



# wwPDB EM Validation Summary Report ⓘ

Apr 23, 2024 – 08:08 am BST

PDB ID : 8RVE  
EMDB ID : EMD-16844  
Title : Vimentin intermediate filament  
Authors : Eibauer, M.; Medalia, O.  
Deposited on : 2024-02-01  
Resolution : 7.20 Å(reported)  
Based on initial model : .

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>.

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

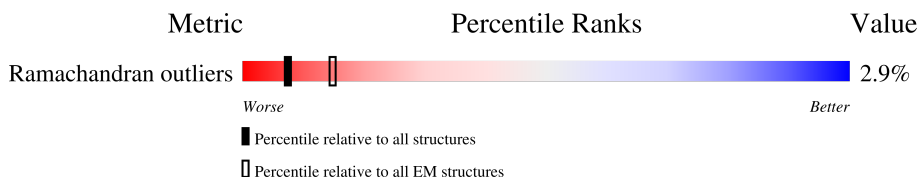
EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 7.20 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)
Ramachandran outliers	154571	4023

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	0	466	6% (Poor fit), 48% (0 outliers), 5% (1 outlier), 46% (Not modelled)
1	1	466	24% (Poor fit), 54% (0 outliers), 2% (1 outlier), 1% (2 outliers), 19% (Not modelled)
1	2	466	22% (Poor fit), 53% (0 outliers), 2% (1 outlier), 1% (2 outliers), 18% (Not modelled)
1	3	466	24% (Poor fit), 37% (0 outliers), 1% (1 outlier), 38% (Not modelled)
1	4	466	28% (Poor fit), 37% (0 outliers), 5% (1 outlier), 30% (Not modelled)
1	5	466	14% (Poor fit), 52% (0 outliers), 2% (1 outlier), 1% (2 outliers), 29% (Not modelled)
1	6	466	14% (Poor fit), 52% (0 outliers), 2% (1 outlier), 1% (2 outliers), 29% (Not modelled)
1	7	466	19% (Poor fit), 27% (0 outliers), 1% (1 outlier), 53% (Not modelled)
1	8	466	22% (Poor fit), 28% (0 outliers), 1% (1 outlier), 49% (Not modelled)
1	9	466	13% (Poor fit), 48% (0 outliers), 5% (1 outlier), 34% (Not modelled)
1	A	466	26% (Poor fit), 53% (0 outliers), 7% (1 outlier), 14% (Not modelled)

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Mol	Chain	Length	Quality of chain
1	AA	466	13% 17% 80%
1	AB	466	14% 19% 79%
1	AC	466	13% 42% 52%
1	AD	466	9% 41% 52%
1	AE	466	8% 9% 89%
1	AF	466	8% 10% 88%
1	AG	466	11% 38% 57%
1	AH	466	11% 38% 57%
1	AI	466	8% 32% 64%
1	AJ	466	10% 31% 64%
1	AK	466	6% 26% 71%
1	AL	466	6% 26% 70%
1	AM	466	5% 15% 83%
1	AN	466	16% 82%
1	AO	466	6% 93%
1	AP	466	6% 92%
1	B	466	26% 52% 6% 42%
1	C	466	29% 56% 5% 40%
1	D	466	30% 55% 40%
1	E	466	5% 6% 93%
1	F	466	7% 92%
1	G	466	6% 9% 89%
1	H	466	6% 10% 88%
1	I	466	5% 14% 83%
1	J	466	8% 16% 82%

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Mol	Chain	Length	Quality of chain
1	K	466	9% 20% 77%
1	L	466	10% 21% 76%
1	M	466	14% 26% 71%
1	N	466	13% 27% 70%
1	O	466	20% 31% 65%
1	P	466	17% 33% 64%
1	Q	466	97%
1	R	466	97%
1	S	466	15% 37% 58%
1	T	466	15% 39% 57%
1	U	466	9% 10% 89%
1	V	466	10% 10% 88%
1	W	466	8% 35% 6% 58%
1	X	466	8% 37% 5% 58%
1	Y	466	15% 20% 79%
1	Z	466	14% 19% 78%
1	a	466	12% 39% 6% 55%
1	b	466	15% 41% 56%
1	c	466	20% 29% 68%
1	d	466	21% 29% 68%
1	e	466	20% 41% 5% 54%
1	f	466	19% 41% 55%
1	g	466	30% 39% 58%
1	h	466	27% 38% 59%
1	i	466	26% 47% 6% 47%

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Mol	Chain	Length	Quality of chain
1	j	466	
1	k	466	
1	l	466	
1	m	466	
1	n	466	
1	o	466	
1	p	466	
1	q	466	
1	r	466	
1	s	466	
1	t	466	
1	u	466	
1	v	466	
1	w	466	
1	x	466	
1	y	466	
1	z	466	

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 54788 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 Vimentin.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	0	253	Total 1012	C 506	N 253	O 253	0	0
1	1	273	Total 1092	C 546	N 273	O 273	0	0
1	2	266	Total 1064	C 532	N 266	O 266	0	0
1	3	191	Total 764	C 382	N 191	O 191	0	0
1	4	195	Total 780	C 390	N 195	O 195	0	0
1	5	267	Total 1068	C 534	N 267	O 267	0	0
1	6	263	Total 1052	C 526	N 263	O 263	0	0
1	7	142	Total 568	C 284	N 142	O 142	0	0
1	8	147	Total 588	C 294	N 147	O 147	0	0
1	9	252	Total 1008	C 504	N 252	O 252	0	0
1	A	281	Total 1124	C 562	N 281	O 281	0	0
1	AA	95	Total 380	C 190	N 95	O 95	0	0
1	AB	100	Total 400	C 200	N 100	O 100	0	0
1	AC	223	Total 892	C 446	N 223	O 223	0	0
1	AD	222	Total 888	C 444	N 222	O 222	0	0
1	AE	49	Total 196	C 98	N 49	O 49	0	0
1	AF	54	Total 216	C 108	N 54	O 54	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	AG	199	Total 796	C 398	N 199	O 199	0	0
1	AH	199	Total 796	C 398	N 199	O 199	0	0
1	AI	167	Total 668	C 334	N 167	O 167	0	0
1	AJ	170	Total 680	C 340	N 170	O 170	0	0
1	AK	136	Total 544	C 272	N 136	O 136	0	0
1	AL	141	Total 564	C 282	N 141	O 141	0	0
1	AM	81	Total 324	C 162	N 81	O 81	0	0
1	AN	85	Total 340	C 170	N 85	O 85	0	0
1	AO	34	Total 136	C 68	N 34	O 34	0	0
1	AP	39	Total 156	C 78	N 39	O 39	0	0
1	B	269	Total 1076	C 538	N 269	O 269	0	0
1	C	281	Total 1124	C 562	N 281	O 281	0	0
1	D	278	Total 1112	C 556	N 278	O 278	0	0
1	E	33	Total 132	C 66	N 33	O 33	0	0
1	F	35	Total 140	C 70	N 35	O 35	0	0
1	G	52	Total 208	C 104	N 52	O 52	0	0
1	H	54	Total 216	C 108	N 54	O 54	0	0
1	I	79	Total 316	C 158	N 79	O 79	0	0
1	J	83	Total 332	C 166	N 83	O 83	0	0
1	K	107	Total 428	C 214	N 107	O 107	0	0
1	L	113	Total 452	C 226	N 113	O 113	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	M	136	Total 544	C 272	N 136	O 136	0	0
1	N	142	Total 568	C 284	N 142	O 142	0	0
1	O	165	Total 660	C 330	N 165	O 165	0	0
1	P	170	Total 680	C 340	N 170	O 170	0	0
1	Q	14	Total 56	C 28	N 14	O 14	0	0
1	R	14	Total 56	C 28	N 14	O 14	0	0
1	S	194	Total 776	C 388	N 194	O 194	0	0
1	T	199	Total 796	C 398	N 199	O 199	0	0
1	U	53	Total 212	C 106	N 53	O 53	0	0
1	V	57	Total 228	C 114	N 57	O 57	0	0
1	W	194	Total 776	C 388	N 194	O 194	0	0
1	X	194	Total 776	C 388	N 194	O 194	0	0
1	Y	99	Total 396	C 198	N 99	O 99	0	0
1	Z	102	Total 408	C 204	N 102	O 102	0	0
1	a	209	Total 836	C 418	N 209	O 209	0	0
1	b	205	Total 820	C 410	N 205	O 205	0	0
1	c	148	Total 592	C 296	N 148	O 148	0	0
1	d	150	Total 600	C 300	N 150	O 150	0	0
1	e	214	Total 856	C 428	N 214	O 214	0	0
1	f	209	Total 836	C 418	N 209	O 209	0	0
1	g	194	Total 776	C 388	N 194	O 194	0	0

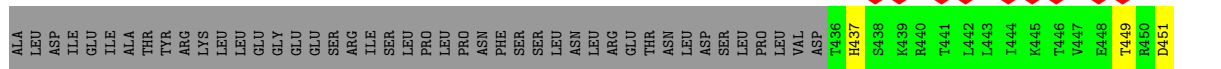
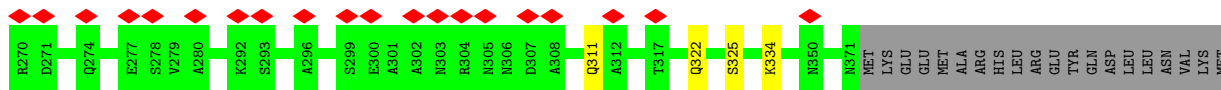
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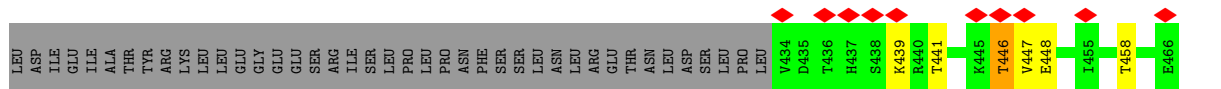
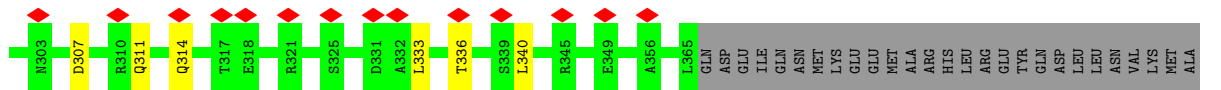
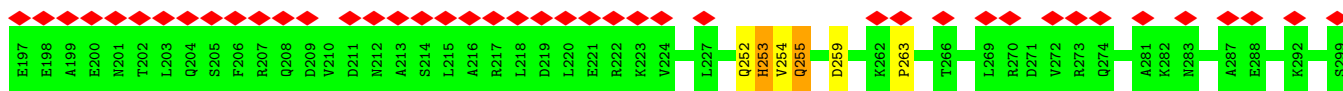
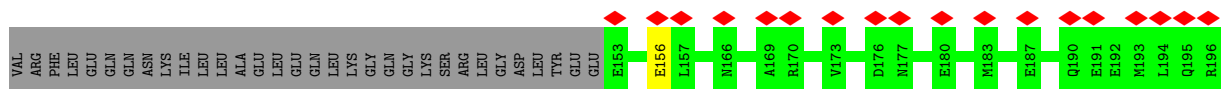
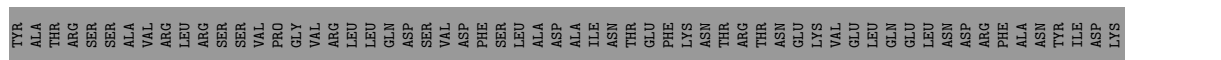
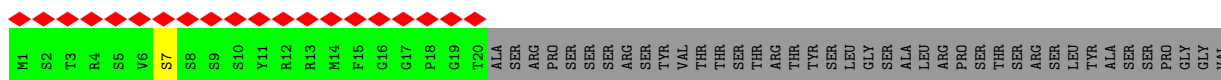
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Mol	Chain	Residues	Atoms				AltConf	Trace
1	h	193	Total	C	N	O	0	0
			772	386	193	193		
1	i	246	Total	C	N	O	0	0
			984	492	246	246		
1	j	237	Total	C	N	O	0	0
			948	474	237	237		
1	k	224	Total	C	N	O	0	0
			896	448	224	224		
1	l	225	Total	C	N	O	0	0
			900	450	225	225		
1	m	265	Total	C	N	O	0	0
			1060	530	265	265		
1	n	253	Total	C	N	O	0	0
			1012	506	253	253		
1	o	254	Total	C	N	O	0	0
			1016	508	254	254		
1	p	253	Total	C	N	O	0	0
			1012	506	253	253		
1	q	283	Total	C	N	O	0	0
			1132	566	283	283		
1	r	278	Total	C	N	O	0	0
			1112	556	278	278		
1	s	277	Total	C	N	O	0	0
			1108	554	277	277		
1	t	266	Total	C	N	O	0	0
			1064	532	266	266		
1	u	258	Total	C	N	O	0	0
			1032	516	258	258		
1	v	254	Total	C	N	O	0	0
			1016	508	254	254		
1	w	259	Total	C	N	O	0	0
			1036	518	259	259		
1	x	250	Total	C	N	O	0	0
			1000	500	250	250		
1	y	224	Total	C	N	O	0	0
			896	448	224	224		
1	z	228	Total	C	N	O	0	0
			912	456	228	228		

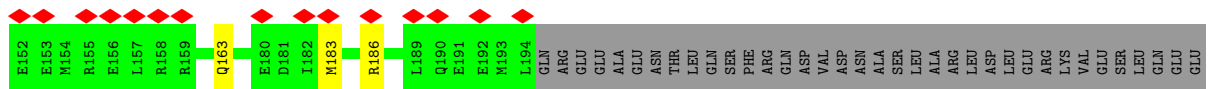
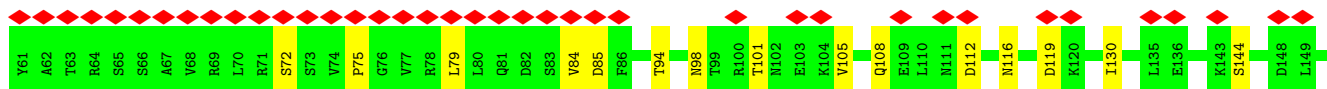
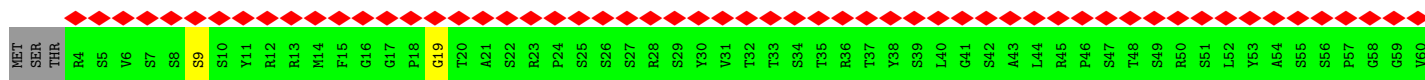




• Molecule 1: Vimentin



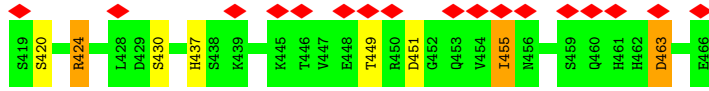
• Molecule 1: Vimentin



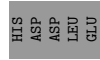
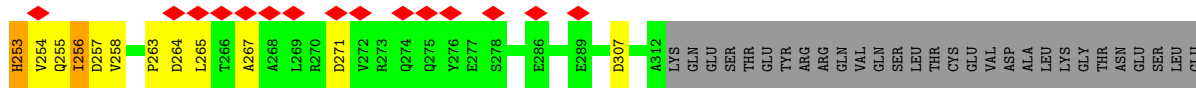
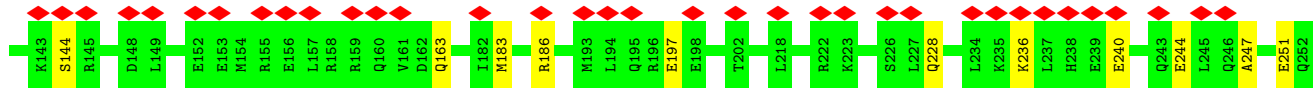
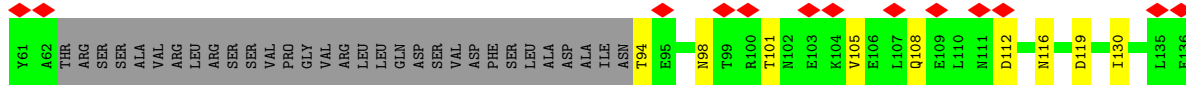
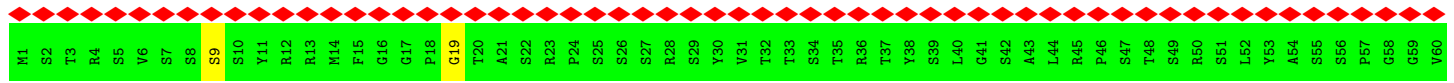




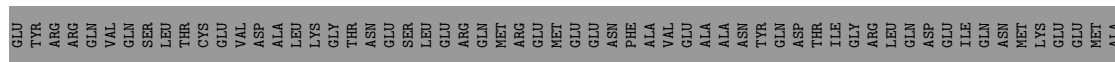
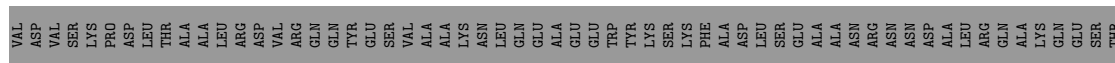
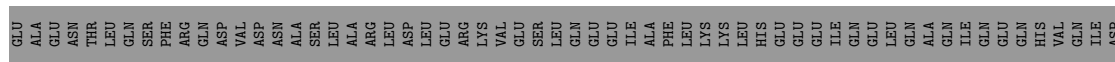
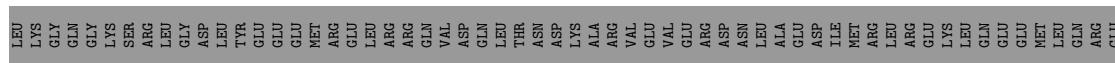
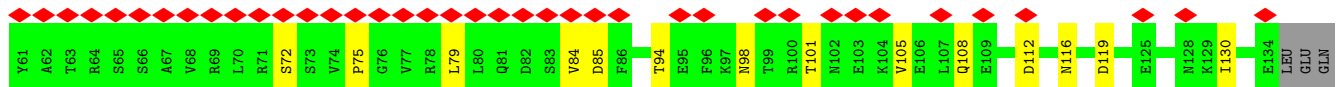
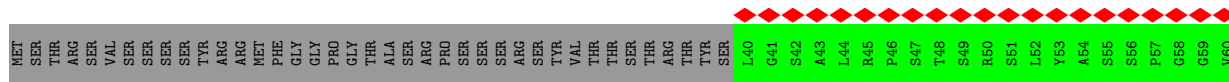




• Molecule 1: Vimentin



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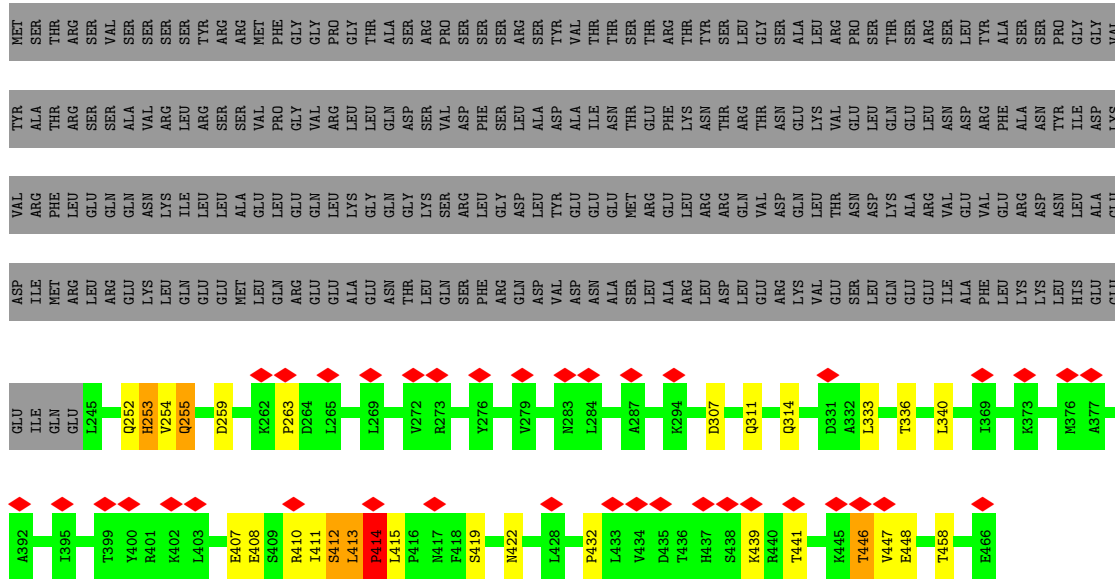
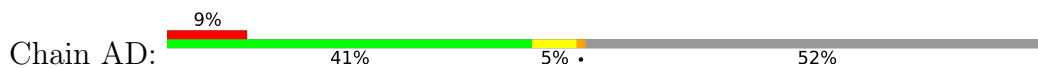




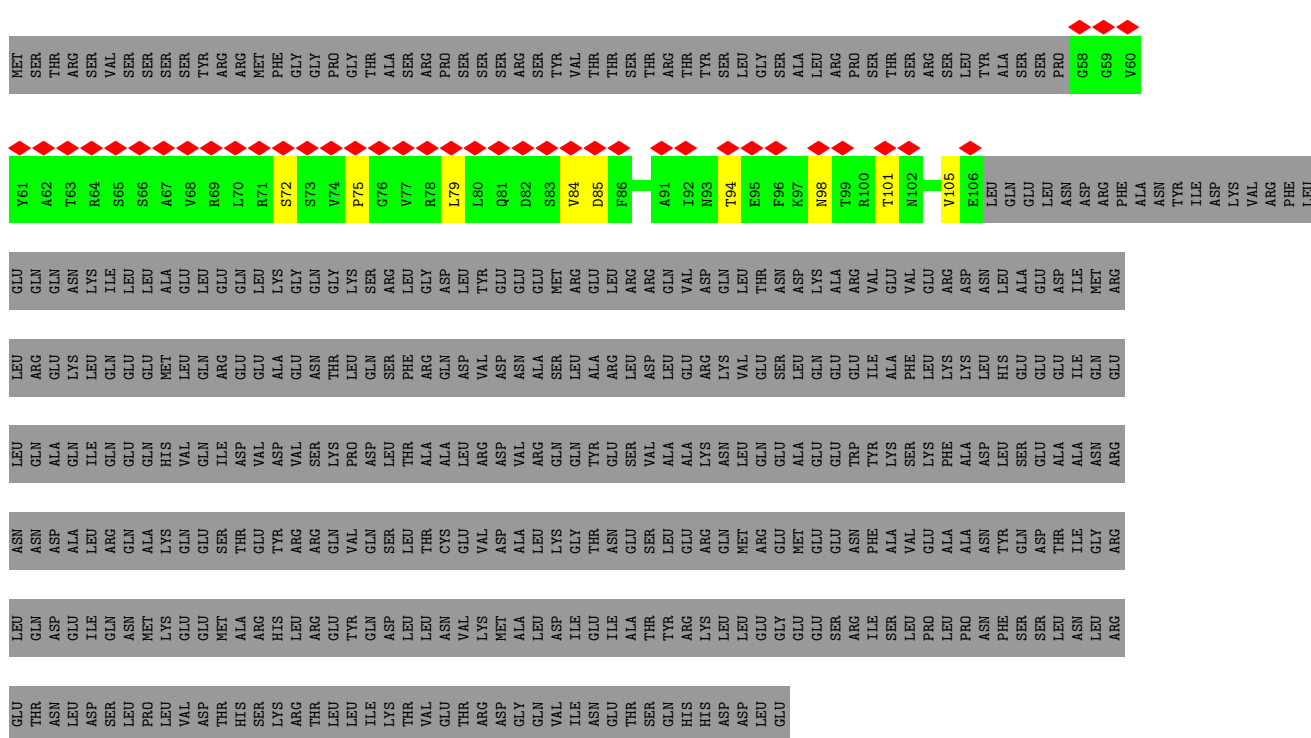




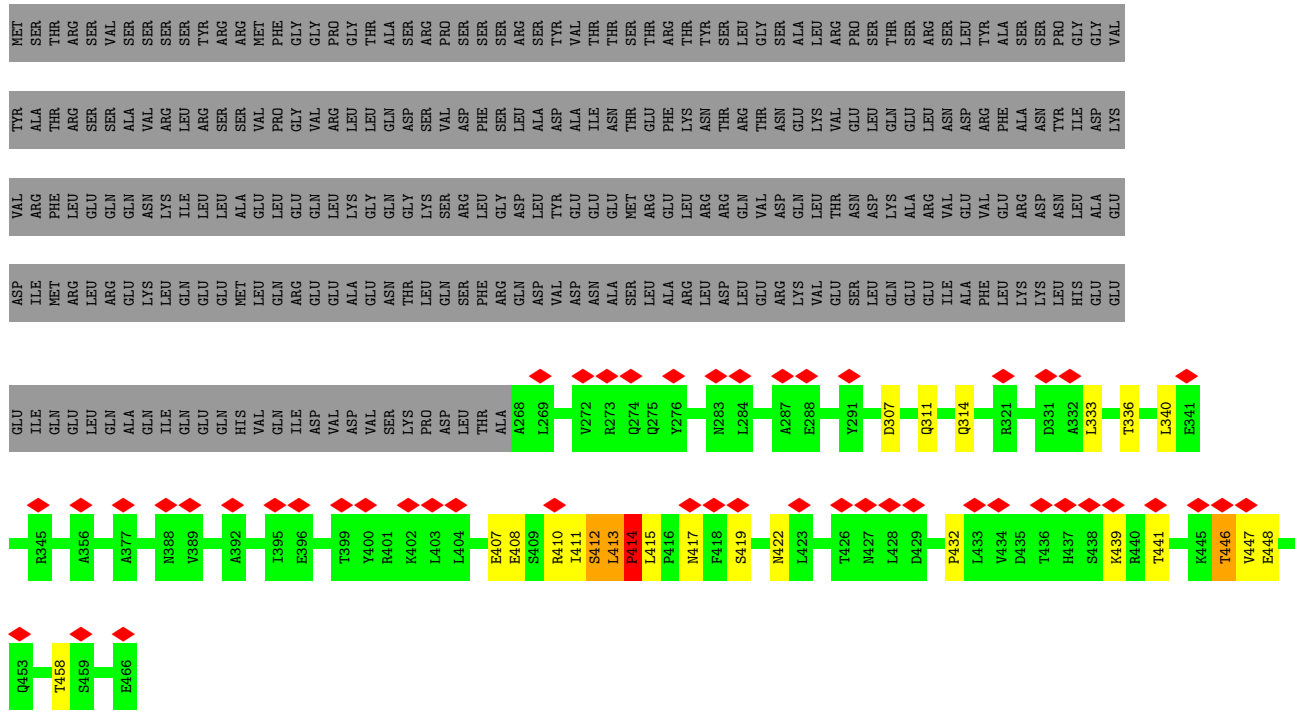
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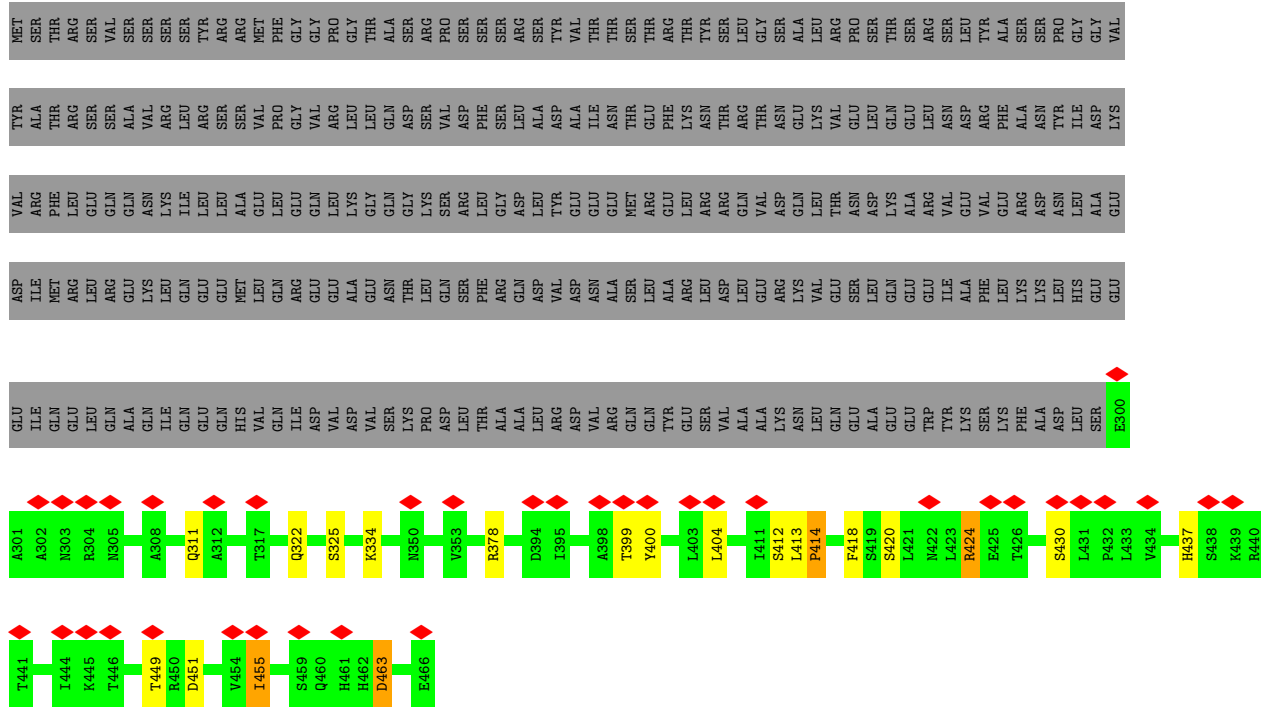
• Molecule 1: Vimentin





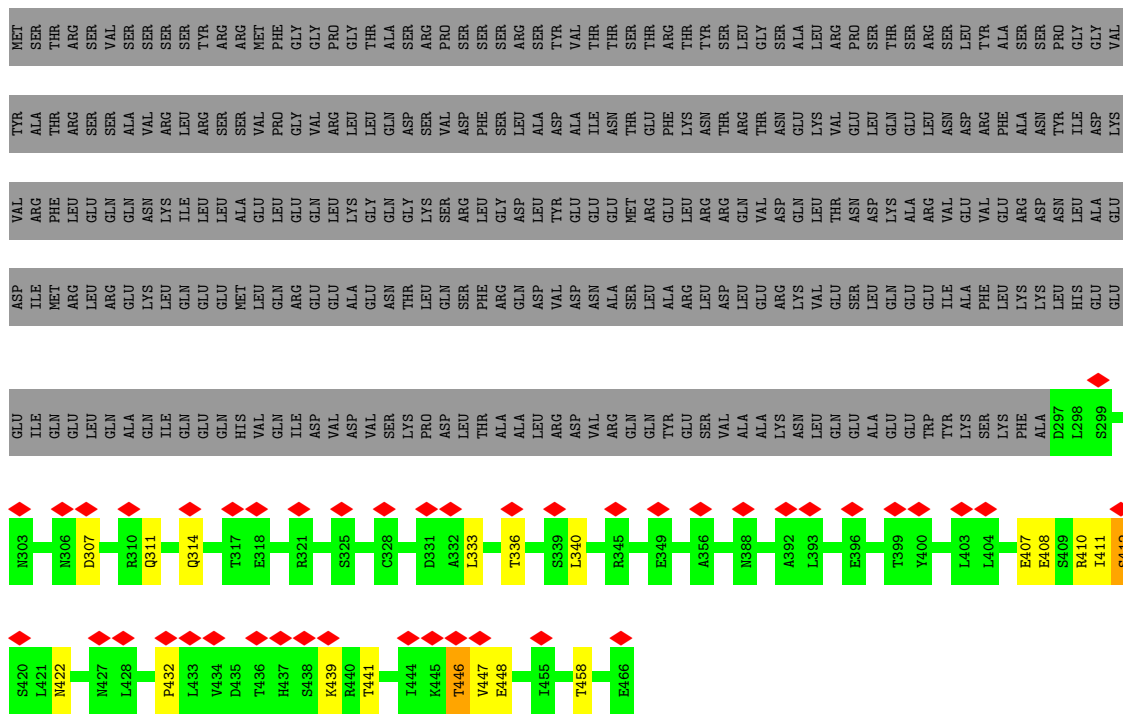


• Molecule 1: Vimentin

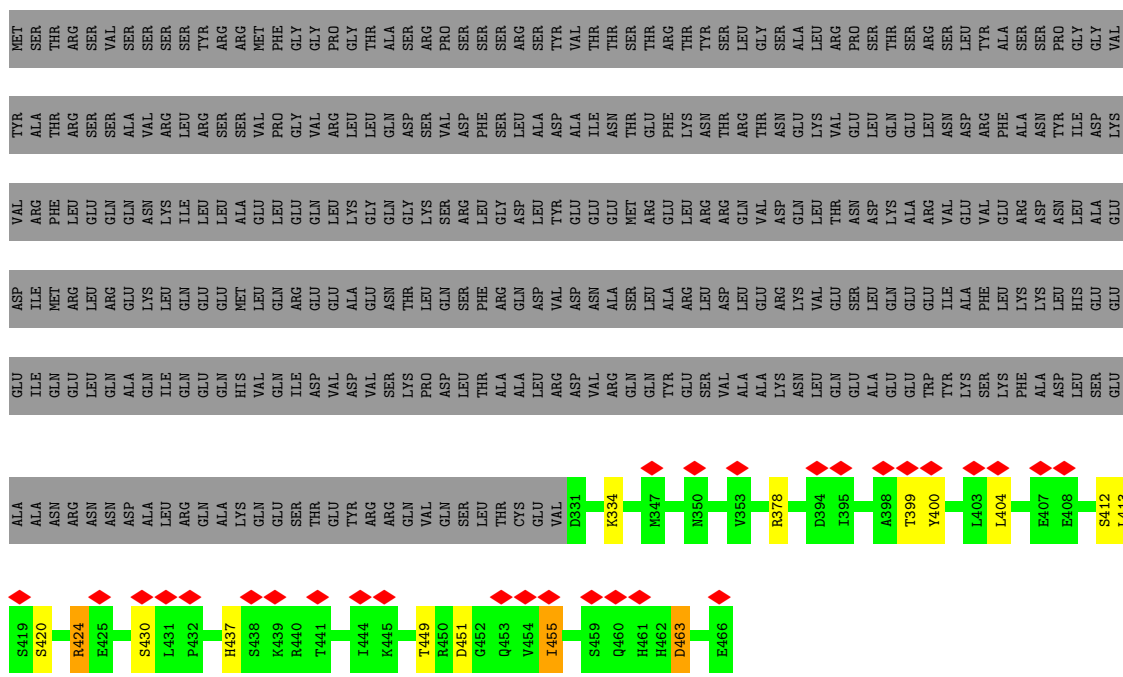


• Molecule 1: Vimentin



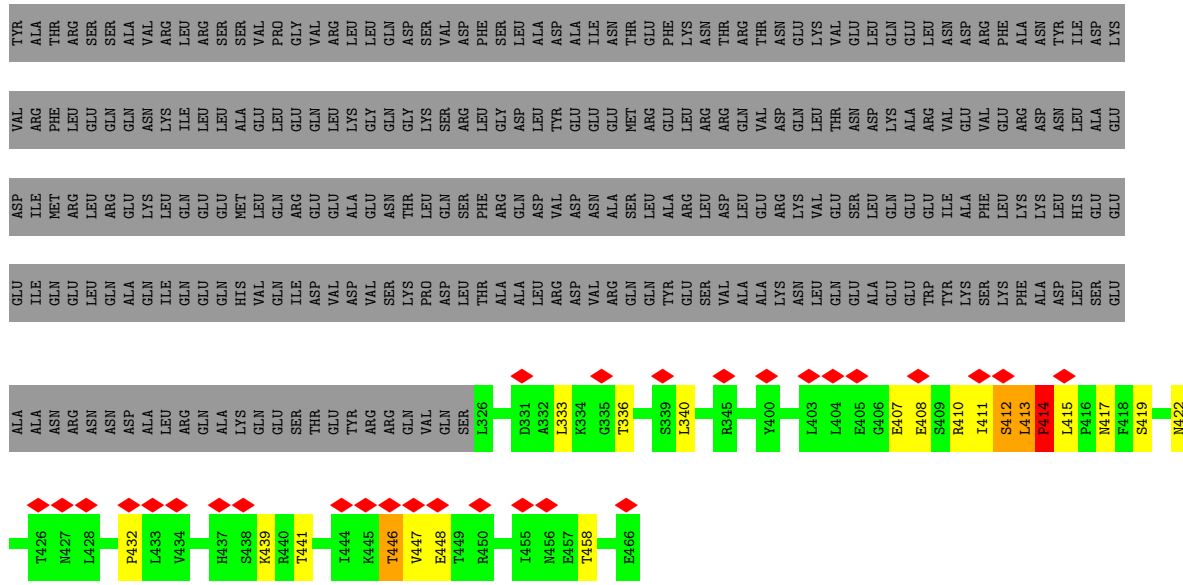


• Molecule 1: Vimentin

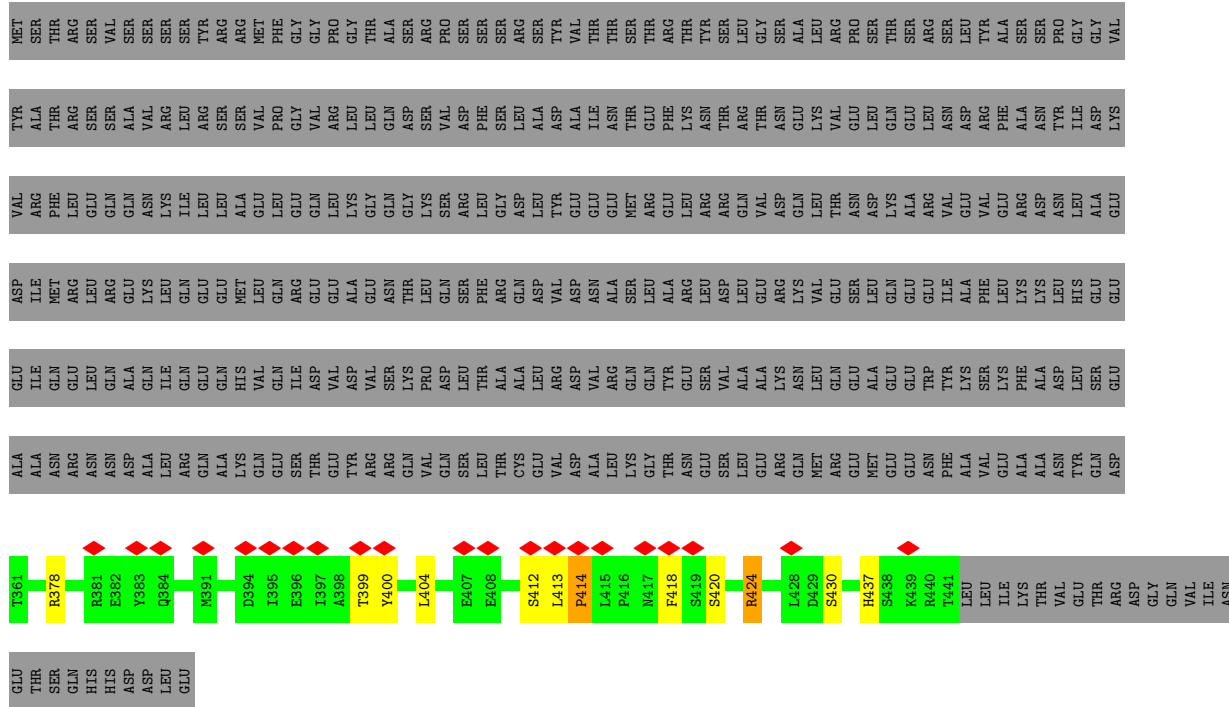


• Molecule 1: Vimentin

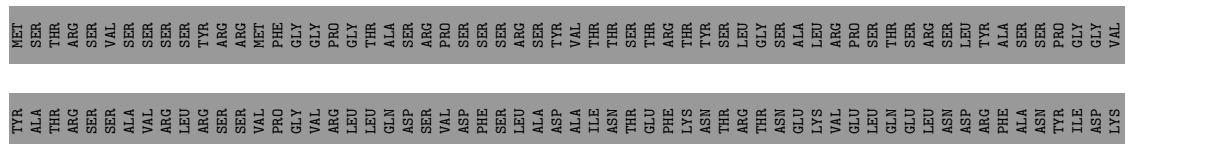


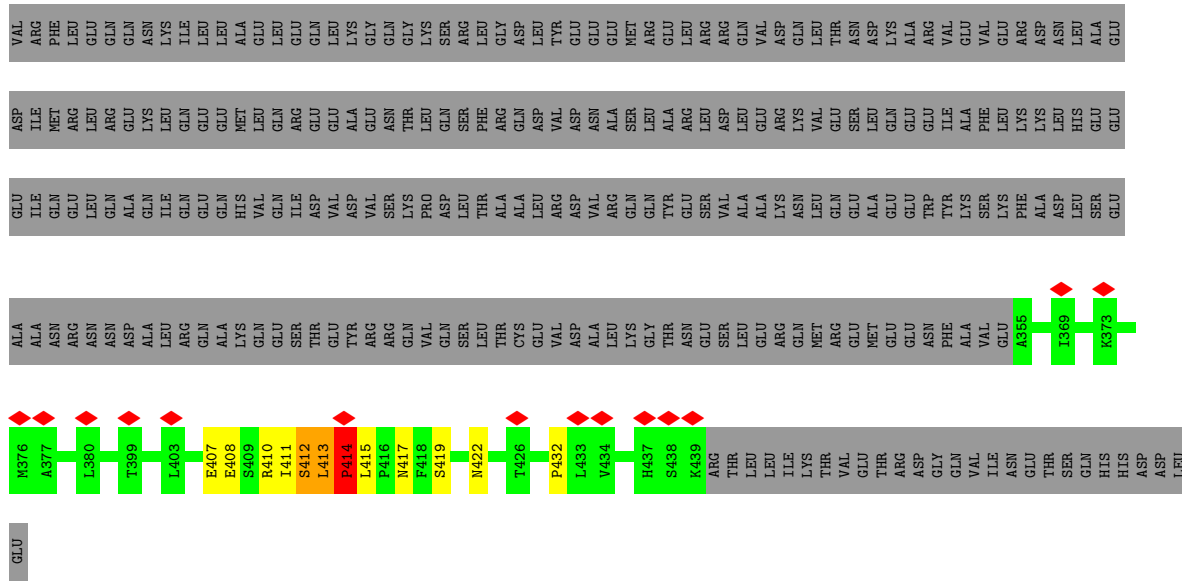


● Molecule 1: Vimentin

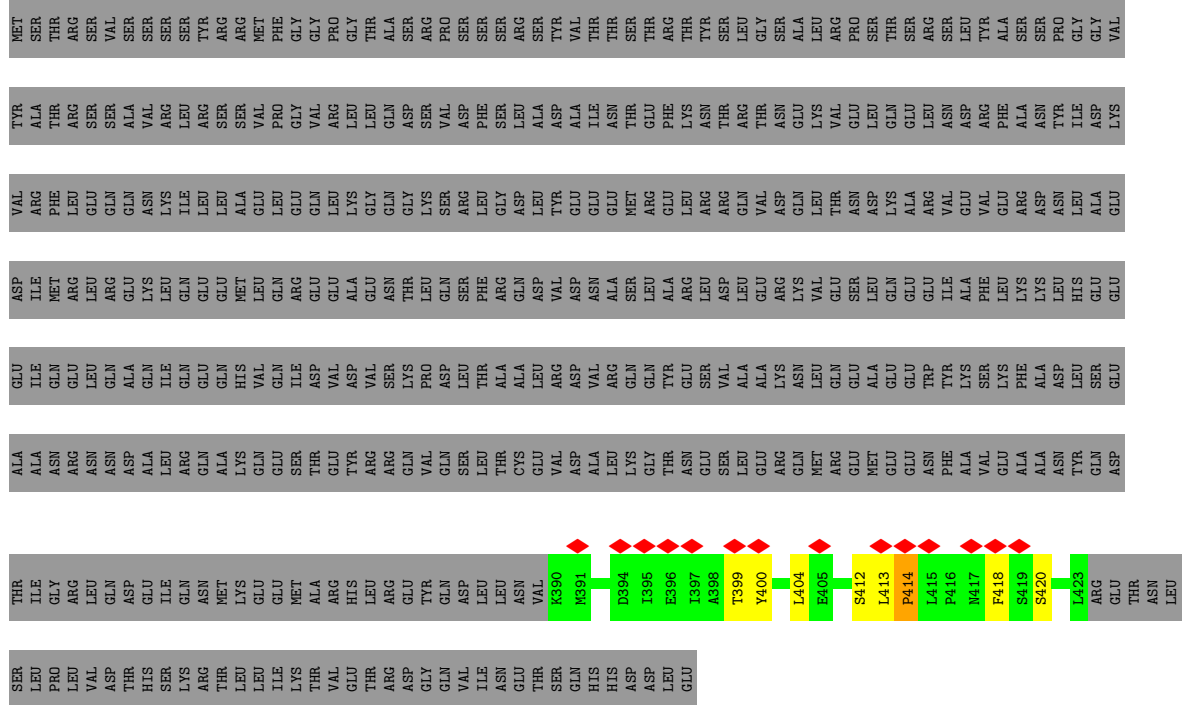


● Molecule 1: Vimentin

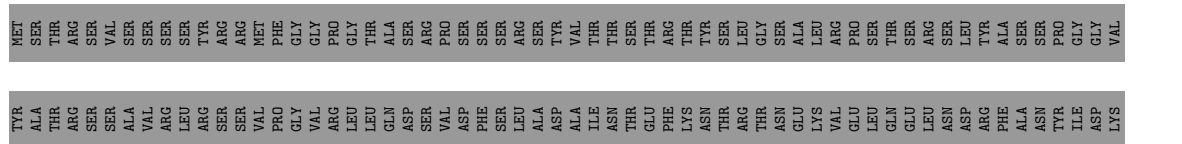




• Molecule 1: Vimentin



• Molecule 1: Vimentin



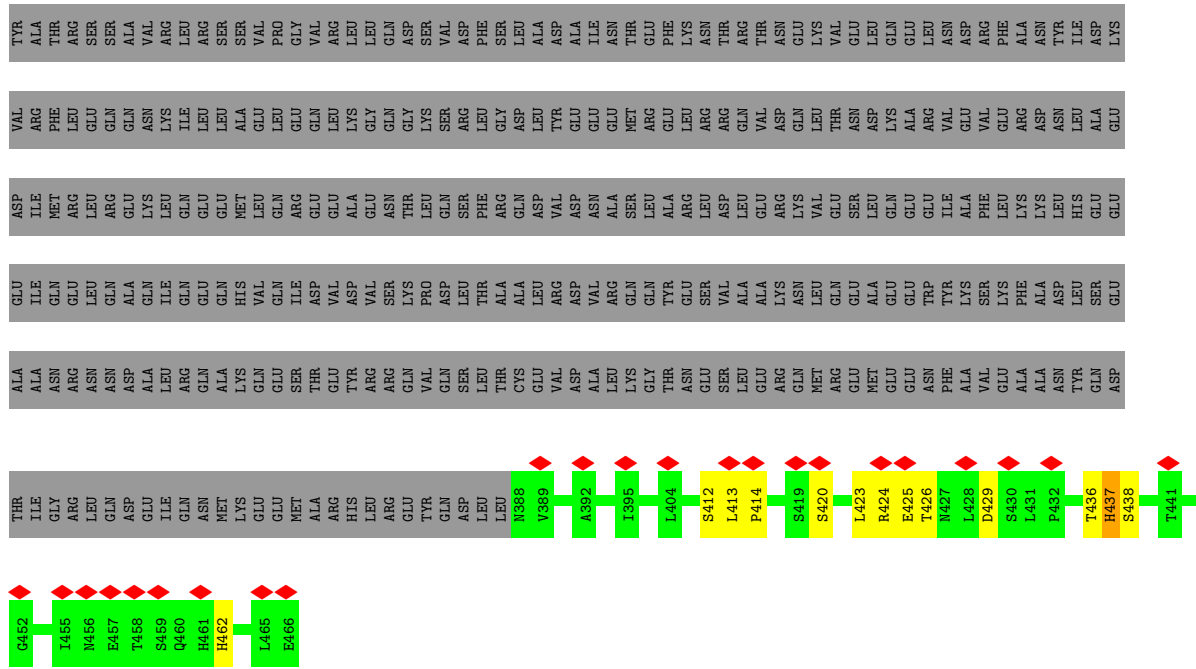




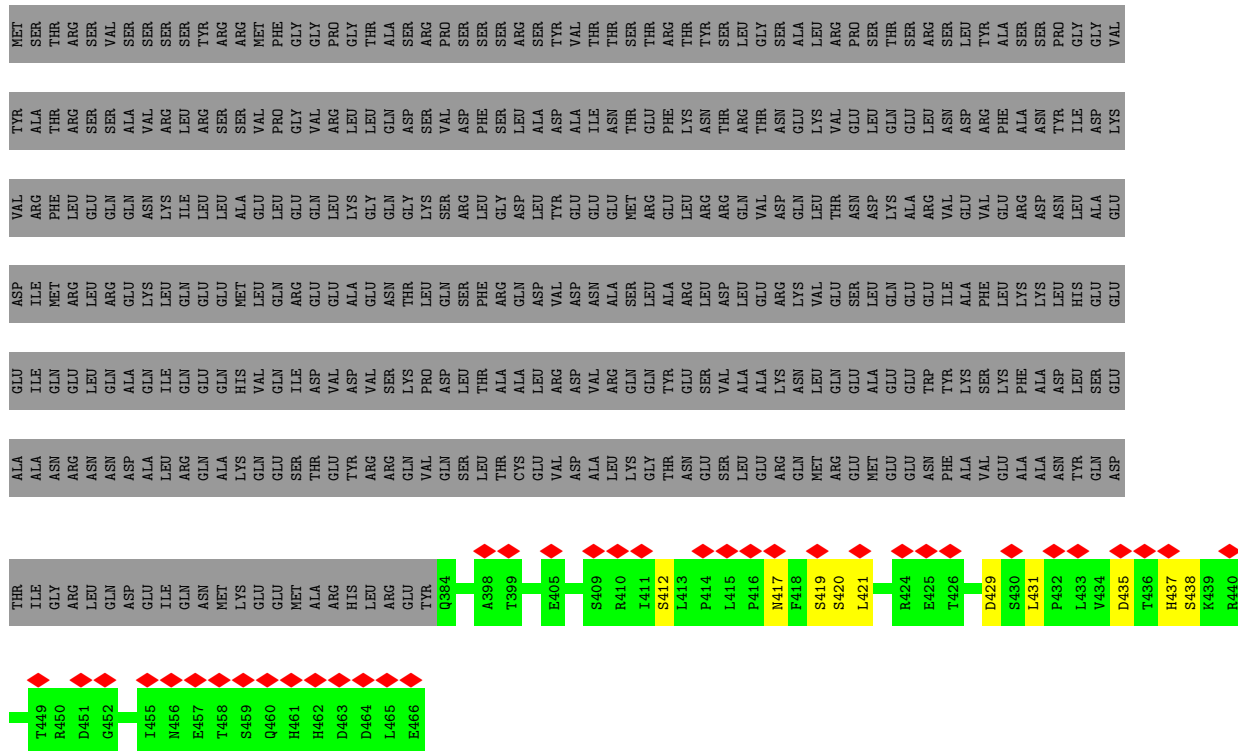








• Molecule 1: Vimentin



• Molecule 1: Vimentin





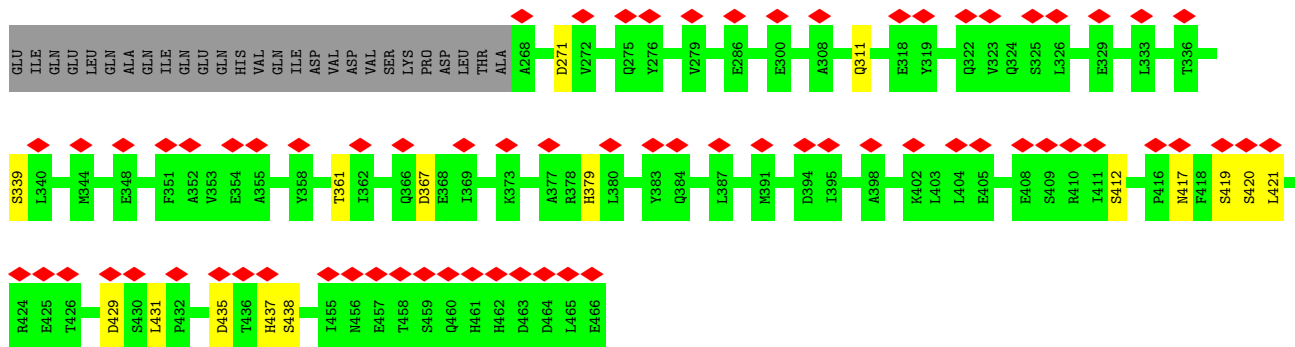








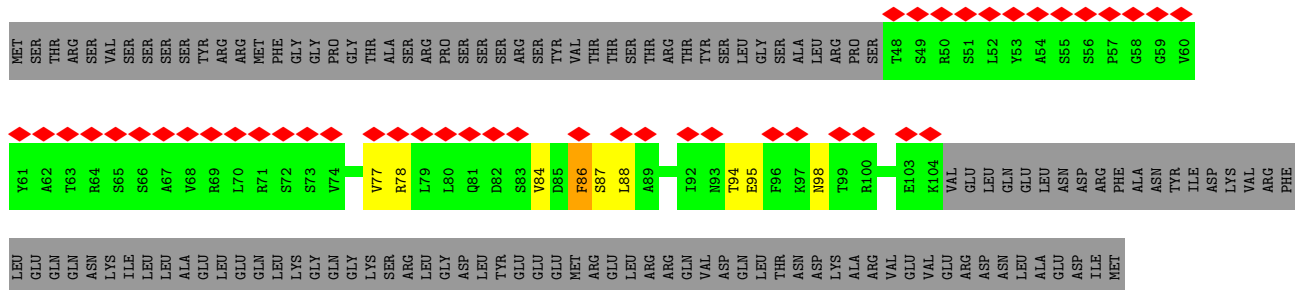




• Molecule 1: Vimentin



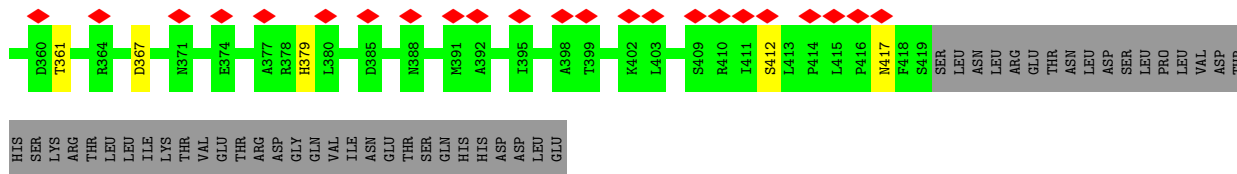
• Molecule 1: Vimentin



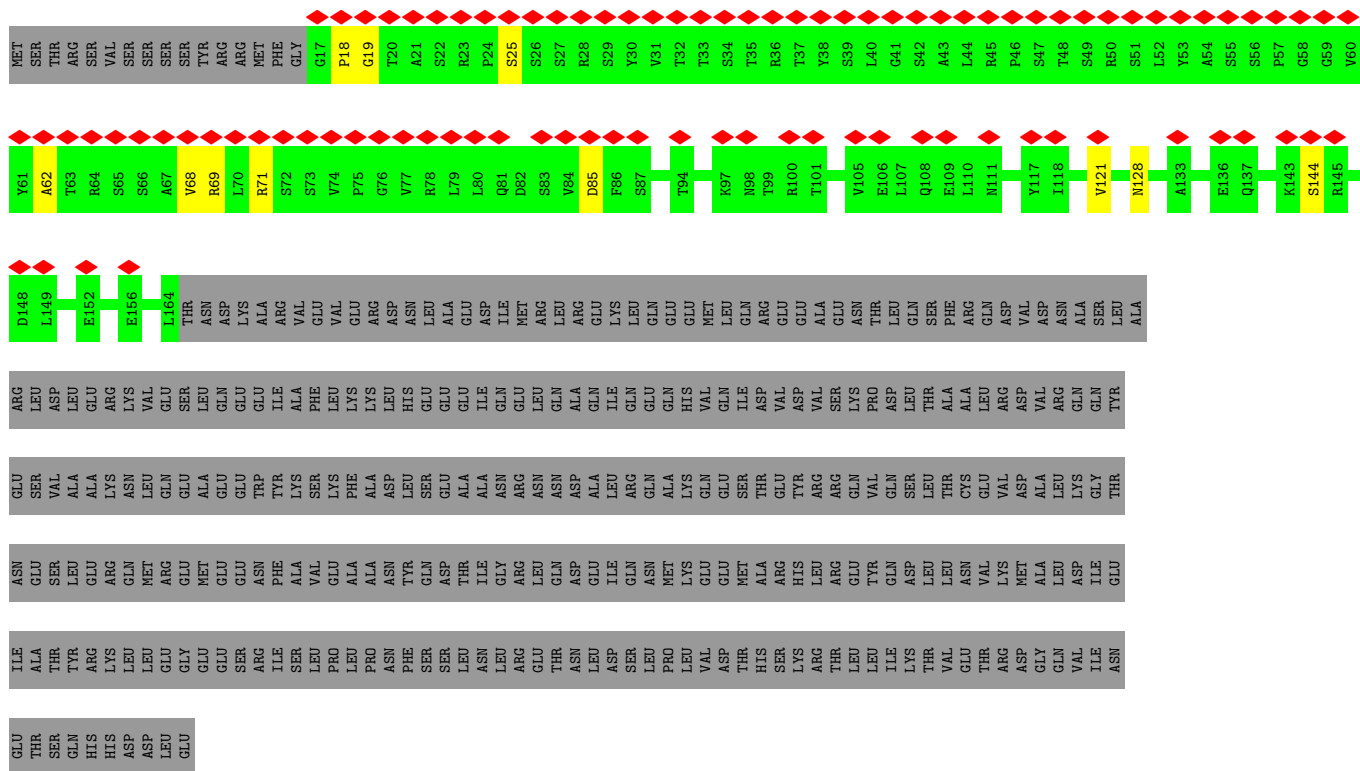




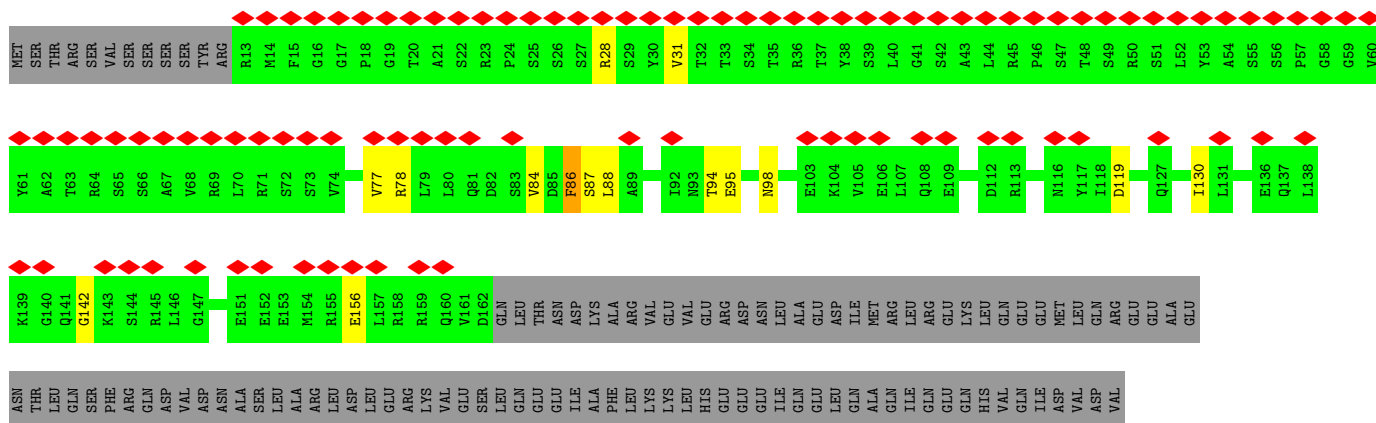




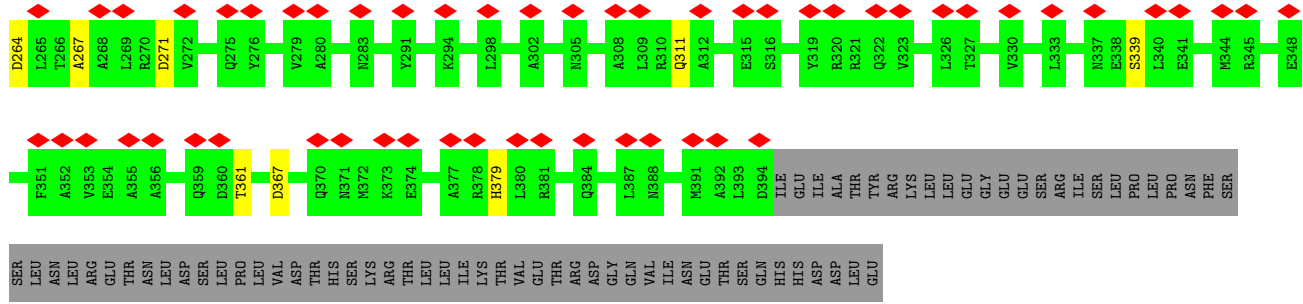
• Molecule 1: Vimentin



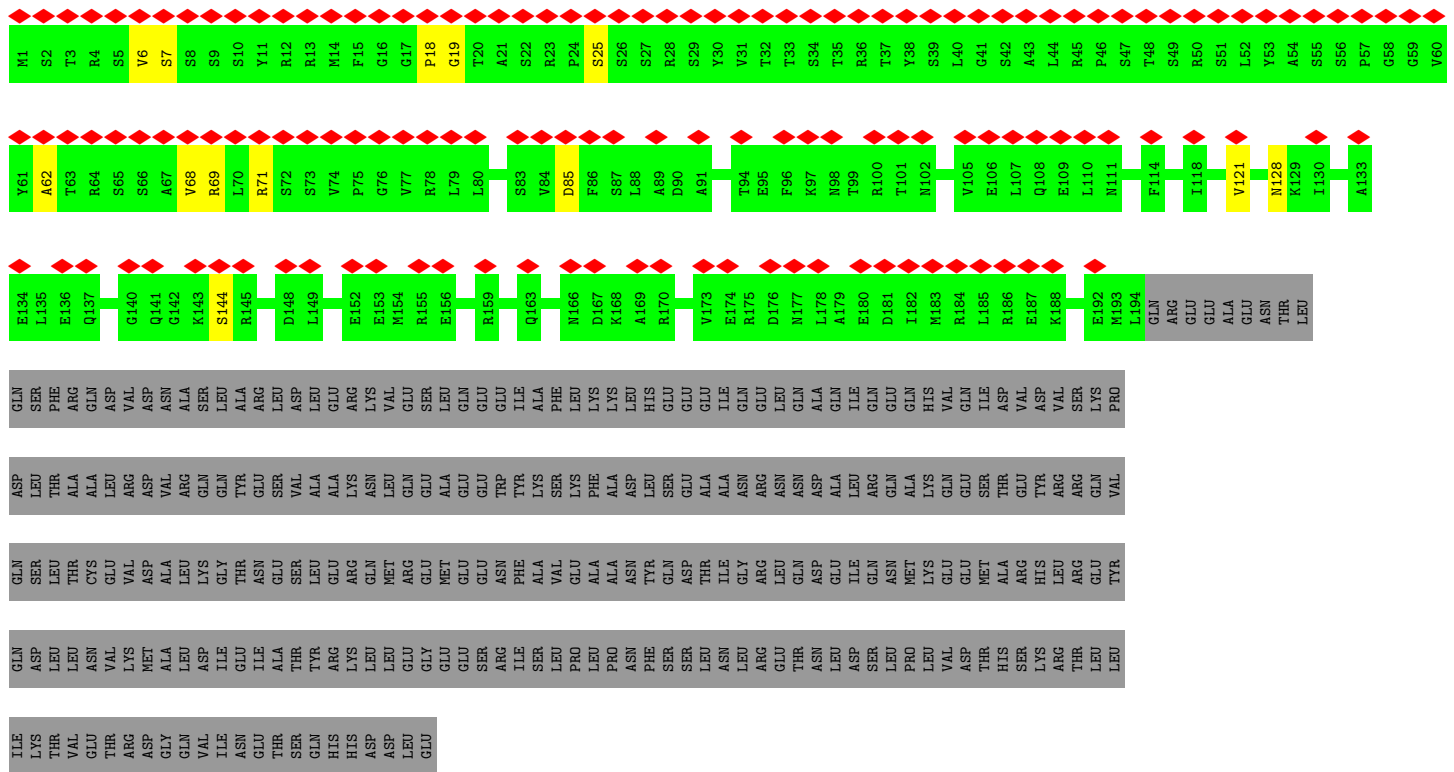
• Molecule 1: Vimentin



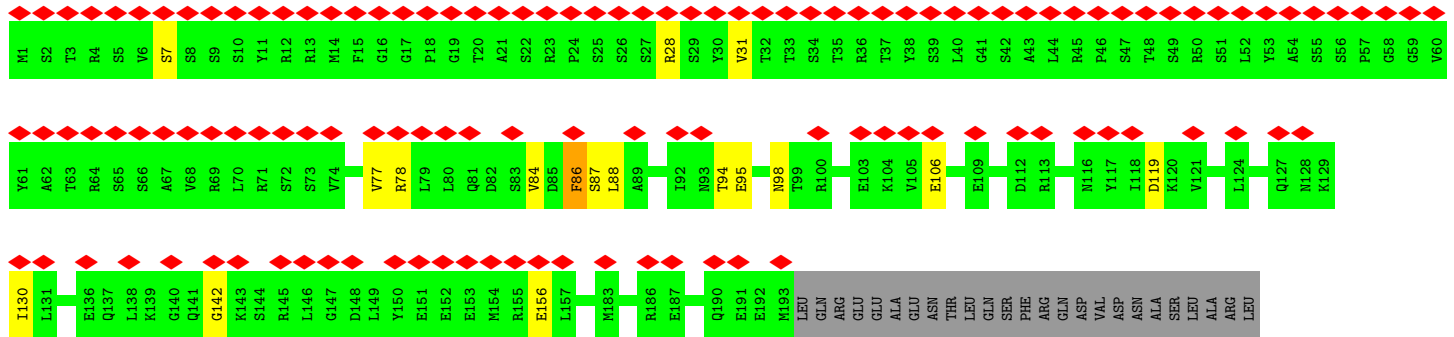




● Molecule 1: Vimentin



● Molecule 1: Vimentin

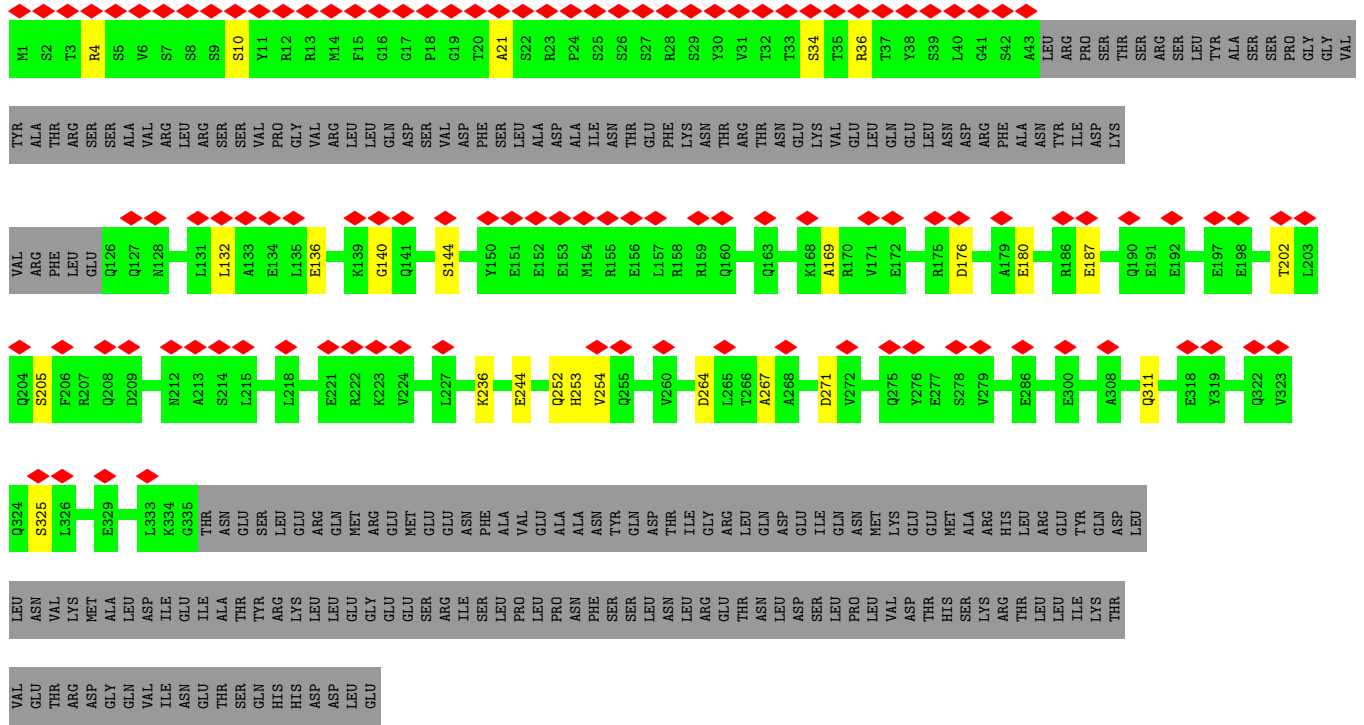




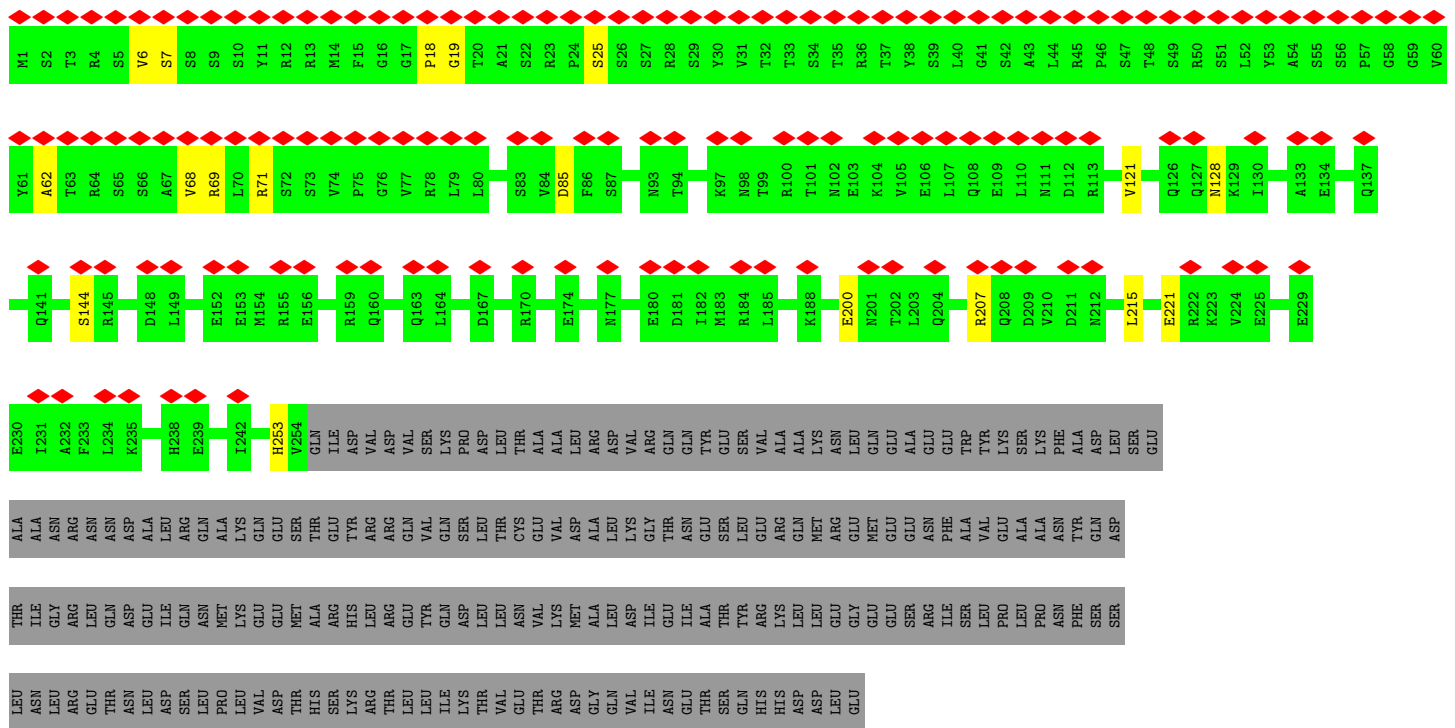






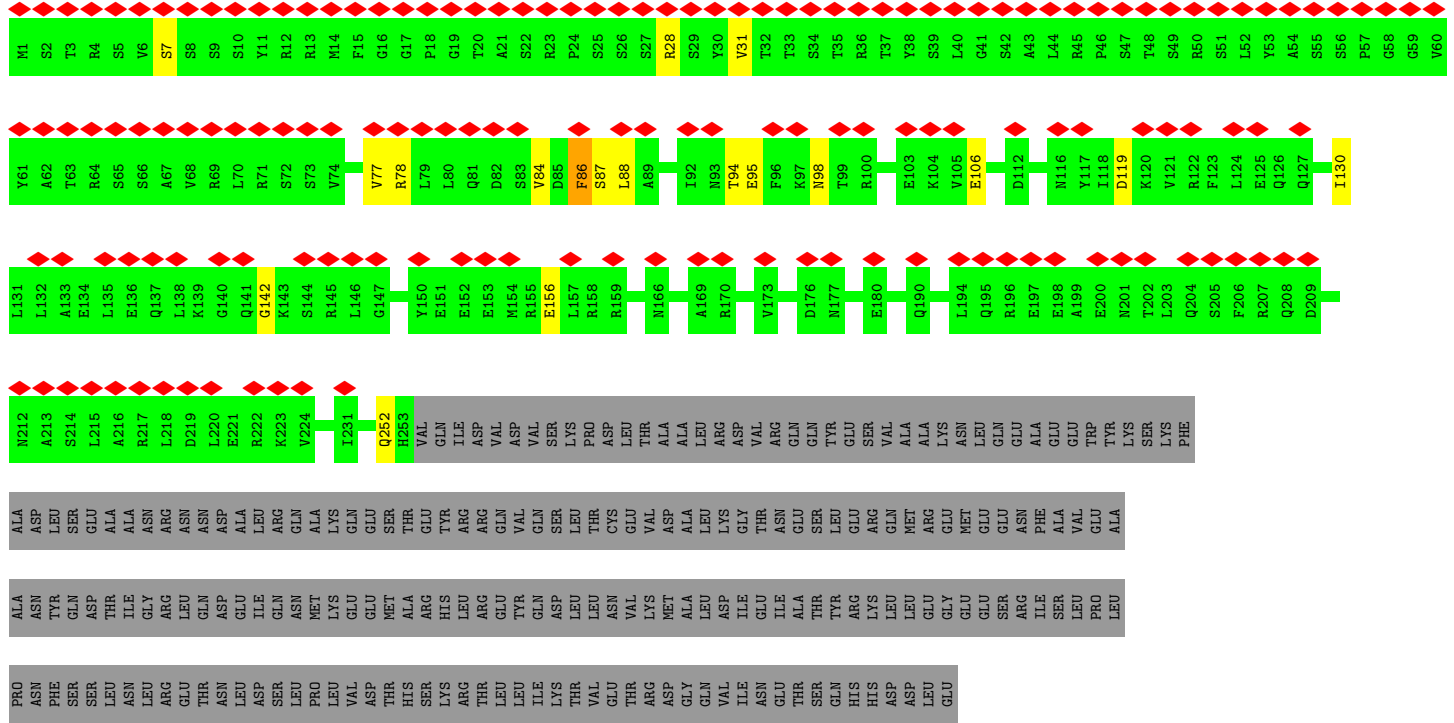


• Molecule 1: Vimentin

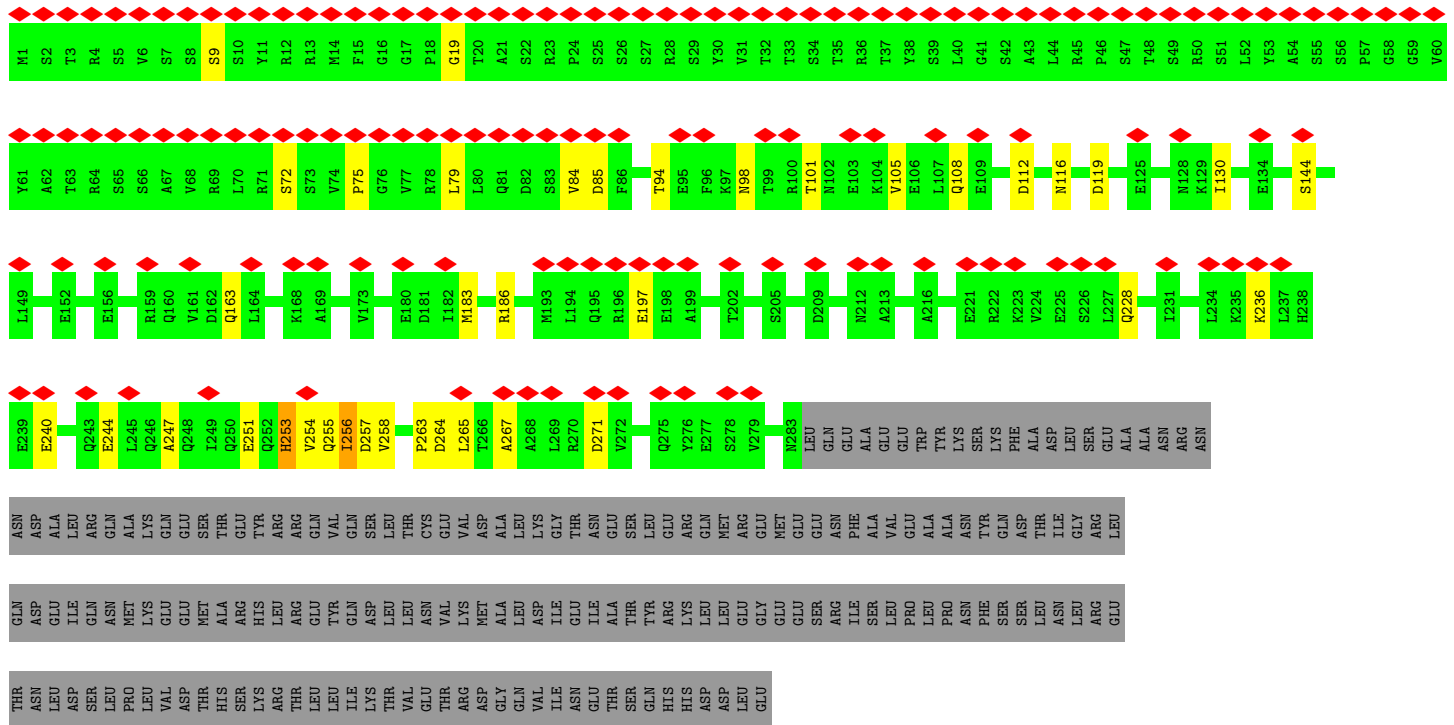


• Molecule 1: Vimentin



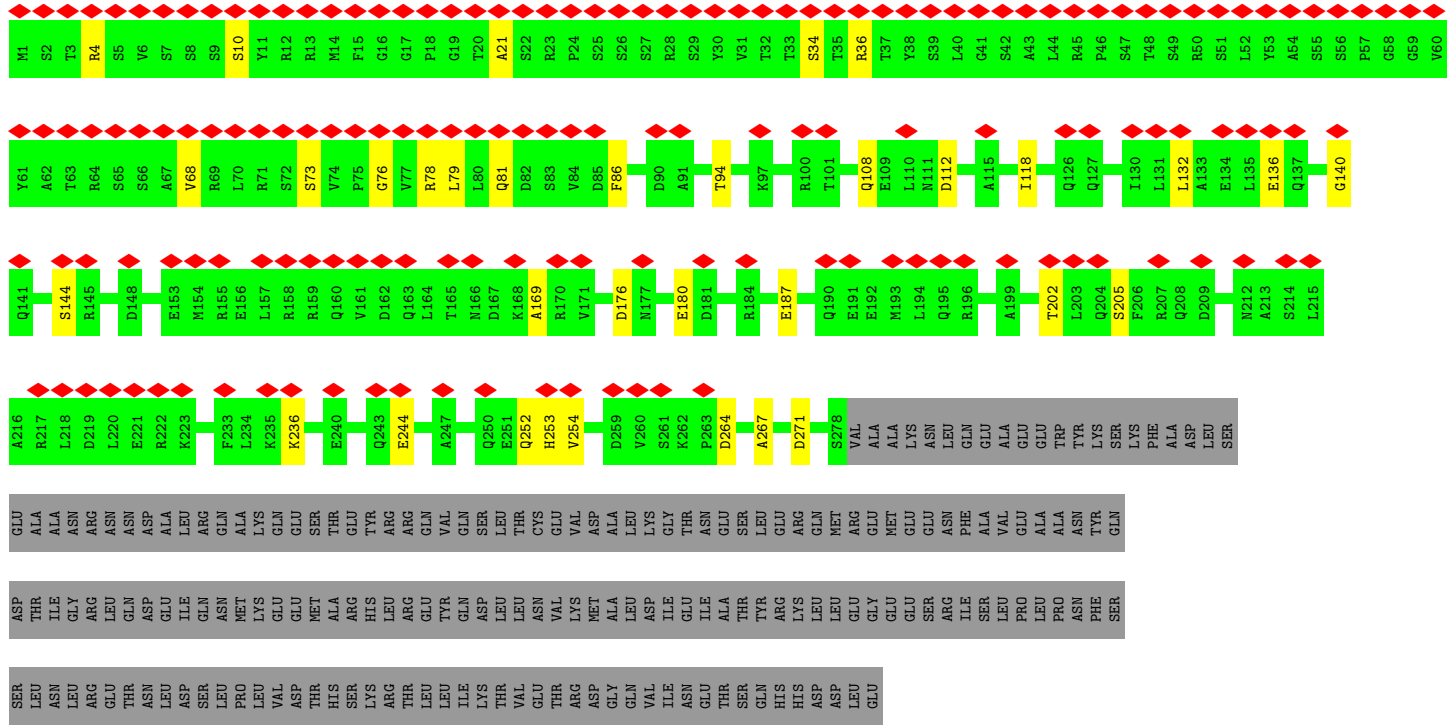


• Molecule 1: Vimentin

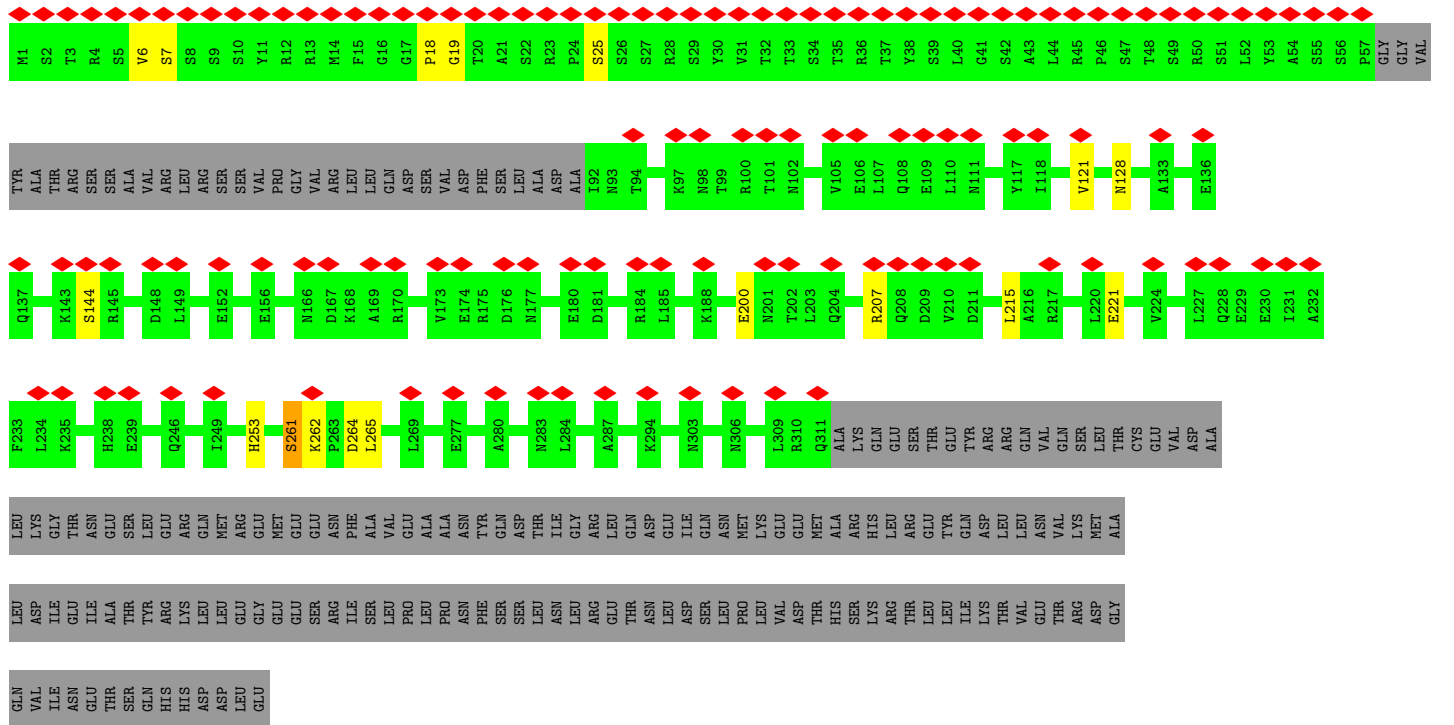


• Molecule 1: Vimentin



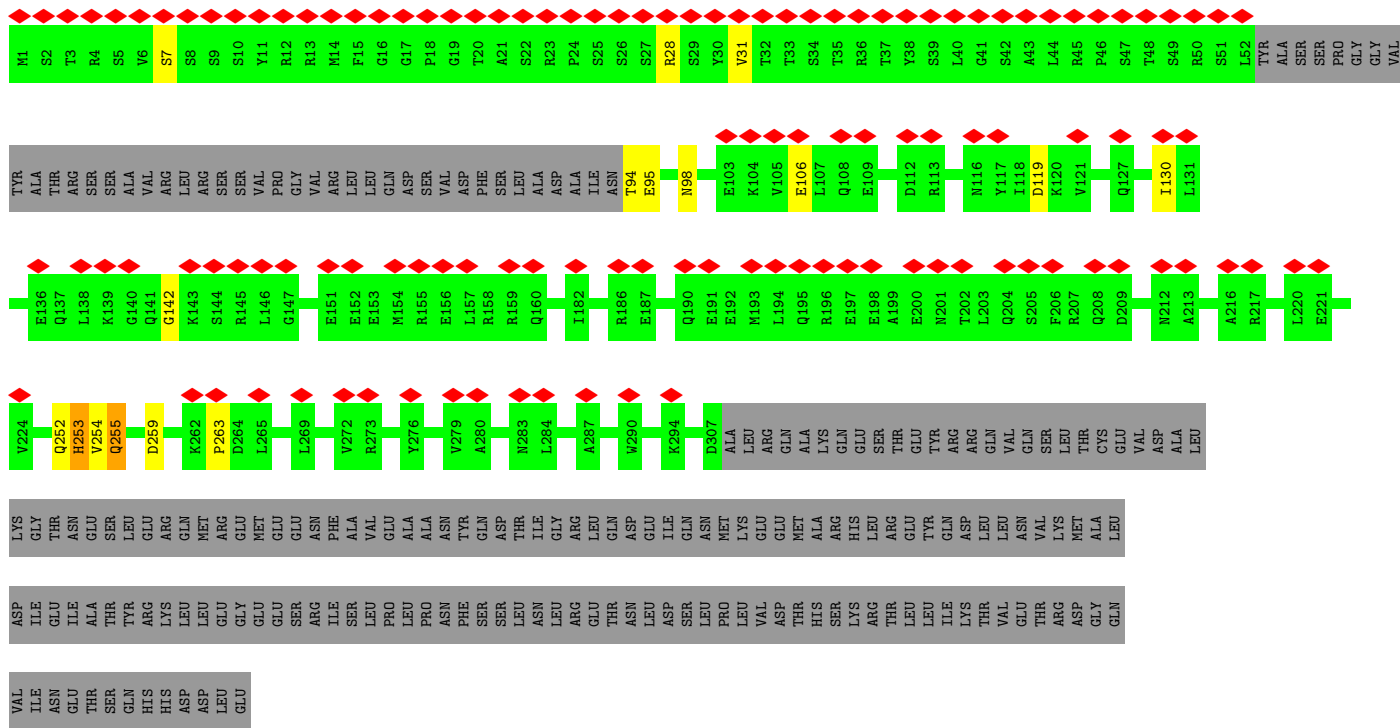


• Molecule 1: Vimentin

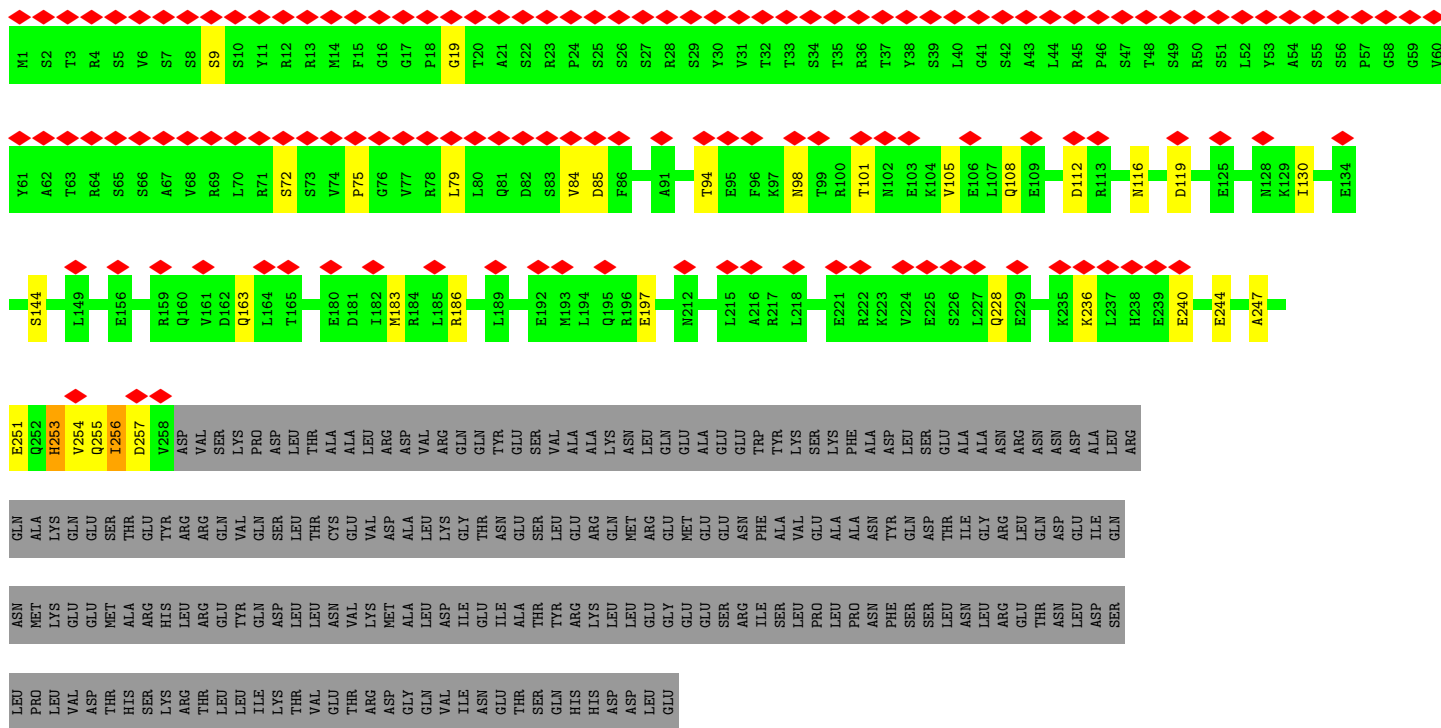


• Molecule 1: Vimentin



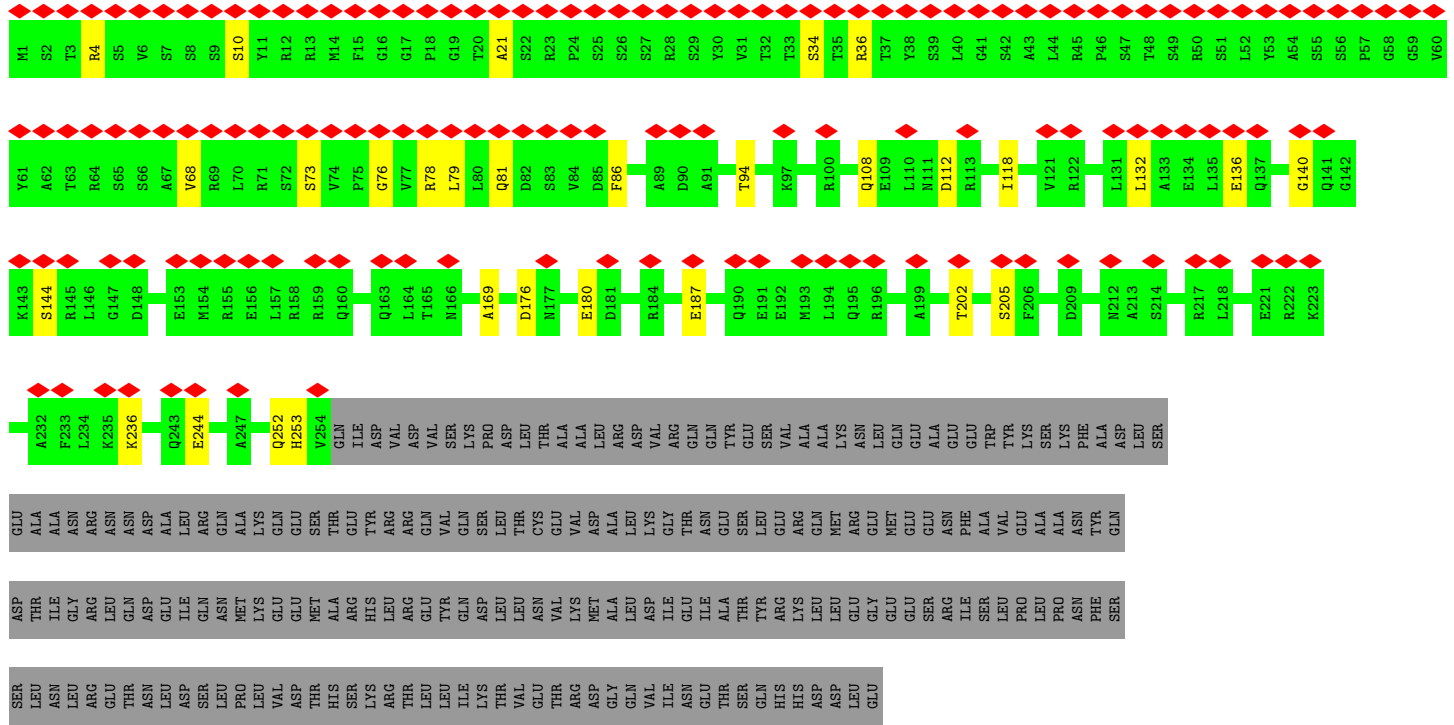


● Molecule 1: Vimentin

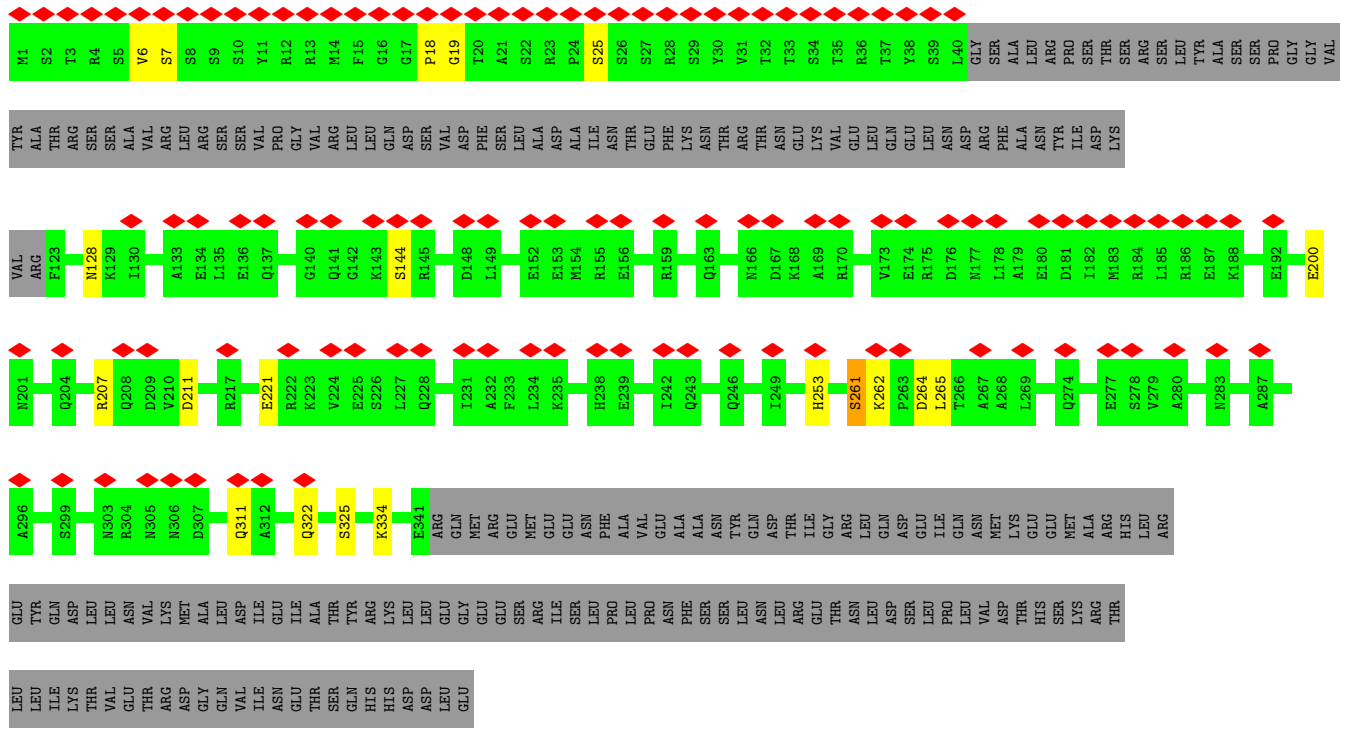


● Molecule 1: Vimentin



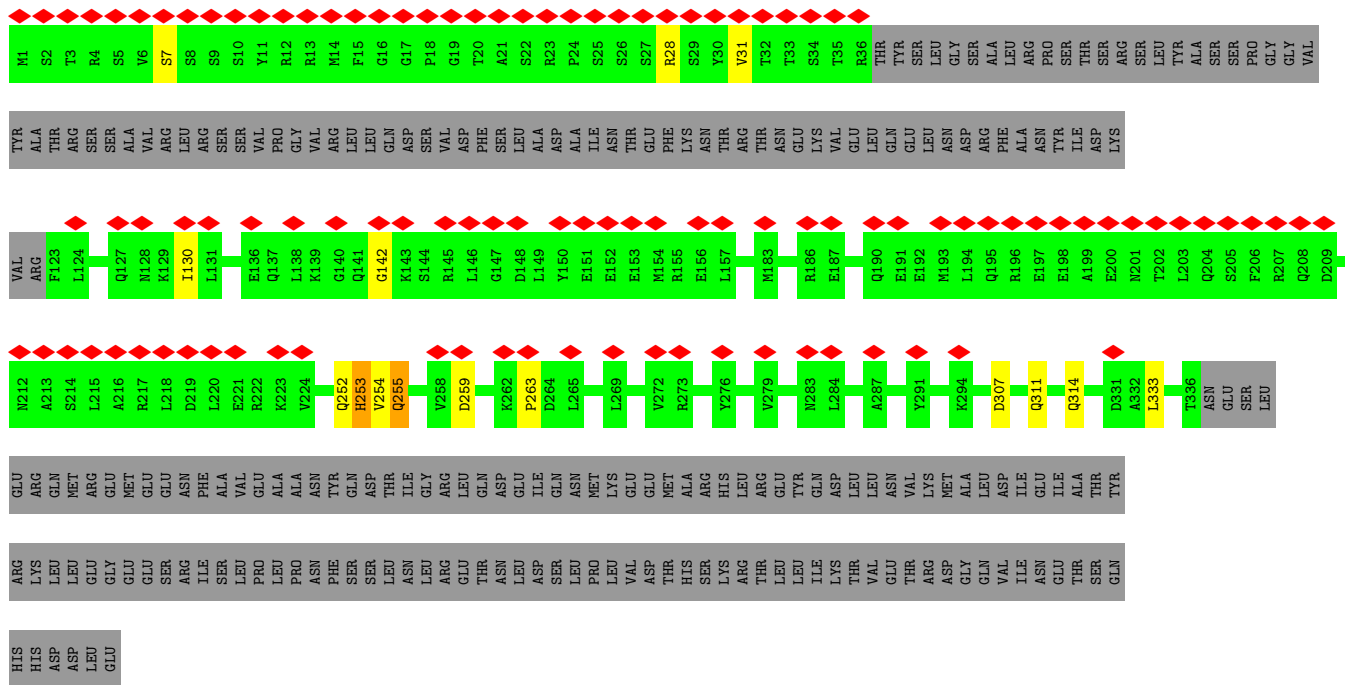


• Molecule 1: Vimentin

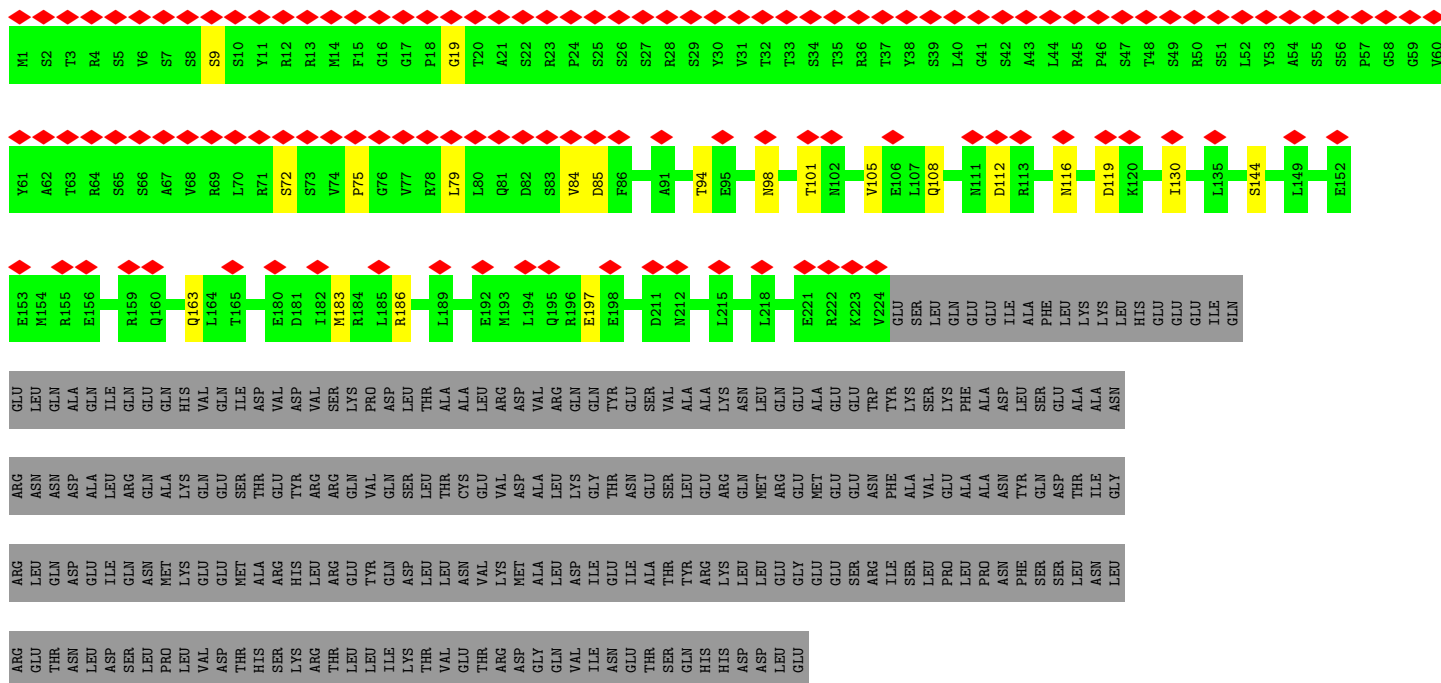
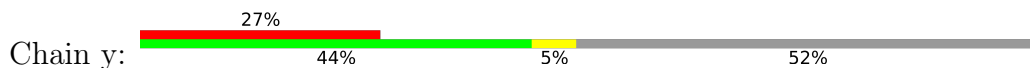


• Molecule 1: Vimentin

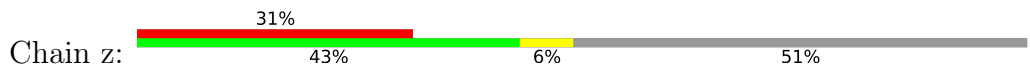




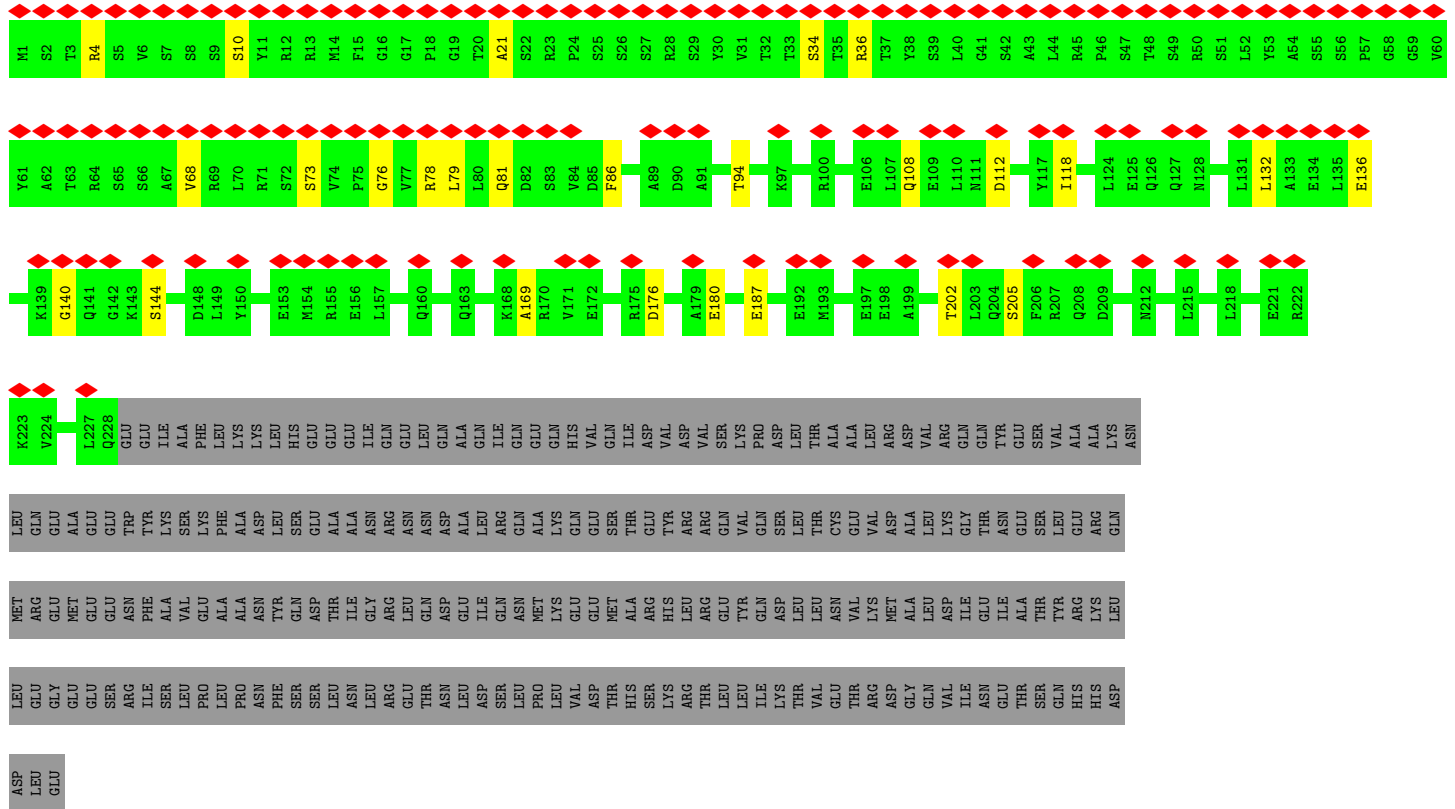
● Molecule 1: Vimentin



● Molecule 1: Vimentin







## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=73.7308°, rise=42.461 Å, axial sym=C1	Depositor
Number of segments used	236920	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 ( $e^-/\text{Å}^2$ )	62	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.016	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	380.798, 380.798, 380.798	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0021, 1.0021, 1.0021	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	0	0.58	0/1011	1.05	7/1262 (0.6%)
1	1	0.81	1/1088 (0.1%)	1.76	3/1353 (0.2%)
1	2	0.46	0/1061	0.94	3/1321 (0.2%)
1	3	0.50	0/763	0.90	0/952
1	4	0.47	0/779	0.90	0/972
1	5	0.81	1/1065 (0.1%)	1.80	4/1326 (0.3%)
1	6	0.45	0/1050	0.94	3/1309 (0.2%)
1	7	0.49	0/567	0.88	0/707
1	8	0.47	0/587	0.89	0/732
1	9	0.84	1/1006 (0.1%)	1.87	4/1254 (0.3%)
1	A	0.54	0/1122	1.01	2/1399 (0.1%)
1	AA	0.49	0/379	0.91	0/472
1	AB	0.47	0/399	0.93	0/497
1	AC	0.88	1/890 (0.1%)	1.96	4/1109 (0.4%)
1	AD	0.60	0/887	1.09	7/1107 (0.6%)
1	AE	0.51	0/195	0.90	0/242
1	AF	0.48	0/215	0.97	0/267
1	AG	0.47	0/795	1.01	1/992 (0.1%)
1	AH	0.61	0/795	1.02	4/992 (0.4%)
1	AI	0.48	0/667	1.04	1/832 (0.1%)
1	AJ	0.64	0/679	1.07	4/847 (0.5%)
1	AK	0.50	0/543	1.09	1/677 (0.1%)
1	AL	0.68	0/563	1.12	4/702 (0.6%)
1	AM	0.52	0/323	1.19	1/402 (0.2%)
1	AN	0.76	0/339	1.18	4/422 (0.9%)
1	AO	0.61	0/135	1.24	0/167
1	AP	1.04	0/155	1.50	4/192 (2.1%)
1	B	0.47	0/1074	0.88	0/1339
1	C	0.81	1/1122 (0.1%)	1.74	3/1399 (0.2%)
1	D	0.45	0/1111	0.92	4/1387 (0.3%)
1	E	0.48	0/131	1.05	1/162 (0.6%)
1	F	0.50	0/139	1.00	0/172
1	G	0.48	0/207	1.11	1/257 (0.4%)
1	H	0.53	0/215	0.95	0/267

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	I	0.49	0/315	1.01	1/392 (0.3%)
1	J	0.50	0/331	0.89	0/412
1	K	0.48	0/427	0.95	1/532 (0.2%)
1	L	0.48	0/451	0.88	0/562
1	M	0.47	0/543	0.90	1/677 (0.1%)
1	N	0.47	0/567	0.84	0/707
1	O	0.46	0/659	0.88	1/822 (0.1%)
1	P	0.46	0/679	0.83	0/847
1	Q	0.49	0/55	0.87	0/67
1	R	0.38	0/55	0.64	0/67
1	S	0.45	0/775	0.86	1/967 (0.1%)
1	T	0.45	0/795	0.81	0/992
1	U	0.49	0/211	0.93	0/262
1	V	0.46	0/227	0.93	1/282 (0.4%)
1	W	0.55	0/775	1.04	3/967 (0.3%)
1	X	0.49	0/775	0.89	0/967
1	Y	0.45	0/395	0.88	0/492
1	Z	0.45	0/407	0.87	1/507 (0.2%)
1	a	0.53	0/835	0.99	2/1042 (0.2%)
1	b	0.46	0/819	0.83	0/1022
1	c	0.45	0/591	0.88	0/737
1	d	0.46	0/599	0.86	1/747 (0.1%)
1	e	0.53	0/855	0.98	2/1067 (0.2%)
1	f	0.45	0/835	0.84	0/1042
1	g	0.46	0/775	0.87	0/967
1	h	0.46	0/771	0.86	1/962 (0.1%)
1	i	0.54	0/982	1.00	2/1224 (0.2%)
1	j	0.46	0/946	0.85	0/1179
1	k	0.46	0/895	0.86	0/1117
1	l	0.45	0/899	0.85	1/1122 (0.1%)
1	m	0.54	0/1058	1.00	2/1319 (0.2%)
1	n	0.48	0/1010	0.87	0/1259
1	o	0.45	0/1015	0.86	0/1267
1	p	0.45	0/1011	0.85	1/1262 (0.1%)
1	q	0.55	0/1131	1.03	2/1412 (0.1%)
1	r	0.49	0/1111	0.92	0/1387
1	s	0.80	1/1105 (0.1%)	1.73	3/1376 (0.2%)
1	t	0.44	0/1062	0.90	3/1324 (0.2%)
1	u	0.55	0/1031	1.03	2/1287 (0.2%)
1	v	0.48	0/1015	0.90	0/1267
1	w	0.82	1/1033 (0.1%)	1.78	3/1286 (0.2%)
1	x	0.44	0/998	0.89	3/1244 (0.2%)
1	y	0.50	0/895	0.90	0/1117

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	z	0.47	0/911	0.89	0/1137
All	All	0.55	7/54687 (0.0%)	1.10	108/68182 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	23
1	1	0	20
1	2	0	16
1	3	0	19
1	4	0	21
1	5	0	22
1	6	0	17
1	7	0	17
1	8	0	16
1	9	0	24
1	A	0	33
1	AA	0	16
1	AB	0	11
1	AC	0	23
1	AD	0	23
1	AE	0	9
1	AF	0	7
1	AG	0	18
1	AH	0	21
1	AI	0	18
1	AJ	0	21
1	AK	0	15
1	AL	0	18
1	AM	0	10
1	AN	0	11
1	AO	0	6
1	AP	0	8
1	B	0	24
1	C	0	15
1	D	0	16
1	E	0	3
1	G	0	11
1	H	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	12
1	J	0	7
1	K	0	13
1	L	0	10
1	M	0	15
1	N	0	11
1	O	0	19
1	P	0	13
1	Q	0	1
1	S	0	19
1	T	0	13
1	U	0	1
1	V	0	6
1	W	0	30
1	X	0	18
1	Y	0	3
1	Z	0	9
1	a	0	25
1	b	0	16
1	c	0	5
1	d	0	10
1	e	0	25
1	f	0	16
1	g	0	7
1	h	0	13
1	i	0	26
1	j	0	18
1	k	0	11
1	l	0	11
1	m	0	26
1	n	0	23
1	o	0	11
1	p	0	13
1	q	0	36
1	r	0	31
1	s	0	14
1	t	0	12
1	u	0	33
1	v	0	27
1	w	0	17
1	x	0	11
1	y	0	20

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	z	0	23
All	All	0	1217

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	261	SER	C-N	-22.08	0.83	1.34
1	5	261	SER	C-N	-22.08	0.83	1.34
1	9	261	SER	C-N	-22.08	0.83	1.34
1	s	261	SER	C-N	-22.08	0.83	1.34
1	C	261	SER	C-N	-22.08	0.83	1.34

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	261	SER	O-C-N	-53.36	37.32	122.70
1	5	261	SER	O-C-N	-53.36	37.33	122.70
1	w	261	SER	O-C-N	-53.35	37.34	122.70
1	9	261	SER	O-C-N	-53.35	37.34	122.70
1	C	261	SER	O-C-N	-53.34	37.35	122.70

There are no chirality outliers.

5 of 1217 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	253	HIS	Peptide
1	0	255	GLN	Mainchain
1	0	263	PRO	Peptide
1	0	307	ASP	Mainchain
1	0	311	GLN	Mainchain

## 5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles

### 5.3.1 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 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	0	251/466 (54%)	220 (88%)	19 (8%)	12 (5%)	2	21
1	1	265/466 (57%)	234 (88%)	25 (9%)	6 (2%)	6	34
1	2	260/466 (56%)	238 (92%)	14 (5%)	8 (3%)	4	27
1	3	189/466 (41%)	156 (82%)	29 (15%)	4 (2%)	7	36
1	4	193/466 (41%)	162 (84%)	26 (14%)	5 (3%)	5	31
1	5	261/466 (56%)	228 (87%)	28 (11%)	5 (2%)	8	38
1	6	259/466 (56%)	237 (92%)	14 (5%)	8 (3%)	4	27
1	7	140/466 (30%)	117 (84%)	21 (15%)	2 (1%)	11	46
1	8	145/466 (31%)	128 (88%)	14 (10%)	3 (2%)	7	36
1	9	248/466 (53%)	210 (85%)	31 (12%)	7 (3%)	5	30
1	A	277/466 (59%)	241 (87%)	29 (10%)	7 (2%)	5	32
1	AA	93/466 (20%)	77 (83%)	15 (16%)	1 (1%)	14	52
1	AB	98/466 (21%)	85 (87%)	11 (11%)	2 (2%)	7	38
1	AC	219/466 (47%)	181 (83%)	31 (14%)	7 (3%)	4	26
1	AD	220/466 (47%)	189 (86%)	19 (9%)	12 (6%)	2	19
1	AE	47/466 (10%)	36 (77%)	10 (21%)	1 (2%)	7	36
1	AF	52/466 (11%)	40 (77%)	10 (19%)	2 (4%)	3	24
1	AG	197/466 (42%)	168 (85%)	23 (12%)	6 (3%)	4	28
1	AH	197/466 (42%)	172 (87%)	17 (9%)	8 (4%)	3	22
1	AI	165/466 (35%)	136 (82%)	23 (14%)	6 (4%)	3	25
1	AJ	168/466 (36%)	143 (85%)	17 (10%)	8 (5%)	2	21
1	AK	134/466 (29%)	105 (78%)	23 (17%)	6 (4%)	2	22
1	AL	139/466 (30%)	115 (83%)	16 (12%)	8 (6%)	1	18
1	AM	79/466 (17%)	63 (80%)	12 (15%)	4 (5%)	2	19
1	AN	83/466 (18%)	68 (82%)	11 (13%)	4 (5%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AO	32/466 (7%)	25 (78%)	3 (9%)	4 (12%)	0	5
1	AP	37/466 (8%)	26 (70%)	7 (19%)	4 (11%)	0	8
1	B	265/466 (57%)	240 (91%)	21 (8%)	4 (2%)	10	46
1	C	277/466 (59%)	236 (85%)	32 (12%)	9 (3%)	4	26
1	D	276/466 (59%)	243 (88%)	24 (9%)	9 (3%)	4	26
1	E	31/466 (7%)	19 (61%)	11 (36%)	1 (3%)	4	26
1	F	33/466 (7%)	26 (79%)	4 (12%)	3 (9%)	1	11
1	G	50/466 (11%)	31 (62%)	18 (36%)	1 (2%)	7	38
1	H	52/466 (11%)	36 (69%)	11 (21%)	5 (10%)	0	10
1	I	77/466 (16%)	55 (71%)	19 (25%)	3 (4%)	3	23
1	J	81/466 (17%)	65 (80%)	11 (14%)	5 (6%)	1	17
1	K	105/466 (22%)	83 (79%)	19 (18%)	3 (3%)	4	29
1	L	111/466 (24%)	95 (86%)	11 (10%)	5 (4%)	2	22
1	M	134/466 (29%)	112 (84%)	19 (14%)	3 (2%)	6	35
1	N	140/466 (30%)	124 (89%)	11 (8%)	5 (4%)	3	25
1	O	163/466 (35%)	141 (86%)	19 (12%)	3 (2%)	8	40
1	P	168/466 (36%)	152 (90%)	11 (6%)	5 (3%)	4	28
1	Q	12/466 (3%)	6 (50%)	4 (33%)	2 (17%)	0	3
1	R	12/466 (3%)	9 (75%)	2 (17%)	1 (8%)	1	12
1	S	192/466 (41%)	170 (88%)	19 (10%)	3 (2%)	9	44
1	T	197/466 (42%)	181 (92%)	11 (6%)	5 (2%)	5	32
1	U	51/466 (11%)	37 (72%)	10 (20%)	4 (8%)	1	13
1	V	55/466 (12%)	43 (78%)	9 (16%)	3 (6%)	2	19
1	W	192/466 (41%)	172 (90%)	13 (7%)	7 (4%)	3	25
1	X	192/466 (41%)	175 (91%)	11 (6%)	6 (3%)	4	27
1	Y	97/466 (21%)	78 (80%)	15 (16%)	4 (4%)	3	22
1	Z	100/466 (22%)	84 (84%)	13 (13%)	3 (3%)	4	28
1	a	207/466 (44%)	194 (94%)	7 (3%)	6 (3%)	4	29
1	b	203/466 (44%)	196 (97%)	6 (3%)	1 (0%)	29	69
1	c	146/466 (31%)	119 (82%)	21 (14%)	6 (4%)	3	22
1	d	148/466 (32%)	124 (84%)	19 (13%)	5 (3%)	3	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	e	212/466 (46%)	202 (95%)	7 (3%)	3 (1%)	11	46
1	f	207/466 (44%)	201 (97%)	5 (2%)	1 (0%)	29	69
1	g	192/466 (41%)	161 (84%)	24 (12%)	7 (4%)	3	25
1	h	191/466 (41%)	164 (86%)	22 (12%)	5 (3%)	5	31
1	i	242/466 (52%)	217 (90%)	19 (8%)	6 (2%)	5	32
1	j	233/466 (50%)	212 (91%)	18 (8%)	3 (1%)	12	48
1	k	222/466 (48%)	190 (86%)	24 (11%)	8 (4%)	3	25
1	l	223/466 (48%)	196 (88%)	22 (10%)	5 (2%)	6	35
1	m	261/466 (56%)	230 (88%)	25 (10%)	6 (2%)	6	34
1	n	249/466 (53%)	226 (91%)	19 (8%)	4 (2%)	9	44
1	o	252/466 (54%)	220 (87%)	24 (10%)	8 (3%)	4	26
1	p	251/466 (54%)	223 (89%)	22 (9%)	6 (2%)	6	33
1	q	281/466 (60%)	236 (84%)	37 (13%)	8 (3%)	5	30
1	r	276/466 (59%)	240 (87%)	30 (11%)	6 (2%)	6	35
1	s	271/466 (58%)	243 (90%)	23 (8%)	5 (2%)	8	40
1	t	262/466 (56%)	240 (92%)	16 (6%)	6 (2%)	6	34
1	u	256/466 (55%)	216 (84%)	35 (14%)	5 (2%)	7	38
1	v	252/466 (54%)	219 (87%)	28 (11%)	5 (2%)	7	38
1	w	253/466 (54%)	230 (91%)	18 (7%)	5 (2%)	7	38
1	x	246/466 (53%)	228 (93%)	12 (5%)	6 (2%)	6	33
1	y	222/466 (48%)	186 (84%)	32 (14%)	4 (2%)	8	40
1	z	226/466 (48%)	195 (86%)	26 (12%)	5 (2%)	6	35
All	All	13495/36348 (37%)	11721 (87%)	1387 (10%)	387 (3%)	7	29

5 of 387 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	413	LEU
1	0	414	PRO
1	1	18	PRO
1	1	265	LEU
1	5	265	LEU

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

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	2
1	5	2
1	9	2
1	AC	2
1	C	2
1	s	2
1	w	2

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	263:PRO	C	264:ASP	N	2.24
1	5	263:PRO	C	264:ASP	N	2.24
1	9	263:PRO	C	264:ASP	N	2.24
1	AC	263:PRO	C	264:ASP	N	2.24
1	C	263:PRO	C	264:ASP	N	2.24

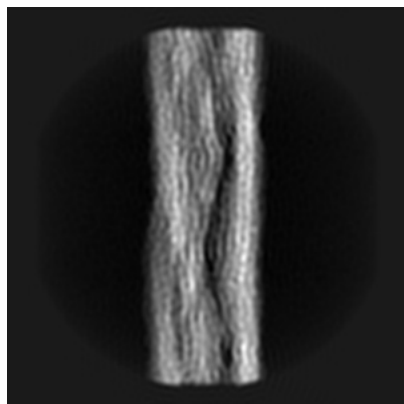
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16844. These allow visual inspection of the internal detail of the map and identification of artifacts.

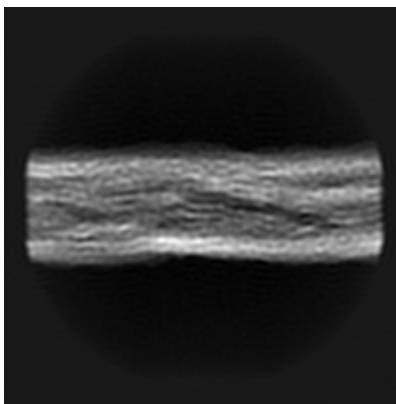
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



X

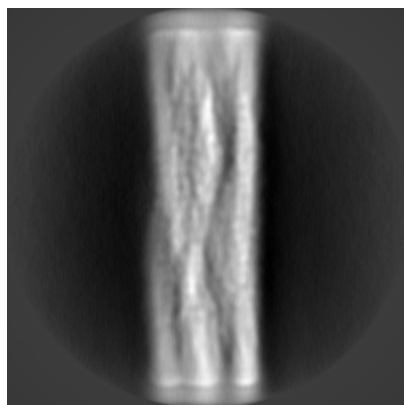


Y

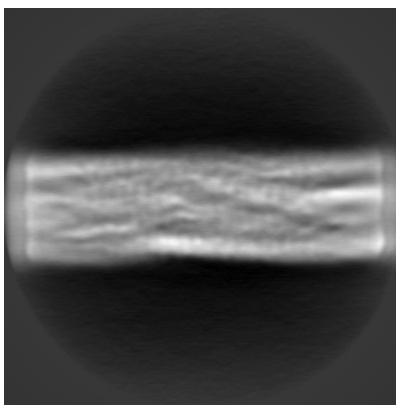


Z

#### 6.1.2 Raw map



X



Y

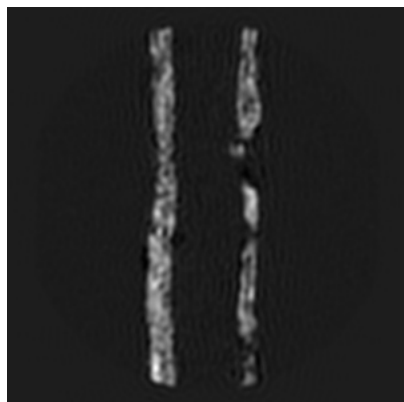


Z

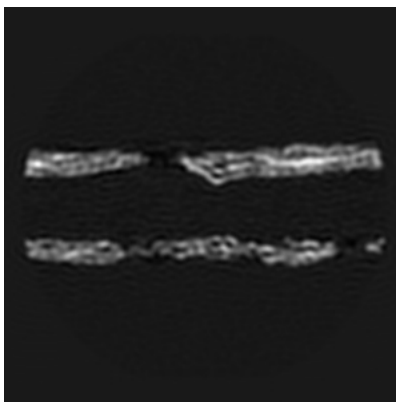
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 190

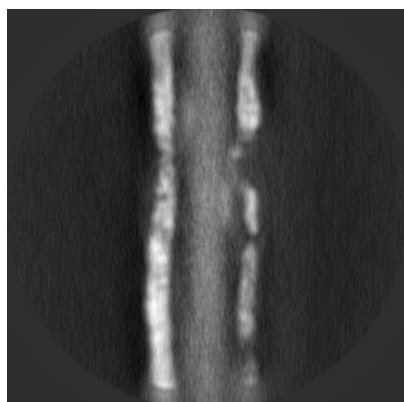


Y Index: 190

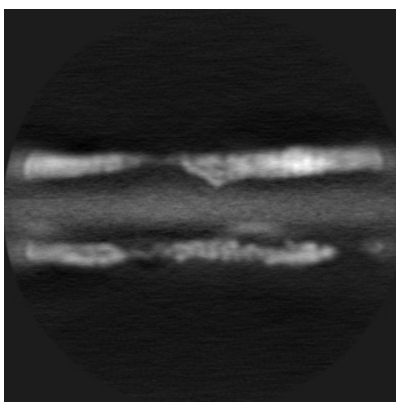


Z Index: 190

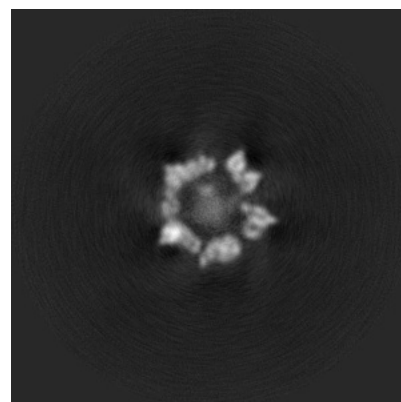
### 6.2.2 Raw map



X Index: 190



Y Index: 190

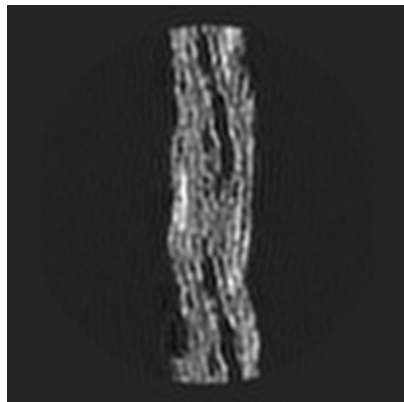


Z Index: 190

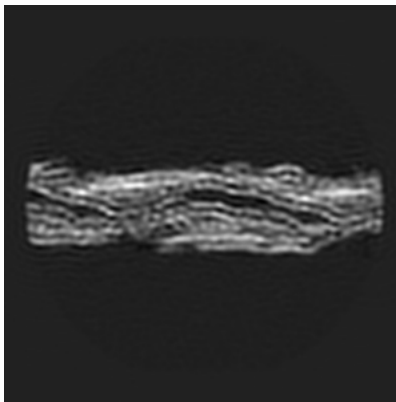
The images above show central slices of the map in three orthogonal directions.

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

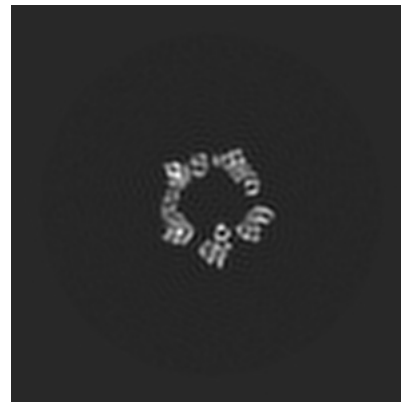
### 6.3.1 Primary map



X Index: 155

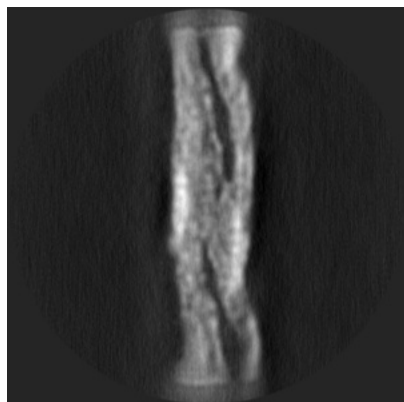


Y Index: 229

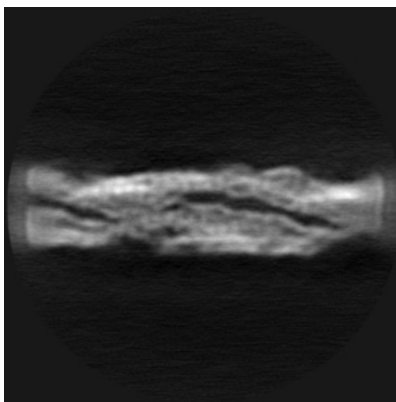


Z Index: 160

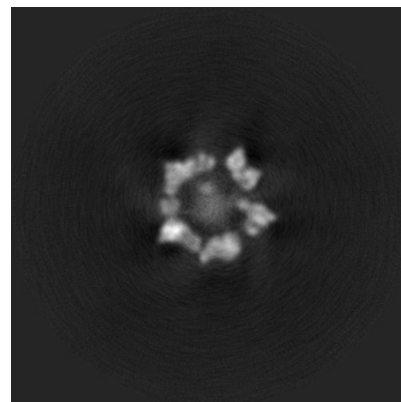
### 6.3.2 Raw map



X Index: 153



Y Index: 229

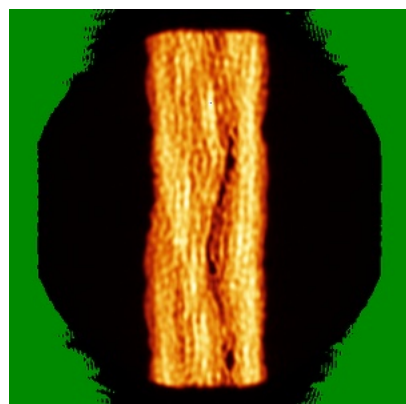


Z Index: 194

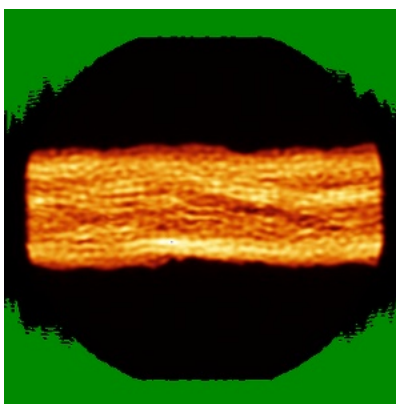
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

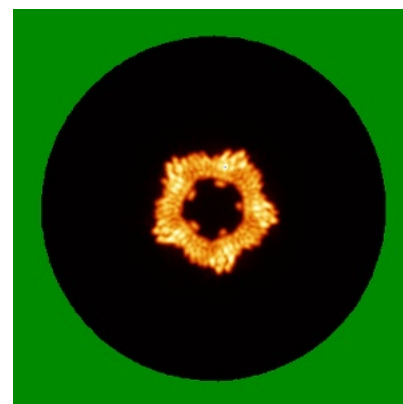
### 6.4.1 Primary map



X

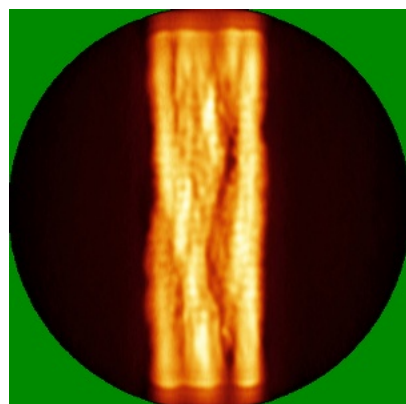


Y

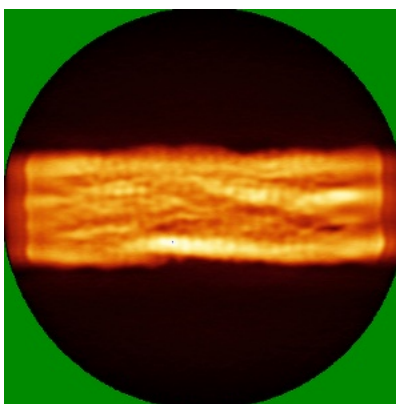


Z

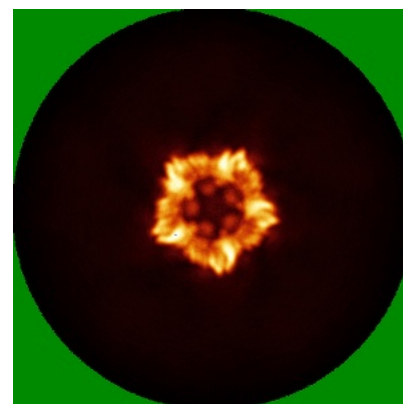
### 6.4.2 Raw map



X



Y



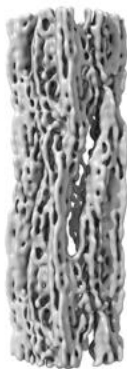
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

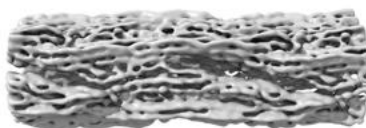


## 6.5 Orthogonal surface views [i](#)

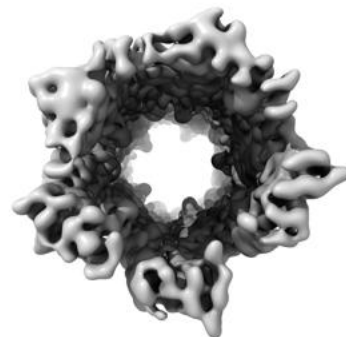
### 6.5.1 Primary map



X



Y



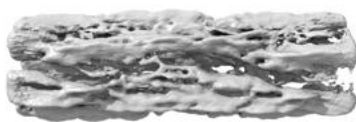
Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

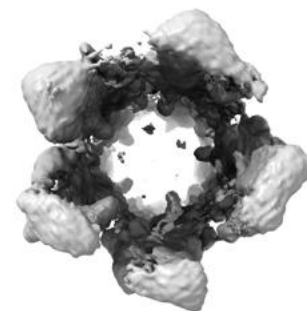
### 6.5.2 Raw map



X



Y



Z

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.

## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

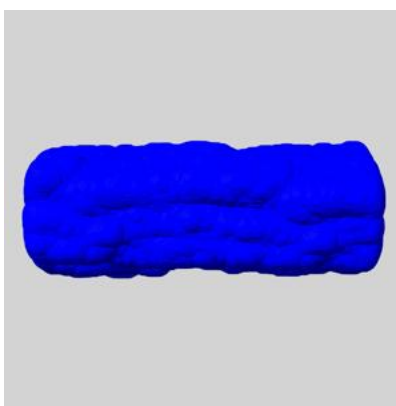
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

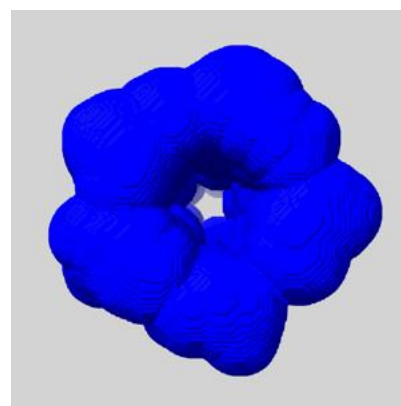
### 6.6.1 emd\_16844\_msk\_1.map [i](#)



X



Y

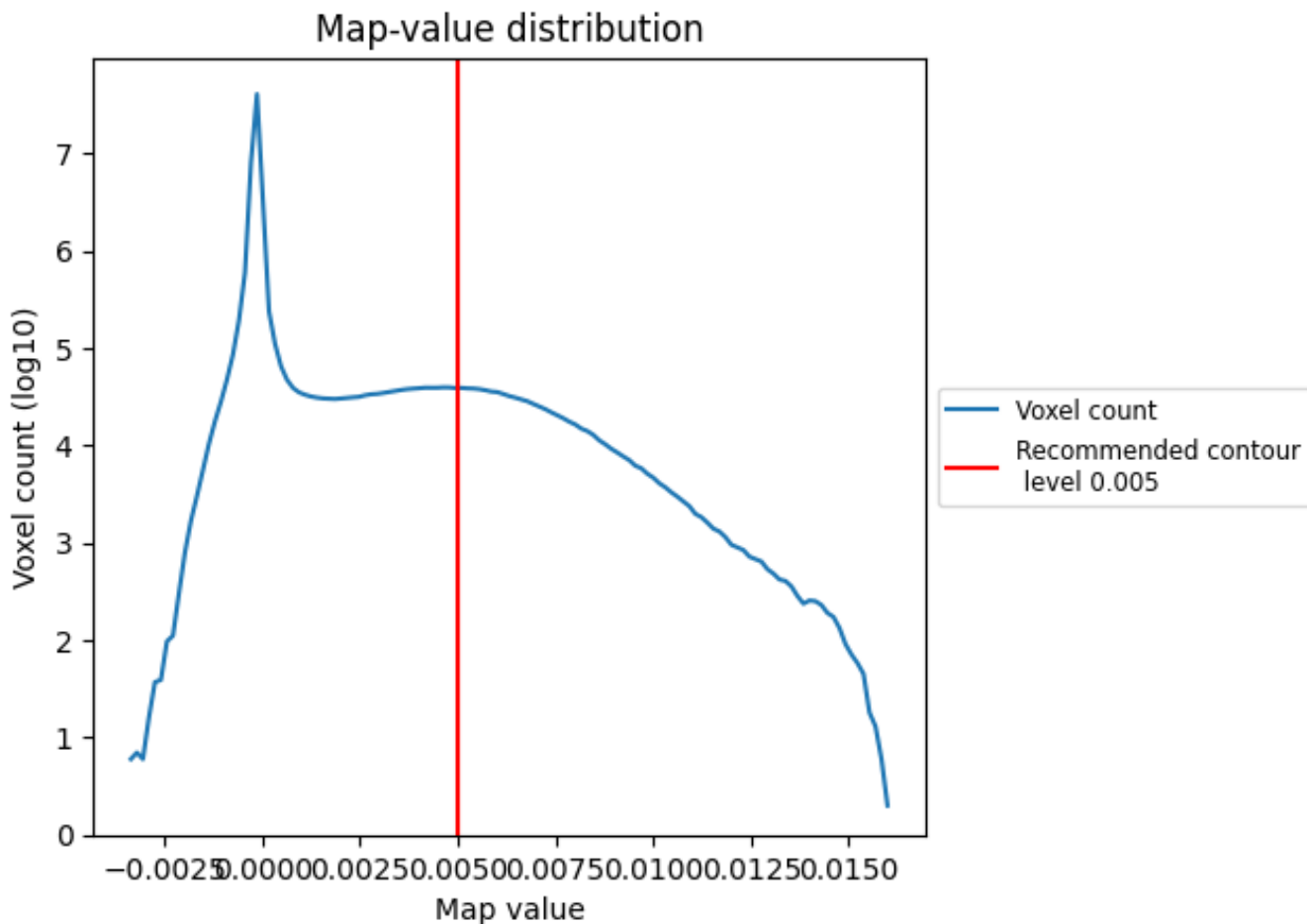


Z

## 7 Map analysis [i](#)

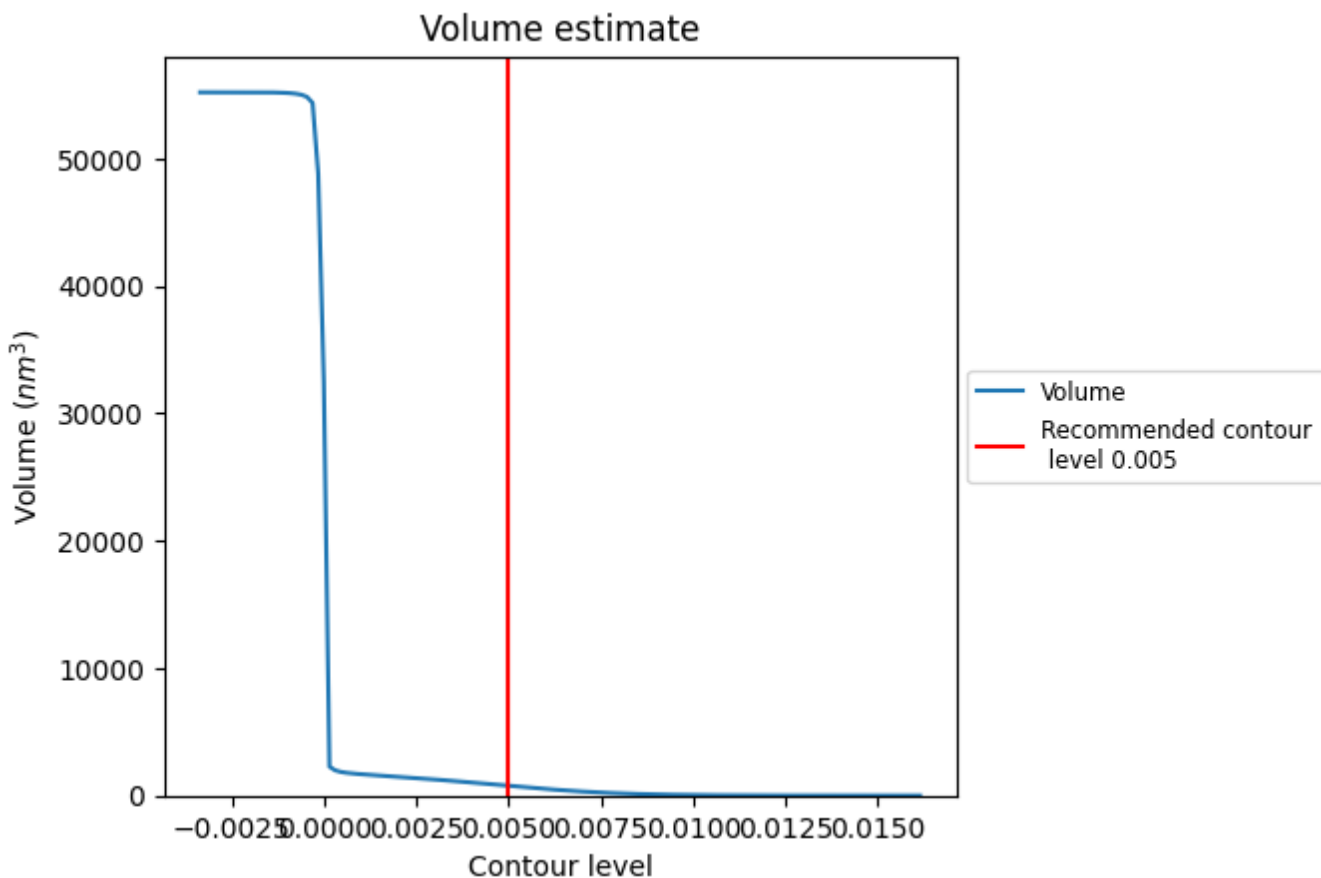
This section contains the results of statistical analysis of the map.

### 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.

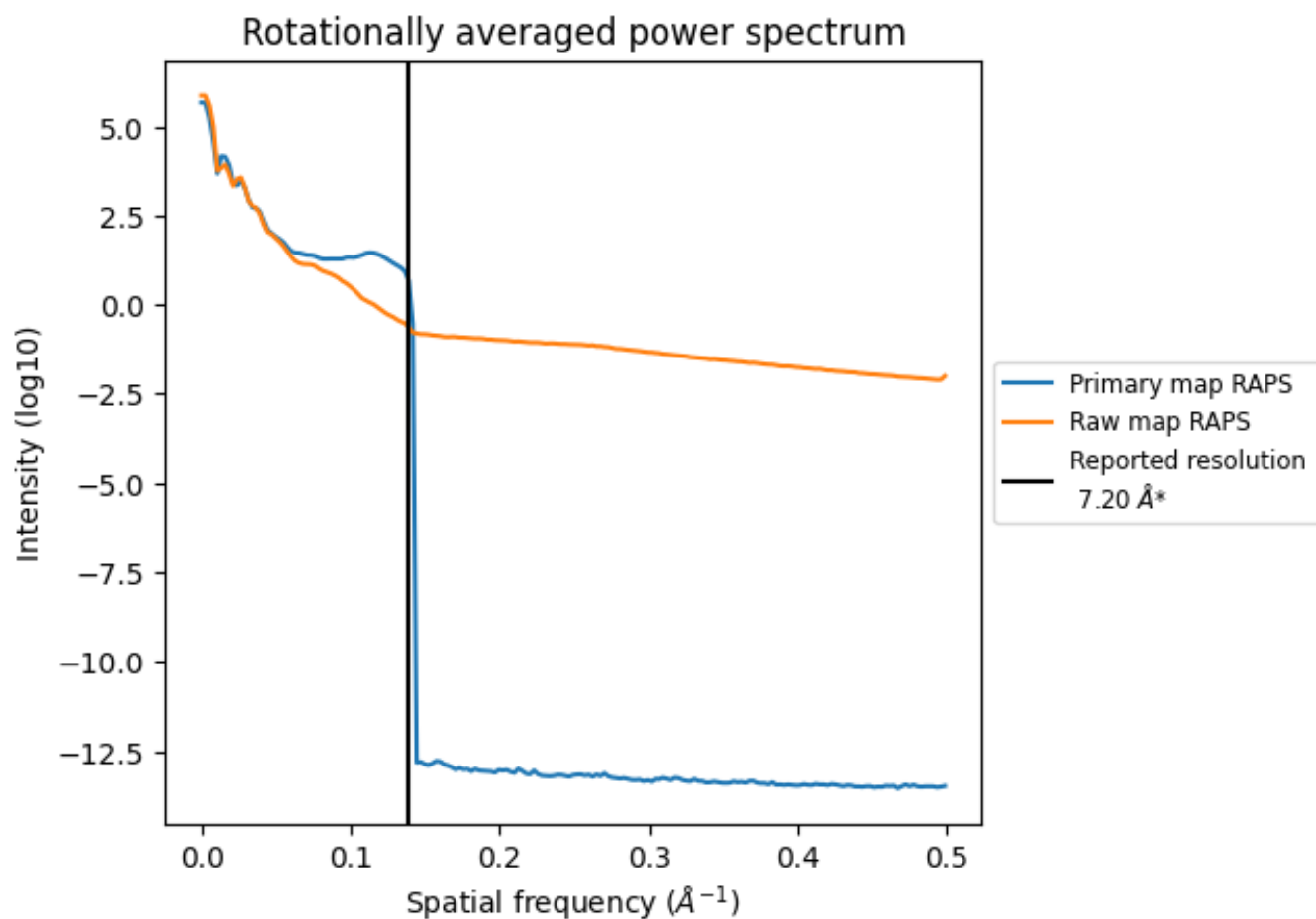
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 768  $\text{nm}^3$ ; this corresponds to an approximate mass of 694 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](#)

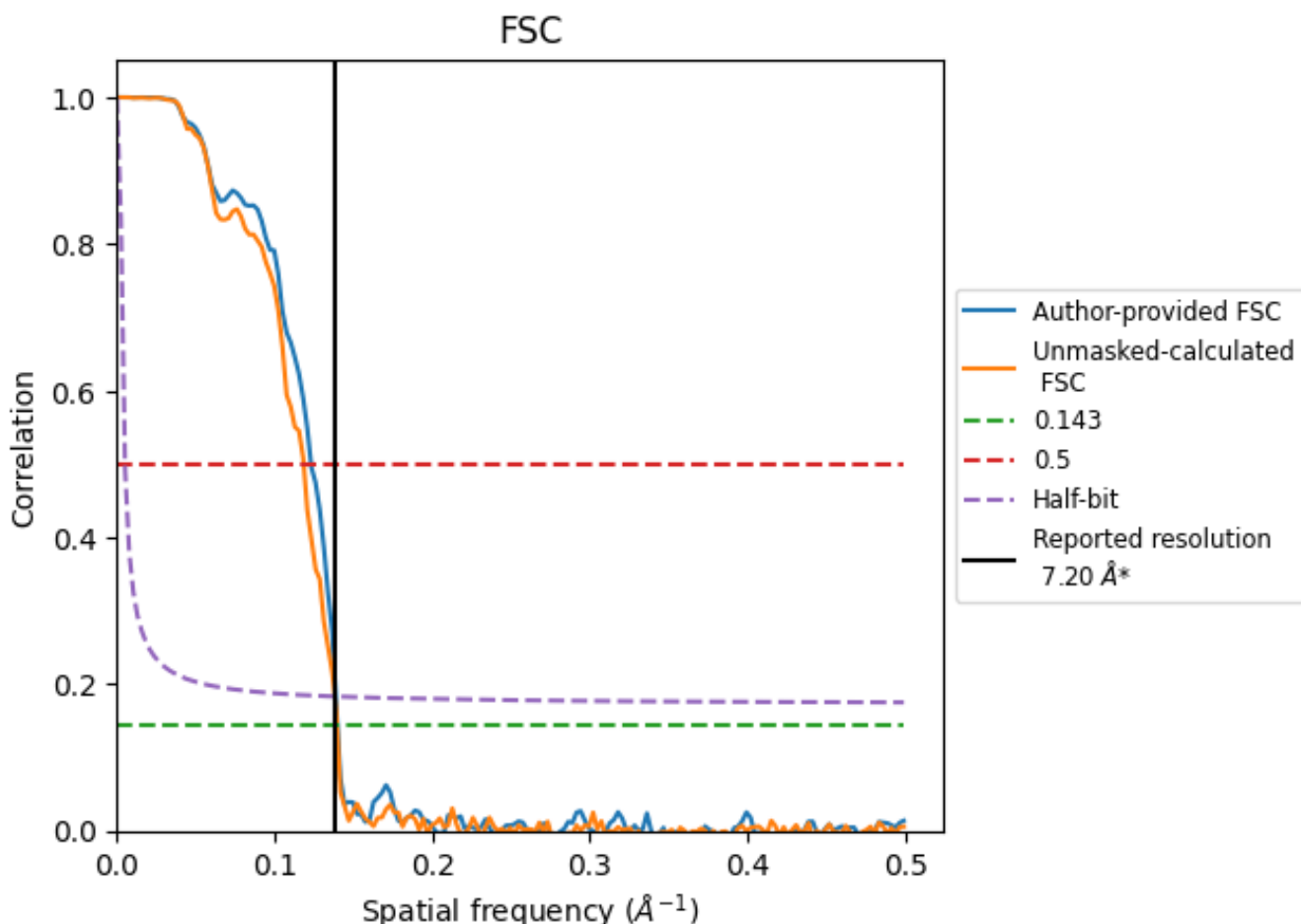


\*Reported resolution corresponds to spatial frequency of 0.139 Å<sup>-1</sup>

## 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 0.139 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

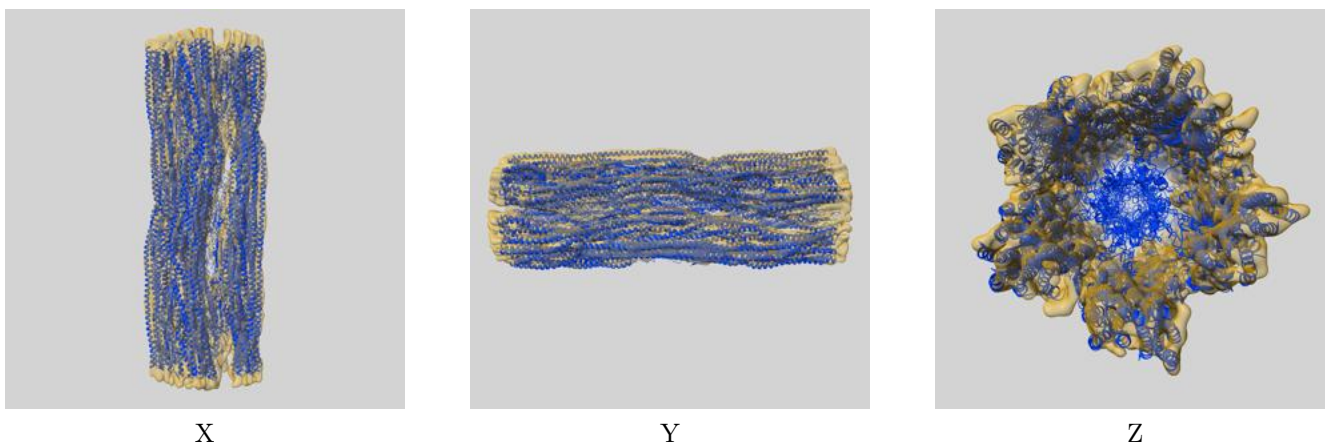
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.20	-	-
Author-provided FSC curve	7.15	8.12	7.20
Unmasked-calculated*	7.16	8.44	7.24

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

This section contains information regarding the fit between EMDB map EMD-16844 and PDB model 8RVE. Per-residue inclusion information can be found in section 3 on page 10.

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



The images above show the 3D surface view of the map at the recommended contour level 0.005 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.

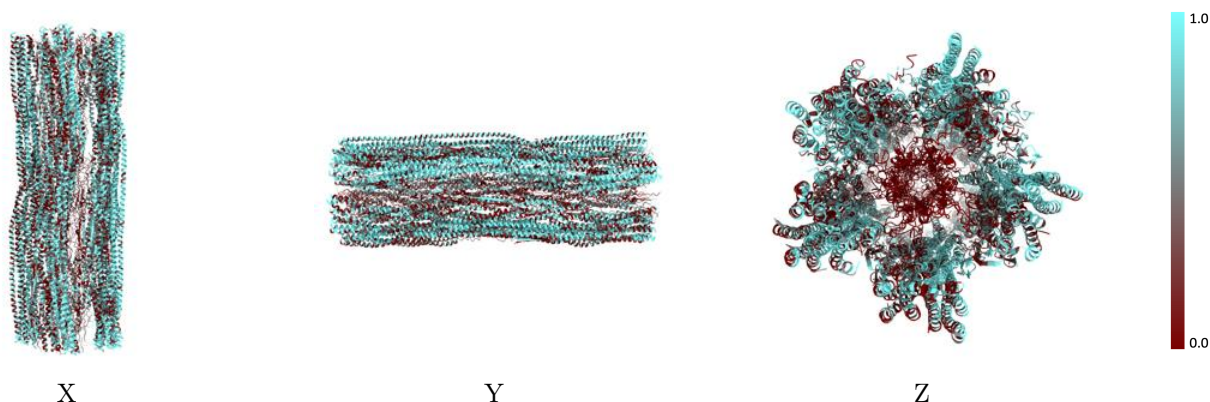


## 9.2 Q-score mapped to coordinate model [\(i\)](#)



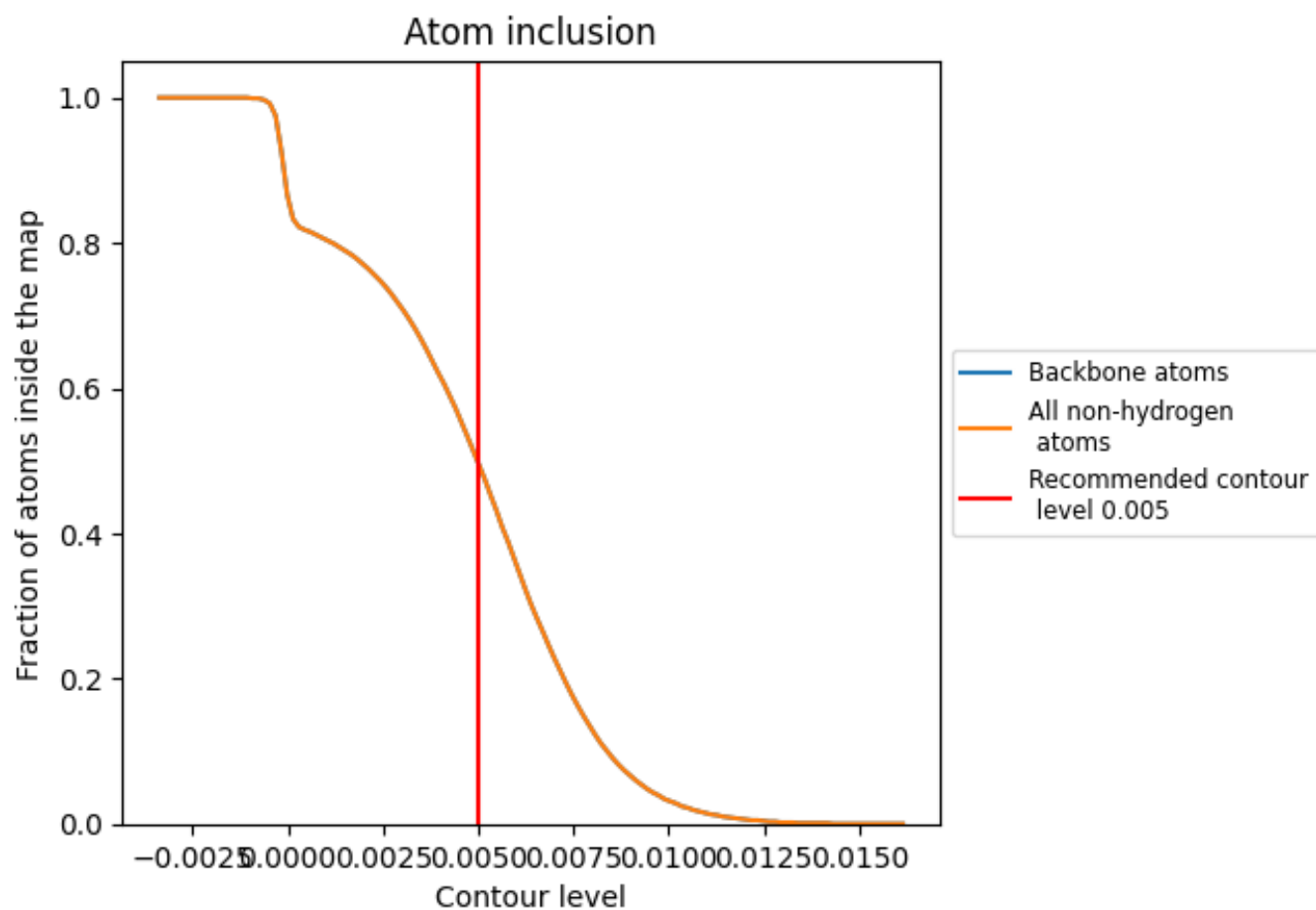
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 50% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4970	 0.0920
0	 0.8250	 0.1680
1	 0.5410	 0.0730
2	 0.5630	 0.0820
3	 0.3770	 0.0510
4	 0.2820	 0.0750
5	 0.6830	 0.0840
6	 0.7030	 0.1090
7	 0.3500	 0.0680
8	 0.2760	 0.0540
9	 0.6940	 0.1300
A	 0.5140	 0.0930
AA	 0.3160	 0.0240
AB	 0.3000	 0.0570
AC	 0.6500	 0.0890
AD	 0.7540	 0.1890
AE	 0.2040	 -0.0010
AF	 0.2590	 0.0200
AG	 0.6810	 0.0890
AH	 0.6870	 0.1600
AI	 0.7200	 0.0860
AJ	 0.6650	 0.0950
AK	 0.7100	 0.0940
AL	 0.7310	 0.1290
AM	 0.6940	 0.1020
AN	 0.7940	 0.1600
AO	 0.5510	 0.0780
AP	 0.6150	 0.1930
B	 0.4970	 0.1110
C	 0.4750	 0.1070
D	 0.4510	 0.0870
E	 0.3560	 0.0870
F	 0.4640	 0.0610
G	 0.4180	 0.1060
H	 0.4310	 0.0640







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*Continued from previous page...*

Chain	Atom inclusion	Q-score
I	 0.6490	 0.1830
J	 0.5060	 0.0960
K	 0.5510	 0.1580
L	 0.5350	 0.1280
M	 0.4780	 0.1290
N	 0.4910	 0.1420
O	 0.4090	 0.1240
P	 0.4590	 0.1490
Q	 0.0540	 0.0500
R	 0.1250	 0.0700
S	 0.5750	 0.1620
T	 0.5680	 0.1650
U	 0.1740	 0.0250
V	 0.1670	 -0.0820
W	 0.7650	 0.2040
X	 0.7730	 0.1980
Y	 0.2830	 0.0730
Z	 0.2870	 0.0490
a	 0.6840	 0.1720
b	 0.6110	 0.1650
c	 0.3140	 0.0730
d	 0.2930	 0.0250
e	 0.5310	 0.1250
f	 0.5020	 0.1390
g	 0.2440	 0.0460
h	 0.3120	 -0.0040
i	 0.4550	 0.0750
j	 0.4950	 0.1140
k	 0.2530	 0.0370
l	 0.2490	 0.0010
m	 0.5130	 0.0800
n	 0.4900	 0.1180
o	 0.3540	 0.0750
p	 0.3580	 0.0410
q	 0.4180	 0.0470
r	 0.3760	 0.0690
s	 0.4700	 0.0930
t	 0.4990	 0.0710
u	 0.4290	 0.0280
v	 0.3550	 0.0400
w	 0.4820	 0.0720
x	 0.5250	 0.0540

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Chain	Atom inclusion	Q-score
y	 0.4100	 0.0390
z	 0.3190	 0.0280