wwPDB EM Validation Summary Report (i)

May 20, 2024 – 06:22 AM JST

PDB ID	:	6LGN
EMDB ID	:	EMD-0881
Title	:	The atomic structure of varicella zoster virus C-capsid
Authors	:	Li, S.; Zheng, Q.
Deposited on	:	2019-12-05
Resolution	:	5.30 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 (i) 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 (i)) were used in the production of this report:

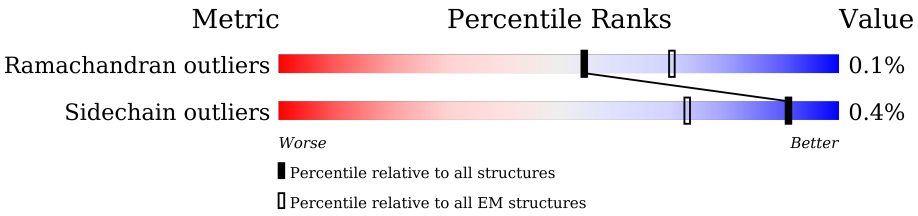
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 5.30 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 >=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 <=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	1396	15% 97% .
1	B	1396	12% 97% .
1	C	1396	13% 97% .
1	E	1396	15% 97% .
1	F	1396	13% 97% .
1	G	1396	14% 92% 7%
1	M	1396	14% 97% .
1	N	1396	12% 97% .
1	O	1396	11% 97% .

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Mol	Chain	Length	Quality of chain
1	P	1396	11% 97%
1	Q	1396	13% 97%
1	R	1396	14% 97%
1	S	1396	11% 97%
1	T	1396	13% 97%
1	U	1396	16% 95% 5%
1	z	1396	16% 43% 57%
2	D	235	42% 57%
2	H	235	42% 58%
2	I	235	43% 57%
2	J	235	43% 57%
2	K	235	43% 57%
2	L	235	43% 57%
2	V	235	43% 57%
2	W	235	42% 57%
2	X	235	43% 57%
2	Y	235	43% 57%
2	Z	235	43% 57%
2	a	235	43% 57%
2	b	235	42% 58%
2	c	235	43% 57%
2	d	235	42% 57%
3	e	483	19% 56% 40%
3	f	483	8% 61% 35%
3	g	483	7% 62% 34%

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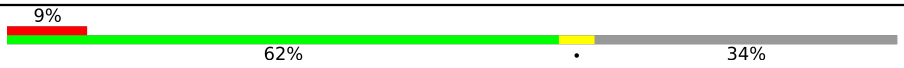
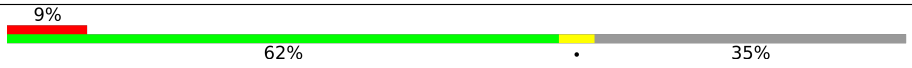
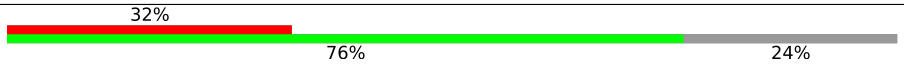
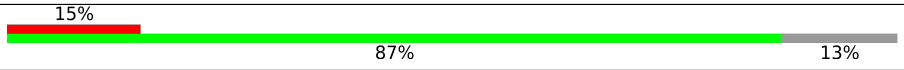
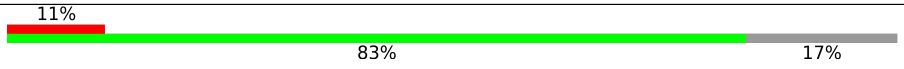
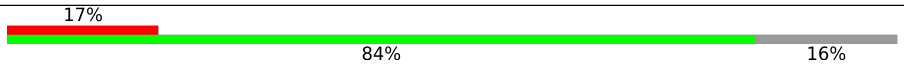
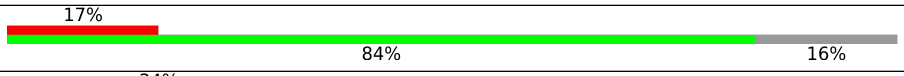
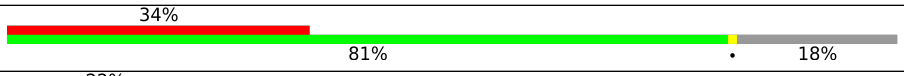
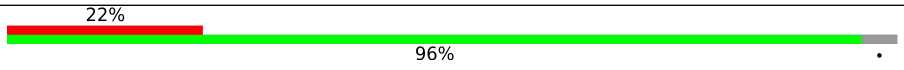
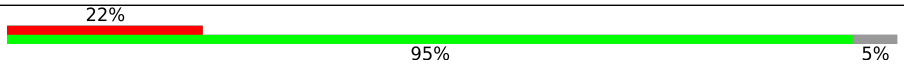
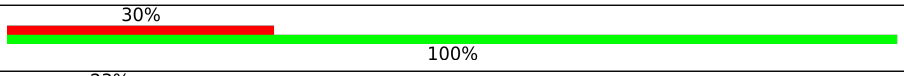
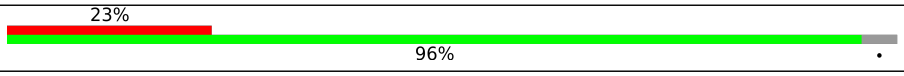
Mol	Chain	Length	Quality of chain
3	h	483	
3	i	483	
4	j	316	
4	k	316	
4	l	316	
4	m	316	
4	n	316	
4	o	316	
4	p	316	
4	q	316	
4	r	316	
4	s	316	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 207987 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	1354	Total	C	N	O	S	0	0
			10592	6695	1880	1949	68		
1	M	1353	Total	C	N	O	S	0	0
			10582	6690	1876	1948	68		
1	N	1353	Total	C	N	O	S	0	0
			10582	6690	1876	1948	68		
1	O	1355	Total	C	N	O	S	0	0
			10600	6701	1881	1950	68		
1	P	1355	Total	C	N	O	S	0	0
			10600	6701	1881	1950	68		
1	Q	1354	Total	C	N	O	S	0	0
			10592	6695	1880	1949	68		
1	R	1353	Total	C	N	O	S	0	0
			10582	6690	1876	1948	68		
1	S	1355	Total	C	N	O	S	0	0
			10600	6701	1881	1950	68		
1	T	1354	Total	C	N	O	S	0	0
			10592	6695	1880	1949	68		
1	U	1331	Total	C	N	O	S	0	0
			10422	6590	1847	1919	66		
1	B	1355	Total	C	N	O	S	0	0
			10600	6701	1881	1950	68		
1	C	1354	Total	C	N	O	S	0	0
			10592	6695	1880	1949	68		
1	E	1353	Total	C	N	O	S	0	0
			10582	6689	1877	1948	68		
1	F	1354	Total	C	N	O	S	0	0
			10592	6695	1880	1949	68		
1	G	1295	Total	C	N	O	S	0	0
			10133	6401	1804	1863	65		
1	z	607	Total	C	N	O	S	0	0
			4709	2970	830	878	31		

- Molecule 2 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	V	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	W	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	X	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	Y	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	Z	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	a	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	b	99	Total	C	N	O	S	0	0
			754	475	142	135	2		
2	c	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	d	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	H	99	Total	C	N	O	S	0	0
			754	475	142	135	2		
2	I	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	J	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	K	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	L	100	Total	C	N	O	S	0	0
			765	481	146	136	2		

- Molecule 3 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	e	289	Total	C	N	O	S	0	0
			2294	1451	411	417	15		
3	f	316	Total	C	N	O	S	0	0
			2492	1574	448	455	15		
3	g	317	Total	C	N	O	S	0	0
			2497	1576	448	458	15		
3	h	317	Total	C	N	O	S	0	0
			2496	1575	448	458	15		
3	i	316	Total	C	N	O	S	0	0
			2490	1572	447	456	15		

- Molecule 4 is a protein called Triplex capsid protein 2.

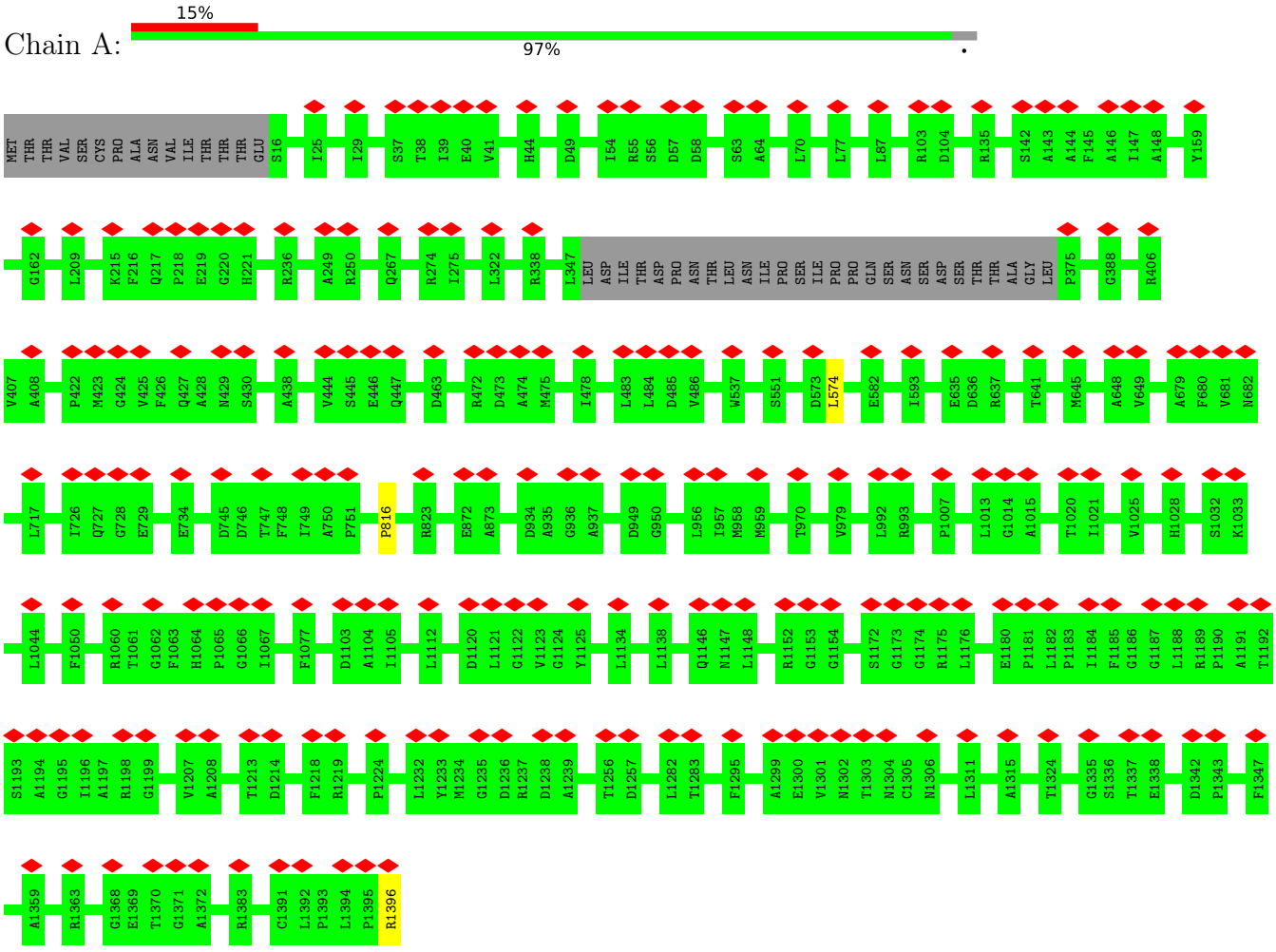
Mol	Chain	Residues	Atoms					AltConf	Trace
4	j	241	Total	C	N	O	S	0	0
			1837	1180	310	337	10		
4	o	258	Total	C	N	O	S	0	0
			1969	1259	334	366	10		
4	k	275	Total	C	N	O	S	0	0
			2090	1336	355	389	10		
4	p	304	Total	C	N	O	S	0	0
			2325	1480	403	429	13		
4	l	263	Total	C	N	O	S	0	0
			2010	1286	342	372	10		
4	q	301	Total	C	N	O	S	0	0
			2307	1469	400	426	12		
4	m	267	Total	C	N	O	S	0	0
			2028	1296	346	376	10		
4	r	315	Total	C	N	O	S	0	0
			2407	1532	420	443	12		
4	n	265	Total	C	N	O	S	0	0
			2019	1291	344	374	10		
4	s	304	Total	C	N	O	S	0	0
			2321	1477	403	429	12		

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.

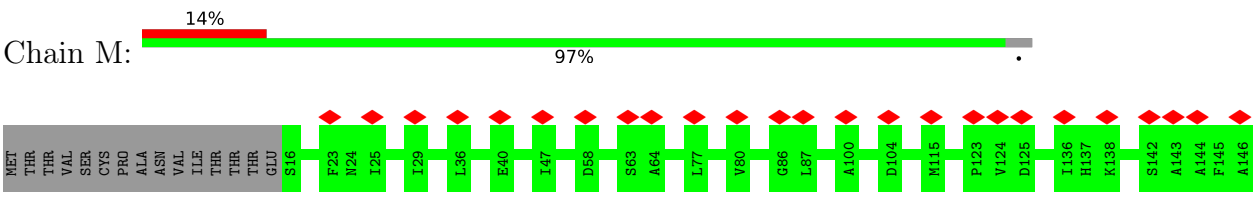
• Molecule 1: Major capsid protein

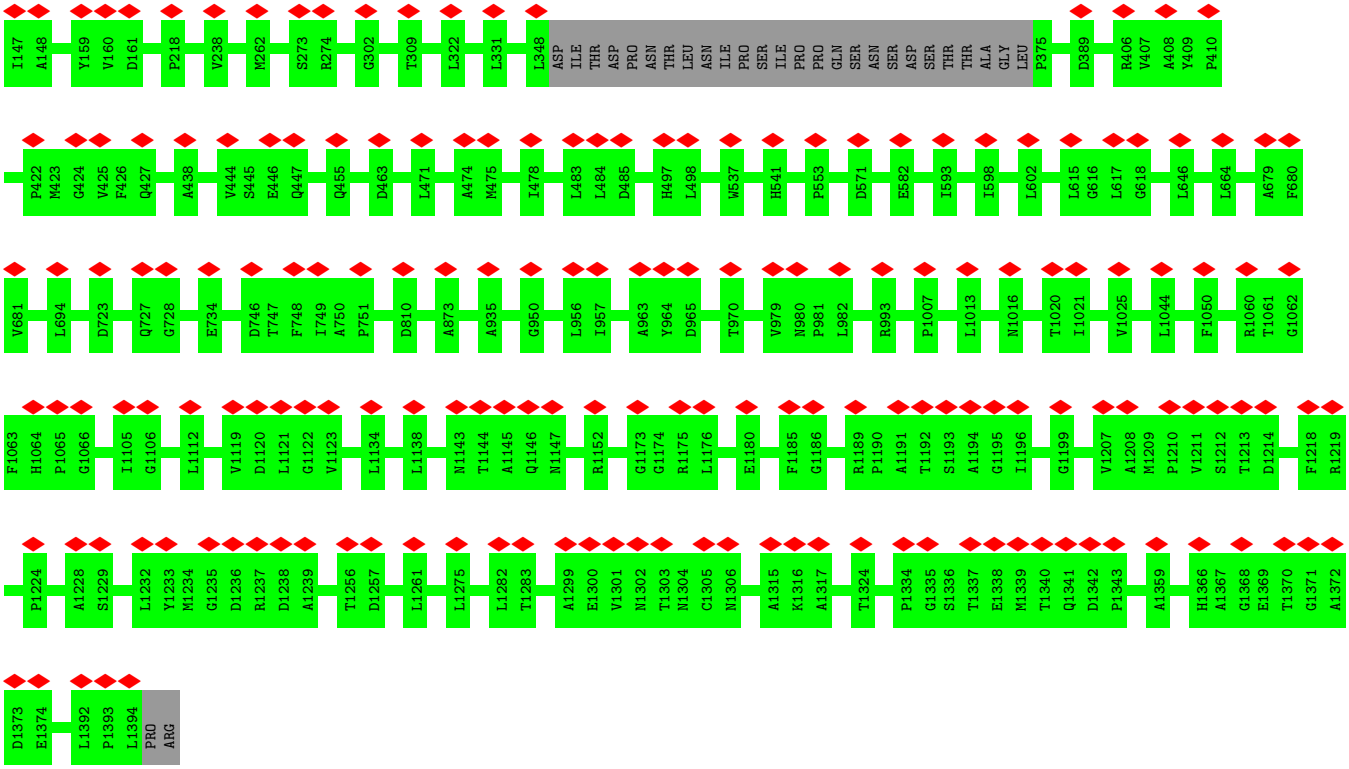
Chain A:



• Molecule 1: Major capsid protein

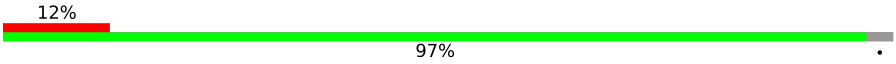
Chain M:

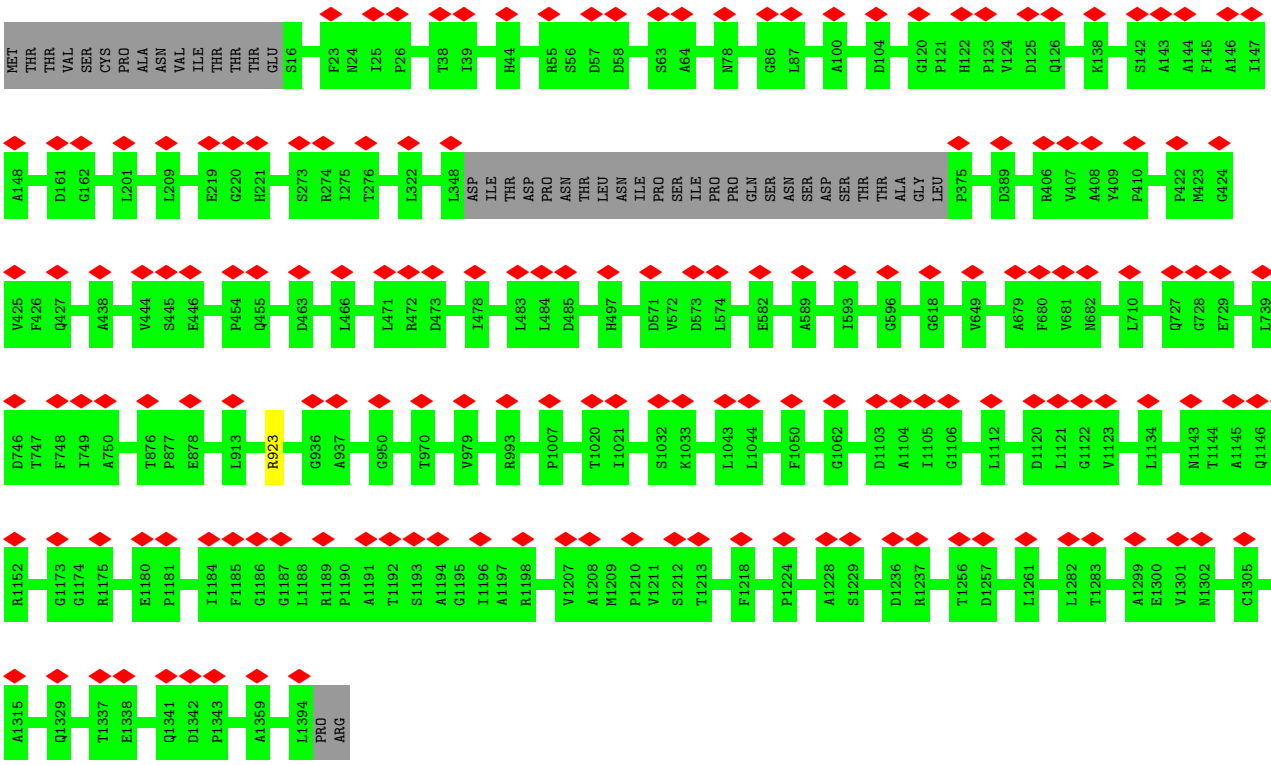




• Molecule 1: Major capsid protein

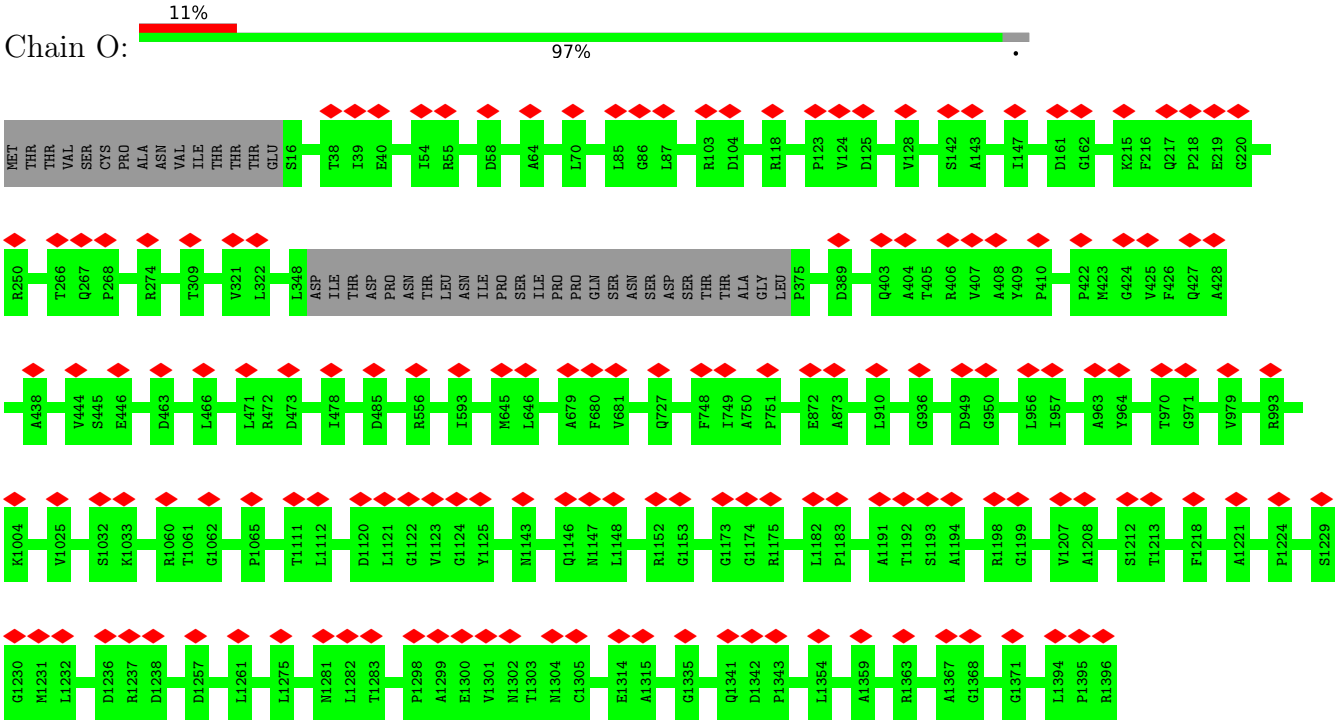
Chain N:





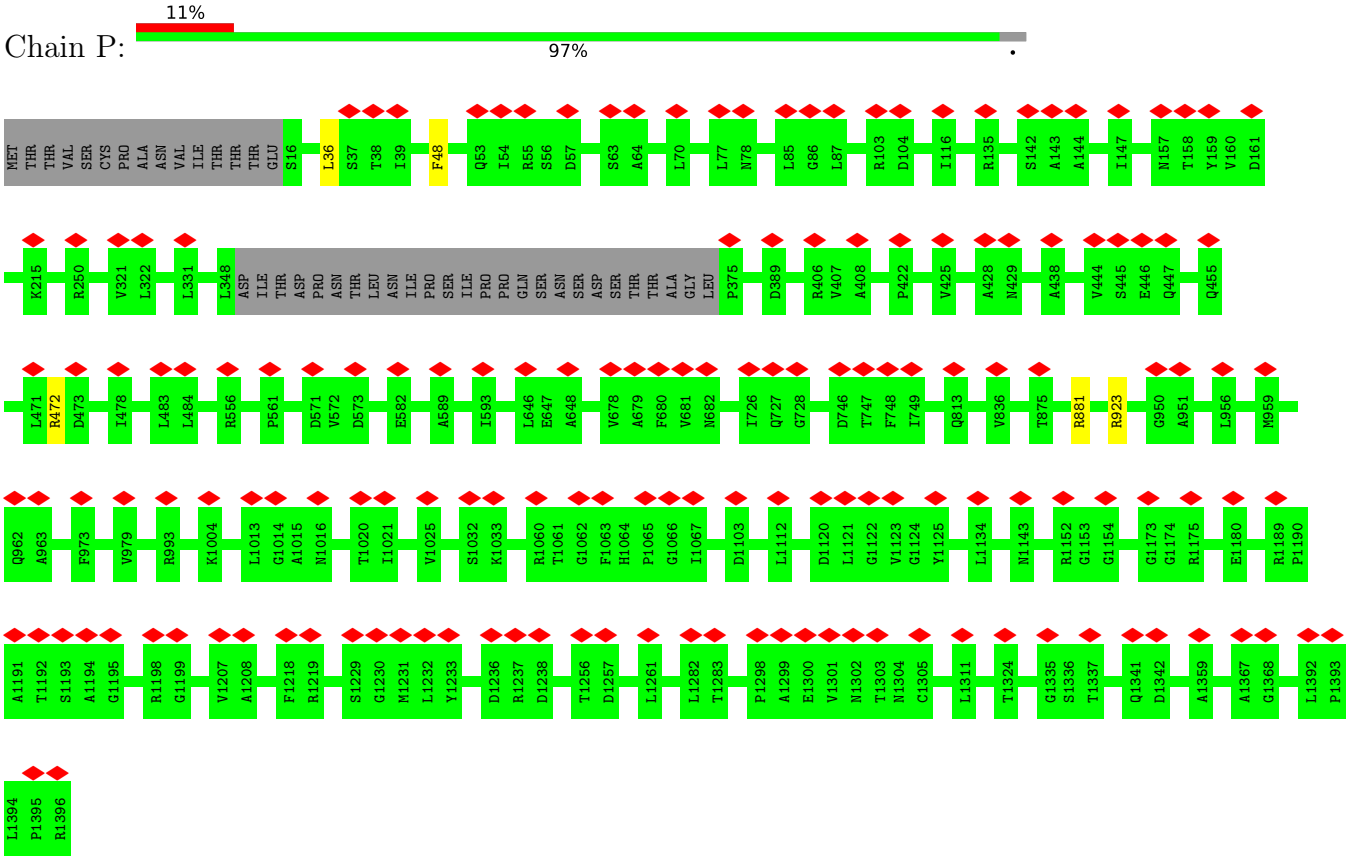
• Molecule 1: Major capsid protein

Chain O:



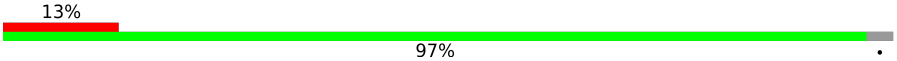
• Molecule 1: Major capsid protein

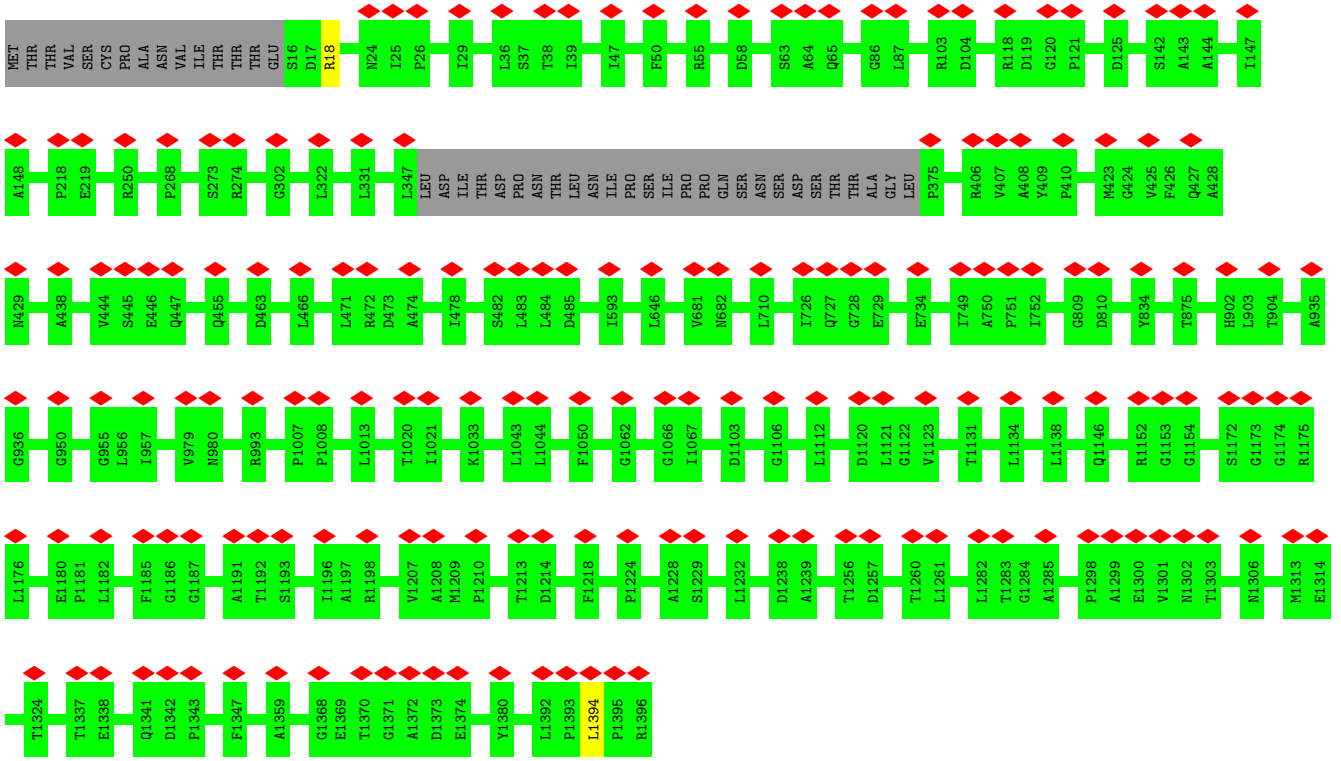
Chain P:



• Molecule 1: Major capsid protein

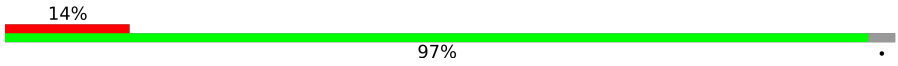
Chain Q:

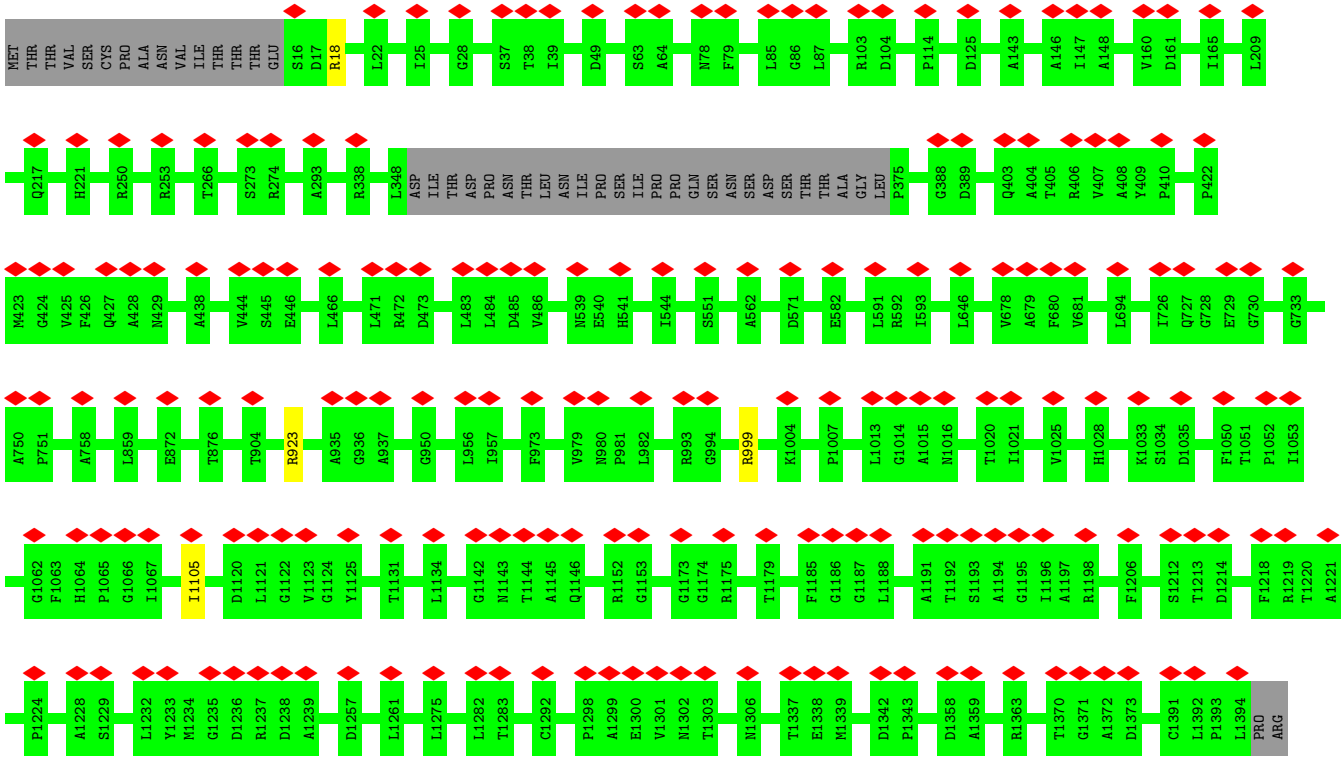




• Molecule 1: Major capsid protein

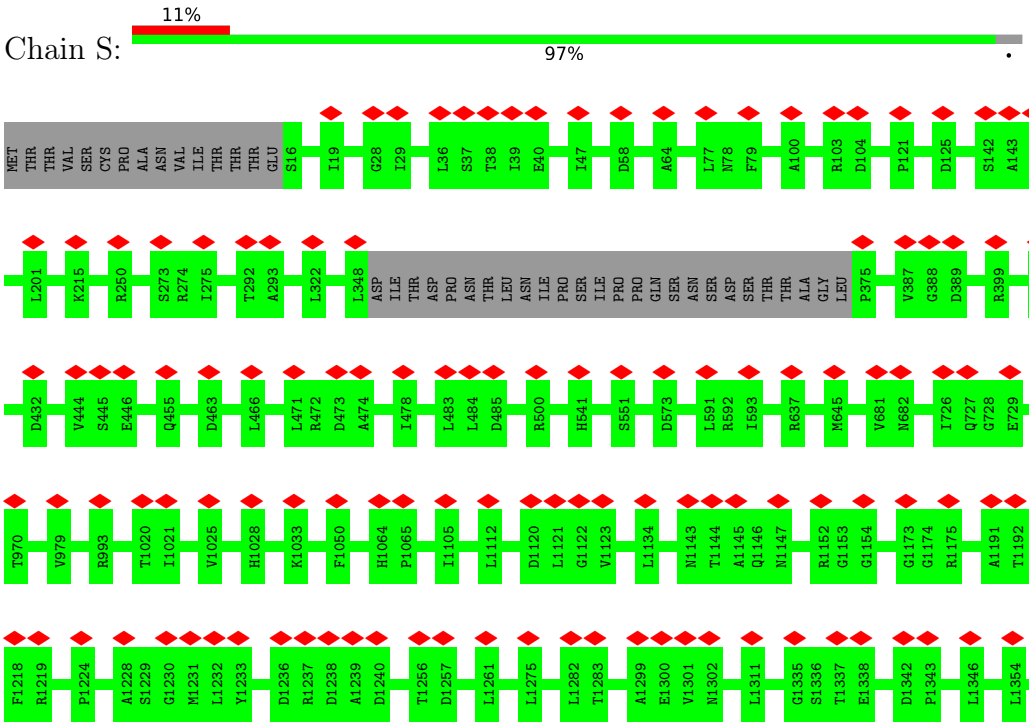
Chain R:





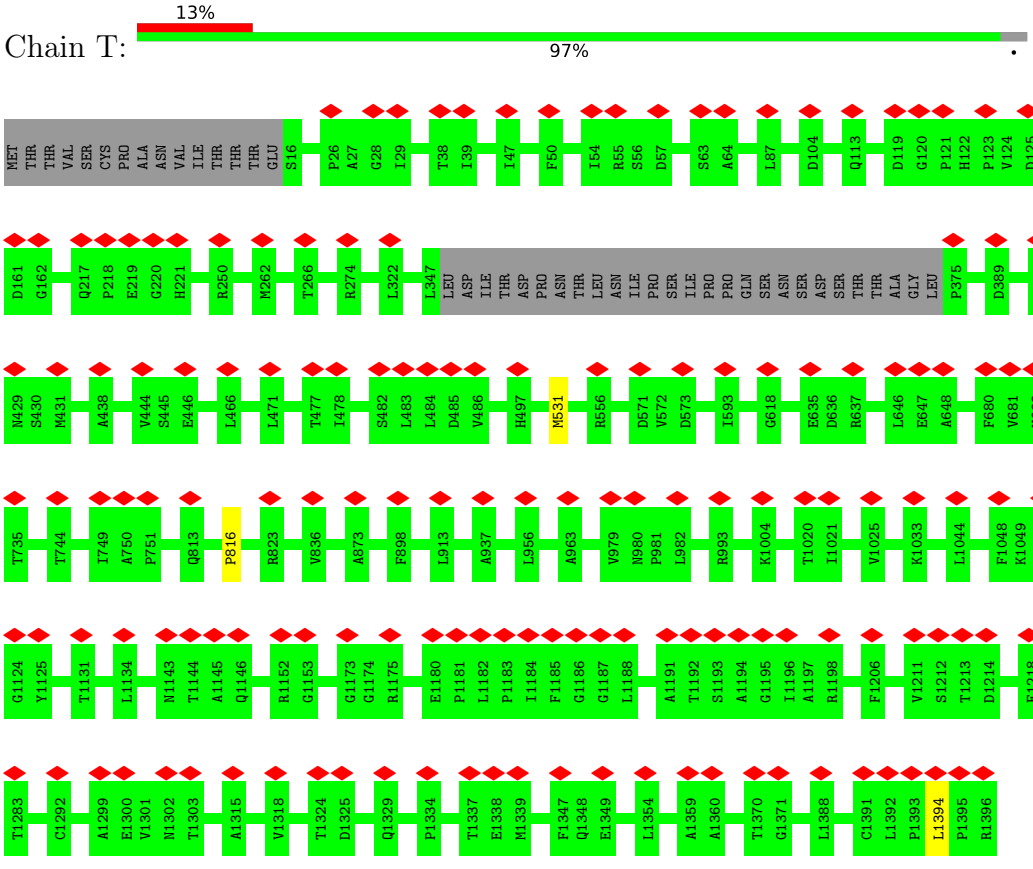
• Molecule 1: Major capsid protein

Chain S:



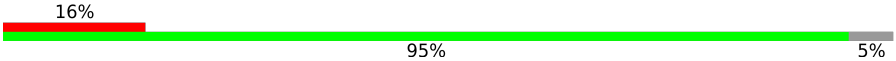
• Molecule 1: Major capsid protein

Chain T:



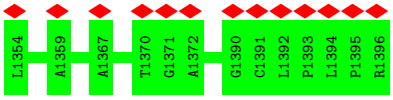
• Molecule 1: Major capsid protein

Chain U:



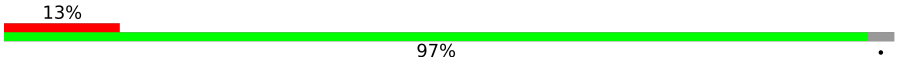
• Molecule 1: Major capsid protein

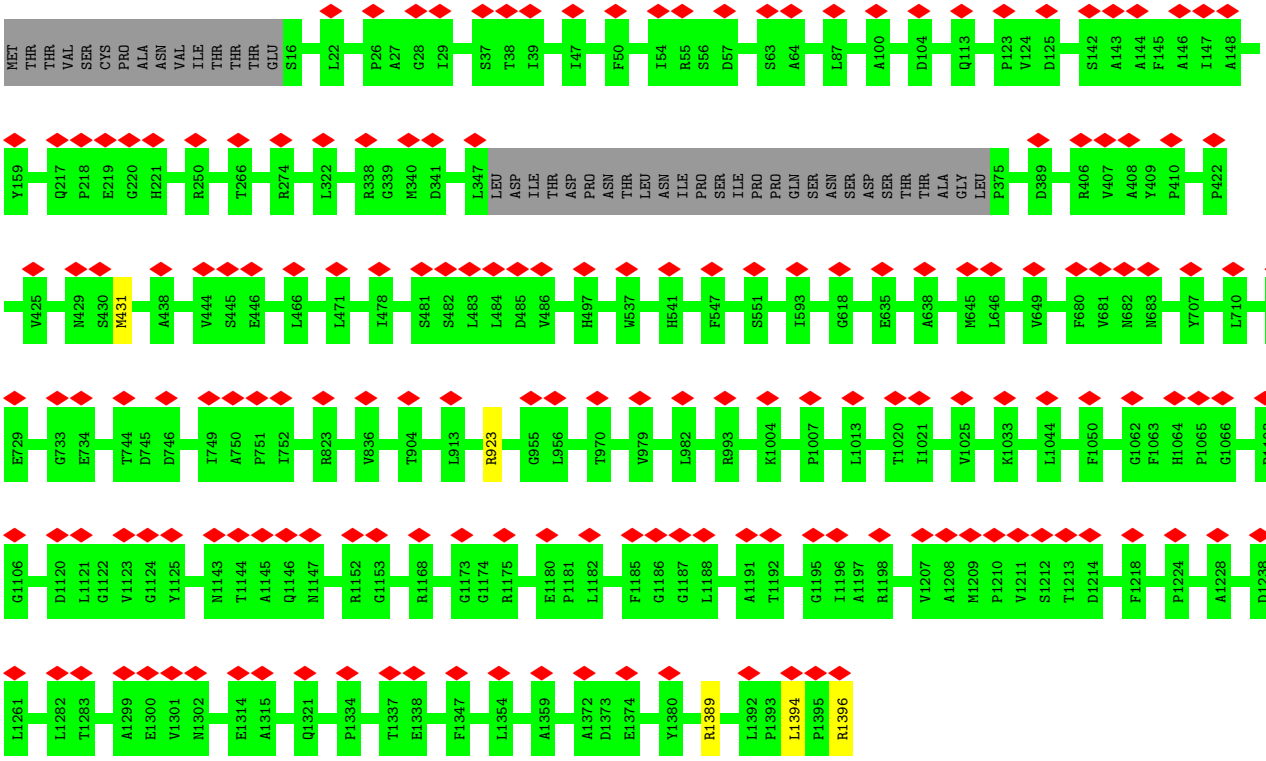
Chain B:



• Molecule 1: Major capsid protein

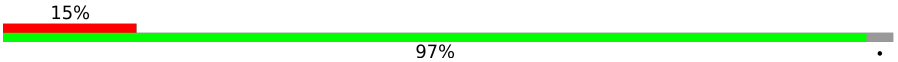
Chain C:

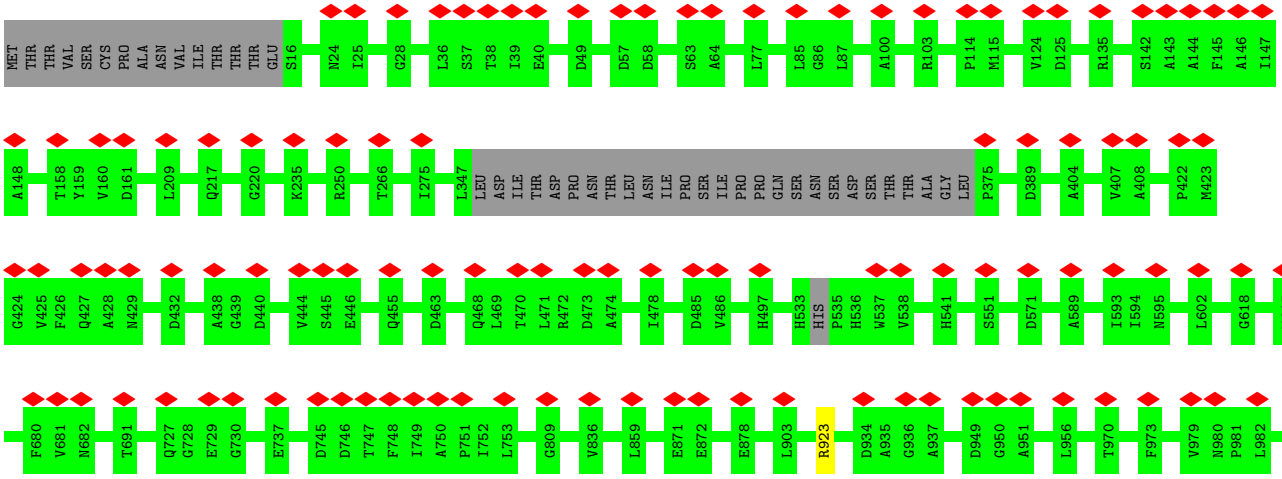


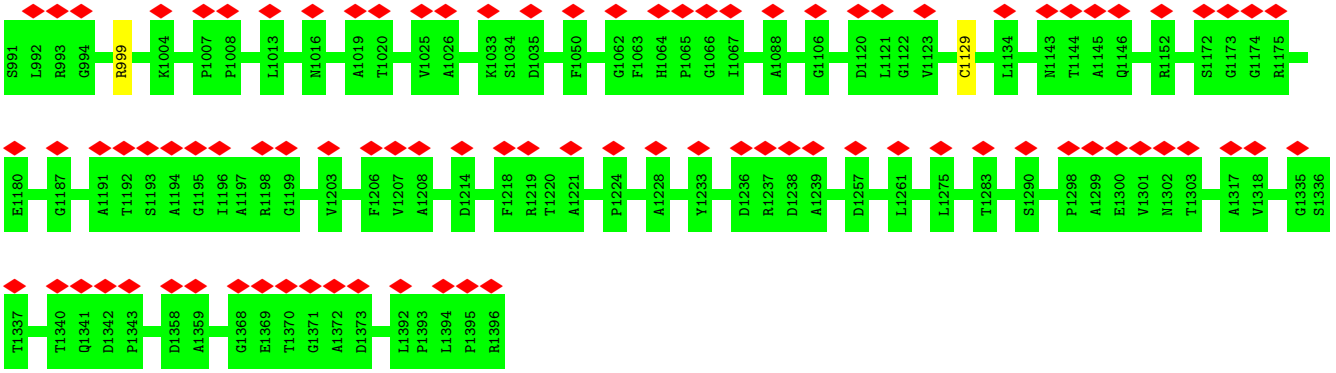


• Molecule 1: Major capsid protein

Chain E:

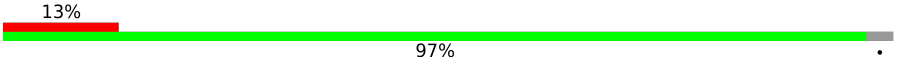


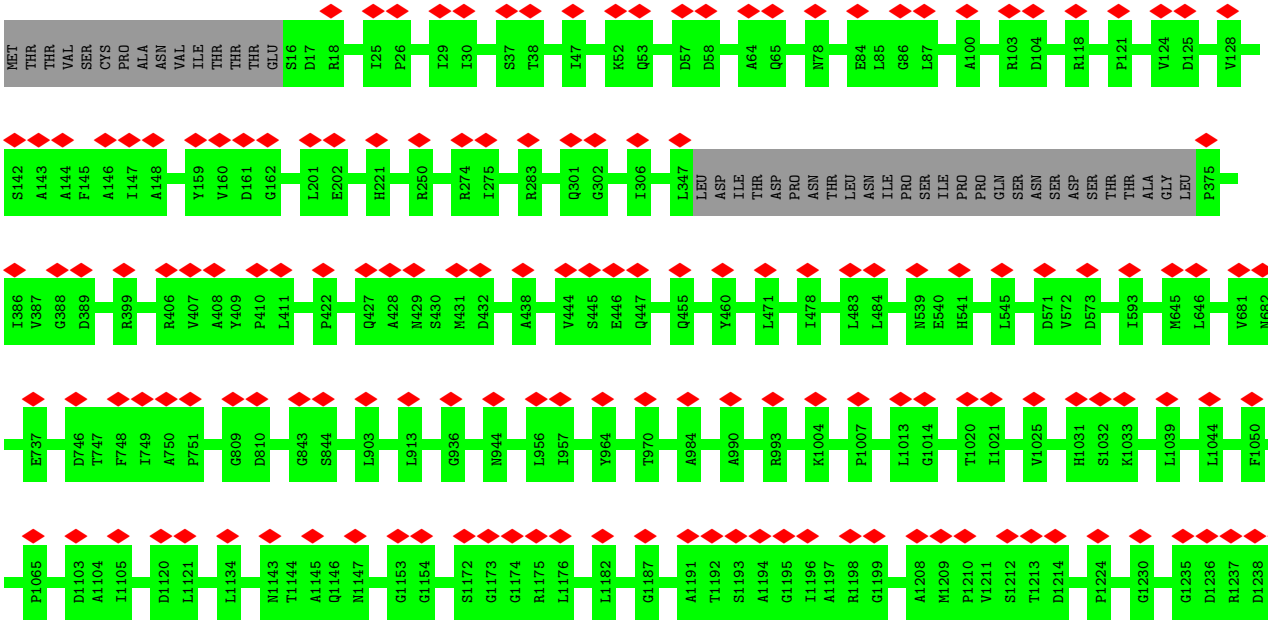




• Molecule 1: Major capsid protein

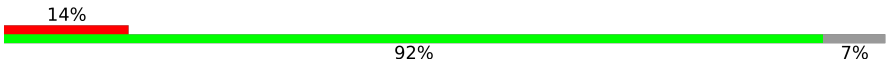
Chain F:

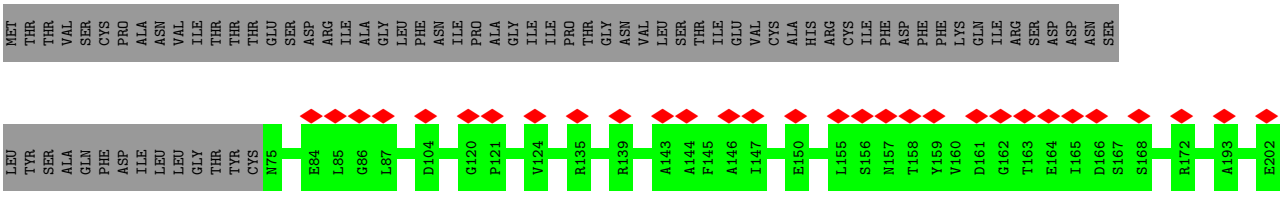


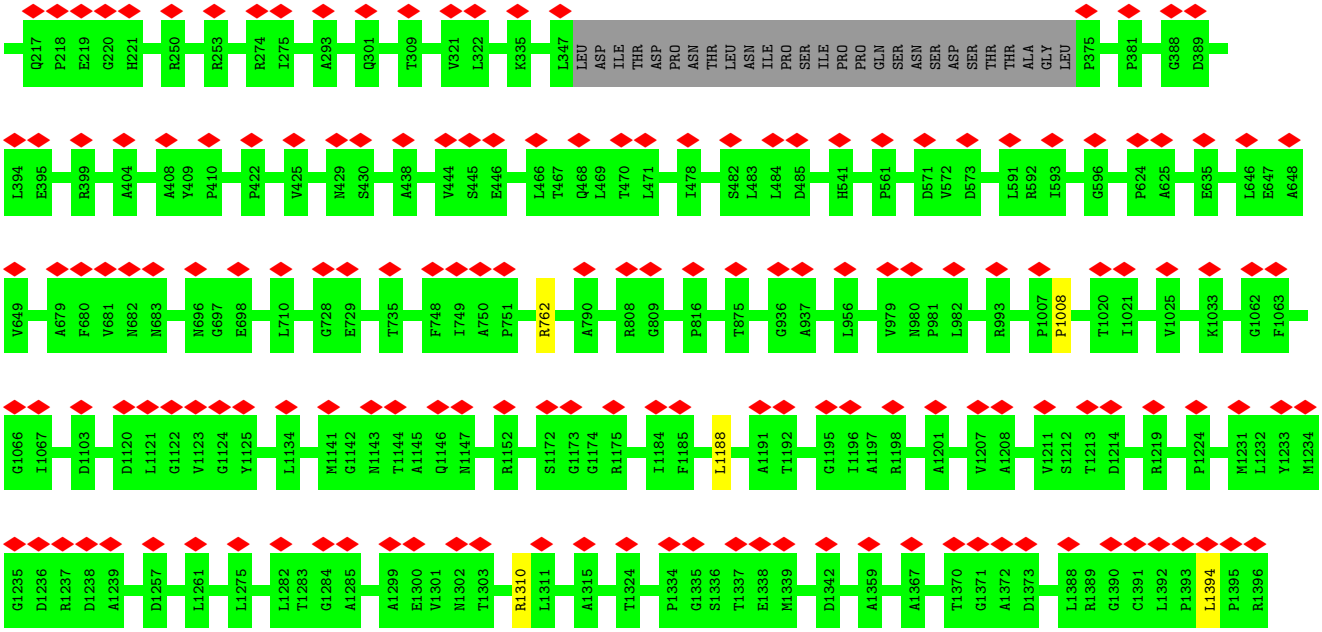


• Molecule 1: Major capsid protein

Chain G:

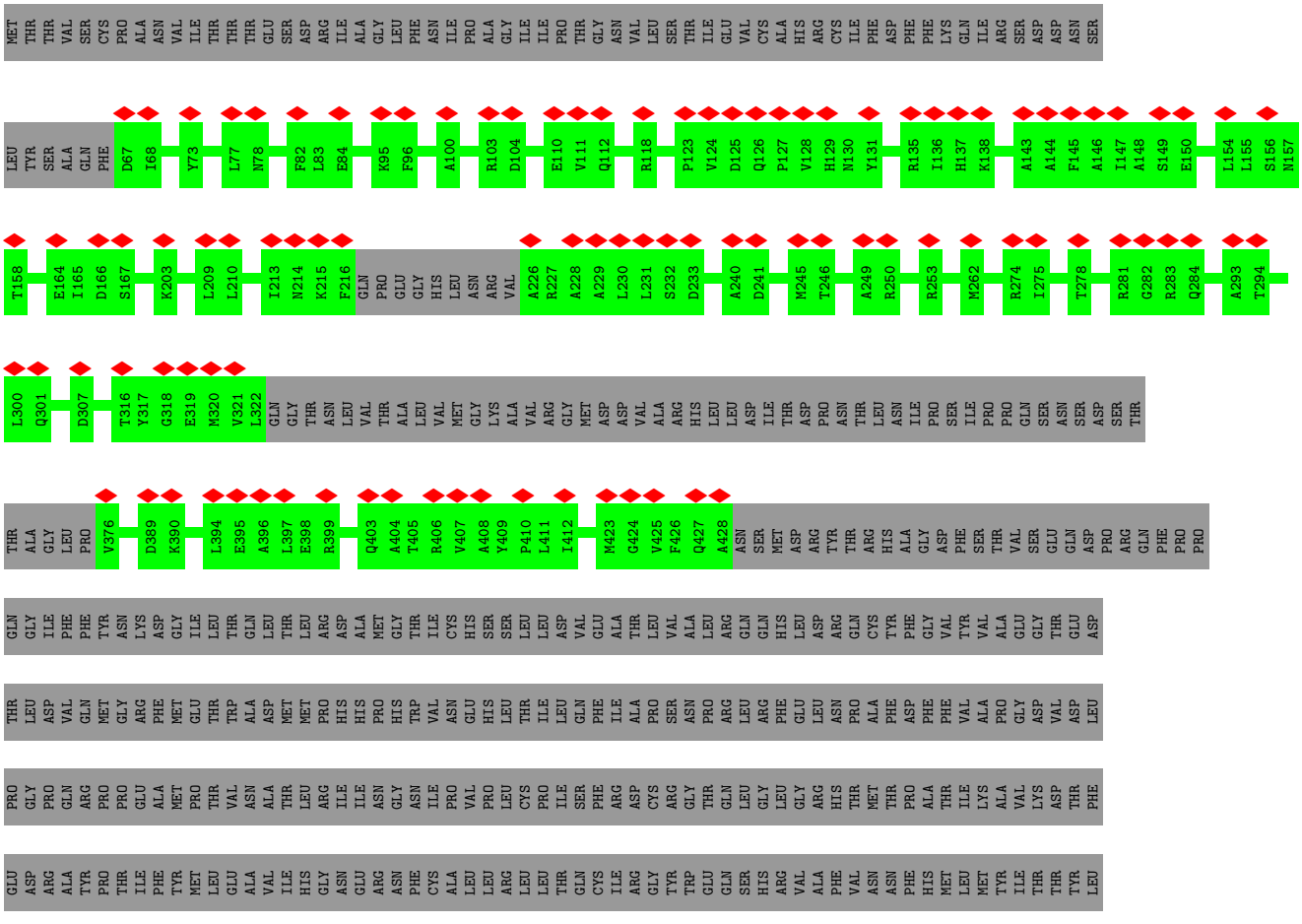


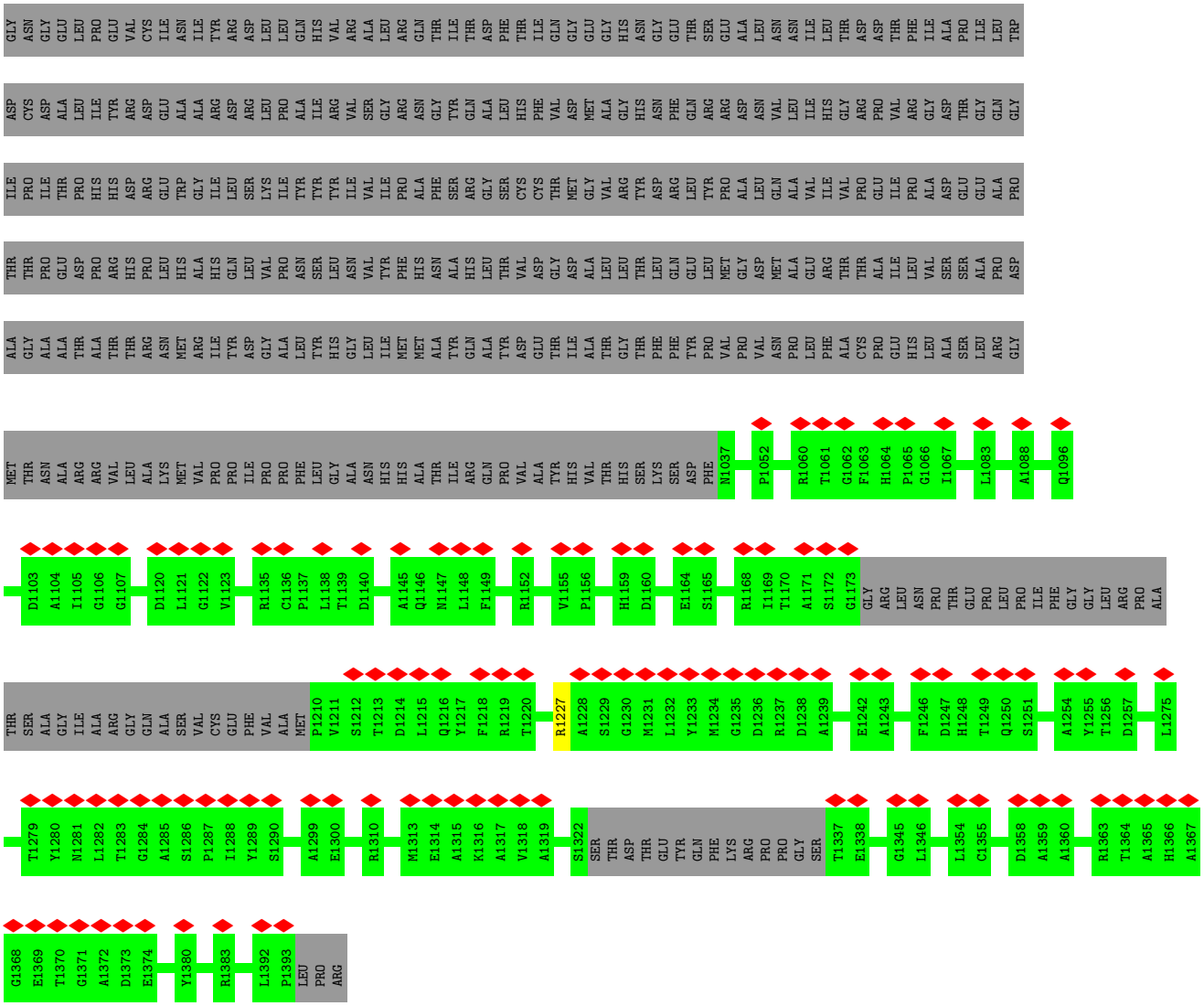




• Molecule 1: Major capsid protein

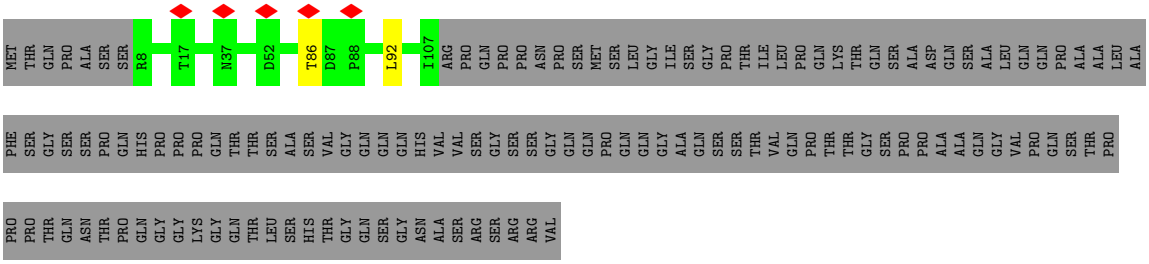
Chain z:





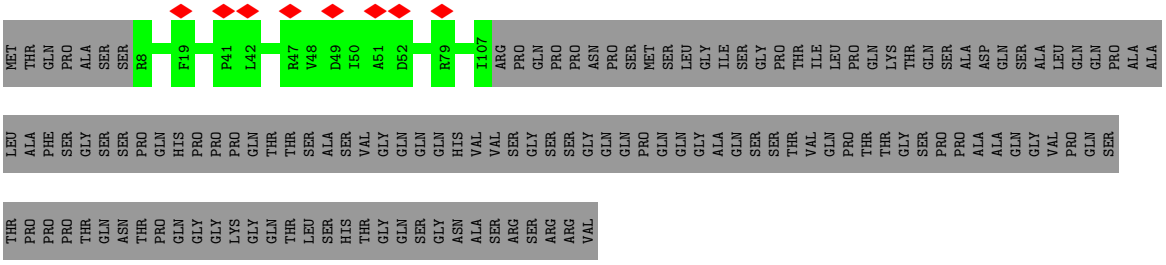
• Molecule 2: Small capsomere-interacting protein

Chain D:



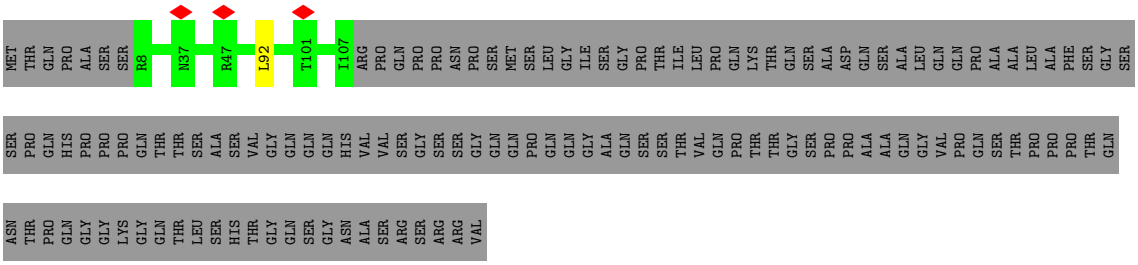
• Molecule 2: Small capsomere-interacting protein

Chain V:



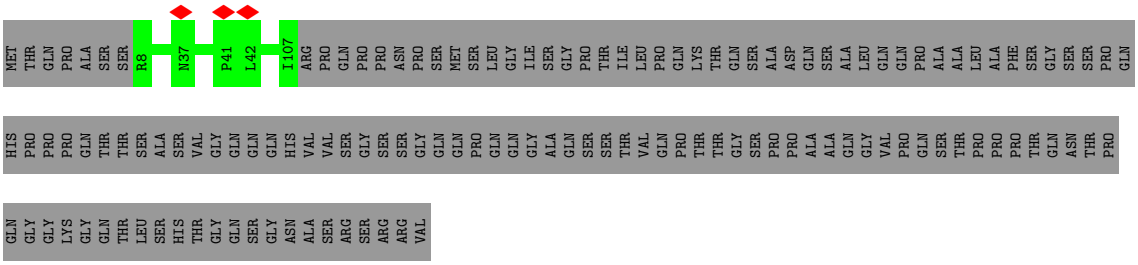
• Molecule 2: Small capsomere-interacting protein

Chain W:



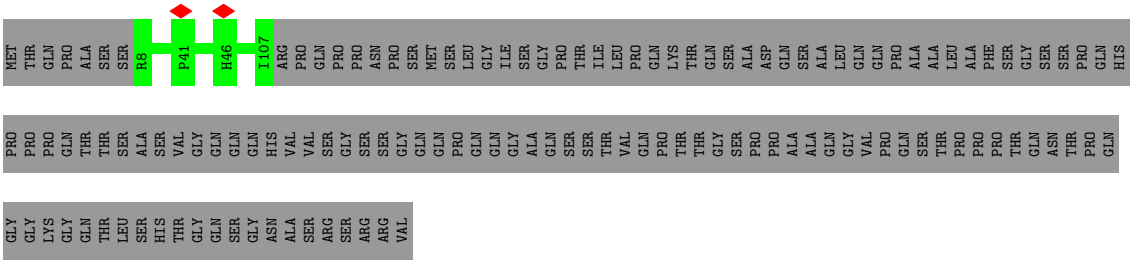
• Molecule 2: Small capsomere-interacting protein

Chain X:



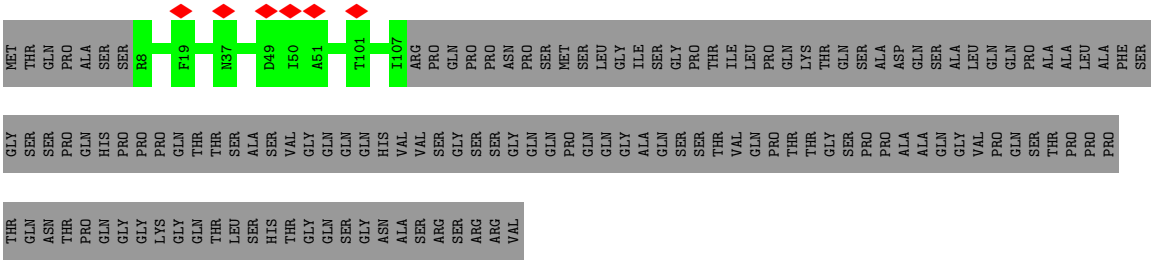
• Molecule 2: Small capsomere-interacting protein

Chain Y:



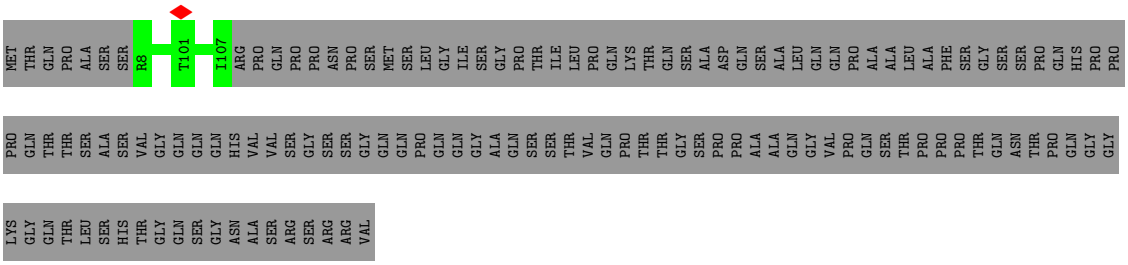
• Molecule 2: Small capsomere-interacting protein

Chain Z:



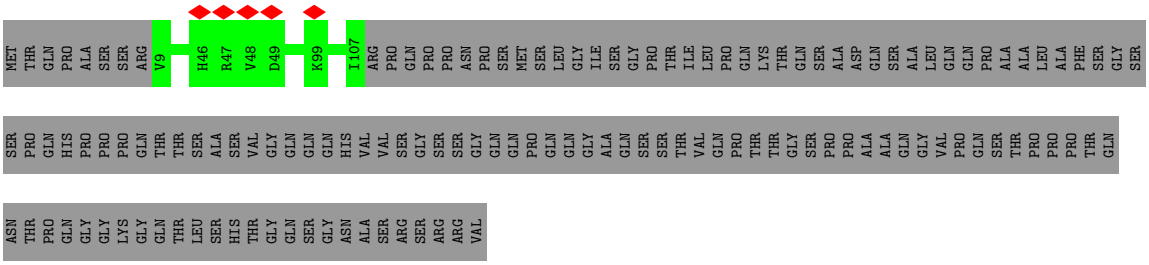
• Molecule 2: Small capsomere-interacting protein

Chain a:



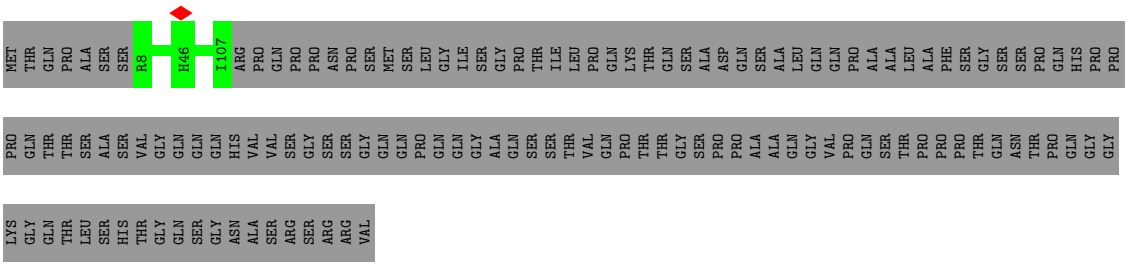
• Molecule 2: Small capsomere-interacting protein

Chain b:



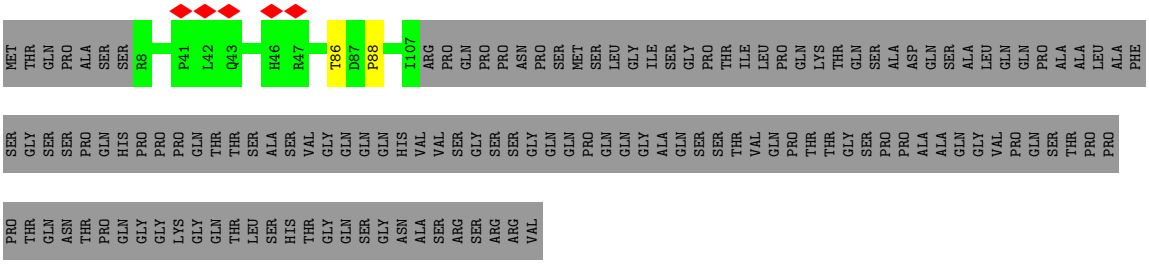
• Molecule 2: Small capsomere-interacting protein

Chain c:



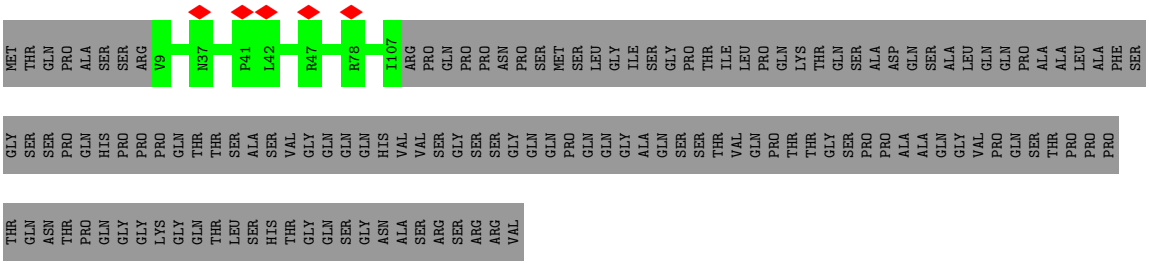
• Molecule 2: Small capsomere-interacting protein

Chain d:



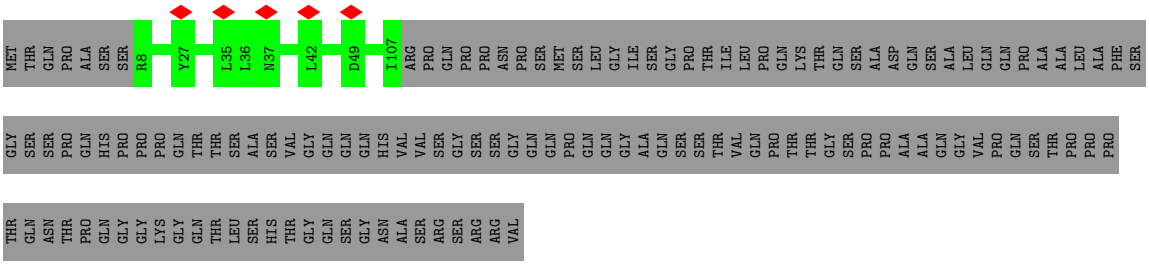
• Molecule 2: Small capsomere-interacting protein

Chain H:



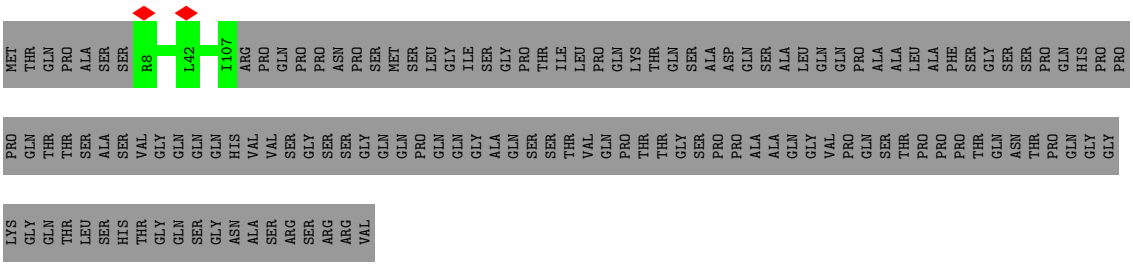
• Molecule 2: Small capsomere-interacting protein

Chain I:



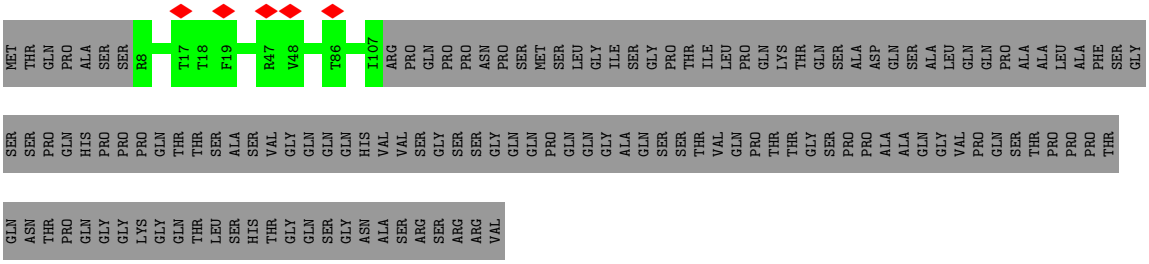
• Molecule 2: Small capsomere-interacting protein

Chain J:



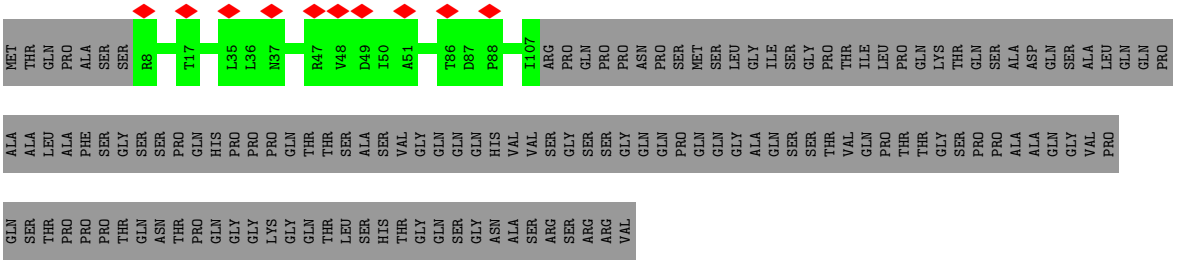
• Molecule 2: Small capsomere-interacting protein

Chain K:



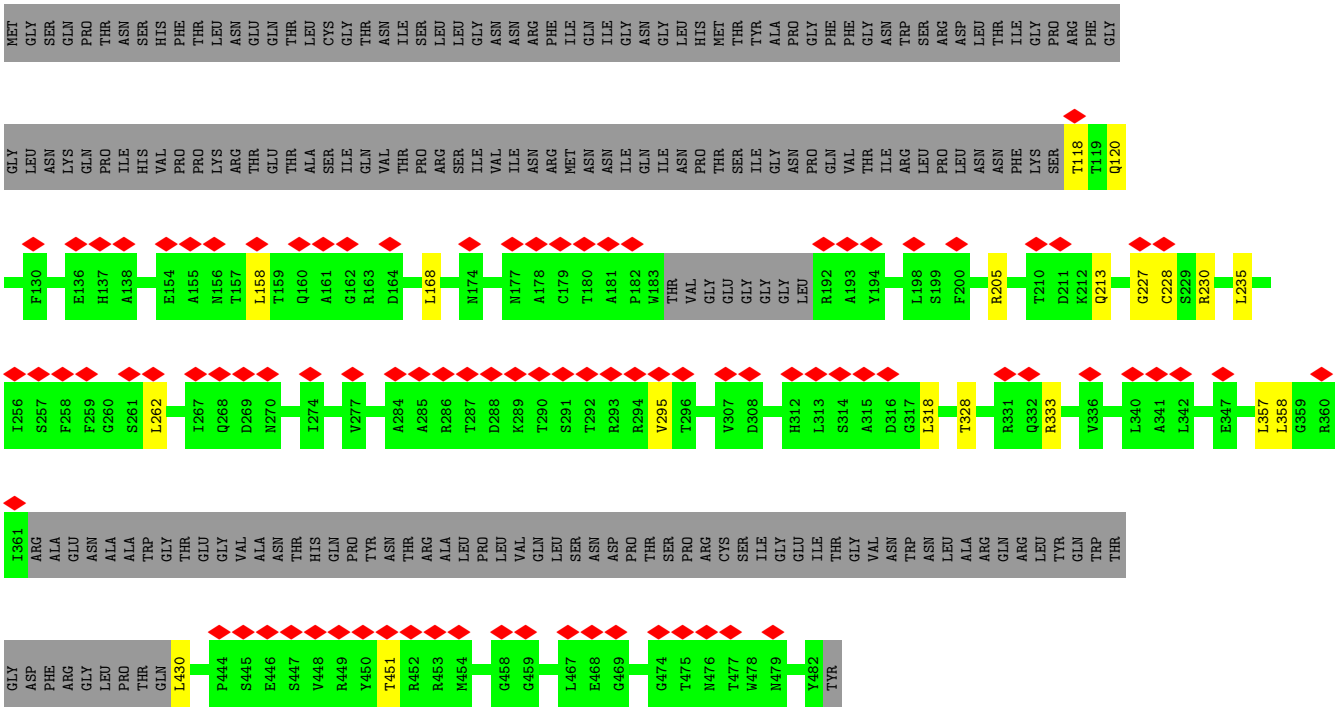
• Molecule 2: Small capsomere-interacting protein

Chain L:



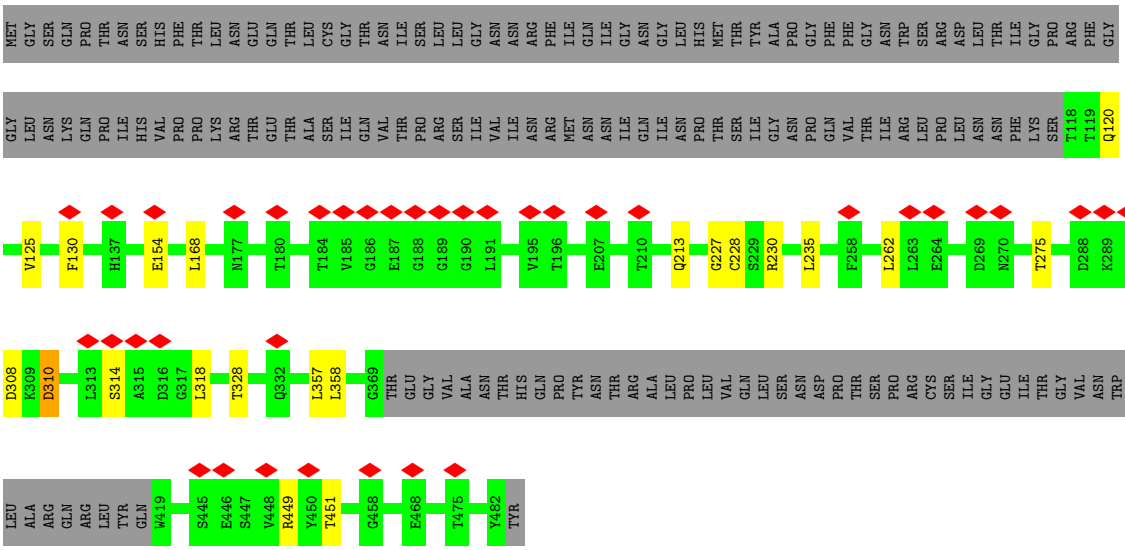
• Molecule 3: Triplex capsid protein 1

Chain e:



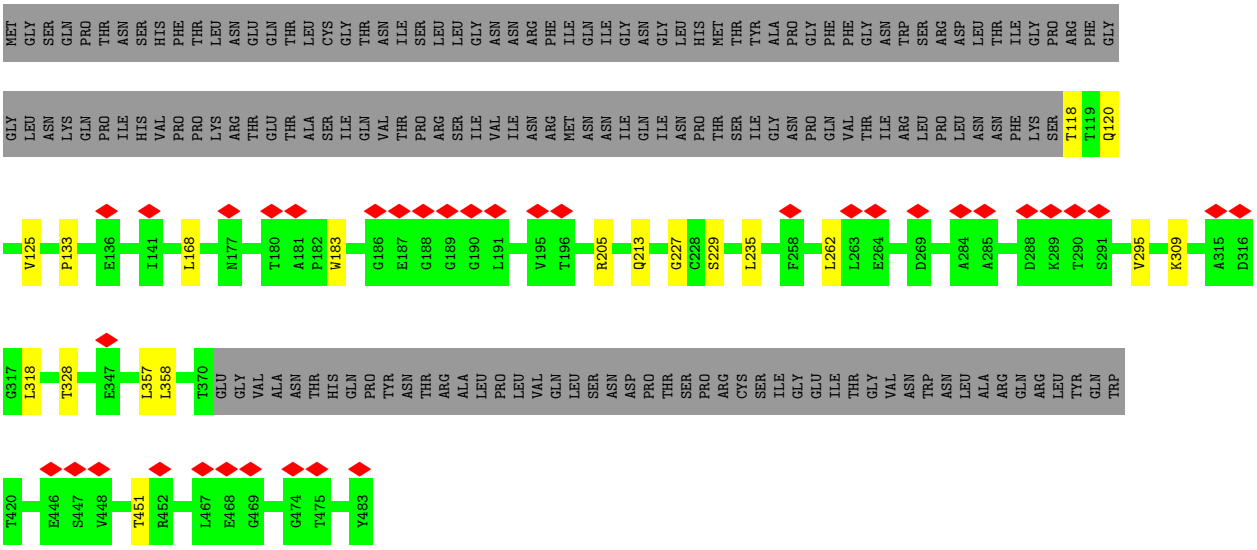
• Molecule 3: Triplex capsid protein 1

Chain f:



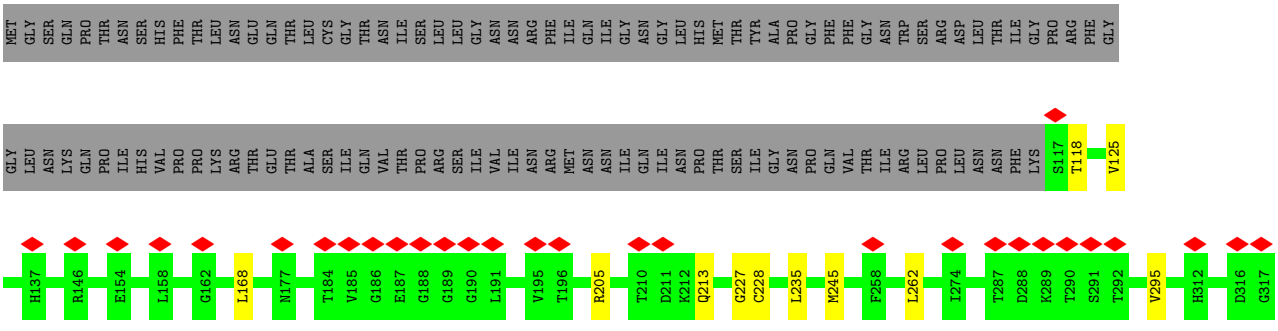
• Molecule 3: Triplex capsid protein 1

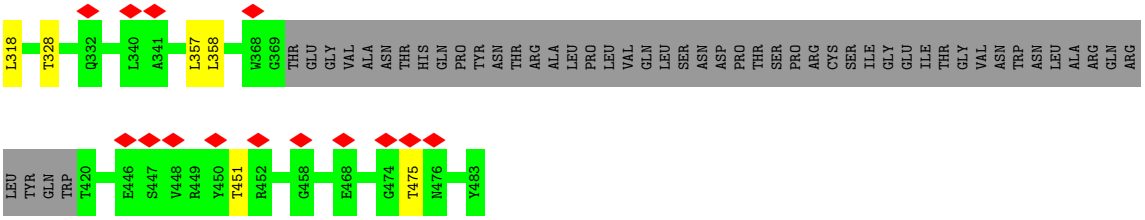
Chain g:



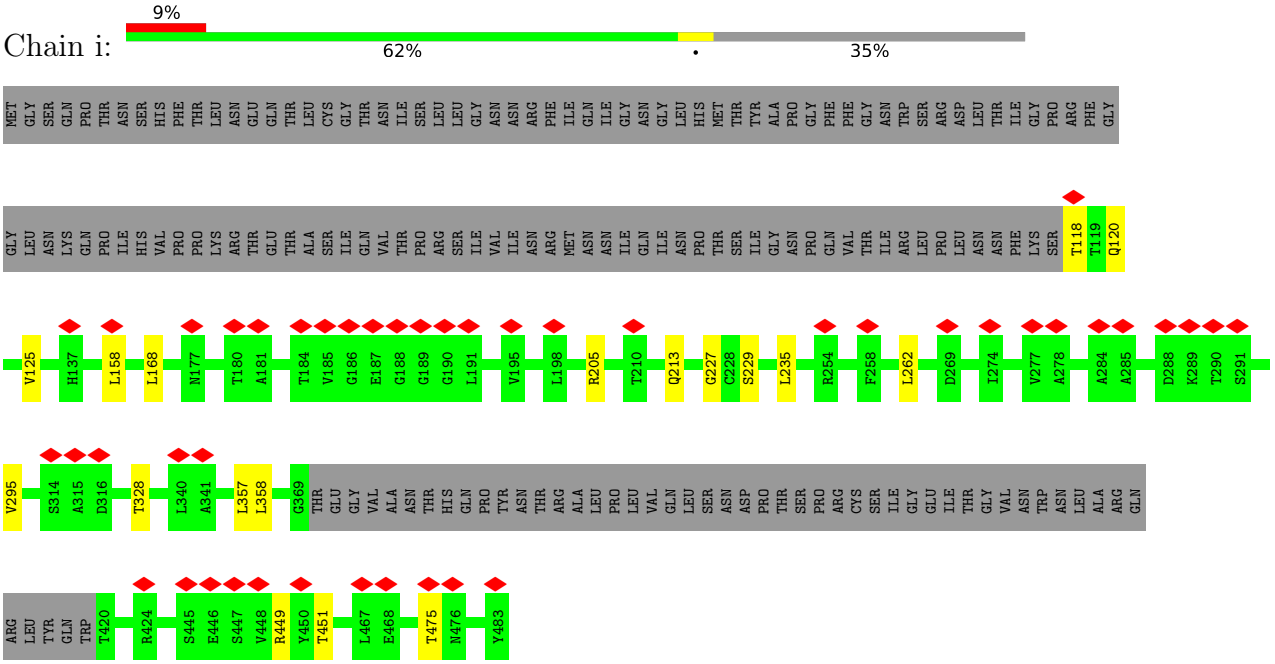
• Molecule 3: Triplex capsid protein 1

Chain h:

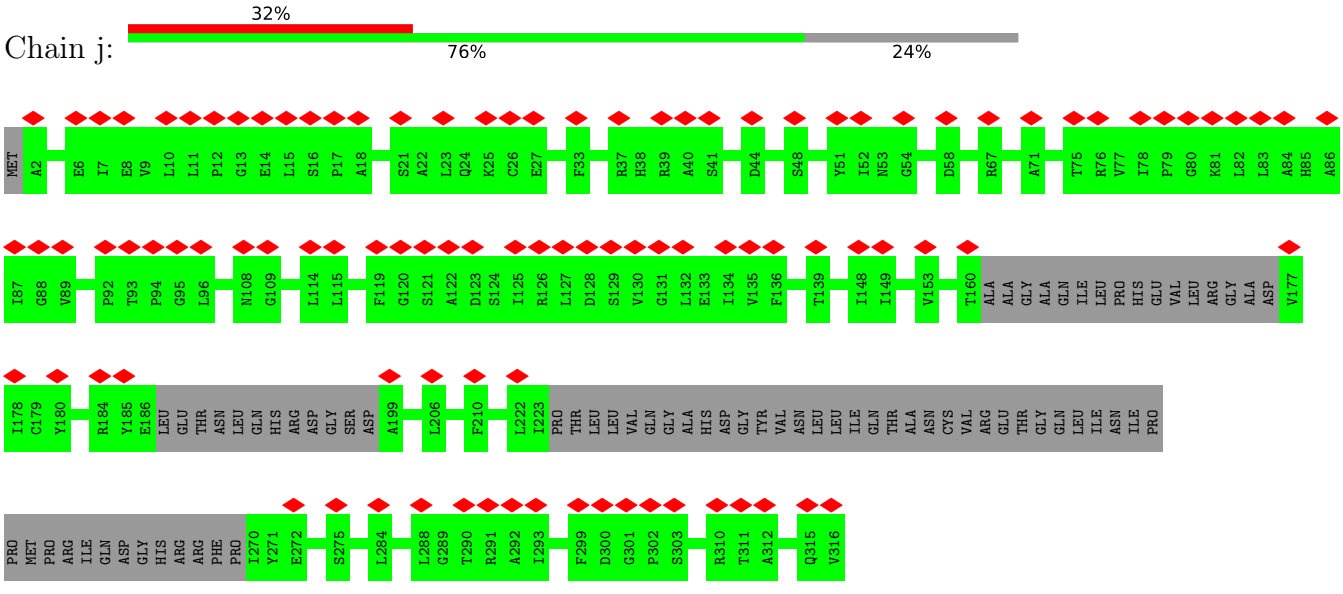




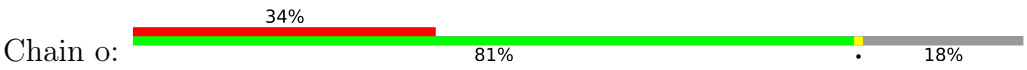
• Molecule 3: Triplex capsid protein 1

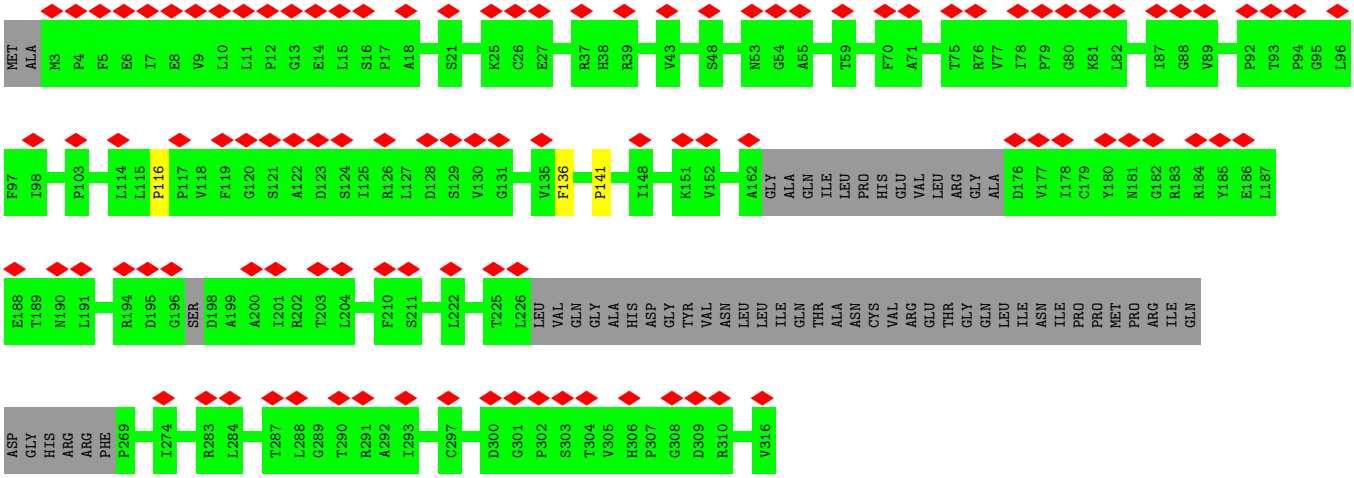


• Molecule 4: Triplex capsid protein 2



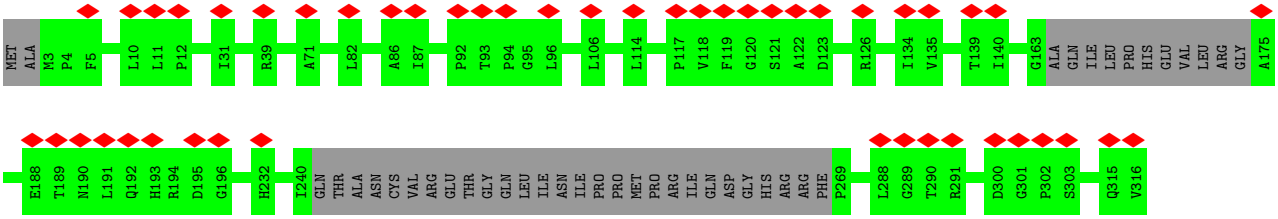
• Molecule 4: Triplex capsid protein 2





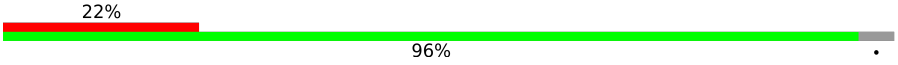
• Molecule 4: Triplex capsid protein 2

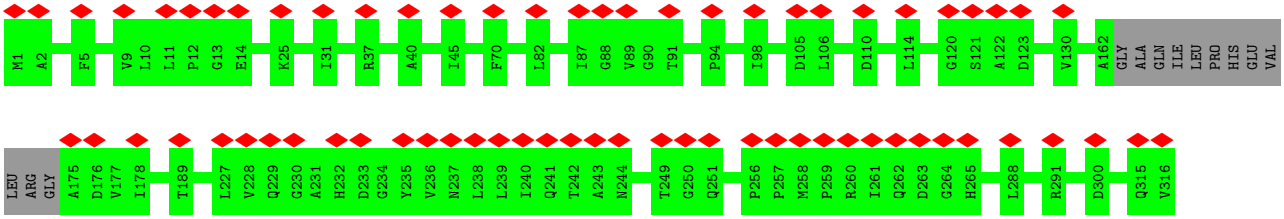
Chain k:



• Molecule 4: Triplex capsid protein 2

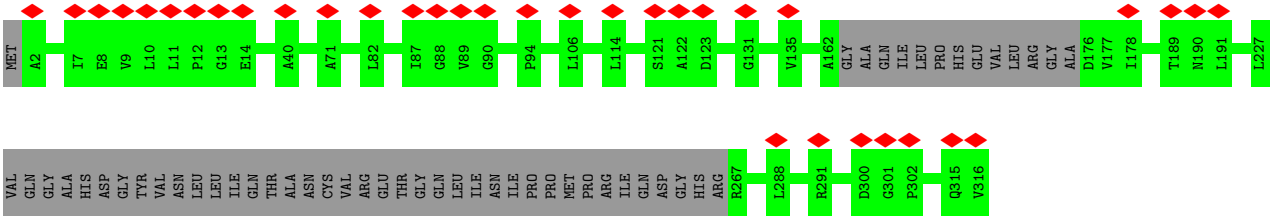
Chain p:





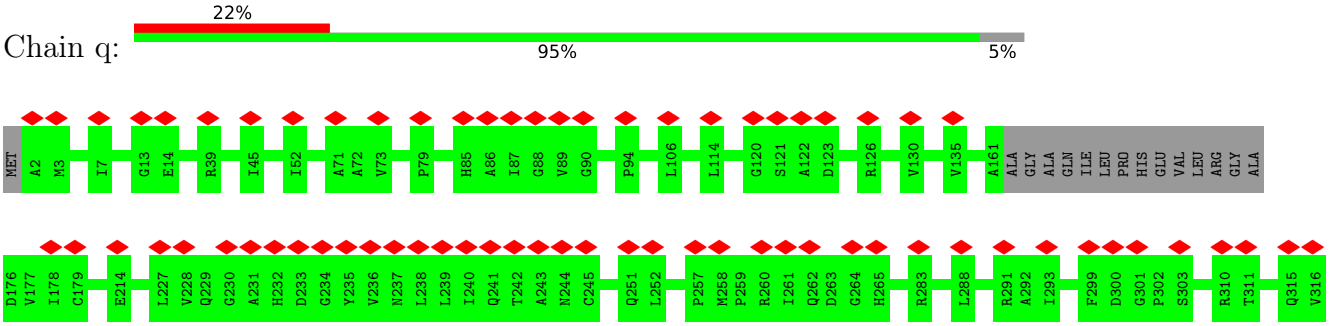
• Molecule 4: Triplex capsid protein 2

Chain l:



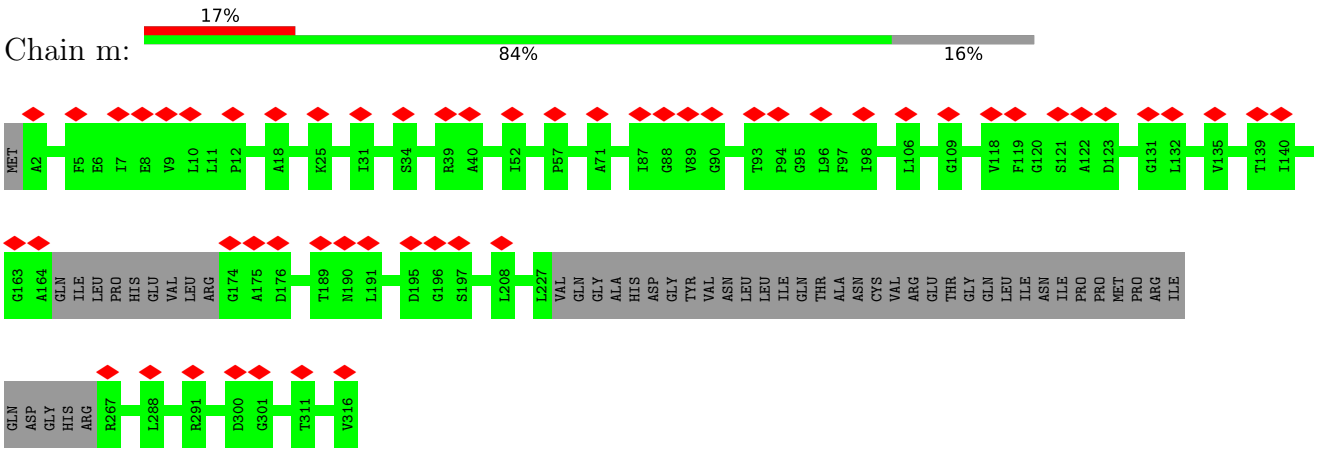
• Molecule 4: Triplex capsid protein 2

Chain q:



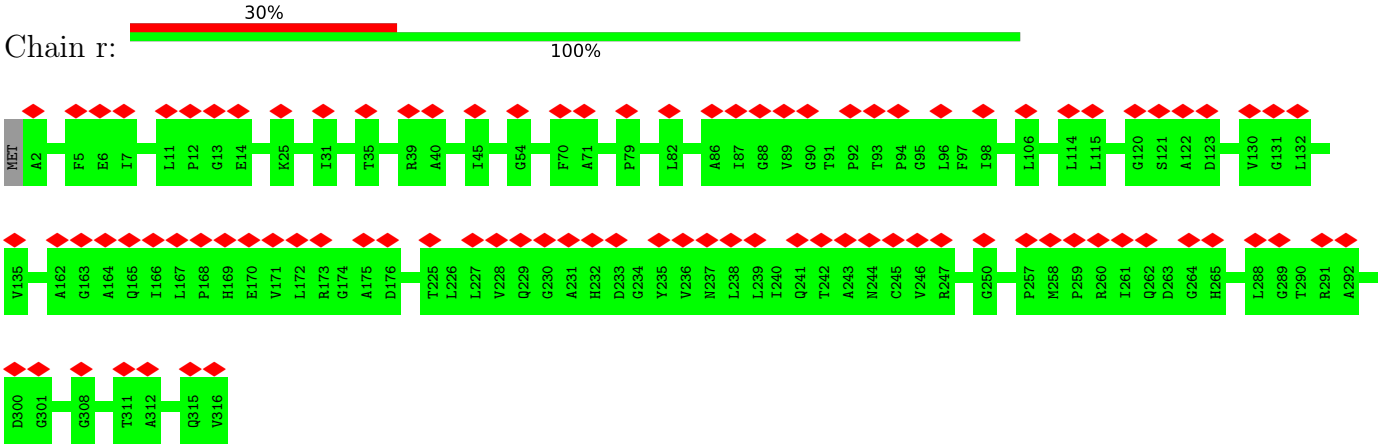
• Molecule 4: Triplex capsid protein 2

Chain m:



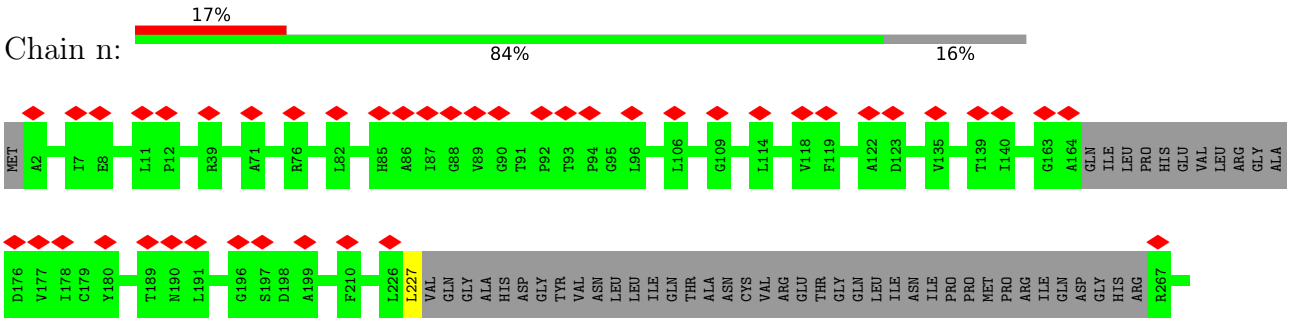
• Molecule 4: Triplex capsid protein 2

Chain r:



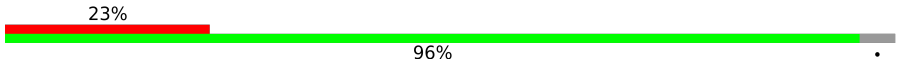
• Molecule 4: Triplex capsid protein 2

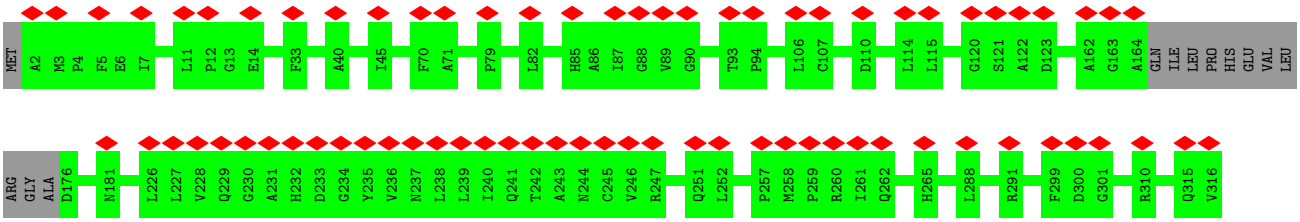
Chain n:



• Molecule 4: Triplex capsid protein 2

Chain s:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2838	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 ($e^-/Å^2$)	56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	13.818	Depositor
Minimum map value	-12.706	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	1.495	Depositor
Recommended contour level	3.0	Depositor
Map size (Å)	1672.9601, 1672.9601, 1672.9601	wwPDB
Map dimensions	1280, 1280, 1280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	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	0.37	0/10846	0.48	1/14767 (0.0%)
1	B	0.32	0/10854	0.47	0/14778
1	C	0.34	0/10846	0.48	0/14767
1	E	0.34	0/10834	0.48	0/14748
1	F	0.31	0/10846	0.48	0/14767
1	G	0.31	0/10377	0.49	1/14130 (0.0%)
1	M	0.37	0/10835	0.48	0/14752
1	N	0.37	0/10835	0.47	0/14752
1	O	0.38	0/10854	0.48	0/14778
1	P	0.37	0/10854	0.49	2/14778 (0.0%)
1	Q	0.38	0/10846	0.48	0/14767
1	R	0.36	0/10835	0.48	0/14752
1	S	0.37	0/10854	0.48	0/14778
1	T	0.37	0/10846	0.48	0/14767
1	U	0.31	0/10675	0.49	0/14536
1	z	0.26	0/4800	0.50	0/6517
2	D	0.28	0/782	0.52	2/1069 (0.2%)
2	H	0.28	0/771	0.47	0/1055
2	I	0.27	0/782	0.46	0/1069
2	J	0.28	0/782	0.47	0/1069
2	K	0.28	0/782	0.48	0/1069
2	L	0.27	0/782	0.48	0/1069
2	V	0.28	0/782	0.46	0/1069
2	W	0.28	0/782	0.50	1/1069 (0.1%)
2	X	0.28	0/782	0.49	0/1069
2	Y	0.28	0/782	0.46	0/1069
2	Z	0.29	0/782	0.47	0/1069
2	a	0.30	0/782	0.47	0/1069
2	b	0.29	0/771	0.48	0/1055
2	c	0.29	0/782	0.49	0/1069
2	d	0.28	0/782	0.51	1/1069 (0.1%)
3	e	0.41	0/2342	0.79	6/3175 (0.2%)
3	f	0.39	0/2547	0.71	4/3456 (0.1%)
3	g	0.45	1/2551 (0.0%)	0.70	6/3461 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	h	0.40	0/2550	0.69	3/3459 (0.1%)
3	i	0.40	0/2544	0.72	5/3451 (0.1%)
4	j	0.29	0/1868	0.49	0/2542
4	k	0.34	0/2127	0.47	0/2898
4	l	0.32	0/2046	0.45	0/2787
4	m	0.34	0/2064	0.47	0/2811
4	n	0.35	0/2055	0.52	1/2799 (0.0%)
4	o	0.32	2/2003 (0.1%)	0.54	0/2727
4	p	0.33	0/2368	0.47	0/3227
4	q	0.33	0/2350	0.47	0/3203
4	r	0.34	0/2453	0.48	0/3345
4	s	0.33	0/2364	0.47	0/3222
All	All	0.35	3/212777 (0.0%)	0.50	33/289704 (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
1	C	0	1
1	F	0	1
1	G	0	1
1	Q	0	1
1	T	0	2
3	g	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	g	133	PRO	N-CD	11.16	1.63	1.47
4	o	141	PRO	N-CD	5.75	1.55	1.47
4	o	116	PRO	N-CD	-5.23	1.40	1.47

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	e	430	LEU	N-CA-C	8.80	134.76	111.00
4	n	227	LEU	CB-CA-C	-7.83	95.33	110.20
1	P	881	ARG	C-N-CA	7.72	141.01	121.70
3	h	358	LEU	N-CA-CB	6.20	122.79	110.40

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Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	f	358	LEU	N-CA-CB	6.18	122.76	110.40

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1394	LEU	Mainchain
1	F	1394	LEU	Mainchain
1	Q	1394	LEU	Mainchain
1	T	1394	LEU	Mainchain
1	T	531	MET	Peptide

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	1350/1396 (97%)	1184 (88%)	165 (12%)	1 (0%)	51 85
1	B	1351/1396 (97%)	1191 (88%)	160 (12%)	0	100 100
1	C	1350/1396 (97%)	1194 (88%)	156 (12%)	0	100 100
1	E	1347/1396 (96%)	1185 (88%)	162 (12%)	0	100 100
1	F	1350/1396 (97%)	1191 (88%)	159 (12%)	0	100 100
1	G	1291/1396 (92%)	1135 (88%)	155 (12%)	1 (0%)	51 85
1	M	1349/1396 (97%)	1206 (89%)	143 (11%)	0	100 100
1	N	1349/1396 (97%)	1207 (90%)	142 (10%)	0	100 100
1	O	1351/1396 (97%)	1201 (89%)	150 (11%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	P	1351/1396 (97%)	1221 (90%)	129 (10%)	1 (0%)	51 85
1	Q	1350/1396 (97%)	1210 (90%)	140 (10%)	0	100 100
1	R	1349/1396 (97%)	1194 (88%)	154 (11%)	1 (0%)	51 85
1	S	1351/1396 (97%)	1206 (89%)	145 (11%)	0	100 100
1	T	1350/1396 (97%)	1194 (88%)	155 (12%)	1 (0%)	51 85
1	U	1327/1396 (95%)	1167 (88%)	160 (12%)	0	100 100
1	z	595/1396 (43%)	505 (85%)	90 (15%)	0	100 100
2	D	98/235 (42%)	79 (81%)	19 (19%)	0	100 100
2	H	97/235 (41%)	78 (80%)	19 (20%)	0	100 100
2	I	98/235 (42%)	79 (81%)	19 (19%)	0	100 100
2	J	98/235 (42%)	79 (81%)	19 (19%)	0	100 100
2	K	98/235 (42%)	82 (84%)	16 (16%)	0	100 100
2	L	98/235 (42%)	76 (78%)	22 (22%)	0	100 100
2	V	98/235 (42%)	75 (76%)	23 (24%)	0	100 100
2	W	98/235 (42%)	79 (81%)	19 (19%)	0	100 100
2	X	98/235 (42%)	84 (86%)	14 (14%)	0	100 100
2	Y	98/235 (42%)	76 (78%)	22 (22%)	0	100 100
2	Z	98/235 (42%)	80 (82%)	18 (18%)	0	100 100
2	a	98/235 (42%)	78 (80%)	20 (20%)	0	100 100
2	b	97/235 (41%)	82 (84%)	15 (16%)	0	100 100
2	c	98/235 (42%)	78 (80%)	20 (20%)	0	100 100
2	d	98/235 (42%)	77 (79%)	20 (20%)	1 (1%)	15 54
3	e	283/483 (59%)	261 (92%)	19 (7%)	3 (1%)	14 52
3	f	312/483 (65%)	289 (93%)	19 (6%)	4 (1%)	12 48
3	g	313/483 (65%)	289 (92%)	23 (7%)	1 (0%)	41 76
3	h	313/483 (65%)	290 (93%)	20 (6%)	3 (1%)	15 54
3	i	312/483 (65%)	290 (93%)	20 (6%)	2 (1%)	25 65
4	j	233/316 (74%)	213 (91%)	20 (9%)	0	100 100
4	k	269/316 (85%)	238 (88%)	31 (12%)	0	100 100
4	l	257/316 (81%)	225 (88%)	32 (12%)	0	100 100
4	m	261/316 (83%)	229 (88%)	32 (12%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	n	259/316 (82%)	231 (89%)	28 (11%)	0	100	100
4	o	250/316 (79%)	226 (90%)	24 (10%)	0	100	100
4	p	300/316 (95%)	278 (93%)	22 (7%)	0	100	100
4	q	297/316 (94%)	266 (90%)	31 (10%)	0	100	100
4	r	313/316 (99%)	289 (92%)	24 (8%)	0	100	100
4	s	300/316 (95%)	275 (92%)	25 (8%)	0	100	100
All	All	26501/31436 (84%)	23462 (88%)	3020 (11%)	19 (0%)	54	85

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	48	PHE
3	e	227	GLY
3	f	227	GLY
3	g	227	GLY
3	h	227	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	1143/1182 (97%)	1142 (100%)	1 (0%)	93	97
1	B	1144/1182 (97%)	1144 (100%)	0	100	100
1	C	1143/1182 (97%)	1139 (100%)	4 (0%)	92	95
1	E	1142/1182 (97%)	1139 (100%)	3 (0%)	92	95
1	F	1143/1182 (97%)	1143 (100%)	0	100	100
1	G	1092/1182 (92%)	1090 (100%)	2 (0%)	93	96
1	M	1142/1182 (97%)	1142 (100%)	0	100	100
1	N	1142/1182 (97%)	1141 (100%)	1 (0%)	93	97
1	O	1144/1182 (97%)	1144 (100%)	0	100	100
1	P	1144/1182 (97%)	1142 (100%)	2 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Q	1143/1182 (97%)	1142 (100%)	1 (0%)	93 97
1	R	1142/1182 (97%)	1139 (100%)	3 (0%)	92 95
1	S	1144/1182 (97%)	1144 (100%)	0	100 100
1	T	1143/1182 (97%)	1143 (100%)	0	100 100
1	U	1125/1182 (95%)	1123 (100%)	2 (0%)	93 96
1	z	511/1182 (43%)	510 (100%)	1 (0%)	93 96
2	D	79/189 (42%)	79 (100%)	0	100 100
2	H	78/189 (41%)	78 (100%)	0	100 100
2	I	79/189 (42%)	79 (100%)	0	100 100
2	J	79/189 (42%)	79 (100%)	0	100 100
2	K	79/189 (42%)	79 (100%)	0	100 100
2	L	79/189 (42%)	79 (100%)	0	100 100
2	V	79/189 (42%)	79 (100%)	0	100 100
2	W	79/189 (42%)	79 (100%)	0	100 100
2	X	79/189 (42%)	79 (100%)	0	100 100
2	Y	79/189 (42%)	79 (100%)	0	100 100
2	Z	79/189 (42%)	79 (100%)	0	100 100
2	a	79/189 (42%)	79 (100%)	0	100 100
2	b	78/189 (41%)	78 (100%)	0	100 100
2	c	79/189 (42%)	79 (100%)	0	100 100
2	d	79/189 (42%)	79 (100%)	0	100 100
3	e	245/410 (60%)	235 (96%)	10 (4%)	30 55
3	f	262/410 (64%)	247 (94%)	15 (6%)	20 47
3	g	263/410 (64%)	251 (95%)	12 (5%)	27 52
3	h	263/410 (64%)	252 (96%)	11 (4%)	30 54
3	i	262/410 (64%)	251 (96%)	11 (4%)	30 54
4	j	205/267 (77%)	205 (100%)	0	100 100
4	k	232/267 (87%)	232 (100%)	0	100 100
4	l	224/267 (84%)	224 (100%)	0	100 100
4	m	224/267 (84%)	224 (100%)	0	100 100
4	n	224/267 (84%)	224 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	o	220/267 (82%)	219 (100%)	1 (0%)	88 93
4	p	258/267 (97%)	258 (100%)	0	100 100
4	q	257/267 (96%)	257 (100%)	0	100 100
4	r	266/267 (100%)	266 (100%)	0	100 100
4	s	257/267 (96%)	257 (100%)	0	100 100
All	All	22432/26467 (85%)	22352 (100%)	80 (0%)	91 94

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	h	118	THR
3	i	168	LEU
3	h	168	LEU
3	h	318	LEU
3	i	295	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 428 such sidechains are listed below:

Mol	Chain	Res	Type
2	c	72	HIS
1	C	656	ASN
3	h	273	ASN
1	U	519	GLN
1	B	480	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

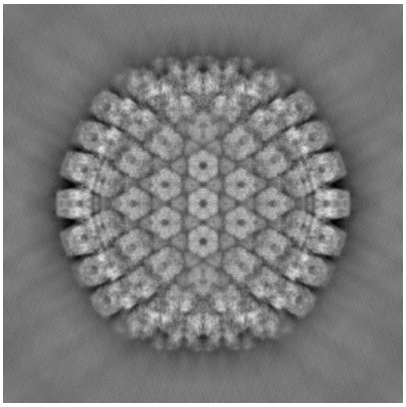
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0881. These allow visual inspection of the internal detail of the map and identification of artifacts.

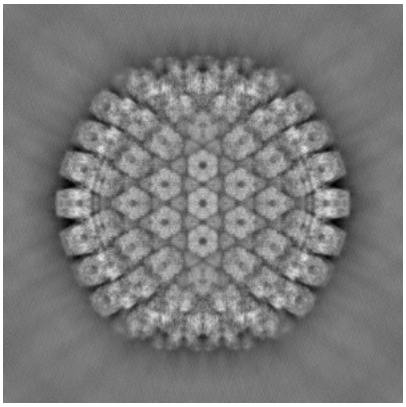
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

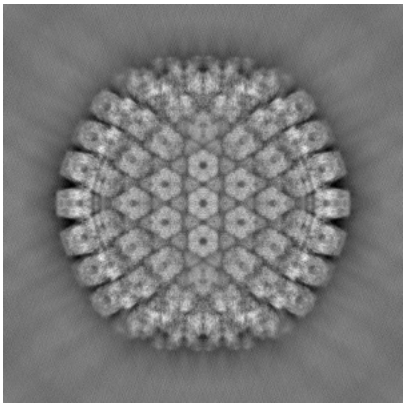
6.1.1 Primary map



X



Y

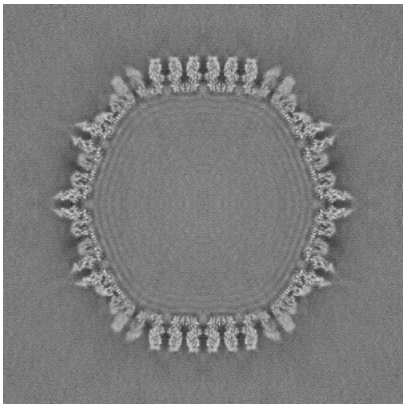


Z

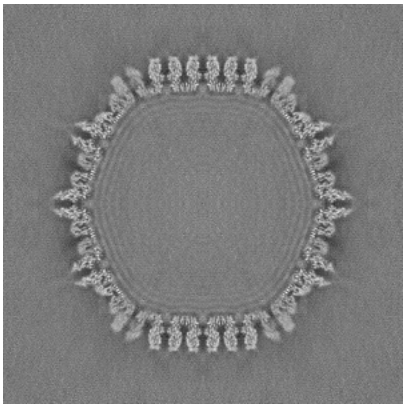
The images above show the map projected in three orthogonal directions.

6.2 Central slices

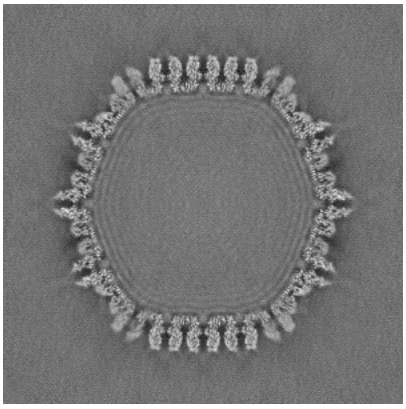
6.2.1 Primary map



X Index: 640



Y Index: 640

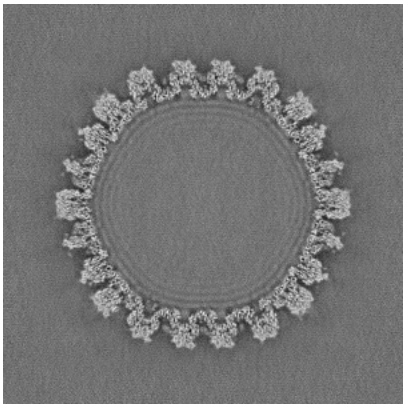


Z Index: 640

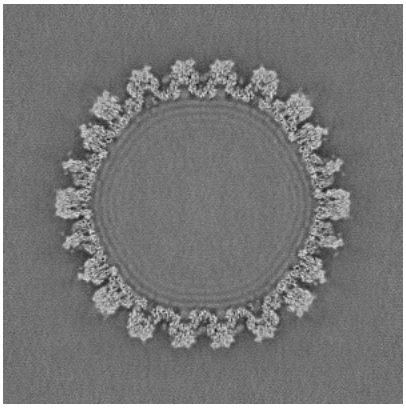
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

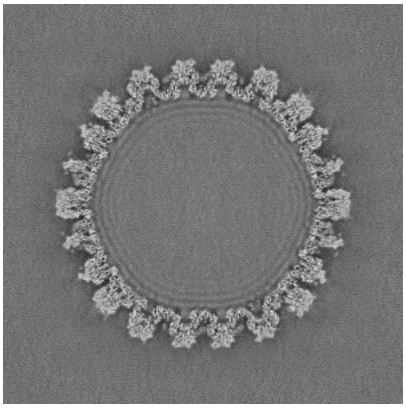
6.3.1 Primary map



X Index: 742



Y Index: 538

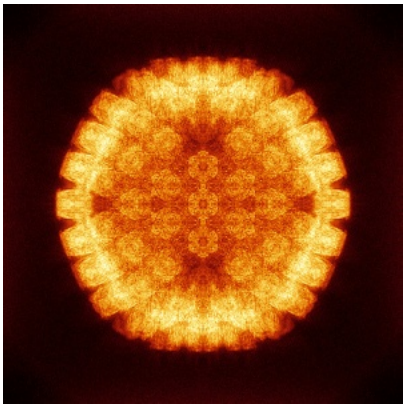


Z Index: 537

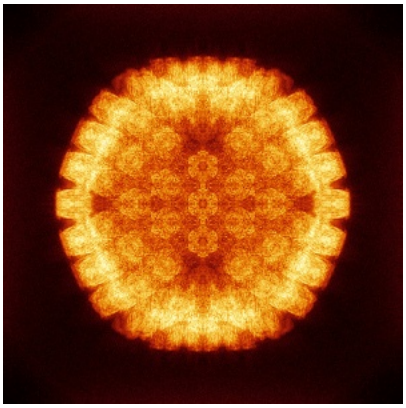
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

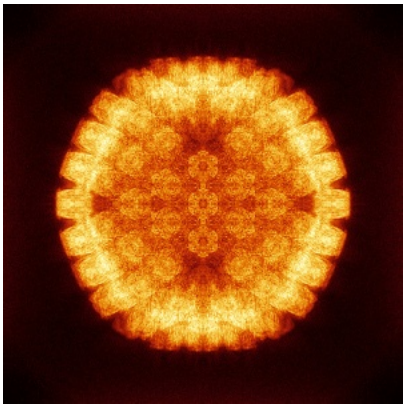
6.4.1 Primary map



X



Y

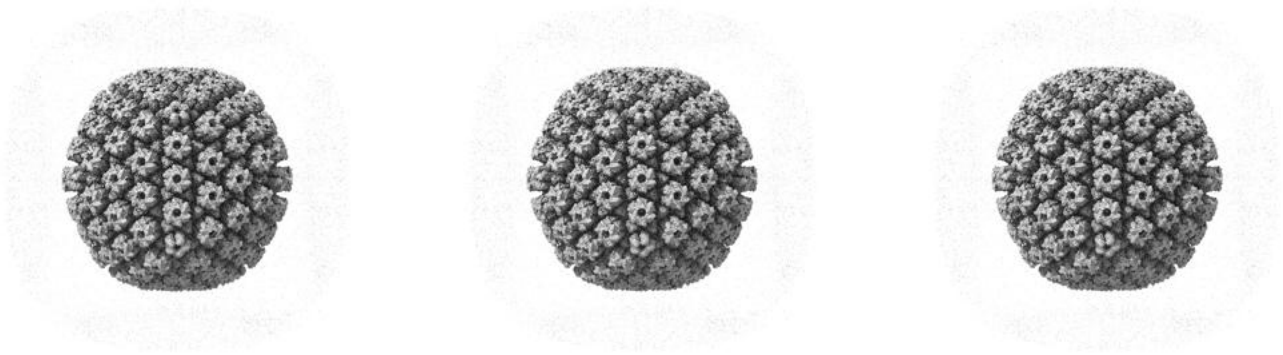


Z

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 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

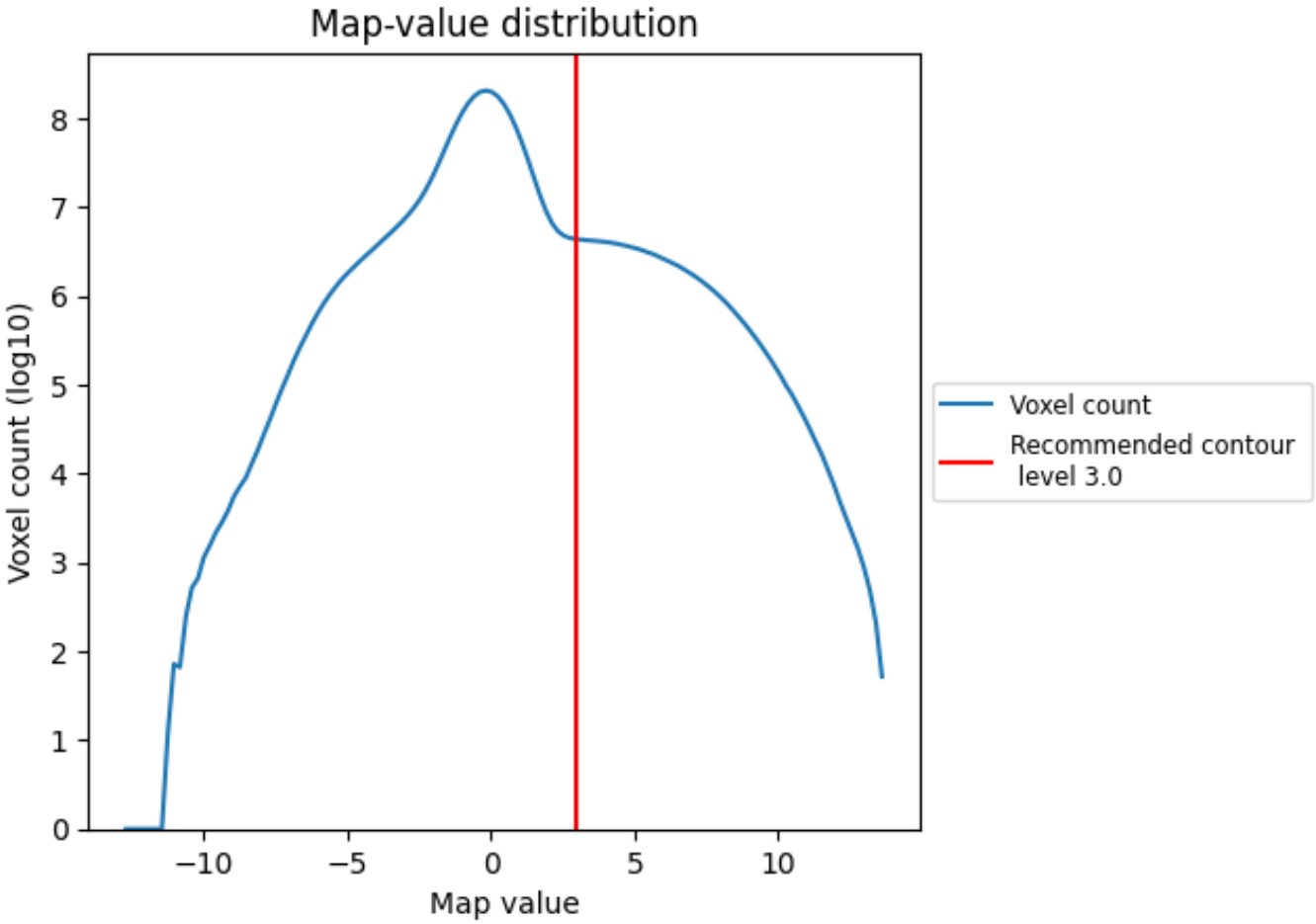
6.6 Mask visualisation (i)

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

7 Map analysis

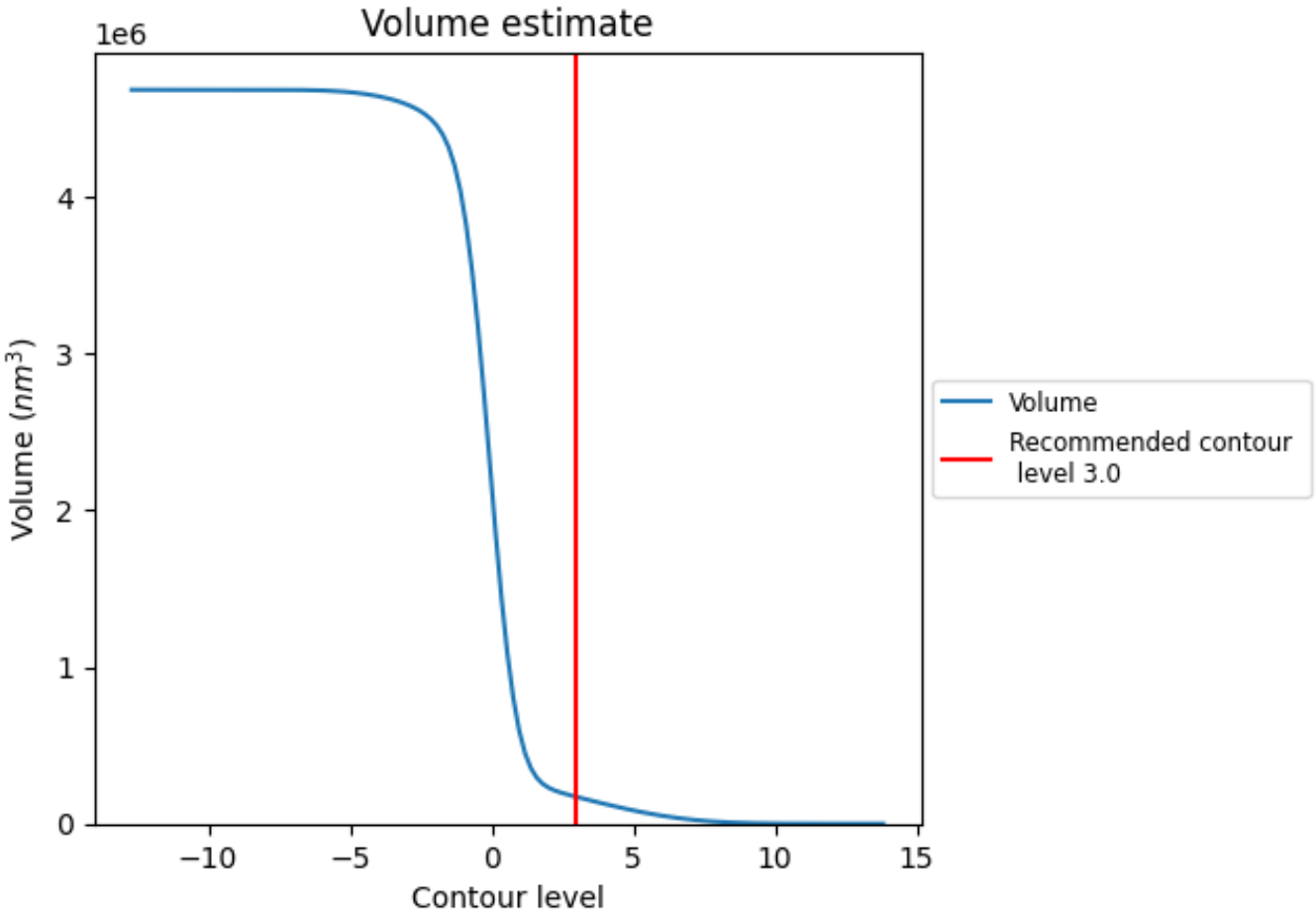
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

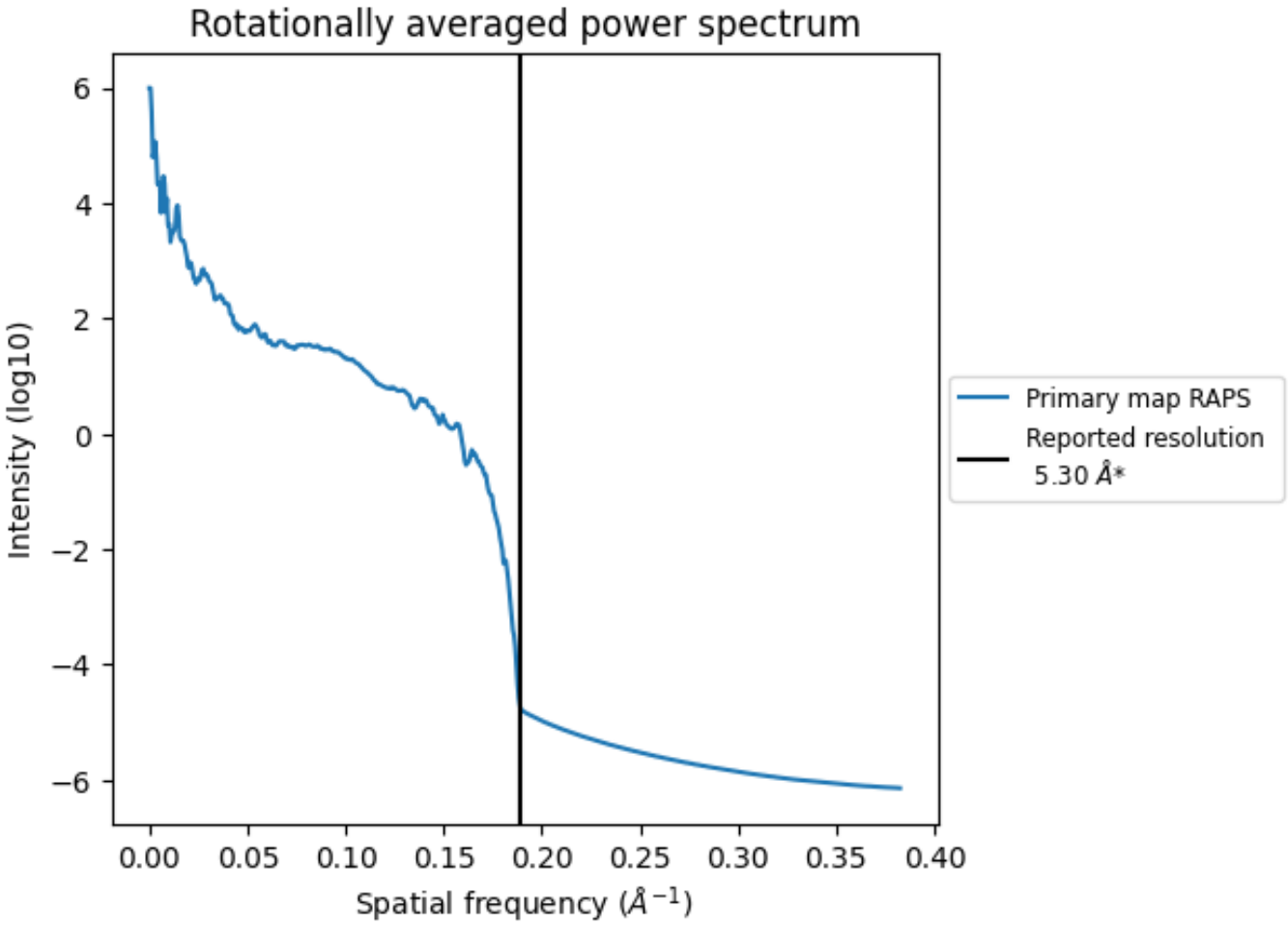
7.2 Volume estimate (i)



The volume at the recommended contour level is 170845 nm^3; this corresponds to an approximate mass of 154328 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 0.189 Å^{-1}

8 Fourier-Shell correlation (i)

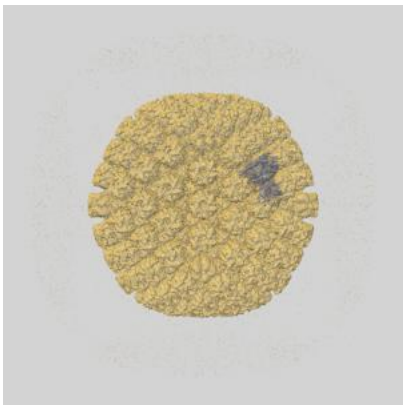
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

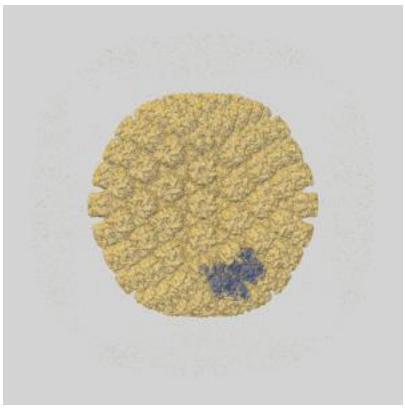
This section contains information regarding the fit between EMDB map EMD-0881 and PDB model 6LGN. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlays

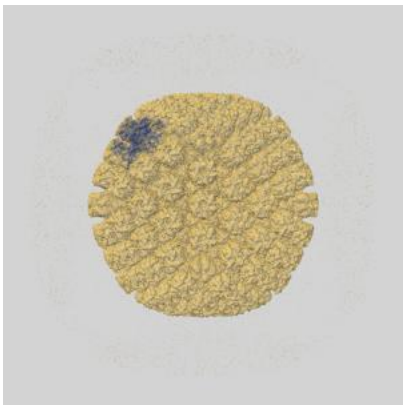
9.1.1 Map-model overlay



X

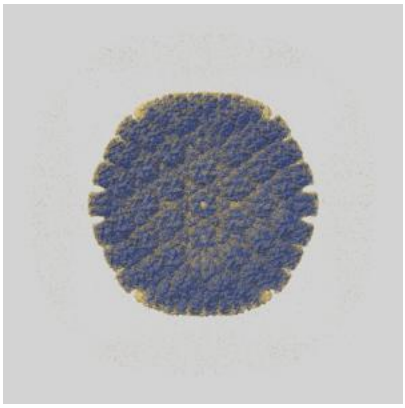


Y

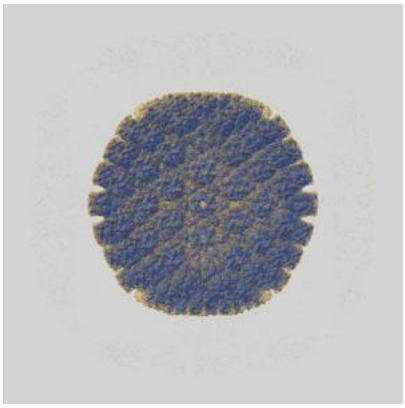


Z

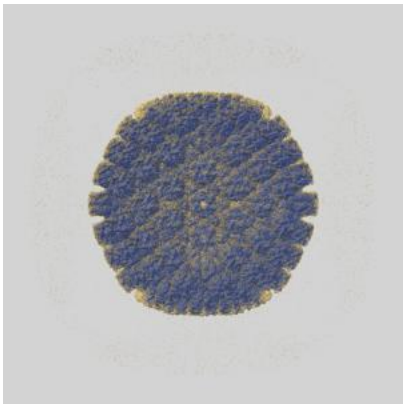
9.1.2 Map-model assembly overlay



X



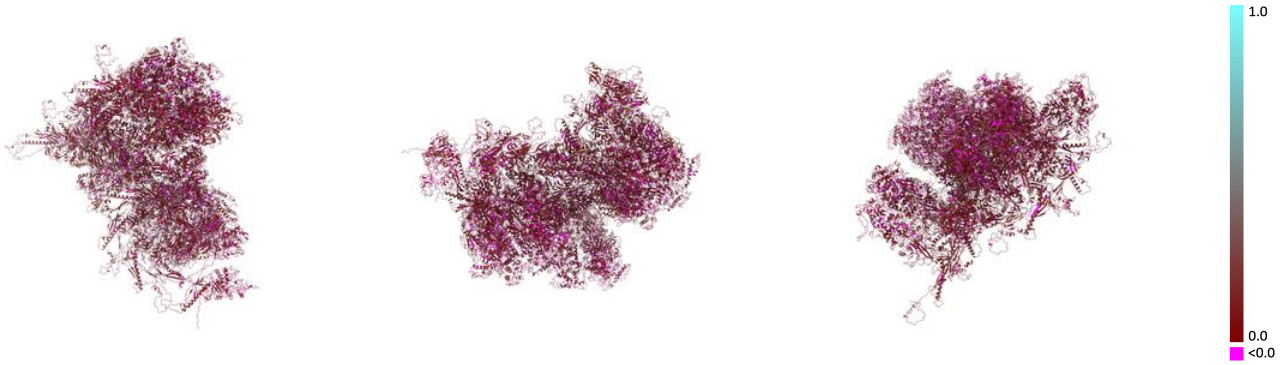
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 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.

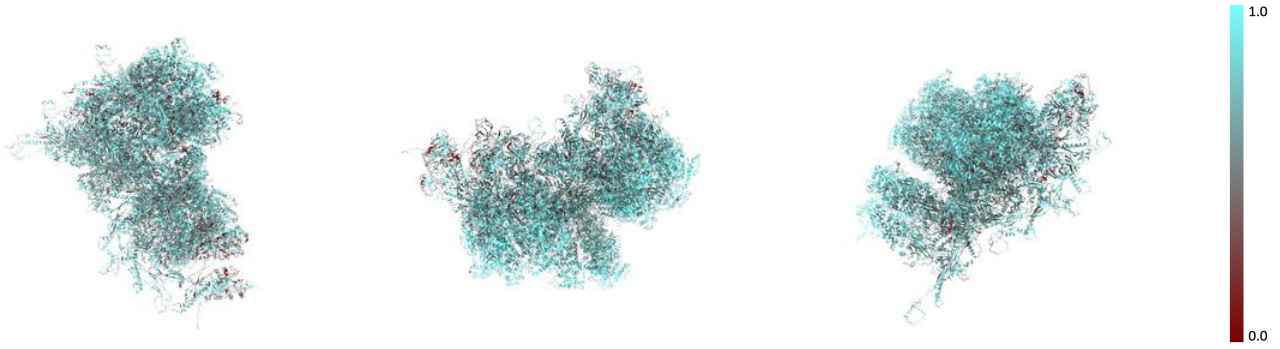
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

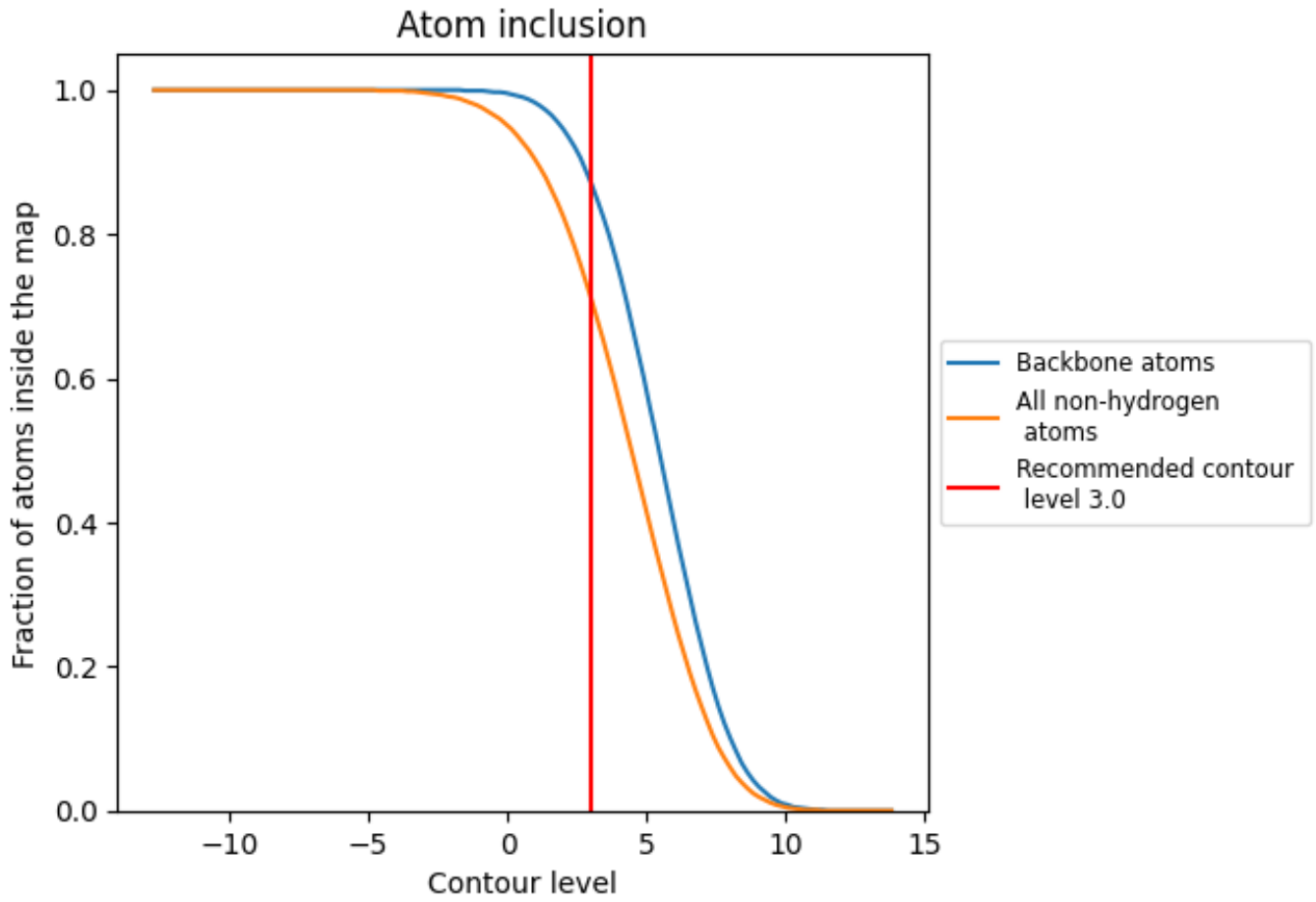
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (3.0).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 71% 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 (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7120	0.1190
A	0.6990	0.1210
B	0.7370	0.1130
C	0.7210	0.1170
D	0.8800	0.1070
E	0.7020	0.1160
F	0.7280	0.1190
G	0.7360	0.1160
H	0.8860	0.1060
I	0.9130	0.1090
J	0.9050	0.1100
K	0.8960	0.1230
L	0.8570	0.1010
M	0.7010	0.1190
N	0.7350	0.1200
O	0.7310	0.1210
P	0.7340	0.1220
Q	0.7240	0.1200
R	0.7070	0.1180
S	0.7300	0.1200
T	0.7230	0.1180
U	0.7100	0.1160
V	0.8420	0.0970
W	0.8990	0.1030
X	0.8810	0.1050
Y	0.8900	0.0780
Z	0.8770	0.0950
a	0.9040	0.0980
b	0.8780	0.0990
c	0.9160	0.1090
d	0.8770	0.0910
e	0.5570	0.1220
f	0.7060	0.1310
g	0.7200	0.1240
h	0.7060	0.1300

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Chain	Atom inclusion	Q-score
i	0.6880	0.1310
j	0.5190	0.1260
k	0.6540	0.1310
l	0.6970	0.1430
m	0.6500	0.1410
n	0.6260	0.1440
o	0.4990	0.1220
p	0.6270	0.1310
q	0.6450	0.1380
r	0.5940	0.1380
s	0.6040	0.1370
z	0.5410	0.1000