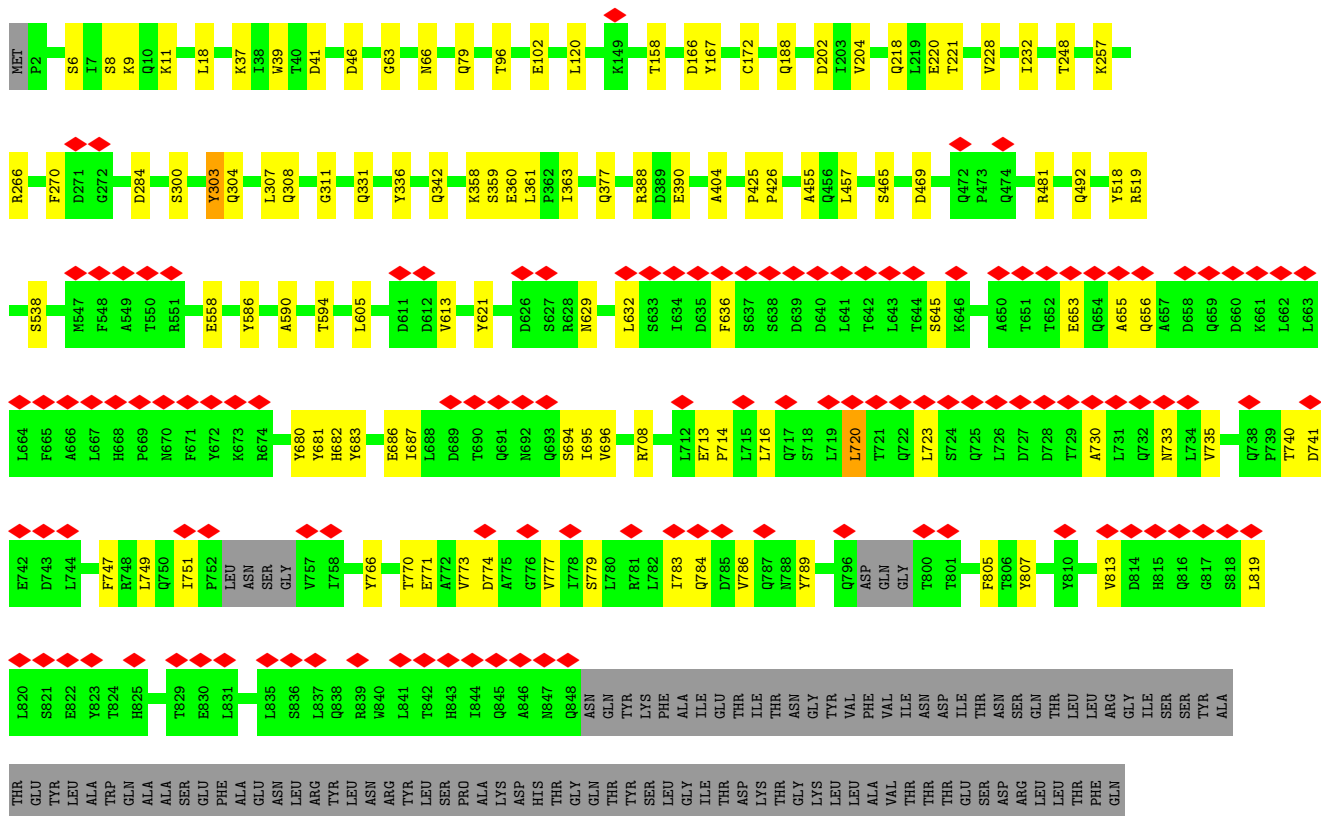
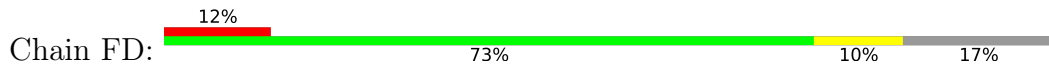
● Molecule 2: All3315 protein



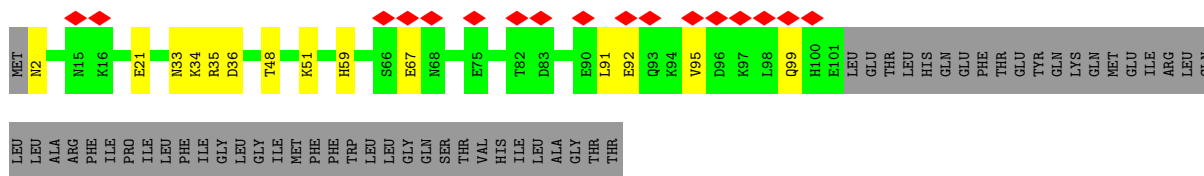




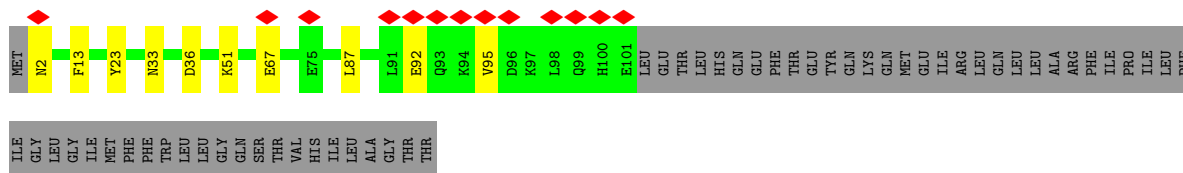
● Molecule 2: All3315 protein



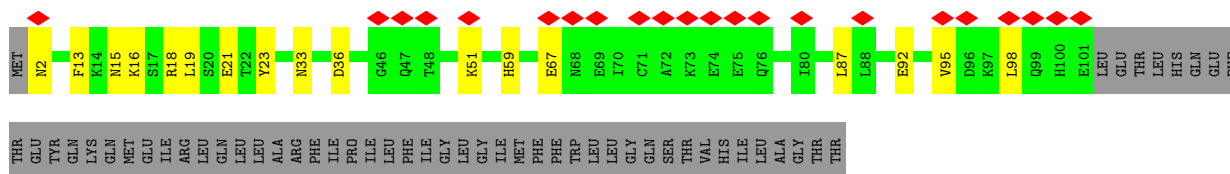




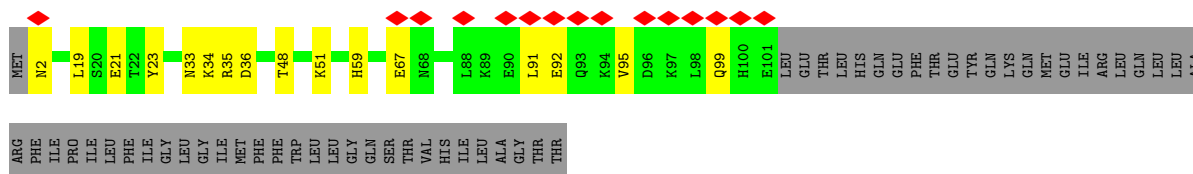
• Molecule 3: All3316 protein



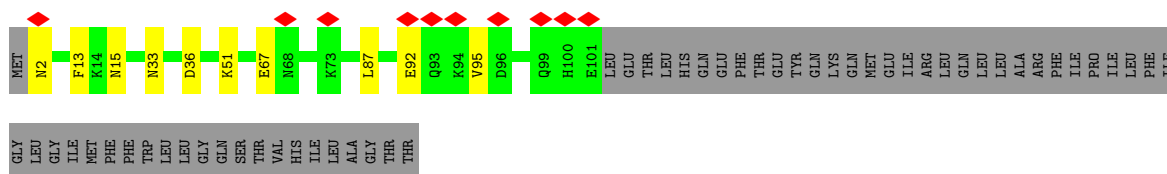
• Molecule 3: All3316 protein



• Molecule 3: All3316 protein



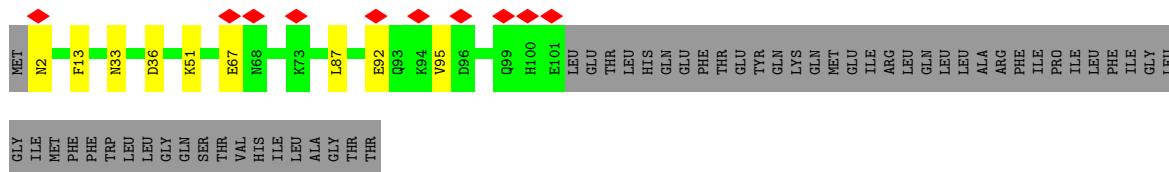
• Molecule 3: All3316 protein



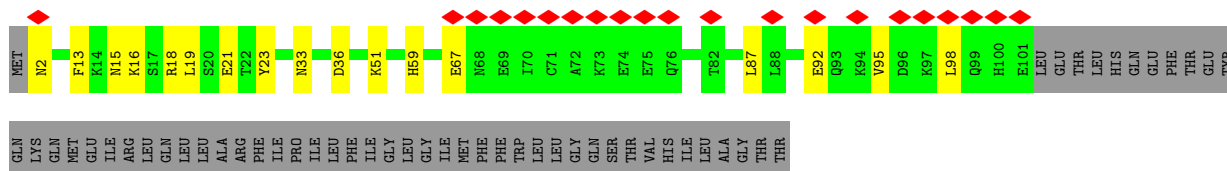
• Molecule 3: All3316 protein



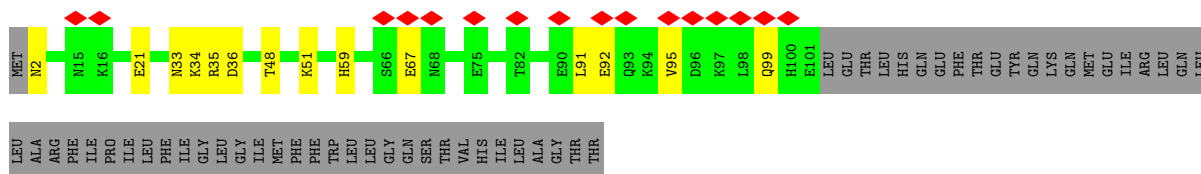




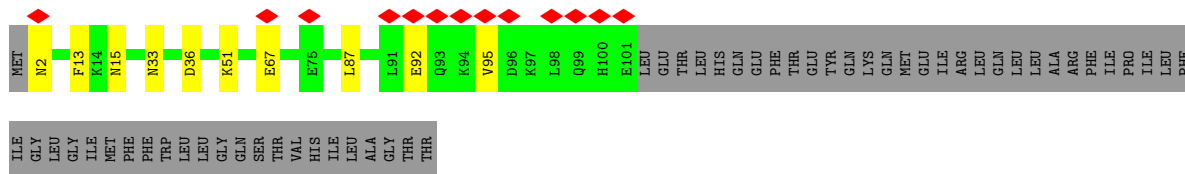
• Molecule 3: All3316 protein



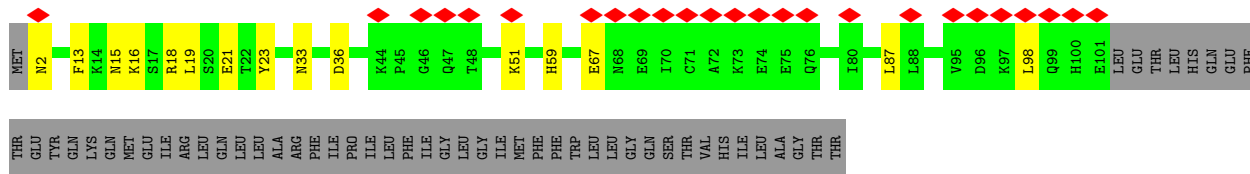
• Molecule 3: All3316 protein



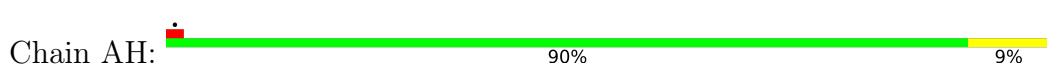
• Molecule 3: All3316 protein

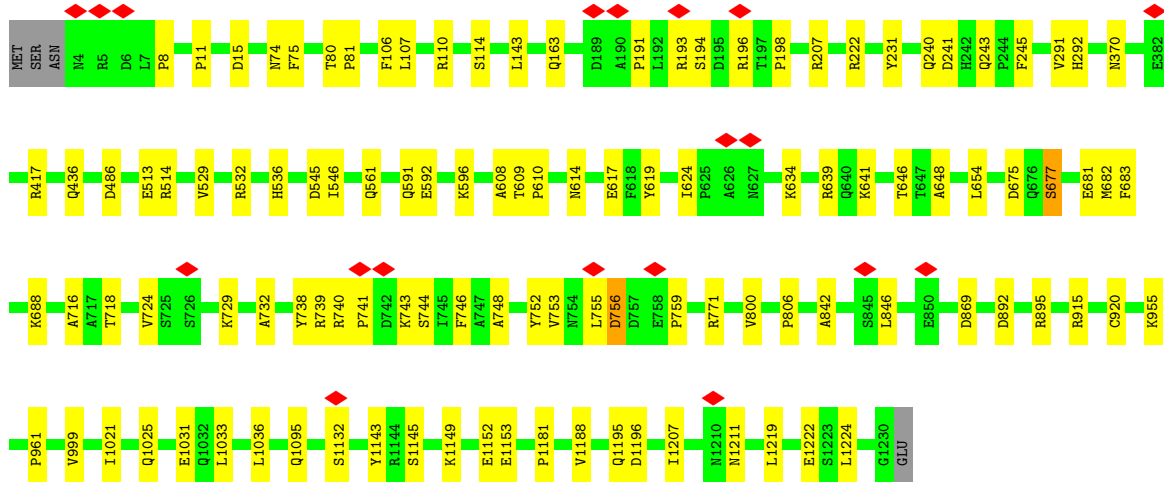


• Molecule 3: All3316 protein

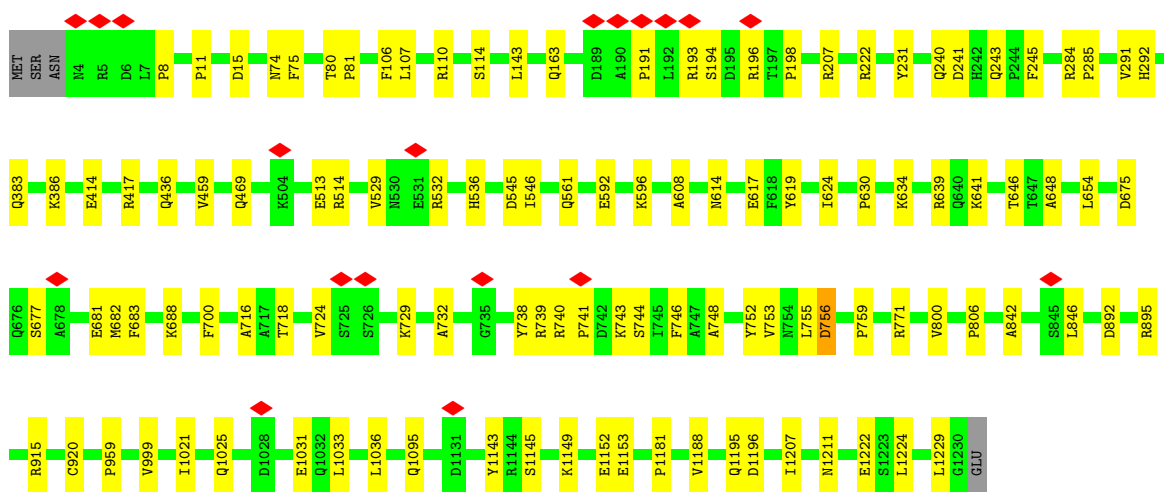
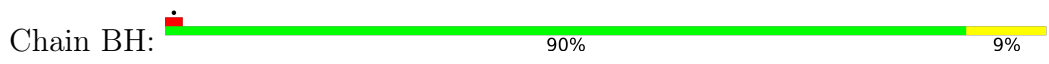


• Molecule 4: All3317 protein

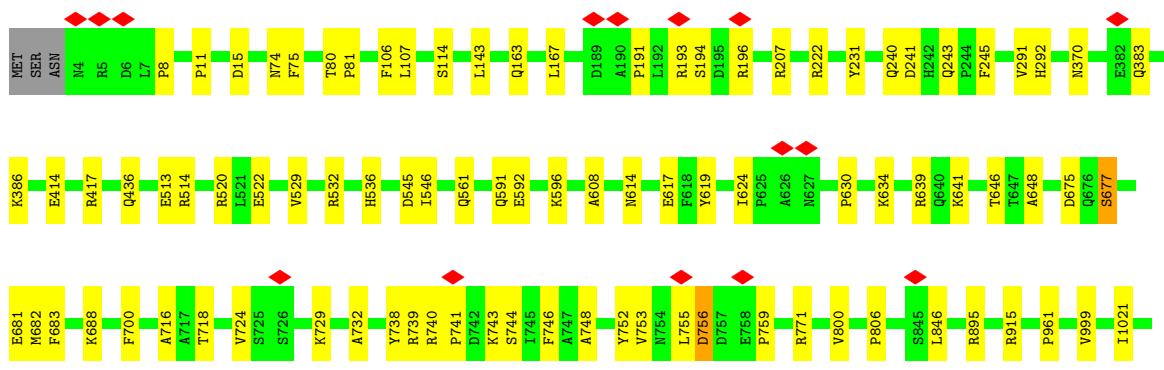


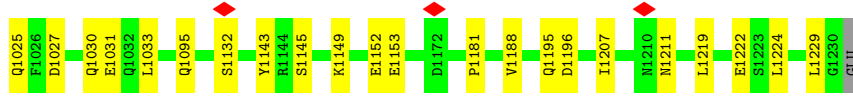


• Molecule 4: All3317 protein

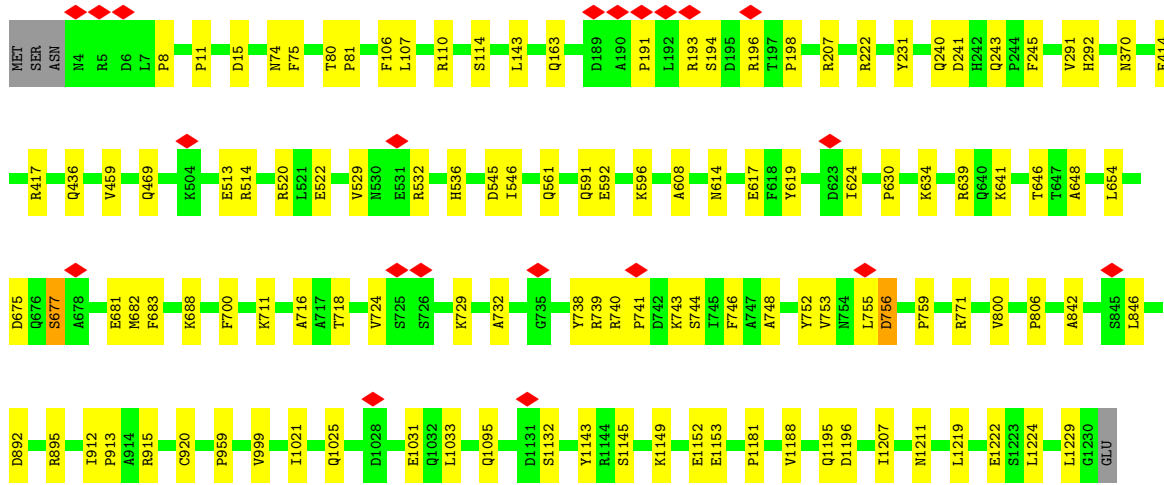


• Molecule 4: All3317 protein

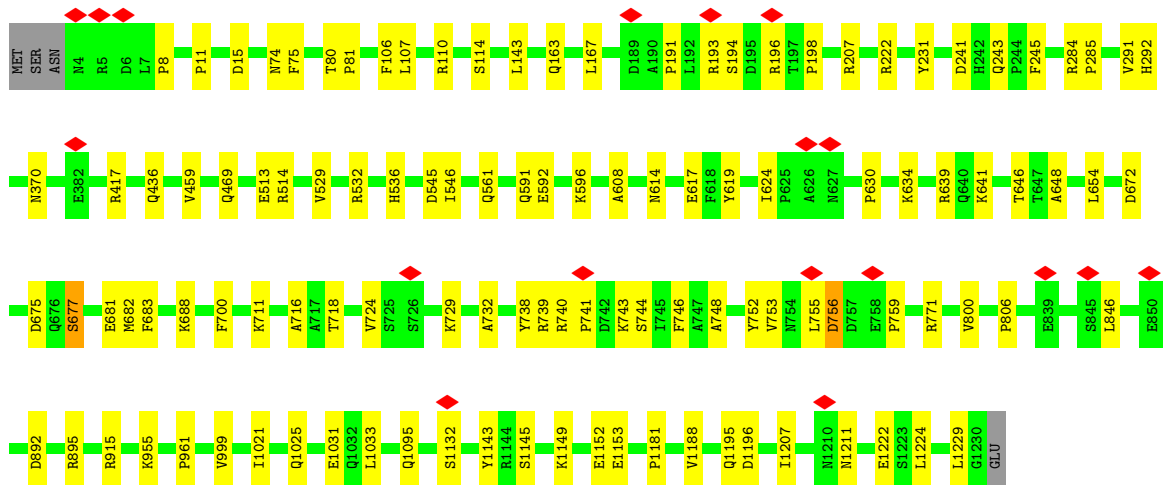




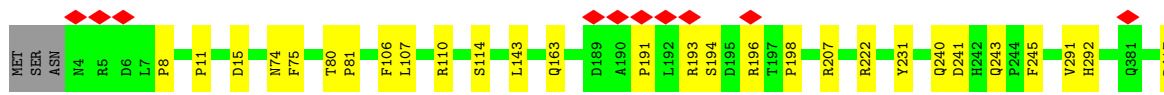
• Molecule 4: All3317 protein

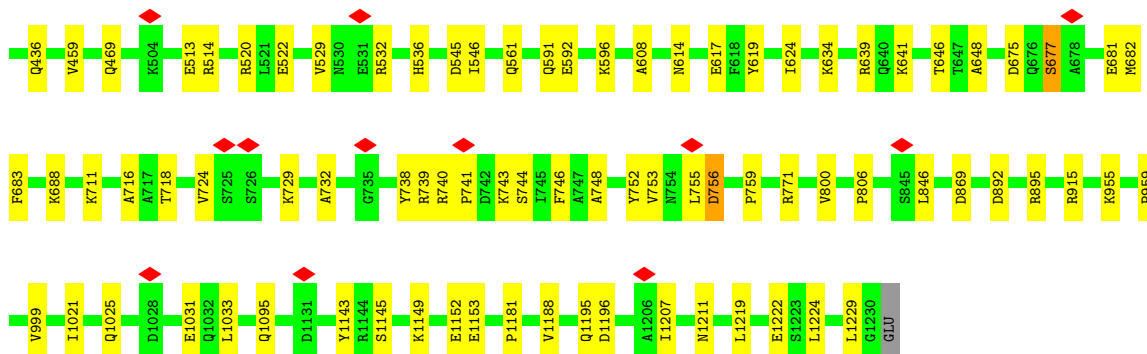


• Molecule 4: All3317 protein



• Molecule 4: All3317 protein





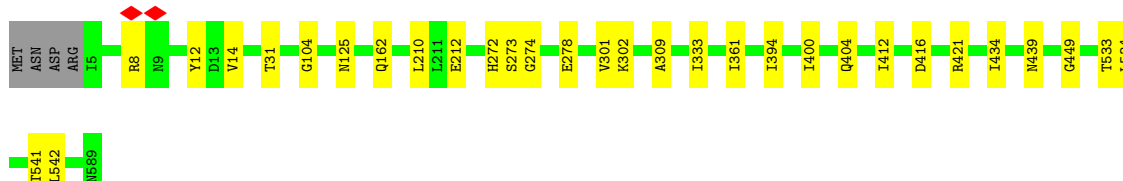
• Molecule 5: All3320 protein



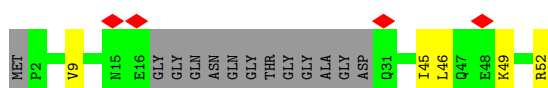
• Molecule 5: All3320 protein



• Molecule 5: All3320 protein



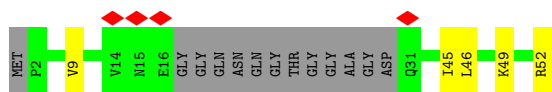
• Molecule 6: Asl3322 protein



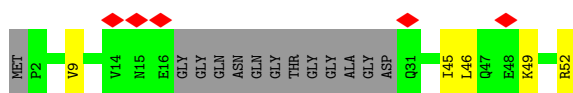
• Molecule 6: Asl3322 protein



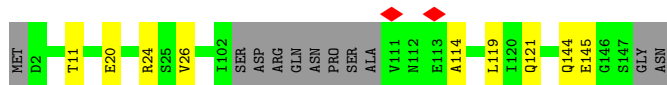
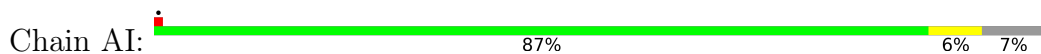




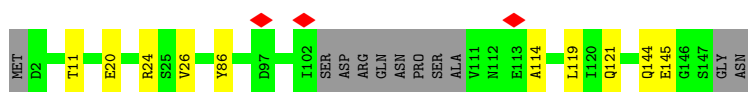
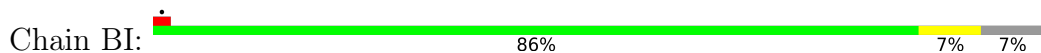
• Molecule 6: Asl3322 protein



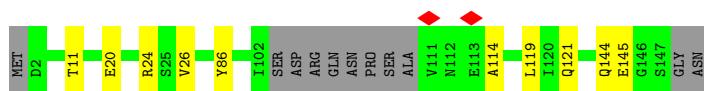
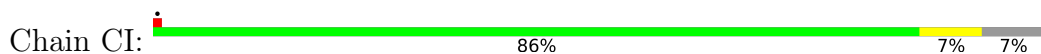
• Molecule 7: All3318 protein



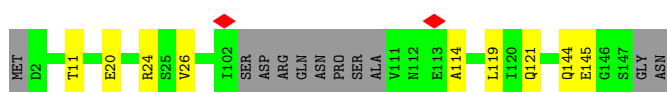
• Molecule 7: All3318 protein



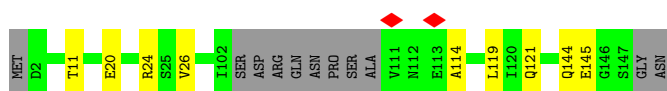
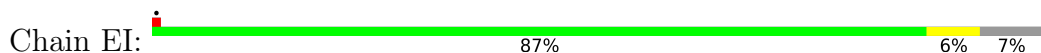
• Molecule 7: All3318 protein



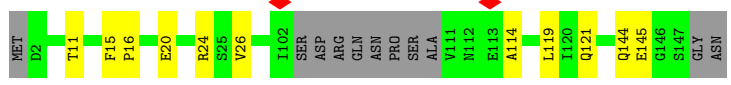
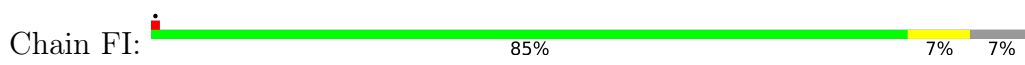
• Molecule 7: All3318 protein



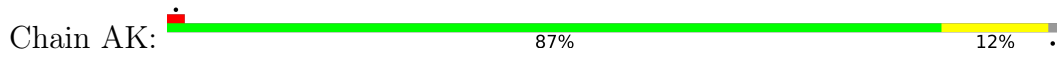
• Molecule 7: All3318 protein



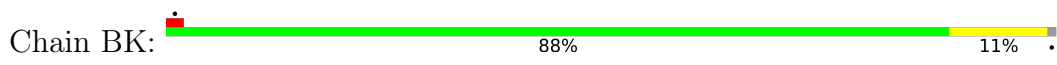
• Molecule 7: All3318 protein



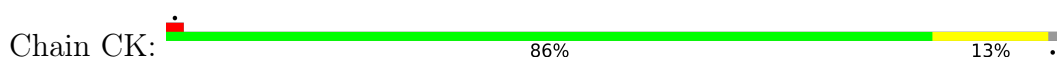
• Molecule 8: All3321 protein



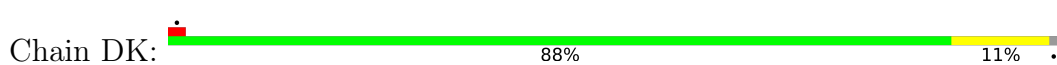
• Molecule 8: All3321 protein



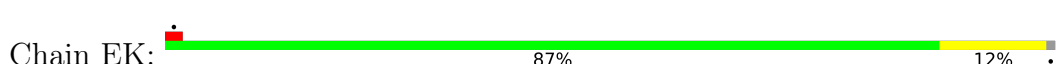
• Molecule 8: All3321 protein



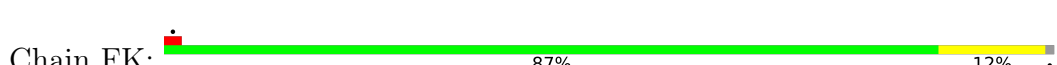
• Molecule 8: All3321 protein



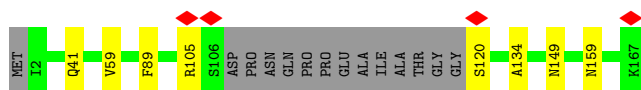
• Molecule 8: All3321 protein



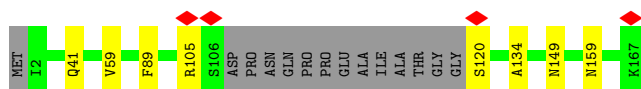
• Molecule 8: All3321 protein



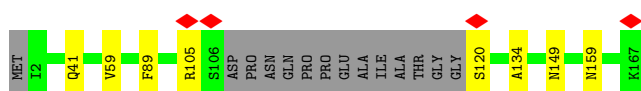
• Molecule 9: All3323 protein



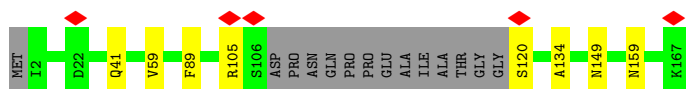
• Molecule 9: All3323 protein



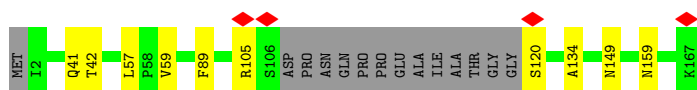
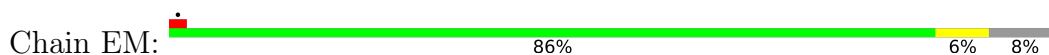
• Molecule 9: All3323 protein



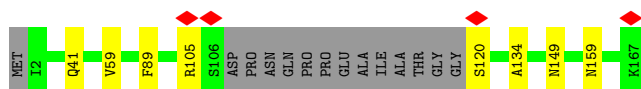
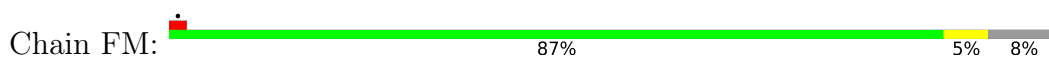
• Molecule 9: All3323 protein



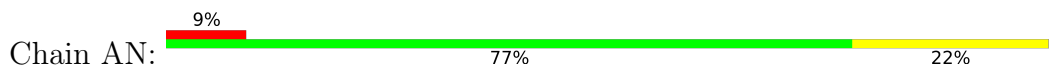
• Molecule 9: All3323 protein

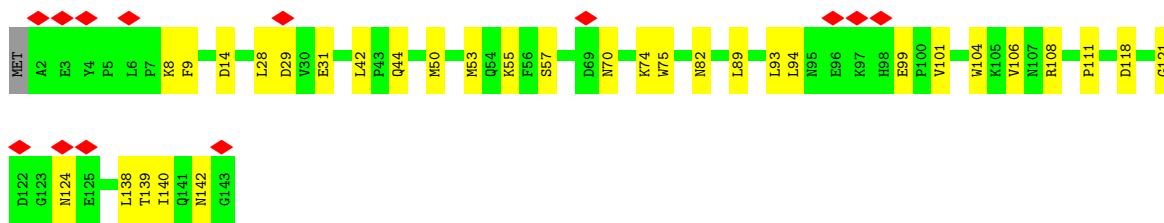


• Molecule 9: All3323 protein

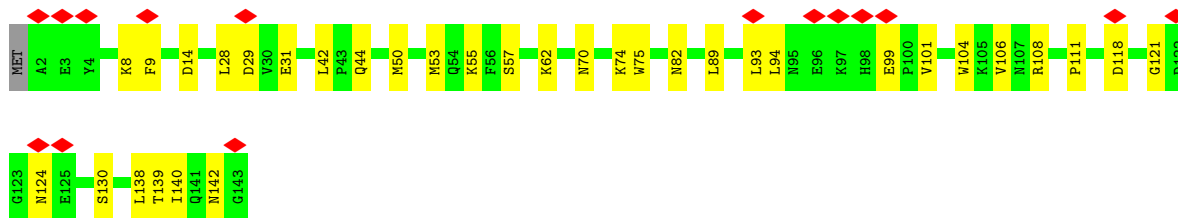
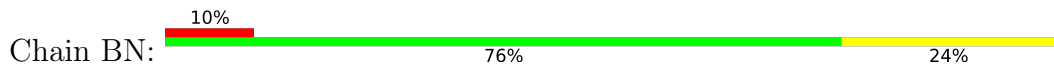


• Molecule 10: All3324 protein

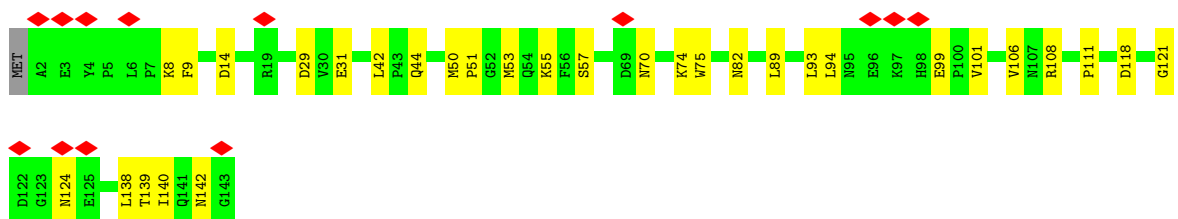
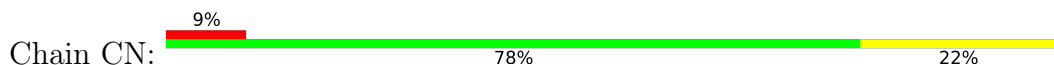




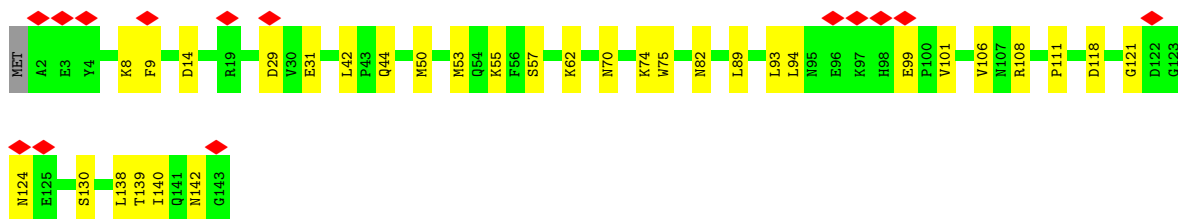
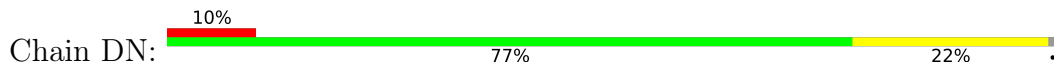
• Molecule 10: All3324 protein



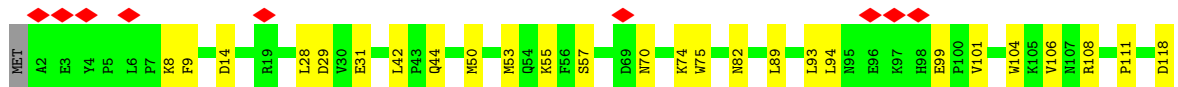
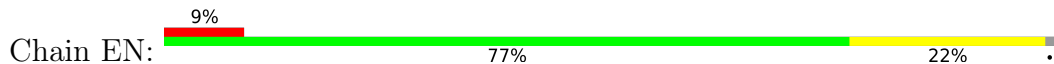
• Molecule 10: All3324 protein

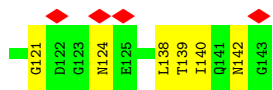


• Molecule 10: All3324 protein

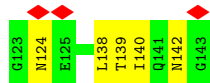
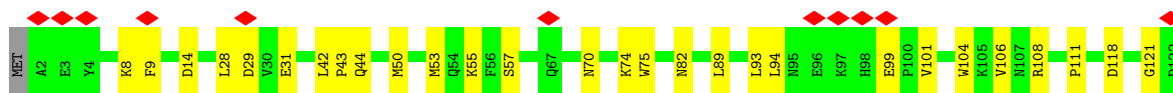
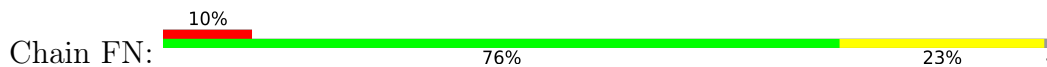


• Molecule 10: All3324 protein





• Molecule 10: All3324 protein



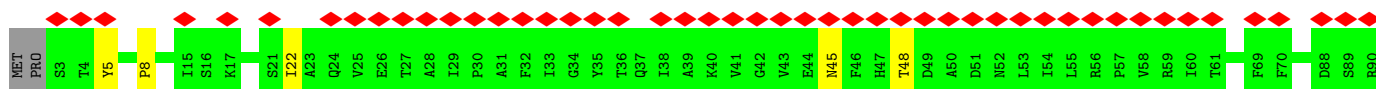
• Molecule 11: All3325 protein



• Molecule 11: All3325 protein

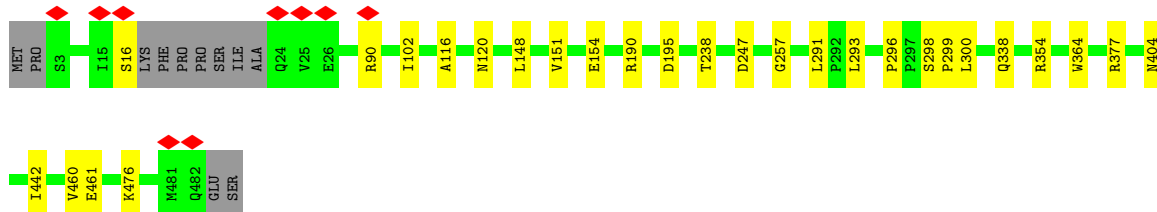


• Molecule 11: All3325 protein

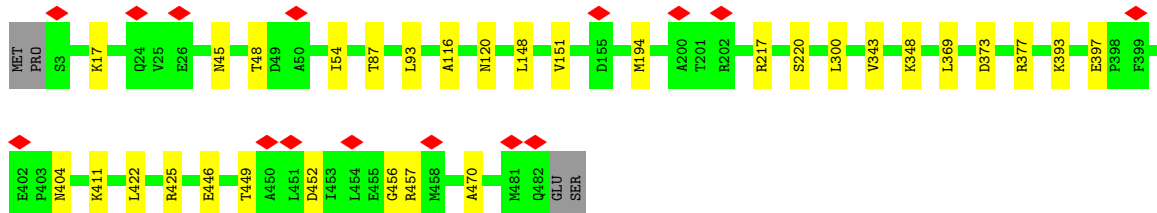




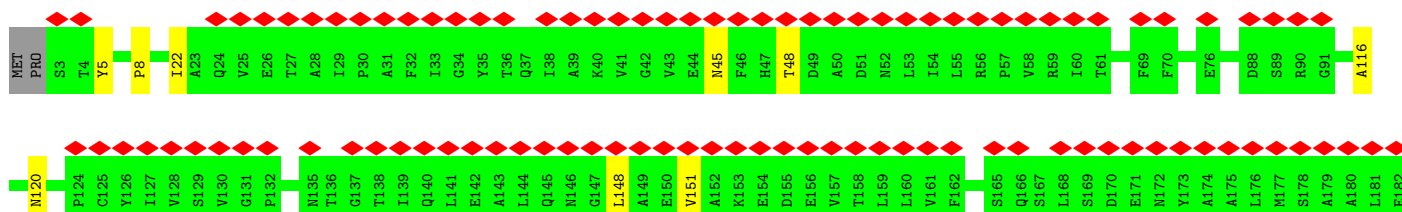
• Molecule 11: All3325 protein

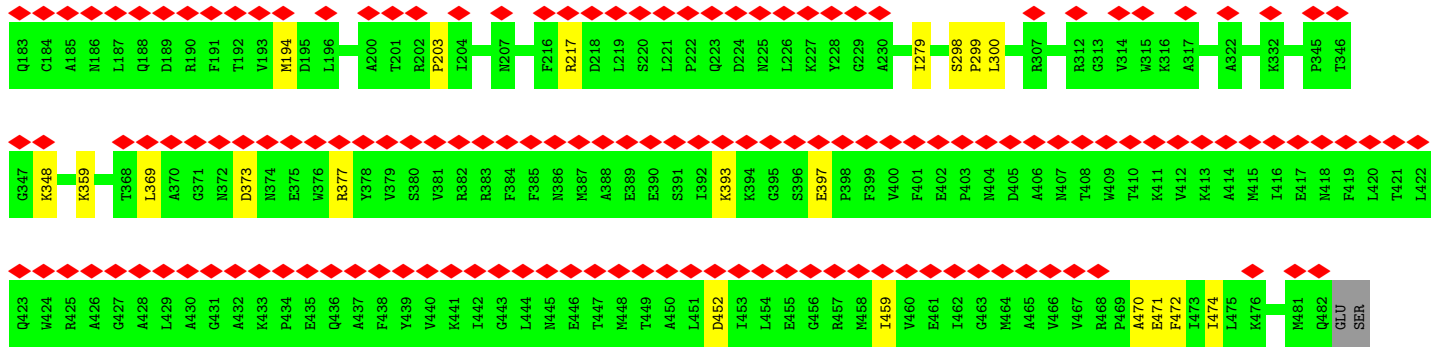


• Molecule 11: All3325 protein

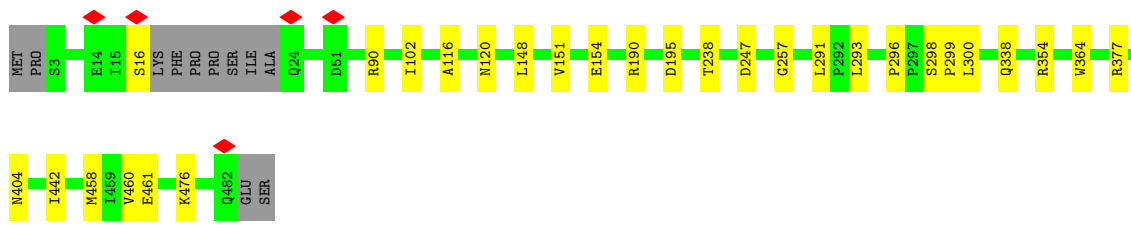


• Molecule 11: All3325 protein

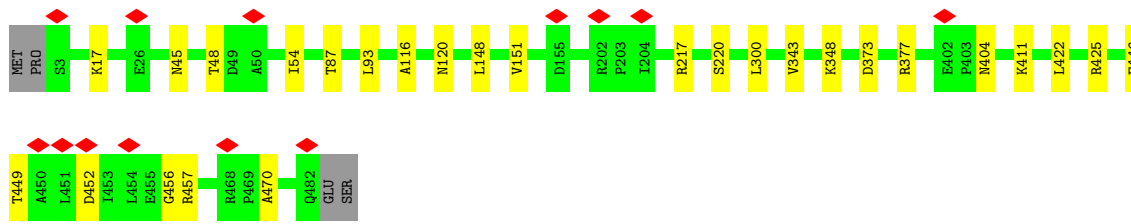




• Molecule 11: All3325 protein

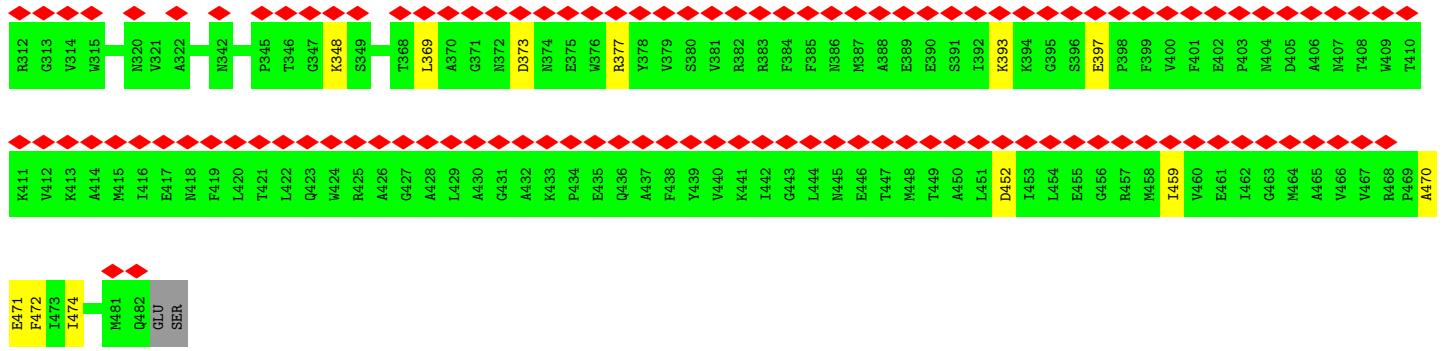


• Molecule 11: All3325 protein



• Molecule 11: All3325 protein





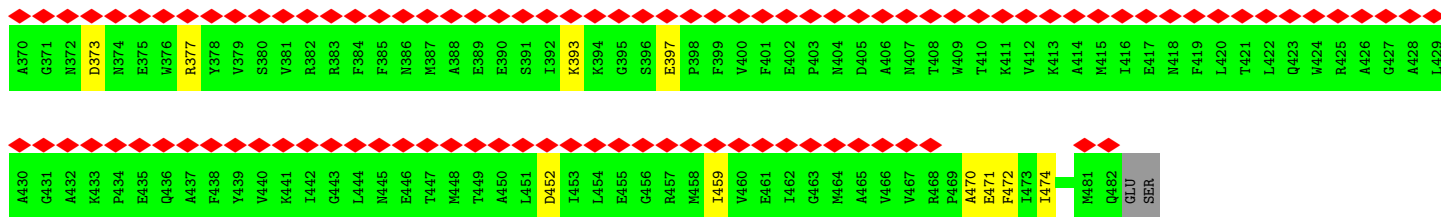
• Molecule 11: All3325 protein



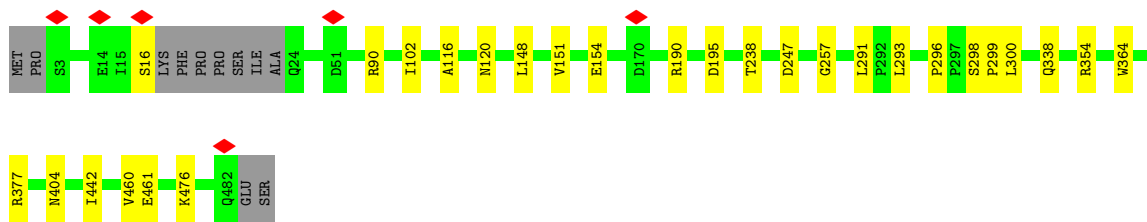
• Molecule 11: All3325 protein



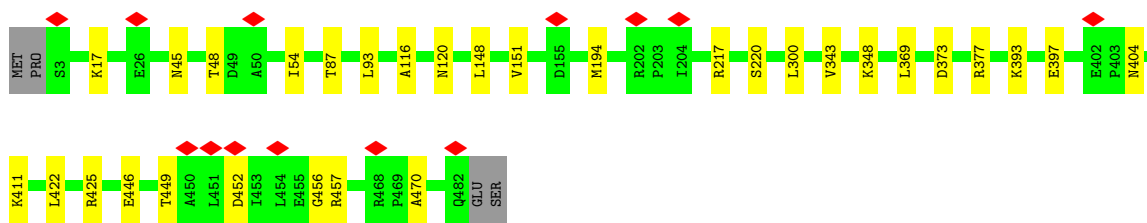




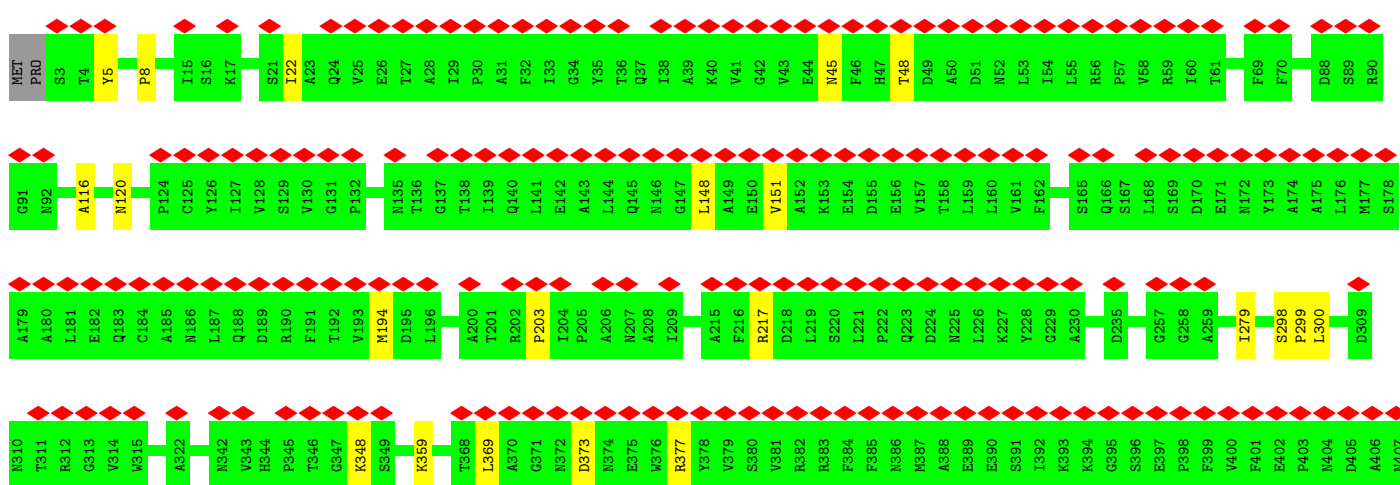
• Molecule 11: All3325 protein

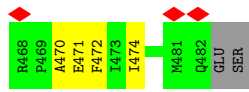
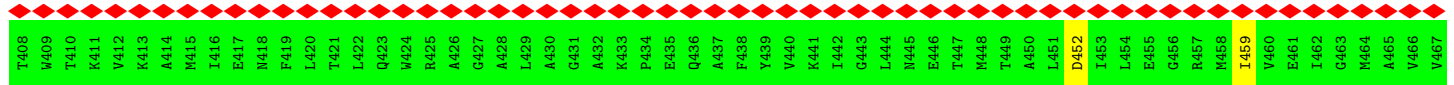


• Molecule 11: All3325 protein



• Molecule 11: All3325 protein

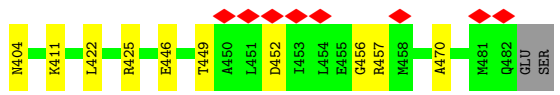
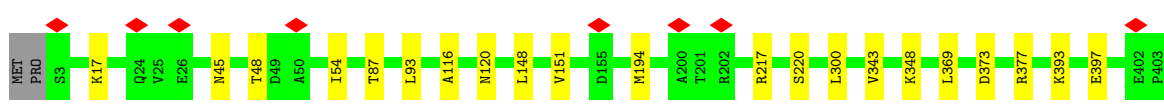




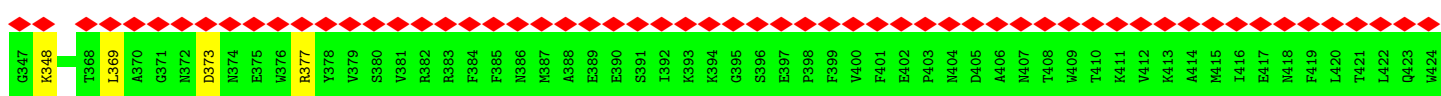
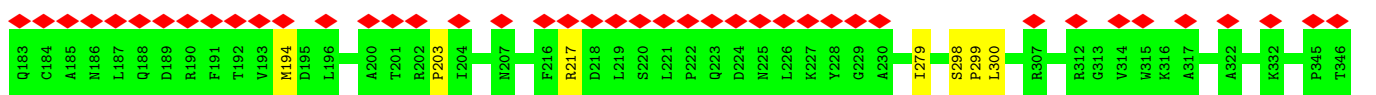
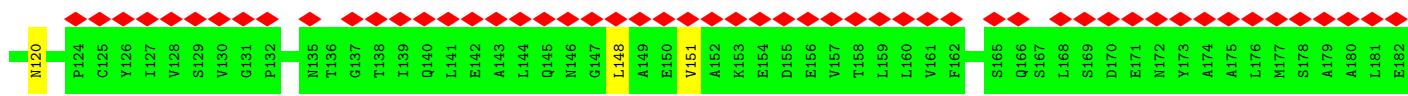
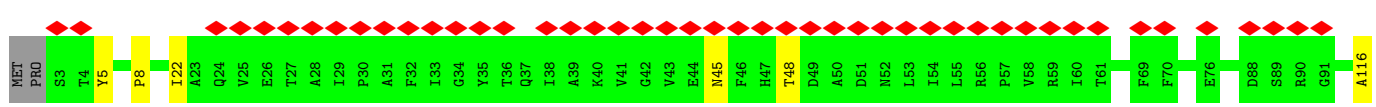
• Molecule 11: All3325 protein



• Molecule 11: All3325 protein



• Molecule 11: All3325 protein



R425	A426	G427	A428	L429	A430	G431	A432	K433	P434	E435	Q436	A437	F438	Y439	V440	K441	I442	G443	L444	N445	E446	T447	M448	T449	A450	L451	D452	I453	L454	E455	G456	R457	M458	I459	V460	E461	I462	G463	M464	A465	V466	V467	R468	P469	A470	E471	F472	I473	I474	L475	K476	M481	Q482	GLU	SER
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	36909	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	52	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.125	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0275	Depositor
Map size ( $\text{\AA}$ )	563.2, 563.2, 563.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1, 1.1, 1.1	Depositor

## 5 Model quality [i](#)

### 5.1 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 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	AA	0.40	0/6041	0.50	0/8212
1	AB	0.38	0/6027	0.48	0/8186
1	AC	0.40	0/5830	0.49	0/7924
1	BA	0.40	0/6041	0.50	0/8212
1	BB	0.38	0/6027	0.48	0/8186
1	BC	0.40	0/5830	0.49	0/7924
1	CA	0.40	0/6041	0.50	0/8212
1	CB	0.38	0/6027	0.48	0/8186
1	CC	0.40	0/5830	0.49	0/7924
1	DA	0.40	0/6041	0.50	0/8212
1	DB	0.38	0/6027	0.48	0/8186
1	DC	0.40	0/5830	0.49	0/7924
1	EA	0.40	0/6041	0.50	0/8212
1	EB	0.38	0/6027	0.48	0/8186
1	EC	0.40	0/5830	0.49	0/7924
1	FA	0.40	0/6041	0.50	0/8212
1	FB	0.38	0/6027	0.48	0/8186
1	FC	0.40	0/5830	0.49	0/7924
2	AD	0.31	0/9323	0.48	0/12684
2	BD	0.31	0/9323	0.48	0/12684
2	CD	0.31	0/9323	0.48	0/12684
2	DD	0.31	0/9323	0.48	0/12684
2	ED	0.31	0/9323	0.48	0/12684
2	FD	0.31	0/9323	0.48	0/12684
3	AE	0.43	0/862	0.53	0/1157
3	AF	0.41	0/862	0.47	0/1157
3	AG	0.41	0/862	0.46	0/1157
3	BE	0.43	0/862	0.53	0/1157
3	BF	0.42	0/862	0.47	0/1157
3	BG	0.41	0/862	0.46	0/1157
3	CE	0.43	0/862	0.53	0/1157
3	CF	0.41	0/862	0.47	0/1157
3	CG	0.41	0/862	0.46	0/1157
3	DE	0.43	0/862	0.53	0/1157

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	DF	0.42	0/862	0.47	0/1157
3	DG	0.41	0/862	0.46	0/1157
3	EE	0.43	0/862	0.53	0/1157
3	EF	0.42	0/862	0.47	0/1157
3	EG	0.41	0/862	0.46	0/1157
3	FE	0.43	0/862	0.53	0/1157
3	FF	0.42	0/862	0.47	0/1157
3	FG	0.41	0/862	0.46	0/1157
4	AH	0.32	0/10021	0.51	0/13644
4	BH	0.32	0/10021	0.51	0/13644
4	CH	0.32	0/10021	0.51	0/13644
4	DH	0.32	0/10021	0.51	0/13644
4	EH	0.32	0/10021	0.51	0/13644
4	FH	0.32	0/10021	0.51	0/13644
5	AJ	0.33	0/4507	0.50	0/6122
5	CJ	0.33	0/4507	0.50	0/6122
5	EJ	0.33	0/4507	0.50	0/6122
6	AL	0.34	0/284	0.60	0/380
6	CL	0.34	0/284	0.60	0/380
6	EL	0.34	0/284	0.61	0/380
7	AI	0.32	0/1116	0.50	0/1513
7	BI	0.32	0/1116	0.50	0/1513
7	CI	0.32	0/1116	0.50	0/1513
7	DI	0.32	0/1116	0.50	0/1513
7	EI	0.32	0/1116	0.50	0/1513
7	FI	0.32	0/1116	0.50	0/1513
8	AK	0.33	0/1942	0.52	0/2623
8	BK	0.32	0/1942	0.51	0/2623
8	CK	0.33	0/1942	0.52	0/2623
8	DK	0.32	0/1942	0.51	0/2623
8	EK	0.33	0/1942	0.52	0/2623
8	FK	0.32	0/1942	0.51	0/2623
9	AM	0.32	0/1282	0.54	0/1737
9	BM	0.32	0/1282	0.54	0/1737
9	CM	0.32	0/1282	0.54	0/1737
9	DM	0.32	0/1282	0.54	0/1737
9	EM	0.32	0/1282	0.54	0/1737
9	FM	0.32	0/1282	0.54	0/1737
10	AN	0.38	0/1181	0.55	0/1601
10	BN	0.38	0/1181	0.55	0/1601
10	CN	0.38	0/1181	0.55	0/1601
10	DN	0.38	0/1181	0.55	0/1601
10	EN	0.38	0/1181	0.55	0/1601

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
10	FN	0.38	0/1181	0.55	0/1601
11	AO	0.34	0/3738	0.51	0/5085
11	AP	0.32	0/3795	0.50	0/5165
11	AQ	0.33	0/3795	0.51	0/5165
11	BO	0.34	0/3738	0.51	0/5085
11	BP	0.32	0/3795	0.50	0/5165
11	BQ	0.33	0/3795	0.51	0/5165
11	CO	0.34	0/3738	0.51	0/5085
11	CP	0.32	0/3795	0.50	0/5165
11	CQ	0.33	0/3795	0.51	0/5165
11	DO	0.34	0/3738	0.51	0/5085
11	DP	0.32	0/3795	0.50	0/5165
11	DQ	0.33	0/3795	0.51	0/5165
11	EO	0.34	0/3738	0.51	0/5085
11	EP	0.32	0/3795	0.50	0/5165
11	EQ	0.33	0/3795	0.51	0/5165
11	FO	0.34	0/3738	0.51	0/5085
11	FP	0.32	0/3795	0.50	0/5165
11	FQ	0.33	0/3795	0.51	0/5165
All	All	0.35	0/354435	0.50	0/481566

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	5899	0	5787	56	0
1	AB	5886	0	5764	48	0
1	AC	5690	0	5581	37	0
1	BA	5899	0	5787	56	0
1	BB	5886	0	5764	47	0
1	BC	5690	0	5581	41	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CA	5899	0	5787	58	0
1	CB	5886	0	5764	43	0
1	CC	5690	0	5581	39	0
1	DA	5899	0	5787	55	0
1	DB	5886	0	5764	43	0
1	DC	5690	0	5581	36	0
1	EA	5899	0	5787	53	0
1	EB	5886	0	5764	49	0
1	EC	5690	0	5581	39	0
1	FA	5899	0	5787	55	0
1	FB	5886	0	5764	50	0
1	FC	5690	0	5581	37	0
2	AD	9112	0	8875	116	0
2	BD	9112	0	8875	110	0
2	CD	9112	0	8875	109	0
2	DD	9112	0	8875	116	0
2	ED	9112	0	8875	112	0
2	FD	9112	0	8875	111	0
3	AE	845	0	828	11	0
3	AF	845	0	828	9	0
3	AG	845	0	829	17	0
3	BE	845	0	828	12	0
3	BF	845	0	828	9	0
3	BG	845	0	829	17	0
3	CE	845	0	828	13	0
3	CF	845	0	828	9	0
3	CG	845	0	829	18	0
3	DE	845	0	828	12	0
3	DF	845	0	828	9	0
3	DG	845	0	829	16	0
3	EE	845	0	828	12	0
3	EF	845	0	828	8	0
3	EG	845	0	829	17	0
3	FE	845	0	828	12	0
3	FF	845	0	828	9	0
3	FG	845	0	829	16	0
4	AH	9792	0	9799	103	0
4	BH	9792	0	9799	101	0
4	CH	9792	0	9799	100	0
4	DH	9792	0	9799	106	0
4	EH	9792	0	9799	103	0
4	FH	9792	0	9799	99	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AJ	4438	0	4441	27	0
5	CJ	4438	0	4441	29	0
5	EJ	4438	0	4441	29	0
6	AL	285	0	304	5	0
6	CL	285	0	304	5	0
6	EL	285	0	304	6	0
7	AI	1098	0	1086	11	0
7	BI	1098	0	1086	12	0
7	CI	1098	0	1086	12	0
7	DI	1098	0	1086	11	0
7	EI	1098	0	1086	11	0
7	FI	1098	0	1086	12	0
8	AK	1898	0	1868	31	0
8	BK	1898	0	1868	25	0
8	CK	1898	0	1868	32	0
8	DK	1898	0	1868	24	0
8	EK	1898	0	1868	28	0
8	FK	1898	0	1868	26	0
9	AM	1254	0	1251	4	0
9	BM	1254	0	1251	4	0
9	CM	1254	0	1251	4	0
9	DM	1254	0	1251	4	0
9	EM	1254	0	1251	5	0
9	FM	1254	0	1251	4	0
10	AN	1152	0	1119	31	0
10	BN	1152	0	1119	32	0
10	CN	1152	0	1119	31	0
10	DN	1152	0	1119	30	0
10	EN	1152	0	1119	30	0
10	FN	1152	0	1119	32	0
11	AO	3663	0	3628	21	0
11	AP	3716	0	3686	30	0
11	AQ	3716	0	3686	25	0
11	BO	3663	0	3628	21	0
11	BP	3716	0	3686	32	0
11	BQ	3716	0	3686	24	0
11	CO	3663	0	3628	22	0
11	CP	3716	0	3686	28	0
11	CQ	3716	0	3686	26	0
11	DO	3663	0	3628	21	0
11	DP	3716	0	3686	29	0
11	DQ	3716	0	3686	24	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	EO	3663	0	3628	21	0
11	EP	3716	0	3686	32	0
11	EQ	3716	0	3686	25	0
11	FO	3663	0	3628	22	0
11	FP	3716	0	3686	31	0
11	FQ	3716	0	3686	24	0
All	All	346635	0	341925	2730	0

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 4.

The worst 5 of 2730 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AD:783:ILE:C	2:AD:783:ILE:HD12	2.22	0.60
2:BD:783:ILE:C	2:BD:783:ILE:HD12	2.22	0.60
2:ED:783:ILE:C	2:ED:783:ILE:HD12	2.22	0.60
2:DD:783:ILE:C	2:DD:783:ILE:HD12	2.22	0.60
4:DH:739:ARG:HA	4:DH:744:SER:O	2.02	0.60

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM 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	AA	721/1476 (49%)	690 (96%)	31 (4%)	0	100	100
1	AB	712/1476 (48%)	686 (96%)	26 (4%)	0	100	100
1	AC	688/1476 (47%)	667 (97%)	21 (3%)	0	100	100
1	BA	721/1476 (49%)	690 (96%)	31 (4%)	0	100	100
1	BB	712/1476 (48%)	686 (96%)	26 (4%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BC	688/1476 (47%)	667 (97%)	21 (3%)	0	100	100
1	CA	721/1476 (49%)	690 (96%)	31 (4%)	0	100	100
1	CB	712/1476 (48%)	686 (96%)	26 (4%)	0	100	100
1	CC	688/1476 (47%)	667 (97%)	21 (3%)	0	100	100
1	DA	721/1476 (49%)	690 (96%)	31 (4%)	0	100	100
1	DB	712/1476 (48%)	686 (96%)	26 (4%)	0	100	100
1	DC	688/1476 (47%)	667 (97%)	21 (3%)	0	100	100
1	EA	721/1476 (49%)	690 (96%)	31 (4%)	0	100	100
1	EB	712/1476 (48%)	686 (96%)	26 (4%)	0	100	100
1	EC	688/1476 (47%)	667 (97%)	21 (3%)	0	100	100
1	FA	721/1476 (49%)	690 (96%)	31 (4%)	0	100	100
1	FB	712/1476 (48%)	686 (96%)	26 (4%)	0	100	100
1	FC	688/1476 (47%)	667 (97%)	21 (3%)	0	100	100
2	AD	1099/1335 (82%)	1075 (98%)	24 (2%)	0	100	100
2	BD	1099/1335 (82%)	1075 (98%)	24 (2%)	0	100	100
2	CD	1099/1335 (82%)	1075 (98%)	24 (2%)	0	100	100
2	DD	1099/1335 (82%)	1075 (98%)	24 (2%)	0	100	100
2	ED	1099/1335 (82%)	1075 (98%)	24 (2%)	0	100	100
2	FD	1099/1335 (82%)	1075 (98%)	24 (2%)	0	100	100
3	AE	98/154 (64%)	93 (95%)	5 (5%)	0	100	100
3	AF	98/154 (64%)	94 (96%)	4 (4%)	0	100	100
3	AG	98/154 (64%)	94 (96%)	4 (4%)	0	100	100
3	BE	98/154 (64%)	93 (95%)	5 (5%)	0	100	100
3	BF	98/154 (64%)	94 (96%)	4 (4%)	0	100	100
3	BG	98/154 (64%)	94 (96%)	4 (4%)	0	100	100
3	CE	98/154 (64%)	93 (95%)	5 (5%)	0	100	100
3	CF	98/154 (64%)	94 (96%)	4 (4%)	0	100	100
3	CG	98/154 (64%)	94 (96%)	4 (4%)	0	100	100
3	DE	98/154 (64%)	93 (95%)	5 (5%)	0	100	100
3	DF	98/154 (64%)	94 (96%)	4 (4%)	0	100	100
3	DG	98/154 (64%)	94 (96%)	4 (4%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	EE	98/154 (64%)	93 (95%)	5 (5%)	0	100	100
3	EF	98/154 (64%)	94 (96%)	4 (4%)	0	100	100
3	EG	98/154 (64%)	94 (96%)	4 (4%)	0	100	100
3	FE	98/154 (64%)	93 (95%)	5 (5%)	0	100	100
3	FF	98/154 (64%)	94 (96%)	4 (4%)	0	100	100
3	FG	98/154 (64%)	94 (96%)	4 (4%)	0	100	100
4	AH	1225/1231 (100%)	1186 (97%)	39 (3%)	0	100	100
4	BH	1225/1231 (100%)	1186 (97%)	39 (3%)	0	100	100
4	CH	1225/1231 (100%)	1186 (97%)	39 (3%)	0	100	100
4	DH	1225/1231 (100%)	1186 (97%)	39 (3%)	0	100	100
4	EH	1225/1231 (100%)	1185 (97%)	40 (3%)	0	100	100
4	FH	1225/1231 (100%)	1186 (97%)	39 (3%)	0	100	100
5	AJ	583/589 (99%)	571 (98%)	12 (2%)	0	100	100
5	CJ	583/589 (99%)	571 (98%)	12 (2%)	0	100	100
5	EJ	583/589 (99%)	571 (98%)	12 (2%)	0	100	100
6	AL	33/50 (66%)	32 (97%)	1 (3%)	0	100	100
6	CL	33/50 (66%)	32 (97%)	1 (3%)	0	100	100
6	EL	33/50 (66%)	32 (97%)	1 (3%)	0	100	100
7	AI	134/149 (90%)	131 (98%)	3 (2%)	0	100	100
7	BI	134/149 (90%)	131 (98%)	3 (2%)	0	100	100
7	CI	134/149 (90%)	131 (98%)	3 (2%)	0	100	100
7	DI	134/149 (90%)	131 (98%)	3 (2%)	0	100	100
7	EI	134/149 (90%)	131 (98%)	3 (2%)	0	100	100
7	FI	134/149 (90%)	131 (98%)	3 (2%)	0	100	100
8	AK	230/234 (98%)	224 (97%)	6 (3%)	0	100	100
8	BK	230/234 (98%)	223 (97%)	7 (3%)	0	100	100
8	CK	230/234 (98%)	223 (97%)	7 (3%)	0	100	100
8	DK	230/234 (98%)	223 (97%)	7 (3%)	0	100	100
8	EK	230/234 (98%)	224 (97%)	6 (3%)	0	100	100
8	FK	230/234 (98%)	223 (97%)	7 (3%)	0	100	100
9	AM	149/167 (89%)	145 (97%)	4 (3%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	BM	149/167 (89%)	145 (97%)	4 (3%)	0	100	100
9	CM	149/167 (89%)	145 (97%)	4 (3%)	0	100	100
9	DM	149/167 (89%)	145 (97%)	4 (3%)	0	100	100
9	EM	149/167 (89%)	145 (97%)	4 (3%)	0	100	100
9	FM	149/167 (89%)	145 (97%)	4 (3%)	0	100	100
10	AN	140/143 (98%)	131 (94%)	9 (6%)	0	100	100
10	BN	140/143 (98%)	131 (94%)	9 (6%)	0	100	100
10	CN	140/143 (98%)	131 (94%)	9 (6%)	0	100	100
10	DN	140/143 (98%)	131 (94%)	9 (6%)	0	100	100
10	EN	140/143 (98%)	131 (94%)	9 (6%)	0	100	100
10	FN	140/143 (98%)	131 (94%)	9 (6%)	0	100	100
11	AO	469/484 (97%)	456 (97%)	13 (3%)	0	100	100
11	AP	478/484 (99%)	471 (98%)	7 (2%)	0	100	100
11	AQ	478/484 (99%)	472 (99%)	6 (1%)	0	100	100
11	BO	469/484 (97%)	456 (97%)	13 (3%)	0	100	100
11	BP	478/484 (99%)	471 (98%)	7 (2%)	0	100	100
11	BQ	478/484 (99%)	472 (99%)	6 (1%)	0	100	100
11	CO	469/484 (97%)	456 (97%)	13 (3%)	0	100	100
11	CP	478/484 (99%)	471 (98%)	7 (2%)	0	100	100
11	CQ	478/484 (99%)	472 (99%)	6 (1%)	0	100	100
11	DO	469/484 (97%)	456 (97%)	13 (3%)	0	100	100
11	DP	478/484 (99%)	471 (98%)	7 (2%)	0	100	100
11	DQ	478/484 (99%)	472 (99%)	6 (1%)	0	100	100
11	EO	469/484 (97%)	456 (97%)	13 (3%)	0	100	100
11	EP	478/484 (99%)	471 (98%)	7 (2%)	0	100	100
11	EQ	478/484 (99%)	472 (99%)	6 (1%)	0	100	100
11	FO	469/484 (97%)	456 (97%)	13 (3%)	0	100	100
11	FP	478/484 (99%)	471 (98%)	7 (2%)	0	100	100
11	FQ	478/484 (99%)	472 (99%)	6 (1%)	0	100	100
All	All	42750/59523 (72%)	41494 (97%)	1256 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM 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	AA	650/1306 (50%)	649 (100%)	1 (0%)	93	98
1	AB	647/1306 (50%)	645 (100%)	2 (0%)	92	96
1	AC	623/1306 (48%)	619 (99%)	4 (1%)	86	94
1	BA	650/1306 (50%)	649 (100%)	1 (0%)	93	98
1	BB	647/1306 (50%)	645 (100%)	2 (0%)	92	96
1	BC	623/1306 (48%)	619 (99%)	4 (1%)	86	94
1	CA	650/1306 (50%)	649 (100%)	1 (0%)	93	98
1	CB	647/1306 (50%)	645 (100%)	2 (0%)	92	96
1	CC	623/1306 (48%)	619 (99%)	4 (1%)	86	94
1	DA	650/1306 (50%)	649 (100%)	1 (0%)	93	98
1	DB	647/1306 (50%)	645 (100%)	2 (0%)	92	96
1	DC	623/1306 (48%)	619 (99%)	4 (1%)	86	94
1	EA	650/1306 (50%)	649 (100%)	1 (0%)	93	98
1	EB	647/1306 (50%)	645 (100%)	2 (0%)	92	96
1	EC	623/1306 (48%)	619 (99%)	4 (1%)	86	94
1	FA	650/1306 (50%)	649 (100%)	1 (0%)	93	98
1	FB	647/1306 (50%)	645 (100%)	2 (0%)	92	96
1	FC	623/1306 (48%)	619 (99%)	4 (1%)	86	94
2	AD	1000/1195 (84%)	998 (100%)	2 (0%)	93	98
2	BD	1000/1195 (84%)	998 (100%)	2 (0%)	93	98
2	CD	1000/1195 (84%)	998 (100%)	2 (0%)	93	98
2	DD	1000/1195 (84%)	998 (100%)	2 (0%)	93	98
2	ED	1000/1195 (84%)	998 (100%)	2 (0%)	93	98
2	FD	1000/1195 (84%)	998 (100%)	2 (0%)	93	98
3	AE	95/143 (66%)	95 (100%)	0	100	100
3	AF	95/143 (66%)	95 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AG	95/143 (66%)	95 (100%)	0	100	100
3	BE	95/143 (66%)	95 (100%)	0	100	100
3	BF	95/143 (66%)	95 (100%)	0	100	100
3	BG	95/143 (66%)	95 (100%)	0	100	100
3	CE	95/143 (66%)	95 (100%)	0	100	100
3	CF	95/143 (66%)	95 (100%)	0	100	100
3	CG	95/143 (66%)	95 (100%)	0	100	100
3	DE	95/143 (66%)	95 (100%)	0	100	100
3	DF	95/143 (66%)	95 (100%)	0	100	100
3	DG	95/143 (66%)	95 (100%)	0	100	100
3	EE	95/143 (66%)	95 (100%)	0	100	100
3	EF	95/143 (66%)	95 (100%)	0	100	100
3	EG	95/143 (66%)	95 (100%)	0	100	100
3	FE	95/143 (66%)	95 (100%)	0	100	100
3	FF	95/143 (66%)	95 (100%)	0	100	100
3	FG	95/143 (66%)	95 (100%)	0	100	100
4	AH	1071/1075 (100%)	1067 (100%)	4 (0%)	91	95
4	BH	1071/1075 (100%)	1067 (100%)	4 (0%)	91	95
4	CH	1071/1075 (100%)	1067 (100%)	4 (0%)	91	95
4	DH	1071/1075 (100%)	1067 (100%)	4 (0%)	91	95
4	EH	1071/1075 (100%)	1067 (100%)	4 (0%)	91	95
4	FH	1071/1075 (100%)	1067 (100%)	4 (0%)	91	95
5	AJ	471/475 (99%)	471 (100%)	0	100	100
5	CJ	471/475 (99%)	471 (100%)	0	100	100
5	EJ	471/475 (99%)	471 (100%)	0	100	100
6	AL	32/38 (84%)	32 (100%)	0	100	100
6	CL	32/38 (84%)	32 (100%)	0	100	100
6	EL	32/38 (84%)	32 (100%)	0	100	100
7	AI	123/132 (93%)	123 (100%)	0	100	100
7	BI	123/132 (93%)	123 (100%)	0	100	100
7	CI	123/132 (93%)	123 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	DI	123/132 (93%)	123 (100%)	0	100	100
7	EI	123/132 (93%)	123 (100%)	0	100	100
7	FI	123/132 (93%)	123 (100%)	0	100	100
8	AK	209/211 (99%)	208 (100%)	1 (0%)	88	95
8	BK	209/211 (99%)	208 (100%)	1 (0%)	88	95
8	CK	209/211 (99%)	208 (100%)	1 (0%)	88	95
8	DK	209/211 (99%)	208 (100%)	1 (0%)	88	95
8	EK	209/211 (99%)	208 (100%)	1 (0%)	88	95
8	FK	209/211 (99%)	208 (100%)	1 (0%)	88	95
9	AM	143/153 (94%)	142 (99%)	1 (1%)	84	94
9	BM	143/153 (94%)	142 (99%)	1 (1%)	84	94
9	CM	143/153 (94%)	142 (99%)	1 (1%)	84	94
9	DM	143/153 (94%)	142 (99%)	1 (1%)	84	94
9	EM	143/153 (94%)	142 (99%)	1 (1%)	84	94
9	FM	143/153 (94%)	142 (99%)	1 (1%)	84	94
10	AN	125/126 (99%)	125 (100%)	0	100	100
10	BN	125/126 (99%)	125 (100%)	0	100	100
10	CN	125/126 (99%)	125 (100%)	0	100	100
10	DN	125/126 (99%)	125 (100%)	0	100	100
10	EN	125/126 (99%)	125 (100%)	0	100	100
10	FN	125/126 (99%)	125 (100%)	0	100	100
11	AO	392/402 (98%)	392 (100%)	0	100	100
11	AP	398/402 (99%)	398 (100%)	0	100	100
11	AQ	398/402 (99%)	398 (100%)	0	100	100
11	BO	392/402 (98%)	392 (100%)	0	100	100
11	BP	398/402 (99%)	398 (100%)	0	100	100
11	BQ	398/402 (99%)	398 (100%)	0	100	100
11	CO	392/402 (98%)	392 (100%)	0	100	100
11	CP	398/402 (99%)	398 (100%)	0	100	100
11	CQ	398/402 (99%)	398 (100%)	0	100	100
11	DO	392/402 (98%)	392 (100%)	0	100	100

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	DP	398/402 (99%)	398 (100%)	0	100	100
11	DQ	398/402 (99%)	398 (100%)	0	100	100
11	EO	392/402 (98%)	392 (100%)	0	100	100
11	EP	398/402 (99%)	398 (100%)	0	100	100
11	EQ	398/402 (99%)	398 (100%)	0	100	100
11	FO	392/402 (98%)	392 (100%)	0	100	100
11	FP	398/402 (99%)	398 (100%)	0	100	100
11	FQ	398/402 (99%)	398 (100%)	0	100	100
All	All	37893/52209 (73%)	37803 (100%)	90 (0%)	93	98

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	DH	999	VAL
4	EH	756	ASP
9	DM	89	PHE
1	EC	456	TYR
1	FA	610	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 331 such sidechains are listed below:

Mol	Chain	Res	Type
1	EB	131	ASN
1	FA	552	ASN
1	EC	499	HIS
4	EH	381	GLN
2	FD	87	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

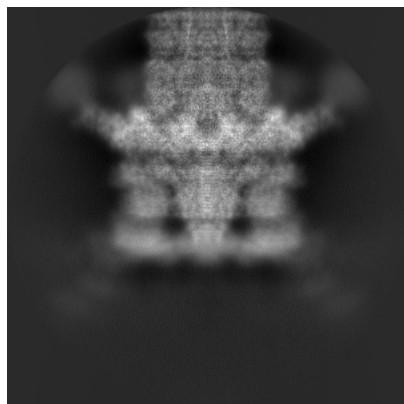
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12029. These allow visual inspection of the internal detail of the map and identification of artifacts.

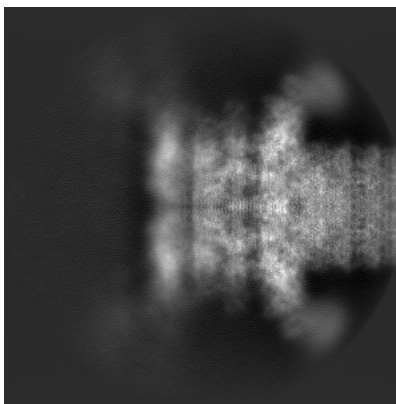
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

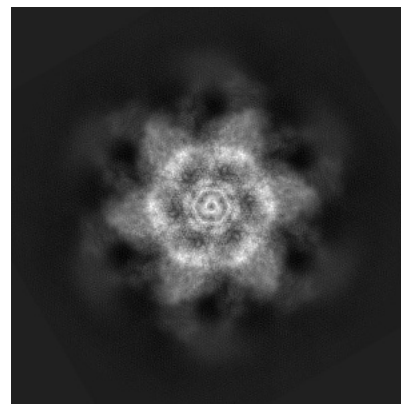
#### 6.1.1 Primary map



X

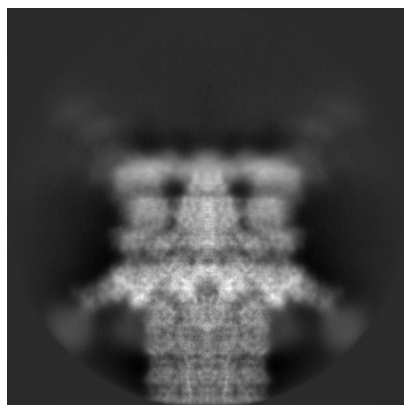


Y

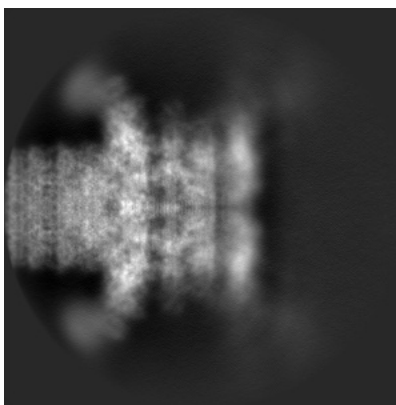


Z

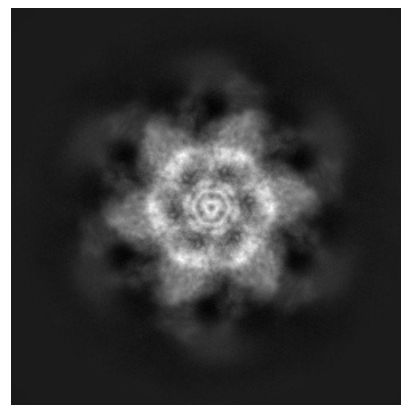
#### 6.1.2 Raw map



X



Y

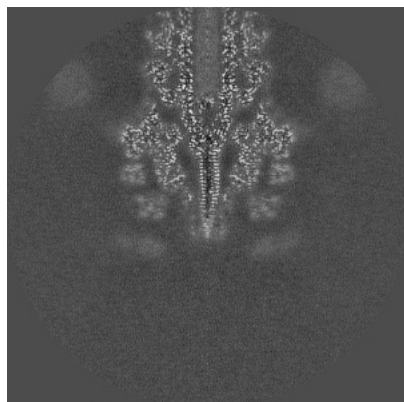


Z

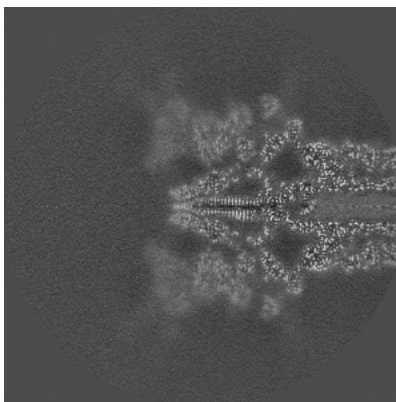
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

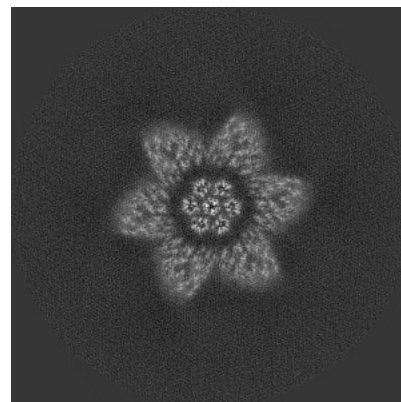
### 6.2.1 Primary map



X Index: 256

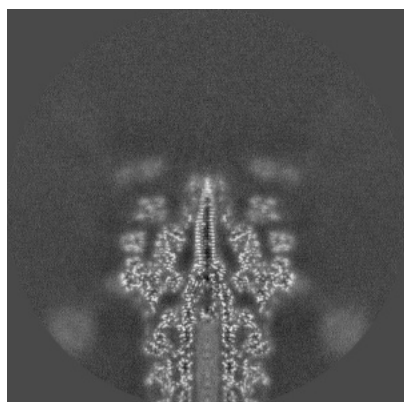


Y Index: 256

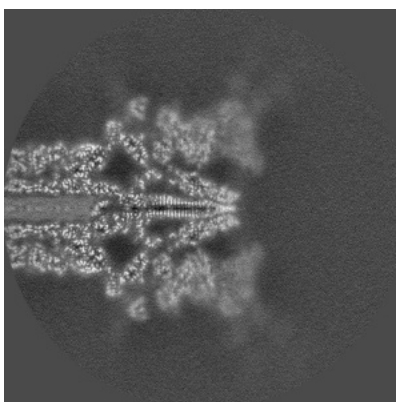


Z Index: 256

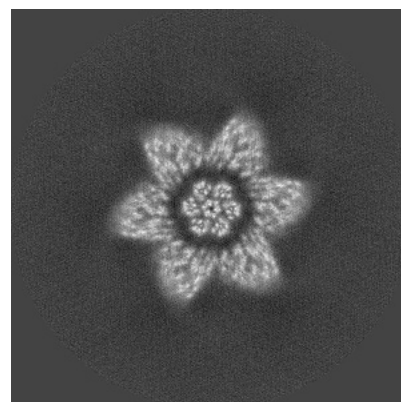
### 6.2.2 Raw map



X Index: 256



Y Index: 256

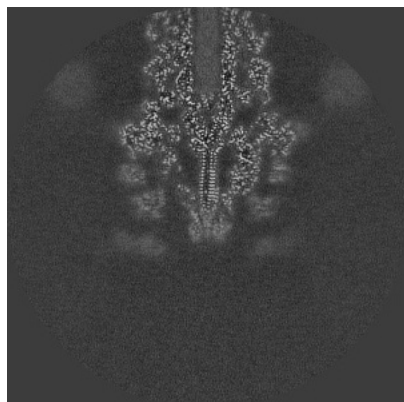


Z Index: 256

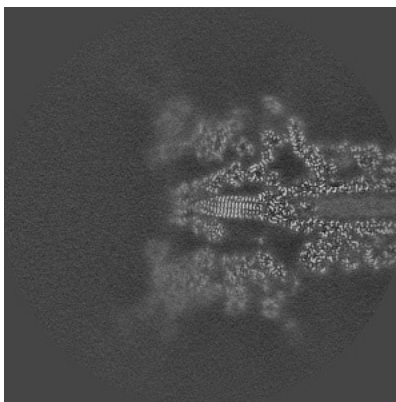
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

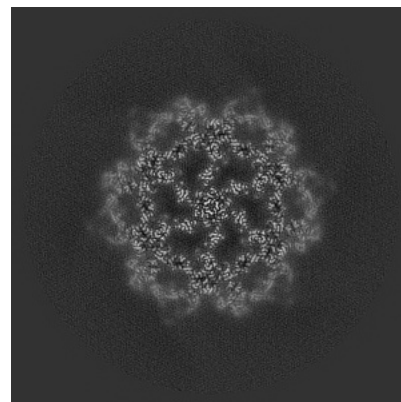
### 6.3.1 Primary map



X Index: 252

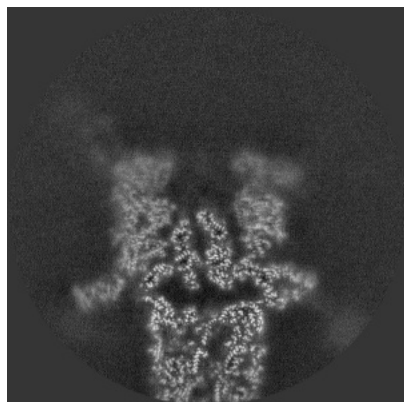


Y Index: 249

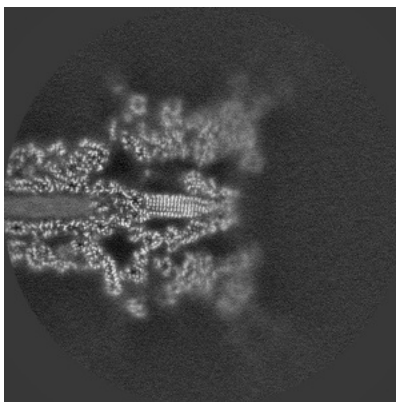


Z Index: 349

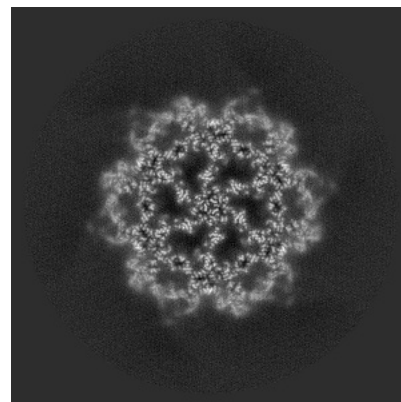
### 6.3.2 Raw map



X Index: 216



Y Index: 262

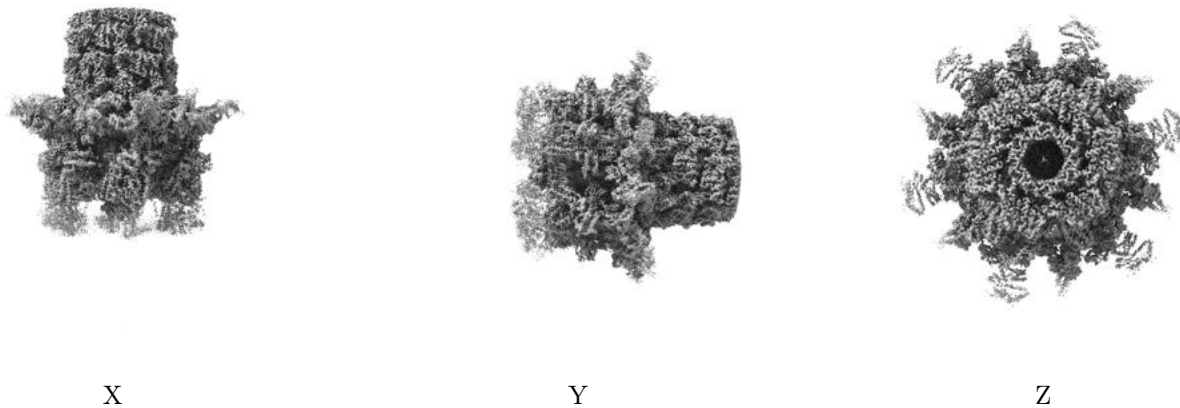


Z Index: 162

The images above show the largest variance slices of the map in three orthogonal directions.

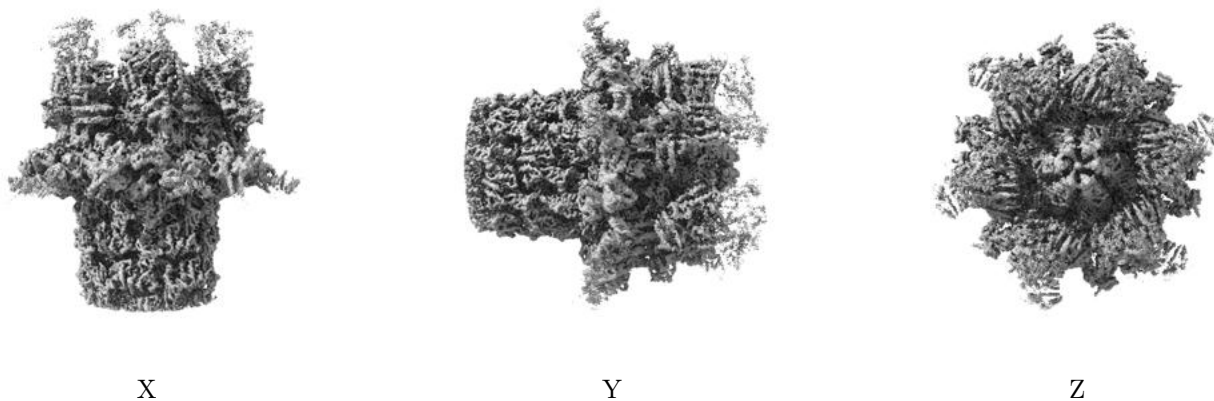
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0275. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

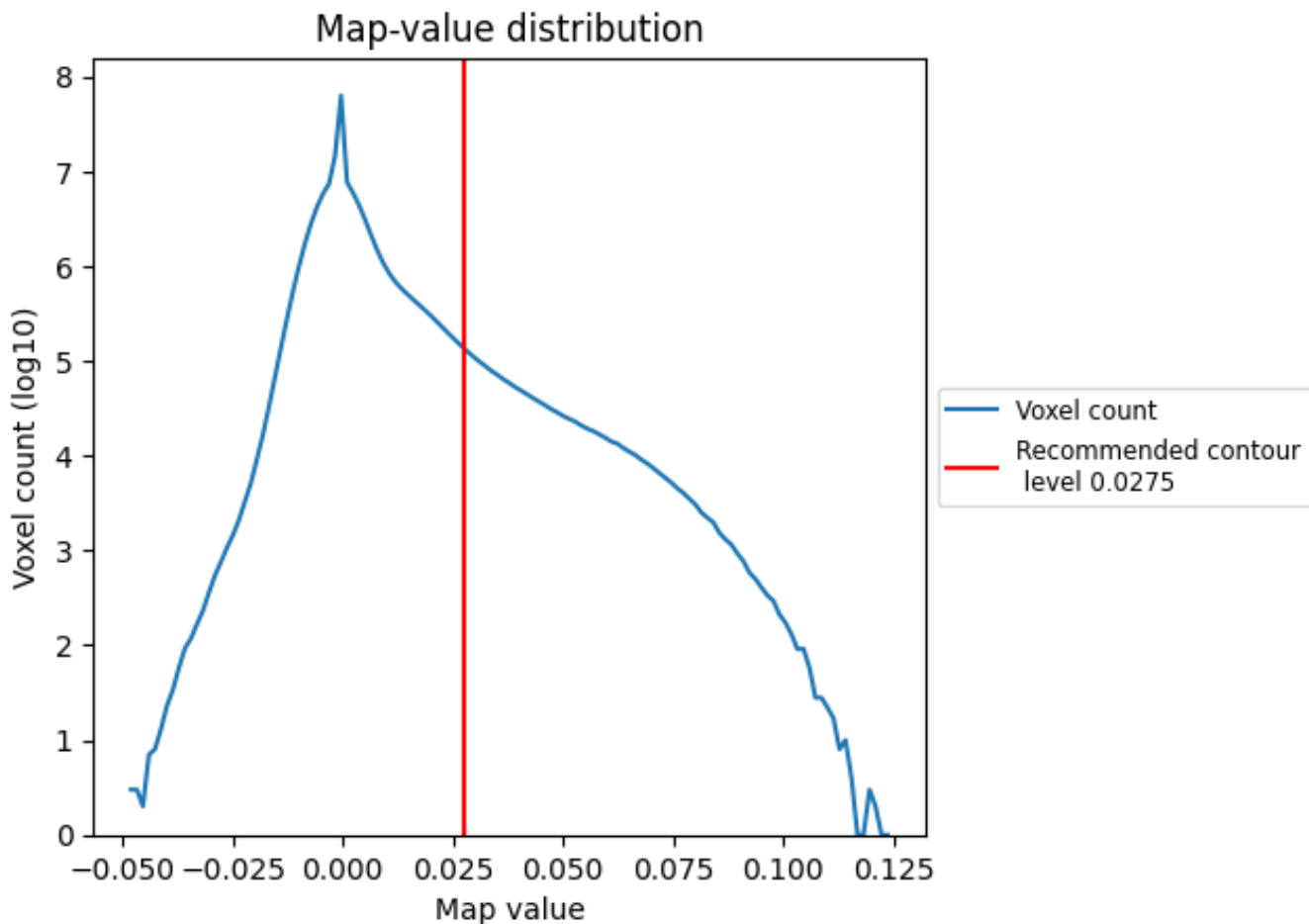
## 6.5 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

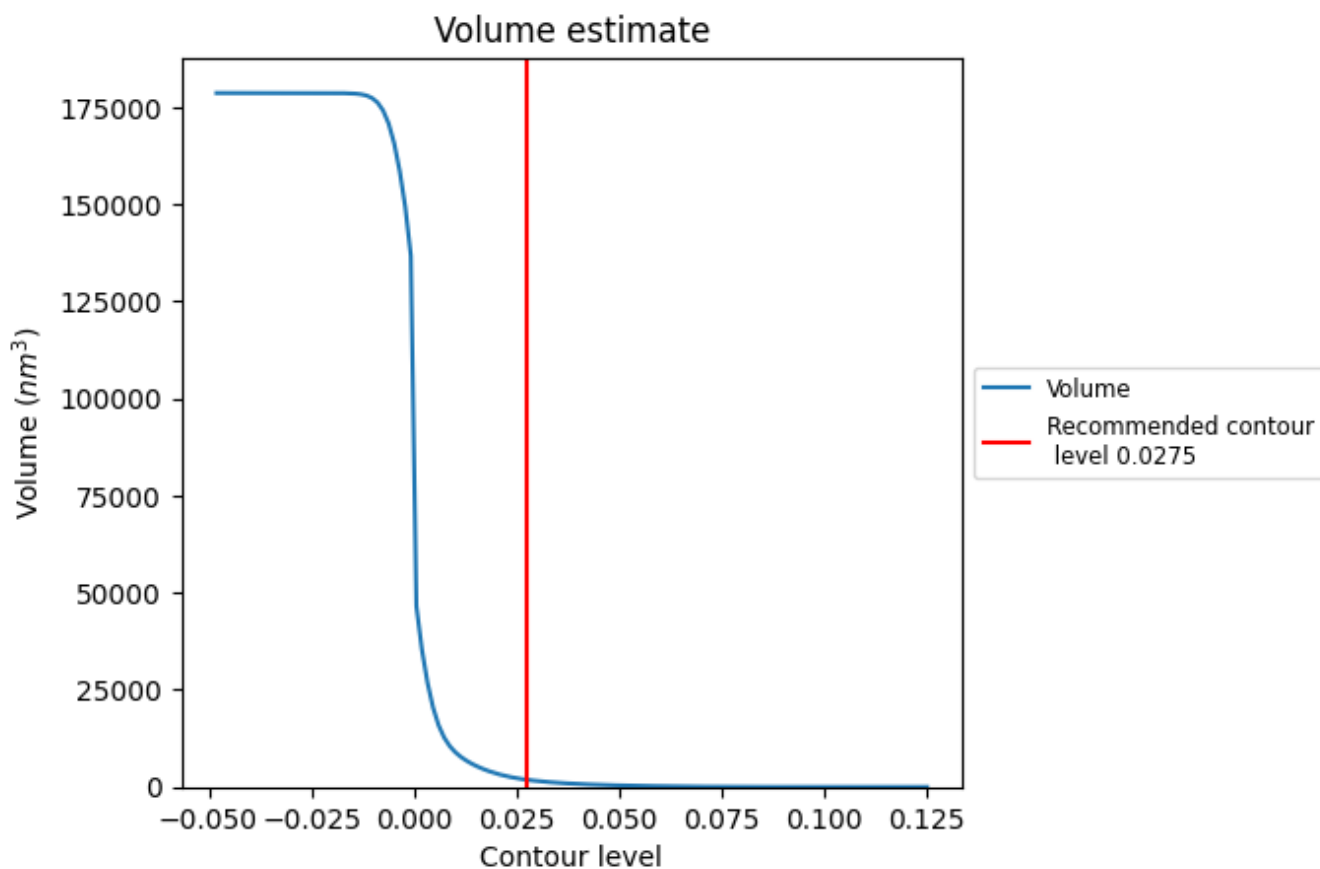
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [\(i\)](#)

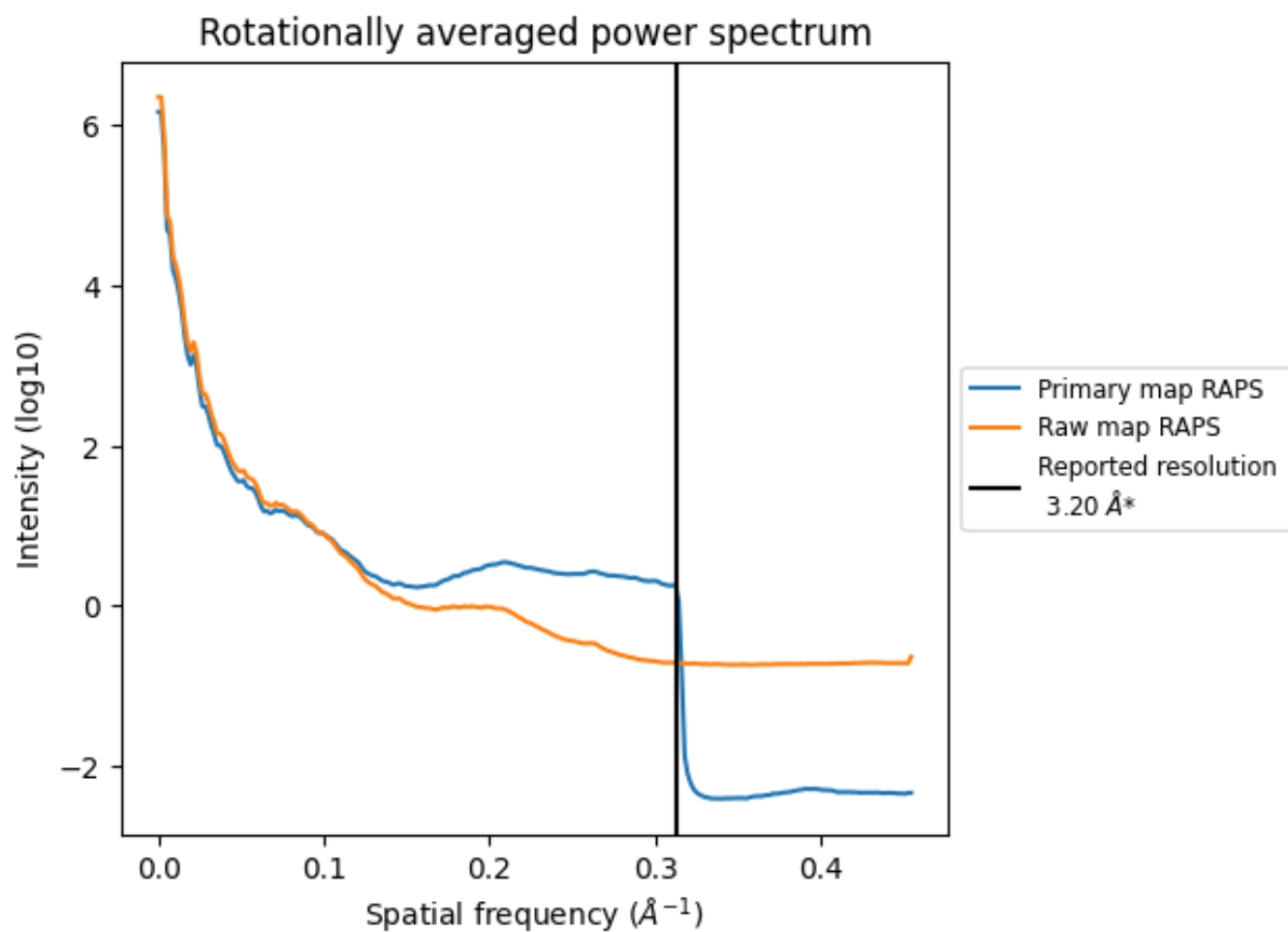


The volume at the recommended contour level is 1849  $\text{nm}^3$ ; this corresponds to an approximate mass of 1670 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum i

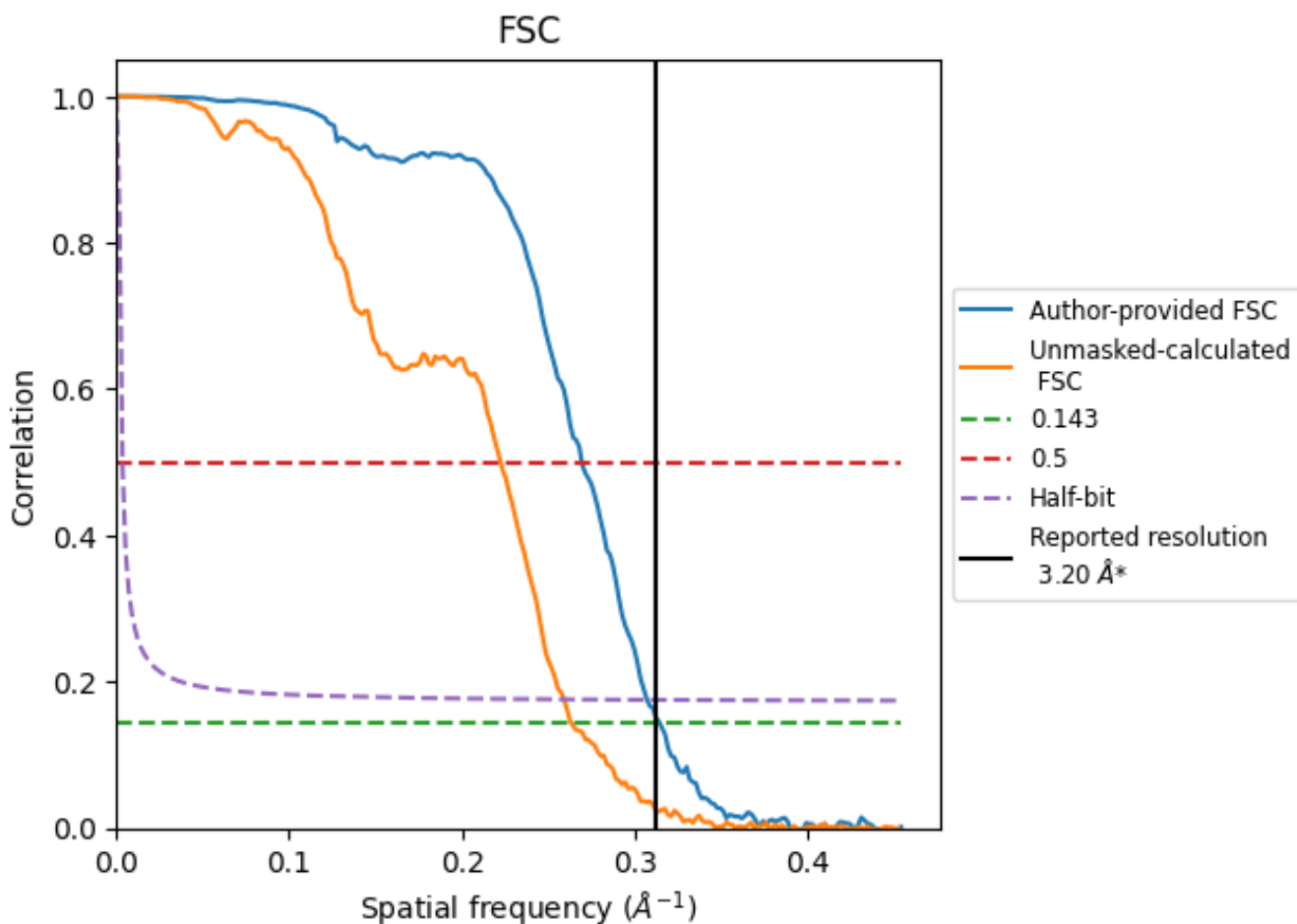


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates

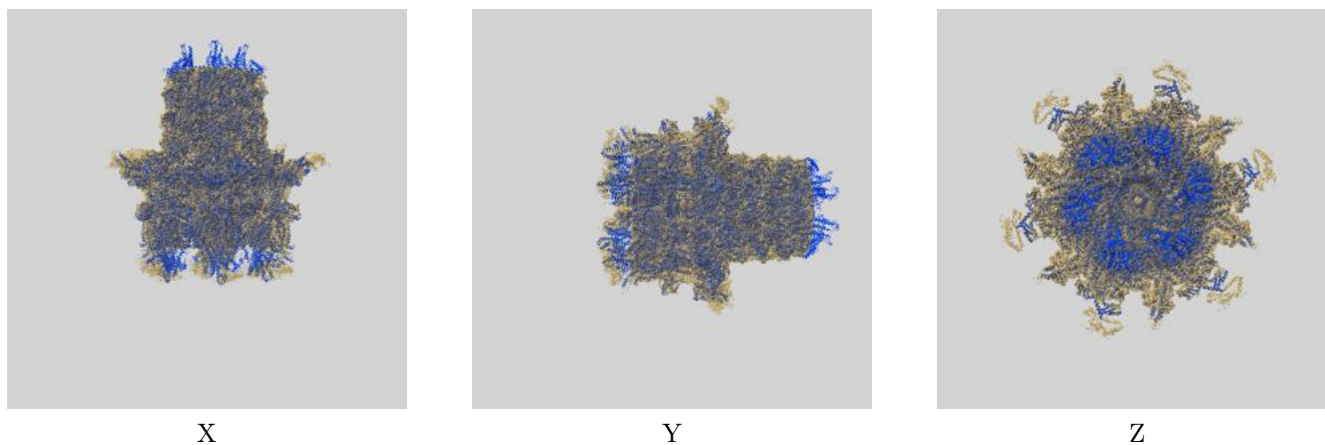
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.71	3.25
Unmasked-calculated*	3.79	4.49	3.86

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.79 differs from the reported value 3.2 by more than 10 %

## 9 Map-model fit [i](#)

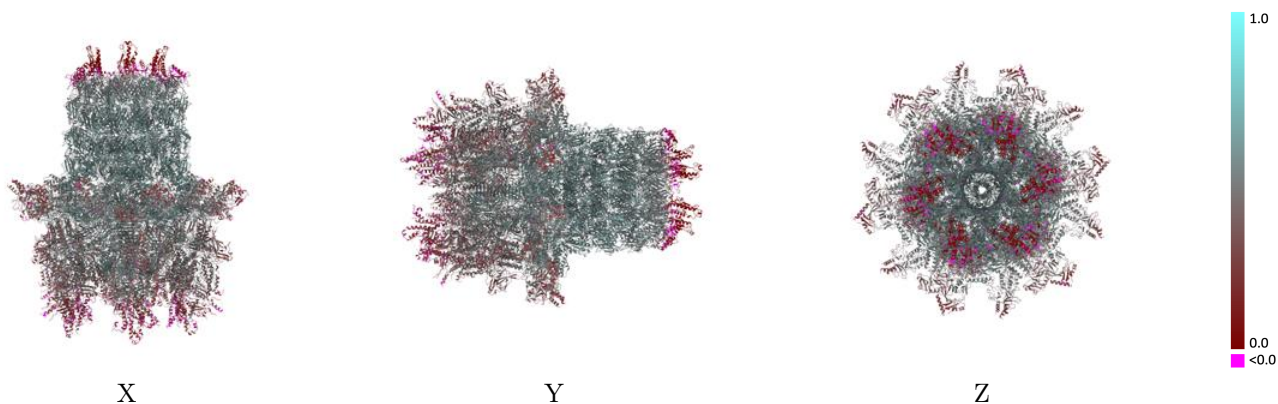
This section contains information regarding the fit between EMDB map EMD-12029 and PDB model 7B5H. Per-residue inclusion information can be found in section 3 on page 13.

### 9.1 Map-model overlay [i](#)



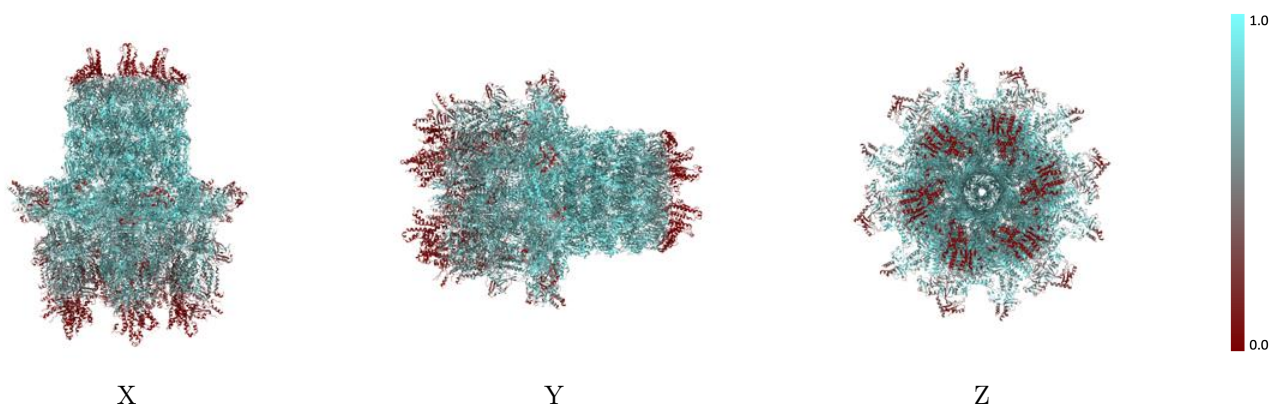
The images above show the 3D surface view of the map at the recommended contour level 0.0275 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



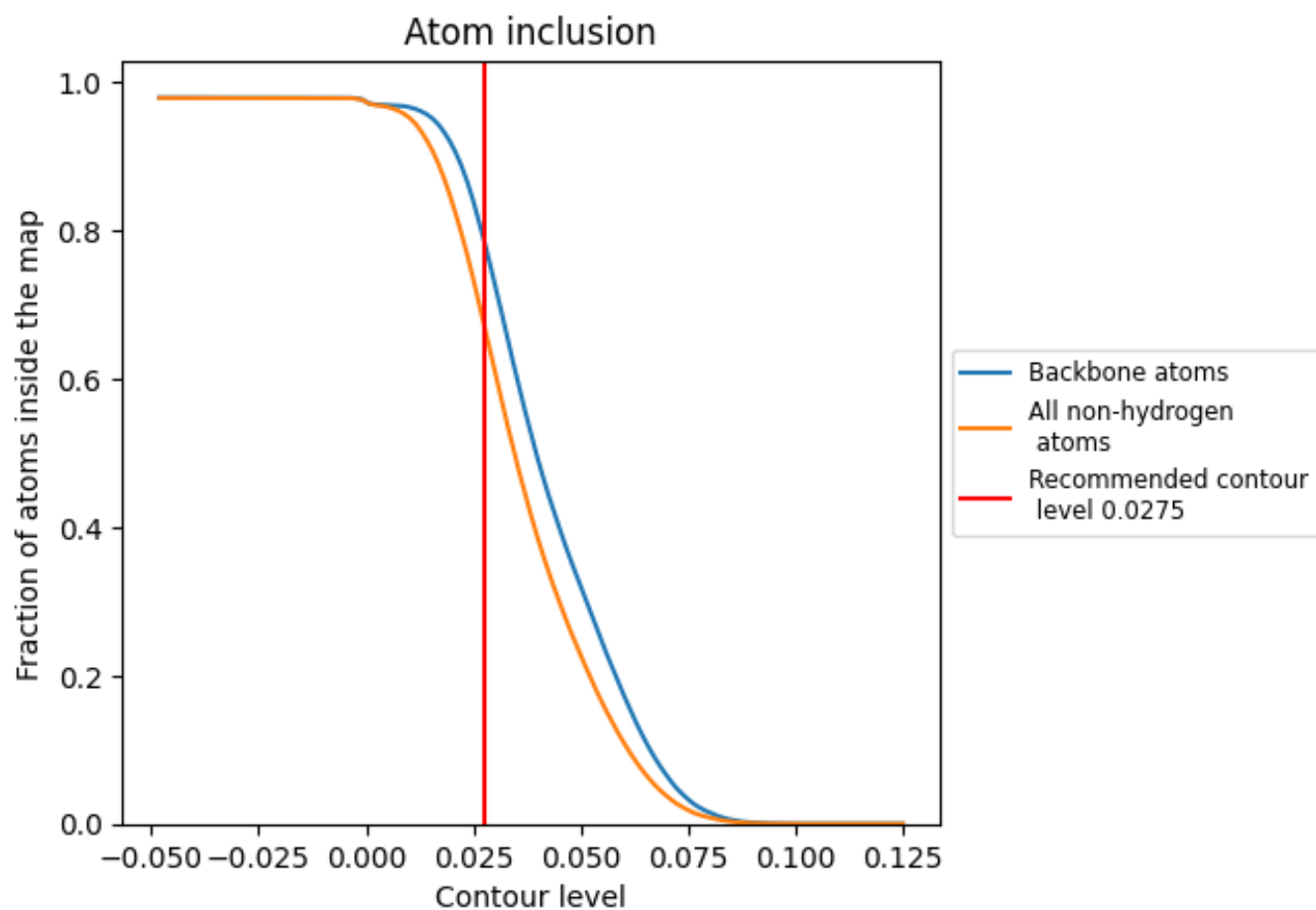
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0275).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0275) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6730	 0.4590
AA	 0.4526	 0.3810
AB	 0.4454	 0.3390
AC	 0.4952	 0.3720
AD	 0.7382	 0.4730
AE	 0.6957	 0.4270
AF	 0.6715	 0.3870
AG	 0.6316	 0.3600
AH	 0.8617	 0.5540
AI	 0.8567	 0.5680
AJ	 0.9083	 0.5950
AK	 0.8782	 0.5810
AL	 0.6762	 0.5460
AM	 0.8325	 0.5670
AN	 0.6941	 0.4970
AO	 0.8642	 0.5660
AP	 0.7945	 0.5380
AQ	 0.3398	 0.2670
BA	 0.4517	 0.3790
BB	 0.4455	 0.3510
BC	 0.5030	 0.3730
BD	 0.7353	 0.4740
BE	 0.6643	 0.4080
BF	 0.6763	 0.3740
BG	 0.6401	 0.3790
BH	 0.8577	 0.5500
BI	 0.8605	 0.5640
BK	 0.8776	 0.5810
BM	 0.8228	 0.5660
BN	 0.6861	 0.4980
BO	 0.8515	 0.5610
BP	 0.7882	 0.5350
BQ	 0.3450	 0.2620
CA	 0.4555	 0.3780
CB	 0.4426	 0.3390



*Continued on next page...*









































*Continued from previous page...*

Chain	Atom inclusion	Q-score
CC	0.4936	0.3720
CD	0.7399	0.4730
CE	0.6920	0.4310
CF	0.6836	0.3920
CG	0.6389	0.3620
CH	0.8607	0.5510
CI	0.8558	0.5660
CJ	0.9065	0.5930
CK	0.8744	0.5790
CL	0.6726	0.5420
CM	0.8341	0.5690
CN	0.6879	0.4990
CO	0.8665	0.5640
CP	0.7945	0.5370
CQ	0.3371	0.2660
DA	0.4545	0.3760
DB	0.4476	0.3510
DC	0.5066	0.3740
DD	0.7388	0.4740
DE	0.6739	0.4100
DF	0.6715	0.3740
DG	0.6401	0.3760
DH	0.8596	0.5500
DI	0.8595	0.5640
DK	0.8824	0.5850
DM	0.8252	0.5700
DN	0.6835	0.5030
DO	0.8551	0.5620
DP	0.7948	0.5340
DQ	0.3456	0.2650
EA	0.4531	0.3810
EB	0.4414	0.3380
EC	0.4934	0.3710
ED	0.7409	0.4710
EE	0.6993	0.4290
EF	0.6787	0.3890
EG	0.6353	0.3600
EH	0.8609	0.5510
EI	0.8502	0.5670
EJ	0.9076	0.5930
EK	0.8776	0.5820
EL	0.6762	0.5470

*Continued on next page...*



*Continued from previous page...*

Chain	Atom inclusion	Q-score
EM	 0.8301	 0.5720
EN	 0.6897	 0.5000
EO	 0.8623	 0.5640
EP	 0.7923	 0.5360
EQ	 0.3338	 0.2650
FA	 0.4541	 0.3790
FB	 0.4449	 0.3500
FC	 0.5075	 0.3740
FD	 0.7330	 0.4740
FE	 0.6655	 0.4120
FF	 0.6691	 0.3790
FG	 0.6353	 0.3770
FH	 0.8590	 0.5520
FI	 0.8614	 0.5630
FK	 0.8792	 0.5810
FM	 0.8179	 0.5670
FN	 0.6799	 0.5000
FO	 0.8548	 0.5630
FP	 0.7937	 0.5360
FQ	 0.3434	 0.2640