



## Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 12:35 AM EST

PDB ID : 6Q1F  
EMDB ID : EMD-20557  
Title : Atomic structure of the Human Herpesvirus 6B Capsid and Capsid-Associated Tegument Complexes  
Authors : Zhang, Y.B.; Liu, W.; Li, Z.H.; Kumar, V.; Alvarez-Cabrera, A.L.; Leibovitch, E.; Cui, Y.X.; Mei, Y.; Bi, G.Q.; Jacobson, S.; Zhou, Z.H.  
Deposited on : 2019-08-03  
Resolution : 9.00 Å(reported)

This is a Full wwPDB EM Validation 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:

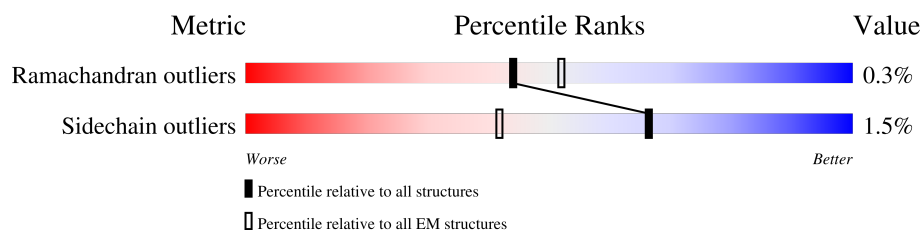
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 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 9.00 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
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	1345	<div> <div>39%</div> <div>99%</div> </div>
1	B	1345	<div> <div>41%</div> <div>98%</div> </div>
1	C	1345	<div> <div>42%</div> <div>97%</div> </div>
1	D	1345	<div> <div>38%</div> <div>98%</div> </div>
1	E	1345	<div> <div>37%</div> <div>98%</div> </div>
1	F	1345	<div> <div>43%</div> <div>98%</div> </div>
1	G	1345	<div> <div>42%</div> <div>98%</div> </div>
1	H	1345	<div> <div>34%</div> <div>98%</div> </div>
1	I	1345	<div> <div>40%</div> <div>99%</div> </div>

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Mol	Chain	Length	Quality of chain
1	q	1345	<div>54%</div> <div>95%</div> <div>..</div>
1	r	1345	<div>49%</div> <div>99%</div> <div>.</div>
1	s	1345	<div>47%</div> <div>99%</div> <div>.</div>
1	t	1345	<div>45%</div> <div>99%</div> <div>.</div>
1	u	1345	<div>49%</div> <div>99%</div> <div>.</div>
1	v	1345	<div>51%</div> <div>96%</div> <div>..</div>
1	w	1345	<div>77%</div> <div>92%</div> <div>. 7%</div>
2	e	858	<div>27%</div> <div>31%</div> <div>.</div> <div>69%</div>
2	f	858	<div>28%</div> <div>31%</div> <div>.</div> <div>69%</div>
2	g	858	<div>25%</div> <div>30%</div> <div>.</div> <div>69%</div>
2	h	858	<div>29%</div> <div>31%</div> <div>.</div> <div>69%</div>
2	i	858	<div>26%</div> <div>30%</div> <div>.</div> <div>69%</div>
2	j	858	<div>29%</div> <div>30%</div> <div>.</div> <div>69%</div>
2	k	858	<div>25%</div> <div>30%</div> <div>.</div> <div>69%</div>
2	l	858	<div>30%</div> <div>30%</div> <div>.</div> <div>69%</div>
2	m	858	<div>24%</div> <div>31%</div> <div>.</div> <div>69%</div>
2	n	858	<div>22%</div> <div>30%</div> <div>.</div> <div>69%</div>
2	o	858	<div>21%</div> <div>30%</div> <div>.</div> <div>69%</div>
2	p	858	<div>25%</div> <div>31%</div> <div>.</div> <div>69%</div>
3	1	89	<div>45%</div> <div>67%</div> <div>.</div> <div>31%</div>
3	2	89	<div>53%</div> <div>67%</div> <div>.</div> <div>31%</div>
3	3	89	<div>61%</div> <div>67%</div> <div>.</div> <div>31%</div>
3	4	89	<div>65%</div> <div>64%</div> <div>.</div> <div>35%</div>
3	J	89	<div>48%</div> <div>65%</div> <div>..</div> <div>31%</div>
3	K	89	<div>47%</div> <div>67%</div> <div>.</div> <div>31%</div>

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Mol	Chain	Length	Quality of chain
3	L	89	
3	M	89	
3	N	89	
3	O	89	
3	P	89	
3	Q	89	
3	R	89	
3	x	89	
3	y	89	
3	z	89	
4	5	299	
4	S	299	
4	T	299	
4	U	299	
4	V	299	
5	6	296	
5	7	296	
5	W	296	
5	X	296	
5	Y	296	
5	Z	296	
5	a	296	
5	b	296	
5	c	296	
5	d	296	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 238552 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	B	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	C	1325	Total	C	N	O	S	0	0
			10552	6709	1792	1991	60		
1	D	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	E	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	F	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	G	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	H	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	I	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	q	1296	Total	C	N	O	S	0	0
			10313	6561	1751	1942	59		
1	r	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	s	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	t	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	u	1344	Total	C	N	O	S	0	0
			10690	6797	1814	2018	61		
1	v	1301	Total	C	N	O	S	0	0
			10331	6564	1759	1948	60		
1	w	1248	Total	C	N	O	S	0	0
			9933	6324	1691	1860	58		

- Molecule 2 is a protein called Large structural phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	e	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	f	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	g	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	h	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	i	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	j	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	k	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	l	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	m	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	n	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	o	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	p	269	Total 2224	C 1417	N 376	O 426	S 5	0	0

- Molecule 3 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	61	Total 483	C 308	N 89	O 83	S 3	0	0
3	K	61	Total 483	C 308	N 89	O 83	S 3	0	0
3	L	61	Total 483	C 308	N 89	O 83	S 3	0	0
3	M	61	Total 483	C 308	N 89	O 83	S 3	0	0
3	N	61	Total 483	C 308	N 89	O 83	S 3	0	0
3	O	61	Total 483	C 308	N 89	O 83	S 3	0	0
3	P	61	Total 483	C 308	N 89	O 83	S 3	0	0
3	Q	61	Total 483	C 308	N 89	O 83	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	x	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	y	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	z	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	1	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	2	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	3	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	4	58	Total	C	N	O	S	0	0
			456	292	85	76	3		

- Molecule 4 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	251	Total	C	N	O	S	0	0
			2023	1306	327	376	14		
4	S	299	Total	C	N	O	S	0	0
			2398	1542	395	446	15		
4	T	299	Total	C	N	O	S	0	0
			2398	1542	395	446	15		
4	U	299	Total	C	N	O	S	0	0
			2398	1542	395	446	15		
4	V	299	Total	C	N	O	S	0	0
			2398	1542	395	446	15		

- Molecule 5 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	282	Total	C	N	O	S	0	0
			2226	1422	370	415	19		
5	W	296	Total	C	N	O	S	0	0
			2337	1486	393	437	21		
5	X	296	Total	C	N	O	S	0	0
			2337	1486	393	437	21		
5	Y	296	Total	C	N	O	S	0	0
			2337	1486	393	437	21		

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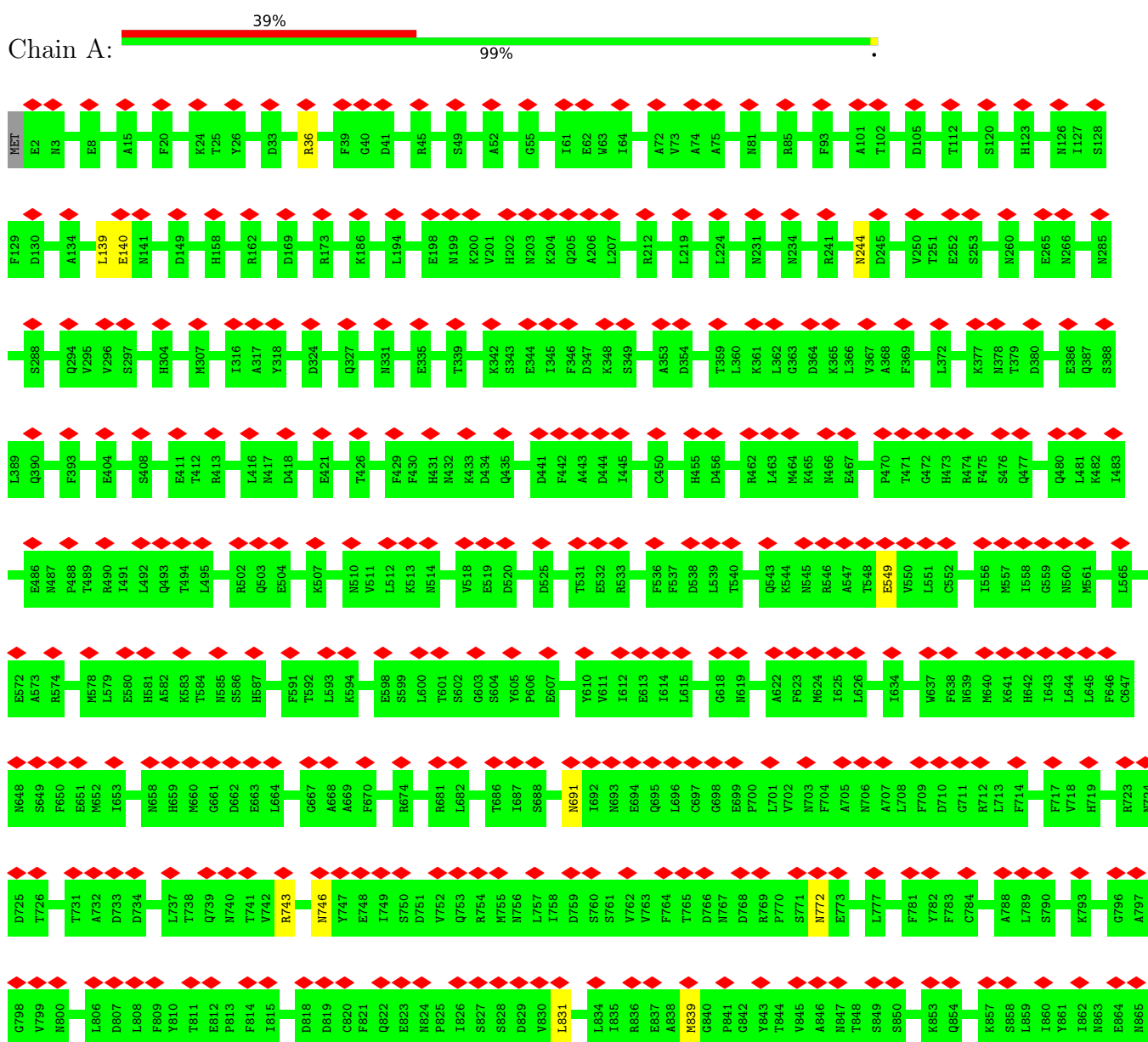
Mol	Chain	Residues	Atoms					AltConf	Trace
5	Z	296	Total	C	N	O	S	0	0
			2337	1486	393	437	21		
5	7	296	Total	C	N	O	S	0	0
			2337	1486	393	437	21		
5	a	295	Total	C	N	O	S	0	0
			2329	1481	392	436	20		
5	b	295	Total	C	N	O	S	0	0
			2329	1481	392	436	20		
5	c	295	Total	C	N	O	S	0	0
			2329	1481	392	436	20		
5	d	295	Total	C	N	O	S	0	0
			2329	1481	392	436	20		



### 3 Residue-property plots

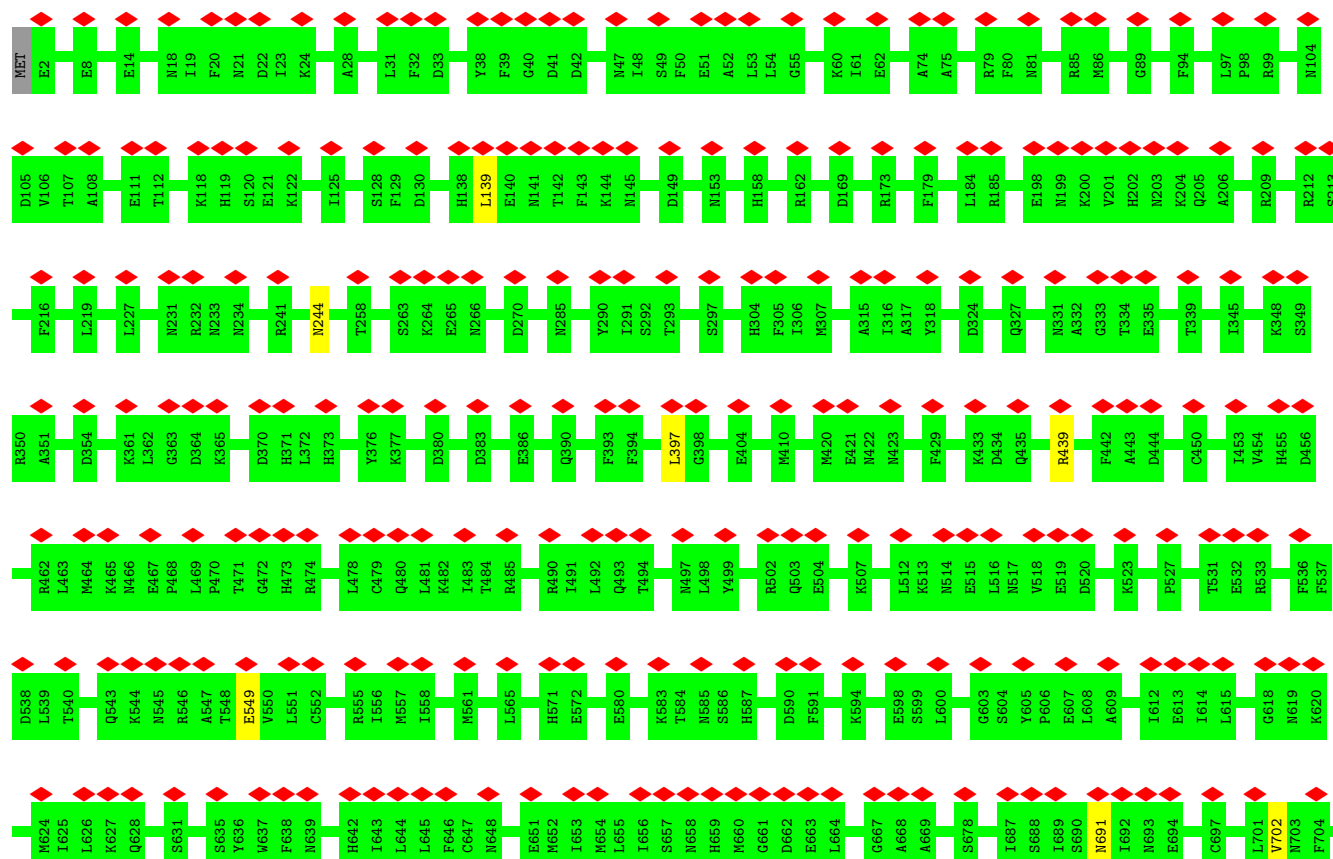
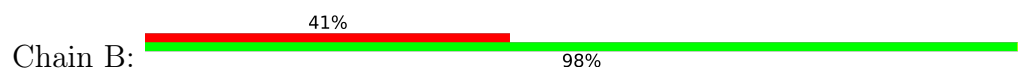
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

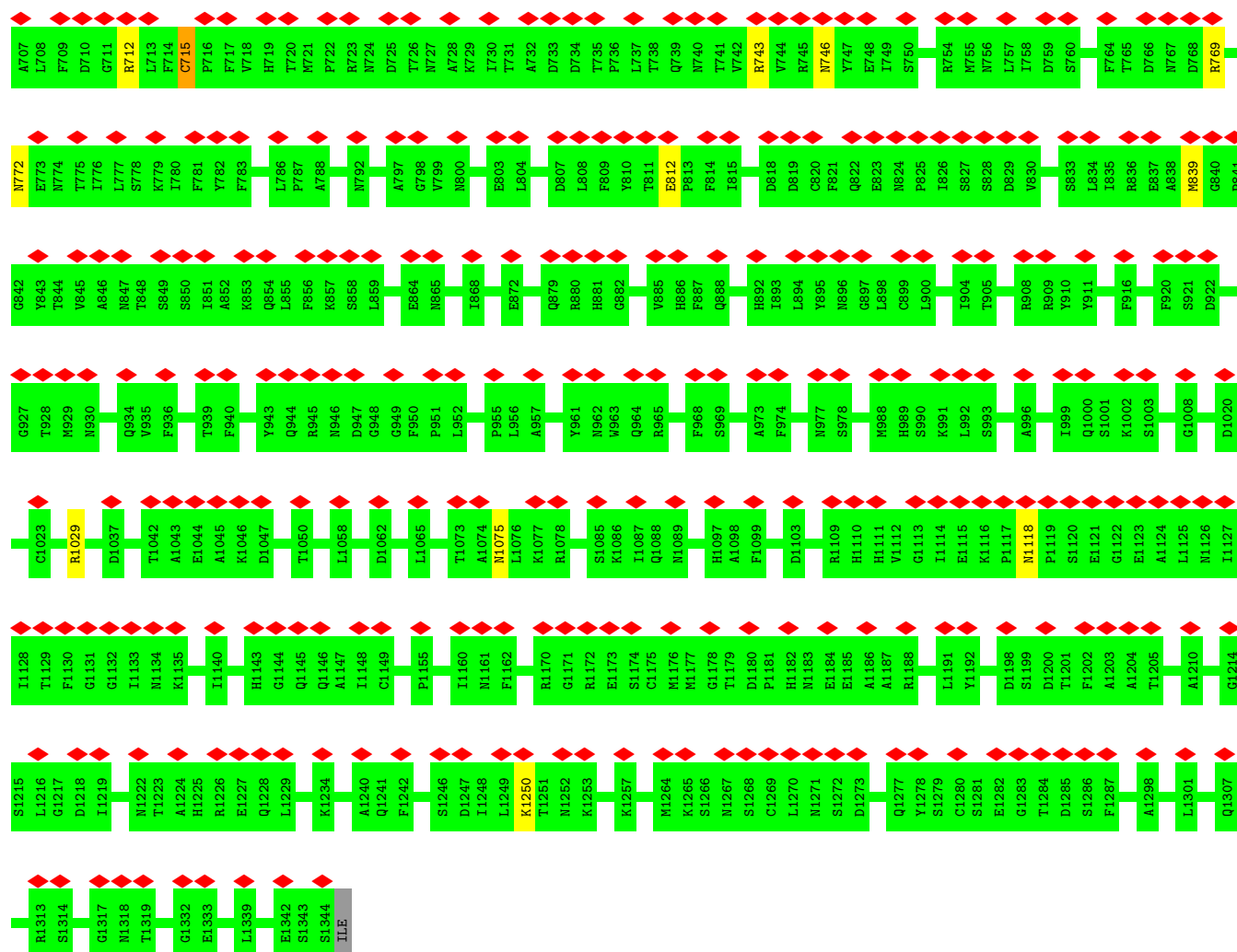
- Molecule 1: Major capsid protein



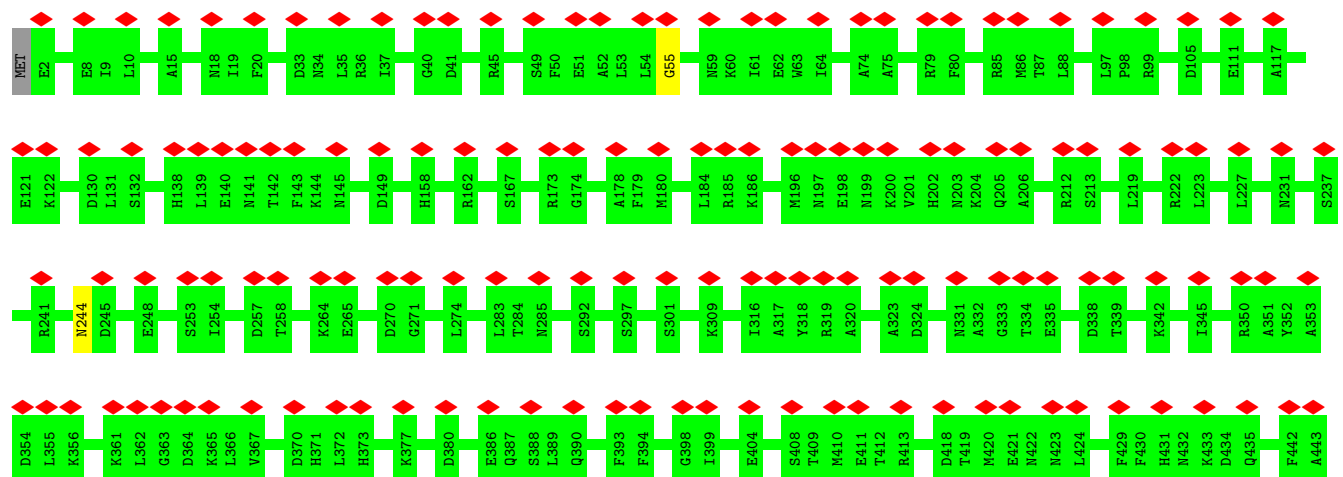
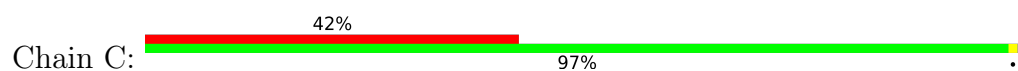


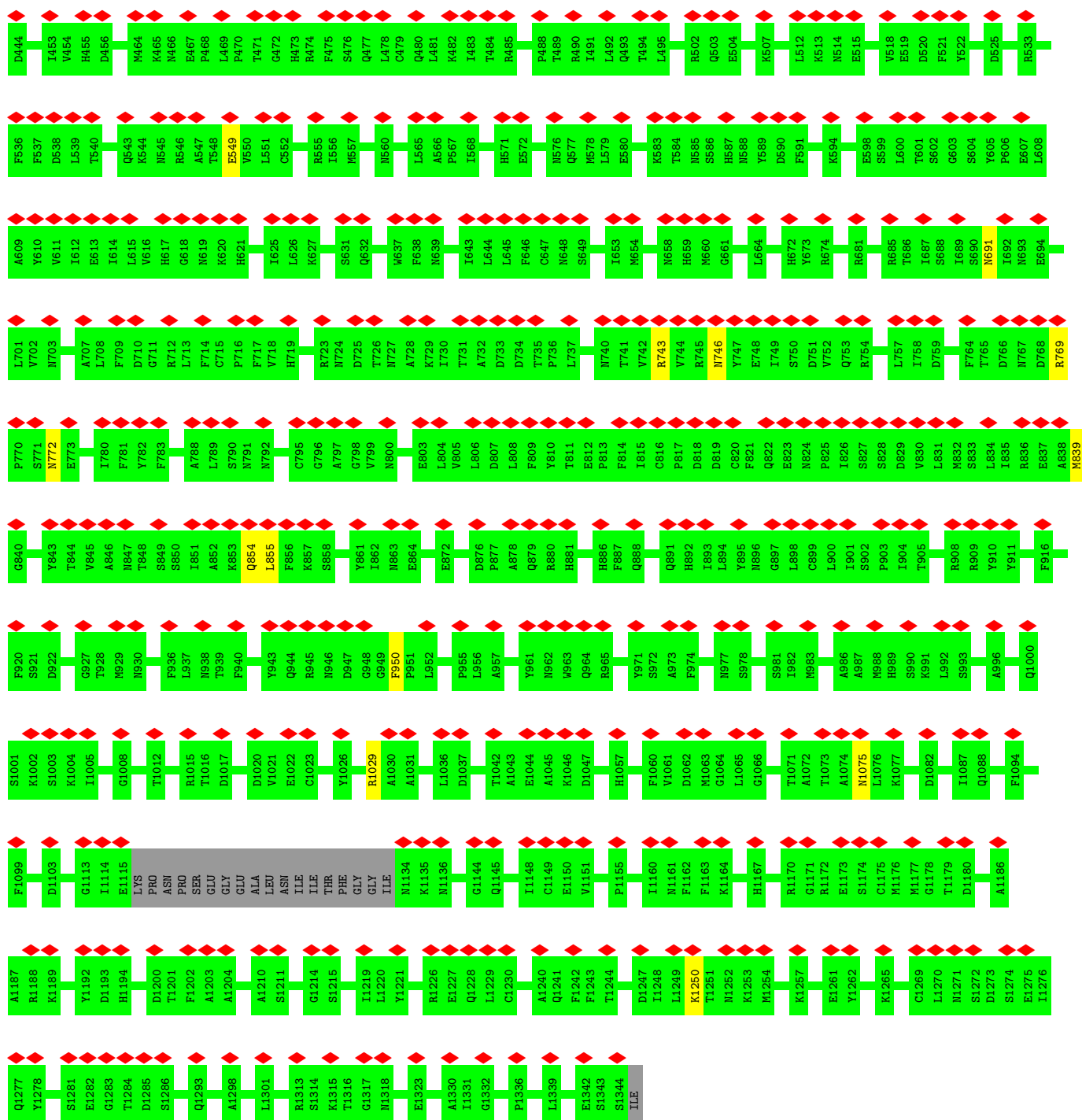
• Molecule 1: Major capsid protein



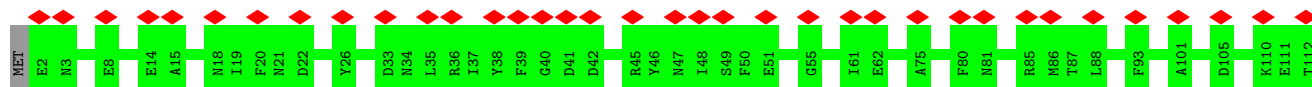
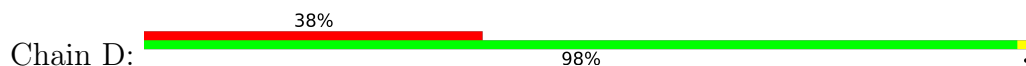


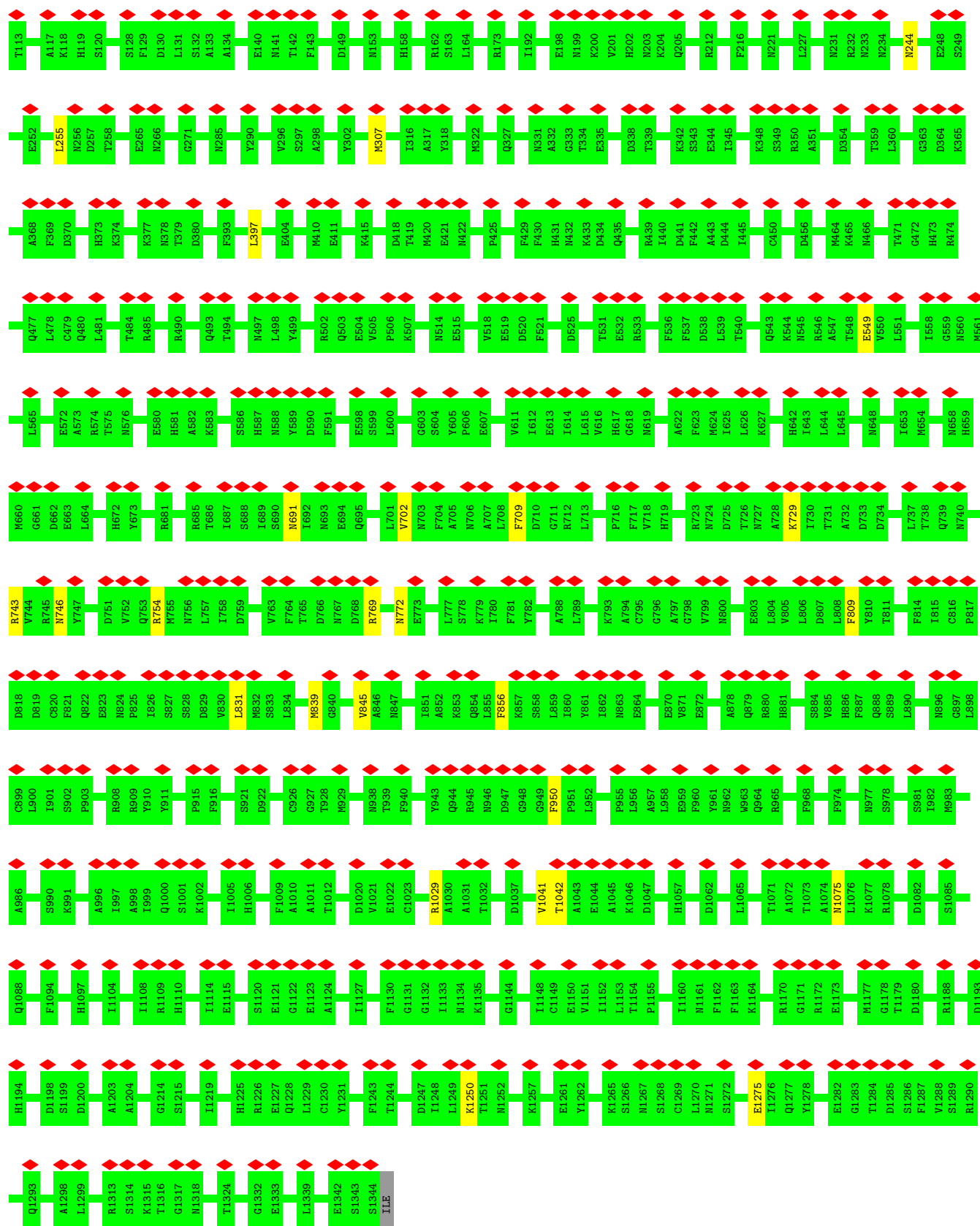
• Molecule 1: Major capsid protein



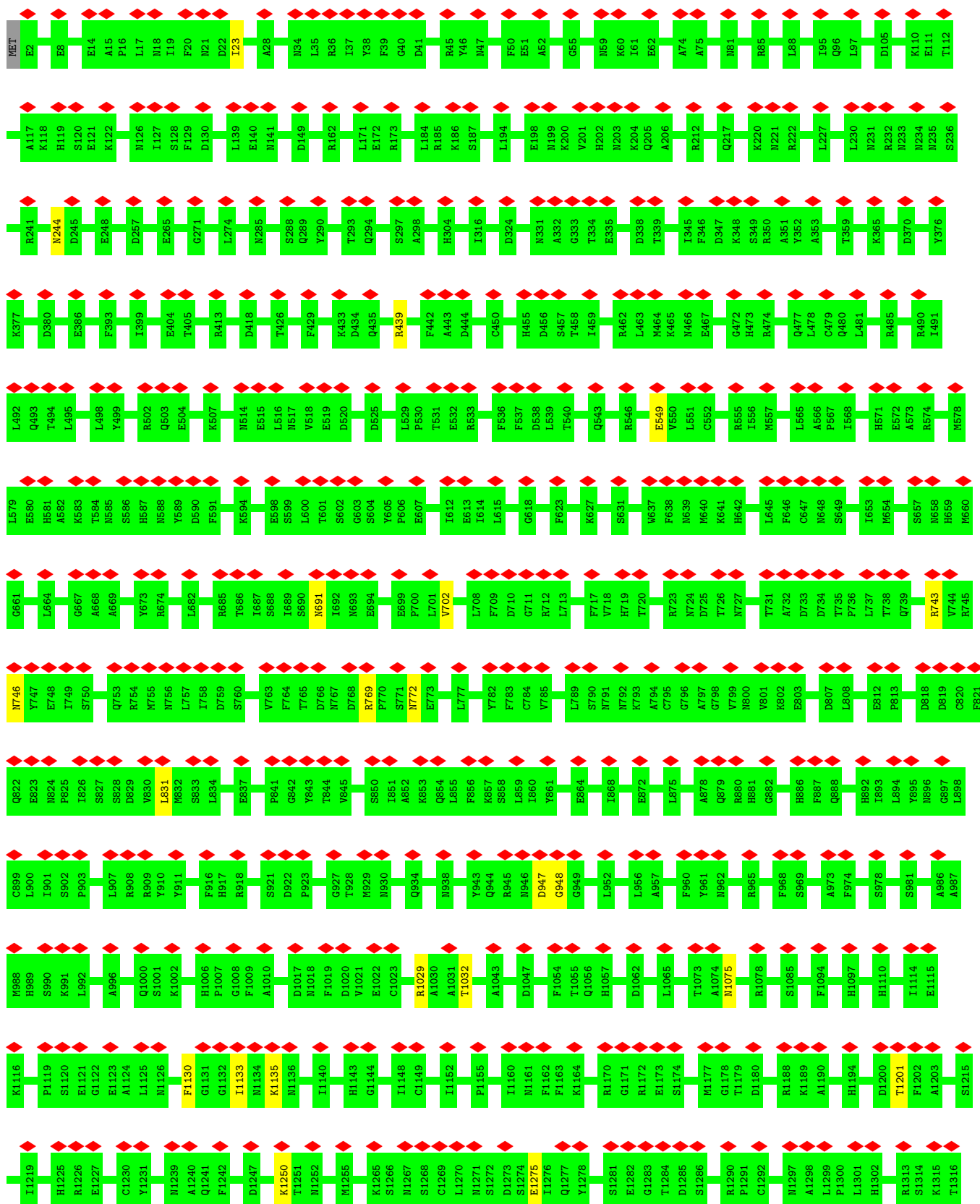


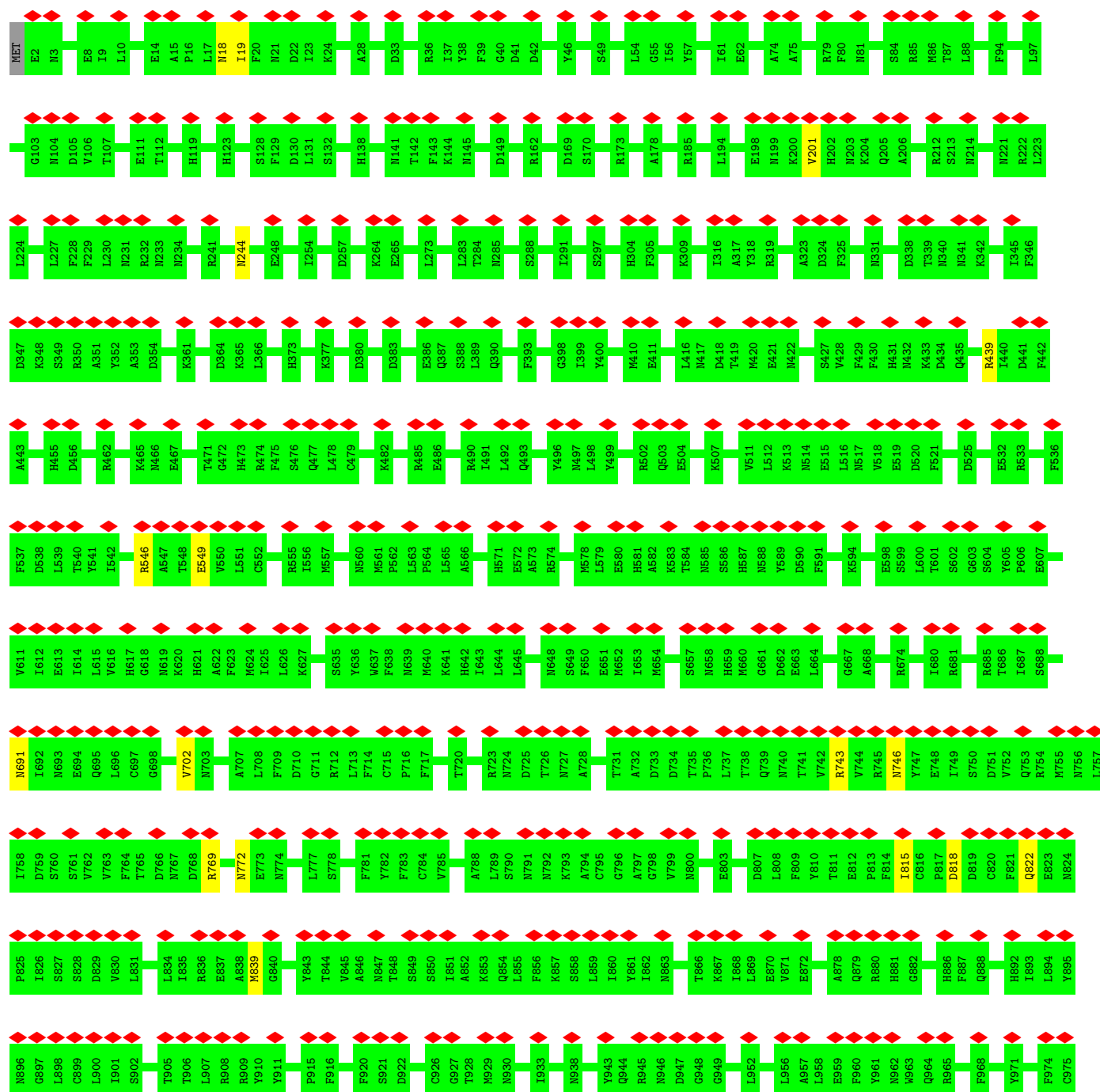
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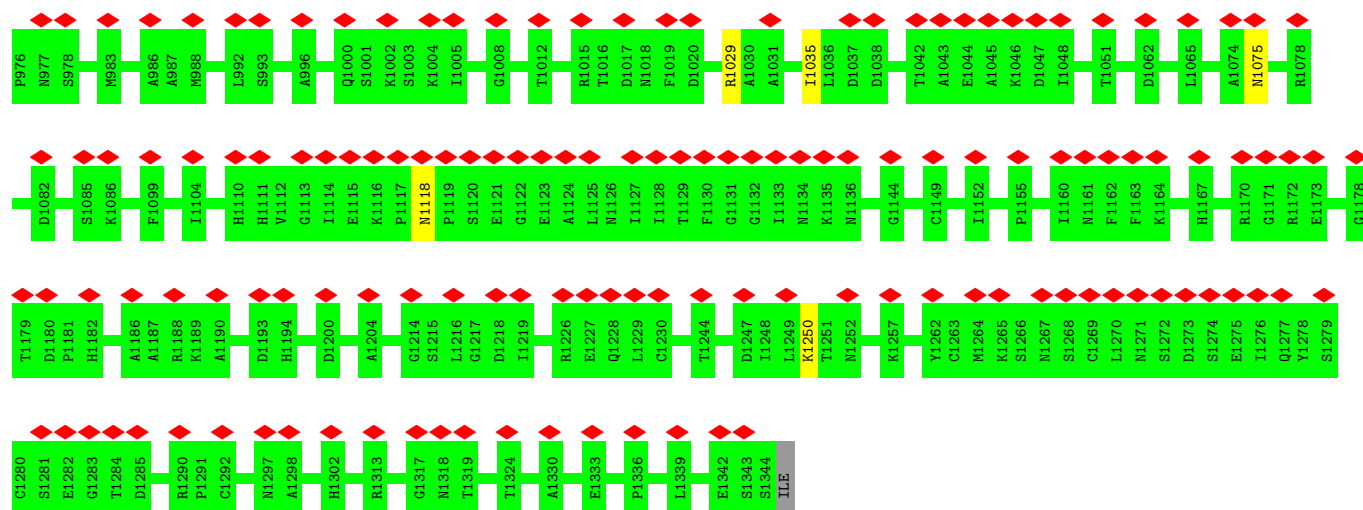




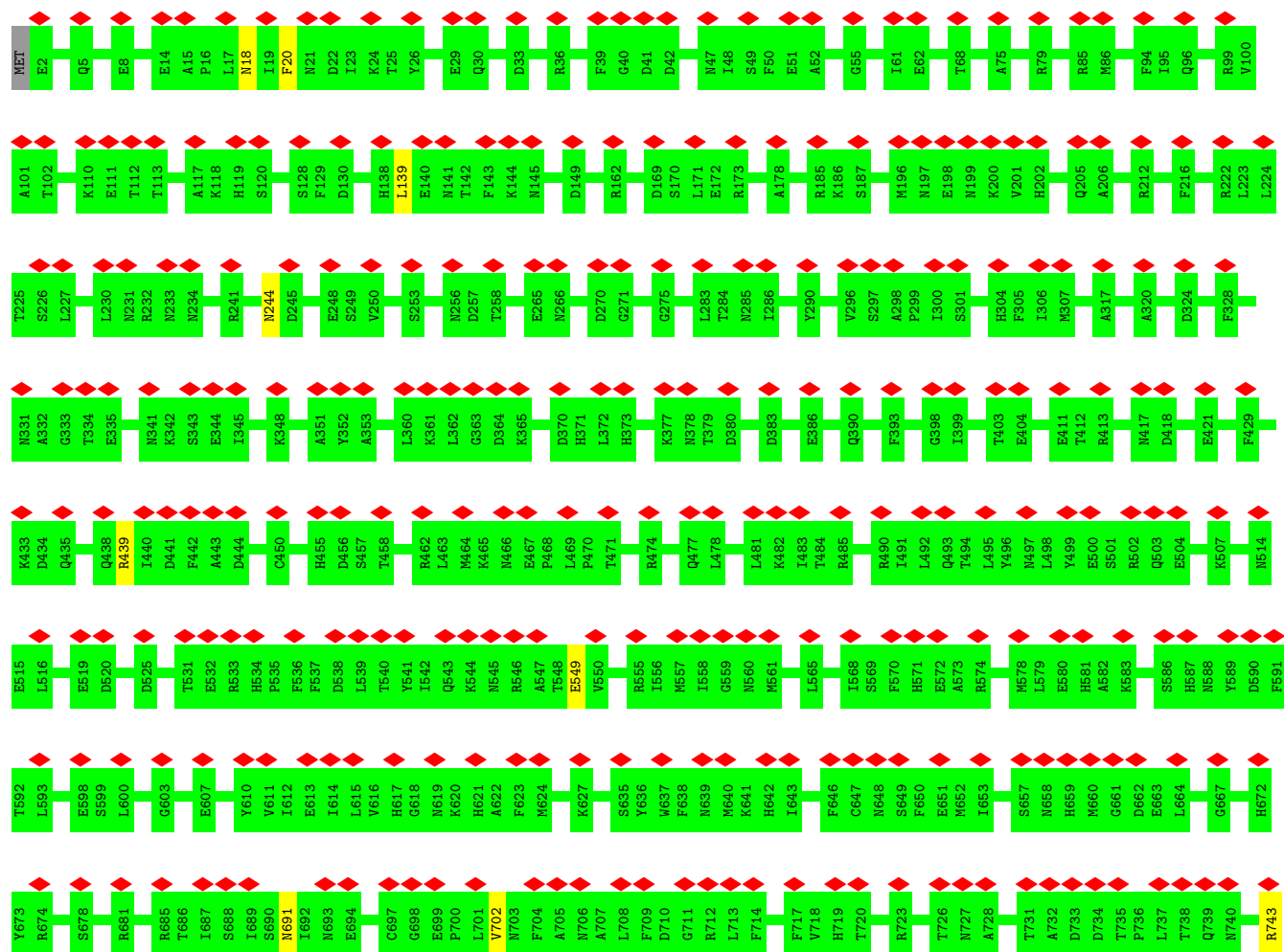
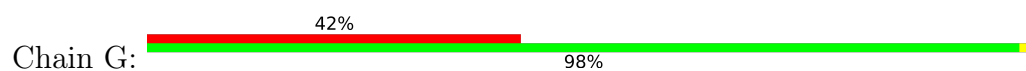
- Molecule 1: Major capsid protein



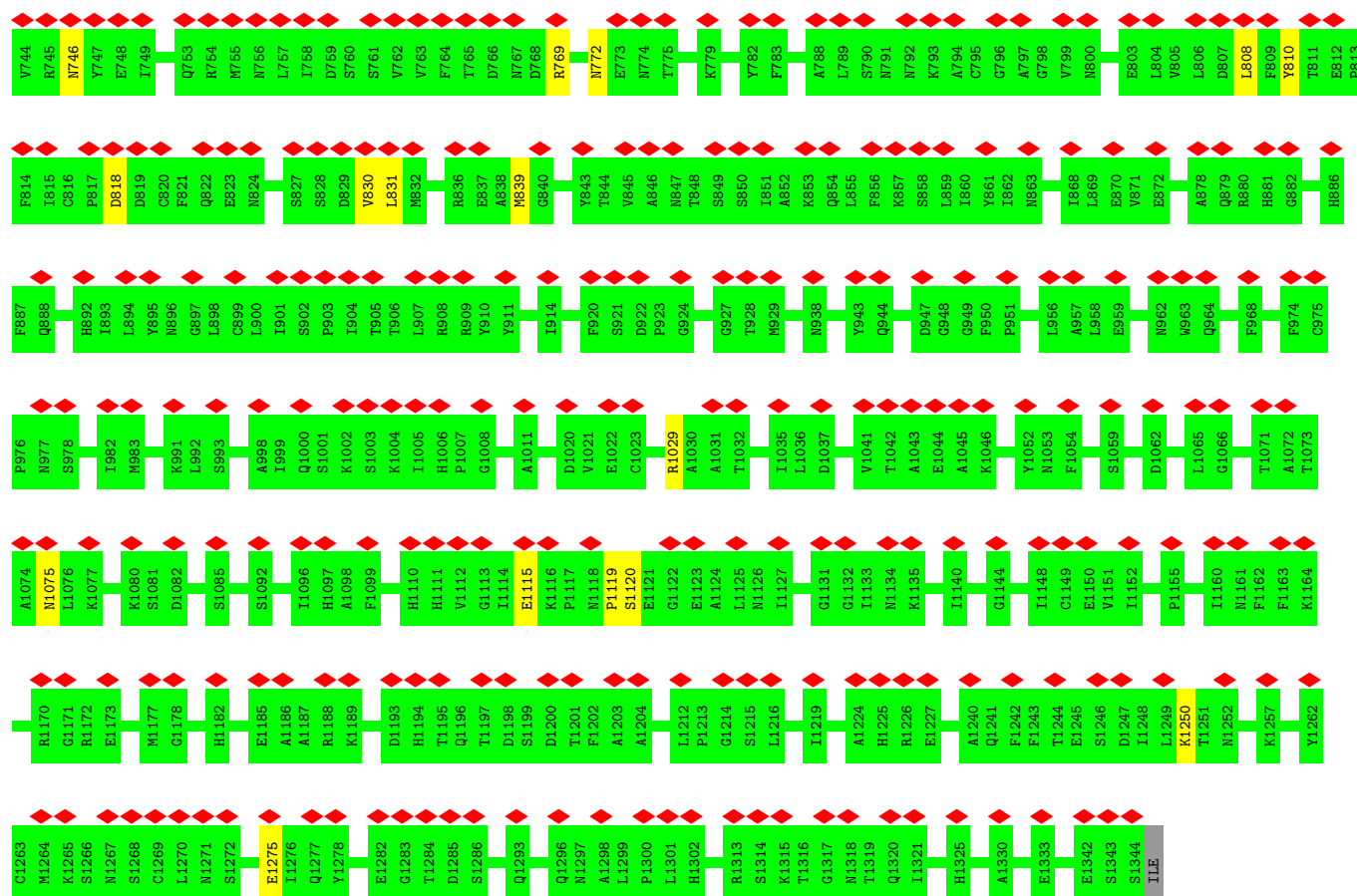




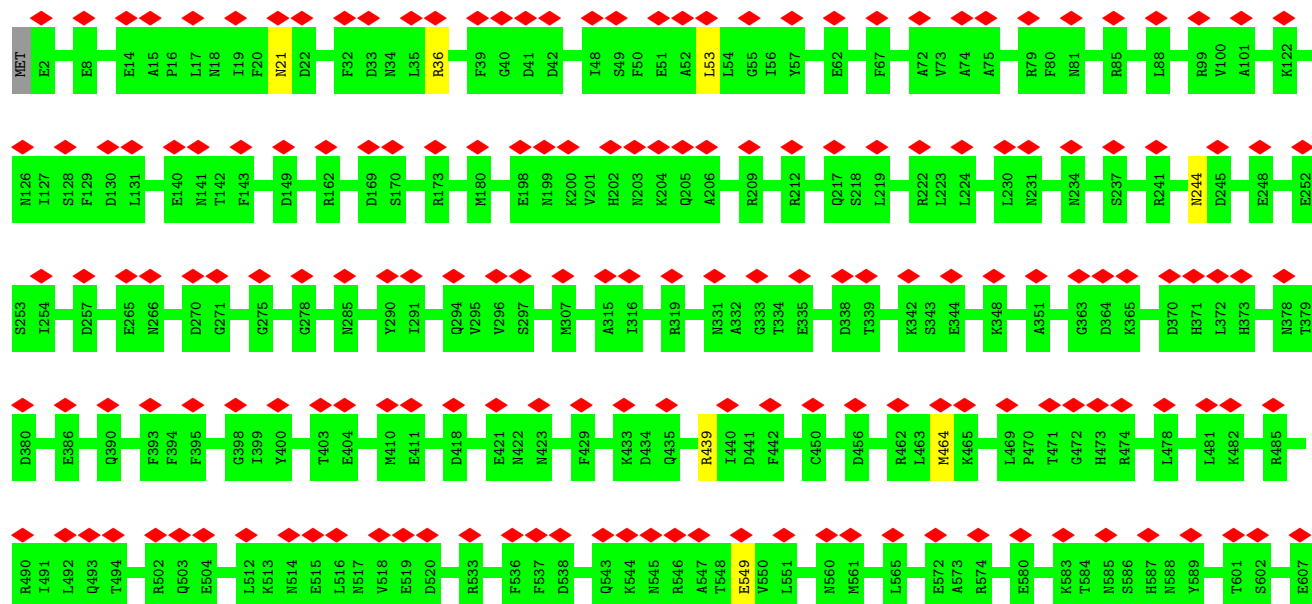
• Molecule 1: Major capsid protein

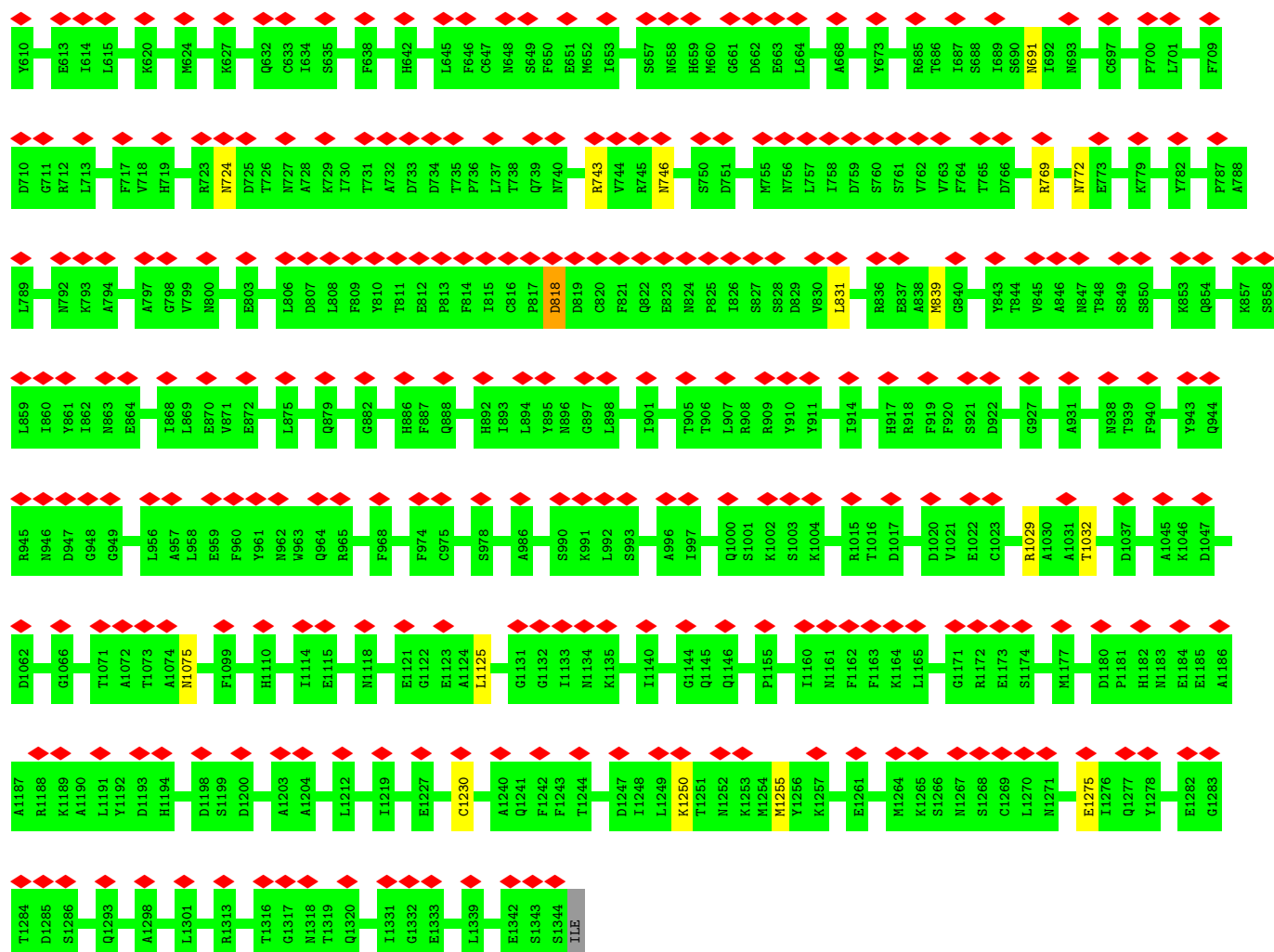




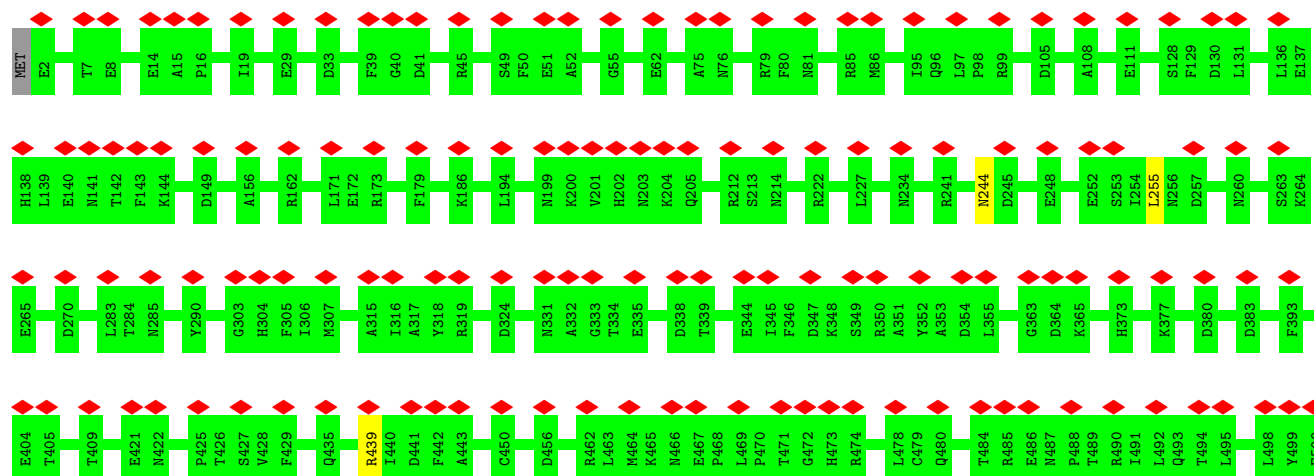
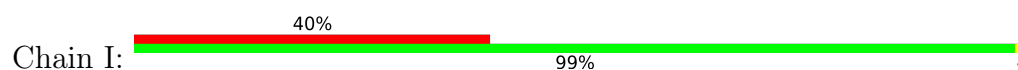


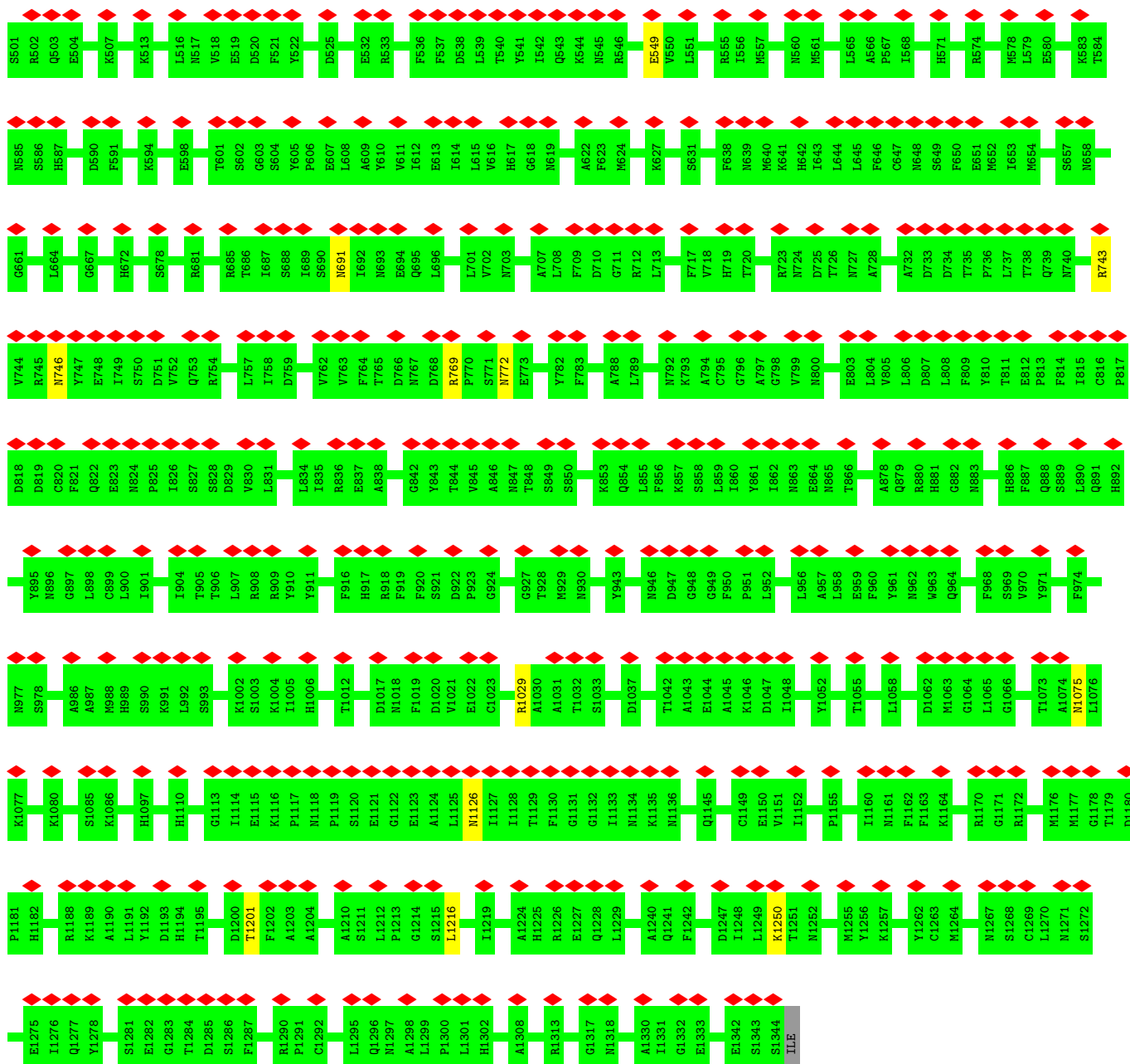
• Molecule 1: Major capsid protein



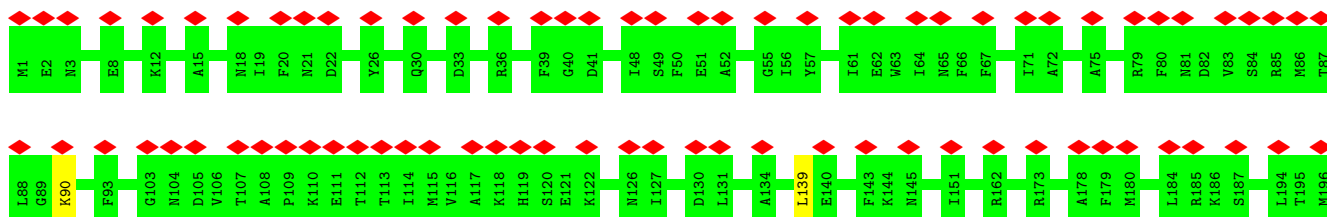


• Molecule 1: Major capsid protein

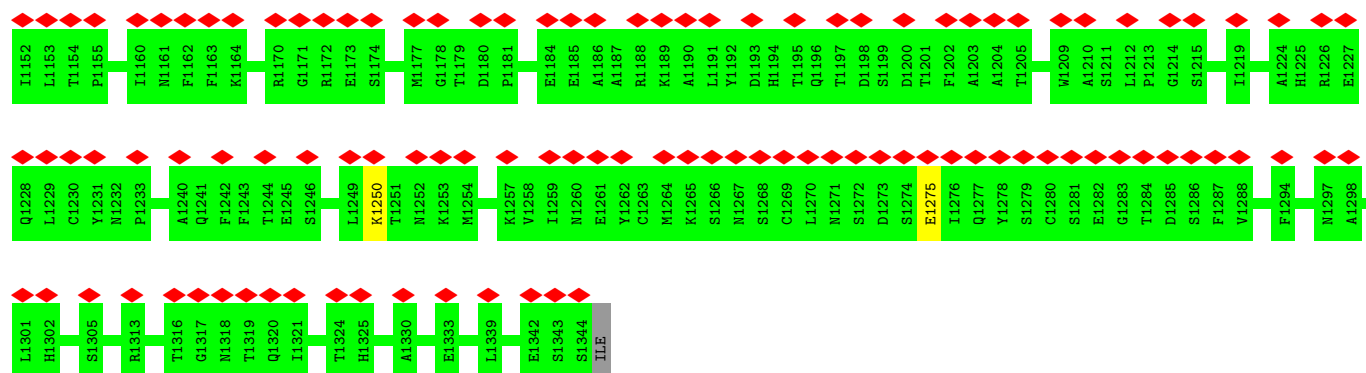




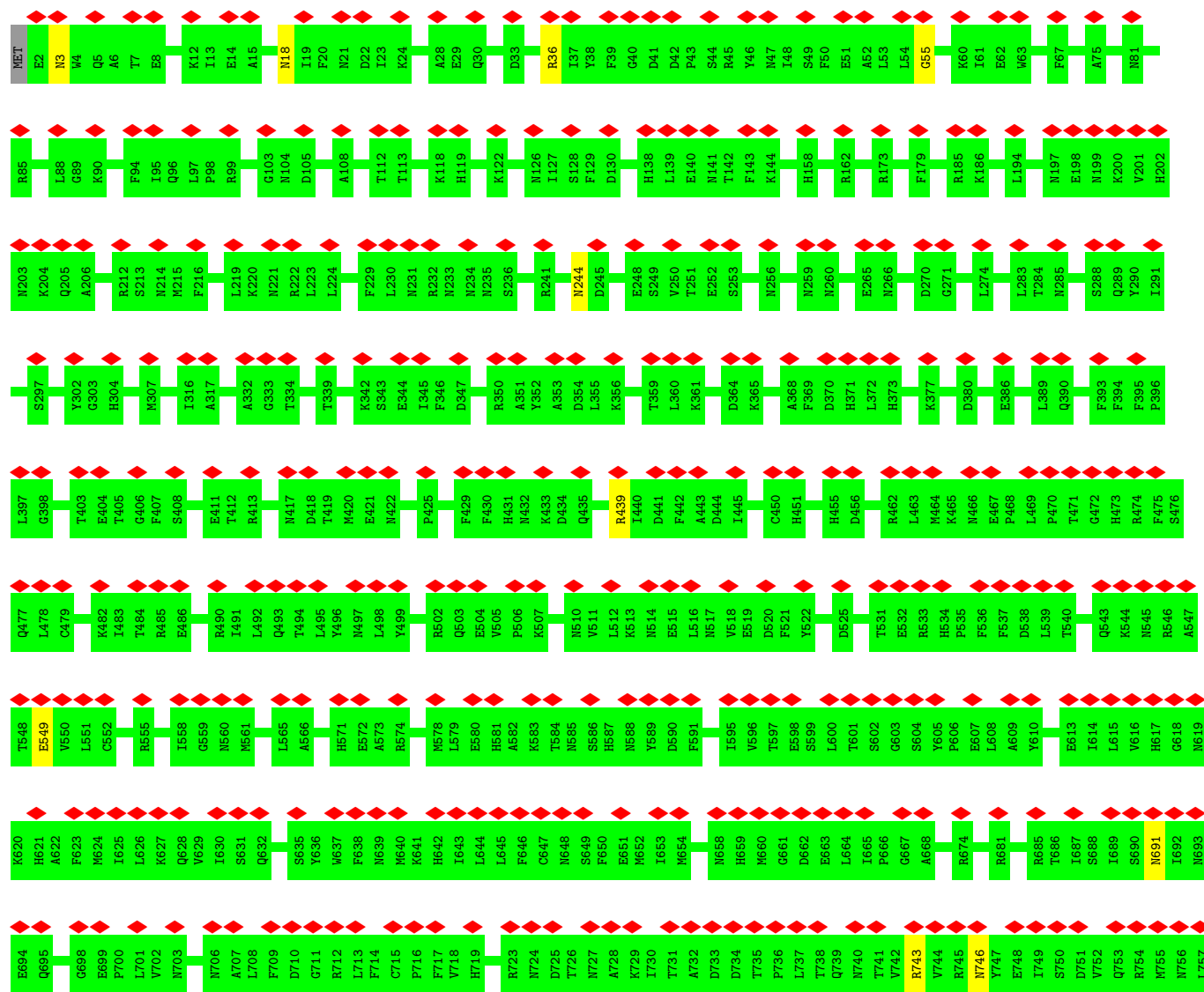
• Molecule 1: Major capsid protein

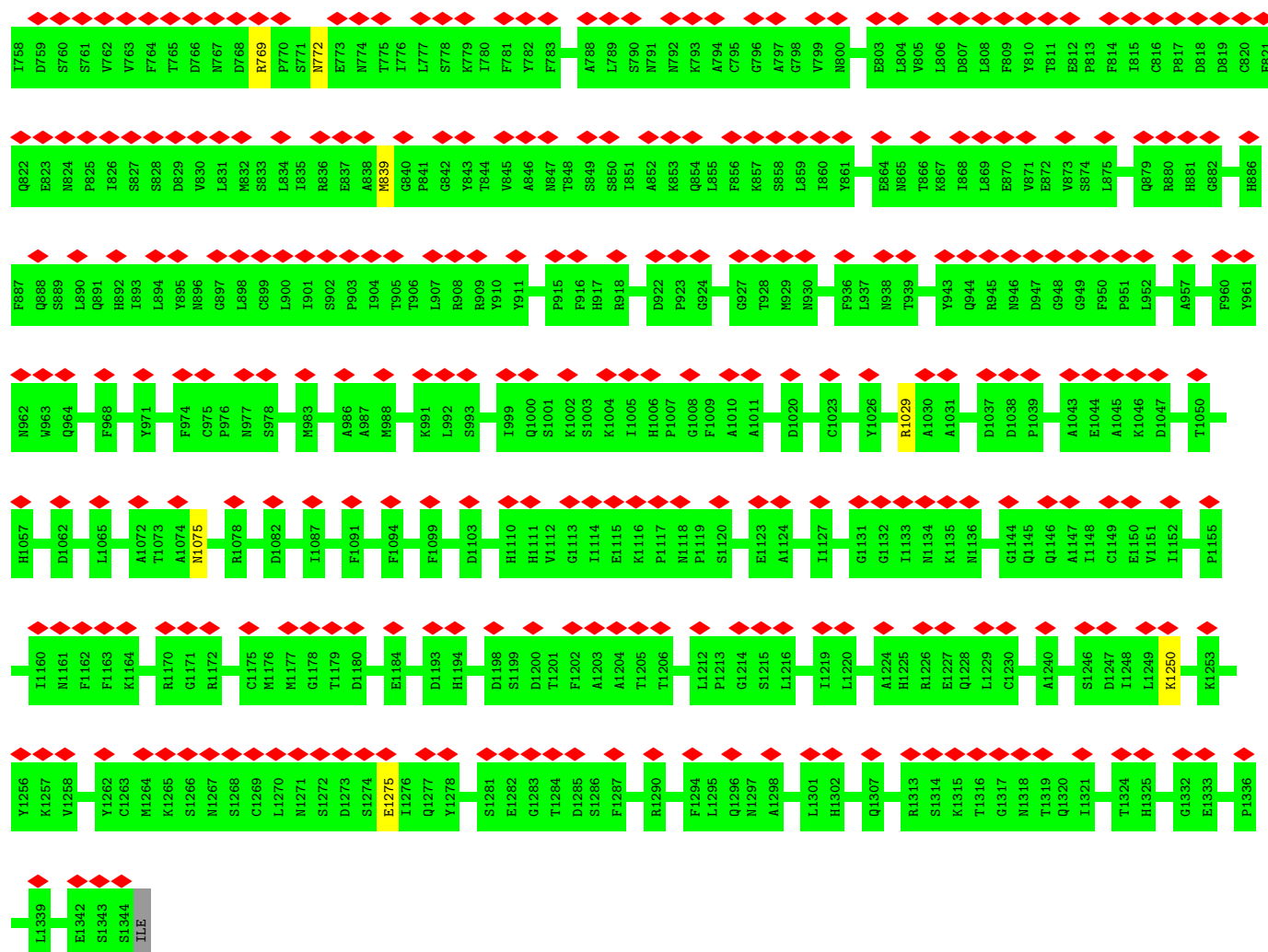


T1073	A1074	N1075	L1076	K1077	K1080	S1081	D1082	M1083	G1084	S1085	K1086	F1094	P1095	I1096	H1097	R1109	H1110	H1111	V1112	G1113	I1114	E1115	K1116	P1117	N1118	P1119	S1120	E1121	G1122	E1123	A1124	L1125	N1126	I1127	I1128	F1130	G1131	G1132	I1133	N1134	K1135	N1136	P1137	S1138	S1139	I1140	L1141	D1062	M1063	G1064	L1065	G1066	F1067	C1149			
A987	M988	H989	S990	K991	L992	S993	P994	V995	A996	I997	A998	I999	Q1000	S1001	K1002	S1003	K1004	I1005	H1006	P1007	G1008	F1009	A1010	A1011	T1012	D1017	D1020	Y1021	E1022	R1029	A1030	A1031	L1036	D1037	D1038	P1039	T1040	A1043	E1044	A1045	K1046	D1047	T1055	F1060	V1061	D1062	M1063	G1064	L1065	G1066	F1067						
E837	A838	M839	G840	P841	C842	Y843	T844	V845	A846	N847	T848	S849	S850	T851	A852	K853	Q854	L855	F856	K857	S858	L859	T860	N863	E864	N865	T866	K867	L868	L869	E872	A876	Q879	R880	H881	Q882	N883	S884	V885	H886	F887	Q888	S889	L890	P891	H892	T893	L894	Y895	P976	N977	S978	L979	A986			
E773	L777	S778	K779	L780	F781	Y782	F783	C784	V785	L786	F787	A788	L789	N792	K793	A794	C795	G796	A797	V798	V799	N800	K802	E803	L806	D807	L808	F809	Y810	T811	E812	P813	F814	I815	C816	P817	D818	D819	C820	F821	Q822	E823	N824	P825	L826	S827	S828	D829	N830	L831	N832	L834	I835	R836			
L713	F714	C715	P716	F717	L718	H719	T720	H721	P722	R723	M724	D725	T726	N727	A728	K729	L730	T731	A732	D733	D734	T735	P736	L737	T738	Q739	N740	T741	V742	R743	R745	N746	Y747	E748	L749	S750	D751	V752	Q753	R754	M755	N756	L757	T758	D759	S760	S761	V762	V763	F764	T765	D766	N767	D768	R769	P770	N772
K641	H642	L643	L644	L645	C646	C647	N648	S649	F650	E651	M652	L653	M654	N658	H659	M660	G661	D662	E663	L664	G667	H672	Y673	R674	S678	R681	K684	R685	T686	L687	S688	L689	S690	N691	L692	N693	E694	Q695	L696	C697	L701	V702	N703	F704	A705	N706	A707	L708	F709	D710	G711	R712					
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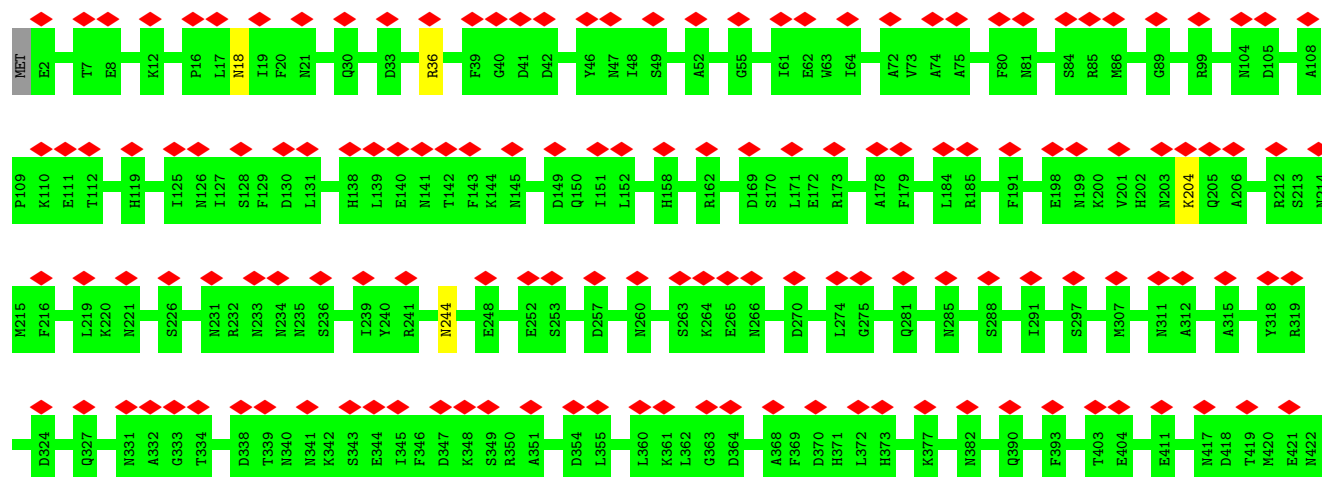


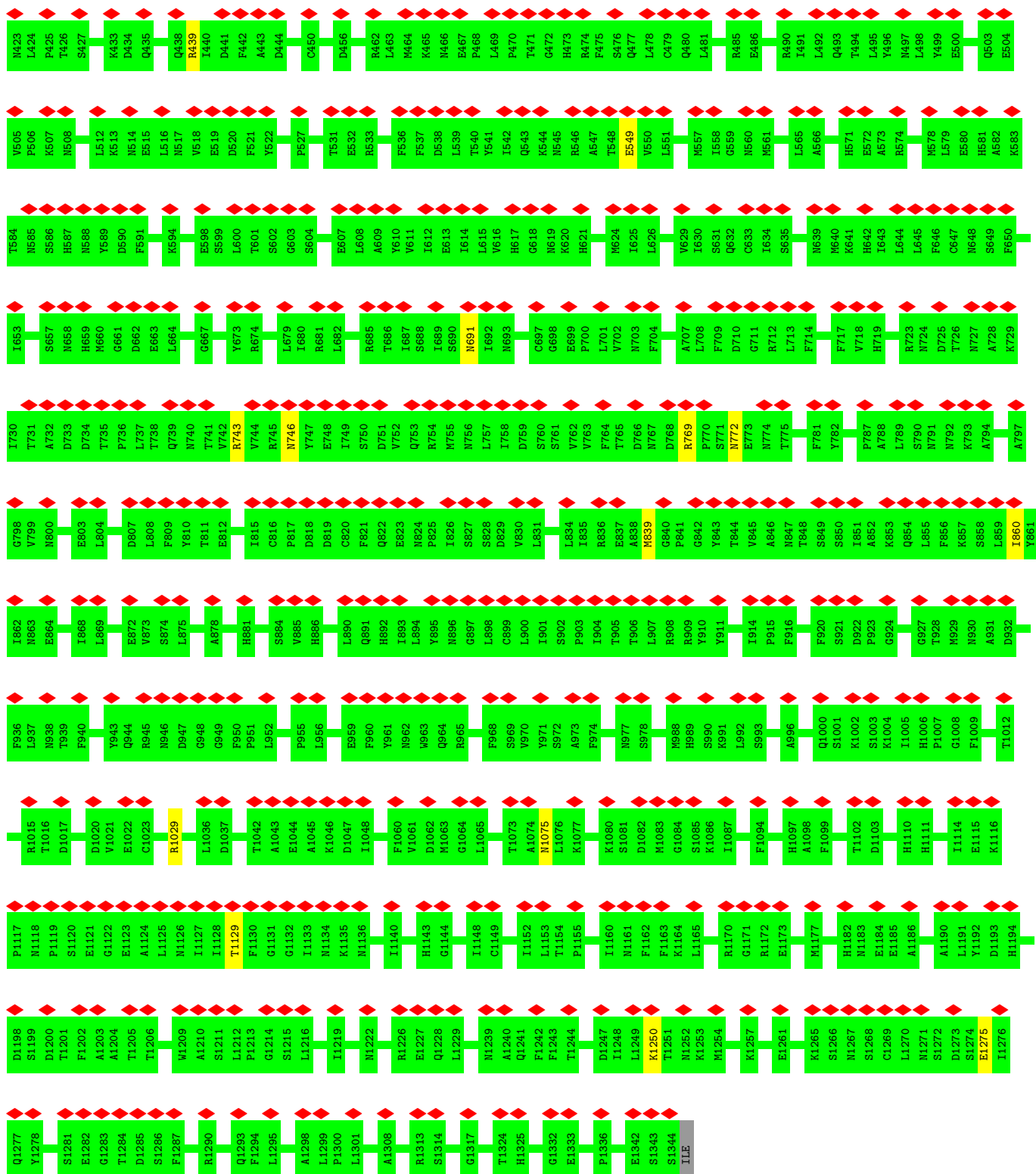
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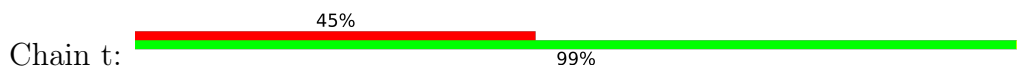


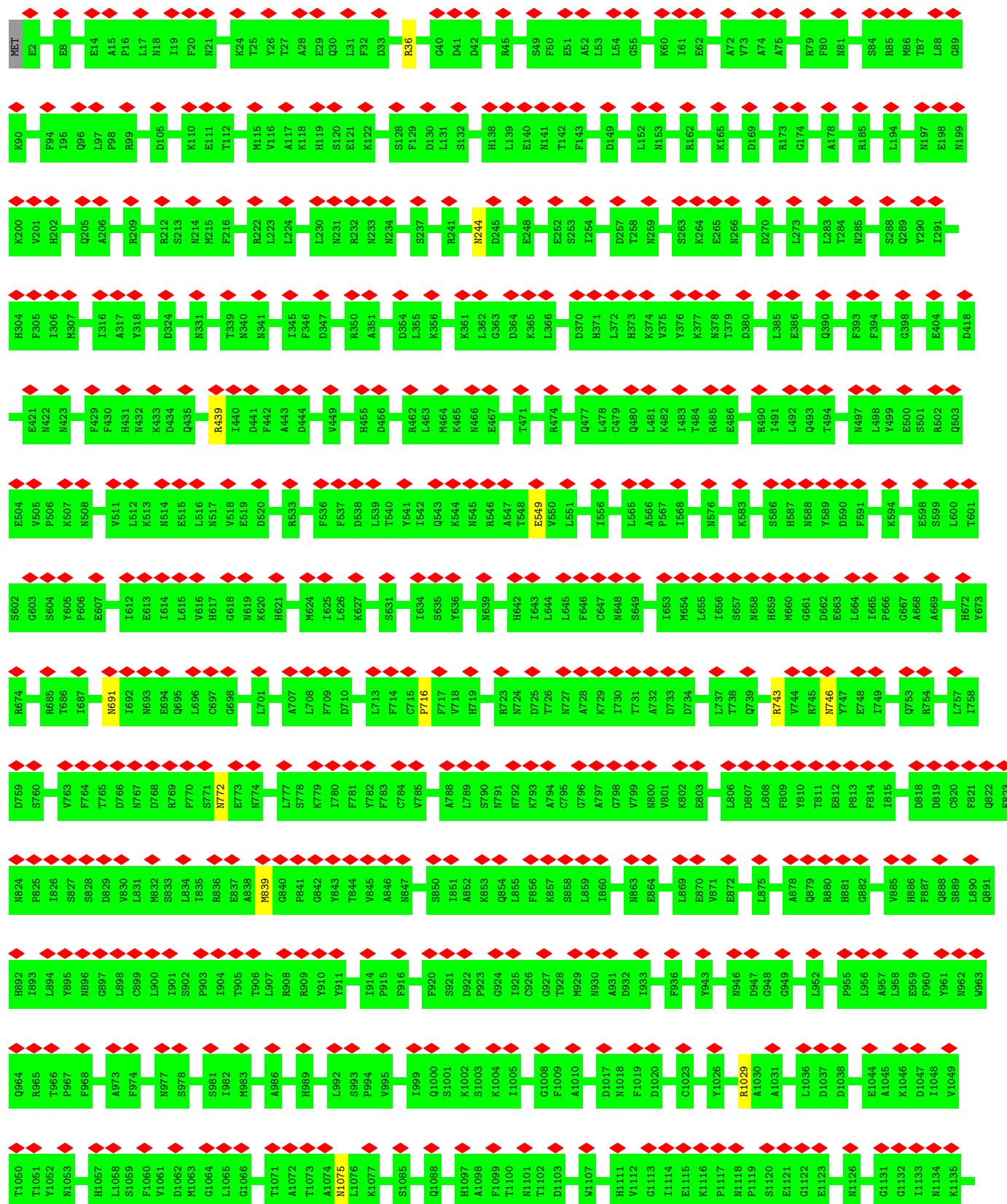
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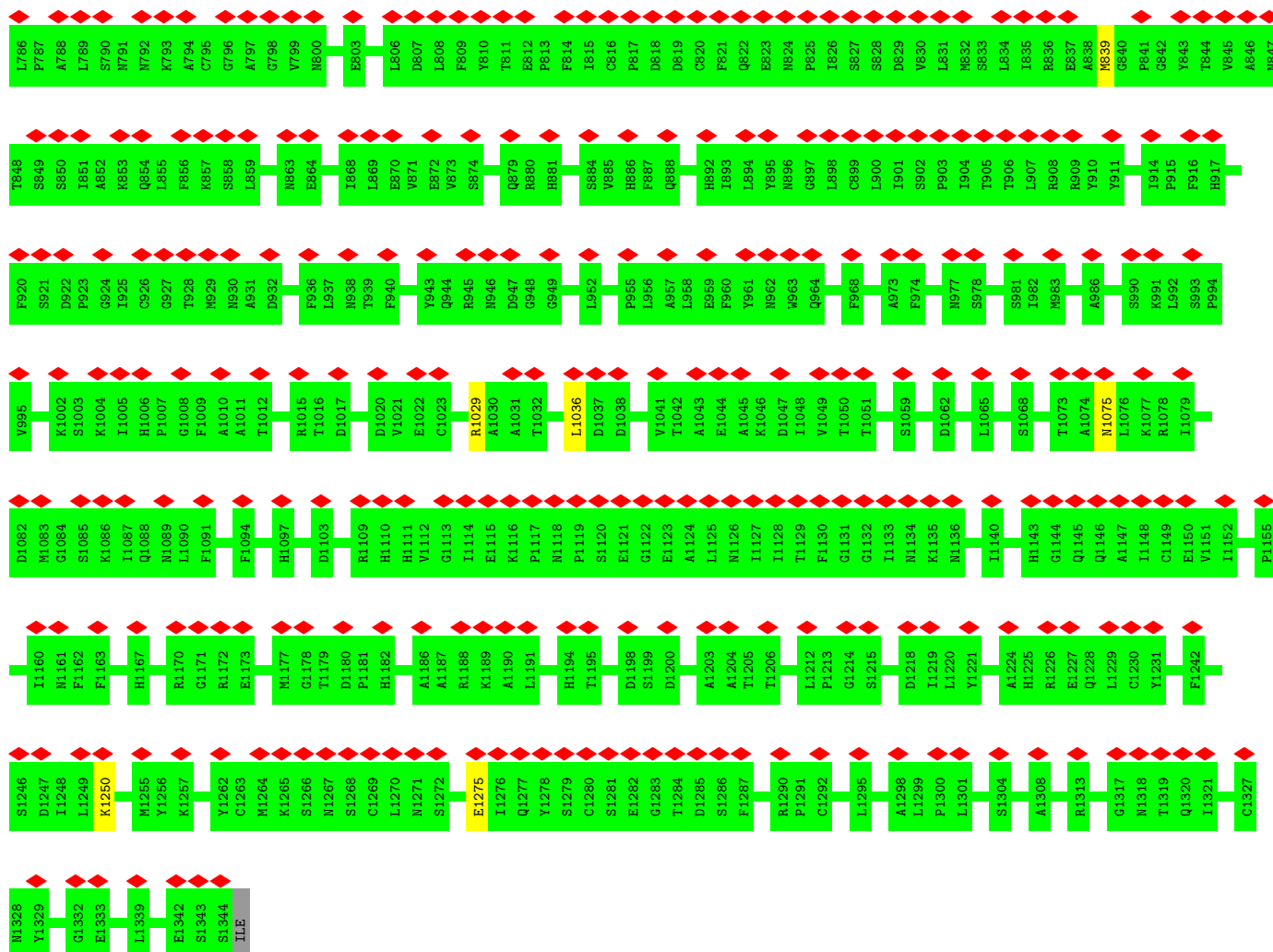
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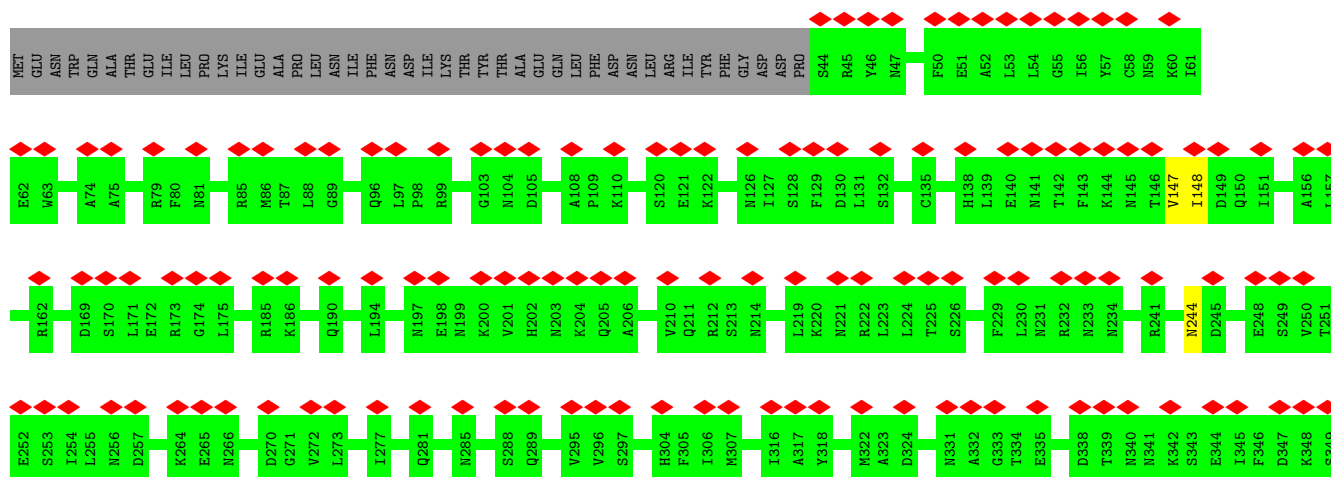








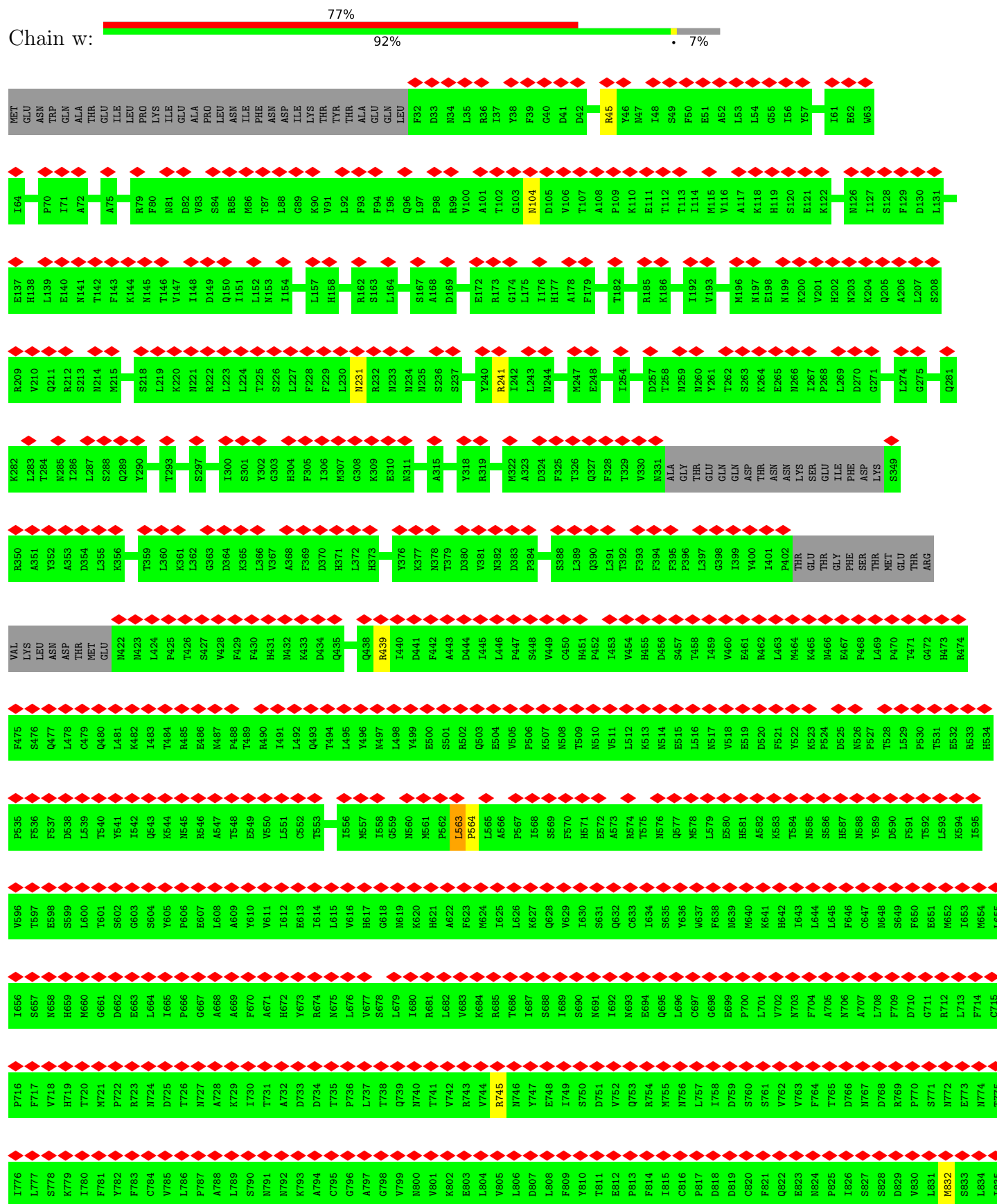
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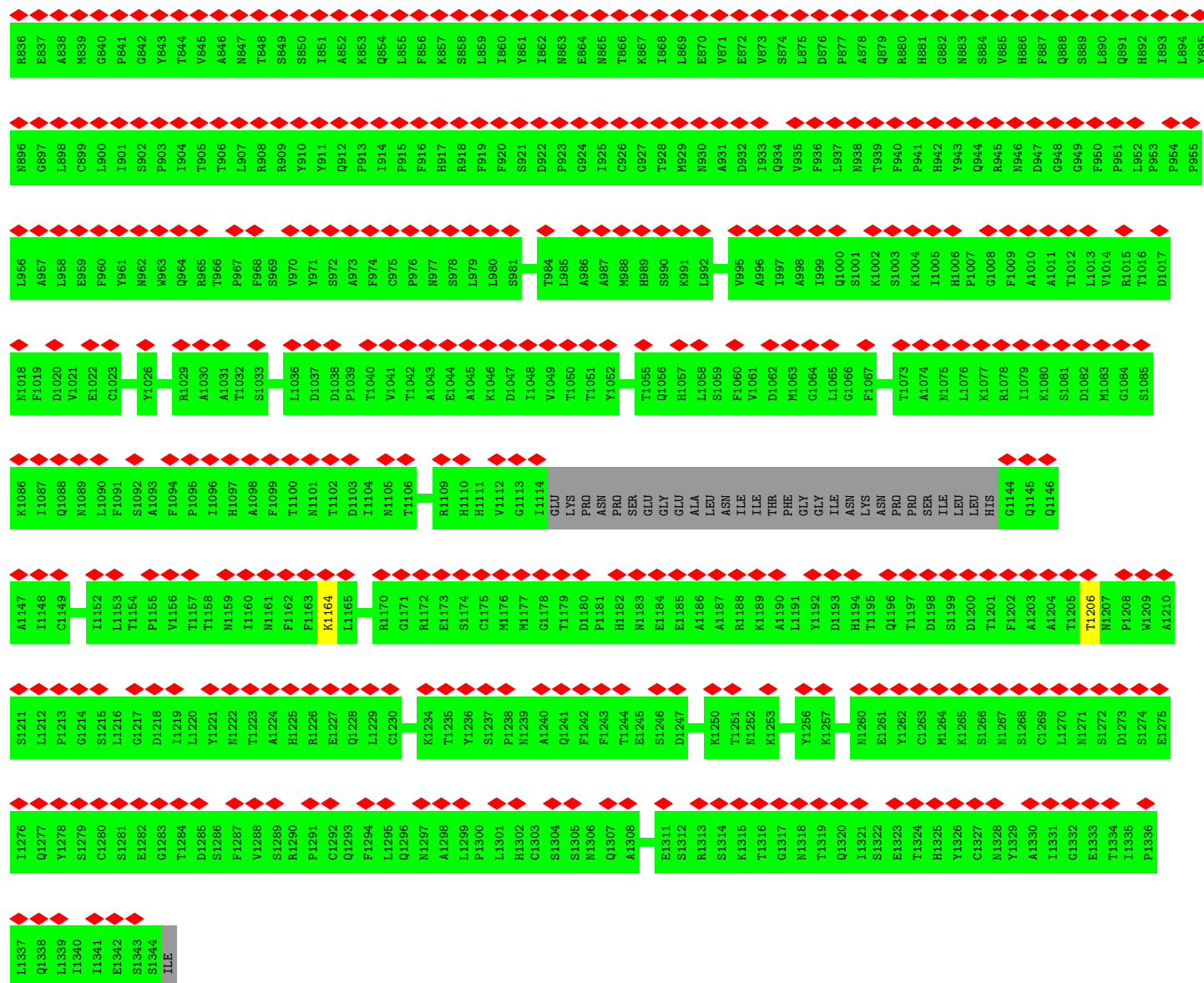


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## ● Molecule 1: Major capsid protein

Chain w:





• Molecule 2: Large structural phosphoprotein





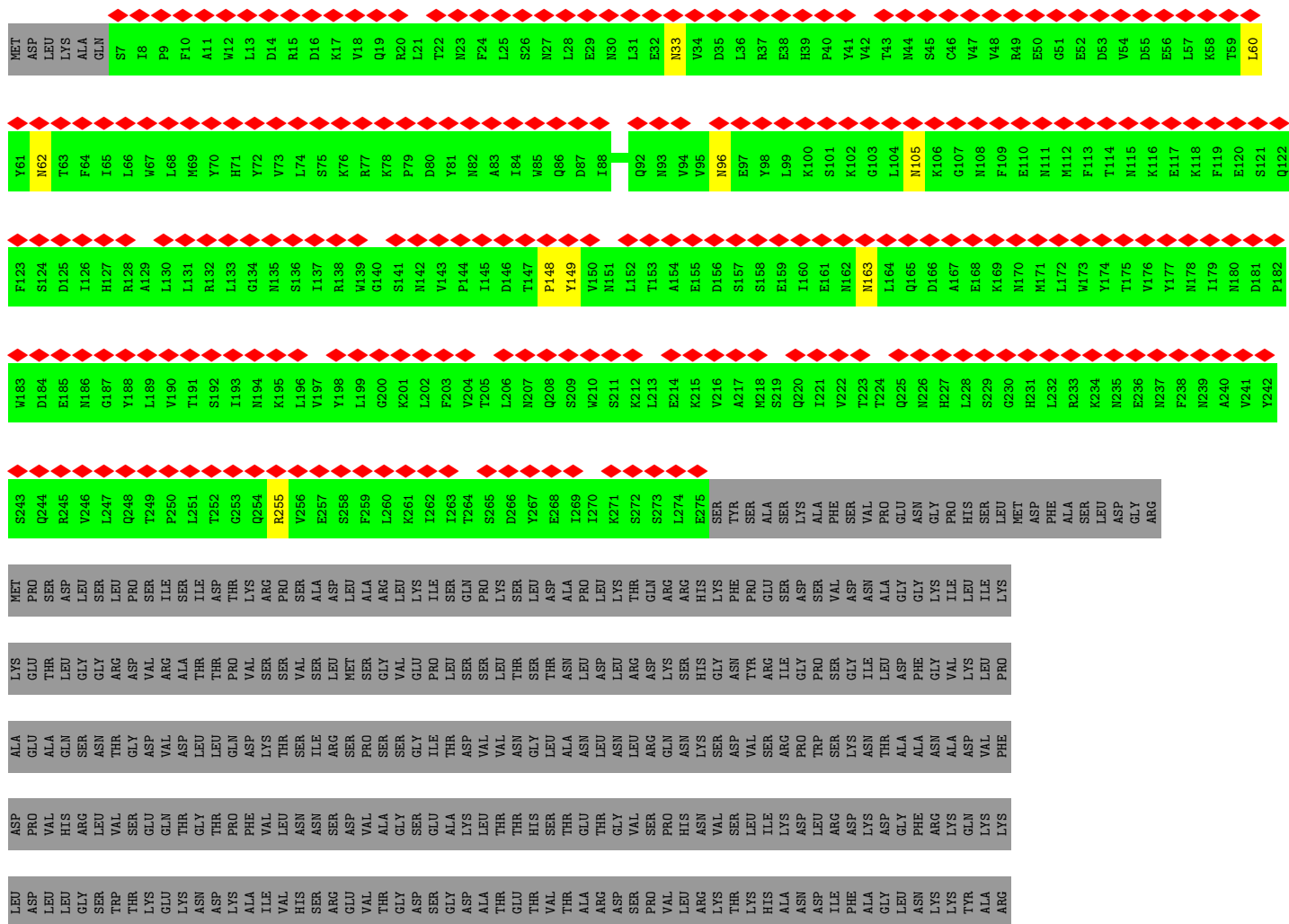




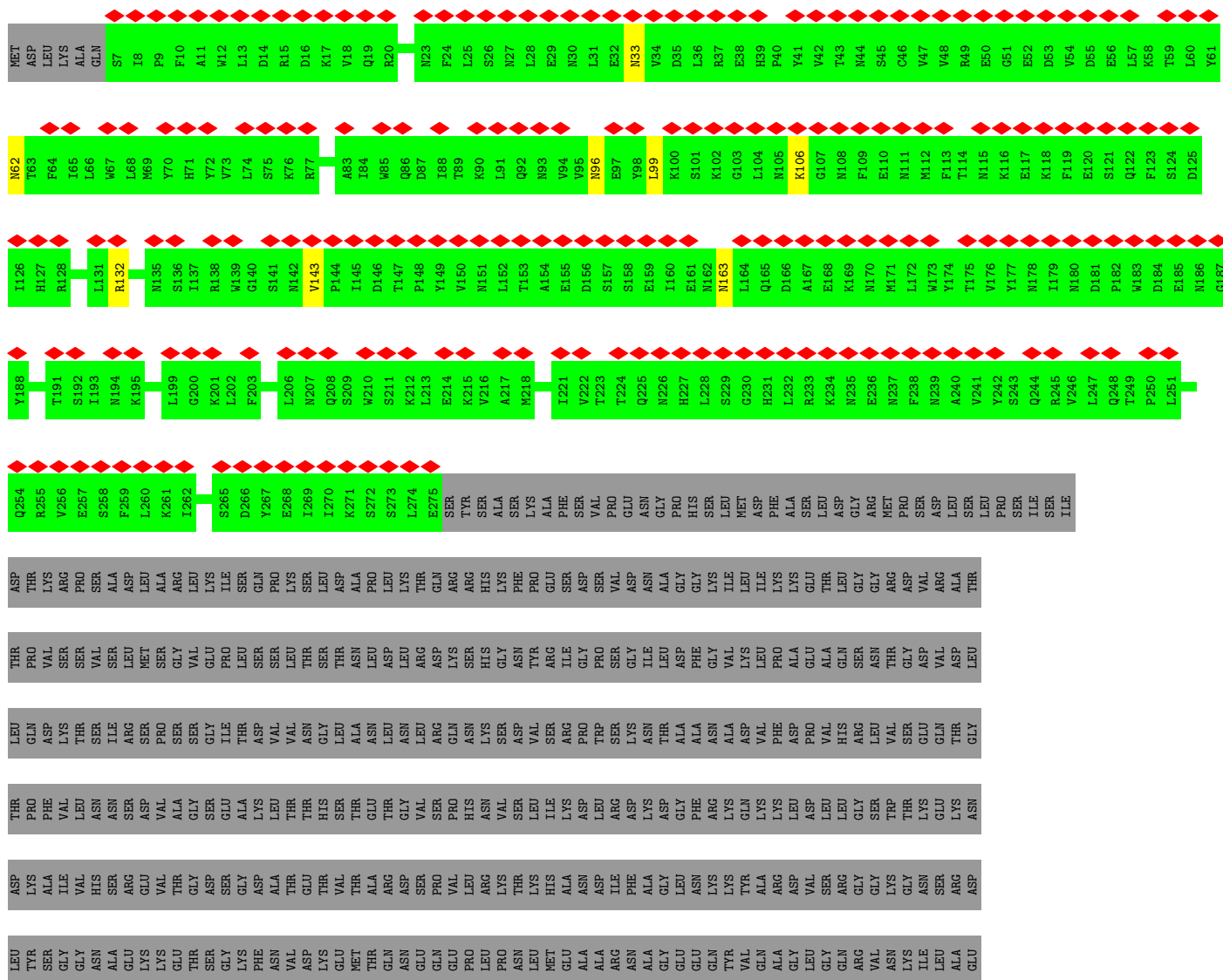


- Molecule 2: Large structural phosphoprotein

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- Molecule 2: Large structural phosphoprotein



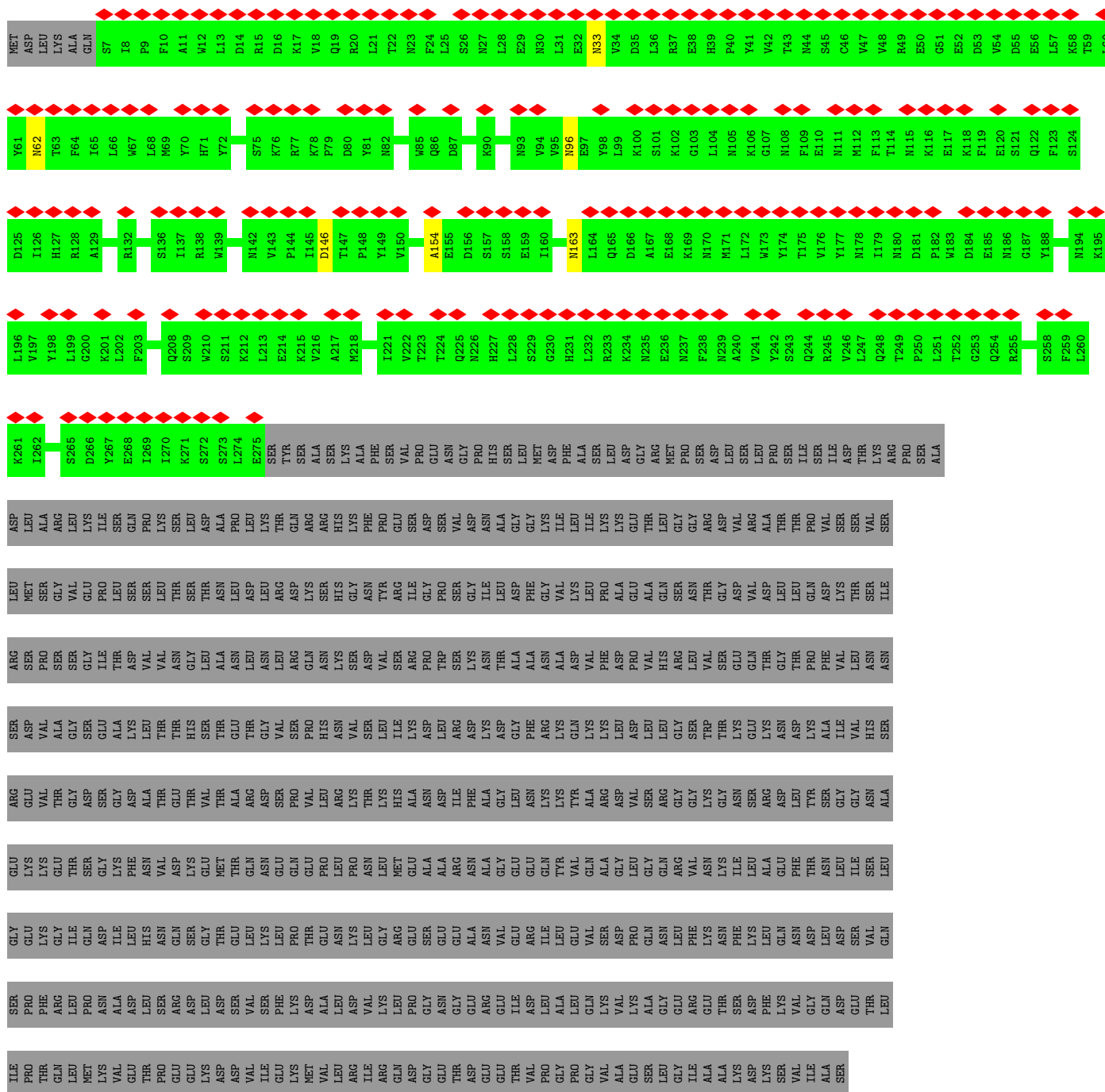
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	ILE	GLN	GLY
	PRO	PRO	LYS
	THR	PHE	GLU
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	LYS	LEU	GLY
	ASP	ASP	THR
	ASP	SER	GLU
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- Molecule 2: Large structural phosphoprotein

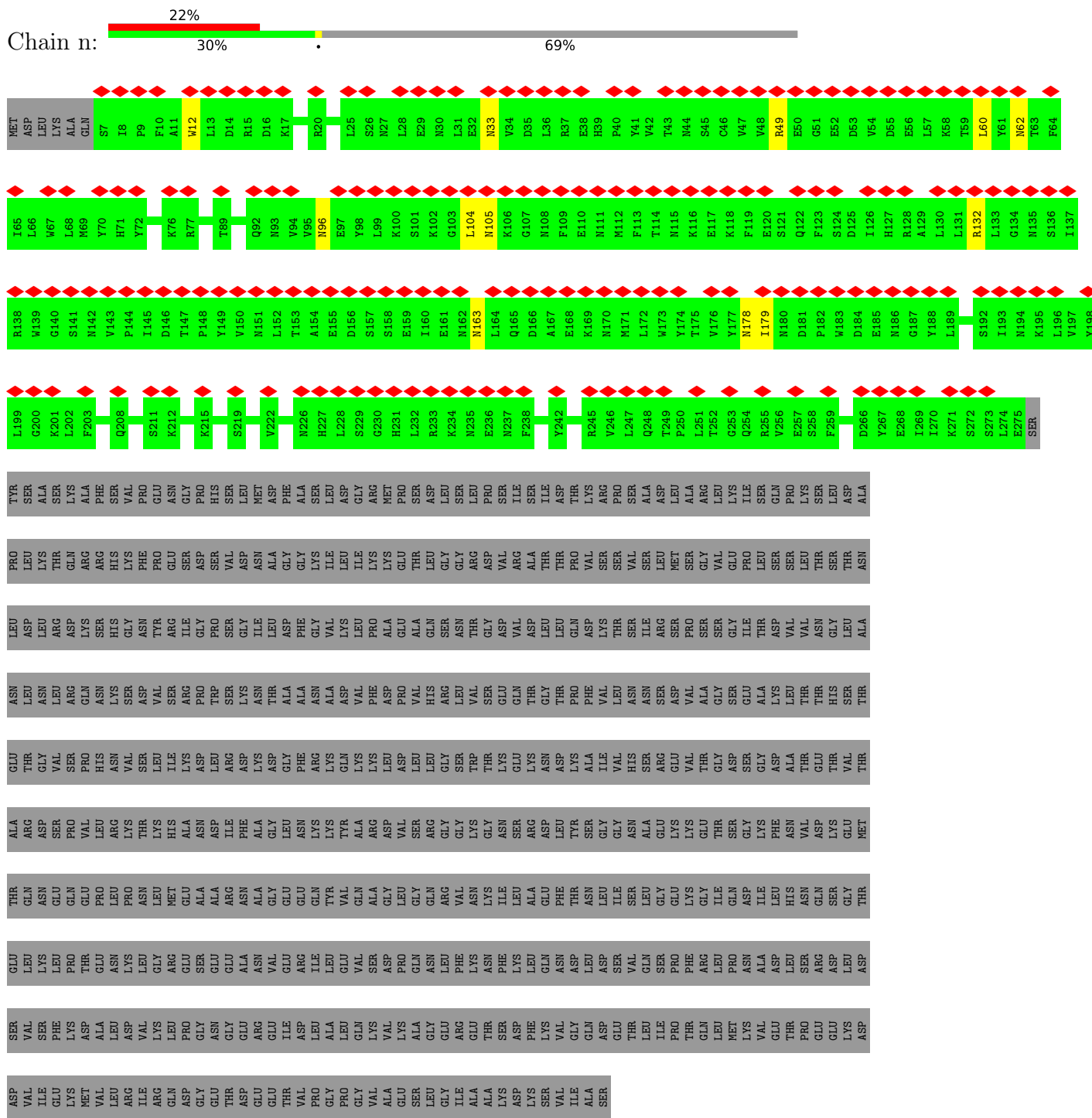
[illegible]

[illegible]

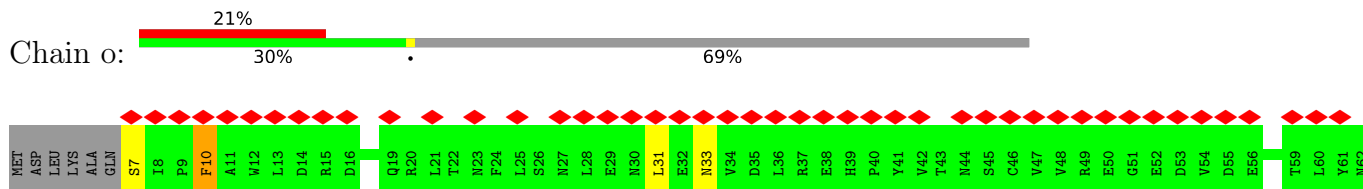
- Molecule 2: Large structural phosphoprotein

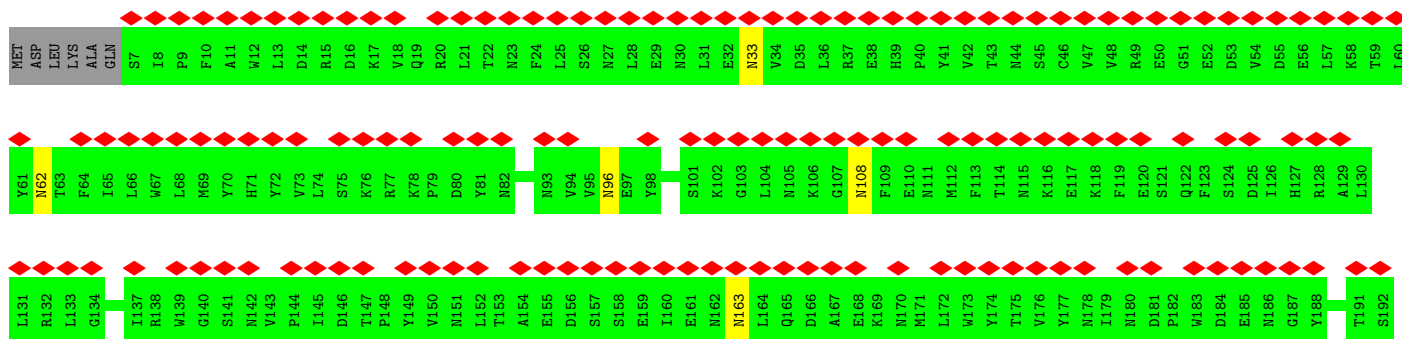
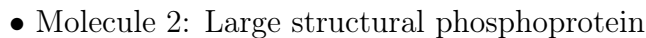


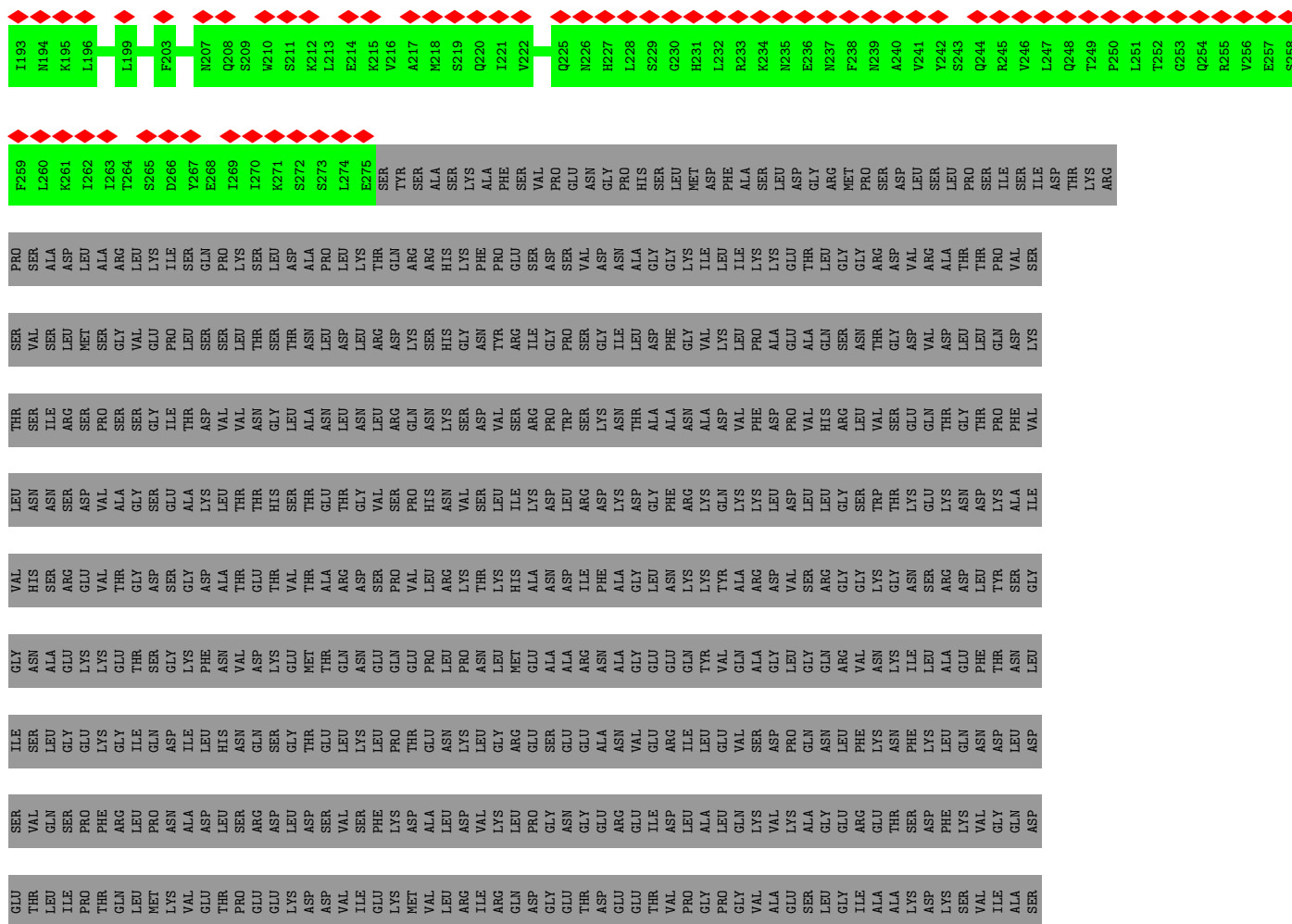
- Molecule 2: Large structural phosphoprotein



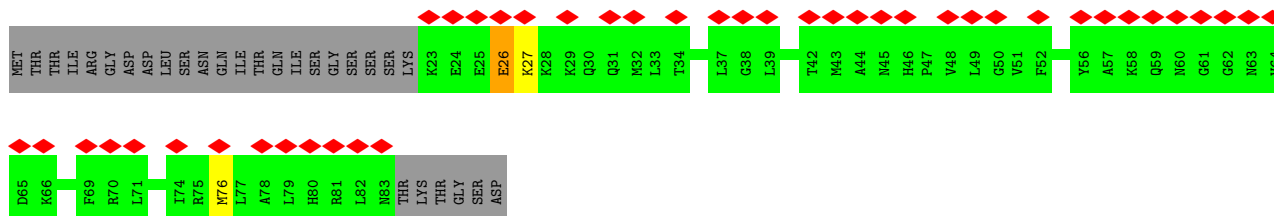
- Molecule 2: Large structural phosphoprotein



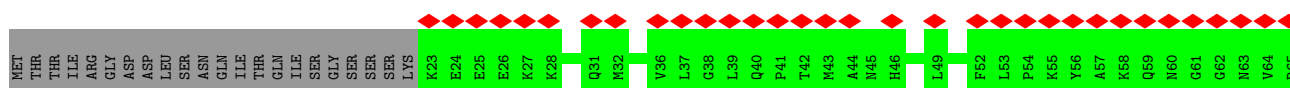




- Molecule 3: Small capsomere-interacting protein



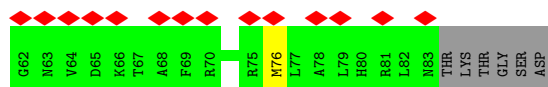
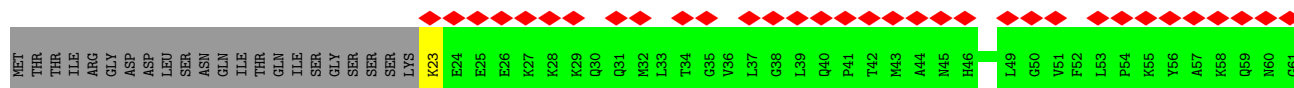
- Molecule 3: Small capsomere-interacting protein



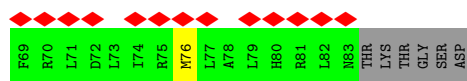
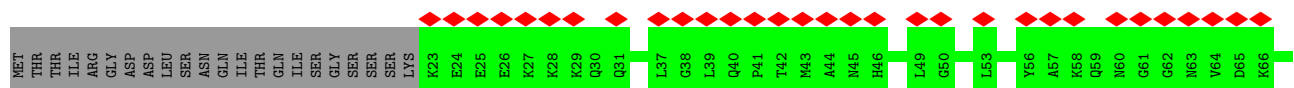




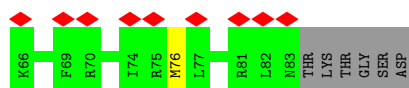
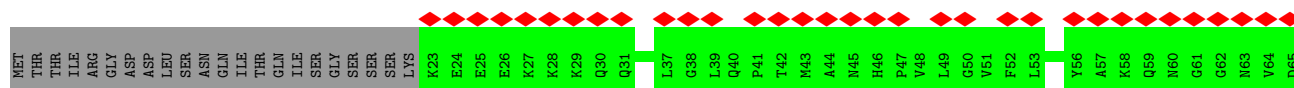
- Molecule 3: Small capsomere-interacting protein



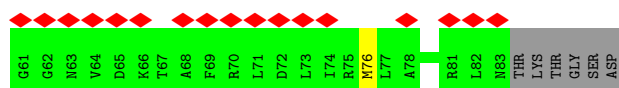
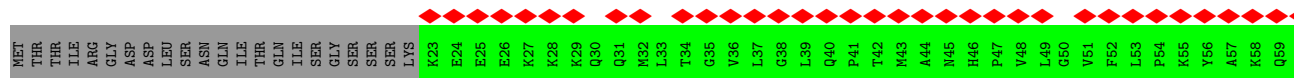
- Molecule 3: Small capsomere-interacting protein



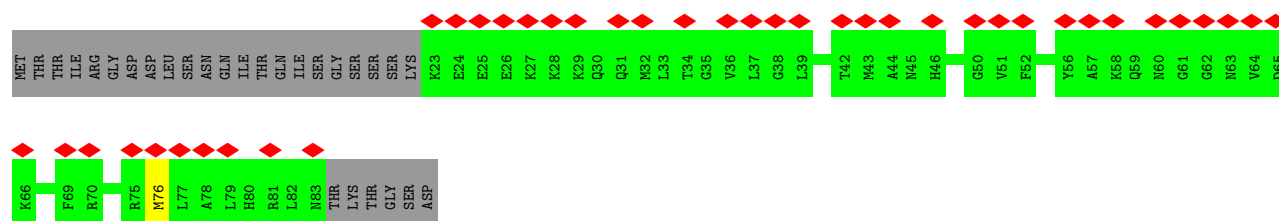
- Molecule 3: Small capsomere-interacting protein



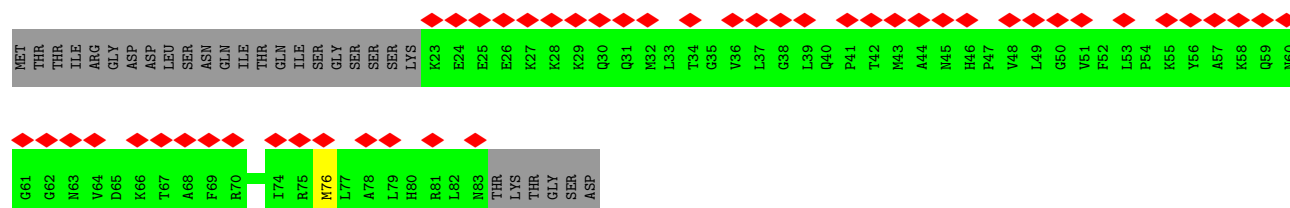
- Molecule 3: Small capsomere-interacting protein



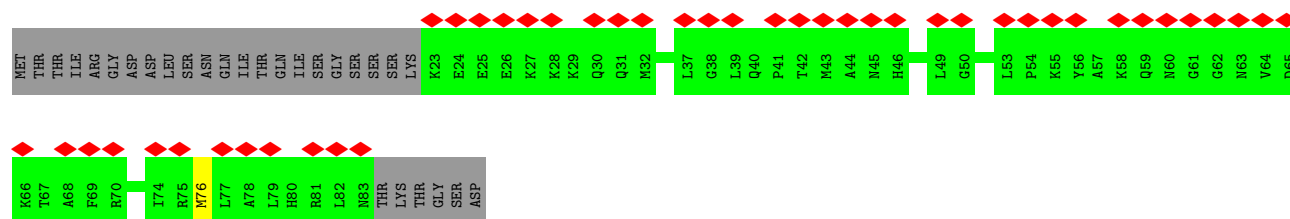
- Molecule 3: Small capsomere-interacting protein



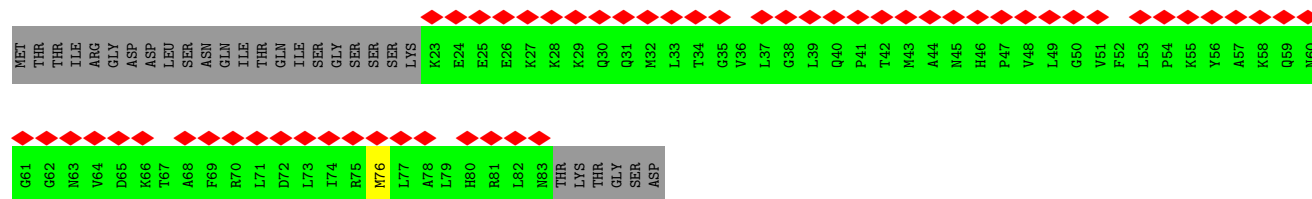
- Molecule 3: Small capsomere-interacting protein



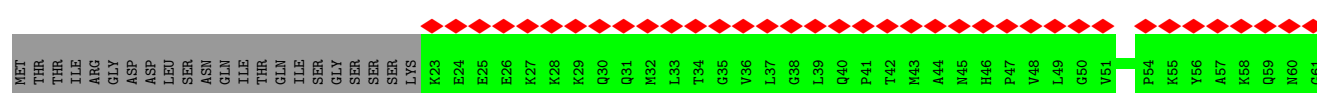
- Molecule 3: Small capsomere-interacting protein

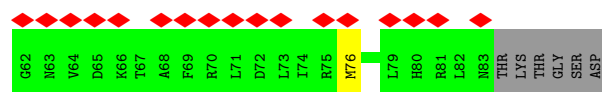


- Molecule 3: Small capsomere-interacting protein

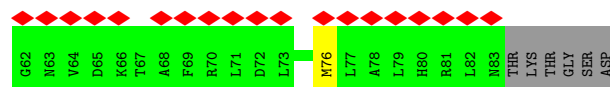
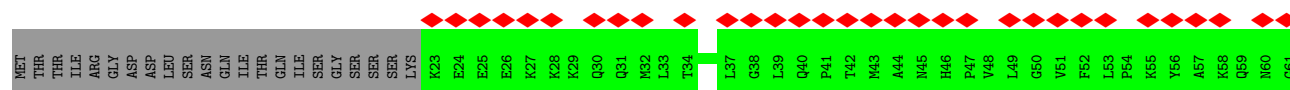


- Molecule 3: Small capsomere-interacting protein

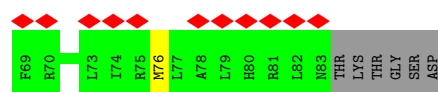
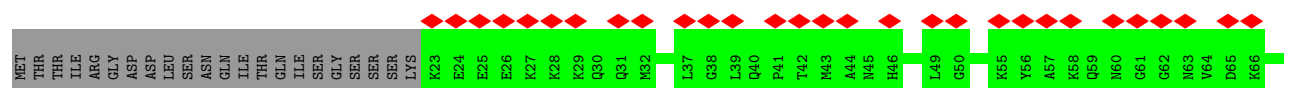




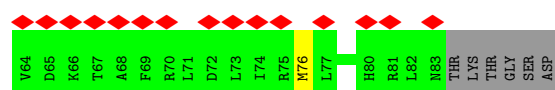
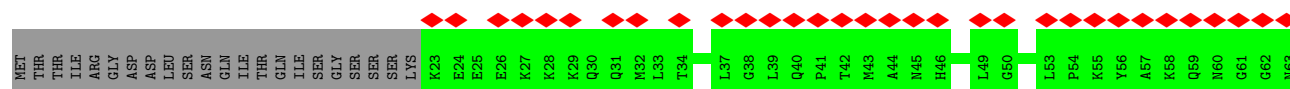
- Molecule 3: Small capsomere-interacting protein



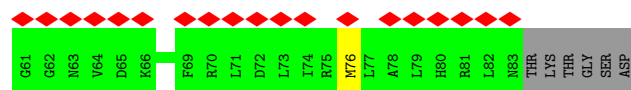
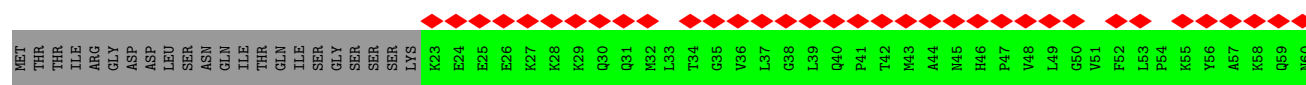
- Molecule 3: Small capsomere-interacting protein



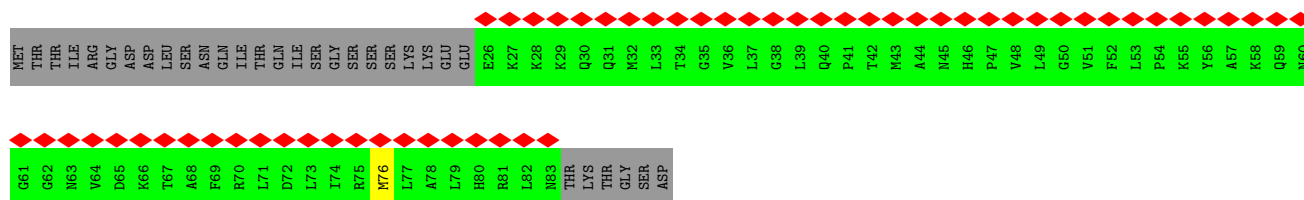
- Molecule 3: Small capsomere-interacting protein



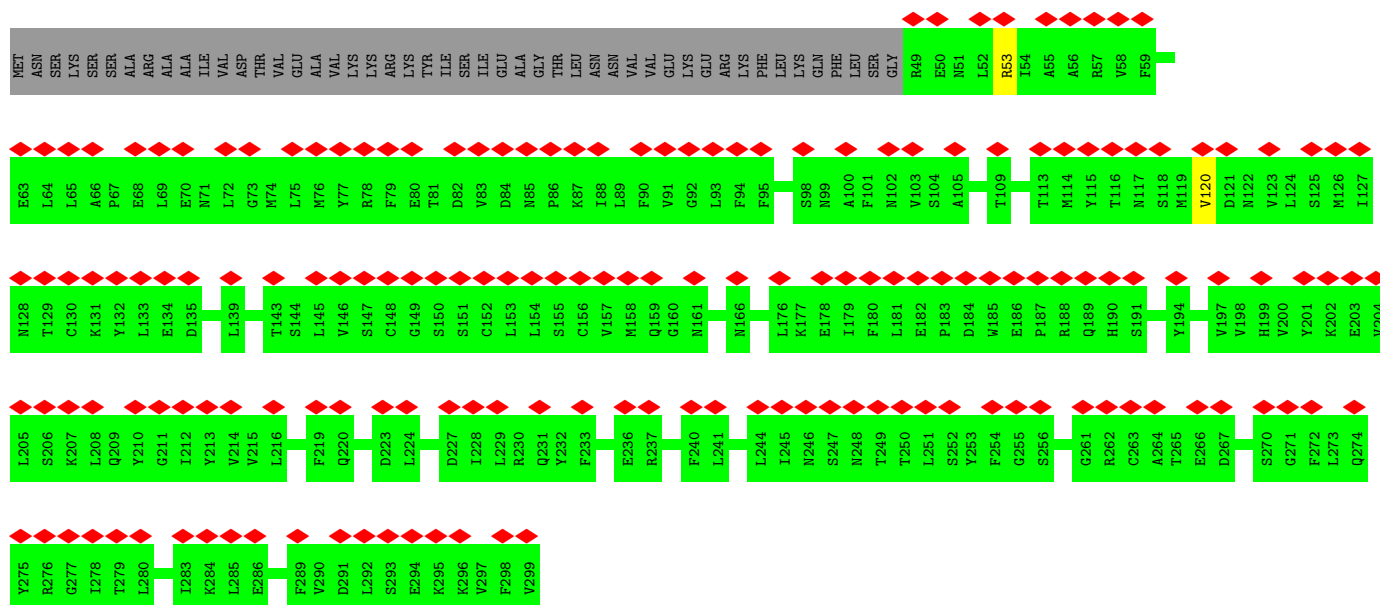
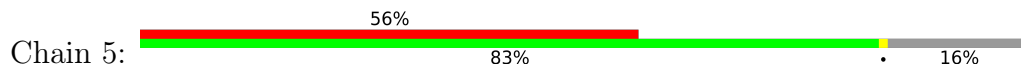
- Molecule 3: Small capsomere-interacting protein



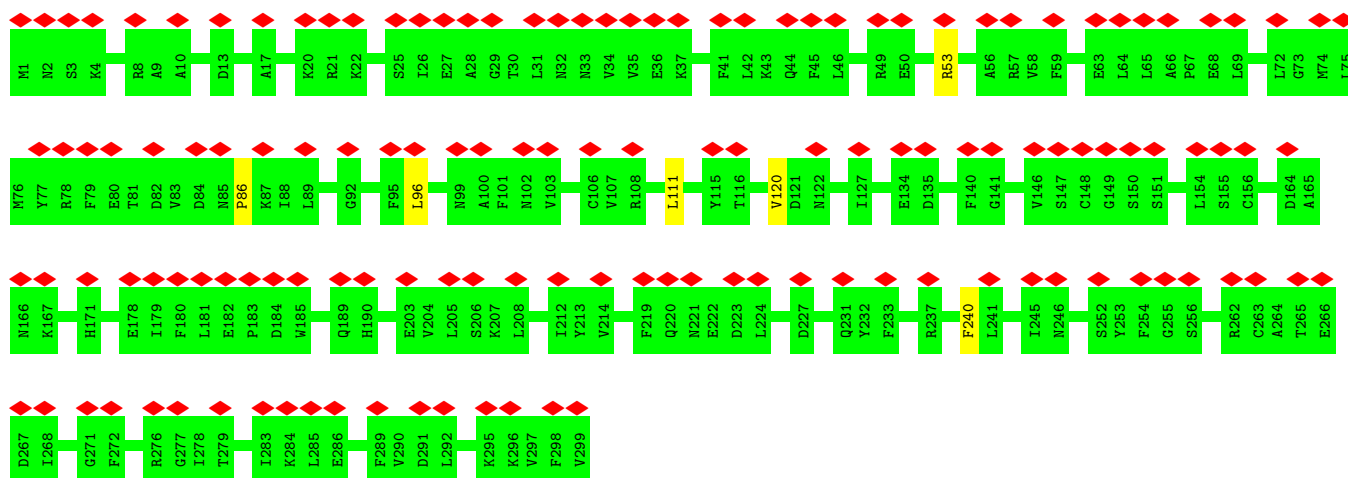
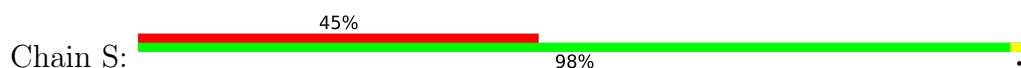
- Molecule 3: Small capsomere-interacting protein



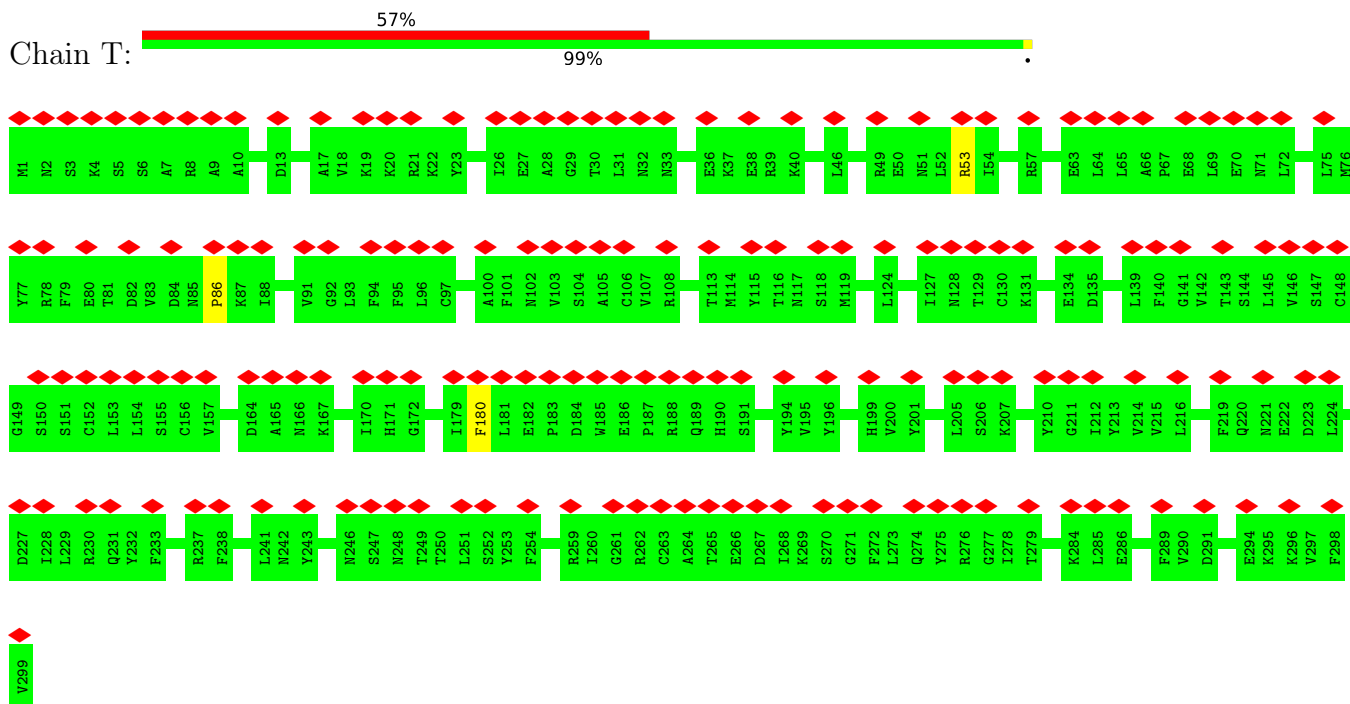
- Molecule 4: Triplex capsid protein 1



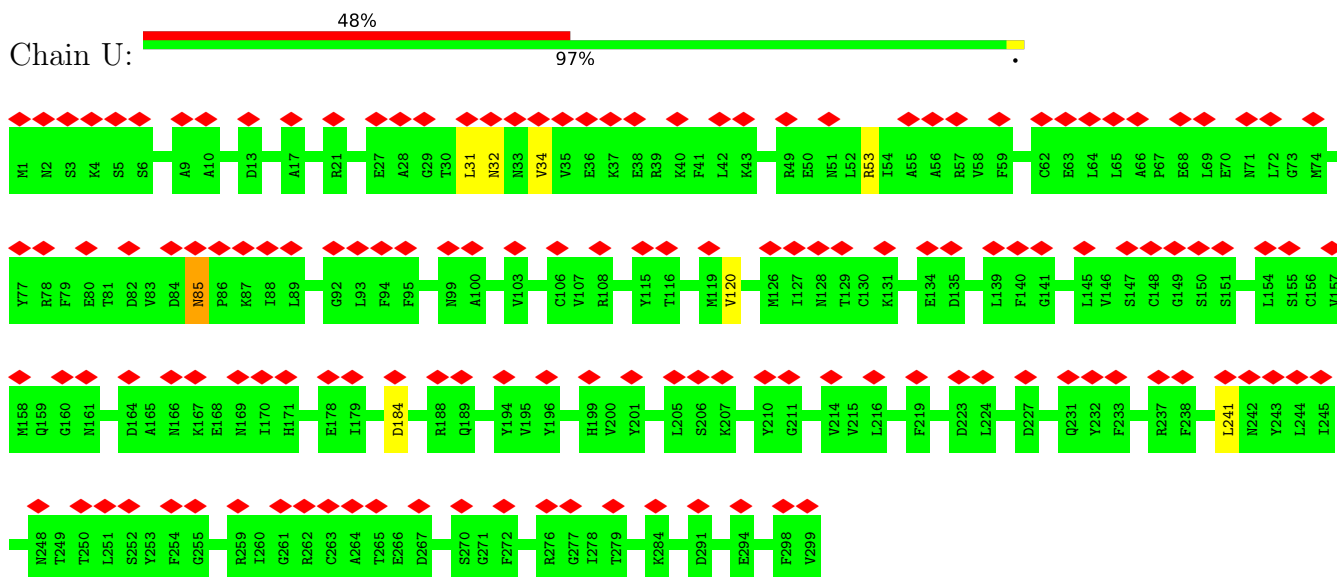
- Molecule 4: Triplex capsid protein 1



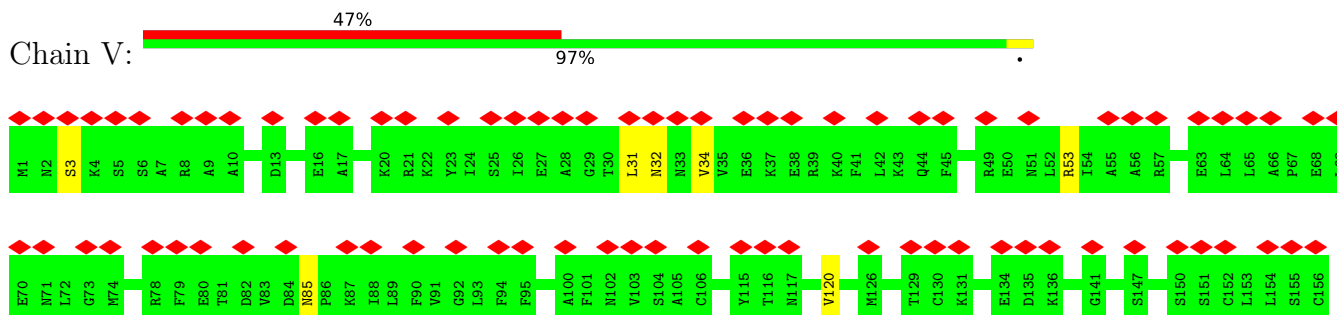
- Molecule 4: Triplex capsid protein 1

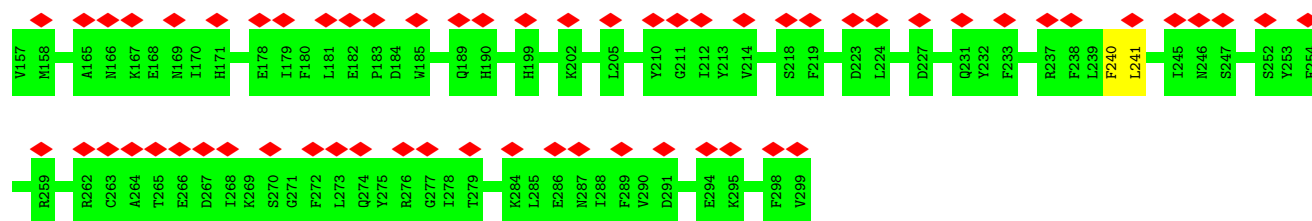


- Molecule 4: Triplex capsid protein 1



- Molecule 4: Triplex capsid protein 1





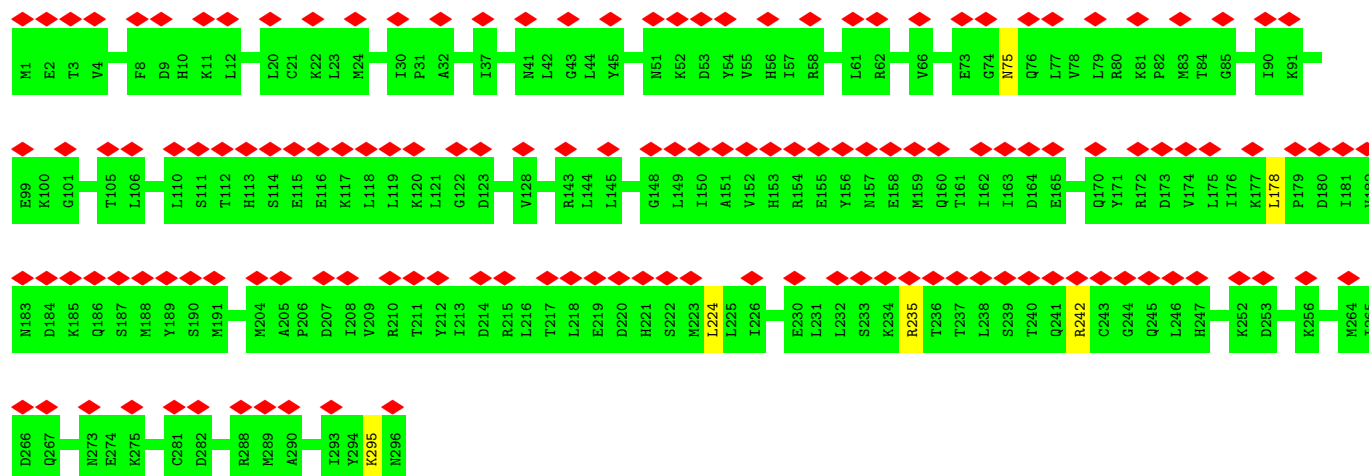
• Molecule 5: Triplex capsid protein 2

Chain 6: 69% 95% 5%

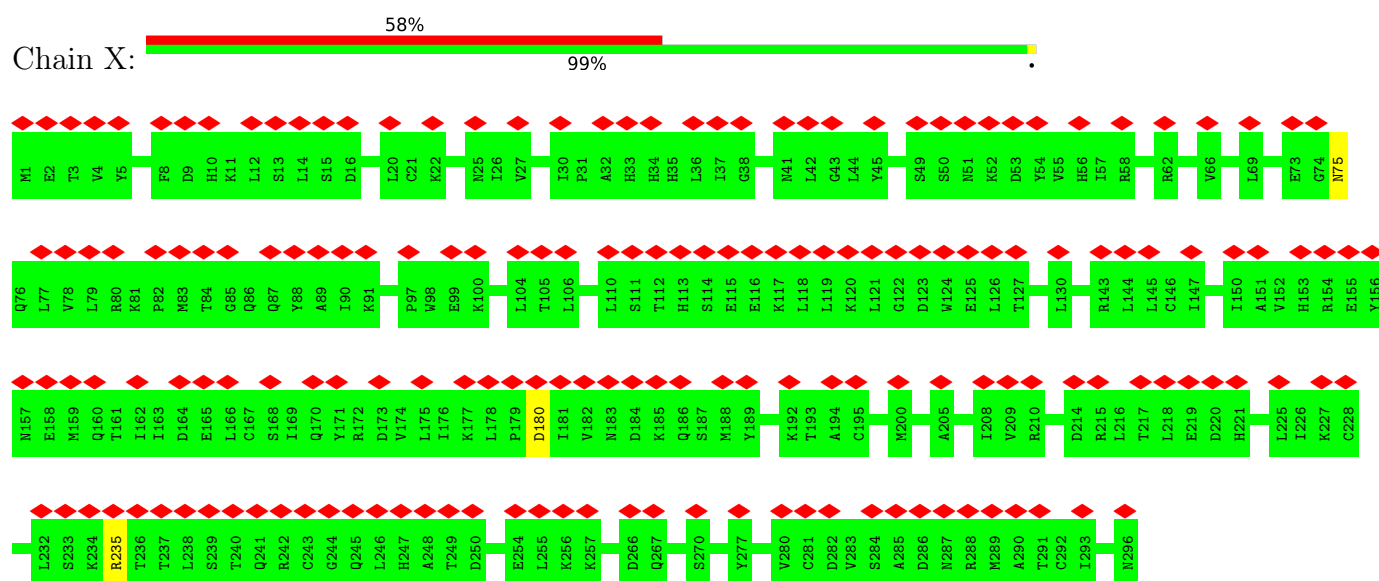


• Molecule 5: Triplex capsid protein 2

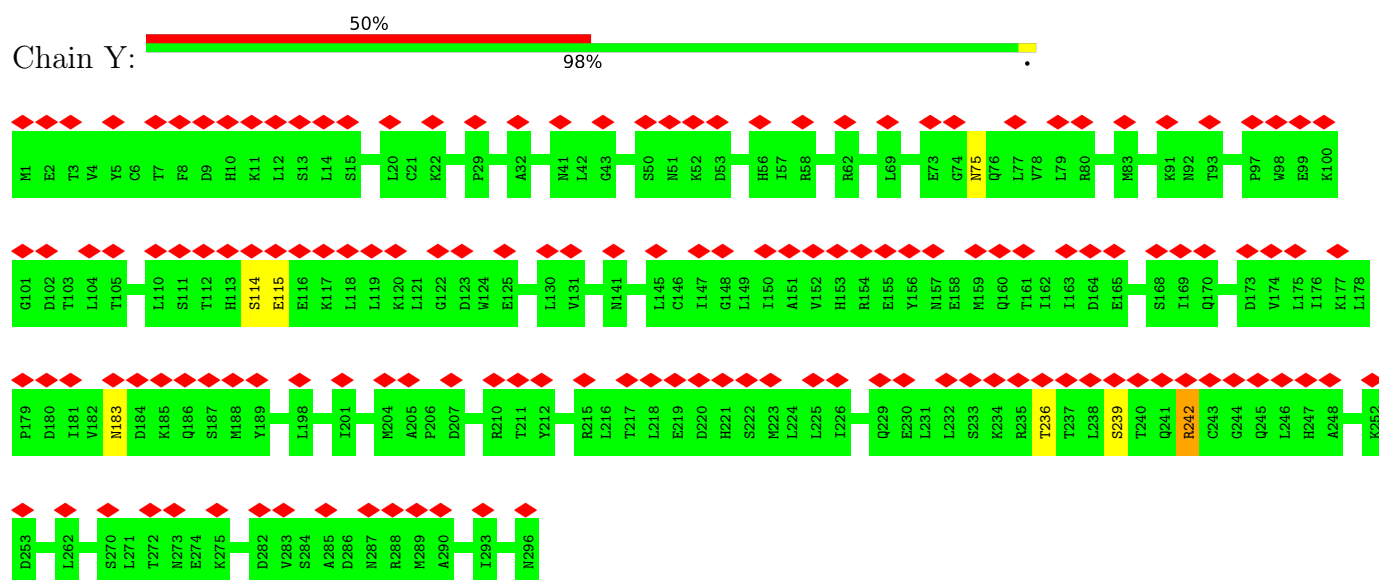
Chain W: 48% 98% 2%



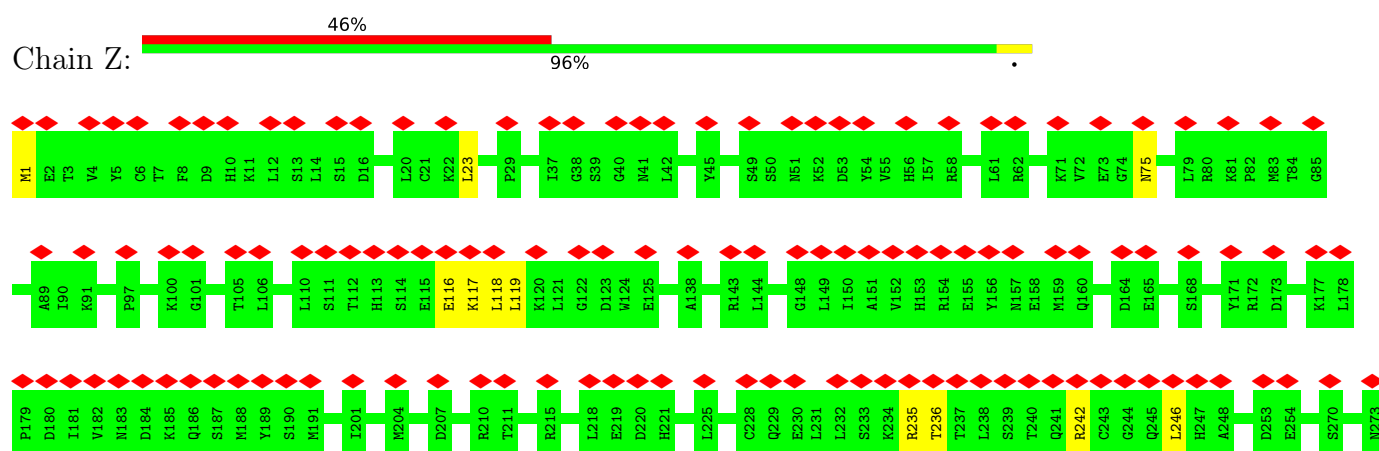
• Molecule 5: Triplex capsid protein 2

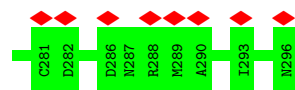


• Molecule 5: Triplex capsid protein 2



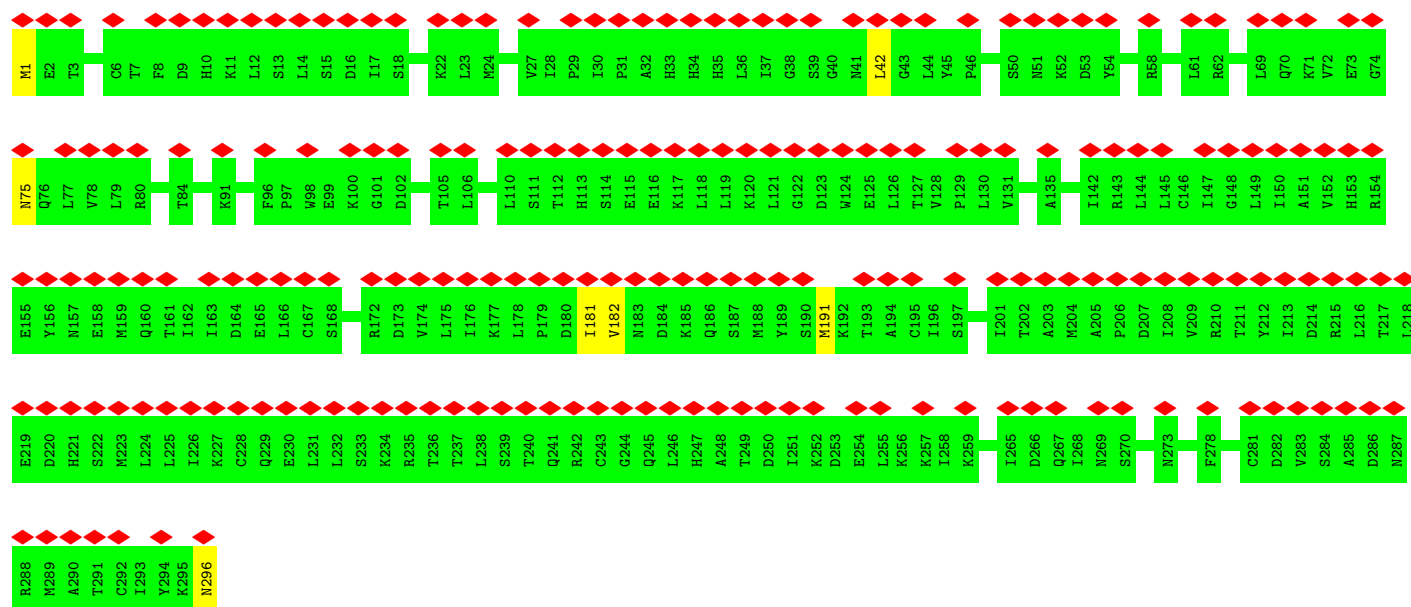
• Molecule 5: Triplex capsid protein 2





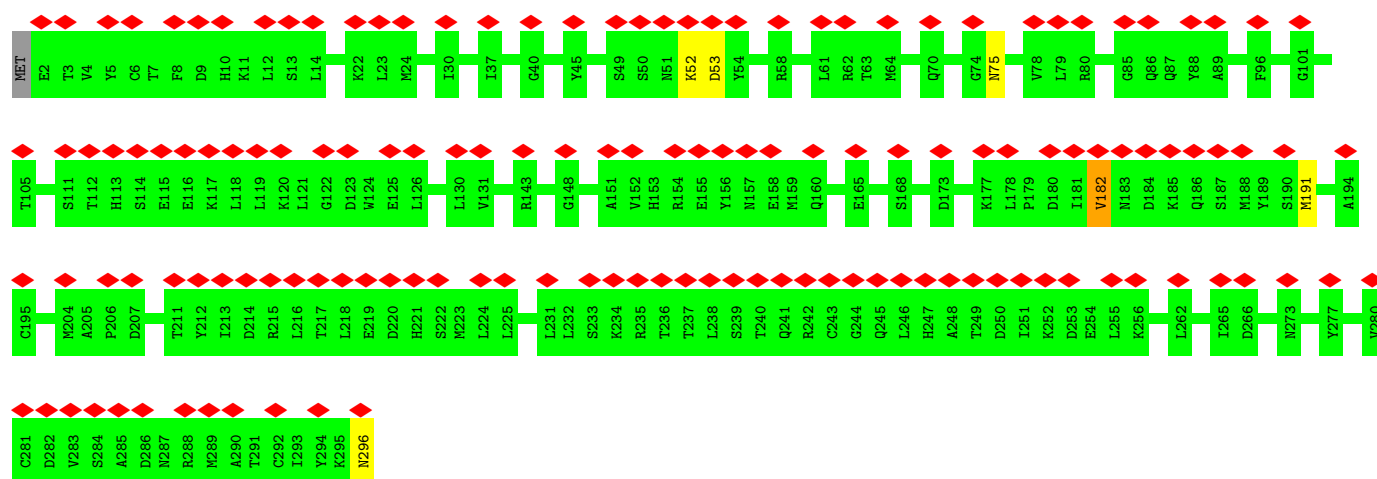
• Molecule 5: Triplex capsid protein 2

Chain 7: 71% 98%



• Molecule 5: Triplex capsid protein 2

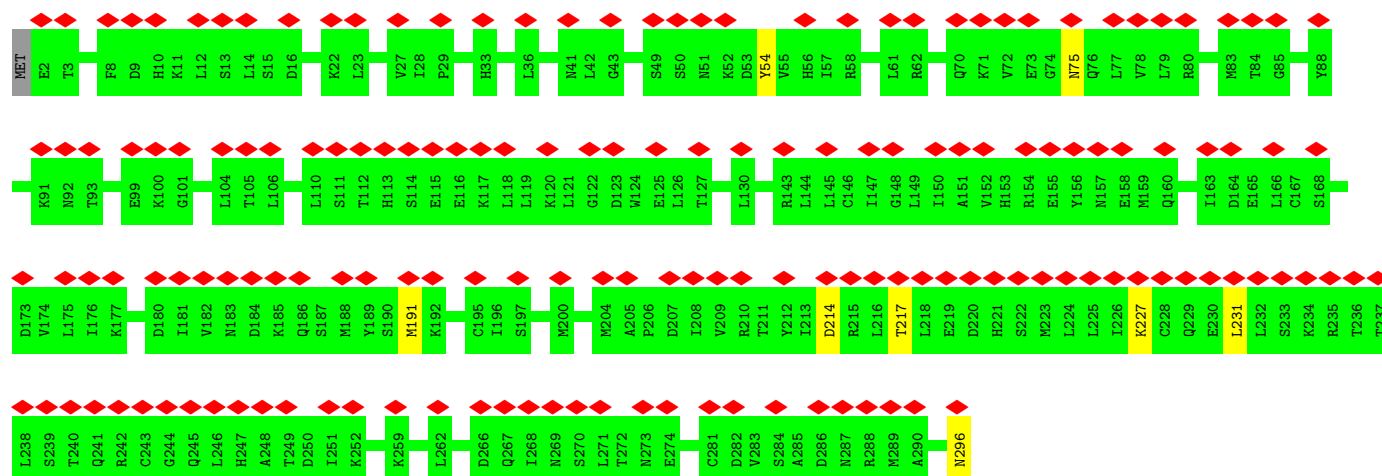
Chain a: 48% 98%



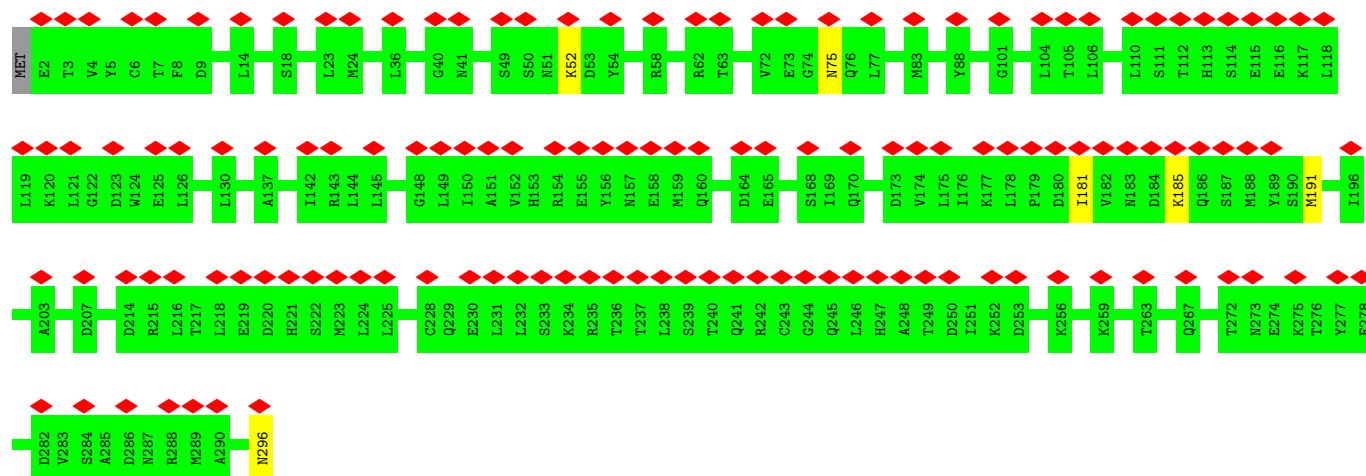
• Molecule 5: Triplex capsid protein 2

Chain b: 54% 97%

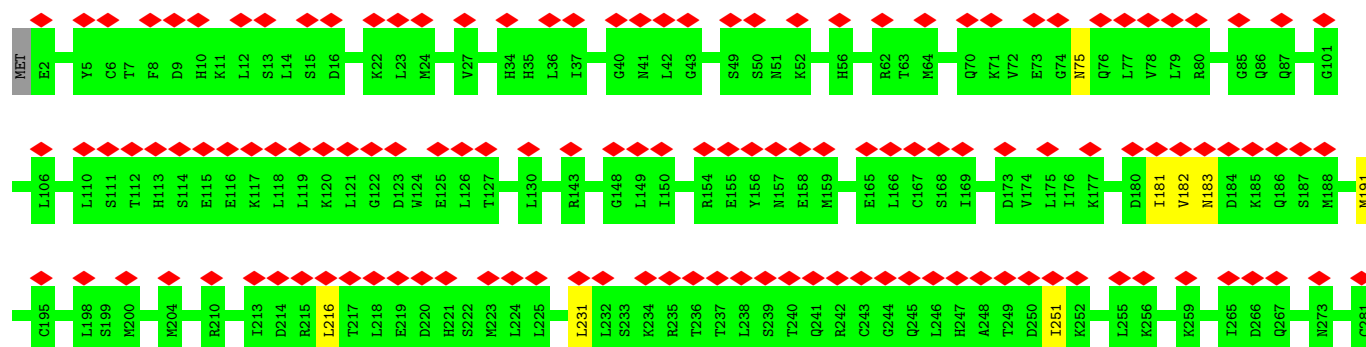


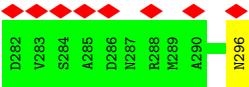


• Molecule 5: Triplex capsid protein 2



• Molecule 5: Triplex capsid protein 2





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	6443	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	23	Depositor
Minimum defocus (nm)	2200	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	64000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.125	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.036	Depositor
Map size (Å)	1388.8, 1388.8, 1388.8	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.17, 2.17, 2.17	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	0.51	0/10927	0.68	0/14860
1	B	0.46	0/10927	0.66	0/14860
1	C	0.46	0/10793	0.63	0/14676
1	D	0.46	0/10927	0.64	1/14860 (0.0%)
1	E	0.50	0/10927	0.66	0/14860
1	F	0.42	0/10927	0.65	0/14860
1	G	0.42	1/10927 (0.0%)	0.66	0/14860
1	H	0.50	0/10927	0.66	0/14860
1	I	0.47	0/10927	0.64	0/14860
1	q	0.42	0/10550	0.64	0/14349
1	r	0.38	0/10927	0.62	0/14860
1	s	0.39	0/10927	0.64	0/14860
1	t	0.40	0/10927	0.63	0/14860
1	u	0.38	0/10935	0.62	0/14870
1	v	0.38	0/10566	0.62	0/14366
1	w	0.38	0/10161	0.66	1/13814 (0.0%)
2	e	0.32	0/2272	0.54	0/3084
2	f	0.34	0/2272	0.62	0/3084
2	g	0.35	0/2272	0.62	0/3084
2	h	0.31	0/2272	0.56	0/3084
2	i	0.32	0/2272	0.63	0/3084
2	j	0.32	0/2272	0.59	0/3084
2	k	0.33	0/2272	0.58	0/3084
2	l	0.32	0/2272	0.57	1/3084 (0.0%)
2	m	0.36	0/2272	0.60	1/3084 (0.0%)
2	n	0.34	0/2272	0.63	1/3084 (0.0%)
2	o	0.40	0/2272	0.66	0/3084
2	p	0.34	0/2272	0.60	0/3084
3	1	0.29	0/490	0.44	0/656
3	2	0.29	0/490	0.44	0/656
3	3	0.28	0/490	0.44	0/656
3	4	0.29	0/463	0.44	0/621
3	J	0.28	0/490	0.44	0/656
3	K	0.28	0/490	0.44	0/656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	L	0.29	0/490	0.44	0/656
3	M	0.29	0/490	0.44	0/656
3	N	0.29	0/490	0.44	0/656
3	O	0.29	0/490	0.44	0/656
3	P	0.29	0/490	0.44	0/656
3	Q	0.28	0/490	0.44	0/656
3	R	0.29	0/490	0.44	0/656
3	x	0.29	0/490	0.44	0/656
3	y	0.29	0/490	0.44	0/656
3	z	0.29	0/490	0.44	0/656
4	5	0.39	0/2062	0.67	0/2793
4	S	0.49	0/2440	0.67	0/3297
4	T	0.48	0/2440	0.70	0/3297
4	U	0.41	0/2440	0.67	0/3297
4	V	0.41	0/2440	0.66	0/3297
5	6	0.39	0/2262	0.67	0/3069
5	7	0.33	0/2374	0.66	0/3219
5	W	0.42	0/2374	0.68	0/3219
5	X	0.38	0/2374	0.62	0/3219
5	Y	0.39	0/2374	0.68	0/3219
5	Z	0.41	0/2374	0.72	0/3219
5	a	0.44	0/2366	0.73	0/3209
5	b	0.44	0/2366	0.73	0/3209
5	c	0.52	0/2366	0.77	0/3209
5	d	0.41	0/2366	0.75	0/3209
All	All	0.42	1/243697 (0.0%)	0.64	5/330985 (0.0%)

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
2	o	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1115	GLU	C-N	-5.30	1.21	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	w	563	LEU	C-N-CD	-8.35	102.23	120.60
2	l	181	ASP	N-CA-C	5.66	126.28	111.00
2	m	154	ALA	N-CA-C	5.37	125.51	111.00
2	n	179	ILE	N-CA-C	-5.11	97.21	111.00
1	D	255	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	o	7	SER	Mainchain

## 5.2 Too-close contacts [i](#)

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

## 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	1341/1345 (100%)	1238 (92%)	102 (8%)	1 (0%)	51	86
1	B	1341/1345 (100%)	1251 (93%)	87 (6%)	3 (0%)	47	81
1	C	1321/1345 (98%)	1239 (94%)	80 (6%)	2 (0%)	47	81
1	D	1341/1345 (100%)	1248 (93%)	89 (7%)	4 (0%)	41	77
1	E	1341/1345 (100%)	1243 (93%)	94 (7%)	4 (0%)	41	77
1	F	1341/1345 (100%)	1243 (93%)	96 (7%)	2 (0%)	51	86
1	G	1341/1345 (100%)	1253 (93%)	83 (6%)	5 (0%)	34	72
1	H	1341/1345 (100%)	1253 (93%)	84 (6%)	4 (0%)	41	77
1	I	1341/1345 (100%)	1242 (93%)	98 (7%)	1 (0%)	51	86
1	q	1292/1345 (96%)	1190 (92%)	99 (8%)	3 (0%)	47	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	r	1341/1345 (100%)	1235 (92%)	103 (8%)	3 (0%)	47	81
1	s	1341/1345 (100%)	1246 (93%)	93 (7%)	2 (0%)	51	86
1	t	1341/1345 (100%)	1240 (92%)	98 (7%)	3 (0%)	47	81
1	u	1342/1345 (100%)	1234 (92%)	106 (8%)	2 (0%)	51	86
1	v	1299/1345 (97%)	1204 (93%)	89 (7%)	6 (0%)	29	69
1	w	1240/1345 (92%)	1141 (92%)	98 (8%)	1 (0%)	51	86
2	e	267/858 (31%)	254 (95%)	13 (5%)	0	100	100
2	f	267/858 (31%)	248 (93%)	16 (6%)	3 (1%)	14	52
2	g	267/858 (31%)	255 (96%)	9 (3%)	3 (1%)	14	52
2	h	267/858 (31%)	248 (93%)	19 (7%)	0	100	100
2	i	267/858 (31%)	245 (92%)	17 (6%)	5 (2%)	8	38
2	j	267/858 (31%)	249 (93%)	16 (6%)	2 (1%)	22	63
2	k	267/858 (31%)	249 (93%)	17 (6%)	1 (0%)	34	72
2	l	267/858 (31%)	247 (92%)	19 (7%)	1 (0%)	34	72
2	m	267/858 (31%)	248 (93%)	18 (7%)	1 (0%)	34	72
2	n	267/858 (31%)	244 (91%)	18 (7%)	5 (2%)	8	38
2	o	267/858 (31%)	247 (92%)	16 (6%)	4 (2%)	10	46
2	p	267/858 (31%)	249 (93%)	18 (7%)	0	100	100
3	1	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	2	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	3	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	4	56/89 (63%)	49 (88%)	7 (12%)	0	100	100
3	J	59/89 (66%)	51 (86%)	7 (12%)	1 (2%)	9	42
3	K	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	L	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	M	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	N	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	O	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	P	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	Q	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	R	59/89 (66%)	52 (88%)	7 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	x	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	y	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	z	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
4	5	249/299 (83%)	226 (91%)	23 (9%)	0	100	100
4	S	297/299 (99%)	269 (91%)	27 (9%)	1 (0%)	41	77
4	T	297/299 (99%)	275 (93%)	21 (7%)	1 (0%)	41	77
4	U	297/299 (99%)	267 (90%)	29 (10%)	1 (0%)	41	77
4	V	297/299 (99%)	268 (90%)	27 (9%)	2 (1%)	22	63
5	6	278/296 (94%)	260 (94%)	18 (6%)	0	100	100
5	7	294/296 (99%)	259 (88%)	32 (11%)	3 (1%)	15	55
5	W	294/296 (99%)	277 (94%)	17 (6%)	0	100	100
5	X	294/296 (99%)	273 (93%)	20 (7%)	1 (0%)	41	77
5	Y	294/296 (99%)	269 (92%)	22 (8%)	3 (1%)	15	55
5	Z	294/296 (99%)	274 (93%)	19 (6%)	1 (0%)	41	77
5	a	293/296 (99%)	262 (89%)	28 (10%)	3 (1%)	15	55
5	b	293/296 (99%)	268 (92%)	24 (8%)	1 (0%)	41	77
5	c	293/296 (99%)	259 (88%)	33 (11%)	1 (0%)	41	77
5	d	293/296 (99%)	258 (88%)	30 (10%)	5 (2%)	9	42
All	All	29747/37695 (79%)	27475 (92%)	2177 (7%)	95 (0%)	44	77

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	55	GLY
1	F	19	ILE
1	G	810	TYR
1	H	21	ASN
1	H	818	ASP
1	v	148	ILE
1	v	810	TYR
1	v	818	ASP
1	w	564	PRO
2	f	178	ASN
2	g	10	PHE
2	i	108	ASN
2	j	149	TYR

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Mol	Chain	Res	Type
2	n	178	ASN
2	o	10	PHE
4	U	85	ASN
4	V	85	ASN
5	X	180	ASP
5	Y	242	ARG
5	Z	116	GLU
5	7	182	VAL
5	a	182	VAL
5	d	182	VAL
1	r	55	GLY
2	i	105	ASN
2	i	150	VAL
4	S	86	PRO
4	T	86	PRO
5	7	191	MET
5	a	52	LYS
5	b	191	MET
5	c	191	MET
5	d	191	MET
1	E	549	GLU
1	G	1120	SER
1	H	549	GLU
1	I	549	GLU
2	f	105	ASN
2	g	11	ALA
2	n	104	LEU
2	n	105	ASN
2	o	149	TYR
3	J	26	GLU
5	a	191	MET
5	d	251	ILE
1	A	549	GLU
1	B	549	GLU
1	C	549	GLU
1	D	549	GLU
1	D	845	VAL
1	E	23	ILE
1	E	948	GLY
1	E	1275	GLU
1	F	549	GLU
1	G	549	GLU

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Mol	Chain	Res	Type
1	G	1119	PRO
1	G	1275	GLU
1	H	1275	GLU
1	q	549	GLU
1	r	1275	GLU
1	t	549	GLU
1	u	549	GLU
1	v	549	GLU
1	v	1275	GLU
2	i	178	ASN
2	n	49	ARG
2	o	144	PRO
5	Y	114	SER
5	Y	115	GLU
1	D	1041	VAL
1	D	1275	GLU
1	r	549	GLU
1	s	549	GLU
1	s	1275	GLU
1	u	1275	GLU
2	i	148	PRO
2	j	148	PRO
2	l	110	GLU
2	m	146	ASP
2	n	12	TRP
5	d	183	ASN
1	q	1275	GLU
1	t	716	PRO
1	t	1275	GLU
2	f	104	LEU
4	V	3	SER
1	B	715	CYS
1	v	147	VAL
1	B	812	GLU
5	7	181	ILE
5	d	181	ILE
2	g	143	VAL
2	o	145	ILE
1	q	716	PRO
2	k	143	VAL

### 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	1218/1220 (100%)	1202 (99%)	16 (1%)	69	81
1	B	1218/1220 (100%)	1201 (99%)	17 (1%)	67	80
1	C	1204/1220 (99%)	1191 (99%)	13 (1%)	73	84
1	D	1218/1220 (100%)	1197 (98%)	21 (2%)	60	78
1	E	1218/1220 (100%)	1200 (98%)	18 (2%)	65	80
1	F	1218/1220 (100%)	1198 (98%)	20 (2%)	62	79
1	G	1218/1220 (100%)	1199 (98%)	19 (2%)	62	79
1	H	1218/1220 (100%)	1197 (98%)	21 (2%)	60	78
1	I	1218/1220 (100%)	1204 (99%)	14 (1%)	73	84
1	q	1180/1220 (97%)	1168 (99%)	12 (1%)	76	86
1	r	1218/1220 (100%)	1204 (99%)	14 (1%)	73	84
1	s	1218/1220 (100%)	1202 (99%)	16 (1%)	69	81
1	t	1218/1220 (100%)	1207 (99%)	11 (1%)	78	87
1	u	1219/1220 (100%)	1205 (99%)	14 (1%)	73	84
1	v	1180/1220 (97%)	1170 (99%)	10 (1%)	81	89
1	w	1133/1220 (93%)	1123 (99%)	10 (1%)	78	87
2	e	253/761 (33%)	247 (98%)	6 (2%)	49	69
2	f	253/761 (33%)	253 (100%)	0	100	100
2	g	253/761 (33%)	246 (97%)	7 (3%)	43	65
2	h	253/761 (33%)	249 (98%)	4 (2%)	62	79
2	i	253/761 (33%)	245 (97%)	8 (3%)	39	61
2	j	253/761 (33%)	246 (97%)	7 (3%)	43	65
2	k	253/761 (33%)	246 (97%)	7 (3%)	43	65
2	l	253/761 (33%)	246 (97%)	7 (3%)	43	65
2	m	253/761 (33%)	249 (98%)	4 (2%)	62	79
2	n	253/761 (33%)	247 (98%)	6 (2%)	49	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	o	253/761 (33%)	247 (98%)	6 (2%)	49	69
2	p	253/761 (33%)	248 (98%)	5 (2%)	55	74
3	1	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	2	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	3	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	4	49/77 (64%)	48 (98%)	1 (2%)	55	74
3	J	52/77 (68%)	49 (94%)	3 (6%)	20	45
3	K	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	L	52/77 (68%)	50 (96%)	2 (4%)	33	57
3	M	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	N	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	O	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	P	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	Q	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	R	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	x	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	y	52/77 (68%)	51 (98%)	1 (2%)	57	75
3	z	52/77 (68%)	51 (98%)	1 (2%)	57	75
4	5	232/273 (85%)	230 (99%)	2 (1%)	78	87
4	S	273/273 (100%)	268 (98%)	5 (2%)	59	77
4	T	273/273 (100%)	271 (99%)	2 (1%)	84	90
4	U	273/273 (100%)	265 (97%)	8 (3%)	42	64
4	V	273/273 (100%)	266 (97%)	7 (3%)	46	66
5	6	261/274 (95%)	260 (100%)	1 (0%)	91	94
5	7	274/274 (100%)	270 (98%)	4 (2%)	65	80
5	W	274/274 (100%)	268 (98%)	6 (2%)	52	71
5	X	274/274 (100%)	272 (99%)	2 (1%)	84	90
5	Y	274/274 (100%)	269 (98%)	5 (2%)	59	77
5	Z	274/274 (100%)	264 (96%)	10 (4%)	35	59
5	a	273/274 (100%)	269 (98%)	4 (2%)	65	80
5	b	273/274 (100%)	266 (97%)	7 (3%)	46	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	c	273/274 (100%)	268 (98%)	5 (2%)	59	77
5	d	273/274 (100%)	269 (98%)	4 (2%)	65	80
All	All	27226/33989 (80%)	26822 (98%)	404 (2%)	66	80

All (404) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	139	LEU
1	A	140	GLU
1	A	244	ASN
1	A	691	ASN
1	A	743	ARG
1	A	746	ASN
1	A	772	ASN
1	A	831	LEU
1	A	839	MET
1	A	950	PHE
1	A	1029	ARG
1	A	1032	THR
1	A	1075	ASN
1	A	1134	ASN
1	A	1250	LYS
1	B	139	LEU
1	B	244	ASN
1	B	397	LEU
1	B	439	ARG
1	B	691	ASN
1	B	702	VAL
1	B	712	ARG
1	B	715	CYS
1	B	743	ARG
1	B	746	ASN
1	B	769	ARG
1	B	772	ASN
1	B	839	MET
1	B	1029	ARG
1	B	1075	ASN
1	B	1118	ASN
1	B	1250	LYS
1	C	244	ASN

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Mol	Chain	Res	Type
1	C	691	ASN
1	C	743	ARG
1	C	746	ASN
1	C	769	ARG
1	C	772	ASN
1	C	839	MET
1	C	854	GLN
1	C	855	LEU
1	C	950	PHE
1	C	1029	ARG
1	C	1075	ASN
1	C	1250	LYS
1	D	244	ASN
1	D	307	MET
1	D	397	LEU
1	D	691	ASN
1	D	702	VAL
1	D	709	PHE
1	D	729	LYS
1	D	743	ARG
1	D	746	ASN
1	D	754	ARG
1	D	769	ARG
1	D	772	ASN
1	D	809	PHE
1	D	831	LEU
1	D	839	MET
1	D	856	PHE
1	D	950	PHE
1	D	1029	ARG
1	D	1042	THR
1	D	1075	ASN
1	D	1250	LYS
1	E	244	ASN
1	E	439	ARG
1	E	691	ASN
1	E	702	VAL
1	E	743	ARG
1	E	746	ASN
1	E	769	ARG
1	E	772	ASN
1	E	831	LEU

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Mol	Chain	Res	Type
1	E	947	ASP
1	E	1029	ARG
1	E	1032	THR
1	E	1075	ASN
1	E	1130	PHE
1	E	1133	ILE
1	E	1135	LYS
1	E	1201	THR
1	E	1250	LYS
1	F	18	ASN
1	F	201	VAL
1	F	244	ASN
1	F	439	ARG
1	F	546	ARG
1	F	691	ASN
1	F	702	VAL
1	F	743	ARG
1	F	746	ASN
1	F	769	ARG
1	F	772	ASN
1	F	815	ILE
1	F	818	ASP
1	F	822	GLN
1	F	839	MET
1	F	1029	ARG
1	F	1035	ILE
1	F	1075	ASN
1	F	1118	ASN
1	F	1250	LYS
1	G	18	ASN
1	G	20	PHE
1	G	139	LEU
1	G	244	ASN
1	G	439	ARG
1	G	691	ASN
1	G	702	VAL
1	G	743	ARG
1	G	746	ASN
1	G	769	ARG
1	G	772	ASN
1	G	808	LEU
1	G	818	ASP

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Mol	Chain	Res	Type
1	G	830	VAL
1	G	831	LEU
1	G	839	MET
1	G	1029	ARG
1	G	1075	ASN
1	G	1250	LYS
1	H	36	ARG
1	H	53	LEU
1	H	244	ASN
1	H	439	ARG
1	H	464	MET
1	H	691	ASN
1	H	724	ASN
1	H	743	ARG
1	H	746	ASN
1	H	769	ARG
1	H	772	ASN
1	H	818	ASP
1	H	831	LEU
1	H	839	MET
1	H	1029	ARG
1	H	1032	THR
1	H	1075	ASN
1	H	1125	LEU
1	H	1230	CYS
1	H	1250	LYS
1	H	1255	MET
1	I	244	ASN
1	I	255	LEU
1	I	439	ARG
1	I	691	ASN
1	I	743	ARG
1	I	746	ASN
1	I	769	ARG
1	I	772	ASN
1	I	1029	ARG
1	I	1075	ASN
1	I	1126	ASN
1	I	1201	THR
1	I	1216	LEU
1	I	1250	LYS
1	q	90	LYS

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Mol	Chain	Res	Type
1	q	139	LEU
1	q	244	ASN
1	q	691	ASN
1	q	746	ASN
1	q	769	ARG
1	q	772	ASN
1	q	831	LEU
1	q	832	MET
1	q	1029	ARG
1	q	1075	ASN
1	q	1250	LYS
1	r	3	ASN
1	r	18	ASN
1	r	36	ARG
1	r	244	ASN
1	r	439	ARG
1	r	691	ASN
1	r	743	ARG
1	r	746	ASN
1	r	769	ARG
1	r	772	ASN
1	r	839	MET
1	r	1029	ARG
1	r	1075	ASN
1	r	1250	LYS
1	s	18	ASN
1	s	36	ARG
1	s	204	LYS
1	s	244	ASN
1	s	439	ARG
1	s	691	ASN
1	s	743	ARG
1	s	746	ASN
1	s	769	ARG
1	s	772	ASN
1	s	839	MET
1	s	860	ILE
1	s	1029	ARG
1	s	1075	ASN
1	s	1129	THR
1	s	1250	LYS
1	t	36	ARG

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Mol	Chain	Res	Type
1	t	244	ASN
1	t	439	ARG
1	t	691	ASN
1	t	743	ARG
1	t	746	ASN
1	t	772	ASN
1	t	839	MET
1	t	1029	ARG
1	t	1075	ASN
1	t	1250	LYS
1	u	1	MET
1	u	36	ARG
1	u	200	LYS
1	u	244	ASN
1	u	691	ASN
1	u	743	ARG
1	u	746	ASN
1	u	769	ARG
1	u	772	ASN
1	u	839	MET
1	u	1029	ARG
1	u	1036	LEU
1	u	1075	ASN
1	u	1250	LYS
1	v	244	ASN
1	v	691	ASN
1	v	743	ARG
1	v	746	ASN
1	v	769	ARG
1	v	772	ASN
1	v	839	MET
1	v	1075	ASN
1	v	1118	ASN
1	v	1250	LYS
1	w	45	ARG
1	w	104	ASN
1	w	231	ASN
1	w	241	ARG
1	w	439	ARG
1	w	563	LEU
1	w	745	ARG
1	w	832	MET

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Mol	Chain	Res	Type
1	w	1164	LYS
1	w	1206	THR
2	e	33	ASN
2	e	62	ASN
2	e	96	ASN
2	e	138	ARG
2	e	163	ASN
2	e	255	ARG
2	g	33	ASN
2	g	62	ASN
2	g	96	ASN
2	g	99	LEU
2	g	106	LYS
2	g	132	ARG
2	g	163	ASN
2	h	33	ASN
2	h	62	ASN
2	h	96	ASN
2	h	163	ASN
2	i	33	ASN
2	i	44	ASN
2	i	49	ARG
2	i	96	ASN
2	i	112	MET
2	i	138	ARG
2	i	163	ASN
2	i	171	MET
2	j	33	ASN
2	j	60	LEU
2	j	62	ASN
2	j	96	ASN
2	j	105	ASN
2	j	163	ASN
2	j	255	ARG
2	k	33	ASN
2	k	62	ASN
2	k	96	ASN
2	k	99	LEU
2	k	106	LYS
2	k	132	ARG
2	k	163	ASN
2	l	31	LEU

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Mol	Chain	Res	Type
2	l	33	ASN
2	l	62	ASN
2	l	96	ASN
2	l	108	ASN
2	l	163	ASN
2	l	180	ASN
2	m	33	ASN
2	m	62	ASN
2	m	96	ASN
2	m	163	ASN
2	n	33	ASN
2	n	60	LEU
2	n	62	ASN
2	n	96	ASN
2	n	132	ARG
2	n	163	ASN
2	o	10	PHE
2	o	31	LEU
2	o	33	ASN
2	o	96	ASN
2	o	132	ARG
2	o	163	ASN
2	p	33	ASN
2	p	62	ASN
2	p	96	ASN
2	p	108	ASN
2	p	163	ASN
3	J	26	GLU
3	J	27	LYS
3	J	76	MET
3	K	76	MET
3	L	23	LYS
3	L	76	MET
3	M	76	MET
3	N	76	MET
3	O	76	MET
3	P	76	MET
3	Q	76	MET
3	R	76	MET
3	x	76	MET
3	y	76	MET
3	z	76	MET

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Mol	Chain	Res	Type
3	1	76	MET
3	2	76	MET
3	3	76	MET
3	4	76	MET
4	5	53	ARG
4	5	120	VAL
4	S	53	ARG
4	S	96	LEU
4	S	111	LEU
4	S	120	VAL
4	S	240	PHE
4	T	53	ARG
4	T	180	PHE
4	U	31	LEU
4	U	32	ASN
4	U	34	VAL
4	U	53	ARG
4	U	85	ASN
4	U	120	VAL
4	U	184	ASP
4	U	241	LEU
4	V	31	LEU
4	V	32	ASN
4	V	34	VAL
4	V	53	ARG
4	V	120	VAL
4	V	240	PHE
4	V	241	LEU
5	6	75	ASN
5	W	75	ASN
5	W	178	LEU
5	W	224	LEU
5	W	235	ARG
5	W	242	ARG
5	W	295	LYS
5	X	75	ASN
5	X	235	ARG
5	Y	75	ASN
5	Y	183	ASN
5	Y	236	THR
5	Y	239	SER
5	Y	242	ARG

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Mol	Chain	Res	Type
5	Z	1	MET
5	Z	23	LEU
5	Z	75	ASN
5	Z	117	LYS
5	Z	118	LEU
5	Z	119	LEU
5	Z	235	ARG
5	Z	236	THR
5	Z	242	ARG
5	Z	246	LEU
5	7	1	MET
5	7	42	LEU
5	7	75	ASN
5	7	296	ASN
5	a	53	ASP
5	a	75	ASN
5	a	182	VAL
5	a	296	ASN
5	b	54	TYR
5	b	75	ASN
5	b	214	ASP
5	b	217	THR
5	b	227	LYS
5	b	231	LEU
5	b	296	ASN
5	c	52	LYS
5	c	75	ASN
5	c	181	ILE
5	c	185	LYS
5	c	296	ASN
5	d	75	ASN
5	d	216	LEU
5	d	231	LEU
5	d	296	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (534) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	ASN
1	A	260	ASN
1	A	294	GLN
1	A	432	ASN

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Mol	Chain	Res	Type
1	A	435	GLN
1	A	438	GLN
1	A	477	GLN
1	A	691	ASN
1	A	727	ASN
1	A	772	ASN
1	A	791	ASN
1	A	863	ASN
1	A	888	GLN
1	A	892	HIS
1	A	896	ASN
1	A	977	ASN
1	A	1000	GLN
1	A	1006	HIS
1	A	1111	HIS
1	B	155	ASN
1	B	211	GLN
1	B	244	ASN
1	B	294	GLN
1	B	387	GLN
1	B	432	ASN
1	B	543	GLN
1	B	581	HIS
1	B	691	ASN
1	B	746	ASN
1	B	772	ASN
1	B	847	ASN
1	B	891	GLN
1	B	896	ASN
1	B	1000	GLN
1	B	1110	HIS
1	B	1111	HIS
1	B	1118	ASN
1	B	1143	HIS
1	B	1159	ASN
1	B	1271	ASN
1	C	244	ASN
1	C	311	ASN
1	C	337	GLN
1	C	432	ASN
1	C	438	GLN
1	C	477	GLN

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Mol	Chain	Res	Type
1	C	543	GLN
1	C	691	ASN
1	C	746	ASN
1	C	772	ASN
1	C	854	GLN
1	C	896	ASN
1	C	1000	GLN
1	C	1168	ASN
1	C	1239	ASN
1	C	1320	GLN
1	C	1325	HIS
1	D	244	ASN
1	D	331	ASN
1	D	435	GLN
1	D	581	HIS
1	D	691	ASN
1	D	739	GLN
1	D	746	ASN
1	D	772	ASN
1	D	891	GLN
1	D	896	ASN
1	D	1000	GLN
1	D	1053	ASN
1	D	1105	ASN
1	D	1111	HIS
1	D	1159	ASN
1	D	1194	HIS
1	D	1325	HIS
1	E	18	ASN
1	E	202	HIS
1	E	244	ASN
1	E	260	ASN
1	E	294	GLN
1	E	378	ASN
1	E	387	GLN
1	E	432	ASN
1	E	435	GLN
1	E	438	GLN
1	E	534	HIS
1	E	543	GLN
1	E	691	ASN
1	E	772	ASN

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Mol	Chain	Res	Type
1	E	791	ASN
1	E	946	ASN
1	E	1000	GLN
1	E	1089	ASN
1	E	1101	ASN
1	E	1111	HIS
1	E	1134	ASN
1	E	1159	ASN
1	E	1239	ASN
1	E	1325	HIS
1	F	18	ASN
1	F	203	ASN
1	F	244	ASN
1	F	294	GLN
1	F	378	ASN
1	F	387	GLN
1	F	432	ASN
1	F	438	GLN
1	F	473	HIS
1	F	543	GLN
1	F	581	HIS
1	F	691	ASN
1	F	746	ASN
1	F	772	ASN
1	F	822	GLN
1	F	847	ASN
1	F	891	GLN
1	F	896	ASN
1	F	938	ASN
1	F	1000	GLN
1	F	1057	HIS
1	F	1097	HIS
1	F	1101	ASN
1	F	1105	ASN
1	F	1111	HIS
1	F	1118	ASN
1	F	1143	HIS
1	G	5	GLN
1	G	18	ASN
1	G	123	HIS
1	G	138	HIS
1	G	155	ASN

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Mol	Chain	Res	Type
1	G	203	ASN
1	G	244	ASN
1	G	294	GLN
1	G	387	GLN
1	G	432	ASN
1	G	438	GLN
1	G	543	GLN
1	G	581	HIS
1	G	691	ASN
1	G	740	ASN
1	G	746	ASN
1	G	772	ASN
1	G	847	ASN
1	G	863	ASN
1	G	888	GLN
1	G	891	GLN
1	G	896	ASN
1	G	938	ASN
1	G	964	GLN
1	G	1000	GLN
1	G	1097	HIS
1	G	1111	HIS
1	G	1134	ASN
1	G	1143	HIS
1	H	244	ASN
1	H	331	ASN
1	H	387	GLN
1	H	435	GLN
1	H	581	HIS
1	H	691	ASN
1	H	724	ASN
1	H	739	GLN
1	H	740	ASN
1	H	746	ASN
1	H	772	ASN
1	H	888	GLN
1	H	896	ASN
1	H	964	GLN
1	H	1000	GLN
1	H	1101	ASN
1	H	1111	HIS
1	H	1159	ASN

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Mol	Chain	Res	Type
1	I	244	ASN
1	I	294	GLN
1	I	432	ASN
1	I	438	GLN
1	I	543	GLN
1	I	581	HIS
1	I	691	ASN
1	I	746	ASN
1	I	772	ASN
1	I	896	ASN
1	I	964	GLN
1	I	1000	GLN
1	I	1101	ASN
1	I	1111	HIS
1	I	1126	ASN
1	I	1159	ASN
1	I	1325	HIS
1	q	203	ASN
1	q	211	GLN
1	q	244	ASN
1	q	294	GLN
1	q	432	ASN
1	q	438	GLN
1	q	543	GLN
1	q	581	HIS
1	q	691	ASN
1	q	746	ASN
1	q	772	ASN
1	q	791	ASN
1	q	891	GLN
1	q	942	HIS
1	q	1000	GLN
1	q	1111	HIS
1	q	1168	ASN
1	q	1182	HIS
1	r	3	ASN
1	r	5	GLN
1	r	21	ASN
1	r	138	HIS
1	r	155	ASN
1	r	244	ASN
1	r	294	GLN

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Mol	Chain	Res	Type
1	r	387	GLN
1	r	432	ASN
1	r	435	GLN
1	r	438	GLN
1	r	543	GLN
1	r	581	HIS
1	r	658	ASN
1	r	691	ASN
1	r	746	ASN
1	r	772	ASN
1	r	847	ASN
1	r	888	GLN
1	r	891	GLN
1	r	1000	GLN
1	r	1111	HIS
1	r	1168	ASN
1	r	1241	GLN
1	r	1325	HIS
1	s	18	ASN
1	s	119	HIS
1	s	138	HIS
1	s	244	ASN
1	s	294	GLN
1	s	378	ASN
1	s	382	ASN
1	s	387	GLN
1	s	432	ASN
1	s	435	GLN
1	s	438	GLN
1	s	543	GLN
1	s	560	ASN
1	s	672	HIS
1	s	691	ASN
1	s	746	ASN
1	s	772	ASN
1	s	847	ASN
1	s	891	GLN
1	s	1000	GLN
1	s	1105	ASN
1	s	1111	HIS
1	s	1168	ASN
1	s	1252	ASN

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Mol	Chain	Res	Type
1	t	145	ASN
1	t	150	GLN
1	t	244	ASN
1	t	294	GLN
1	t	387	GLN
1	t	432	ASN
1	t	438	GLN
1	t	543	GLN
1	t	581	HIS
1	t	691	ASN
1	t	746	ASN
1	t	772	ASN
1	t	847	ASN
1	t	891	GLN
1	t	892	HIS
1	t	1000	GLN
1	t	1111	HIS
1	t	1168	ASN
1	t	1338	GLN
1	u	244	ASN
1	u	294	GLN
1	u	304	HIS
1	u	387	GLN
1	u	432	ASN
1	u	435	GLN
1	u	438	GLN
1	u	543	GLN
1	u	560	ASN
1	u	581	HIS
1	u	672	HIS
1	u	691	ASN
1	u	746	ASN
1	u	772	ASN
1	u	891	GLN
1	u	892	HIS
1	u	896	ASN
1	u	1000	GLN
1	u	1097	HIS
1	u	1101	ASN
1	u	1111	HIS
1	u	1168	ASN
1	v	155	ASN

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Mol	Chain	Res	Type
1	v	211	GLN
1	v	244	ASN
1	v	294	GLN
1	v	331	ASN
1	v	432	ASN
1	v	435	GLN
1	v	438	GLN
1	v	543	GLN
1	v	659	HIS
1	v	691	ASN
1	v	746	ASN
1	v	772	ASN
1	v	888	GLN
1	v	891	GLN
1	v	892	HIS
1	v	1000	GLN
1	v	1111	HIS
1	v	1118	ASN
1	v	1241	GLN
1	v	1325	HIS
1	w	104	ASN
1	w	119	HIS
1	w	141	ASN
1	w	202	HIS
1	w	387	GLN
1	w	432	ASN
1	w	466	ASN
1	w	477	GLN
1	w	514	ASN
1	w	617	HIS
1	w	746	ASN
1	w	847	ASN
1	w	854	GLN
1	w	863	ASN
1	w	879	GLN
1	w	881	HIS
1	w	934	GLN
1	w	964	GLN
1	w	1088	GLN
1	w	1097	HIS
1	w	1182	HIS
1	w	1297	ASN

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Mol	Chain	Res	Type
1	w	1318	ASN
2	e	33	ASN
2	e	71	HIS
2	e	96	ASN
2	f	33	ASN
2	f	71	HIS
2	f	82	ASN
2	f	105	ASN
2	f	163	ASN
2	f	194	ASN
2	f	248	GLN
2	g	33	ASN
2	g	44	ASN
2	g	71	HIS
2	g	92	GLN
2	g	115	ASN
2	g	122	GLN
2	g	163	ASN
2	g	194	ASN
2	h	27	ASN
2	h	30	ASN
2	h	33	ASN
2	h	71	HIS
2	h	92	GLN
2	h	122	GLN
2	h	194	ASN
2	h	237	ASN
2	i	27	ASN
2	i	33	ASN
2	i	39	HIS
2	i	44	ASN
2	i	71	HIS
2	i	96	ASN
2	i	194	ASN
2	j	33	ASN
2	j	71	HIS
2	j	96	ASN
2	j	105	ASN
2	j	163	ASN
2	j	248	GLN
2	k	30	ASN
2	k	33	ASN

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Mol	Chain	Res	Type
2	k	44	ASN
2	k	71	HIS
2	k	92	GLN
2	k	108	ASN
2	k	163	ASN
2	k	239	ASN
2	l	33	ASN
2	l	71	HIS
2	l	92	GLN
2	l	108	ASN
2	l	142	ASN
2	l	163	ASN
2	l	180	ASN
2	l	237	ASN
2	m	33	ASN
2	m	62	ASN
2	m	71	HIS
2	m	92	GLN
2	n	62	ASN
2	n	71	HIS
2	n	92	GLN
2	n	96	ASN
2	n	248	GLN
2	n	254	GLN
2	o	27	ASN
2	o	33	ASN
2	o	44	ASN
2	o	62	ASN
2	o	71	HIS
2	o	92	GLN
2	o	111	ASN
2	p	27	ASN
2	p	30	ASN
2	p	33	ASN
2	p	71	HIS
2	p	108	ASN
2	p	115	ASN
2	p	142	ASN
2	p	186	ASN
3	J	46	HIS
3	J	59	GLN
3	J	60	ASN

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Mol	Chain	Res	Type
3	K	46	HIS
3	K	59	GLN
3	K	60	ASN
3	L	46	HIS
3	L	59	GLN
3	L	60	ASN
3	M	46	HIS
3	M	59	GLN
3	M	60	ASN
3	N	46	HIS
3	N	59	GLN
3	N	60	ASN
3	O	46	HIS
3	O	59	GLN
3	O	60	ASN
3	P	46	HIS
3	P	59	GLN
3	P	60	ASN
3	Q	46	HIS
3	Q	59	GLN
3	Q	60	ASN
3	R	46	HIS
3	R	59	GLN
3	R	60	ASN
3	x	46	HIS
3	x	59	GLN
3	x	60	ASN
3	y	46	HIS
3	y	59	GLN
3	y	60	ASN
3	z	46	HIS
3	z	59	GLN
3	z	60	ASN
3	1	46	HIS
3	1	59	GLN
3	1	60	ASN
3	2	46	HIS
3	2	59	GLN
3	2	60	ASN
3	3	59	GLN
3	3	60	ASN
3	4	46	HIS

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Mol	Chain	Res	Type
3	4	59	GLN
3	4	60	ASN
4	S	193	GLN
4	T	220	GLN
4	T	242	ASN
4	U	122	ASN
4	V	122	ASN
4	V	161	ASN
5	6	34	HIS
5	6	75	ASN
5	6	170	GLN
5	W	34	HIS
5	W	75	ASN
5	W	170	GLN
5	W	221	HIS
5	X	34	HIS
5	X	75	ASN
5	X	170	GLN
5	X	186	GLN
5	X	247	HIS
5	Y	34	HIS
5	Y	75	ASN
5	Y	153	HIS
5	Y	170	GLN
5	Y	183	ASN
5	Y	221	HIS
5	Y	269	ASN
5	Z	34	HIS
5	Z	75	ASN
5	Z	76	GLN
5	Z	153	HIS
5	Z	170	GLN
5	Z	221	HIS
5	Z	269	ASN
5	7	75	ASN
5	7	76	GLN
5	7	113	HIS
5	7	229	GLN
5	7	296	ASN
5	a	51	ASN
5	a	75	ASN
5	a	76	GLN

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Mol	Chain	Res	Type
5	a	87	GLN
5	a	92	ASN
5	a	229	GLN
5	a	296	ASN
5	b	56	HIS
5	b	75	ASN
5	b	87	GLN
5	b	92	ASN
5	b	229	GLN
5	b	267	GLN
5	b	296	ASN
5	c	75	ASN
5	c	113	HIS
5	c	153	HIS
5	c	229	GLN
5	c	247	HIS
5	c	296	ASN
5	d	75	ASN
5	d	87	GLN
5	d	92	ASN
5	d	113	HIS
5	d	157	ASN
5	d	221	HIS
5	d	245	GLN
5	d	247	HIS
5	d	296	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

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.

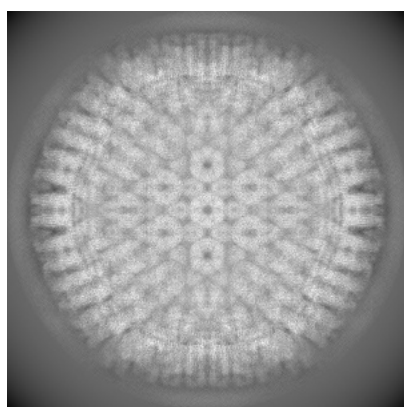
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20557. These allow visual inspection of the internal detail of the map and identification of artifacts.

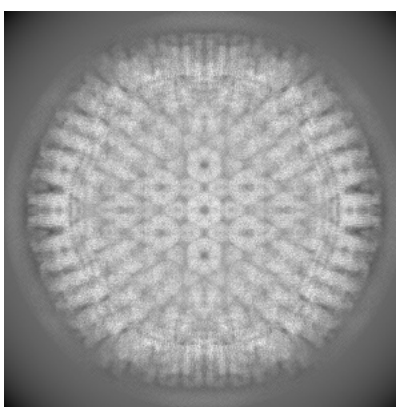
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

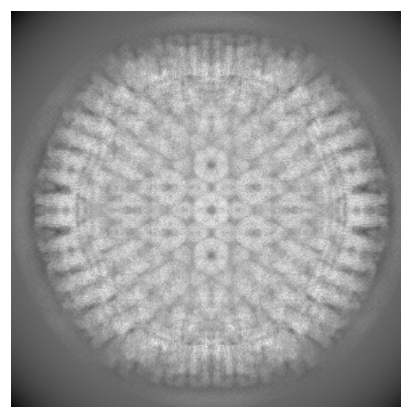
#### 6.1.1 Primary map



X



Y

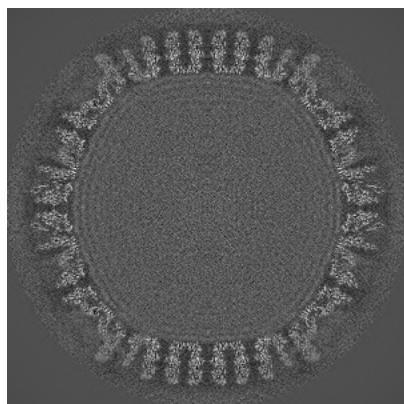


Z

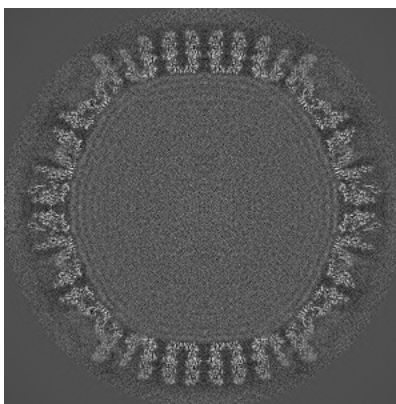
The images above show the map projected in three orthogonal directions.

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

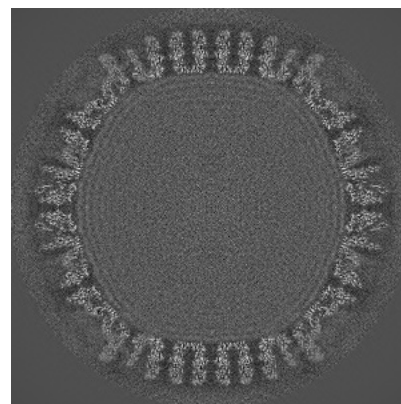
#### 6.2.1 Primary map



X Index: 320



Y Index: 320

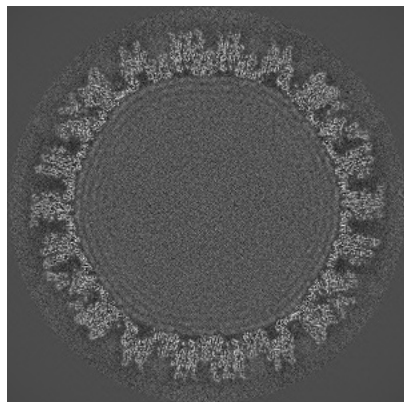


Z Index: 320

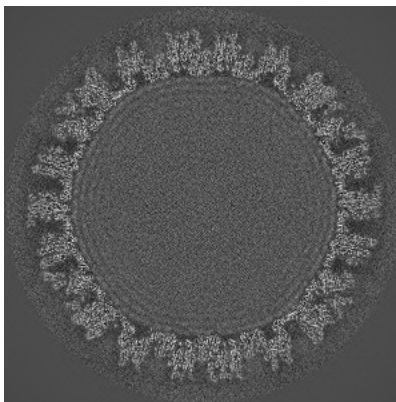
The images above show central slices of the map in three orthogonal directions.

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

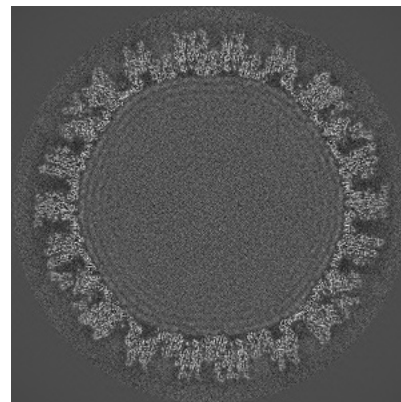
### 6.3.1 Primary map



X Index: 266



Y Index: 266



Z Index: 266

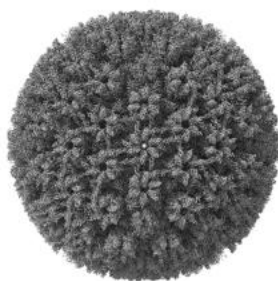
The images above show the largest variance slices of the map in three orthogonal directions.

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

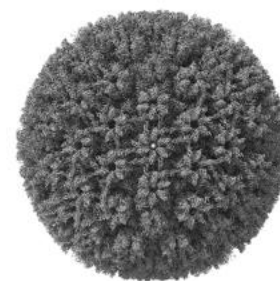
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

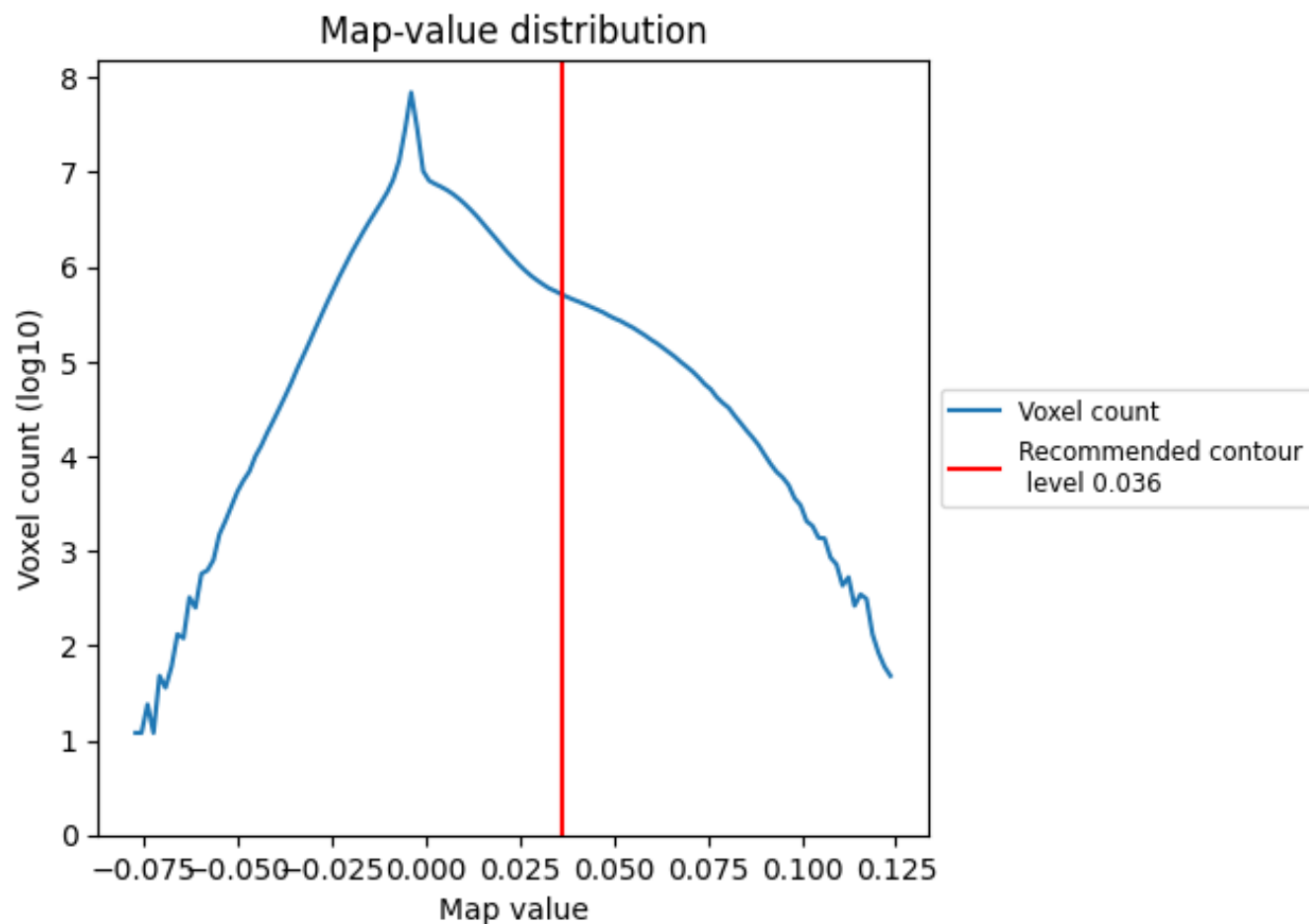
## 6.5 Mask visualisation

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.

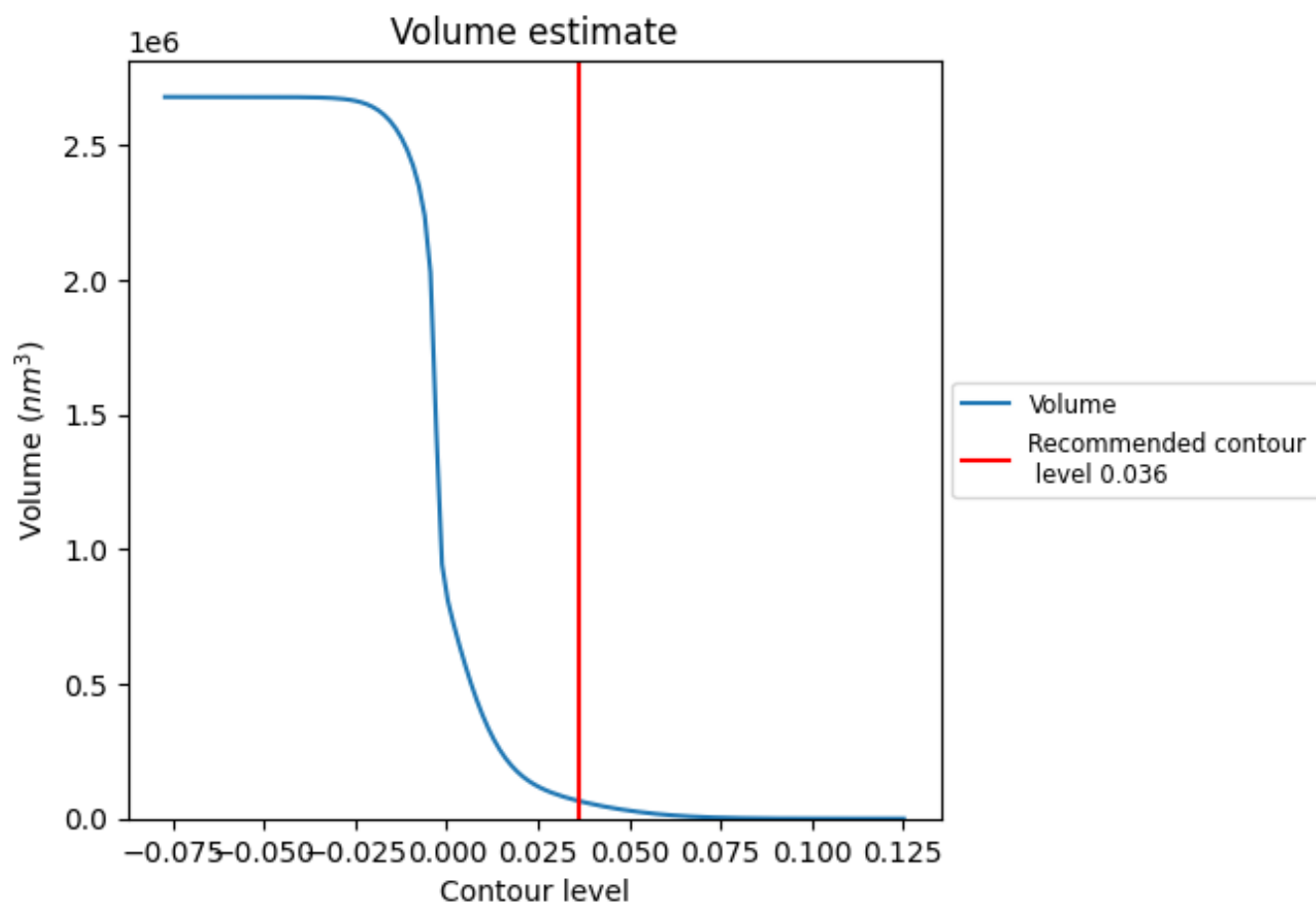
### 7.1 Map-value distribution [i](#)



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.



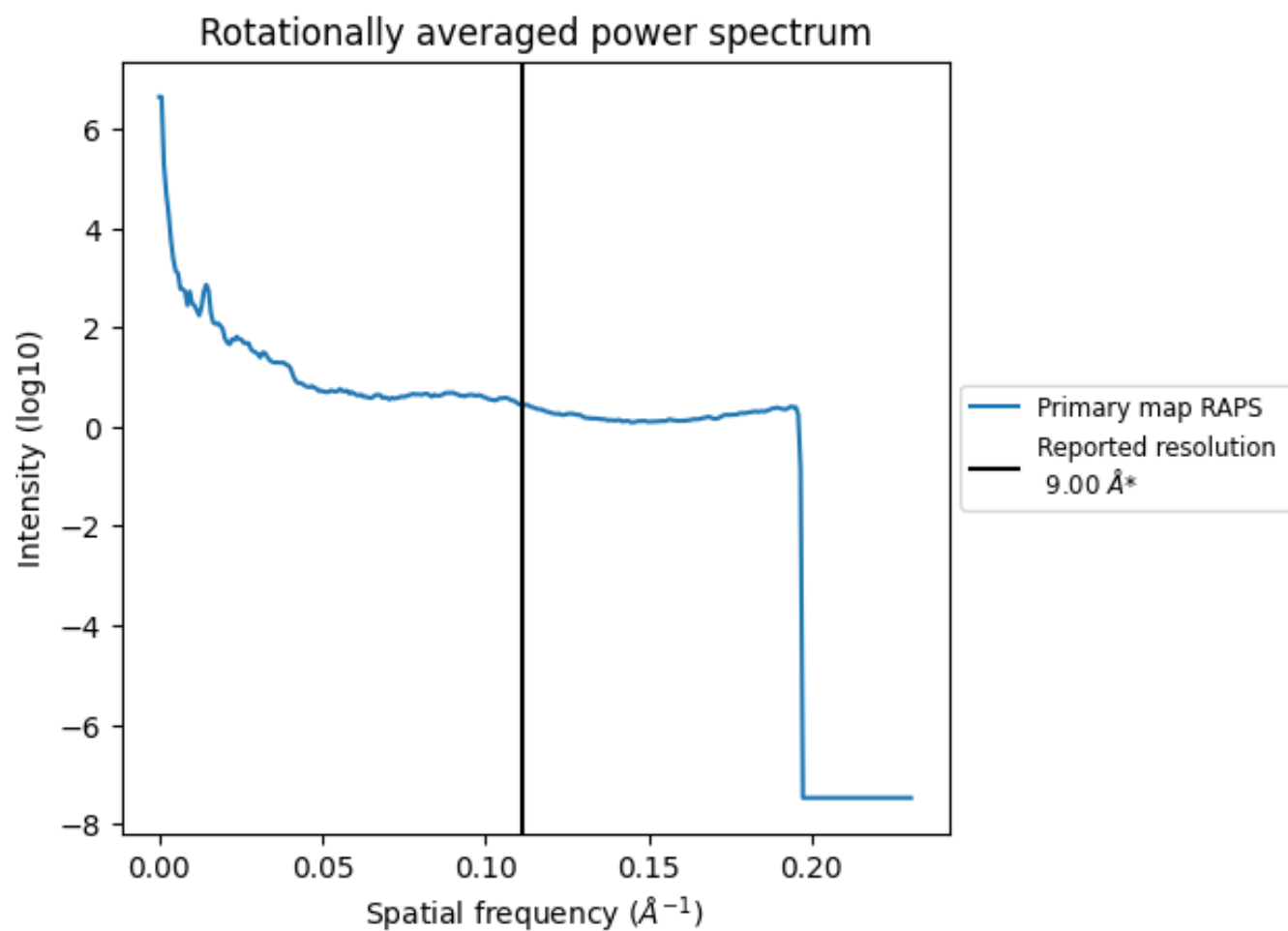
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 66298 nm<sup>3</sup>; this corresponds to an approximate mass of 59889 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 0.111 Å<sup>-1</sup>

## 8 Fourier-Shell correlation ⓘ

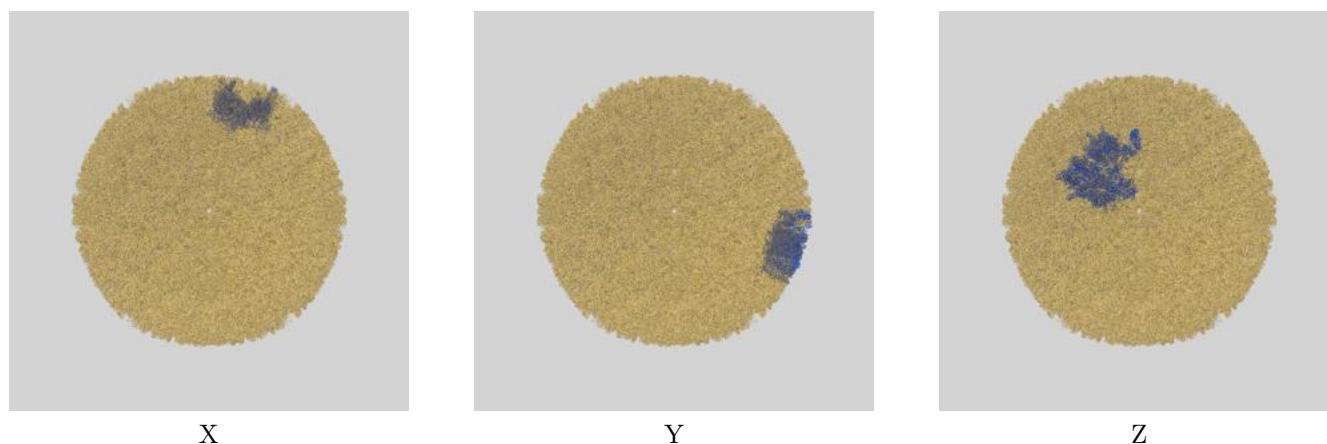
This section was not generated. No FSC curve or half-maps provided.

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

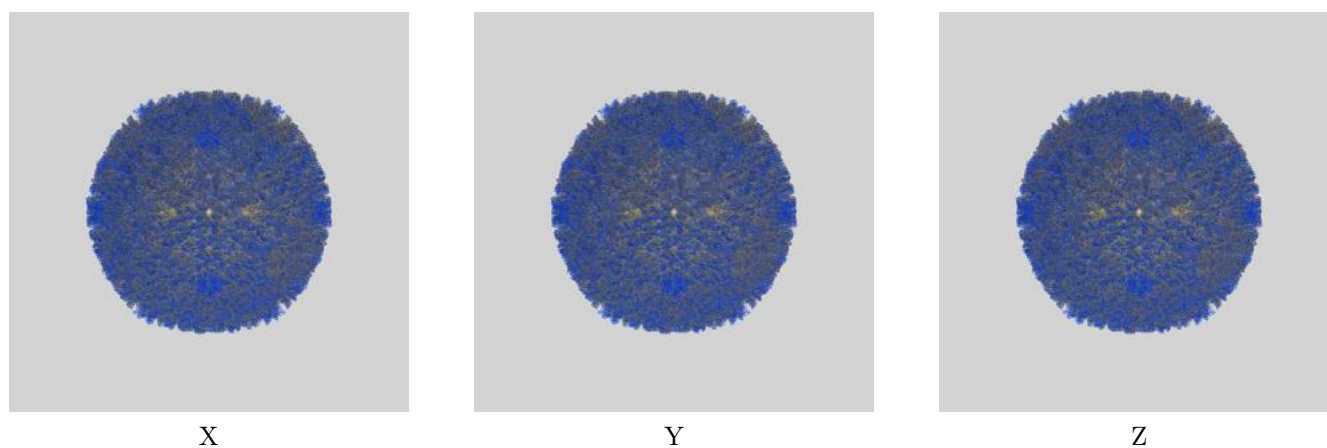
This section contains information regarding the fit between EMDB map EMD-20557 and PDB model 6Q1F. Per-residue inclusion information can be found in section 3 on page 9.

### 9.1 Map-model overlays

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

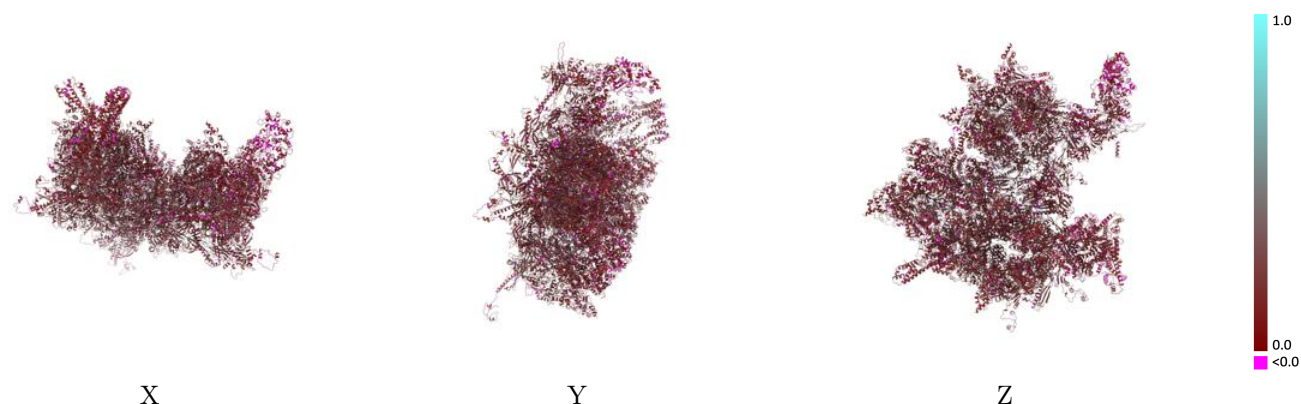


#### 9.1.2 Map-model assembly overlay [i](#)



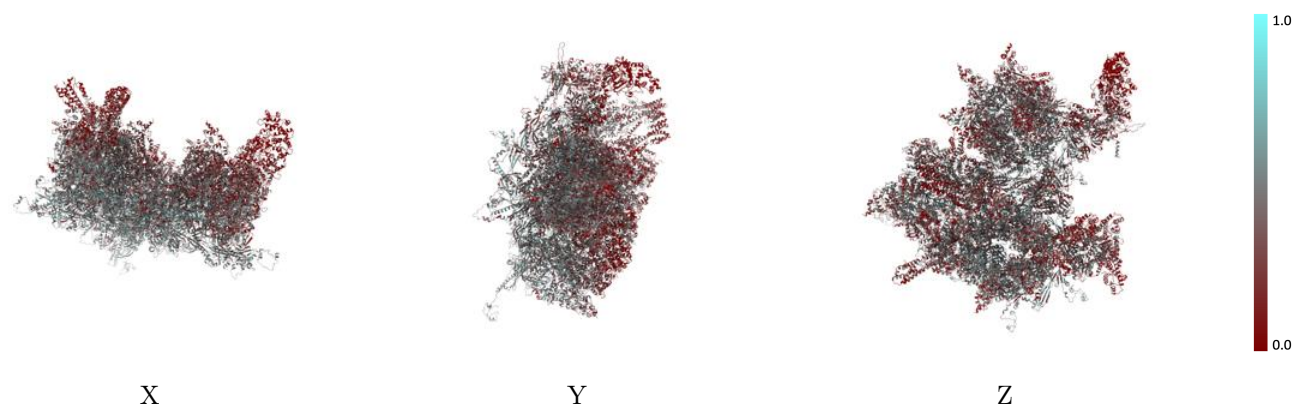
The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



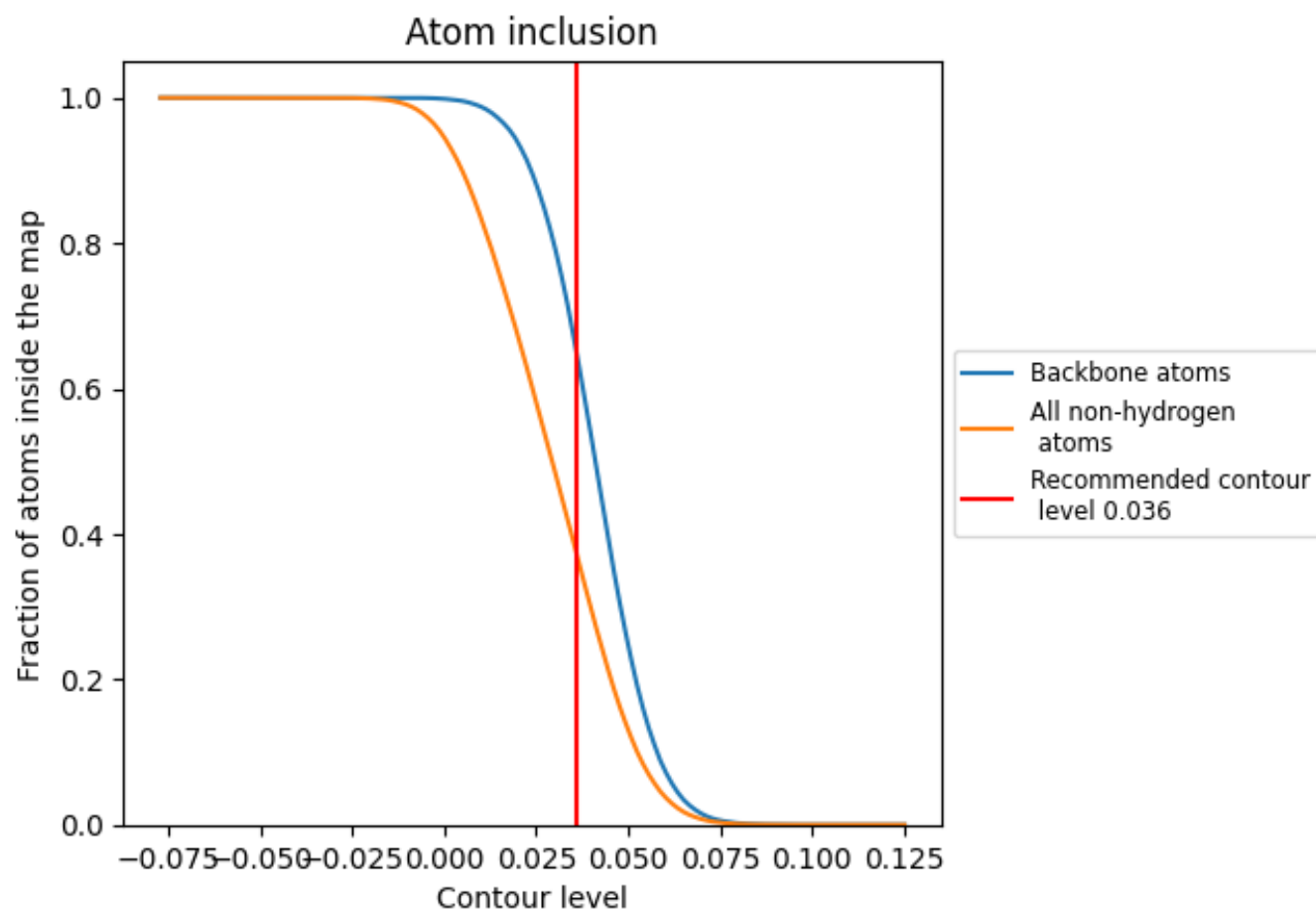
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.036).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 37% 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 (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3730	 0.2130
1	 0.3130	 0.1980
2	 0.2626	 0.1960
3	 0.1555	 0.1720
4	 0.0022	 0.1250
5	 0.3020	 0.2000
6	 0.2609	 0.1820
7	 0.2514	 0.1770
A	 0.4445	 0.2310
B	 0.4324	 0.2250
C	 0.4356	 0.2330
D	 0.4517	 0.2340
E	 0.4519	 0.2330
F	 0.4256	 0.2240
G	 0.4414	 0.2260
H	 0.4618	 0.2370
I	 0.4432	 0.2290
J	 0.2857	 0.1930
K	 0.2752	 0.2050
L	 0.2458	 0.2050
M	 0.2899	 0.1910
N	 0.2605	 0.2000
O	 0.2164	 0.2160
P	 0.2899	 0.1820
Q	 0.2479	 0.1880
R	 0.2794	 0.1850
S	 0.4238	 0.2310
T	 0.3592	 0.2160
U	 0.4064	 0.2300
V	 0.4195	 0.2280
W	 0.3782	 0.2090
X	 0.3296	 0.2030
Y	 0.3682	 0.2050
Z	 0.3843	 0.2100
a	 0.3795	 0.2150



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Chain	Atom inclusion	Q-score
b	 0.3542	 0.2050
c	 0.3908	 0.2110
d	 0.3852	 0.2110
e	 0.1902	 0.1650
f	 0.1627	 0.1710
g	 0.2108	 0.1730
h	 0.1068	 0.1560
i	 0.1962	 0.1750
j	 0.1237	 0.1680
k	 0.2246	 0.1540
l	 0.1049	 0.1590
m	 0.2479	 0.1690
n	 0.2658	 0.1640
o	 0.2993	 0.1730
p	 0.2172	 0.1740
q	 0.3608	 0.2130
r	 0.3995	 0.2230
s	 0.4047	 0.2190
t	 0.4223	 0.2250
u	 0.4019	 0.2170
v	 0.3810	 0.2120
w	 0.1815	 0.1650
x	 0.1408	 0.1800
y	 0.1681	 0.1790
z	 0.2248	 0.1960