



wwPDB EM Validation Summary Report ⓘ

Mar 2, 2024 – 08:06 PM EST

PDB ID : 5TX1
EMDB ID : EMD-8471
Title : Cryo-Electron microscopy structure of species-D human adenovirus 26
Authors : Reddy, V.; Yu, X.; Veesler, D.
Deposited on : 2016-11-15
Resolution : 3.70 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

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.dev70
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

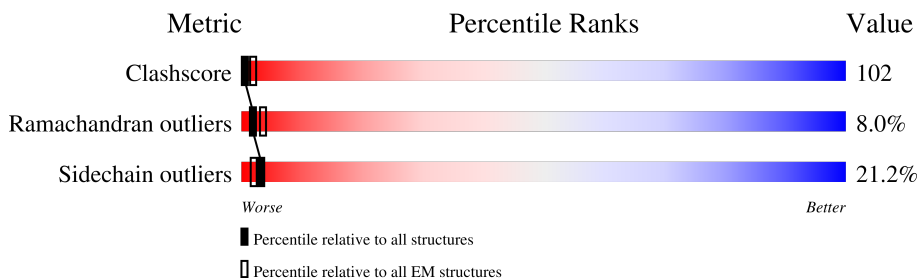
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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 ≥ 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	
1	B	952	
1	C	952	
1	D	952	
1	E	952	
1	F	952	
1	G	952	
1	H	952	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	952	5% 18% 55% 24% .
1	J	952	5% 20% 54% 23% .
1	K	952	. 18% 55% 24% .
1	L	952	5% 20% 55% 22% ..
2	N	497	12% 30% 52% 12% . 5%
3	O	19	84% 32% 58% 11%
4	M	388	57% 33% 51% 11% ..
5	P	134	37% 34% 43% 11% . 10%
5	Q	134	37% 29% 43% 15% . 10%
5	R	134	16% 33% 45% 16% 6%
5	S	134	30% 32% 43% 13% . 10%
6	U	227	. 21% 45% 11% . 21%
6	V	227	. 25% 43% 11% 21%
7	1	31	71% 39% 35% 19% 6%
7	2	31	6% 16% 39% 23% 10% 13%
7	3	31	68% 10% 29% 45% 16%
7	4	31	13% 10% 35% 32% 10% 13%
7	5	31	48% 19% 32% 32% 16%
7	6	31	81% 10% 48% 19% 10% 13%
7	7	31	68% 16% 39% 29% 16%
7	8	31	77% 35% 48% 13% .
7	9	31	74% 16% 39% 19% 10% 16%
8	X	10	80% 50% 50%
8	Y	10	90% 70% 30%
8	Z	10	50% 20% 40% 40%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 105738 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
			Total	C	N	O	S		
1	A	951	7551	4796	1276	1444	35	0	0
1	B	949	7536	4787	1274	1441	34	0	0
1	C	946	7519	4777	1271	1437	34	0	0
1	D	947	7526	4780	1272	1440	34	0	0
1	E	947	7526	4780	1272	1440	34	0	0
1	F	950	7544	4792	1275	1442	35	0	0
1	G	947	7526	4780	1272	1440	34	0	0
1	H	947	7526	4780	1272	1440	34	0	0
1	I	949	7536	4787	1274	1441	34	0	0
1	J	951	7551	4795	1276	1446	34	0	0
1	K	951	7551	4795	1276	1446	34	0	0
1	L	947	7524	4780	1272	1438	34	0	0

- Molecule 2 is a protein called Penton.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	N	473	3803	2416	643	730	14	0	0

- Molecule 3 is a protein called Fiber.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	O	19	Total	C	N	O	0	0
			162	105	27	30		

- Molecule 4 is a protein called PIIIa.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	376	Total	C	N	O	S	0	0
			2938	1832	530	567	9		

- Molecule 5 is a protein called PIX.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	120	Total	C	N	O	S	0	0
			871	535	155	177	4		
5	Q	120	Total	C	N	O	S	0	0
			875	538	155	178	4		
5	R	134	Total	C	N	O	S	0	0
			965	592	169	199	5		
5	S	121	Total	C	N	O	S	0	0
			881	542	156	180	3		

- Molecule 6 is a protein called PVIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	180	Total	C	N	O	S	0	0
			1391	876	239	270	6		
6	V	180	Total	C	N	O	S	0	0
			1391	876	239	270	6		

- Molecule 7 is a protein called PVI.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1	31	Total	C	N	O	S	0	0
			236	146	44	45	1		
7	2	27	Total	C	N	O	S	0	0
			211	132	39	39	1		
7	3	26	Total	C	N	O	S	0	0
			202	127	37	37	1		
7	4	27	Total	C	N	O	S	0	0
			211	132	39	39	1		
7	5	26	Total	C	N	O	S	0	0
			202	127	37	37	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	27	Total	C	N	O	S	0	0
			211	132	39	39	1		
7	7	26	Total	C	N	O	S	0	0
			202	127	37	37	1		
7	8	31	Total	C	N	O	S	0	0
			236	146	44	45	1		
7	9	26	Total	C	N	O	S	0	0
			202	127	37	37	1		

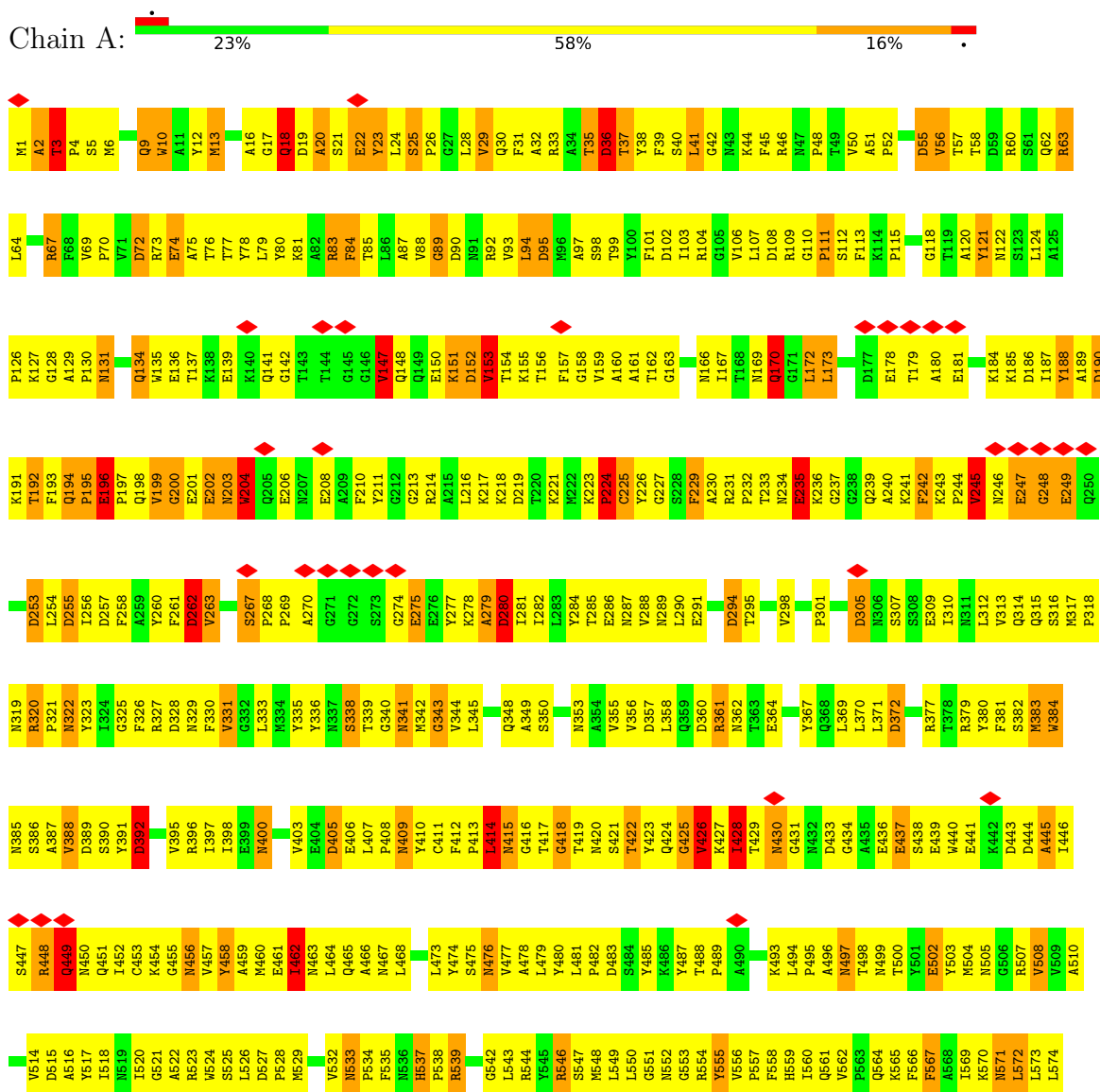
- Molecule 8 is a protein called Unknown.

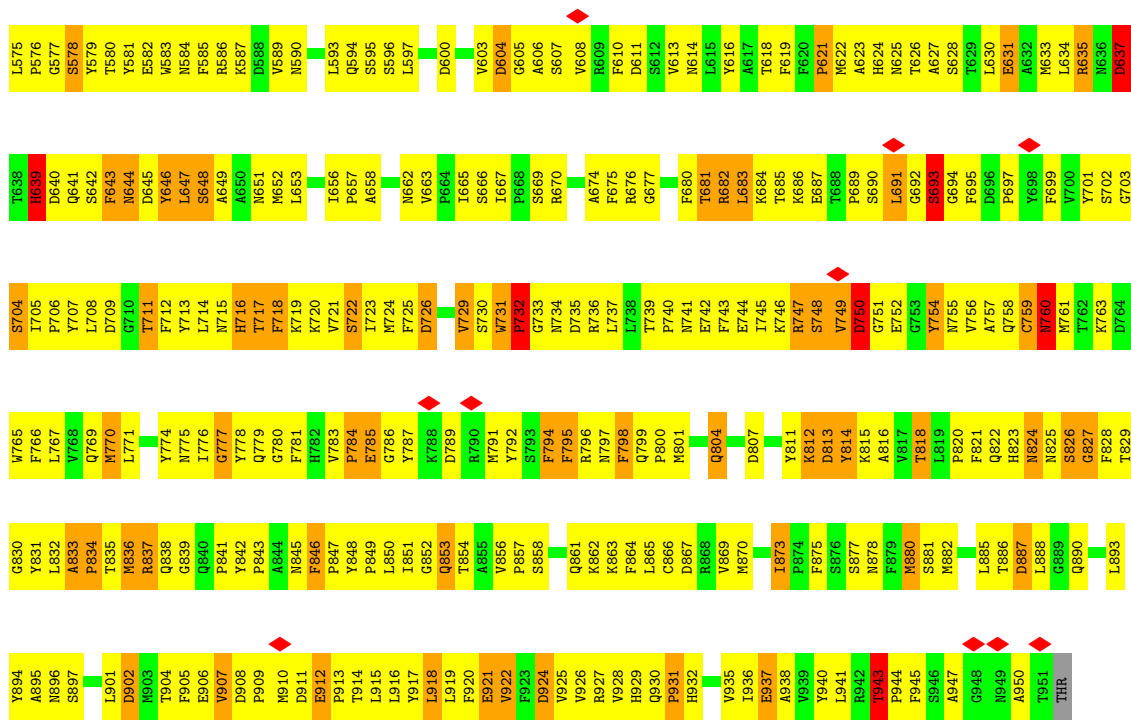
Mol	Chain	Residues	Atoms				AltConf	Trace
8	X	10	Total	C	N	O	0	0
			51	30	10	11		
8	Y	10	Total	C	N	O	0	0
			51	30	10	11		
8	Z	6	Total	C	N	O	0	0
			30	18	6	6		

3 Residue-property plots

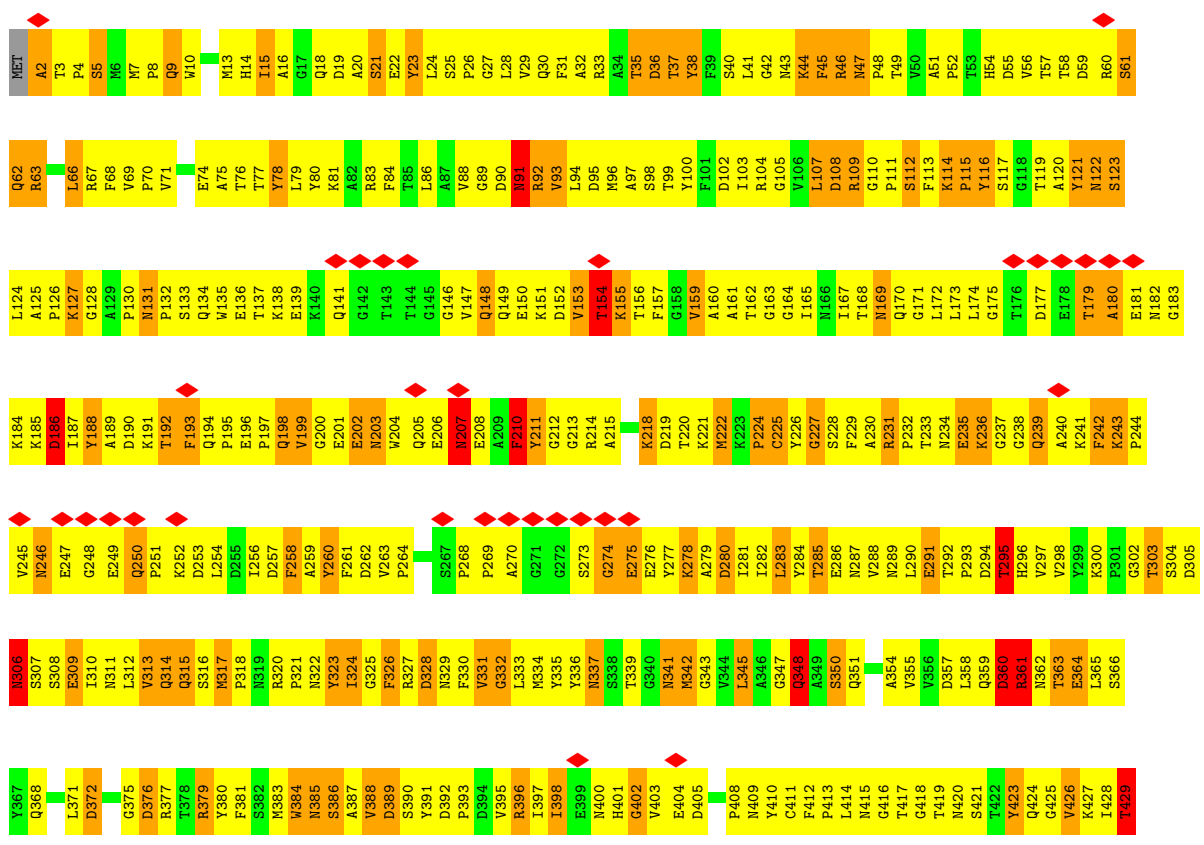
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

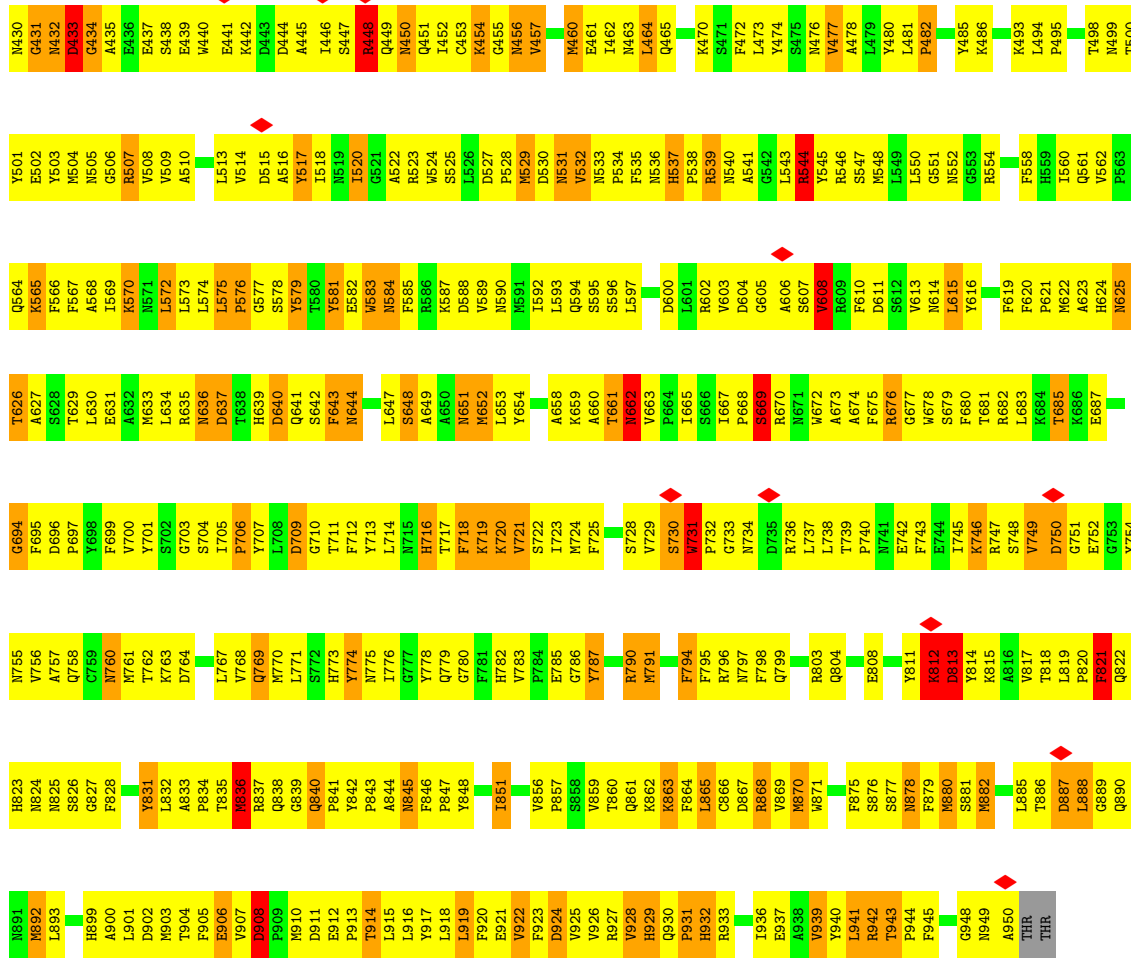
- Molecule 1: Hexon protein



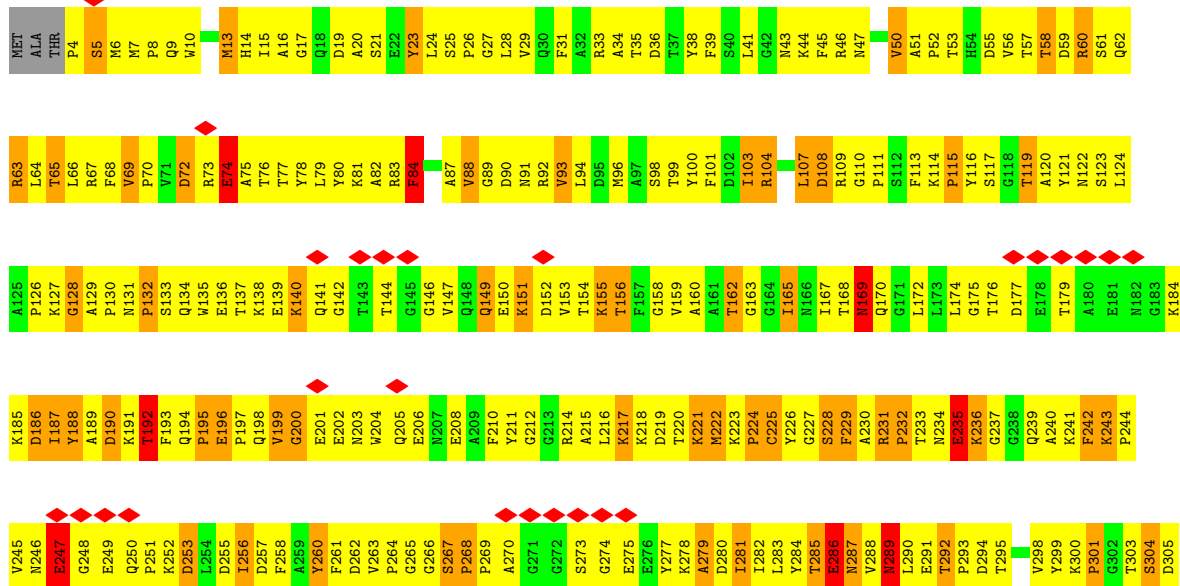
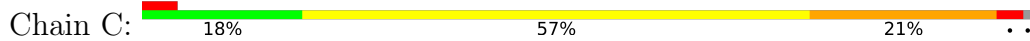


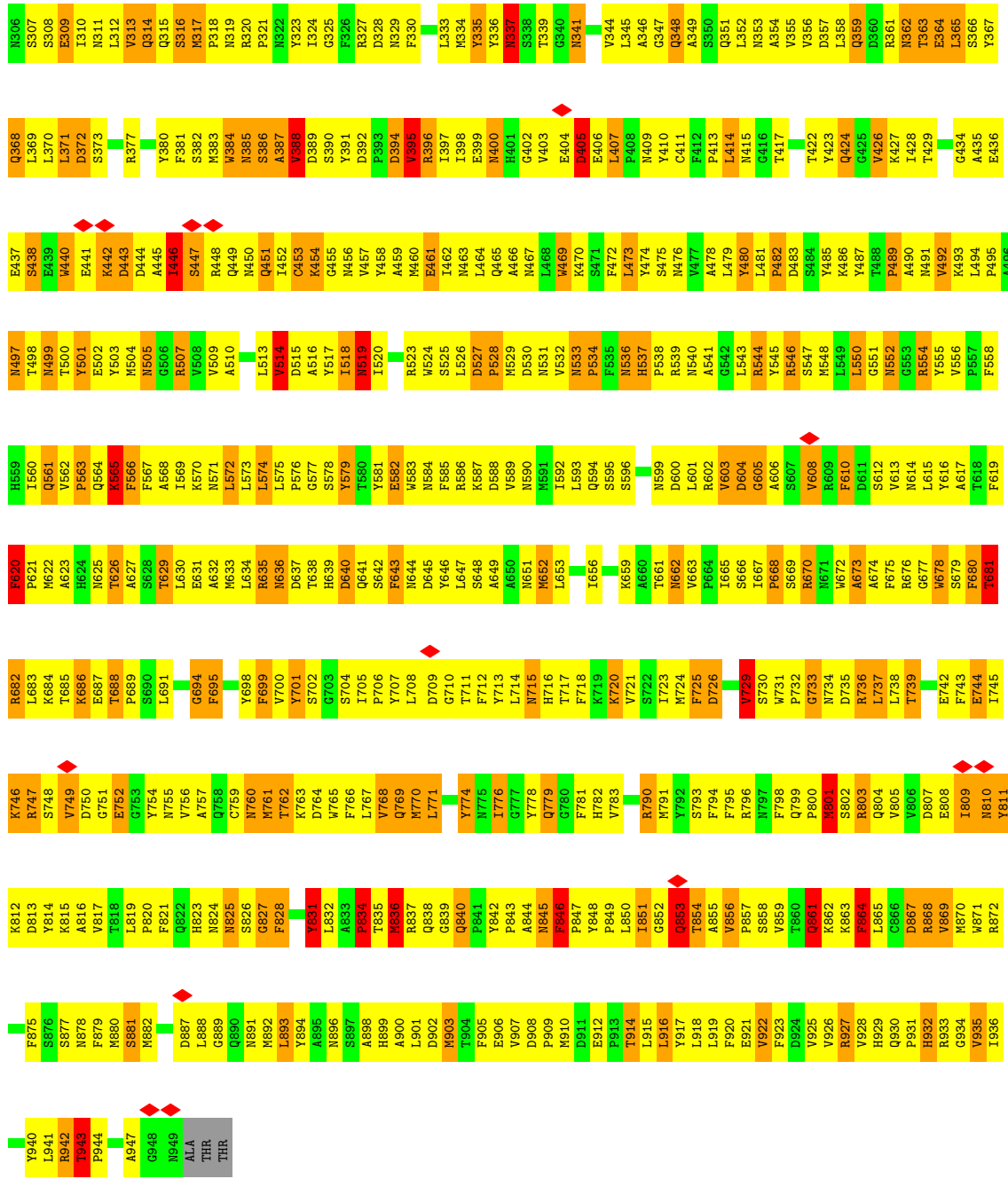
• Molecule 1: Hexon protein



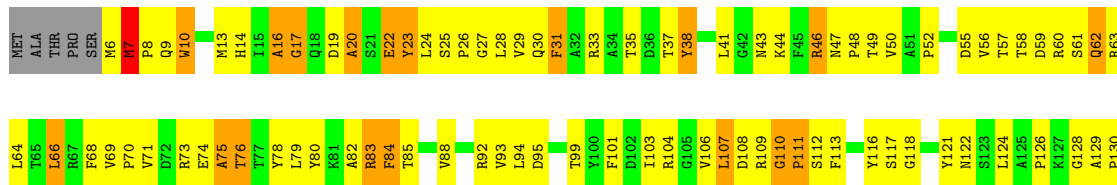
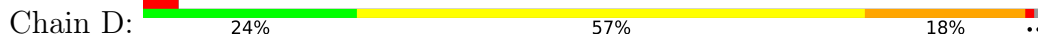


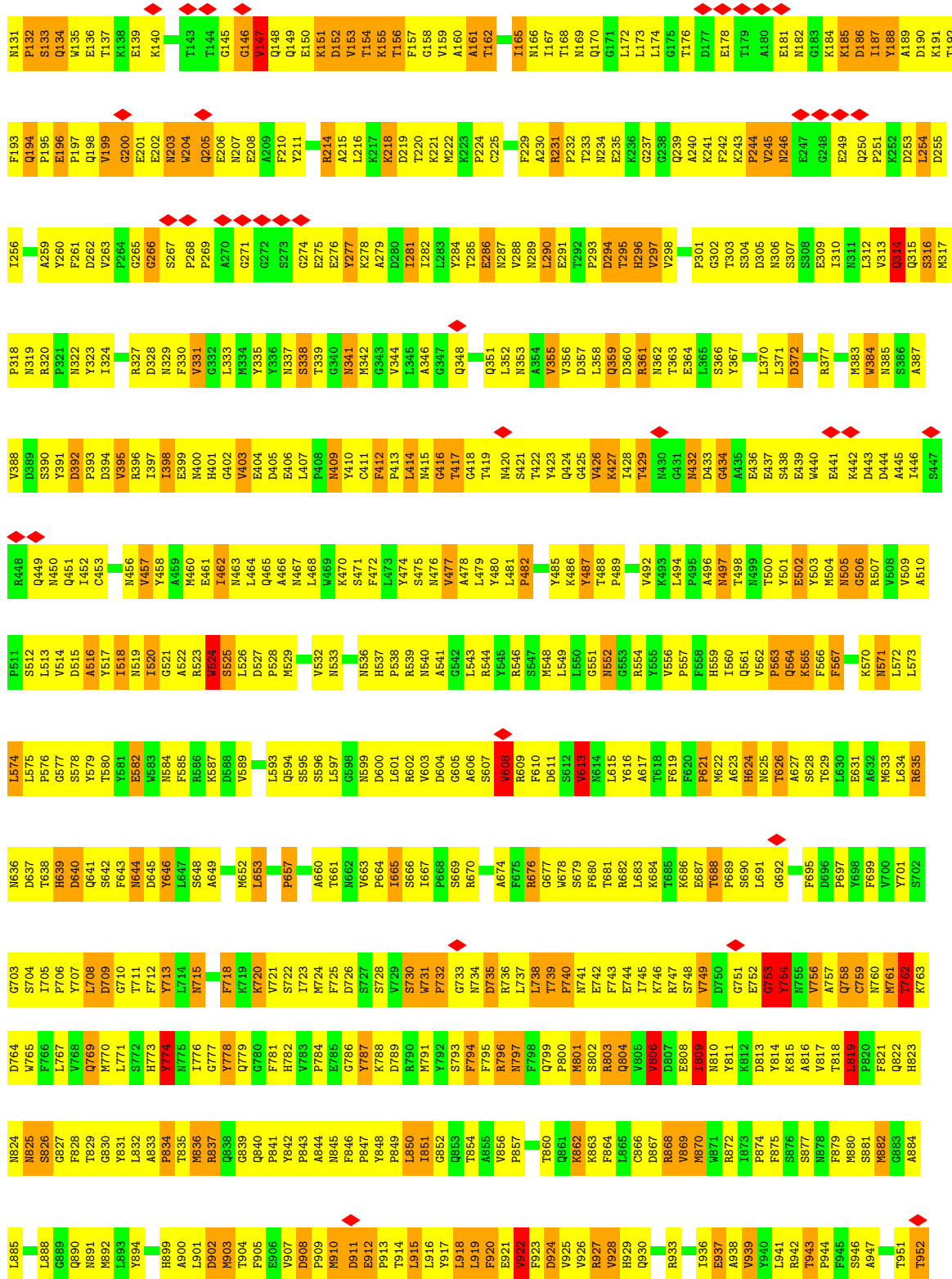
• Molecule 1: Hexon protein



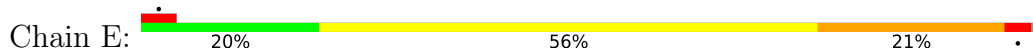


• Molecule 1: Hexon protein

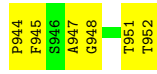




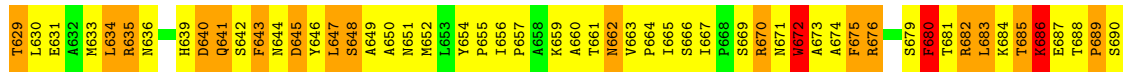
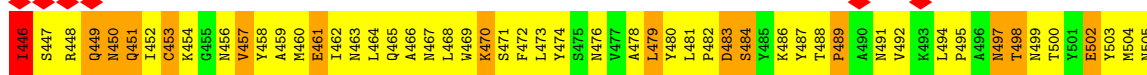
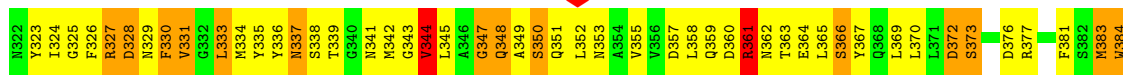
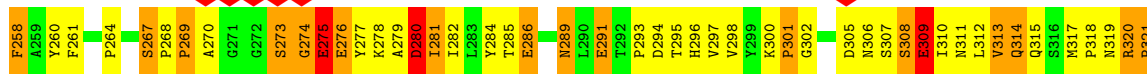
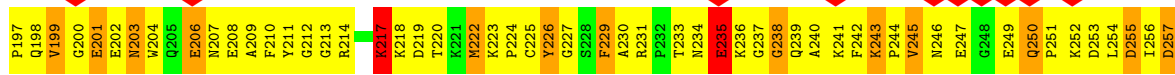
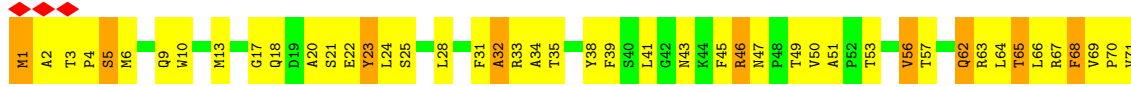
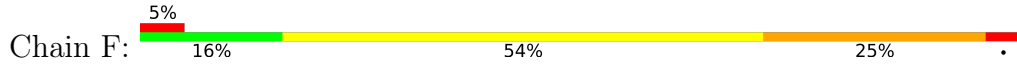
• Molecule 1: Hexon protein

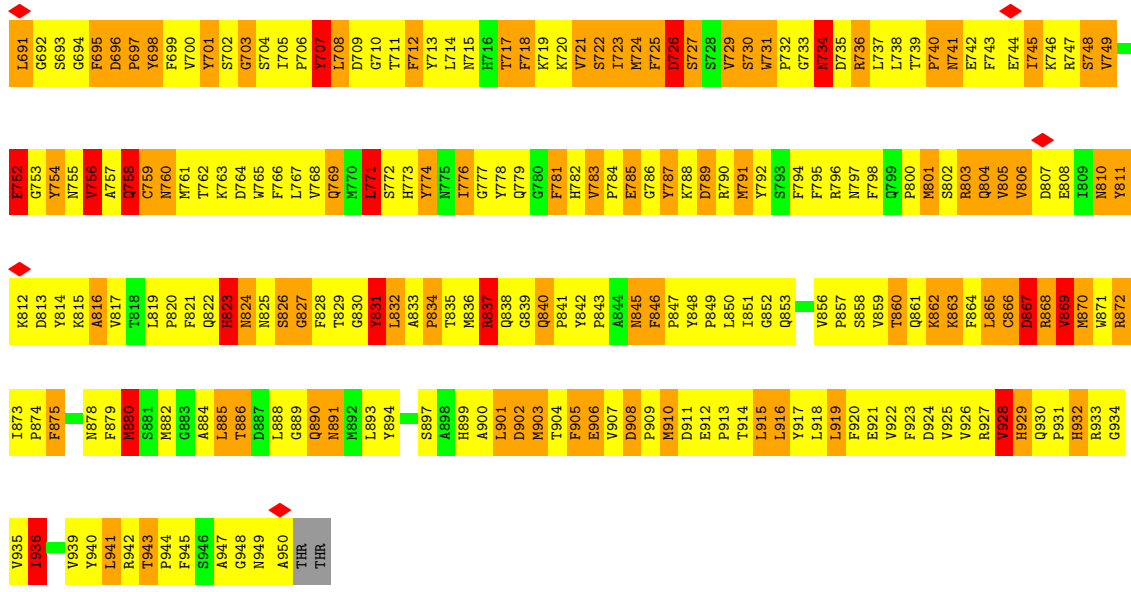


MET	ALA	THR	PRO	SER	M6	M7	P8	Q9	W10	A11	T12	M13	H14	I15	A16	G17	Q18	D19	A20	S21	E22	Y23	L24	S25	P26	G27	L28	V29	Q30	F31	A32	R33	A34	T35	D36	T37	Y38	F39	S40	L41	K44	F45	R46	M47	P48	T49	V50	A51	P52	T53	H54	D55	V56	T57	T58	A59	D60	S61																																																								
Q62	R63	L64	T65	L66	R67	F68	V69	P70	V71	S72	W73	E74	A75	T76	T77	Y78	L79	Y80	K81	A82	E83	F84	T85	L86	A87	V88	G89	D90	M91	R92	V93	L94	D95	M96	A97	S98	T99	Y100	F101	D102	L103	R104	L107	D108	R109	G110	P111	S112	F113	K114	P115	H116	D117	S118	E119	A120	D121	M122																																																								
S123	L124	A125	P126	A129	P130	M131	P132	S133	Q134	W135	E136	T137	K138	E139	T140	Q141	G142	Q205	T143	T144	V147	Q148	Q149	E150	K151	D152	V153	K155	T156	F157	G158	T162	G163	G164	I165	N166	I167	T168	M169	Q170	N234	E235	K236	G237	G238	Q239	A240	K241	F242	A180	E181	N182	G183	K184	K185	D186																																																										
G248	E249	Q250	D253	L254	D255	L256	D257	F258	A259	A260	Y261	F262	V263	P264	G265	G266	S267	P268	P269	A270	G271	G272	S273	G274	E275	E276	Y277	K278	A279	D280	L281	I282	L283	L284	L285	N286	E287	E288	N289	L290	F229	A230	T233	N234	E235	G238	Q239	A240	K241	F242	A180	E181	N182	G183	K184	K185	D186																																																									
E309	T310	N311	L312	V313	Q314	Q315	S316	R317	P318	N319	S320	N321	Y322	Y323	L324	R327	Q328	K329	F330	V331	G332	K333	Y335	Y336	N337	S338	T339	G340	N341	N342	G343	V344	L345	A346	G347	Q348	A349	S350	Q351	L352	N353	A354	V355	V356	D357	T358	Y359	N360	P361	E362	L363	L364	S365	Y366	Q367	D368	N369	L370	S371	L372	G373	Q374	D375	R376	R377	Y378	Y379	Y380	S381	S382	K383	N384	N385	S386	A387	V388	D392	V395	R396	L397	E399	N400	H401	G402	V403	E404	D405	E406	L407	P408	M409	Y410	C411	F412	N415	G416	T417	G418	N420	S421	T422	Y423	Q424	C425	V426	K427	L428	T429	N430	T498	M499	T500	E501	S502
L370	S373	L374	G375	Q376	R377	T378	Y379	Y380	S381	S382	K383	N384	N385	S386	A387	V388	D392	V395	R396	L397	E399	N400	H401	G402	V403	E404	D405	E406	L407	P408	M409	Y410	C411	F412	N415	G416	T417	G418	N420	S421	T422	Y423	Q424	C425	V426	K427	L428	T429	N430	T498	M499	T500	E501	S502																																																												
E439	W440	E441	K442	D443	D444	A445	L446	S447	R448	Q449	Q450	Q451	L452	C453	K454	C455	N456	V457	Y458	A459	N460	D461	L462	N463	Q465	A466	N467	K470	S471	F472	L473	Y474	S475	N476	V477	A478	L479	A480	D483	S484	Y485	K486	Y487	T488	P489	V492	K493	K494	P495	T498	M499	T500	E501	S502																																																												
Y503	M504	G506	R507	V508	Y509	A510	P511	S512	L513	V514	D515	A516	Y517	Y518	Y581	E582	V583	N584	F585	R586	K587	D588	Y589	H590	H591	L592	L593	Q594	S595	S596	L597	G598	N599	D600	L601	R602	V603	D604	G605	A606	S607	B608	R609	F610	V613	N614	L615	V616	A617	T618	F619	F620	L683	P621	A622	A623	N625	O626	K565																																																							
F566	F567	A568	L569	K570	N571	L572	L573	L574	L575	P576	G577	S578	Y579	Y580	Y581	E582	V583	N584	F585	R586	K587	D588	Y589	H590	H591	L592	L593	Q594	S595	S596	L597	G598	N599	D600	L601	R602	V603	D604	G605	A606	S607	B608	R609	F610	V613	N614	L615	V616	A617	T618	F619	F620	L683	P621	A622	A623	N625	O626	K565																																																							
A627	S628	T629	L630	E631	A632	M633	L634	R635	N636	D637	T638	H639	S640	Q641	S642	F643	N644	D645	V646	L647	S648	A649	A650	N651	H652	L653	P657	A658	K659	A660	T661	N662	V663	P664	L665	S666	L667	F668	G669	R670	N671	M672	N673	A674	F675	R676	G677	M678	S679	F680	T681	T682	L683	P621	A622	A623	N625	O626	K565																																																							
S690	L691	G692	R695	D696	F699	S702	T705	P706	L708	D709	G710	T711	F712	Y713	L714	N715	H716	T717	K719	K720	W721	S722	W723	Y724	R725	G726	S727	S728	W729	S730	W731	P732	G733	N734	D735	R736	L737	L738	T739	F740	N741	E742	F743	G744	E745	H746	R747	S748	Y749	D750	G753	Y754																																																														
N755	V756	A757	Q758	C759	N760	M761	T762	K763	D764	W765	F766	L767	M770	L771	S772	R773	T774	N775	Q776	C777	G778	H779	Y780	F781	H782	W783	F784	E785	G786	Y787	K788	D789	R790	M791	Y792	S793	F794	F795	R796	N797	F798	R799	S800	R803	O804	N805	C806	D807	E808	I809	N810	R811	K812	H813	D814	K815	A816																																																									
N816	L817	Q818	C819	T820	H821	H822	H823	N824	N825	S826	G827	F828	H831	L832	A833	P834	T835	M836	R837	Q838	C839	G840	H841	Y842	F843	A844	N845	F846	Y848	R849	L850	H851	G852	Q853	T854	H855	V856	P857	S858	H859	T860	Q861	K862	K863	F864	L865	D866	R867	H868	H869	M870	H871	R872	L873	H874	F875	N876																																																									

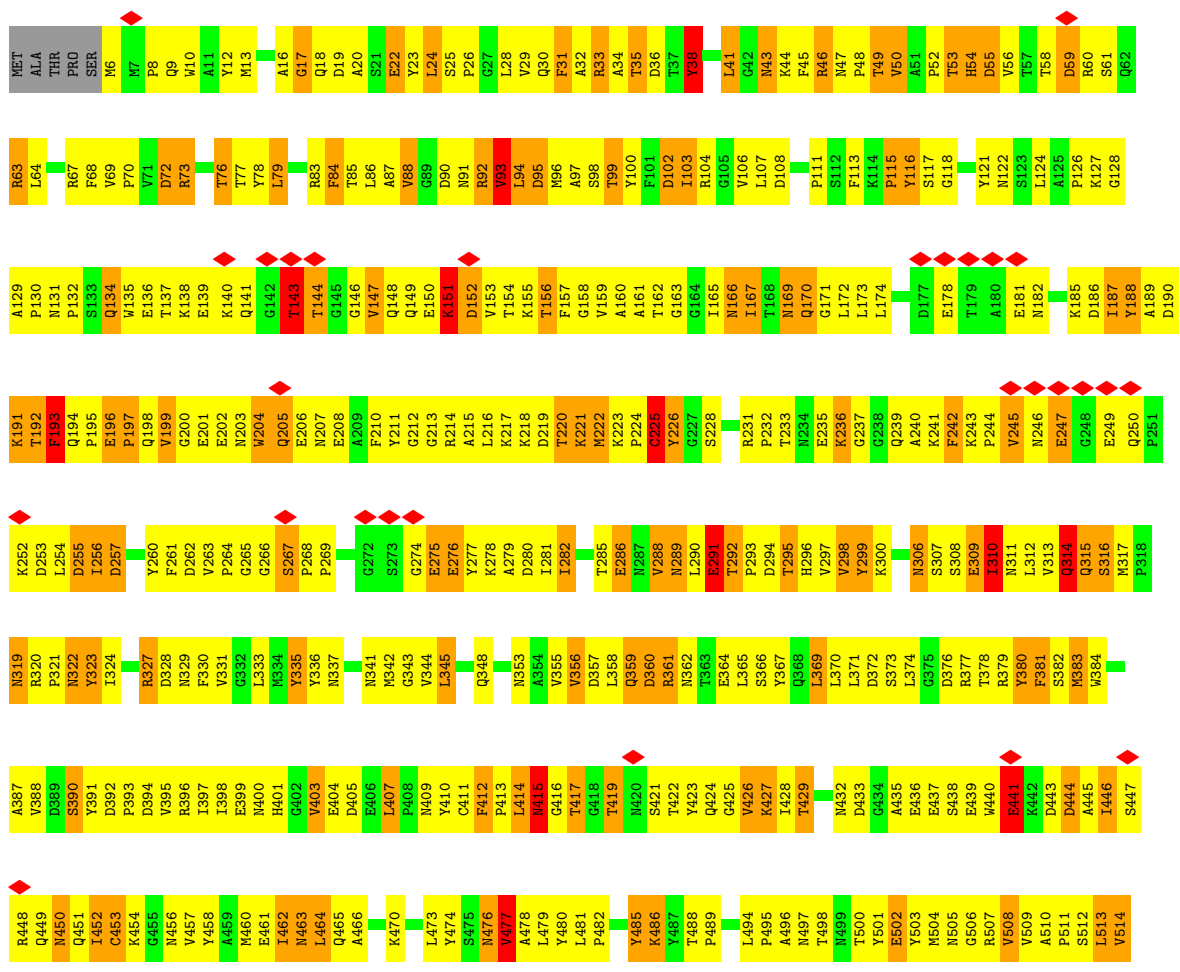


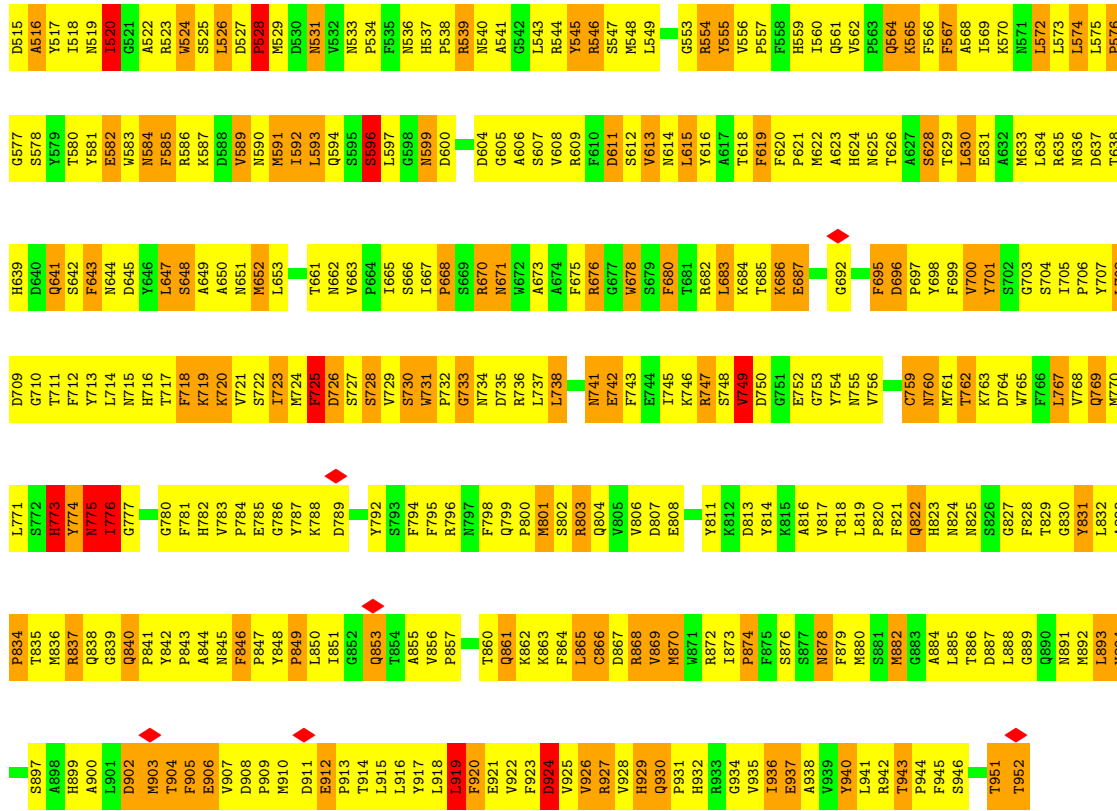
● Molecule 1: Hexon protein



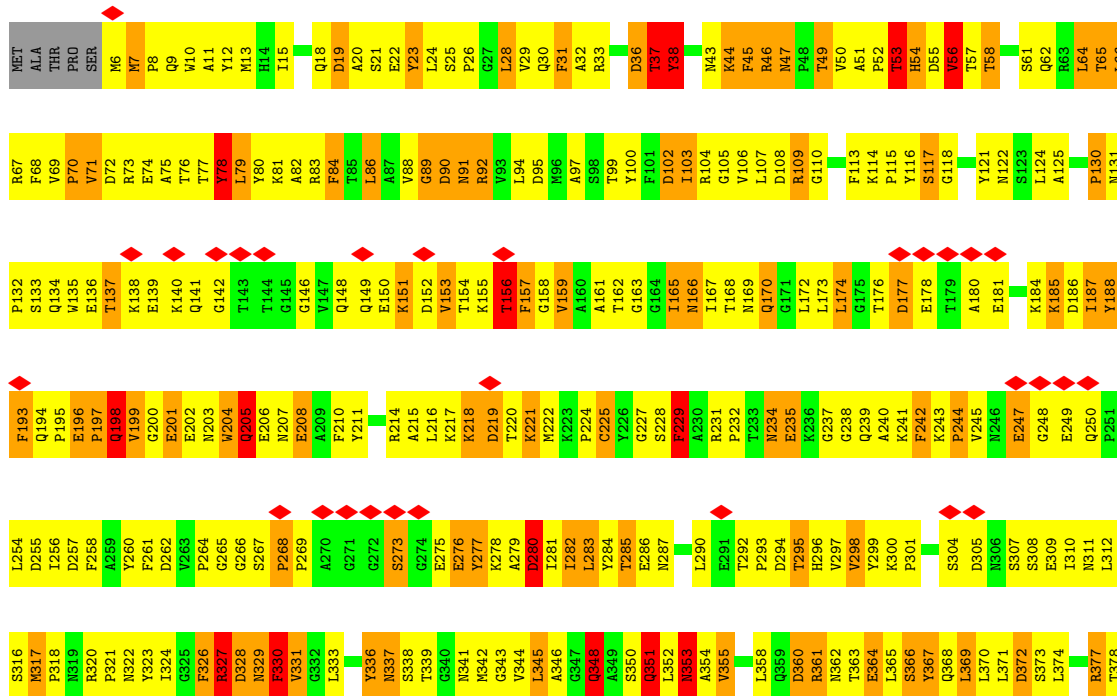
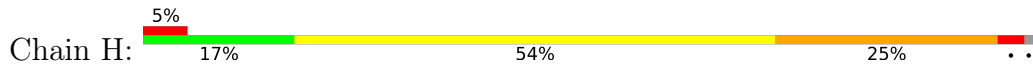


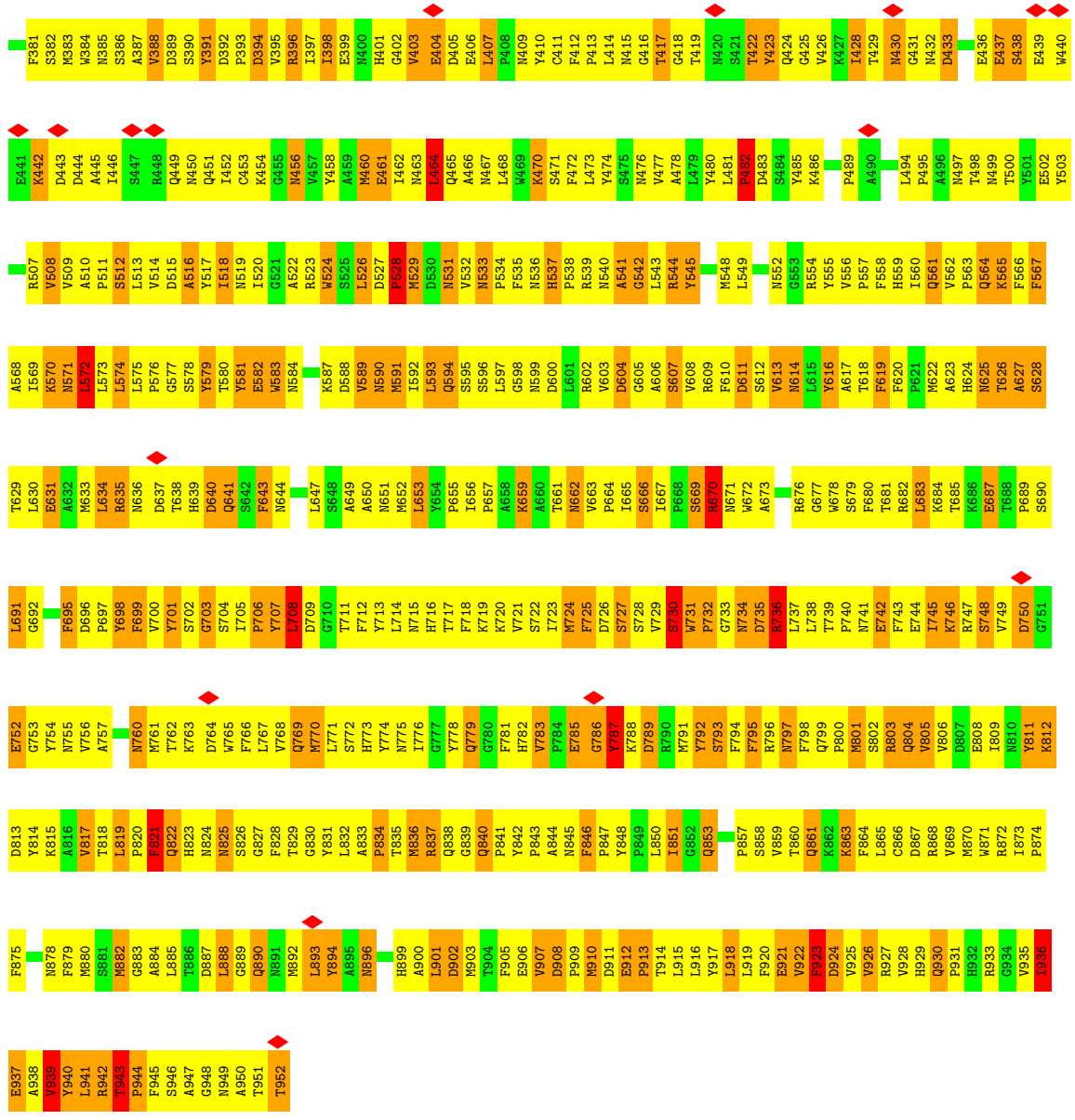
• Molecule 1: Hexon protein



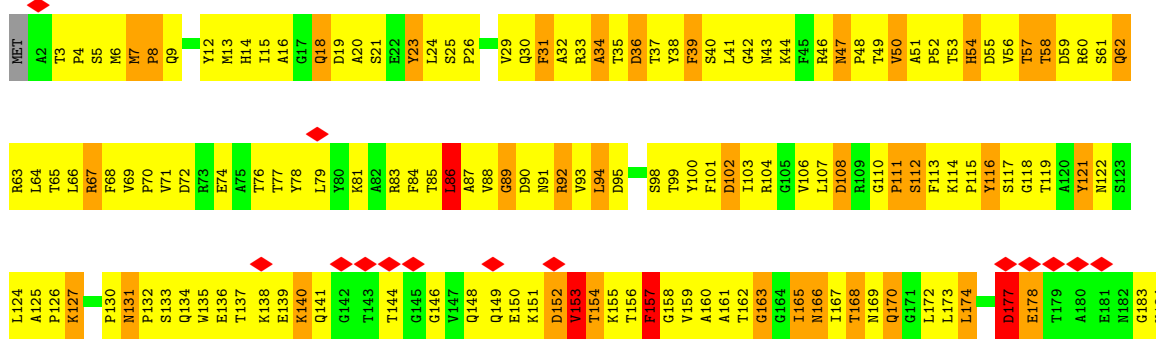
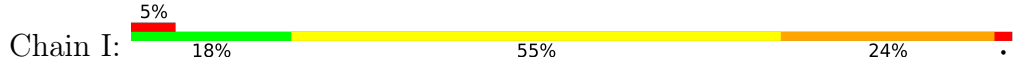


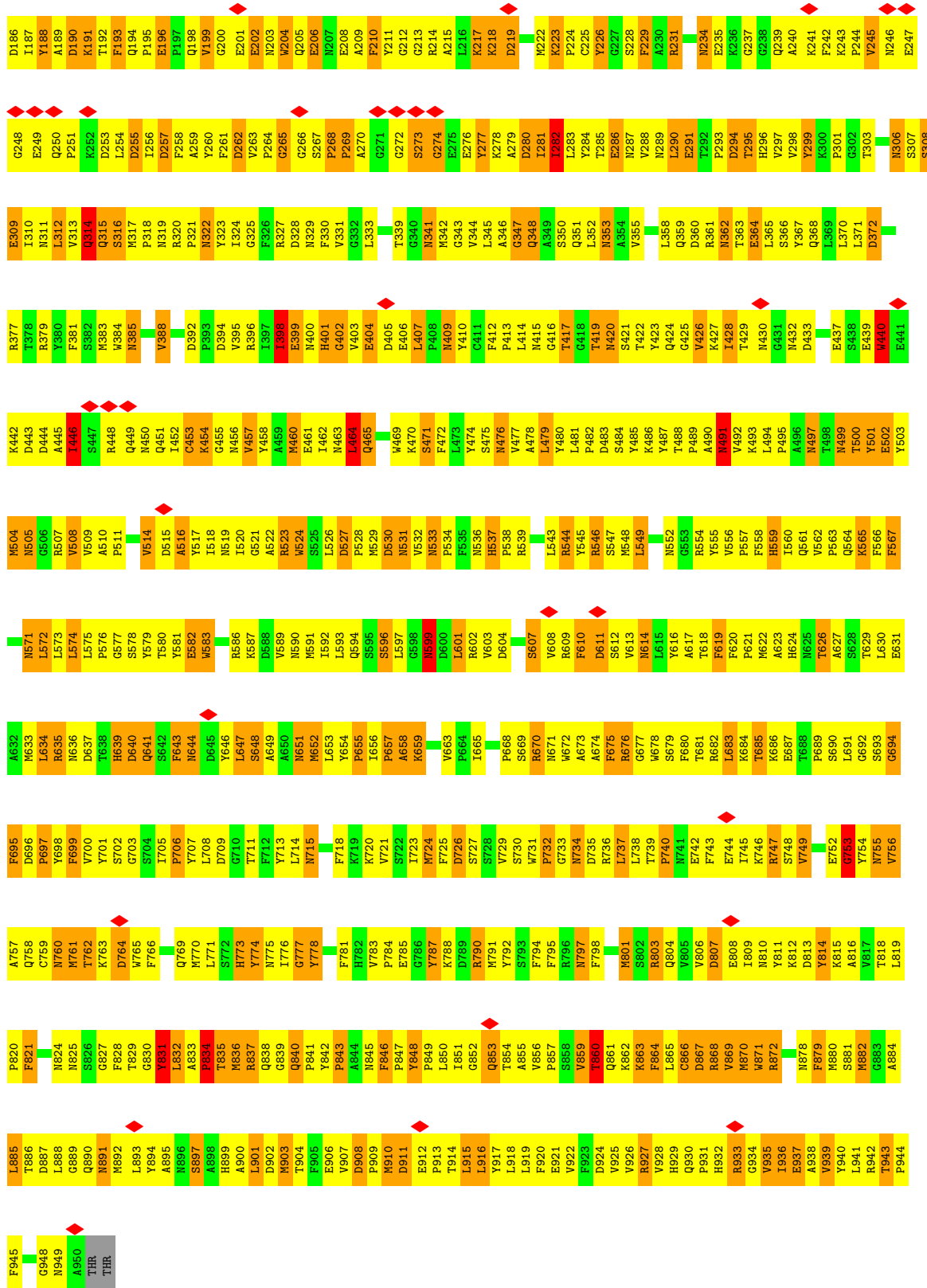
• Molecule 1: Hexon protein



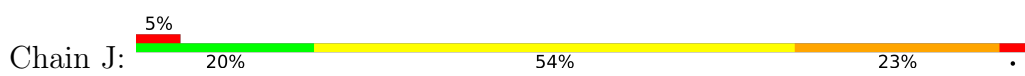


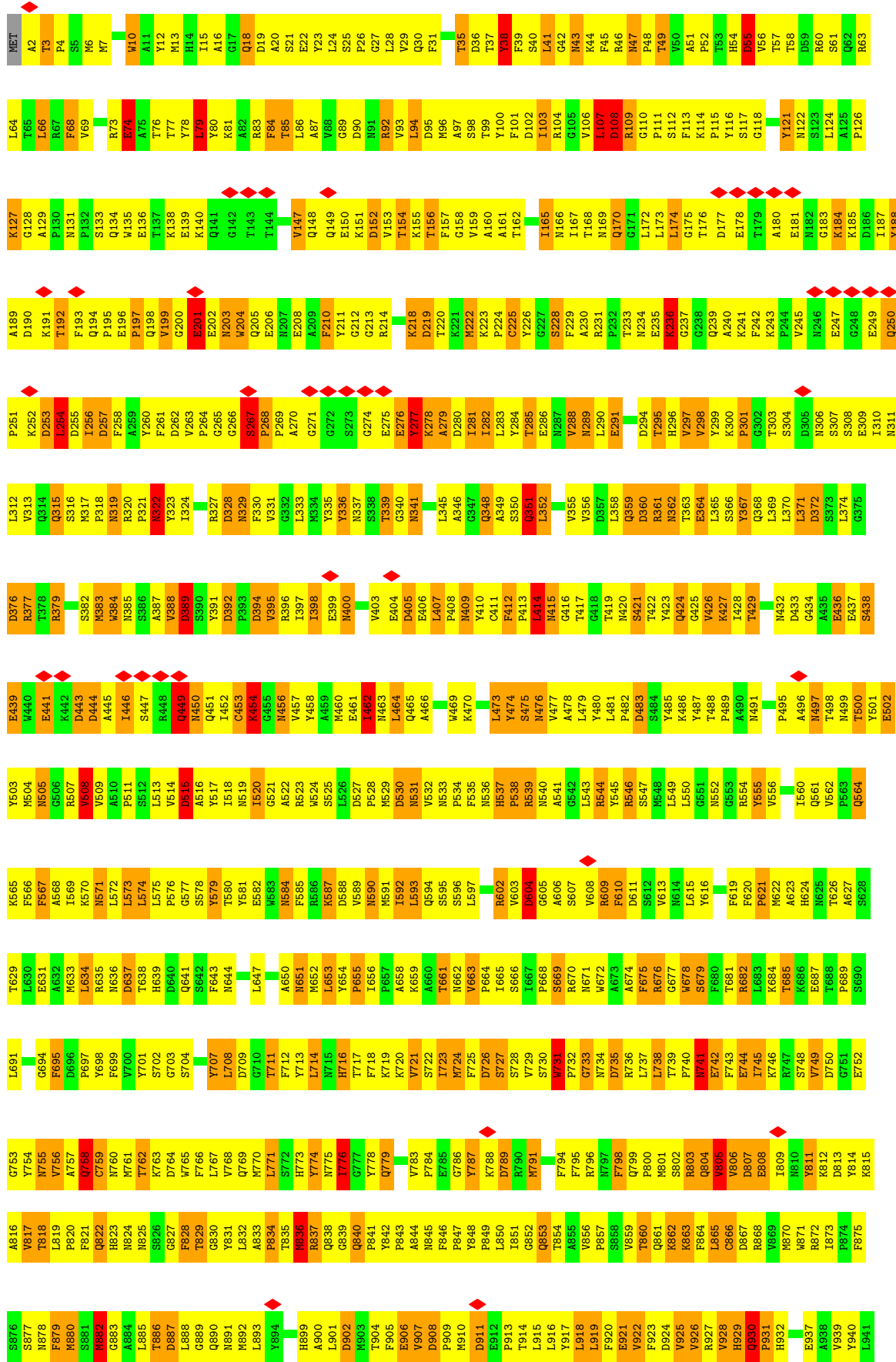
• Molecule 1: Hexon protein

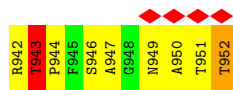




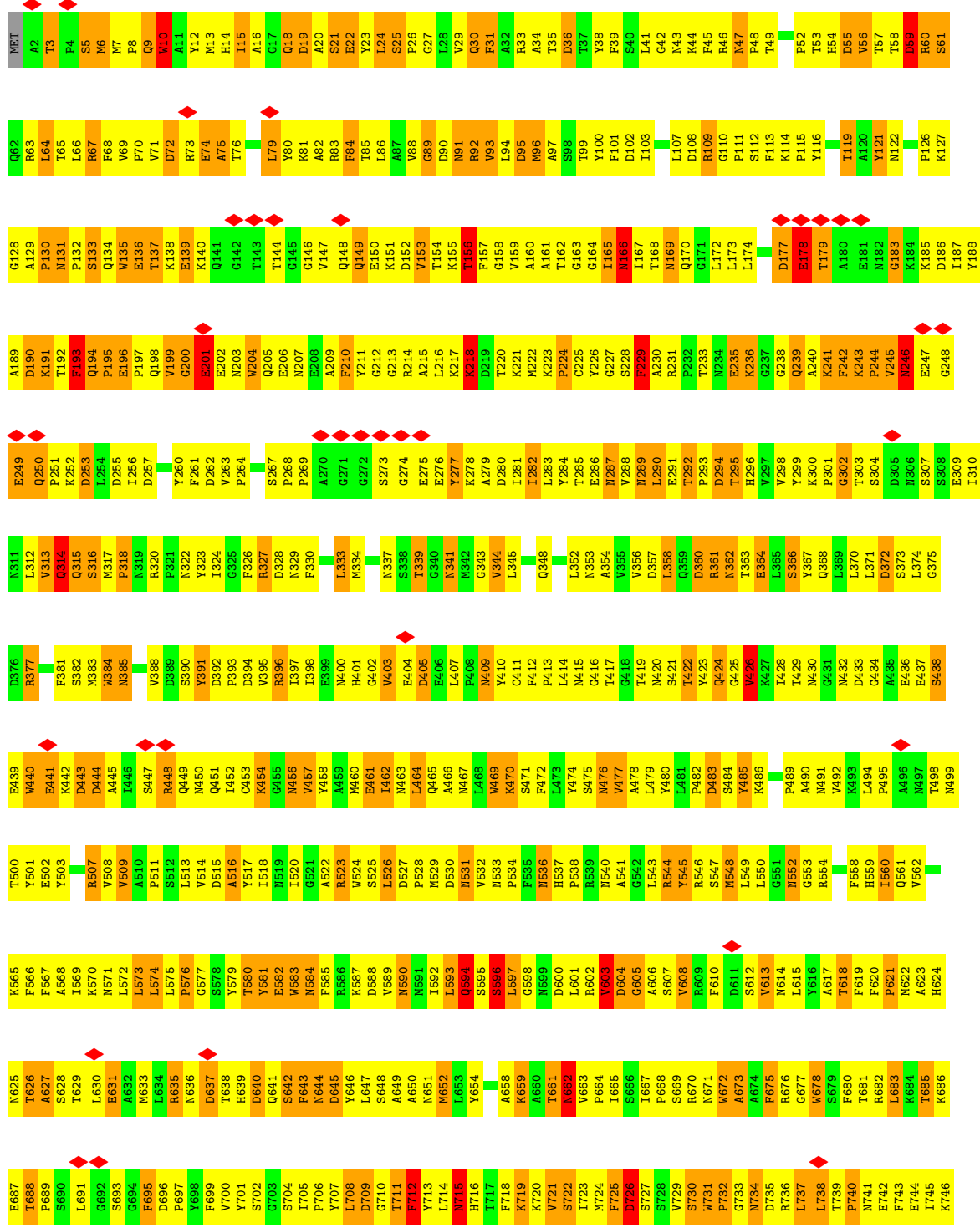
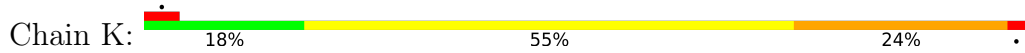
• Molecule 1: Hexon protein

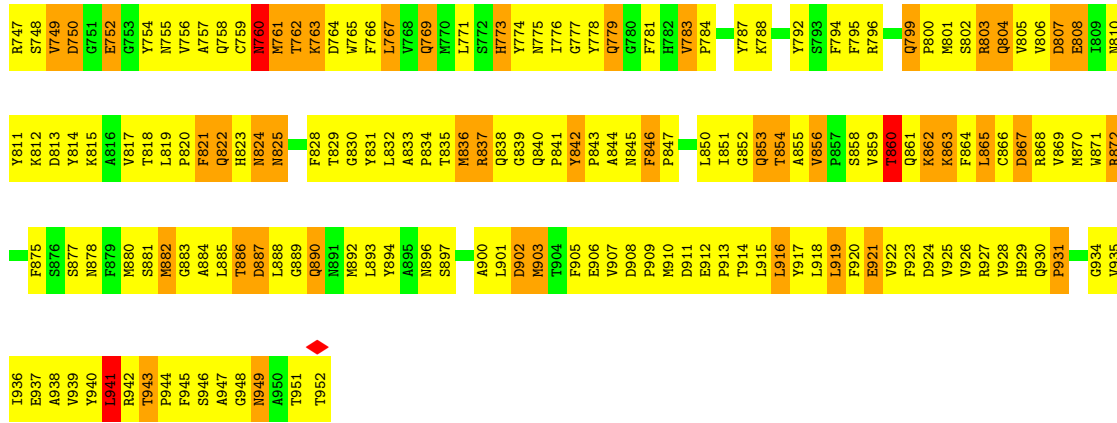




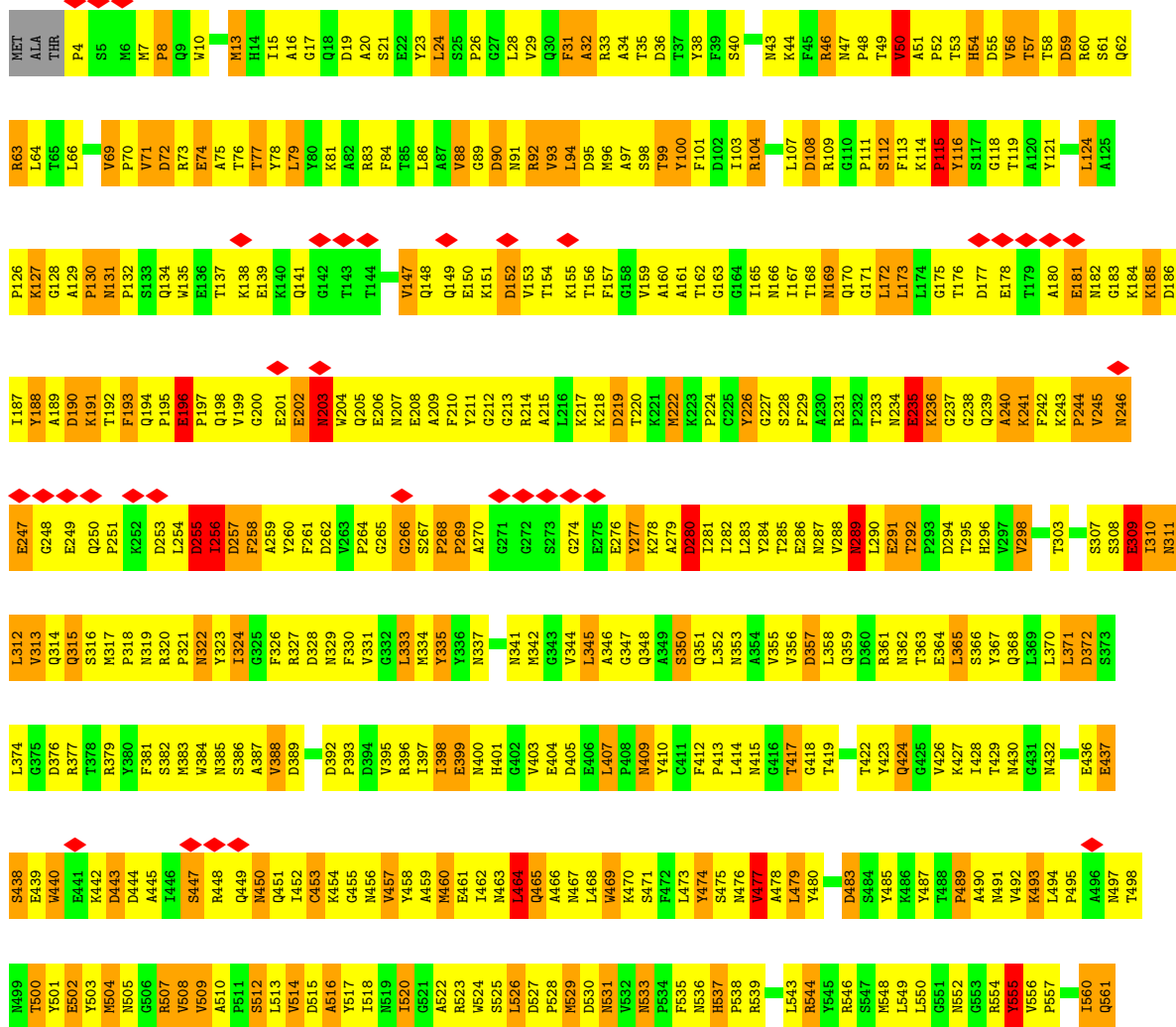
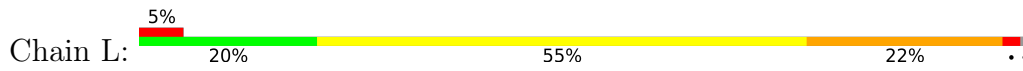


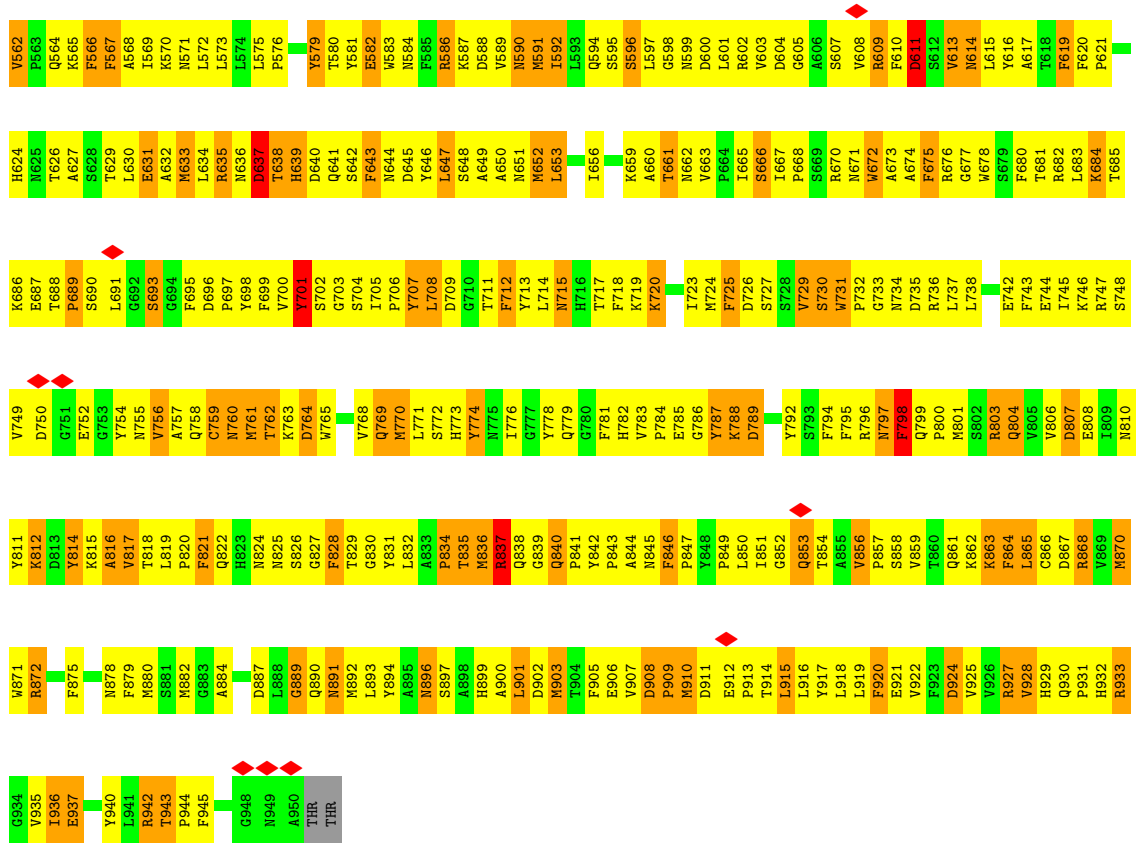
• Molecule 1: Hexon protein



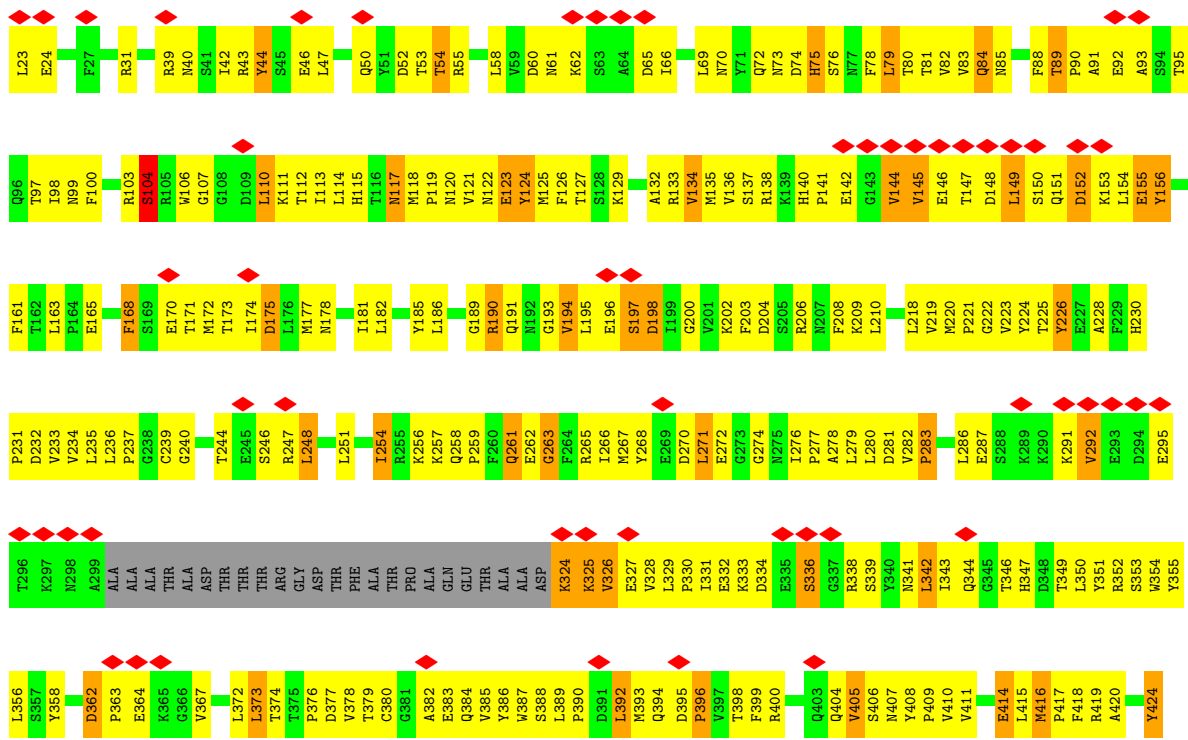


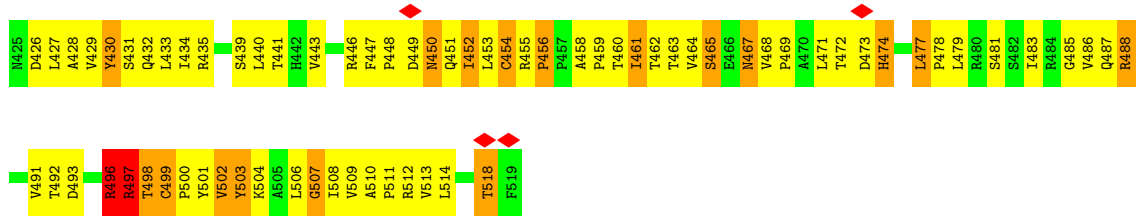
● Molecule 1: Hexon protein



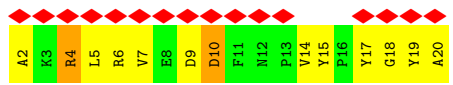
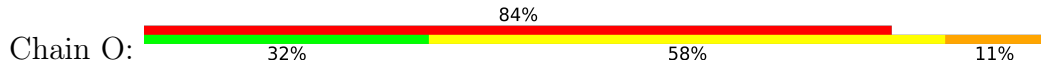


• Molecule 2: Penton

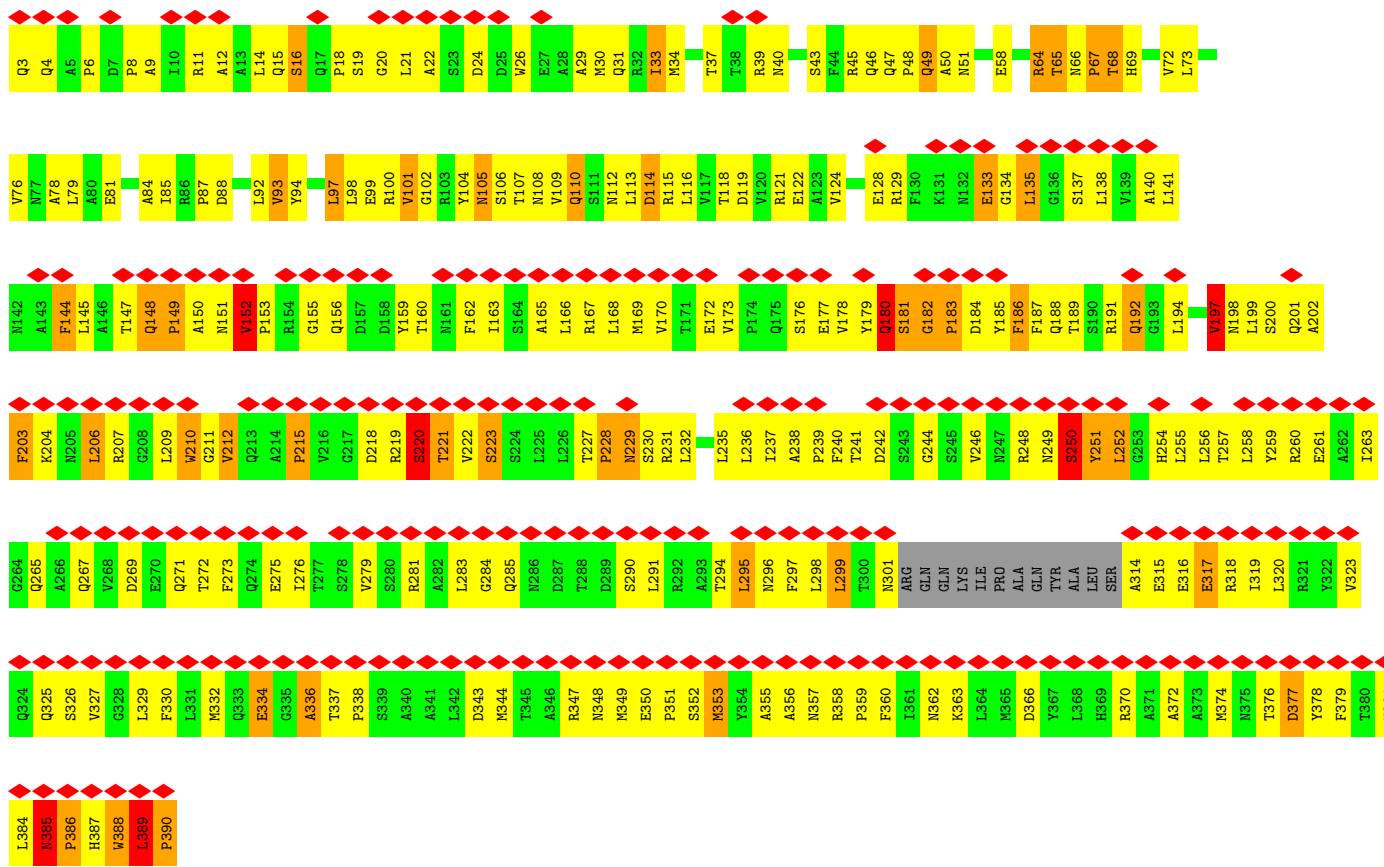




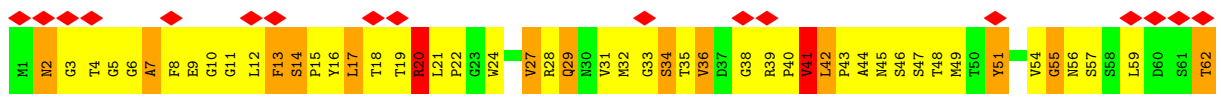
• Molecule 3: Fiber

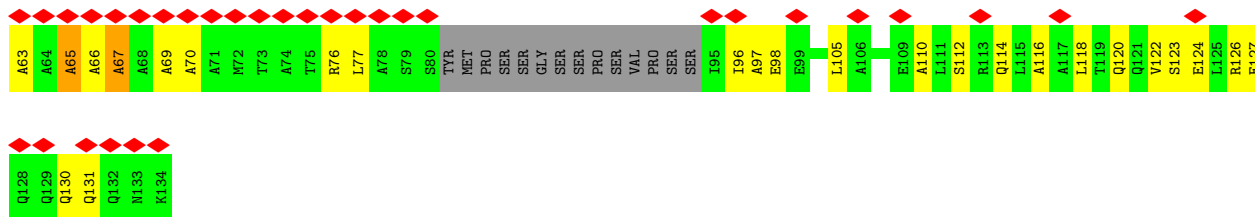


• Molecule 4: PIHa

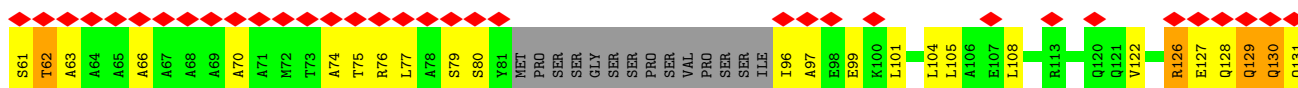
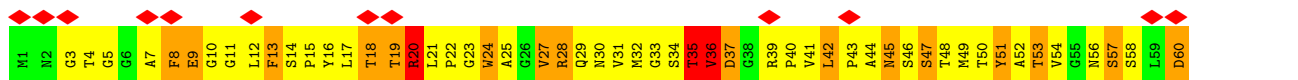


• Molecule 5: PIX

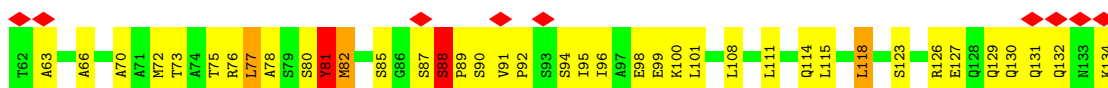
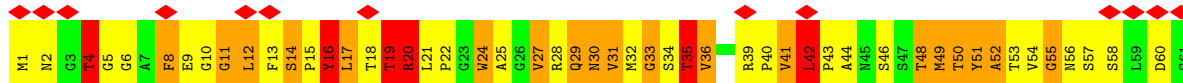




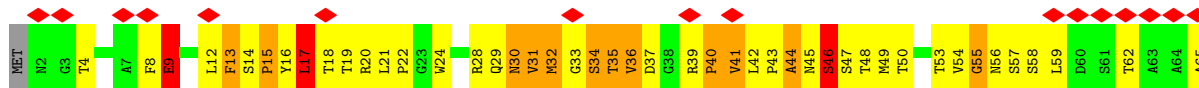
• Molecule 5: PIX



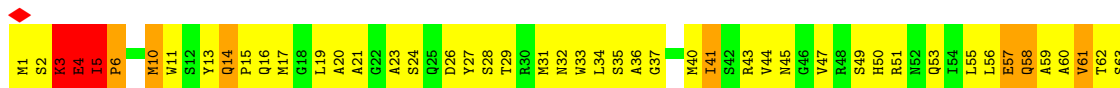
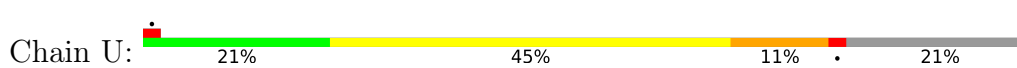
• Molecule 5: PIX

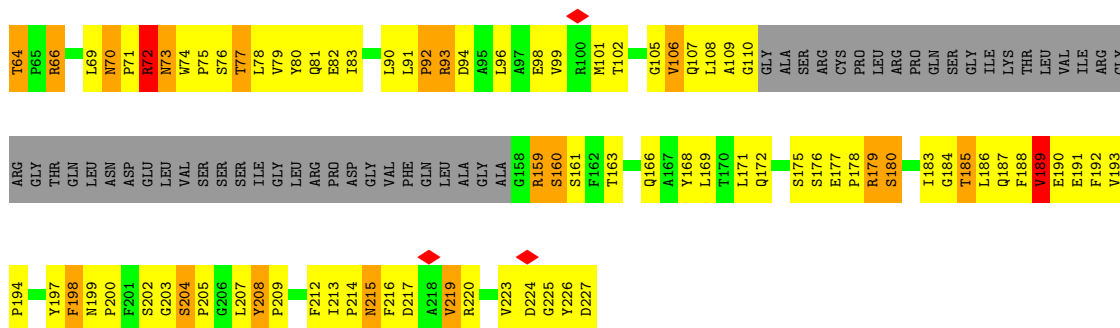


• Molecule 5: PIX

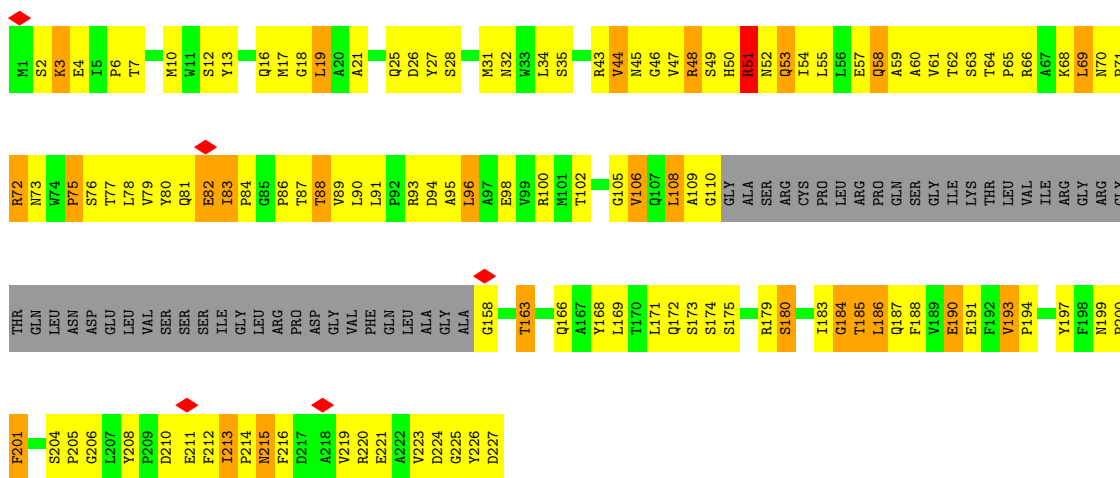


• Molecule 6: PVIII

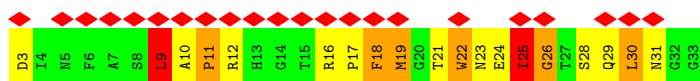




• Molecule 6: PVIII



• Molecule 7: PVI



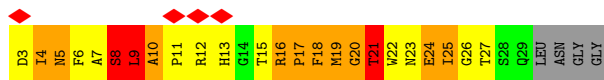
• Molecule 7: PVI



• Molecule 7: PVI



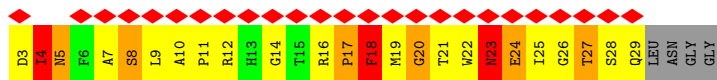
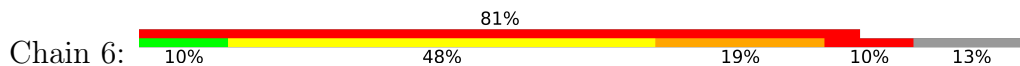
• Molecule 7: PVI



• Molecule 7: PVI



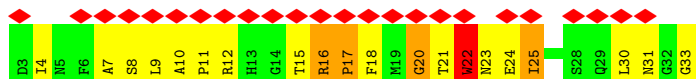
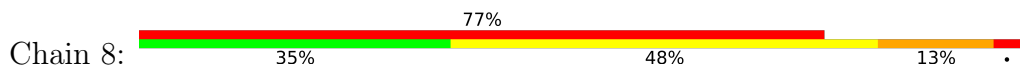
• Molecule 7: PVI



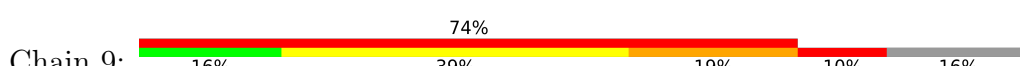
• Molecule 7: PVI



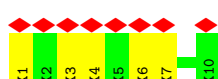
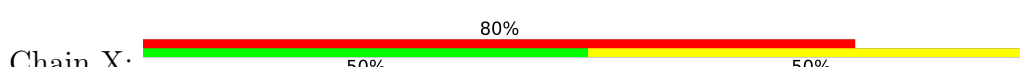
• Molecule 7: PVI



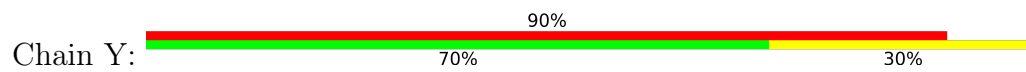
• Molecule 7: PVI



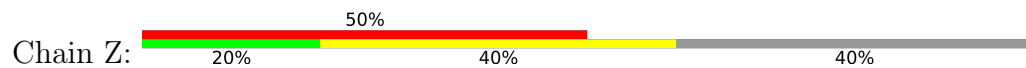
• Molecule 8: Unknown



● Molecule 8: Unknown



● Molecule 8: Unknown



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	19000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	Not provided	
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.115	Depositor
Minimum map value	-0.069	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	1571.9999, 1571.9999, 1571.9999	wwPDB
Map dimensions	1200, 1200, 1200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.31, 1.31, 1.31	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	A	0.73	5/7757 (0.1%)	1.12	54/10551 (0.5%)
1	B	0.95	15/7743 (0.2%)	1.40	81/10534 (0.8%)
1	C	0.80	5/7726 (0.1%)	1.19	52/10509 (0.5%)
1	D	0.82	10/7732 (0.1%)	1.18	47/10517 (0.4%)
1	E	0.90	12/7732 (0.2%)	1.28	78/10517 (0.7%)
1	F	0.86	6/7751 (0.1%)	1.27	70/10544 (0.7%)
1	G	0.92	9/7732 (0.1%)	1.57	70/10517 (0.7%)
1	H	0.92	11/7732 (0.1%)	1.33	69/10517 (0.7%)
1	I	0.78	1/7743 (0.0%)	1.18	53/10534 (0.5%)
1	J	1.01	11/7758 (0.1%)	1.26	49/10554 (0.5%)
1	K	0.84	3/7758 (0.0%)	1.22	55/10554 (0.5%)
1	L	0.77	2/7731 (0.0%)	1.18	45/10516 (0.4%)
2	N	0.71	4/3896 (0.1%)	0.98	15/5302 (0.3%)
3	O	1.04	0/167	1.66	1/225 (0.4%)
4	M	0.75	5/2990 (0.2%)	1.04	20/4067 (0.5%)
5	P	0.86	1/879 (0.1%)	1.44	15/1190 (1.3%)
5	Q	1.04	1/884 (0.1%)	1.45	13/1197 (1.1%)
5	R	0.82	0/978	1.30	13/1328 (1.0%)
5	S	0.78	0/890	1.22	7/1206 (0.6%)
6	U	0.73	0/1428	1.06	2/1946 (0.1%)
6	V	0.68	0/1428	1.01	5/1946 (0.3%)
7	1	1.45	2/242 (0.8%)	1.89	7/326 (2.1%)
7	2	1.20	0/217	1.73	6/294 (2.0%)
7	3	0.92	0/208	1.73	10/282 (3.5%)
7	4	1.26	2/217 (0.9%)	1.66	10/294 (3.4%)
7	5	1.21	0/208	1.71	7/282 (2.5%)
7	6	1.04	0/217	1.56	9/294 (3.1%)
7	7	1.06	1/208 (0.5%)	1.70	5/282 (1.8%)
7	8	1.28	1/242 (0.4%)	1.67	3/326 (0.9%)
7	9	1.16	0/208	1.46	2/282 (0.7%)
All	All	0.86	107/108402 (0.1%)	1.26	873/147433 (0.6%)

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	A	0	2
1	B	0	5
1	C	0	1
1	E	0	2
1	F	0	3
1	G	1	3
1	H	0	2
1	I	0	1
1	J	0	2
1	L	0	2
5	P	0	1
All	All	1	24

The worst 5 of 107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	277	TYR	CB-CG	-49.00	0.78	1.51
1	B	433	ASP	CB-CG	-28.79	0.91	1.51
1	H	328	ASP	CB-CG	-21.23	1.07	1.51
1	G	776	ILE	CB-CG1	-20.98	0.95	1.54
1	D	297	VAL	CB-CG1	19.99	1.94	1.52

The worst 5 of 873 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	774	TYR	CB-CG-CD1	-63.44	82.93	121.00
1	G	774	TYR	CB-CG-CD2	60.92	157.55	121.00
1	B	210	PHE	CB-CG-CD2	-28.19	101.07	120.80
1	J	277	TYR	CA-CB-CG	25.09	161.06	113.40
1	B	210	PHE	CB-CG-CD1	25.02	138.31	120.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	G	776	ILE	CB

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	GLN	Mainchain,Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	429	THR	Mainchain,Peptide
1	B	431	GLY	Mainchain
1	B	432	ASN	Sidechain
1	B	433	ASP	Mainchain

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	A	7551	0	7220	1552	0
1	B	7536	0	7195	2040	0
1	C	7519	0	7187	1985	0
1	D	7526	0	7193	1420	0
1	E	7526	0	7186	1709	0
1	F	7544	0	7214	2019	0
1	G	7526	0	7193	1614	0
1	H	7526	0	7184	1842	0
1	I	7536	0	7203	1663	0
1	J	7551	0	7211	1876	0
1	K	7551	0	7216	1769	0
1	L	7524	0	7194	1819	0
2	N	3803	0	3723	530	0
3	O	162	0	148	25	0
4	M	2938	0	2905	414	0
5	P	871	0	873	278	0
5	Q	875	0	873	338	0
5	R	965	0	962	318	0
5	S	881	0	877	157	0
6	U	1391	0	1342	374	0
6	V	1391	0	1344	199	0
7	1	236	0	219	95	0
7	2	211	0	196	66	0
7	3	202	0	188	68	0
7	4	211	0	196	95	0
7	5	202	0	188	65	0
7	6	211	0	196	74	0
7	7	202	0	188	29	0
7	8	236	0	219	47	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	9	202	0	188	86	0
8	X	51	0	14	6	0
8	Y	51	0	13	3	0
8	Z	30	0	8	9	0
All	All	105738	0	101256	21102	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 102.

The worst 5 of 21102 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)
1:J:162:THR:HG21	1:J:193:PHE:CD2	1.16	1.65
1:A:407:LEU:HD21	1:C:474:TYR:CD2	1.30	1.64
1:F:950:ALA:CB	1:H:893:LEU:HD12	1.19	1.63
1:H:94:LEU:CD1	1:H:619:PHE:CD1	1.80	1.62
1:A:462:ILE:HD12	1:B:411:CYS:SG	1.40	1.61

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	947/952 (100%)	670 (71%)	190 (20%)	87 (9%)	1	9
1	B	947/952 (100%)	714 (75%)	173 (18%)	60 (6%)	1	17
1	C	944/952 (99%)	646 (68%)	207 (22%)	91 (10%)	0	8
1	D	945/952 (99%)	683 (72%)	195 (21%)	67 (7%)	1	15
1	E	945/952 (99%)	705 (75%)	170 (18%)	70 (7%)	1	13
1	F	948/952 (100%)	681 (72%)	178 (19%)	89 (9%)	0	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	945/952 (99%)	684 (72%)	194 (20%)	67 (7%)	1	15
1	H	945/952 (99%)	654 (69%)	216 (23%)	75 (8%)	1	12
1	I	947/952 (100%)	669 (71%)	192 (20%)	86 (9%)	1	9
1	J	949/952 (100%)	672 (71%)	206 (22%)	71 (8%)	1	13
1	K	949/952 (100%)	718 (76%)	160 (17%)	71 (8%)	1	13
1	L	945/952 (99%)	638 (68%)	235 (25%)	72 (8%)	1	13
2	N	469/497 (94%)	366 (78%)	76 (16%)	27 (6%)	1	19
3	O	17/19 (90%)	13 (76%)	3 (18%)	1 (6%)	1	18
4	M	372/388 (96%)	281 (76%)	63 (17%)	28 (8%)	1	13
5	P	116/134 (87%)	84 (72%)	25 (22%)	7 (6%)	1	18
5	Q	116/134 (87%)	89 (77%)	22 (19%)	5 (4%)	2	24
5	R	132/134 (98%)	97 (74%)	26 (20%)	9 (7%)	1	16
5	S	117/134 (87%)	83 (71%)	26 (22%)	8 (7%)	1	16
6	U	176/227 (78%)	131 (74%)	32 (18%)	13 (7%)	1	13
6	V	176/227 (78%)	126 (72%)	36 (20%)	14 (8%)	1	12
7	1	29/31 (94%)	20 (69%)	6 (21%)	3 (10%)	0	7
7	2	25/31 (81%)	15 (60%)	7 (28%)	3 (12%)	0	5
7	3	24/31 (77%)	12 (50%)	7 (29%)	5 (21%)	0	1
7	4	25/31 (81%)	13 (52%)	6 (24%)	6 (24%)	0	0
7	5	24/31 (77%)	14 (58%)	9 (38%)	1 (4%)	3	25
7	6	25/31 (81%)	15 (60%)	3 (12%)	7 (28%)	0	0
7	7	24/31 (77%)	13 (54%)	5 (21%)	6 (25%)	0	0
7	8	29/31 (94%)	20 (69%)	6 (21%)	3 (10%)	0	7
7	9	24/31 (77%)	15 (62%)	4 (17%)	5 (21%)	0	1
All	All	13276/13597 (98%)	9541 (72%)	2678 (20%)	1057 (8%)	2	12

5 of 1057 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ALA
1	A	89	GLY
1	A	151	LYS
1	A	199	VAL
1	A	248	GLY

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	A	817/818 (100%)	696 (85%)	121 (15%)	3	18
1	B	815/818 (100%)	662 (81%)	153 (19%)	1	10
1	C	814/818 (100%)	651 (80%)	163 (20%)	1	8
1	D	814/818 (100%)	675 (83%)	139 (17%)	2	13
1	E	814/818 (100%)	645 (79%)	169 (21%)	1	7
1	F	816/818 (100%)	603 (74%)	213 (26%)	0	4
1	G	814/818 (100%)	616 (76%)	198 (24%)	0	5
1	H	814/818 (100%)	604 (74%)	210 (26%)	0	4
1	I	815/818 (100%)	627 (77%)	188 (23%)	1	6
1	J	817/818 (100%)	609 (74%)	208 (26%)	0	4
1	K	817/818 (100%)	605 (74%)	212 (26%)	0	4
1	L	814/818 (100%)	635 (78%)	179 (22%)	1	6
2	N	428/443 (97%)	370 (86%)	58 (14%)	3	21
3	O	16/16 (100%)	14 (88%)	2 (12%)	4	23
4	M	317/327 (97%)	279 (88%)	38 (12%)	5	25
5	P	89/102 (87%)	77 (86%)	12 (14%)	4	21
5	Q	89/102 (87%)	73 (82%)	16 (18%)	1	11
5	R	102/102 (100%)	81 (79%)	21 (21%)	1	7
5	S	90/102 (88%)	72 (80%)	18 (20%)	1	8
6	U	153/190 (80%)	120 (78%)	33 (22%)	1	7
6	V	153/190 (80%)	124 (81%)	29 (19%)	1	9
7	1	24/24 (100%)	18 (75%)	6 (25%)	0	4
7	2	22/24 (92%)	13 (59%)	9 (41%)	0	0
7	3	21/24 (88%)	15 (71%)	6 (29%)	0	2
7	4	22/24 (92%)	18 (82%)	4 (18%)	1	11
7	5	21/24 (88%)	15 (71%)	6 (29%)	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	6	22/24 (92%)	21 (96%)	1 (4%)	27 57
7	7	21/24 (88%)	20 (95%)	1 (5%)	25 56
7	8	24/24 (100%)	20 (83%)	4 (17%)	2 14
7	9	21/24 (88%)	14 (67%)	7 (33%)	0 1
All	All	11416/11606 (98%)	8992 (79%)	2424 (21%)	3 7

5 of 2424 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	426	VAL
5	R	50	THR
1	K	661	THR
1	K	409	ASN
1	L	596	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 513 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	949	ASN
4	M	15	GLN
1	L	929	HIS
1	F	540	ASN
1	F	456	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	4
1	A	2
1	J	2
1	H	2
1	G	1
1	D	1
1	E	1

The worst 5 of 13 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	179:THR	C	180:ALA	N	2.03
1	B	432:ASN	C	433:ASP	N	1.65
1	B	429:THR	C	430:ASN	N	1.19
1	J	276:GLU	C	277:TYR	N	1.19
1	G	776:ILE	C	777:GLY	N	1.18

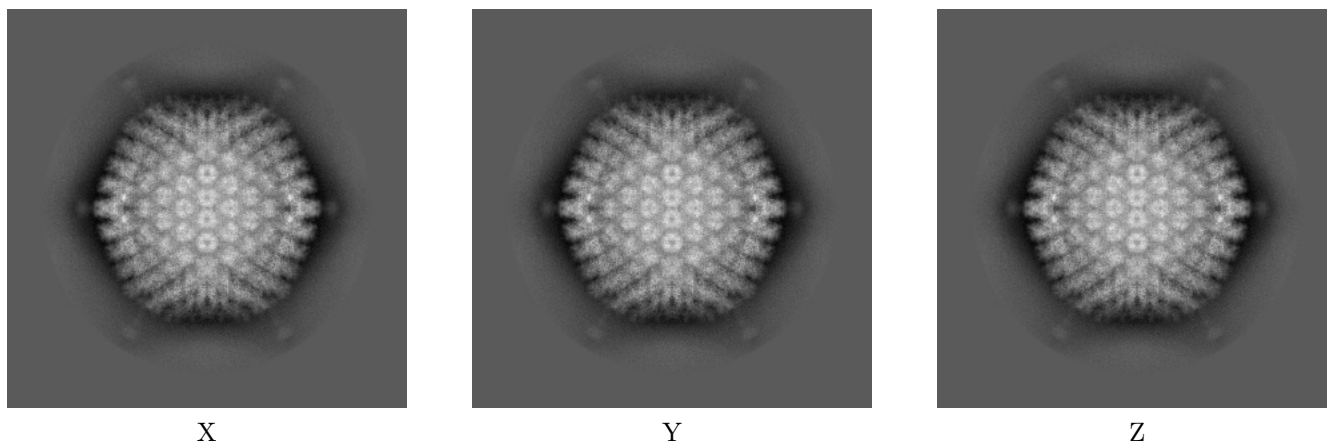
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8471. 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](#)

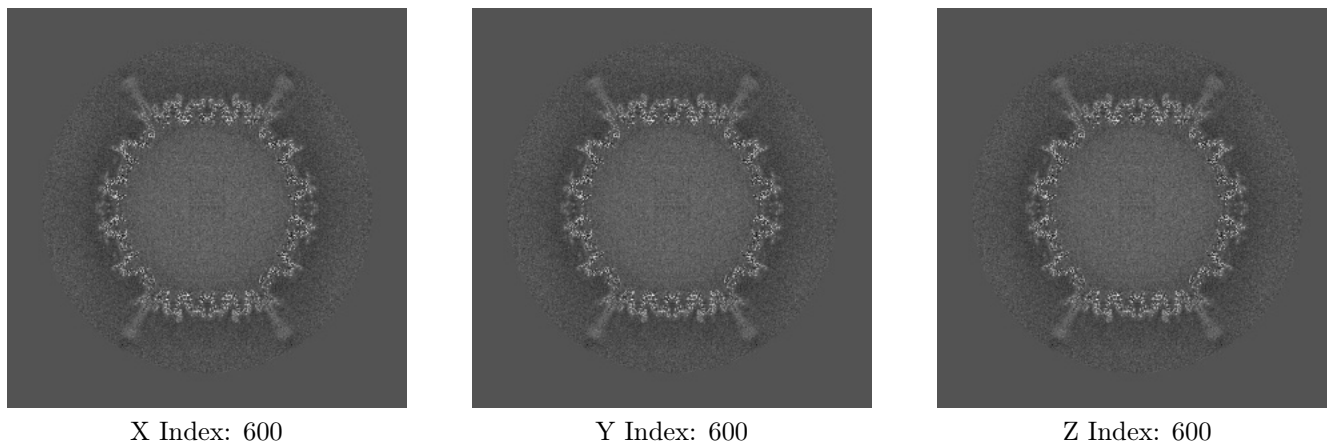
6.1.1 Primary map



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

6.2 Central slices [i](#)

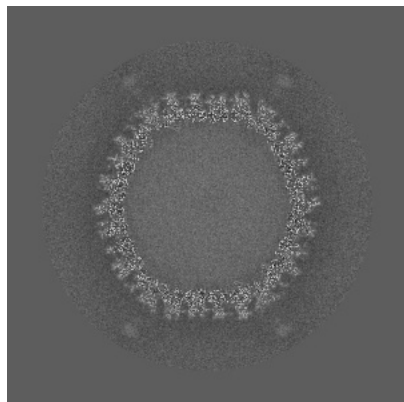
6.2.1 Primary map



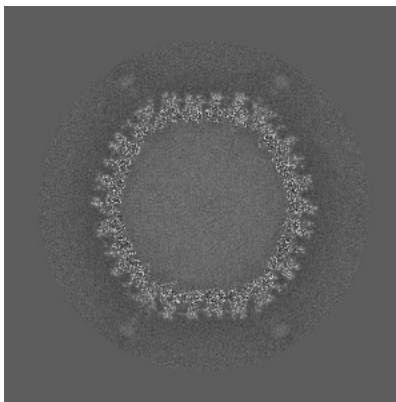
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

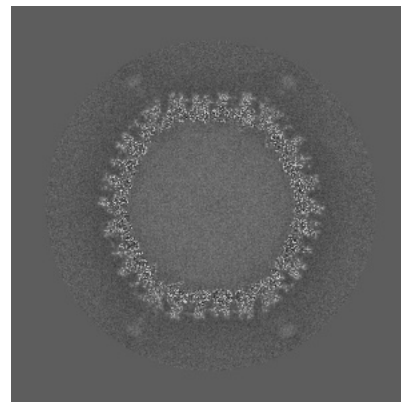
6.3.1 Primary map



X Index: 615



Y Index: 585

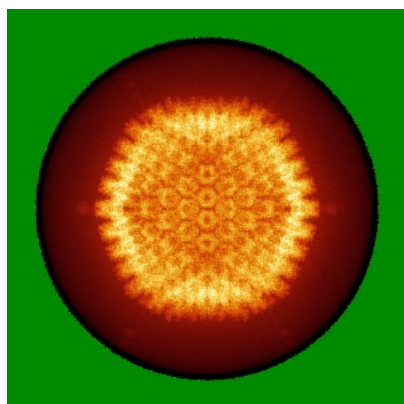


Z Index: 585

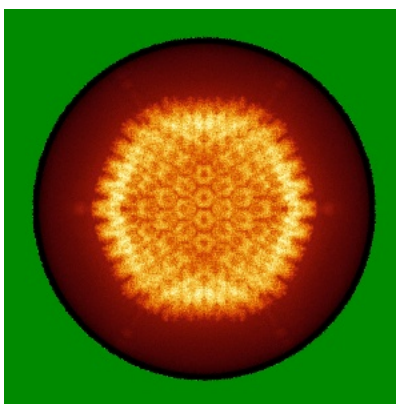
The images above show the largest variance slices of the map in three orthogonal directions.

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

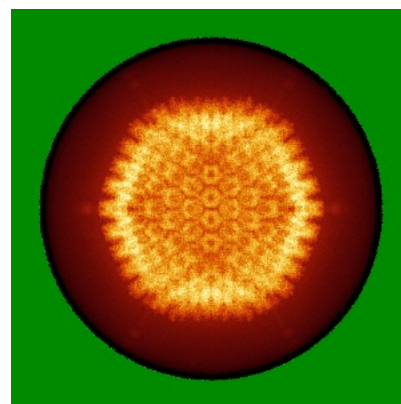
6.4.1 Primary map



X



Y

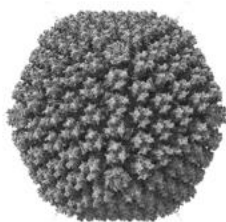


Z

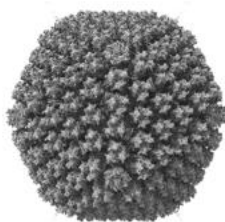
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

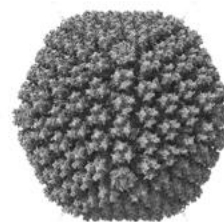
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

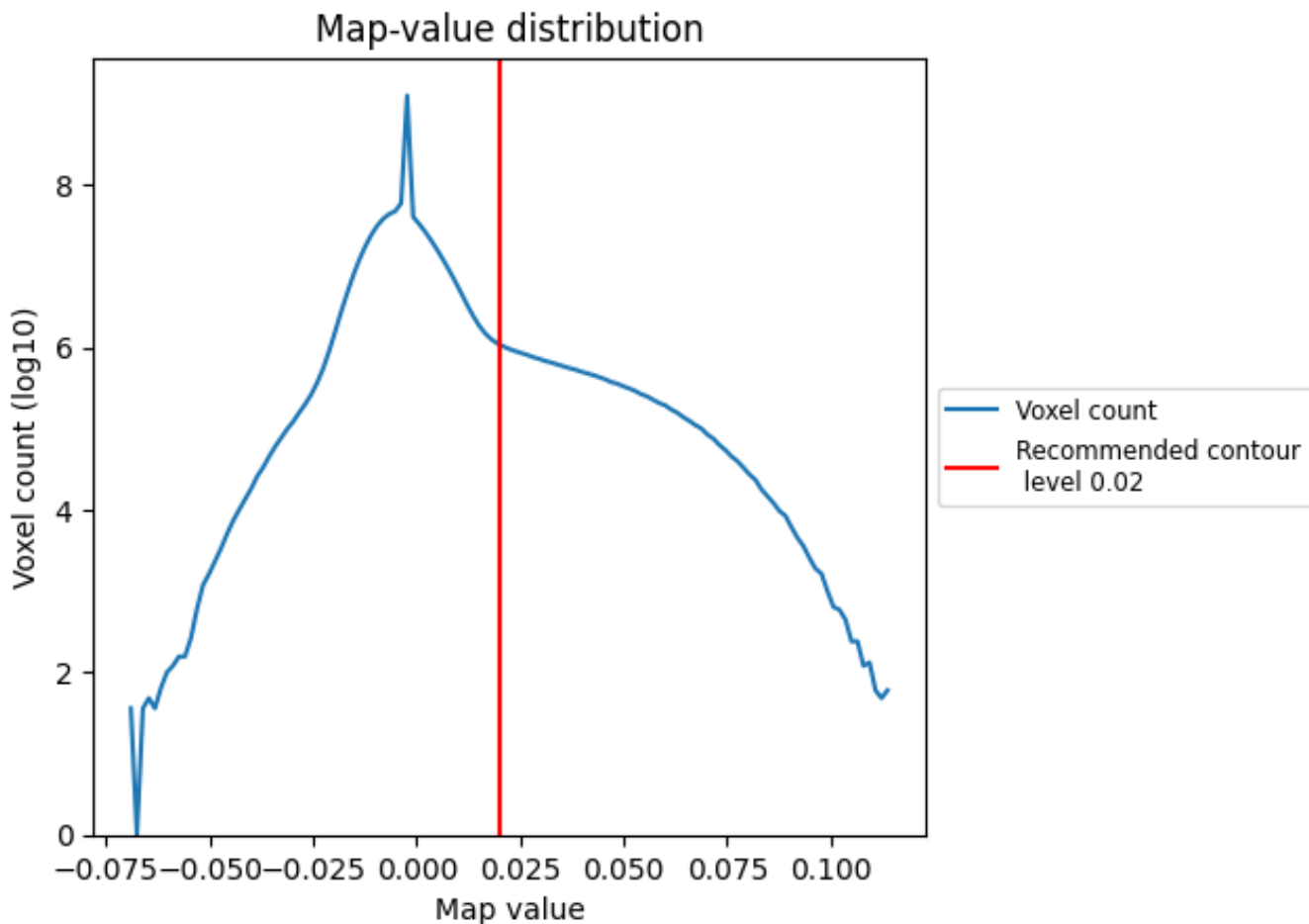
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

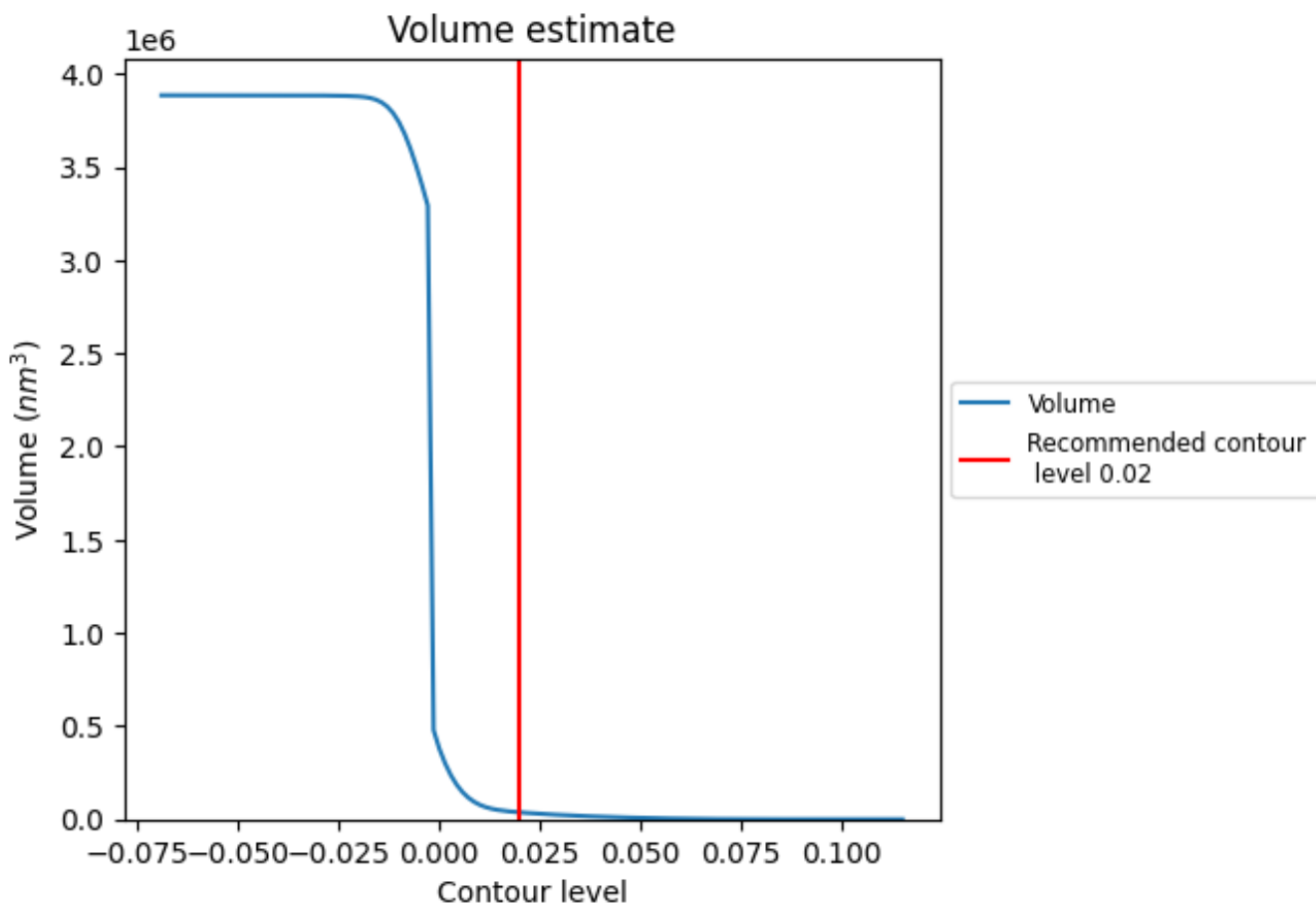
This section contains the results of statistical analysis of the map.

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.

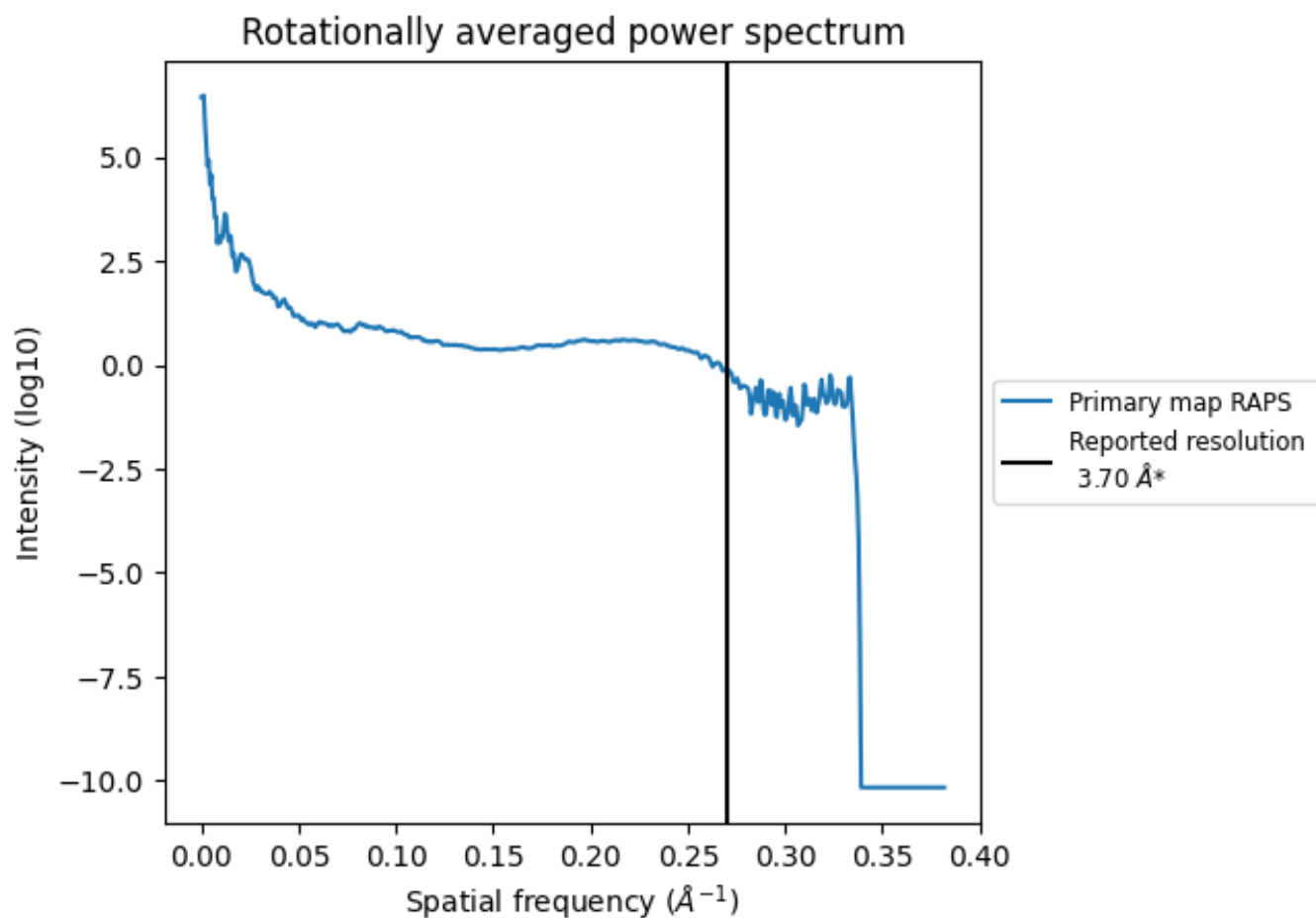
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 37384 nm³; this corresponds to an approximate mass of 33770 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 0.270 Å⁻¹

8 Fourier-Shell correlation

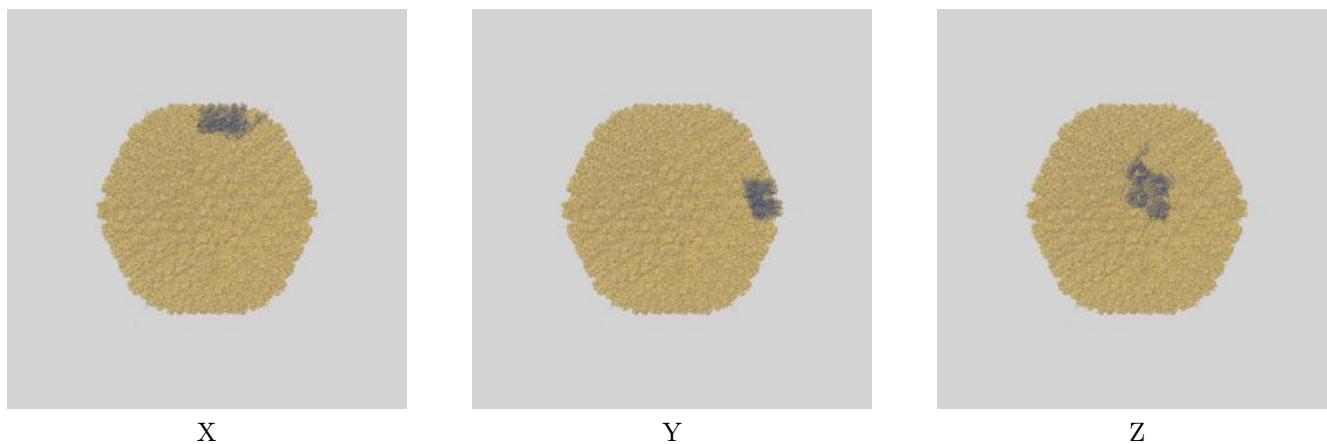
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

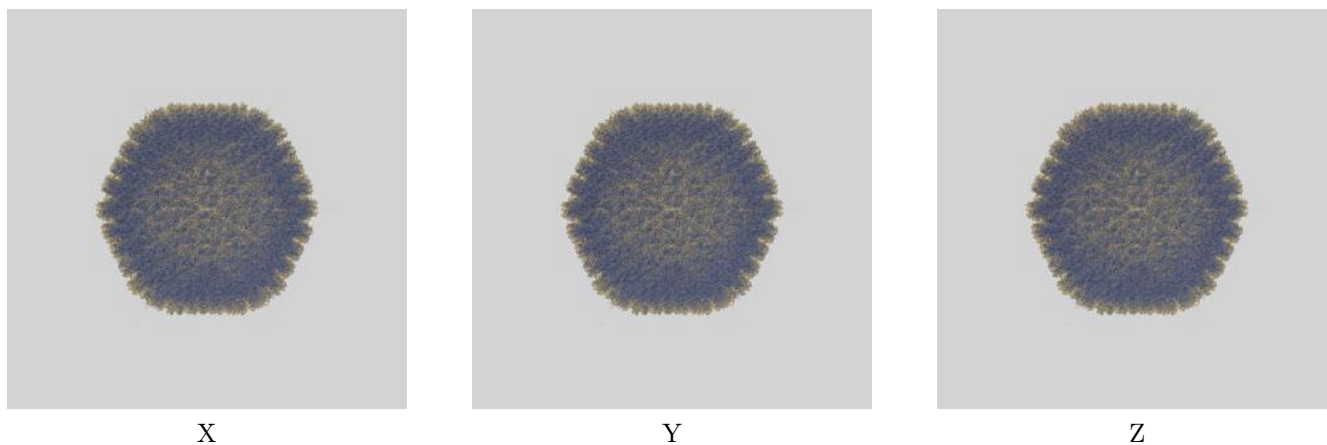
This section contains information regarding the fit between EMDB map EMD-8471 and PDB model 5TX1. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

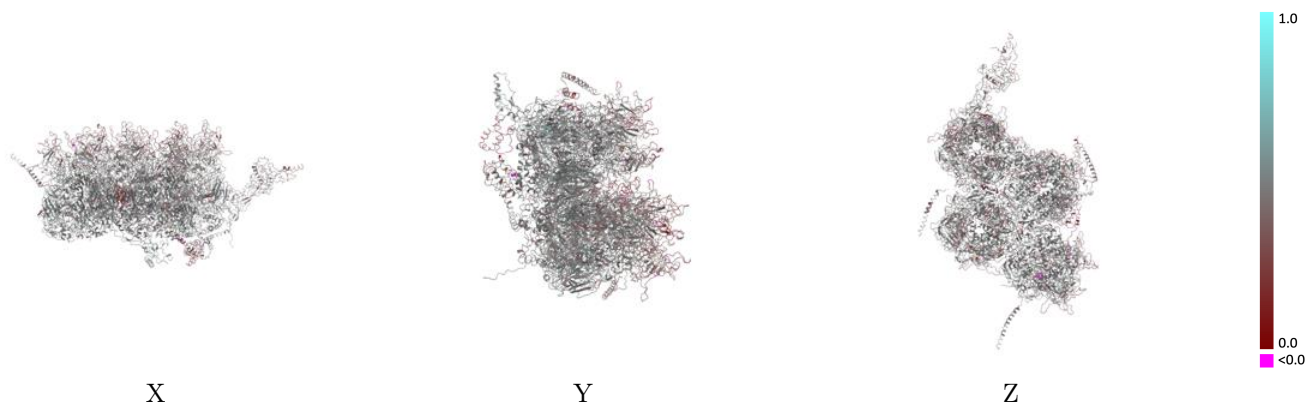


9.1.2 Map-model assembly overlay [i](#)



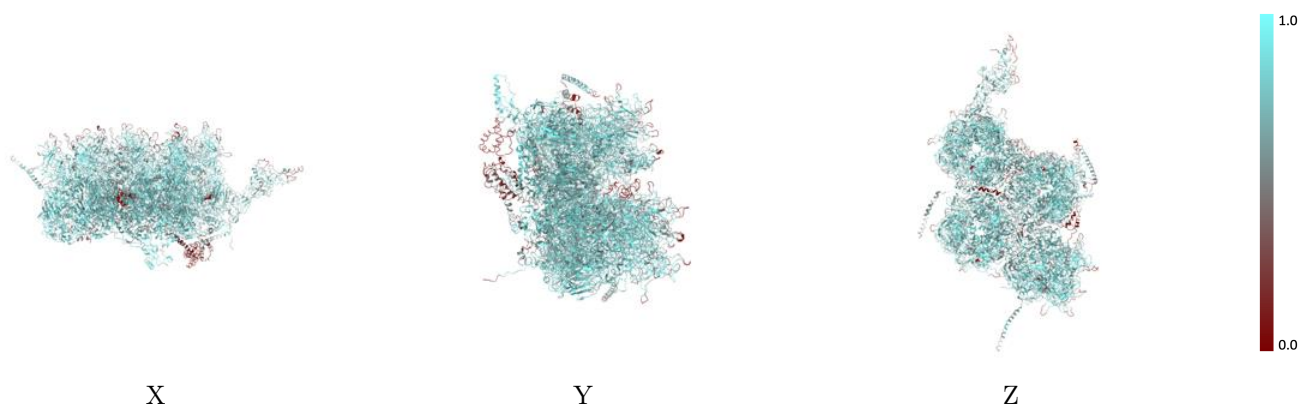
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



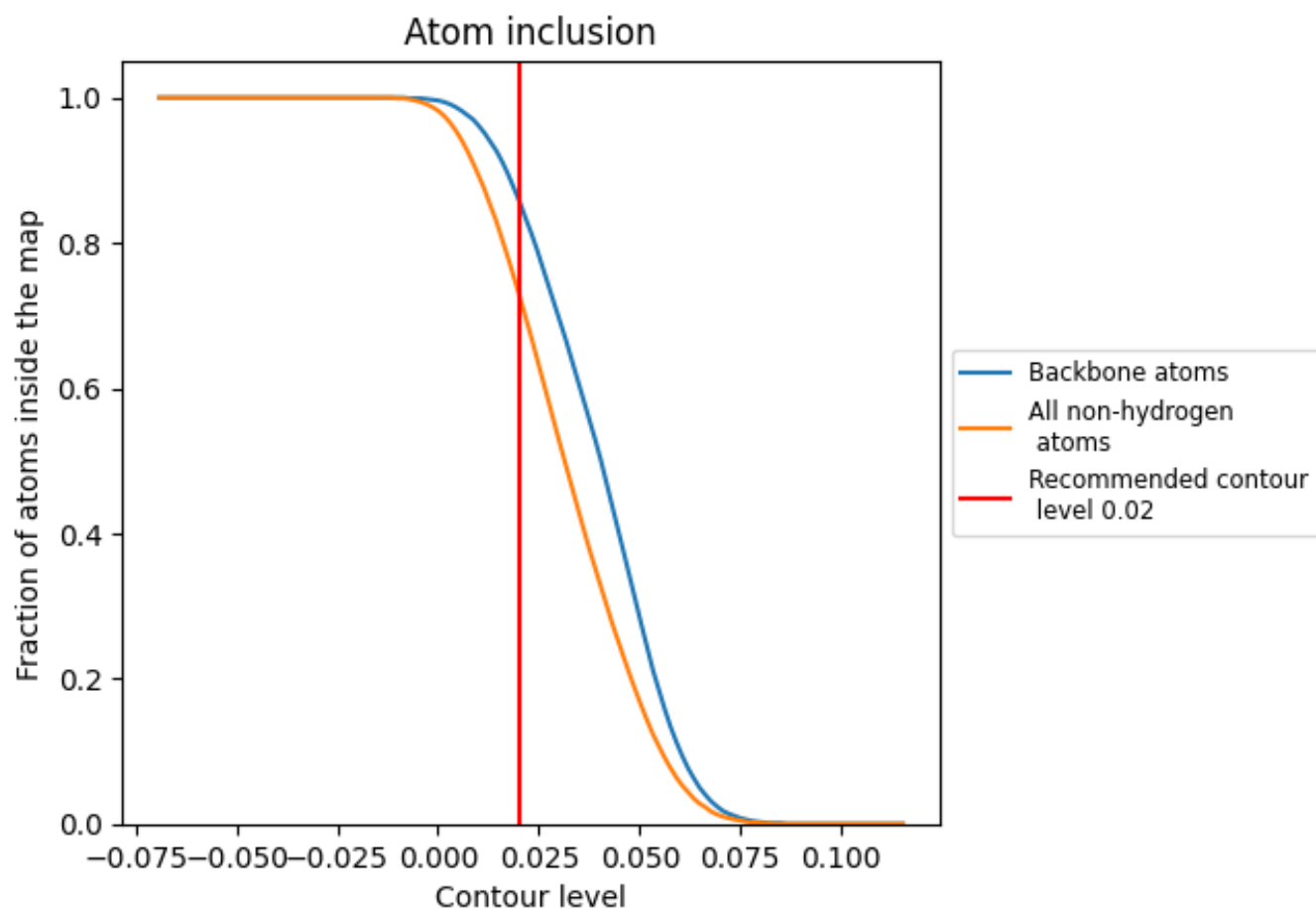
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).





































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 73% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7310	 0.4470
1	 0.2640	 0.3000
2	 0.6410	 0.4160
3	 0.2180	 0.3560
4	 0.6070	 0.3940
5	 0.3250	 0.3850
6	 0.1070	 0.3530
7	 0.2280	 0.3810
8	 0.2380	 0.3470
9	 0.1570	 0.3040
A	 0.7550	 0.4470
B	 0.7530	 0.4360
C	 0.7670	 0.4510
D	 0.7620	 0.4550
E	 0.7620	 0.4530
F	 0.7740	 0.4620
G	 0.7790	 0.4610
H	 0.7740	 0.4610
I	 0.7780	 0.4620
J	 0.7730	 0.4570
K	 0.7670	 0.4530
L	 0.7720	 0.4570
M	 0.3330	 0.3730
N	 0.6280	 0.4240
O	 0.1160	 0.3390
P	 0.4590	 0.3410
Q	 0.4120	 0.3280
R	 0.5920	 0.3940
S	 0.4840	 0.3420
U	 0.7520	 0.4900
V	 0.7690	 0.4900
X	 0.1960	 0.4500
Y	 0.1760	 0.3590
Z	 0.3000	 0.3330

