



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 02:34 PM EST

PDB ID : 7TAU  
EMDB ID : EMD-25786  
Title : Refined capsid structure of human adenovirus D26 at 3.4 Å resolution  
Authors : Reddy, V.S.; Yu, X.; Barry, M.A.  
Deposited on : 2021-12-21  
Resolution : 3.38 Å (reported)  
Based on initial model : 5TX1

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.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

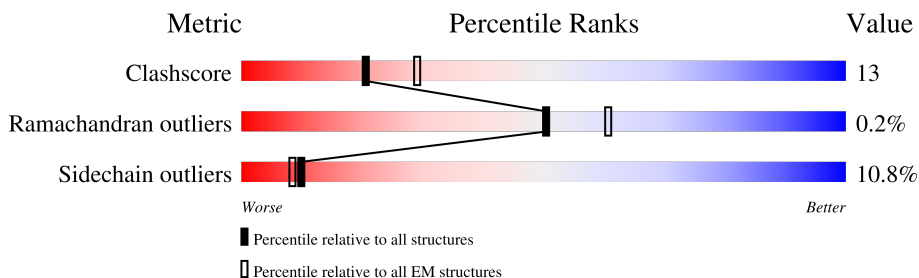
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.38 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	A	952	<div> <div>29%</div> <div>66%</div> <div>29%</div> <div>.</div> </div>
1	B	952	<div> <div>23%</div> <div>61%</div> <div>32%</div> <div>6%</div> </div>
1	C	952	<div> <div>22%</div> <div>65%</div> <div>30%</div> <div>..</div> </div>
1	D	952	<div> <div>30%</div> <div>66%</div> <div>29%</div> <div>..</div> </div>
1	E	952	<div> <div>28%</div> <div>66%</div> <div>30%</div> <div>..</div> </div>
1	F	952	<div> <div>26%</div> <div>64%</div> <div>32%</div> <div>.</div> </div>
1	G	952	<div> <div>31%</div> <div>65%</div> <div>29%</div> <div>5%</div> </div>
1	H	952	<div> <div>28%</div> <div>62%</div> <div>32%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	952	
1	J	952	
1	K	952	
1	L	952	
2	N	519	
3	O	374	
4	M	560	
5	P	134	
5	Q	134	
5	R	134	
5	S	134	
6	U	227	
6	V	227	
7	1	234	
7	2	234	
7	3	234	
7	4	234	
7	5	234	
7	6	234	
7	7	234	
7	8	234	
7	9	234	
8	X	15	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 105672 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 Hexon protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	951	Total	C	N	O	S	0	0
			7551	4796	1276	1444	35		
1	B	949	Total	C	N	O	S	0	0
			7536	4787	1274	1441	34		
1	C	946	Total	C	N	O	S	0	0
			7519	4777	1271	1437	34		
1	D	947	Total	C	N	O	S	0	0
			7526	4780	1272	1440	34		
1	E	947	Total	C	N	O	S	0	0
			7526	4780	1272	1440	34		
1	F	949	Total	C	N	O	S	0	0
			7539	4789	1274	1441	35		
1	G	947	Total	C	N	O	S	0	0
			7526	4780	1272	1440	34		
1	H	947	Total	C	N	O	S	0	0
			7526	4780	1272	1440	34		
1	I	949	Total	C	N	O	S	0	0
			7536	4787	1274	1441	34		
1	J	951	Total	C	N	O	S	0	0
			7551	4795	1276	1446	34		
1	K	950	Total	C	N	O	S	0	0
			7546	4792	1275	1445	34		
1	L	947	Total	C	N	O	S	0	0
			7524	4780	1272	1438	34		

- Molecule 2 is a protein called Penton protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	471	Total	C	N	O	S	0	0
			3786	2404	640	728	14		

- Molecule 3 is a protein called Fiber.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	O	17	Total	C	N	O	0	0
			147	96	24	27		

- Molecule 4 is a protein called Pre-hexon-linking protein IIIa.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	362	Total	C	N	O	S	0	0
			2829	1771	508	541	9		

- Molecule 5 is a protein called PIX.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	122	Total	C	N	O	S	0	0
			889	547	157	181	4		
5	Q	114	Total	C	N	O	S	0	0
			821	508	143	166	4		
5	R	133	Total	C	N	O	S	0	0
			957	587	168	198	4		
5	S	122	Total	C	N	O	S	0	0
			887	545	157	182	3		

- Molecule 6 is a protein called PVIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	190	Total	C	N	O	S	0	0
			1462	919	252	285	6		
6	V	188	Total	C	N	O	S	0	0
			1449	911	250	282	6		

- Molecule 7 is a protein called Pre-protein VI.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1	30	Total	C	N	O	S	0	0
			236	147	43	45	1		
7	2	26	Total	C	N	O	S	0	0
			203	128	38	36	1		
7	3	27	Total	C	N	O	S	0	0
			211	132	40	38	1		
7	4	29	Total	C	N	O	S	0	0
			227	142	42	42	1		
7	5	28	Total	C	N	O	S	0	0
			219	138	41	39	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	27	Total	C	N	O	S	0	0
			211	132	40	38	1		
7	7	27	Total	C	N	O	S	0	0
			211	132	40	38	1		
7	8	29	Total	C	N	O	S	0	0
			227	142	42	42	1		
7	9	28	Total	C	N	O	S	0	0
			219	138	41	39	1		

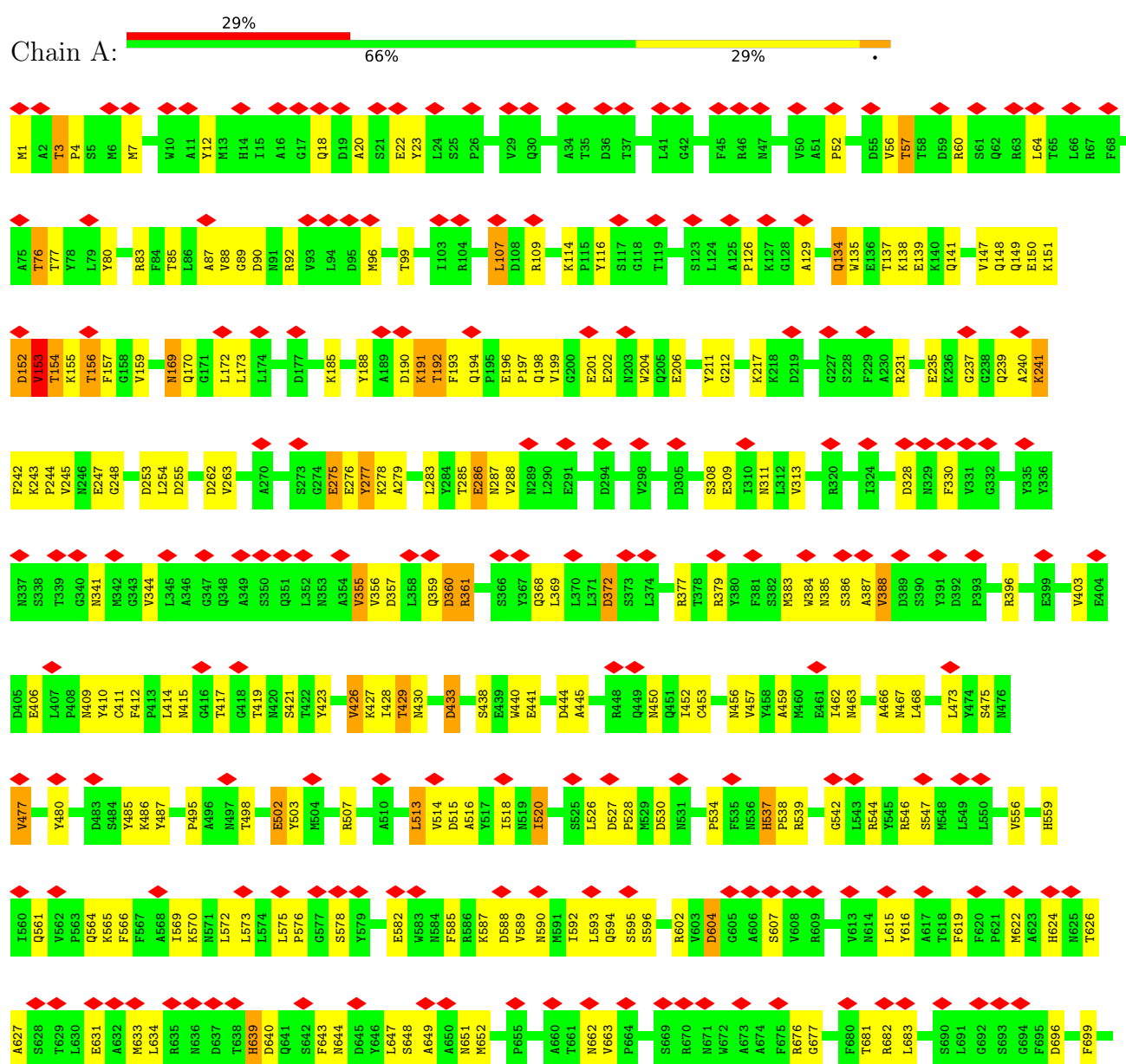
- Molecule 8 is a protein called Unknown fragment.

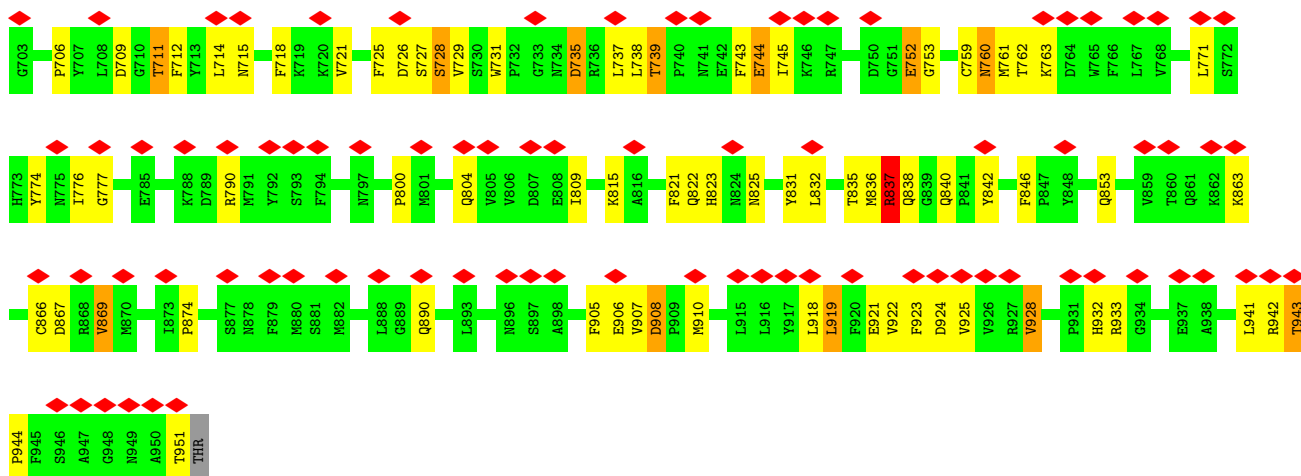
Mol	Chain	Residues	Atoms				AltConf	Trace
8	X	15	Total	C	N	O	0	0
			75	45	15	15		

### 3 Residue-property plots [i](#)

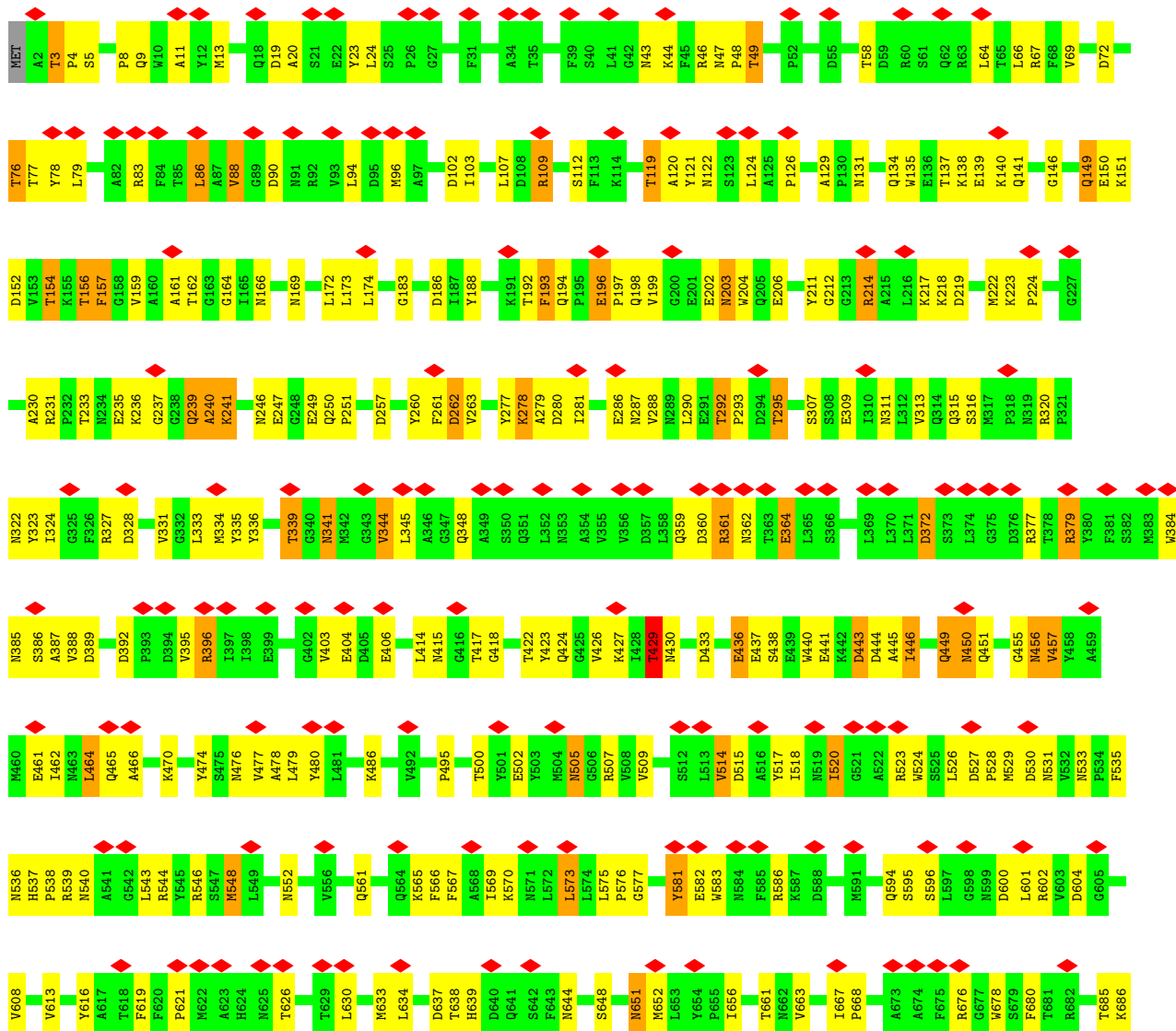
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

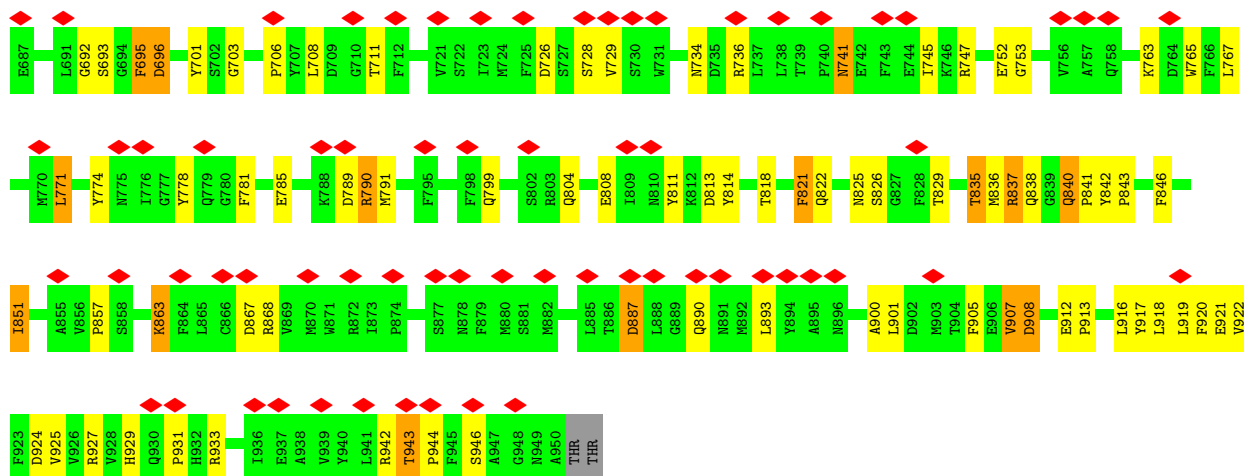
#### • Molecule 1: Hexon protein



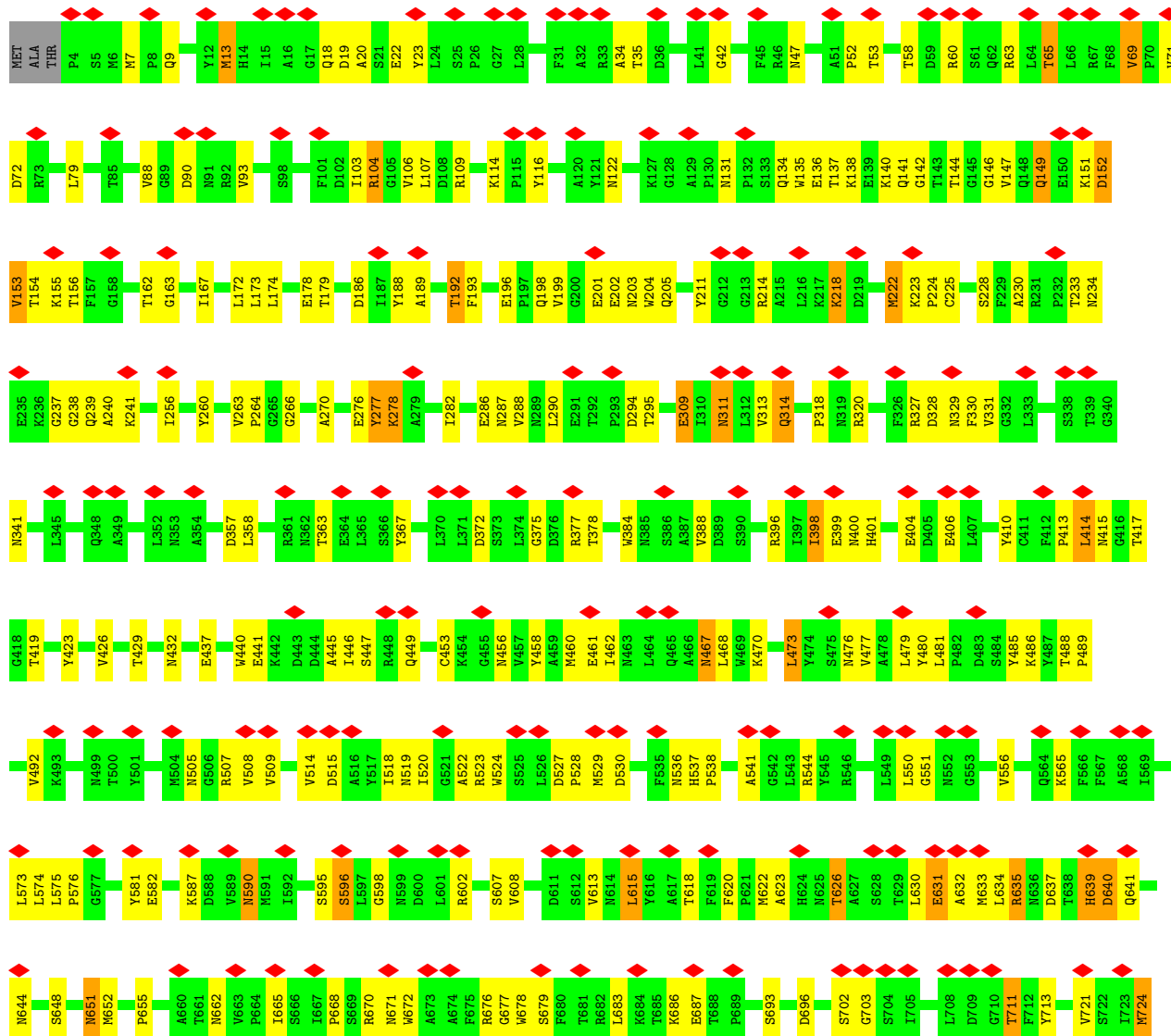


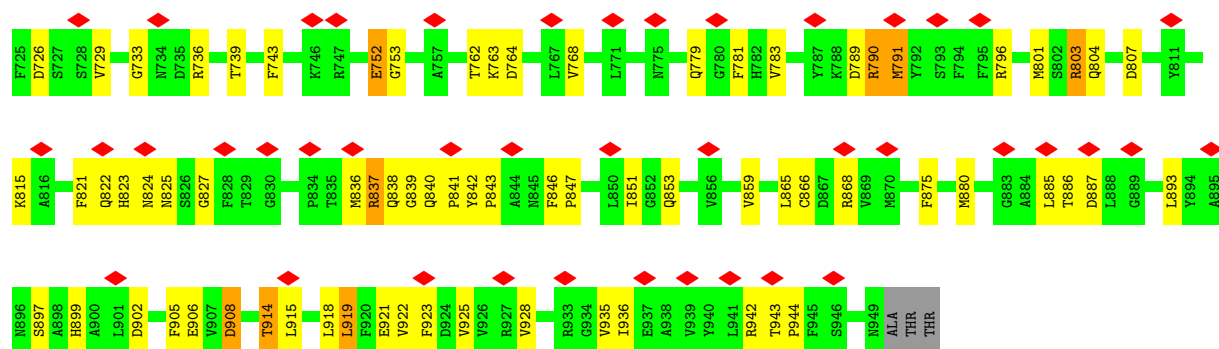
• Molecule 1: Hexon protein



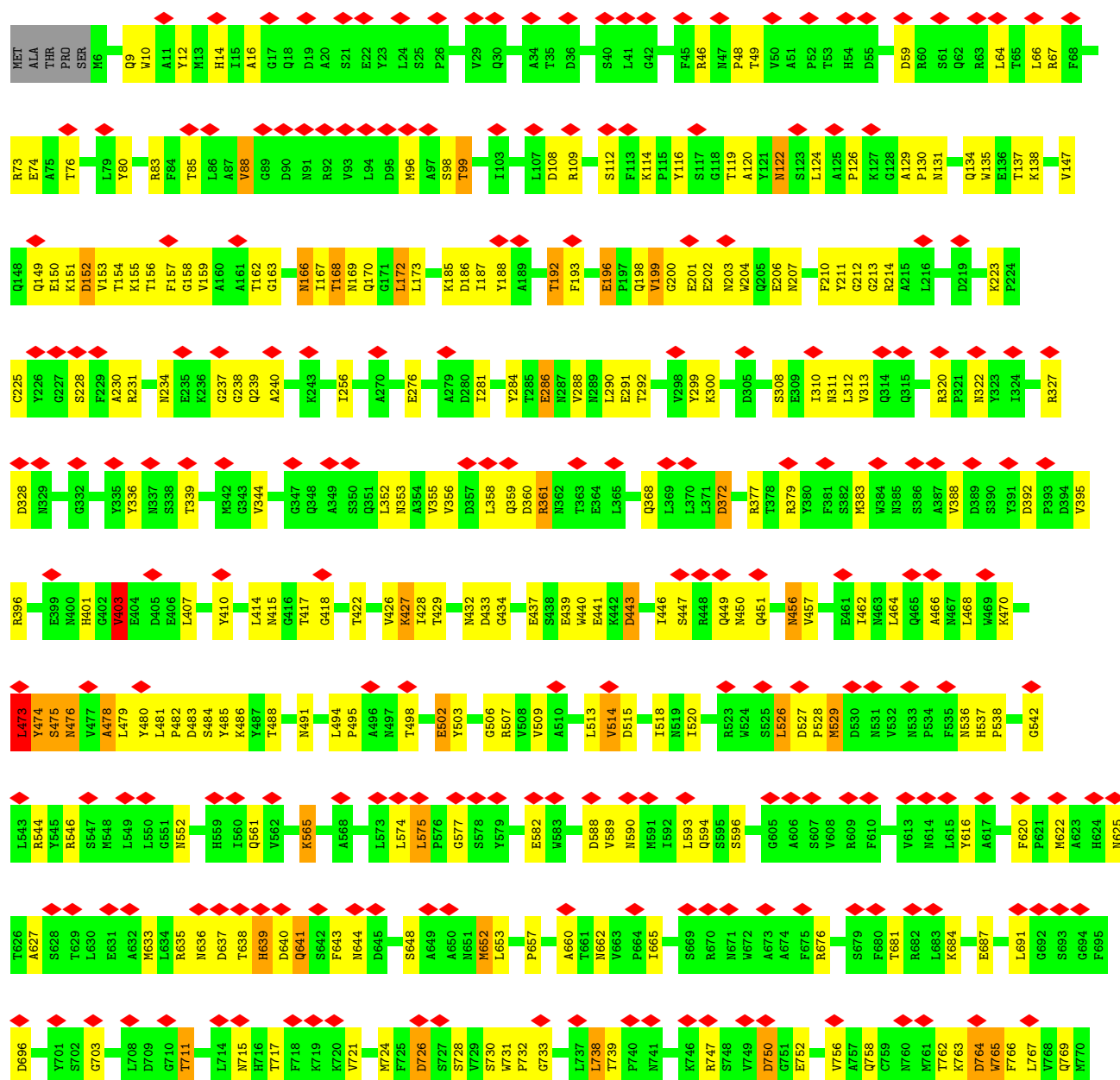


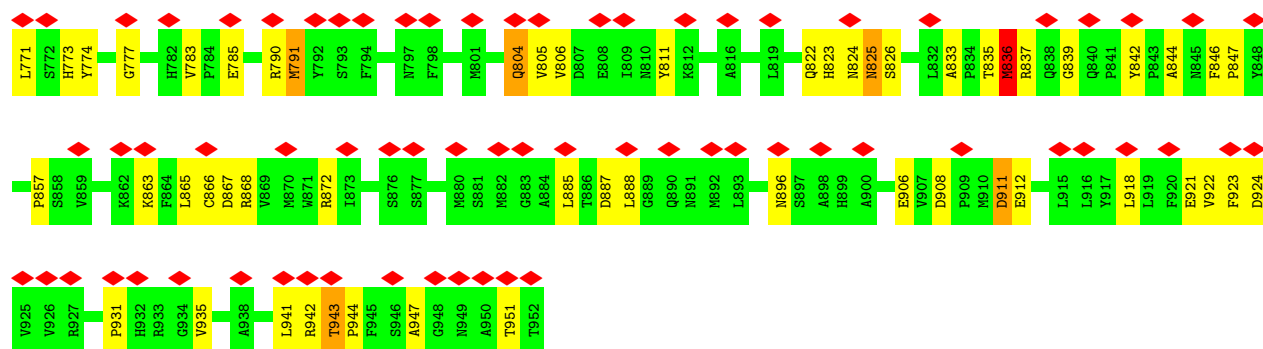
• Molecule 1: Hexon protein



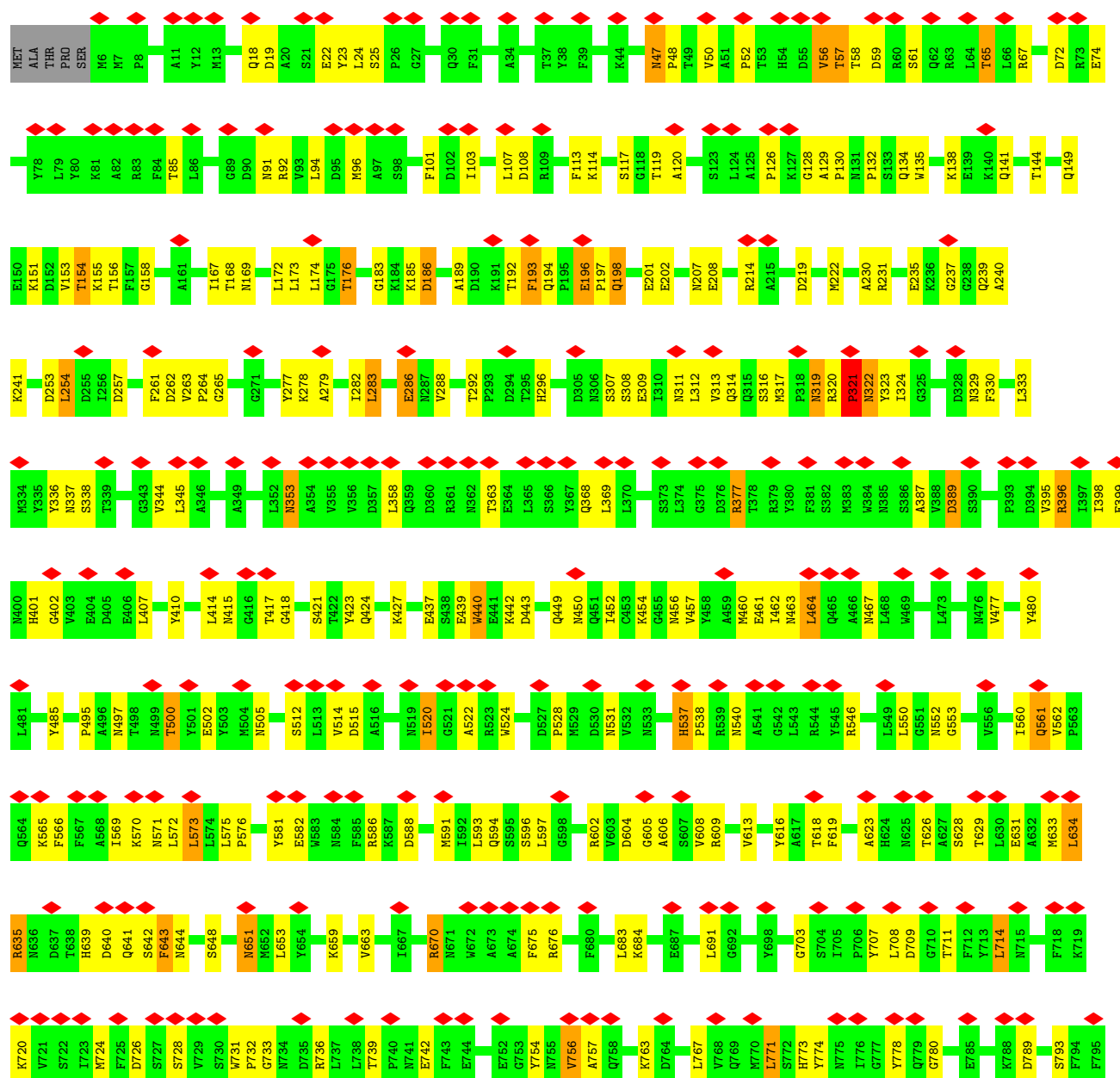


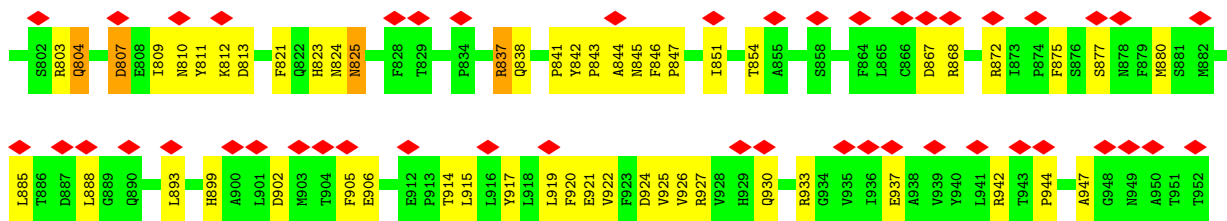
• Molecule 1: Hexon protein



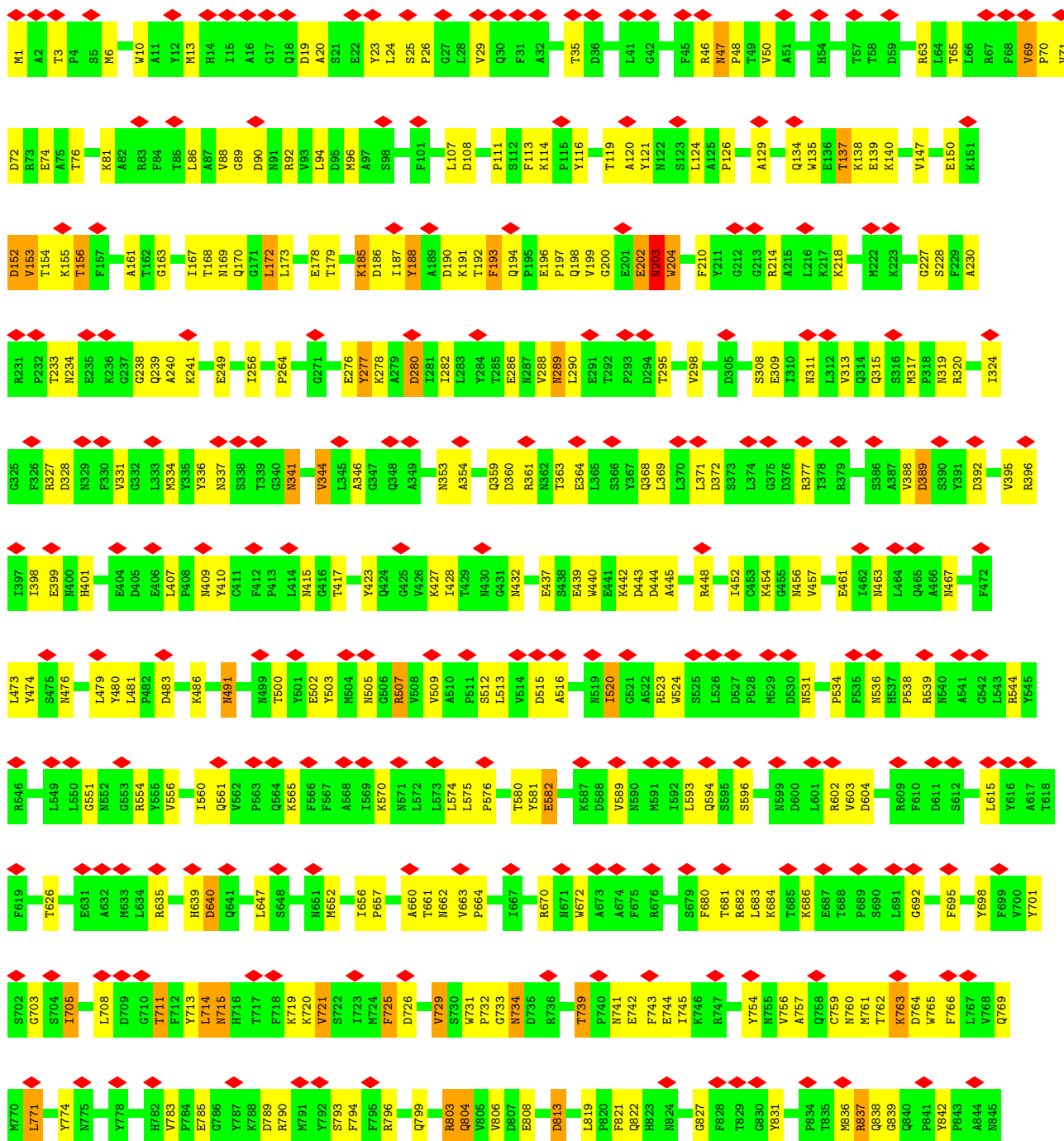


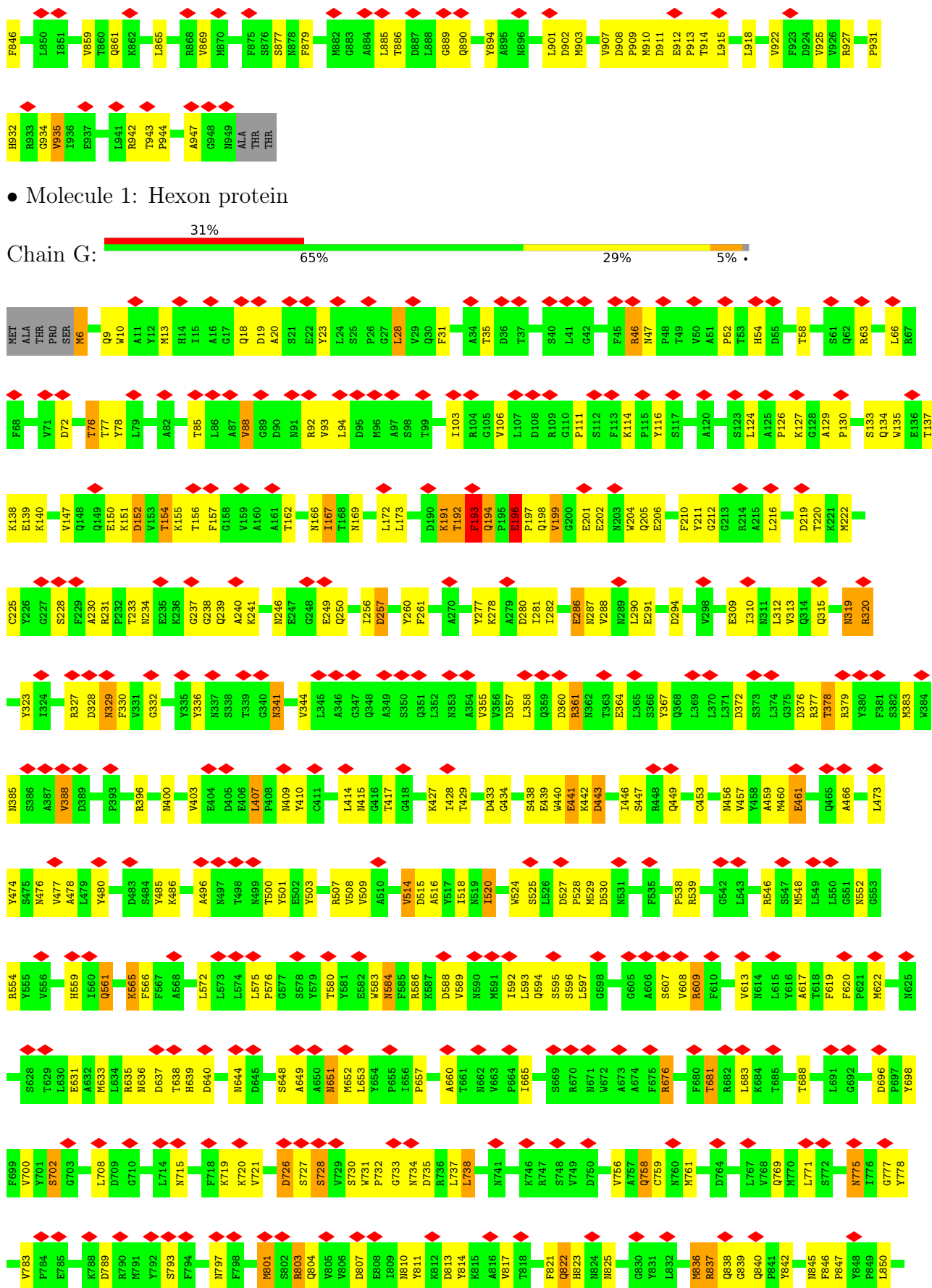
• Molecule 1: Hexon protein

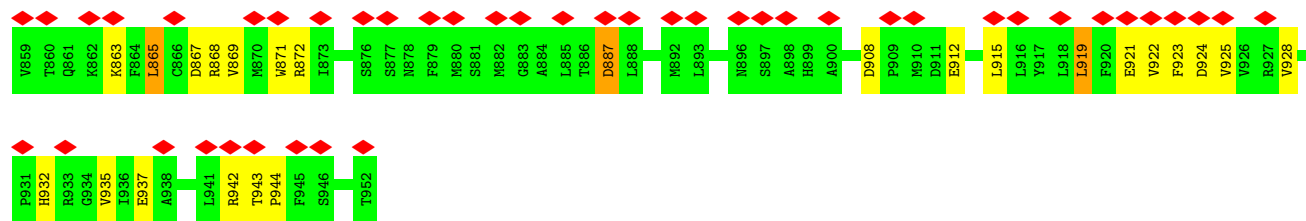




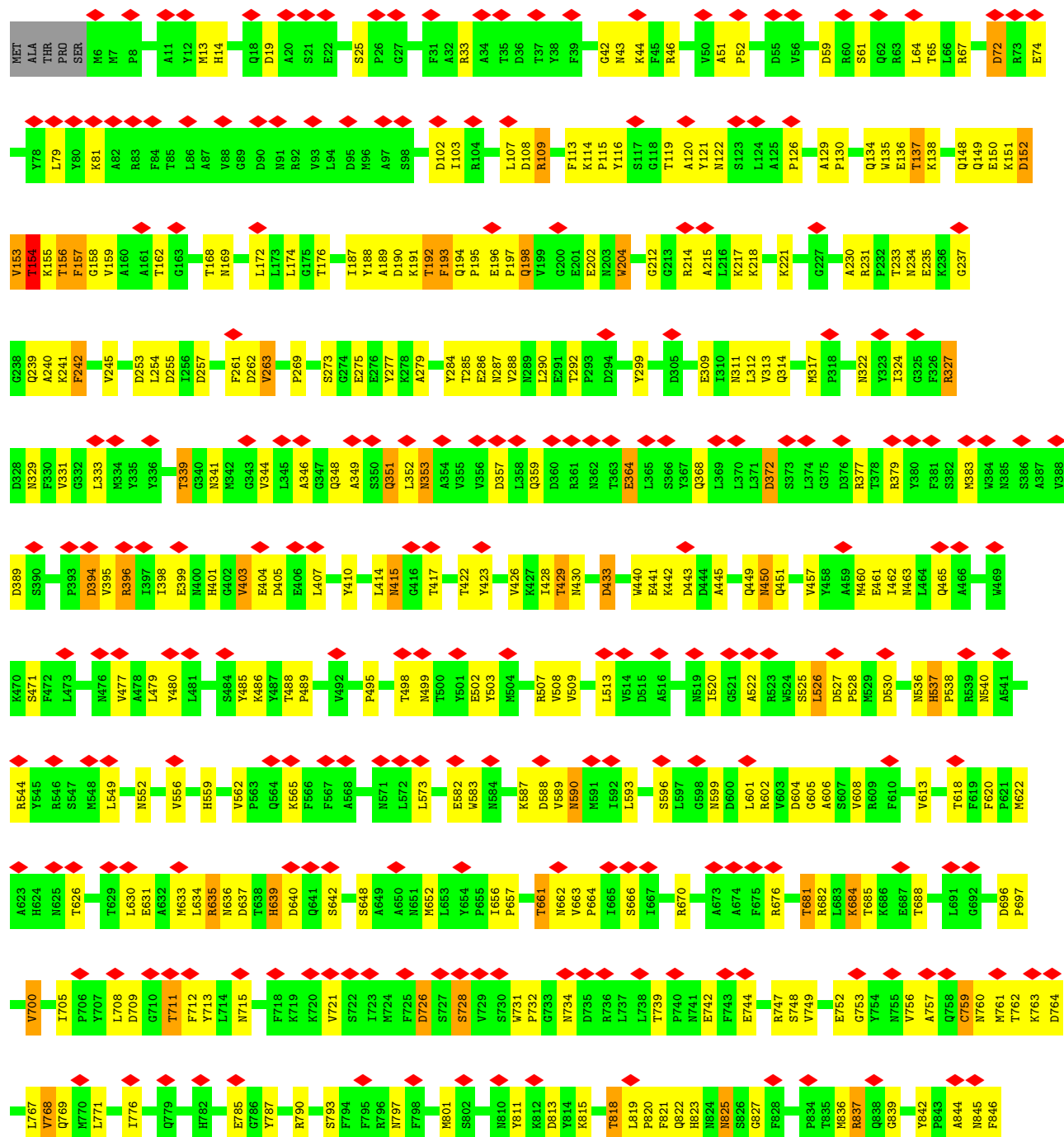
• Molecule 1: Hexon protein

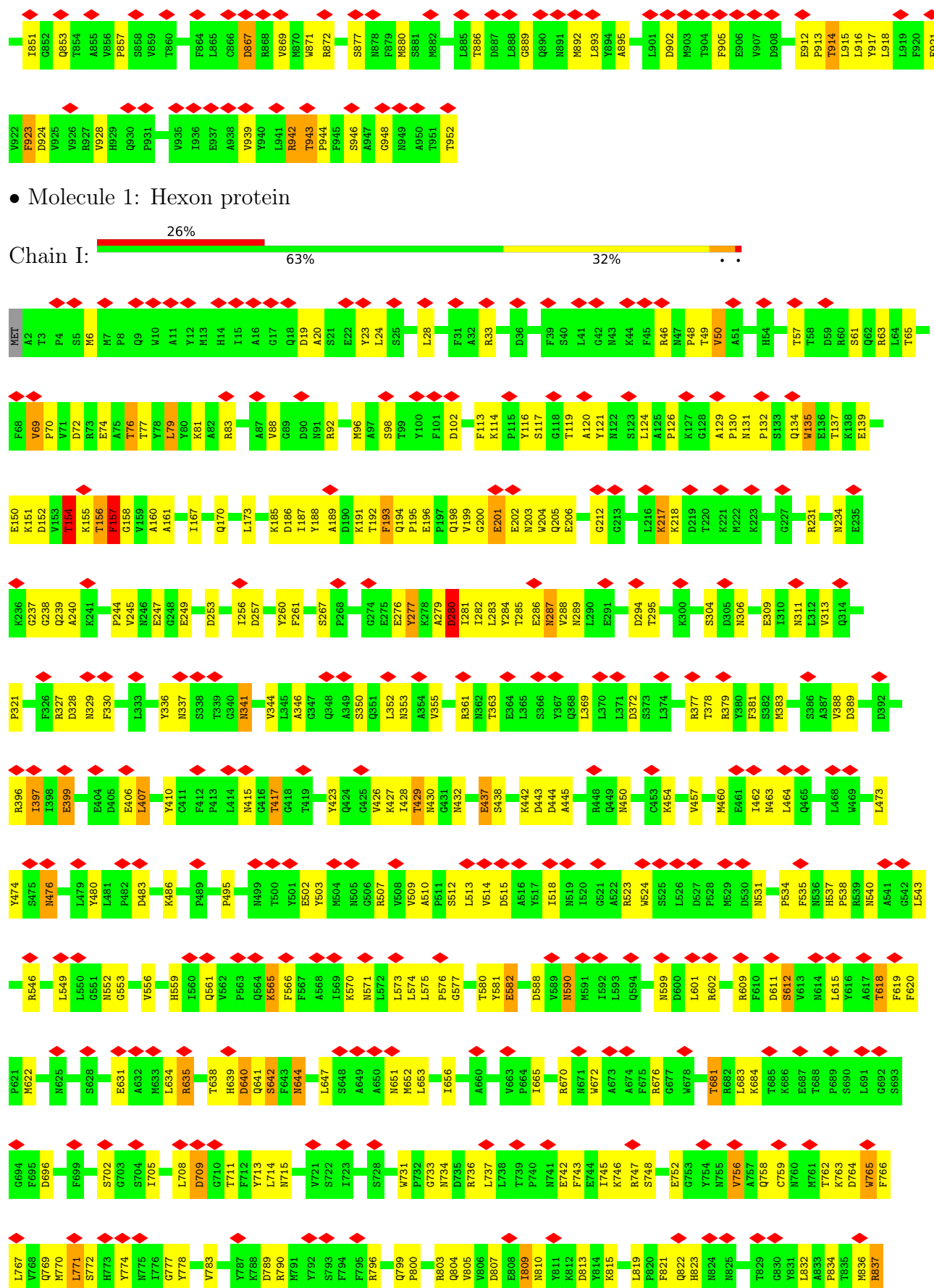


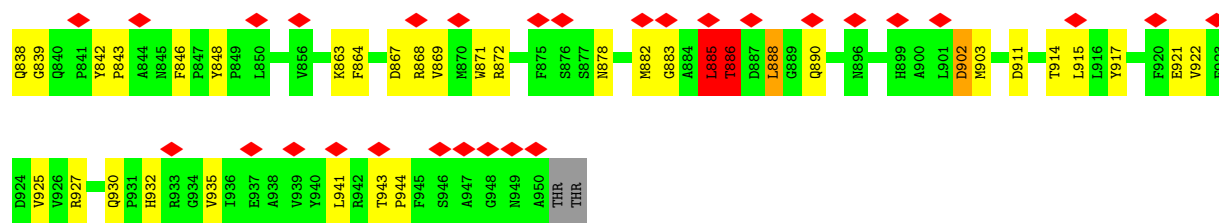




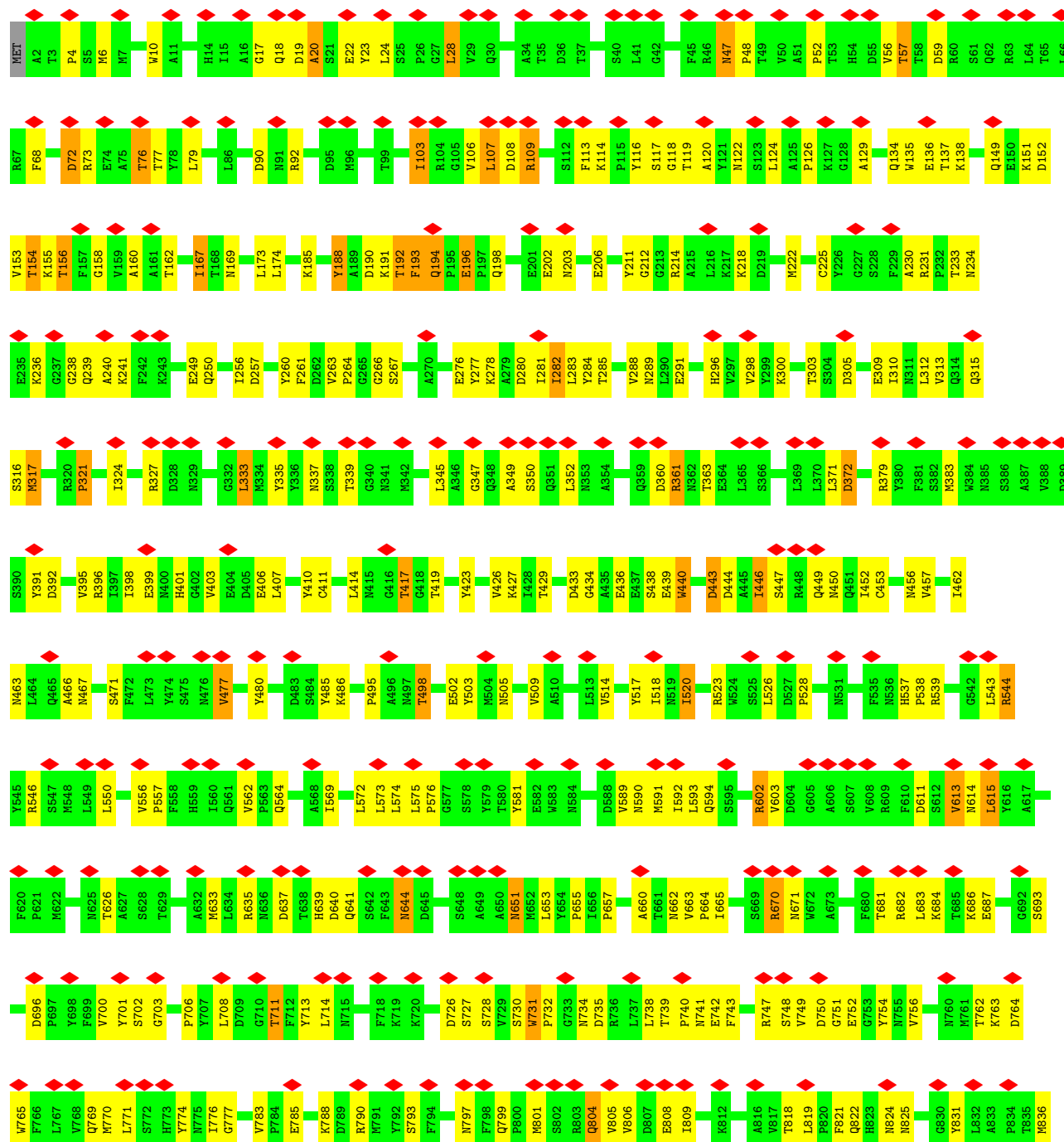
• Molecule 1: Hexon protein

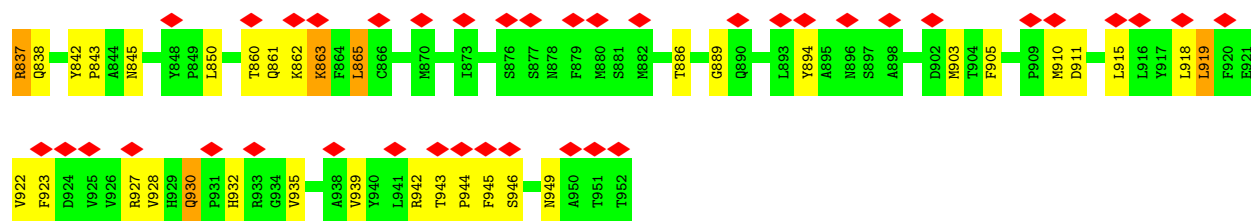




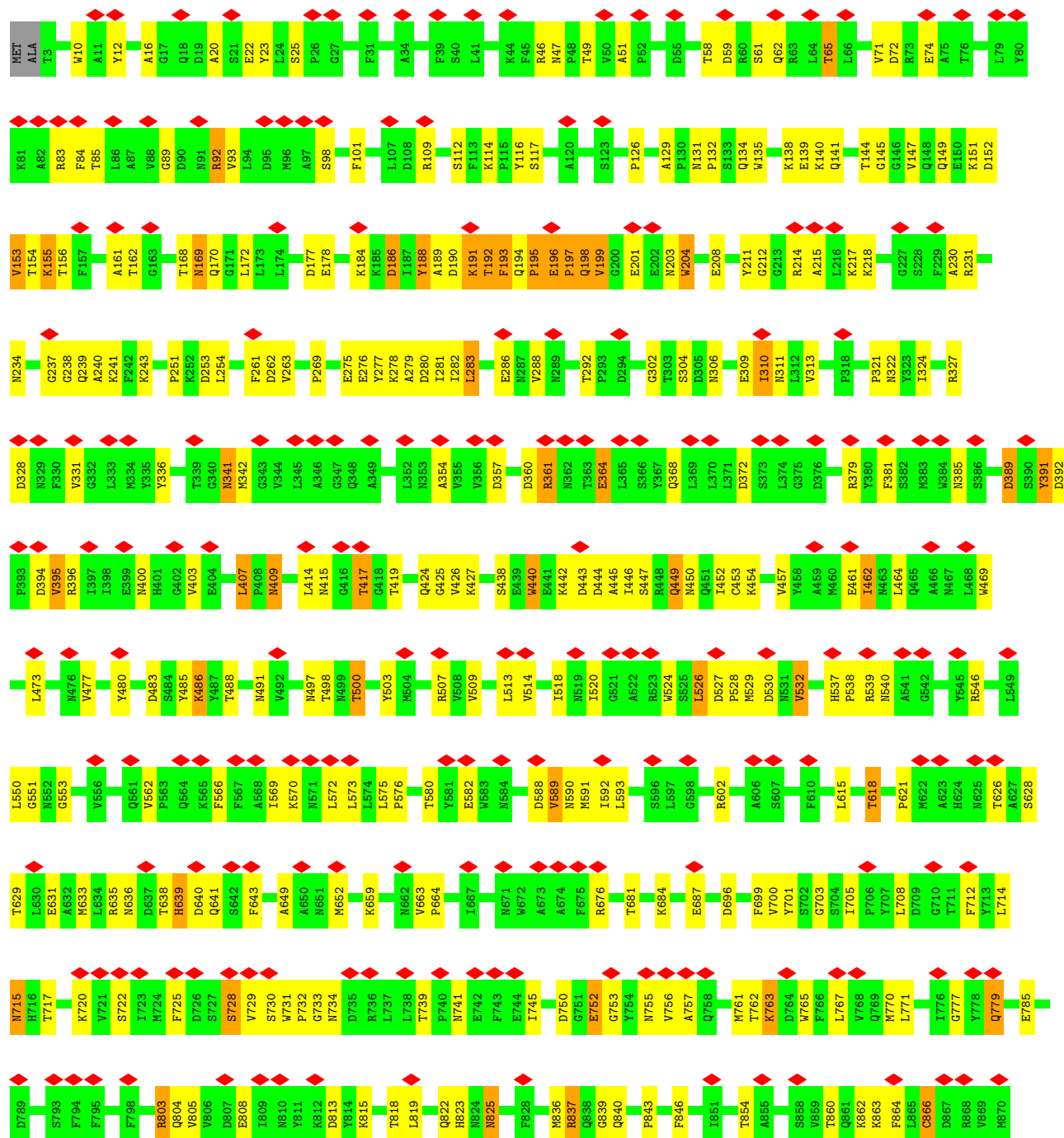


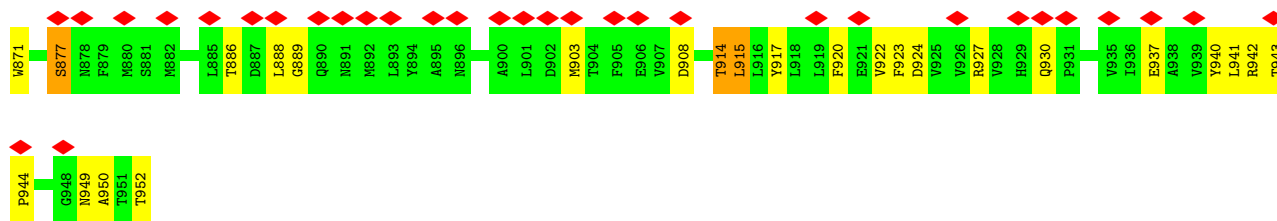
• Molecule 1: Hexon protein



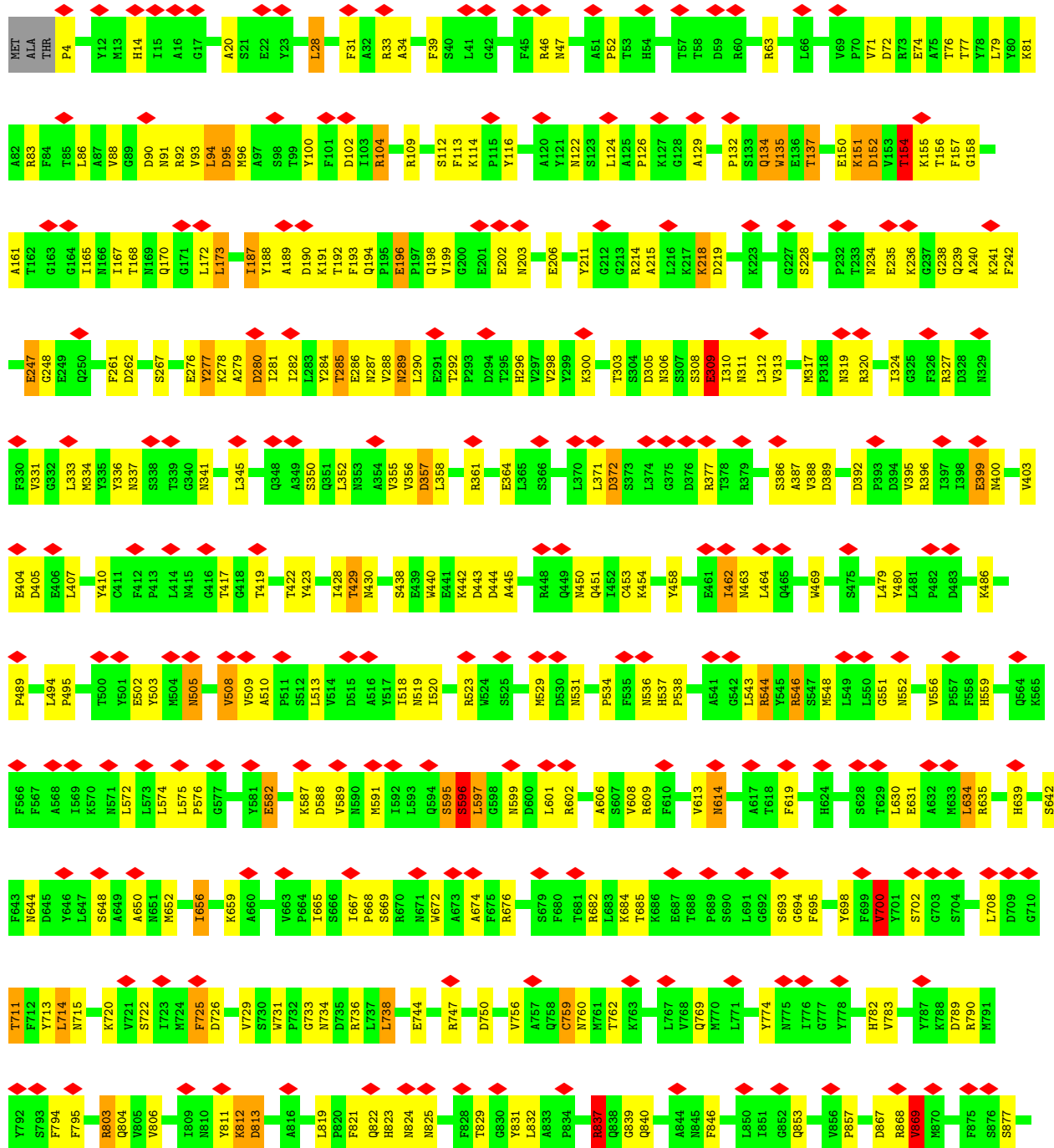


• Molecule 1: Hexon protein



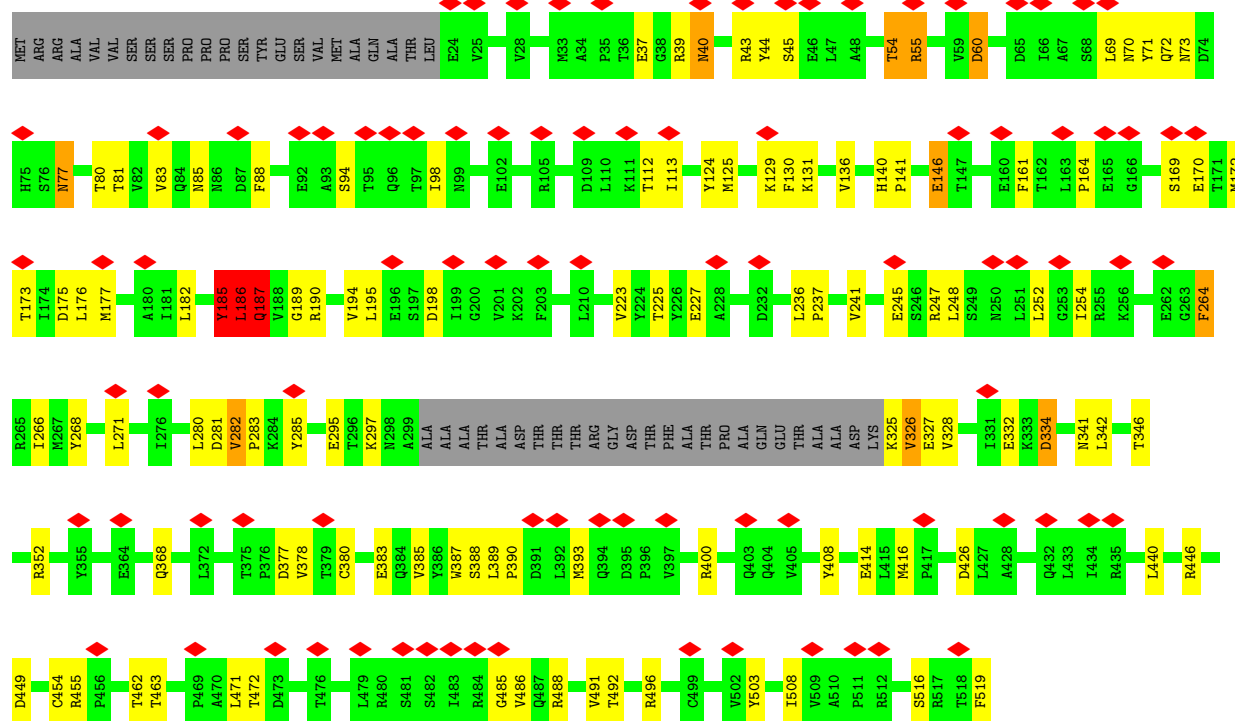


• Molecule 1: Hexon protein

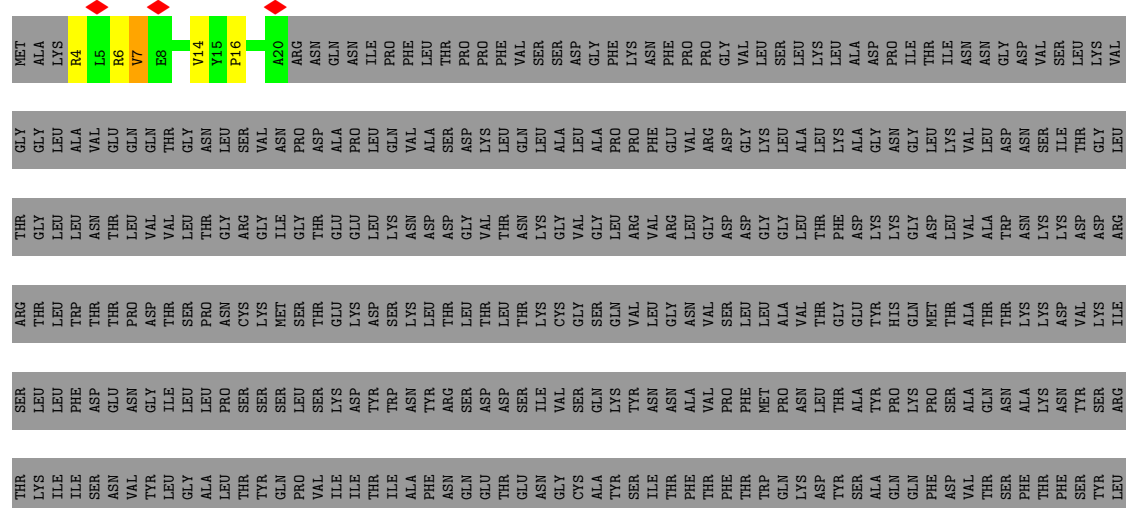




• Molecule 2: Penton protein



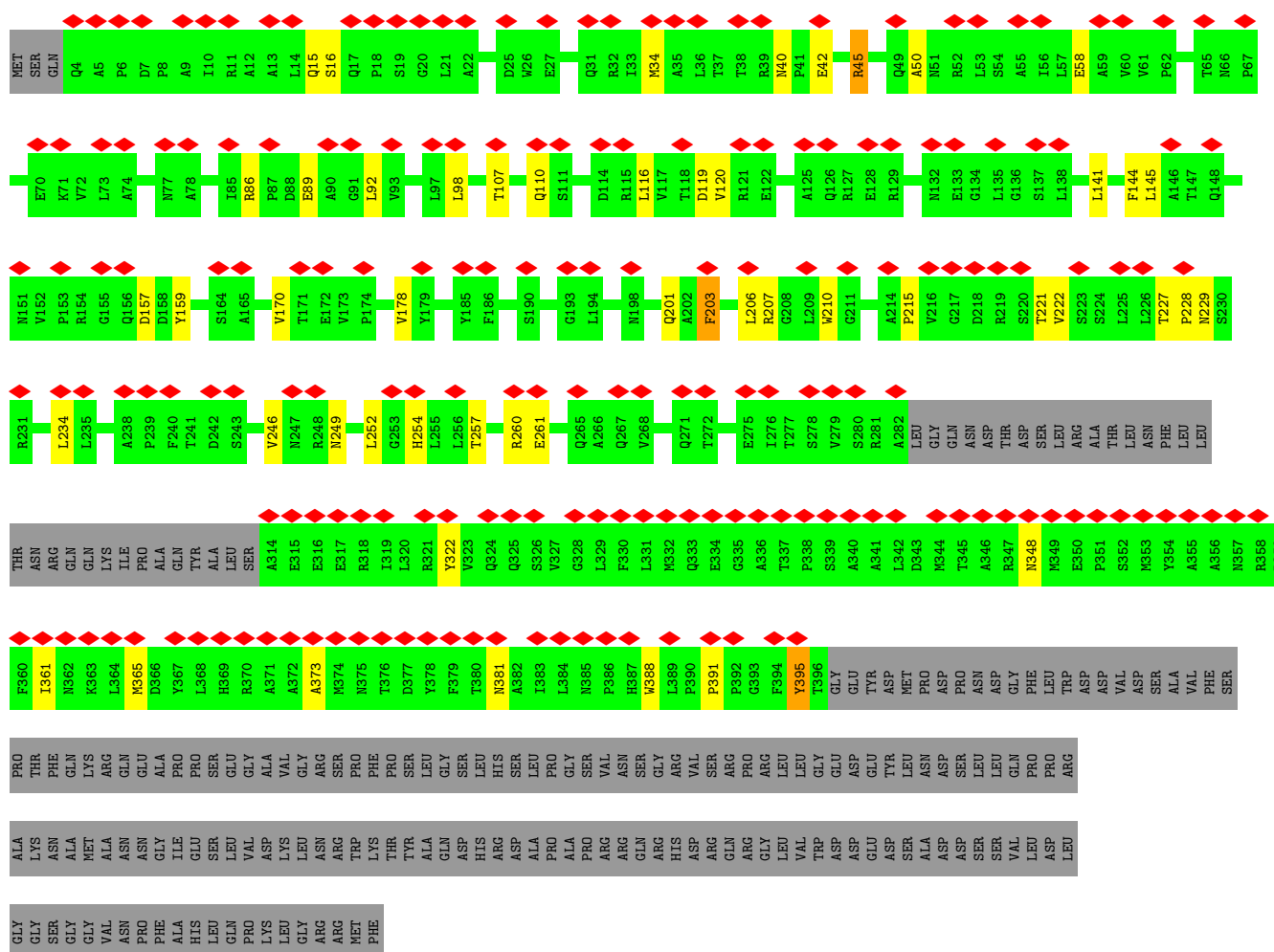
• Molecule 3: Fiber



THR  
GLN  
GLU  
ASN  
LYS  
ASP  
LYS  
ASP

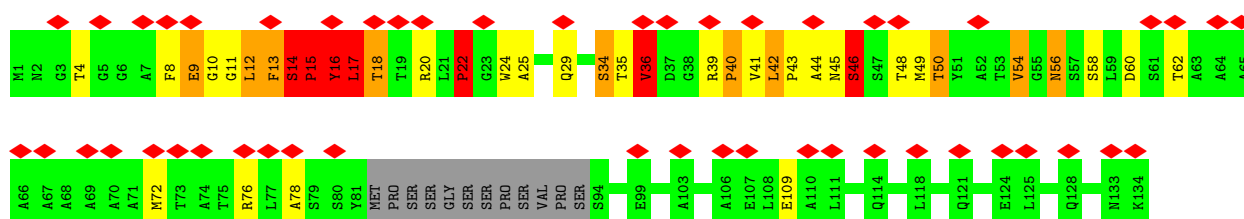
• Molecule 4: Pre-hexon-linking protein IIIa

Chain M: 



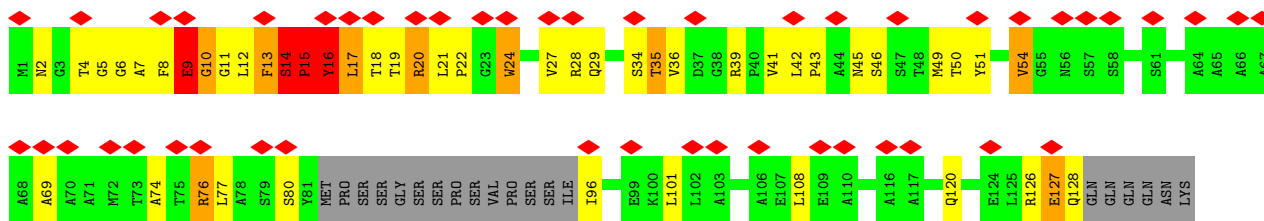
• Molecule 5: PIX

Chain P: 

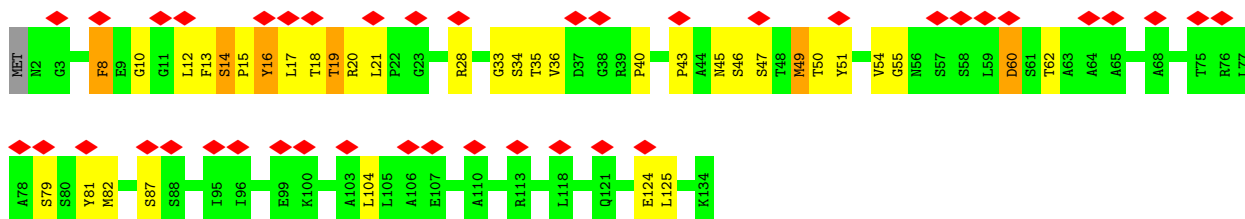
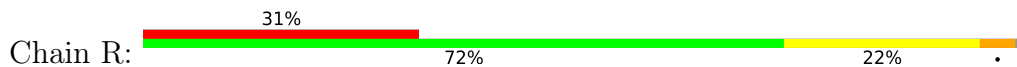


• Molecule 5: PIX

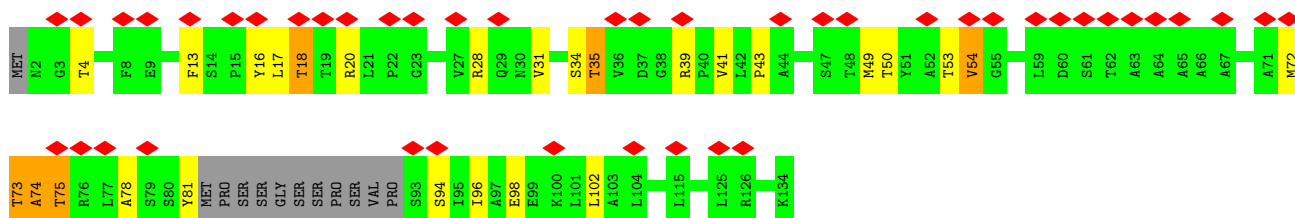
Chain Q: 



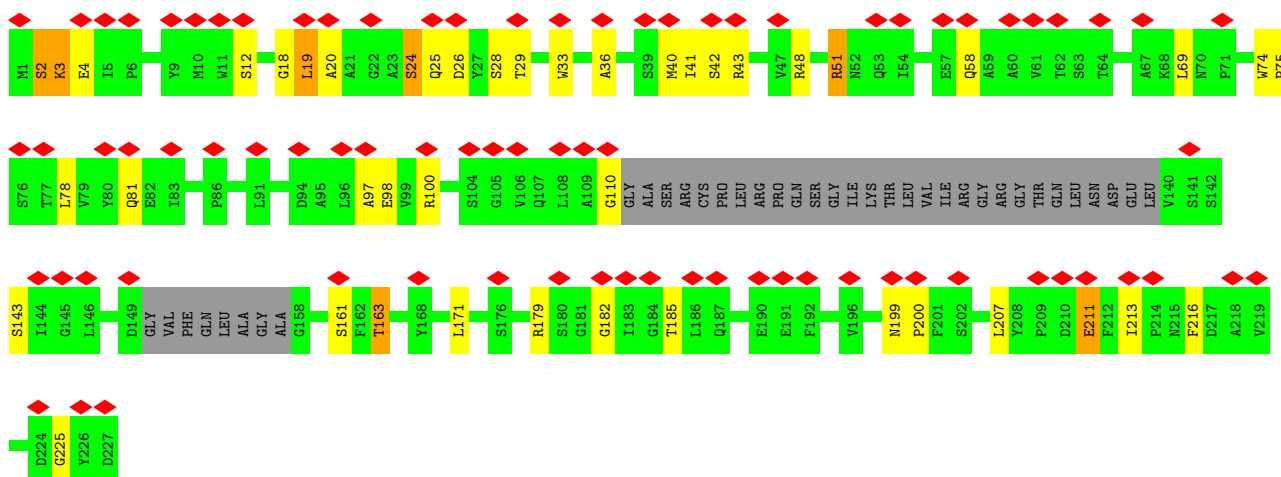
• Molecule 5: PIX



• Molecule 5: PIX



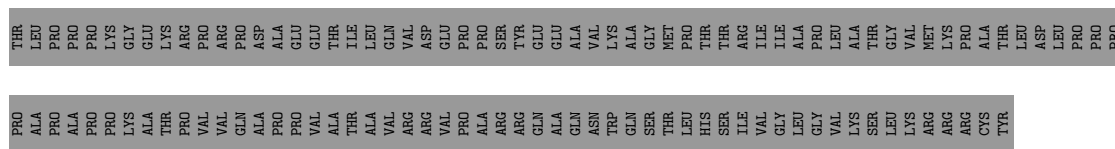
• Molecule 6: PVIII



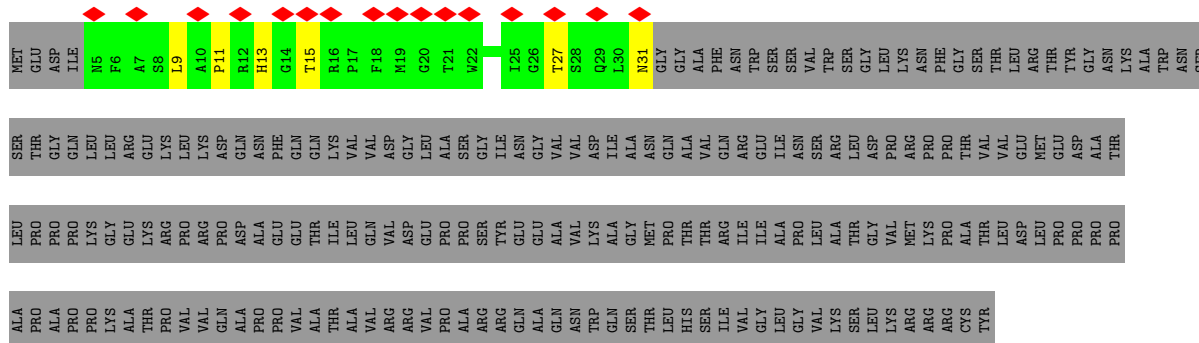
• Molecule 6: PVIII



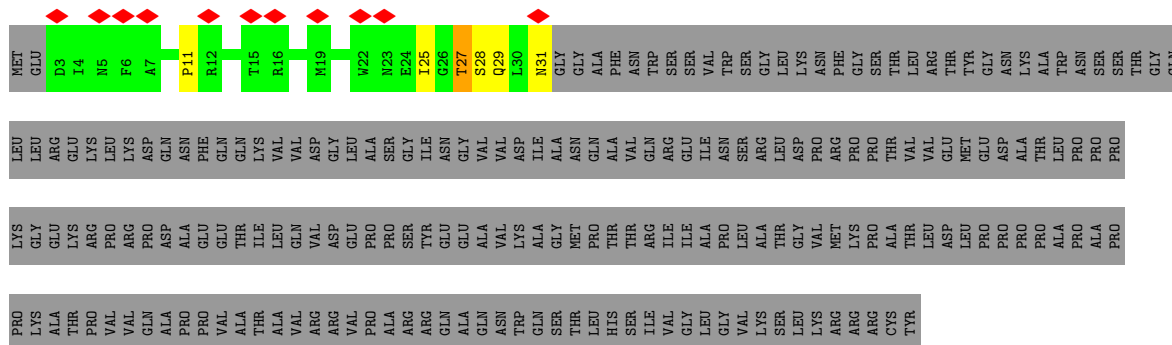




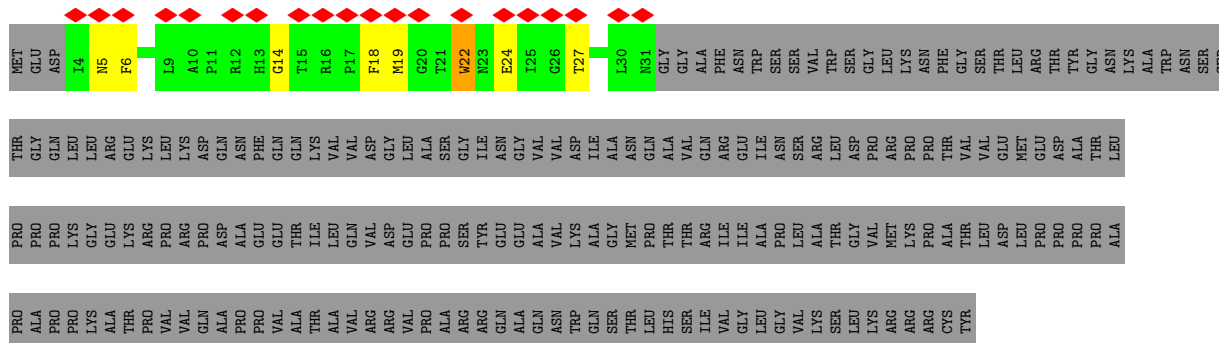
- Molecule 7: Pre-protein VI



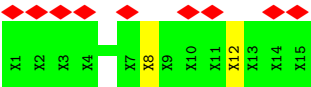
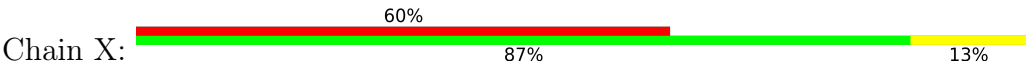
- Molecule 7: Pre-protein VI



- Molecule 7: Pre-protein VI



- Molecule 8: Unknown fragment



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	30834	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	53	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	54.450	Depositor
Minimum map value	-32.776	Depositor
Average map value	-0.056	Depositor
Map value standard deviation	3.692	Depositor
Recommended contour level	1.8	Depositor
Map size ( $\text{\AA}$ )	1089.9199, 1089.9199, 1089.9199	wwPDB
Map dimensions	832, 832, 832	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.31, 1.31, 1.31	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	A	0.46	0/7758	0.52	3/10554 (0.0%)
1	B	0.52	2/7743 (0.0%)	0.56	5/10534 (0.0%)
1	C	0.46	4/7726 (0.1%)	0.51	3/10509 (0.0%)
1	D	0.59	5/7732 (0.1%)	0.57	4/10517 (0.0%)
1	E	0.51	1/7732 (0.0%)	0.54	3/10517 (0.0%)
1	F	0.57	1/7746 (0.0%)	0.57	4/10537 (0.0%)
1	G	0.51	4/7732 (0.1%)	0.53	3/10517 (0.0%)
1	H	0.59	1/7732 (0.0%)	0.58	4/10517 (0.0%)
1	I	0.67	4/7743 (0.1%)	0.62	8/10534 (0.1%)
1	J	0.53	1/7758 (0.0%)	0.55	1/10554 (0.0%)
1	K	0.63	7/7753 (0.1%)	0.58	5/10547 (0.0%)
1	L	0.58	5/7731 (0.1%)	0.58	6/10516 (0.1%)
2	N	0.62	3/3879 (0.1%)	0.60	2/5280 (0.0%)
3	O	0.61	0/152	0.70	1/207 (0.5%)
4	M	0.63	0/2884	0.61	2/3926 (0.1%)
5	P	1.28	11/898 (1.2%)	1.26	14/1216 (1.2%)
5	Q	1.08	9/830 (1.1%)	1.04	11/1127 (1.0%)
5	R	0.29	0/970	0.45	0/1318
5	S	0.42	0/896	0.61	1/1214 (0.1%)
6	U	0.99	4/1499 (0.3%)	0.75	0/2041
6	V	0.34	0/1486	0.44	0/2023
7	1	0.25	0/242	0.51	0/328
7	2	0.89	0/209	1.38	5/283 (1.8%)
7	3	0.26	0/217	0.44	0/294
7	4	0.78	0/233	0.86	1/316 (0.3%)
7	5	0.25	0/225	0.47	0/305
7	6	0.64	0/217	0.73	0/294
7	7	0.27	0/217	0.44	0/294
7	8	0.61	0/233	0.89	2/316 (0.6%)
7	9	0.26	0/225	0.42	0/305
All	All	0.58	62/108398 (0.1%)	0.58	88/147440 (0.1%)

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	D	0	3
1	K	0	1
1	L	0	1
2	N	0	3
4	M	0	1
All	All	0	9

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	15	PRO	CA-C	-9.18	1.34	1.52
5	P	17	LEU	CA-C	-7.49	1.33	1.52
5	Q	17	LEU	CA-C	-7.48	1.33	1.52
5	Q	15	PRO	CA-C	-7.08	1.38	1.52
6	U	12	SER	CA-CB	-7.03	1.42	1.52

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	44	ALA	N-CA-C	-17.22	64.52	111.00
7	2	26	GLY	N-CA-C	15.26	151.25	113.10
1	G	193	PHE	N-CA-C	-11.83	79.06	111.00
5	Q	11	GLY	N-CA-C	-10.93	85.77	113.10
5	P	11	GLY	N-CA-C	-9.76	88.70	113.10

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	474	TYR	Mainchain
1	D	475	SER	Mainchain
1	D	476	ASN	Mainchain
1	K	186	ASP	Mainchain
1	L	595	SER	Mainchain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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	A	7551	0	7226	240	0
1	B	7536	0	7207	265	0
1	C	7519	0	7191	231	0
1	D	7526	0	7197	243	0
1	E	7526	0	7197	227	0
1	F	7539	0	7214	270	0
1	G	7526	0	7197	235	0
1	H	7526	0	7197	263	0
1	I	7536	0	7207	250	0
1	J	7551	0	7221	240	0
1	K	7546	0	7216	242	0
1	L	7524	0	7196	248	0
2	N	3786	0	3699	56	0
3	O	147	0	132	2	0
4	M	2829	0	2795	27	0
5	P	889	0	889	44	0
5	Q	821	0	822	55	0
5	R	957	0	950	44	0
5	S	887	0	882	17	0
6	U	1462	0	1416	32	0
6	V	1449	0	1402	14	0
7	1	236	0	219	7	0
7	2	203	0	192	5	0
7	3	211	0	198	7	0
7	4	227	0	213	8	0
7	5	219	0	209	9	0
7	6	211	0	198	8	0
7	7	211	0	198	1	0
7	8	227	0	213	4	0
7	9	219	0	209	8	0
8	X	75	0	17	1	0
All	All	105672	0	101319	2791	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 13.

The worst 5 of 2791 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)
5:Q:15:PRO:HB2	5:Q:17:LEU:H	1.22	1.01
1:A:154:THR:HG23	1:A:155:LYS:HG2	1.47	0.96
1:K:196:GLU:HG2	1:L:823:HIS:HB3	1.47	0.94
1:K:194:GLN:HB2	1:K:197:PRO:HD2	1.52	0.91
1:I:762:THR:HG22	1:I:763:LYS:N	1.84	0.90

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	A	949/952 (100%)	825 (87%)	121 (13%)	3 (0%)	41	73
1	B	947/952 (100%)	843 (89%)	101 (11%)	3 (0%)	41	73
1	C	944/952 (99%)	803 (85%)	139 (15%)	2 (0%)	47	78
1	D	945/952 (99%)	821 (87%)	122 (13%)	2 (0%)	47	78
1	E	945/952 (99%)	841 (89%)	104 (11%)	0	100	100
1	F	947/952 (100%)	815 (86%)	129 (14%)	3 (0%)	41	73
1	G	945/952 (99%)	817 (86%)	123 (13%)	5 (0%)	29	63
1	H	945/952 (99%)	817 (86%)	127 (13%)	1 (0%)	51	82
1	I	947/952 (100%)	818 (86%)	128 (14%)	1 (0%)	51	82
1	J	949/952 (100%)	830 (88%)	118 (12%)	1 (0%)	51	82
1	K	948/952 (100%)	833 (88%)	115 (12%)	0	100	100
1	L	945/952 (99%)	821 (87%)	120 (13%)	4 (0%)	34	68
2	N	467/519 (90%)	434 (93%)	32 (7%)	1 (0%)	47	78
3	O	15/374 (4%)	13 (87%)	2 (13%)	0	100	100
4	M	358/560 (64%)	344 (96%)	14 (4%)	0	100	100
5	P	118/134 (88%)	96 (81%)	19 (16%)	3 (2%)	5	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Q	110/134 (82%)	84 (76%)	24 (22%)	2 (2%)	8	35
5	R	131/134 (98%)	109 (83%)	22 (17%)	0	100	100
5	S	118/134 (88%)	98 (83%)	18 (15%)	2 (2%)	9	36
6	U	184/227 (81%)	172 (94%)	12 (6%)	0	100	100
6	V	182/227 (80%)	167 (92%)	15 (8%)	0	100	100
7	1	28/234 (12%)	20 (71%)	8 (29%)	0	100	100
7	2	24/234 (10%)	16 (67%)	8 (33%)	0	100	100
7	3	25/234 (11%)	20 (80%)	5 (20%)	0	100	100
7	4	27/234 (12%)	18 (67%)	9 (33%)	0	100	100
7	5	26/234 (11%)	21 (81%)	5 (19%)	0	100	100
7	6	25/234 (11%)	21 (84%)	4 (16%)	0	100	100
7	7	25/234 (11%)	20 (80%)	5 (20%)	0	100	100
7	8	27/234 (12%)	24 (89%)	3 (11%)	0	100	100
7	9	26/234 (11%)	20 (77%)	6 (23%)	0	100	100
All	All	13272/15973 (83%)	11581 (87%)	1658 (12%)	33 (0%)	50	78

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	ASP
1	C	153	VAL
1	D	153	VAL
1	F	153	VAL
1	F	203	ASN

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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	A	817/818 (100%)	741 (91%)	76 (9%)	9	31
1	B	815/818 (100%)	721 (88%)	94 (12%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	814/818 (100%)	724 (89%)	90 (11%)	6	23
1	D	814/818 (100%)	728 (89%)	86 (11%)	6	25
1	E	814/818 (100%)	730 (90%)	84 (10%)	7	27
1	F	816/818 (100%)	733 (90%)	83 (10%)	7	28
1	G	814/818 (100%)	718 (88%)	96 (12%)	5	20
1	H	814/818 (100%)	712 (88%)	102 (12%)	4	18
1	I	815/818 (100%)	723 (89%)	92 (11%)	6	22
1	J	817/818 (100%)	725 (89%)	92 (11%)	6	22
1	K	817/818 (100%)	721 (88%)	96 (12%)	5	20
1	L	814/818 (100%)	720 (88%)	94 (12%)	5	22
2	N	426/462 (92%)	387 (91%)	39 (9%)	9	32
3	O	15/324 (5%)	12 (80%)	3 (20%)	1	4
4	M	304/472 (64%)	291 (96%)	13 (4%)	29	60
5	P	91/102 (89%)	77 (85%)	14 (15%)	2	12
5	Q	83/102 (81%)	70 (84%)	13 (16%)	2	11
5	R	101/102 (99%)	89 (88%)	12 (12%)	5	20
5	S	91/102 (89%)	83 (91%)	8 (9%)	10	34
6	U	162/190 (85%)	154 (95%)	8 (5%)	25	57
6	V	160/190 (84%)	150 (94%)	10 (6%)	18	49
7	1	25/195 (13%)	24 (96%)	1 (4%)	31	61
7	2	21/195 (11%)	12 (57%)	9 (43%)	0	0
7	3	22/195 (11%)	22 (100%)	0	100	100
7	4	24/195 (12%)	21 (88%)	3 (12%)	4	18
7	5	23/195 (12%)	21 (91%)	2 (9%)	10	35
7	6	22/195 (11%)	19 (86%)	3 (14%)	3	16
7	7	22/195 (11%)	17 (77%)	5 (23%)	1	3
7	8	24/195 (12%)	22 (92%)	2 (8%)	11	37
7	9	23/195 (12%)	21 (91%)	2 (9%)	10	35
All	All	11420/13617 (84%)	10188 (89%)	1232 (11%)	10	25

5 of 1232 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	391	TYR
5	P	22	PRO
1	K	638	THR
1	K	389	ASP
1	L	596	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	641	GLN
1	K	62	GLN
1	I	838	GLN
1	J	662	ASN
1	L	840	GLN

### 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.

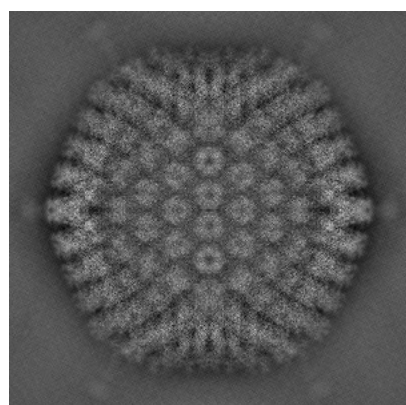
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25786. These allow visual inspection of the internal detail of the map and identification of artifacts.

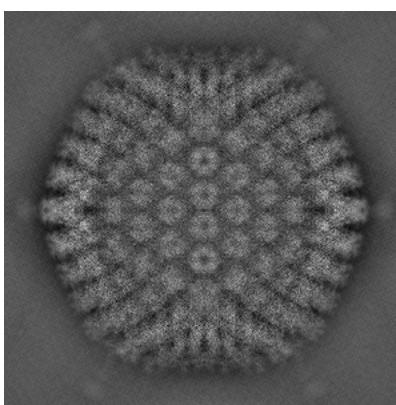
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

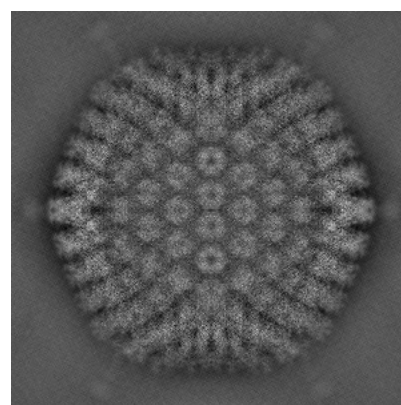
#### 6.1.1 Primary map



X



Y

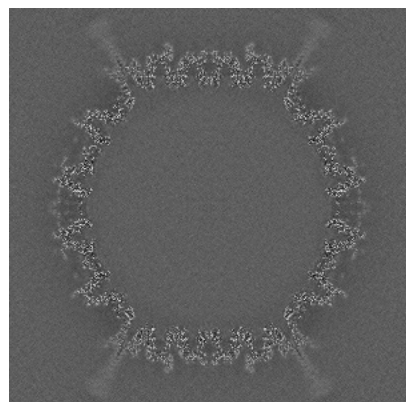


Z

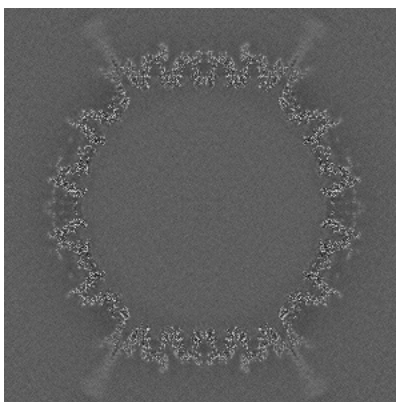
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

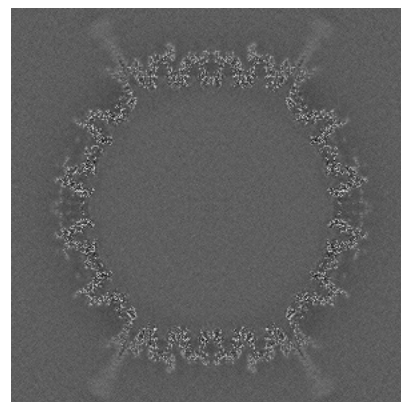
#### 6.2.1 Primary map



X Index: 416



Y Index: 416

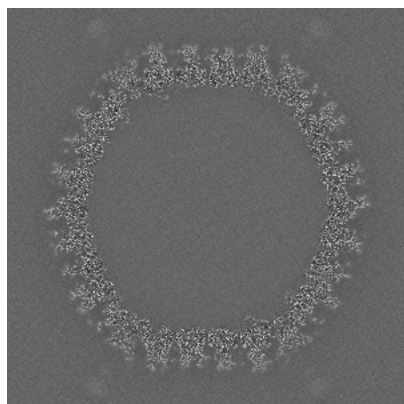


Z Index: 416

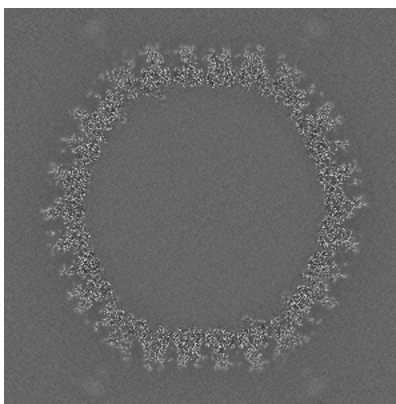
The images above show central slices of the map in three orthogonal directions.

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

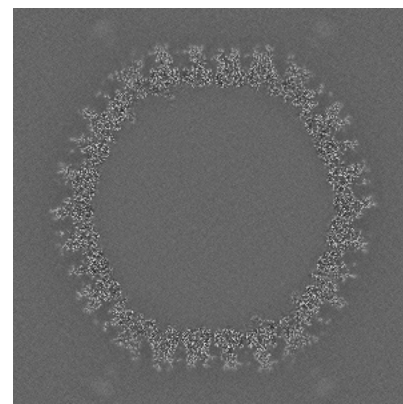
### 6.3.1 Primary map



X Index: 431



Y Index: 431



Z Index: 431

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

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

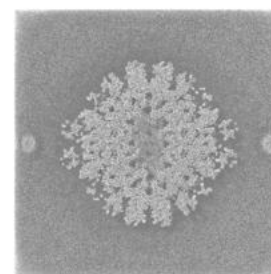
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

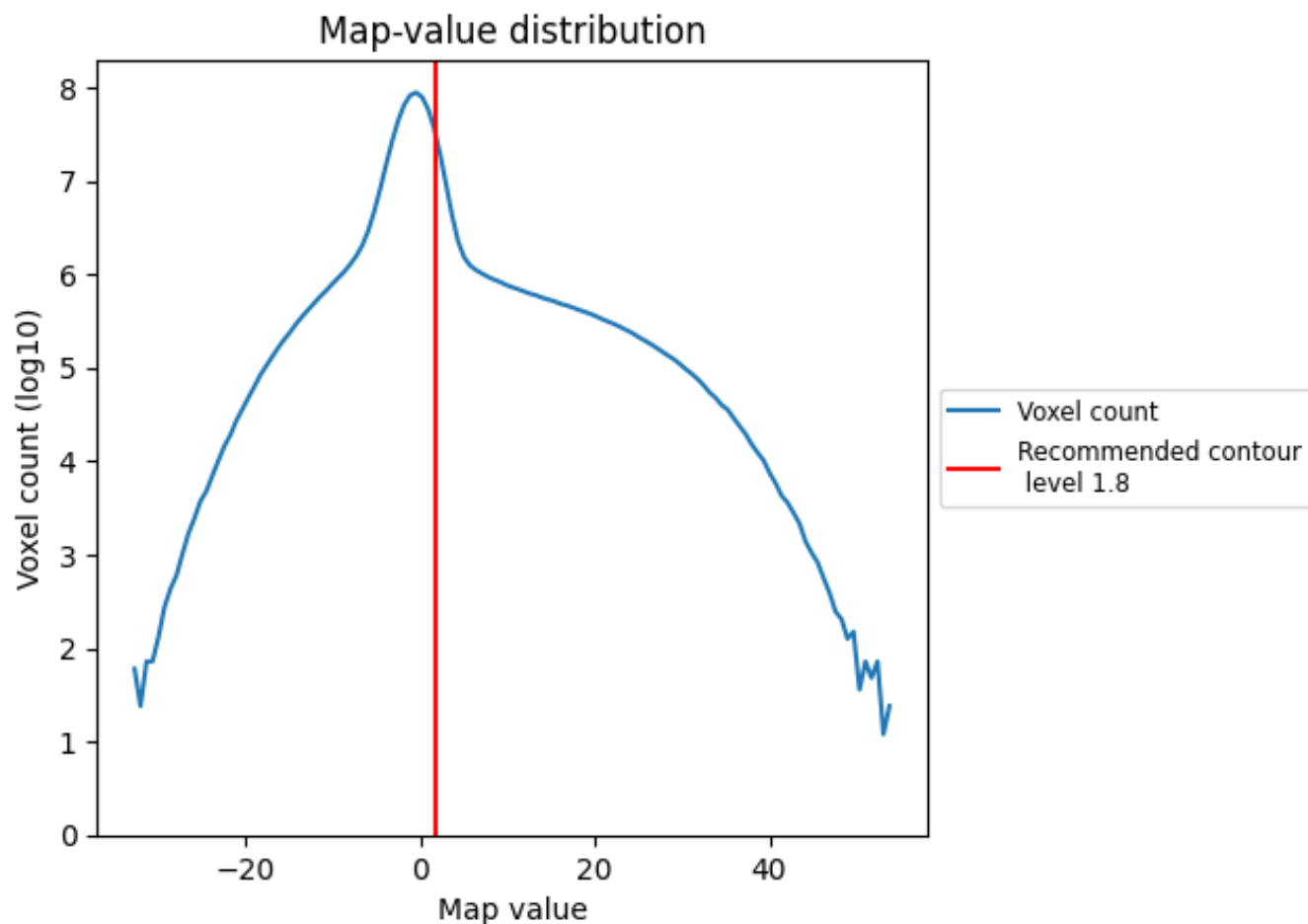
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

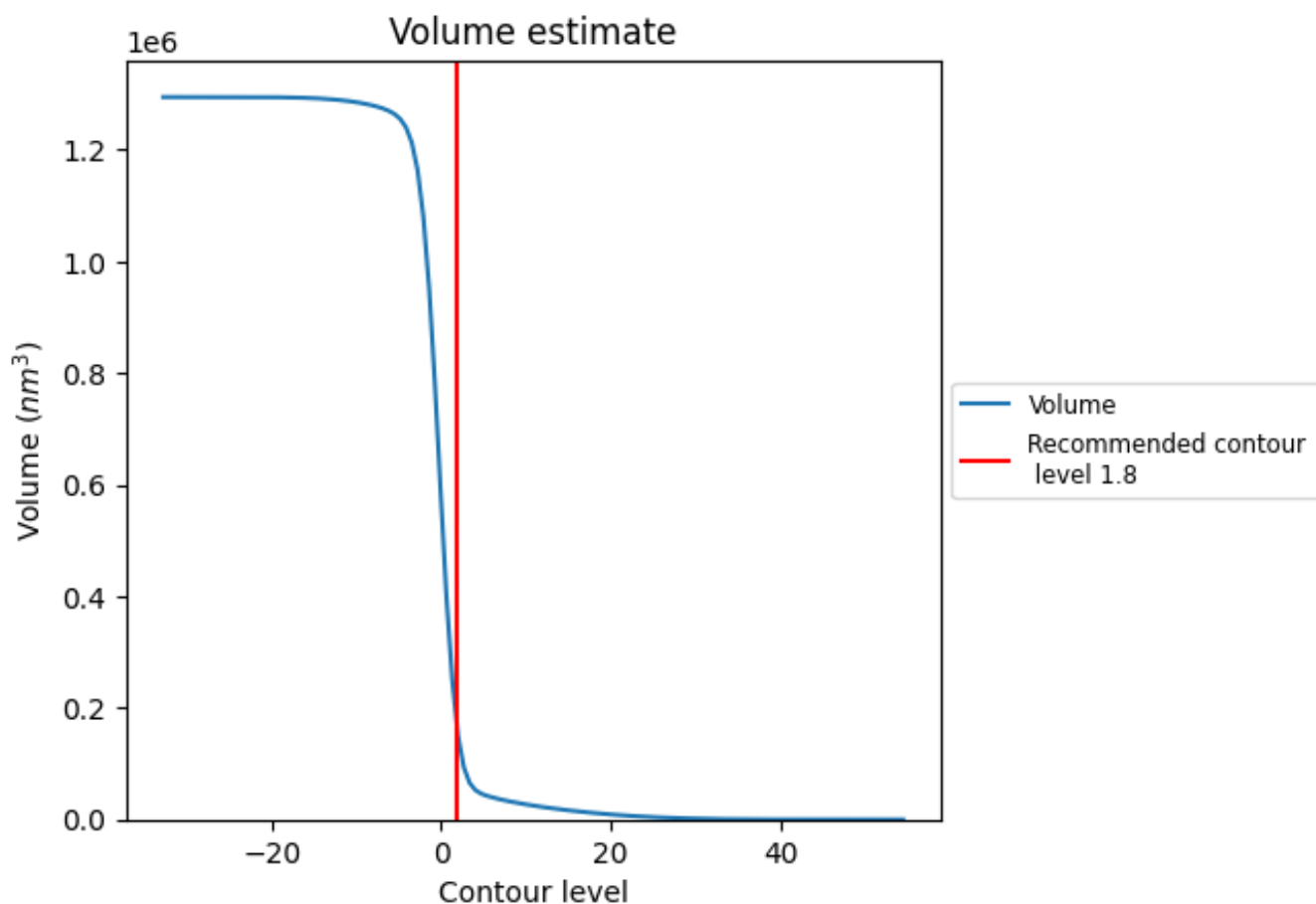
This section contains the results of statistical analysis of the map.

### 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.

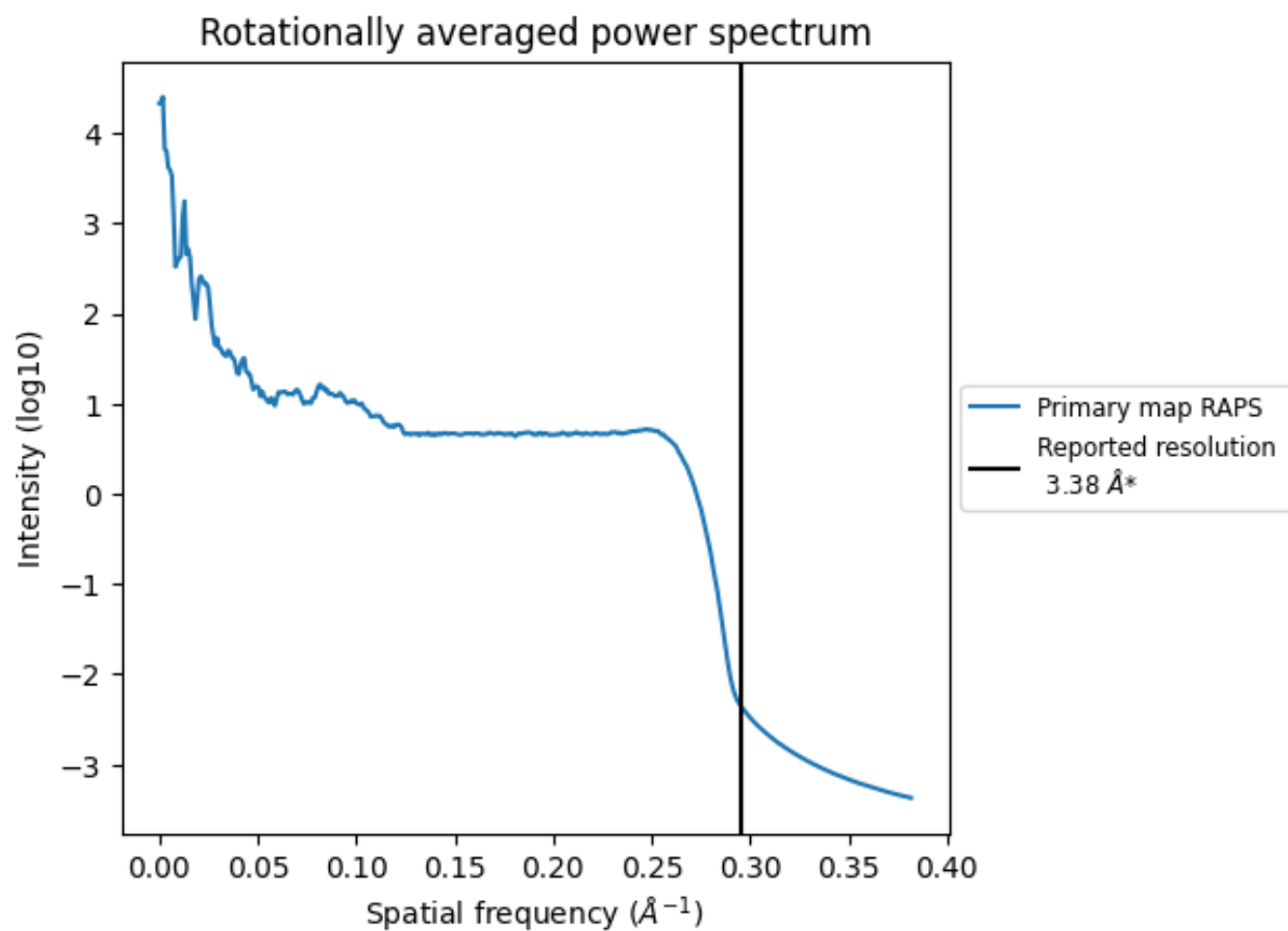
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 176024 nm<sup>3</sup>; this corresponds to an approximate mass of 159007 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 ⓘ

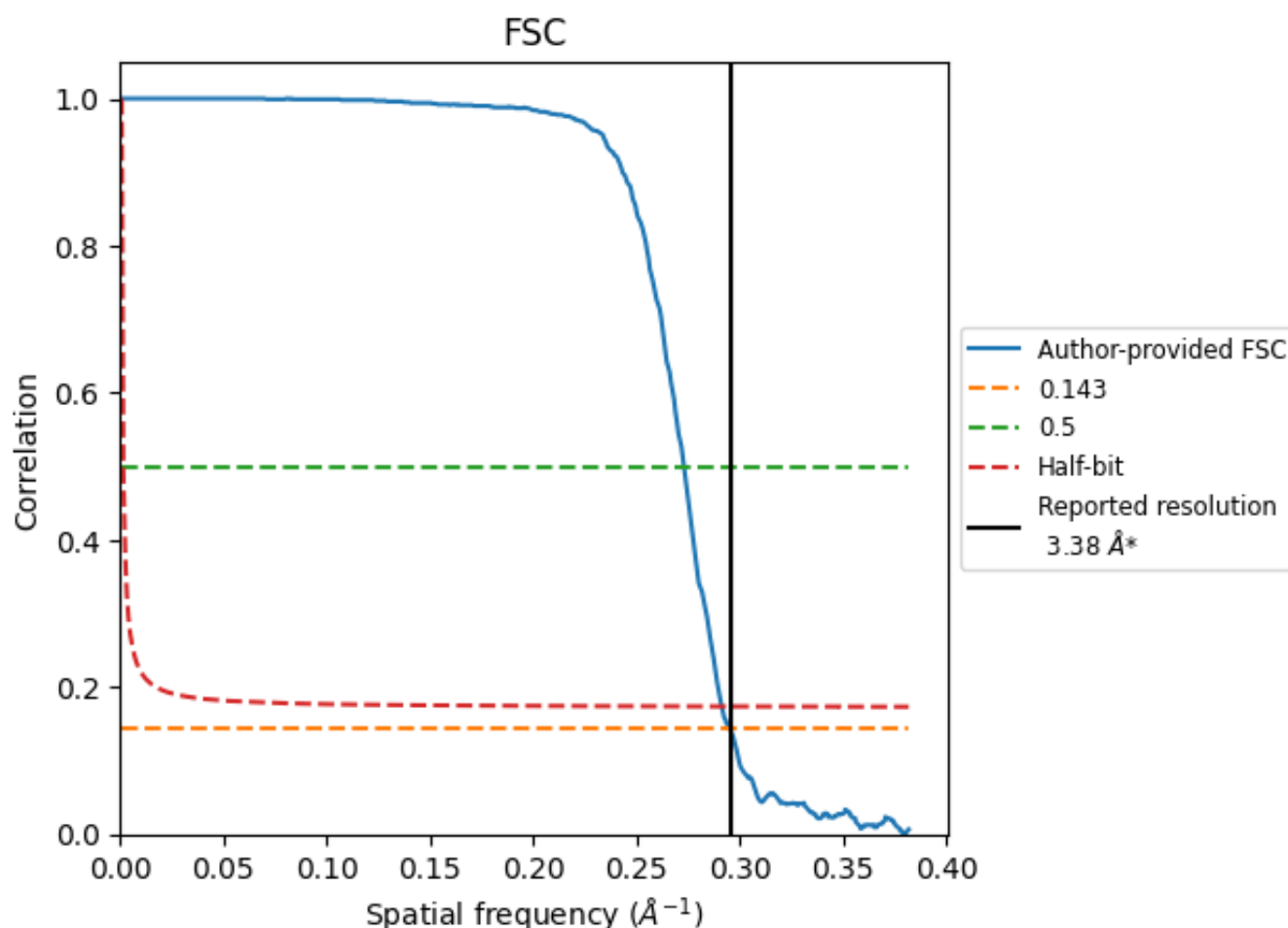


\*Reported resolution corresponds to spatial frequency of 0.296 Å<sup>-1</sup>

## 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 0.296  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.38	-	-
Author-provided FSC curve	3.39	3.66	3.43
Unmasked-calculated*	-	-	-

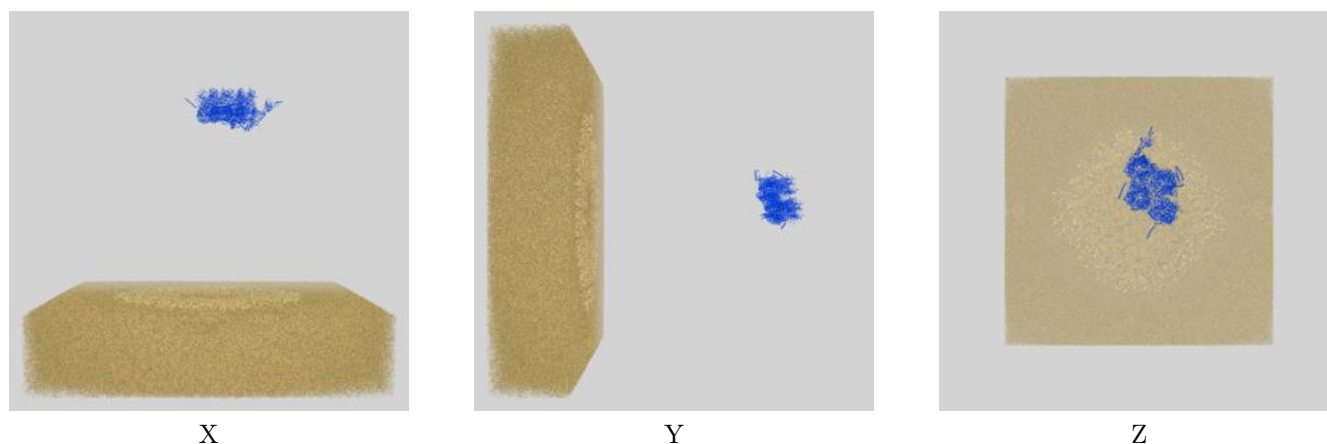
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

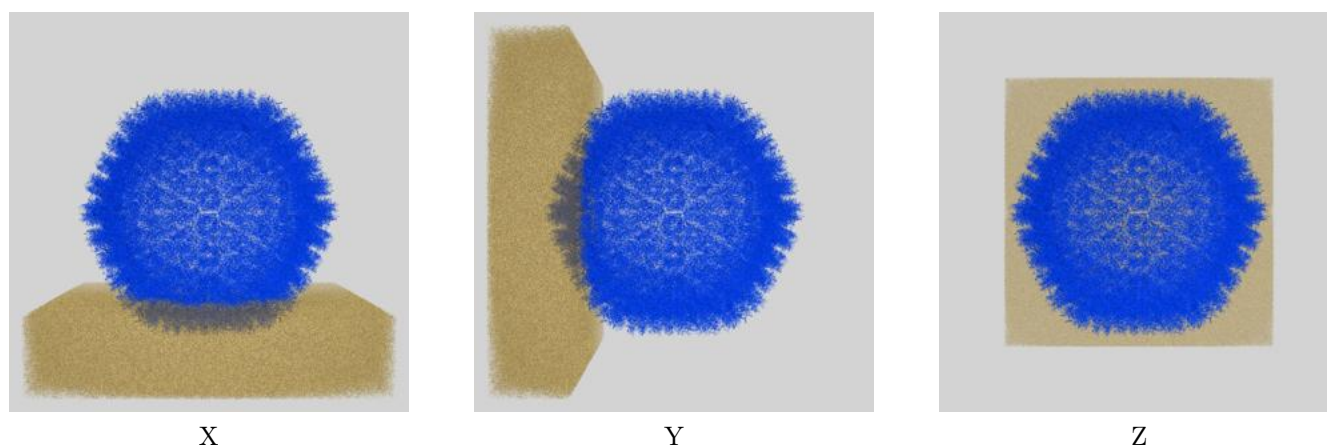
This section contains information regarding the fit between EMDB map EMD-25786 and PDB model 7TAU. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlays

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

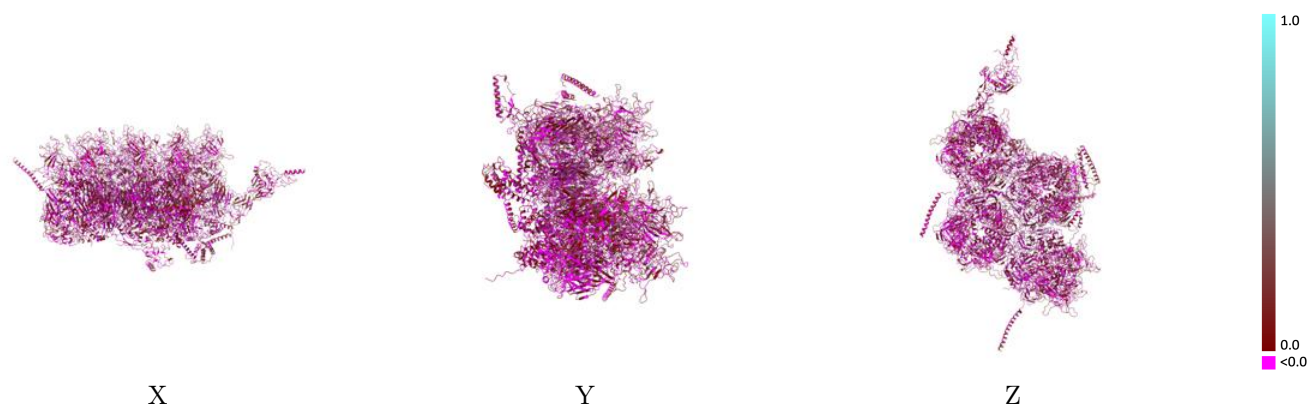


#### 9.1.2 Map-model assembly overlay [i](#)



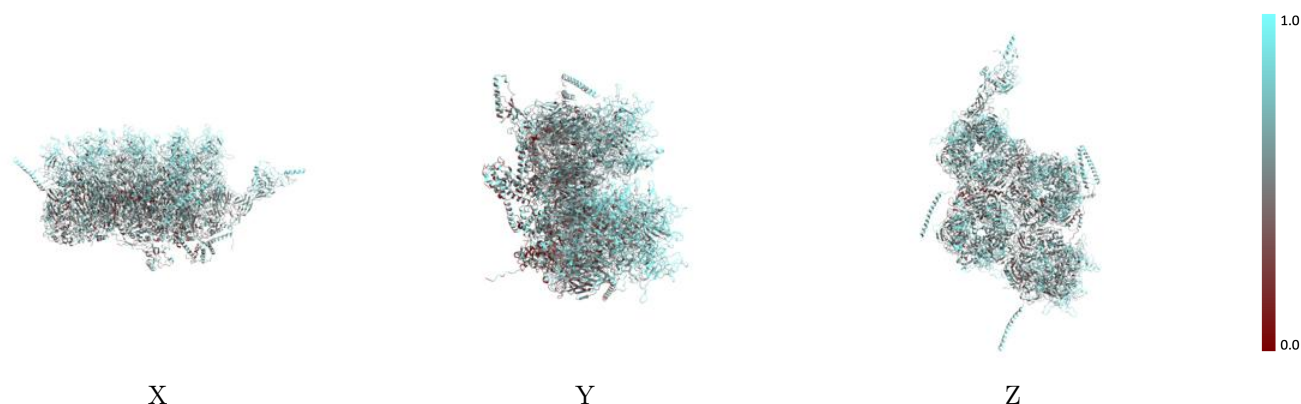
The images above show the 3D surface view of the map at the recommended contour level 1.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



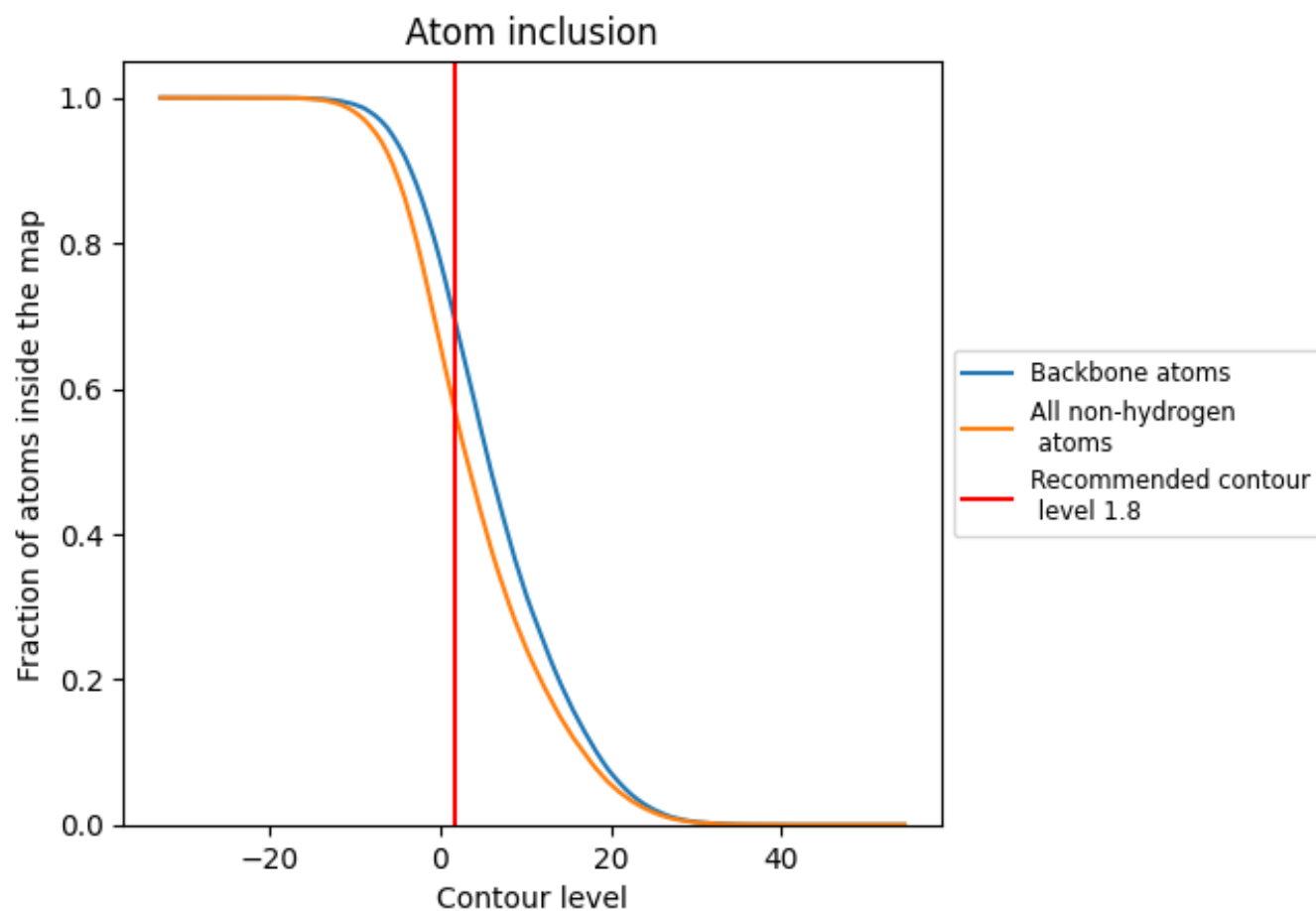
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.8).

































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 57% 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 (1.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5664	 0.0400
1	 0.4156	 0.0680
2	 0.5404	 0.0510
3	 0.3058	 0.0190
4	 0.4595	 0.0290
5	 0.4439	 0.1130
6	 0.2476	 -0.0080
7	 0.3107	 -0.0030
8	 0.4550	 0.0800
9	 0.2804	 0.0020
A	 0.5802	 0.0330
B	 0.6067	 0.0440
C	 0.6045	 0.0580
D	 0.5586	 0.0200
E	 0.5667	 0.0260
F	 0.5716	 0.0430
G	 0.5536	 0.0240
H	 0.5606	 0.0350
I	 0.5723	 0.0460
J	 0.5644	 0.0340
K	 0.5833	 0.0410
L	 0.5977	 0.0630
M	 0.4192	 0.0430
N	 0.6184	 0.0650
O	 0.6071	 0.0450
P	 0.4948	 0.0330
Q	 0.4981	 0.0410
R	 0.5909	 0.1010
S	 0.5316	 0.0800
U	 0.4884	 0.0120
V	 0.4936	 0.0190
X	 0.3600	 0.0470

