



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 05:53 PM UTC

PDB ID : 6M6G / pdb_00006m6g
EMDB ID : EMD-30123
Title : Structure of HSV2 viron capsid portal vertex
Authors : Wang, X.X.; Wang, N.
Deposited on : 2020-03-14
Resolution : 5.39 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

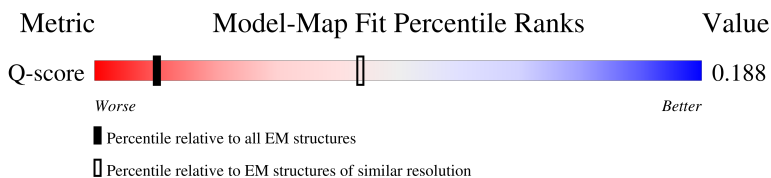
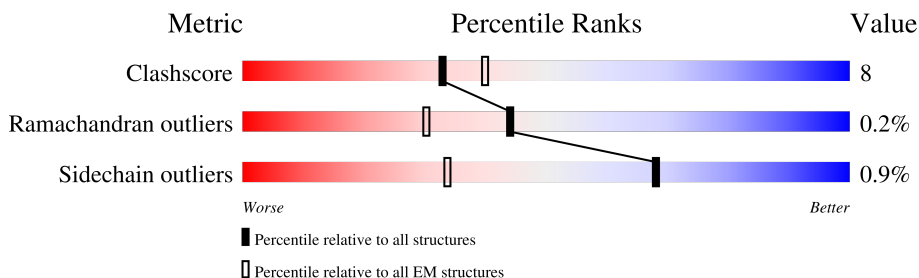
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

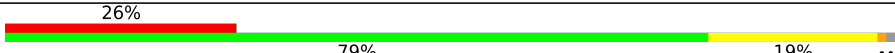
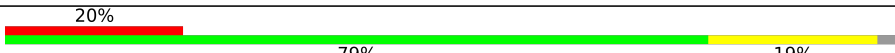
The reported resolution of this entry is 5.39 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	498 (4.90 - 5.87)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	1374	
1	C	1374	
1	D	1374	
1	E	1374	

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Mol	Chain	Length	Quality of chain
1	F	1374	
1	I	1374	
2	G	112	
2	M	112	
2	Q	112	
2	T	112	
2	U	112	
2	V	112	
3	K	318	
3	O	318	
4	L	84	
5	P	87	
6	S	466	
7	k	702	
8	l	585	
8	m	585	
9	n	3122	
9	o	3122	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 78731 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	B	1362	Total	C	N	O	S	0	0
			10198	6475	1847	1821	55		
1	C	1362	Total	C	N	O	S	0	0
			10209	6479	1844	1831	55		
1	D	1362	Total	C	N	O	S	0	0
			10221	6485	1848	1833	55		
1	E	1351	Total	C	N	O	S	0	0
			10162	6452	1837	1818	55		
1	F	1351	Total	C	N	O	S	0	0
			9978	6343	1804	1779	52		
1	I	1319	Total	C	N	O	S	0	0
			9831	6234	1785	1758	54		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	17	MET	ILE	conflict	UNP P89442
B	18	VAL	LEU	conflict	UNP P89442
B	382	LYS	ARG	conflict	UNP P89442
B	986	HIS	ASP	conflict	UNP P89442
C	17	MET	ILE	conflict	UNP P89442
C	18	VAL	LEU	conflict	UNP P89442
C	382	LYS	ARG	conflict	UNP P89442
C	986	HIS	ASP	conflict	UNP P89442
D	17	MET	ILE	conflict	UNP P89442
D	18	VAL	LEU	conflict	UNP P89442
D	382	LYS	ARG	conflict	UNP P89442
D	986	HIS	ASP	conflict	UNP P89442
E	17	MET	ILE	conflict	UNP P89442
E	18	VAL	LEU	conflict	UNP P89442
E	382	LYS	ARG	conflict	UNP P89442
E	986	HIS	ASP	conflict	UNP P89442
F	17	MET	ILE	conflict	UNP P89442
F	18	VAL	LEU	conflict	UNP P89442

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Chain	Residue	Modelled	Actual	Comment	Reference
F	382	LYS	ARG	conflict	UNP P89442
F	986	HIS	ASP	conflict	UNP P89442
I	17	MET	ILE	conflict	UNP P89442
I	18	VAL	LEU	conflict	UNP P89442
I	382	LYS	ARG	conflict	UNP P89442
I	986	HIS	ASP	conflict	UNP P89442

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	101	Total	C	N	O	S	0	0
			772	488	143	139	2		
2	M	101	Total	C	N	O	S	0	0
			772	488	143	139	2		
2	Q	101	Total	C	N	O	S	0	0
			772	488	143	139	2		
2	T	101	Total	C	N	O	S	0	0
			772	488	143	139	2		
2	U	101	Total	C	N	O	S	0	0
			772	488	143	139	2		
2	V	101	Total	C	N	O	S	0	0
			772	488	143	139	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	22	THR	MET	conflict	UNP G9I257
M	22	THR	MET	conflict	UNP G9I257
Q	22	THR	MET	conflict	UNP G9I257
T	22	THR	MET	conflict	UNP G9I257
U	22	THR	MET	conflict	UNP G9I257
V	22	THR	MET	conflict	UNP G9I257

- Molecule 3 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	299	Total	C	N	O	S	0	0
			2078	1341	373	357	7		
3	O	307	Total	C	N	O	S	0	0
			2175	1405	392	370	8		

- Molecule 4 is a protein called coiled coils.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	L	84	Total	C	N	O	0	0
			420	252	84	84		

- Molecule 5 is a protein called Coiled coils.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	P	87	Total	C	N	O	0	0
			435	261	87	87		

- Molecule 6 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	279	Total	C	N	O	S	0	0
			1975	1264	354	341	16		

- Molecule 7 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	k	553	Total	C	N	O	S	0	0
			4233	2695	773	748	17		

- Molecule 8 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	l	94	Total	C	N	O	S	0	0
			770	493	139	136	2		
8	m	80	Total	C	N	O		0	0
			648	411	123	114			

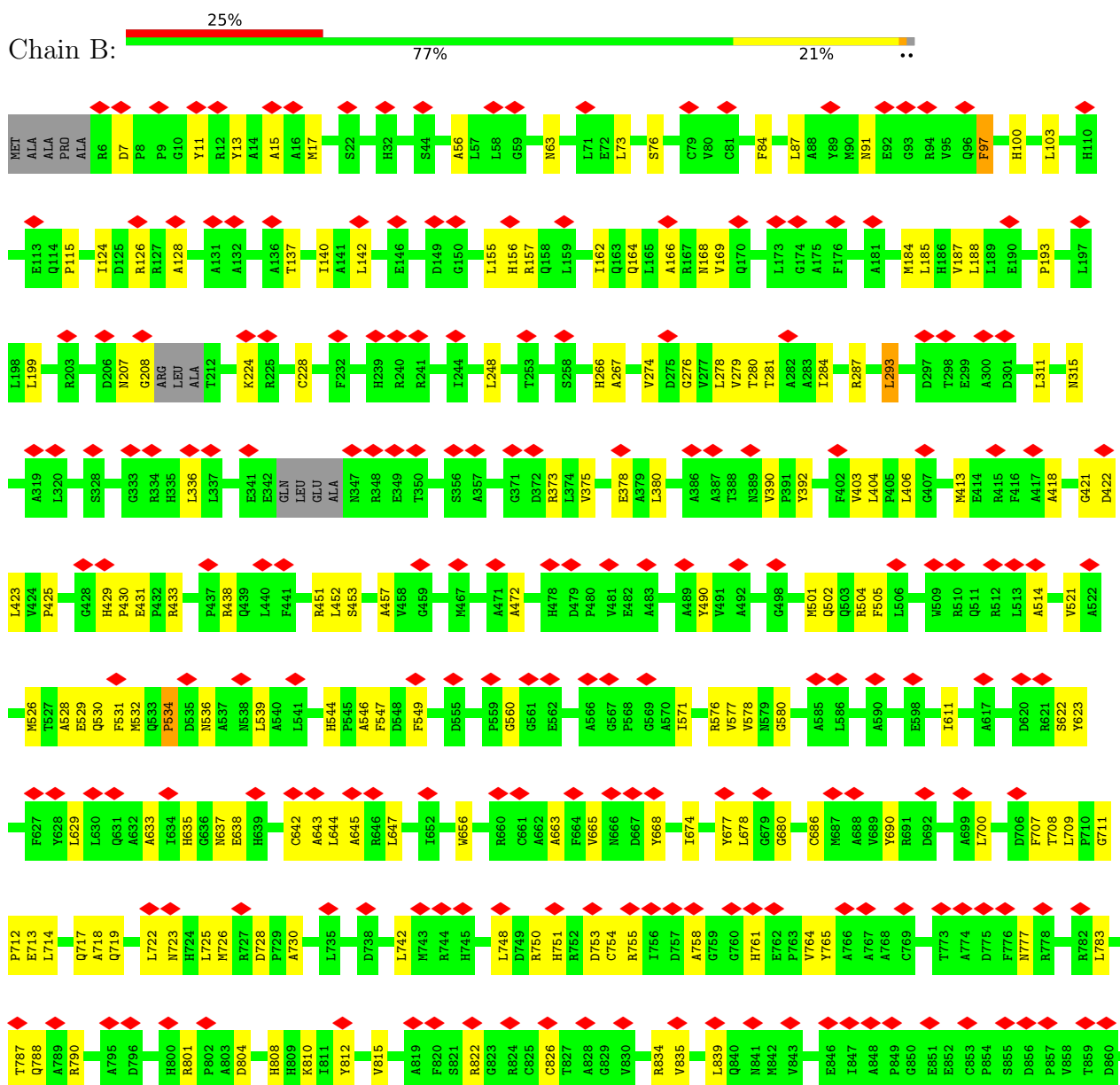
- Molecule 9 is a protein called Large tegument protein deneddylase.

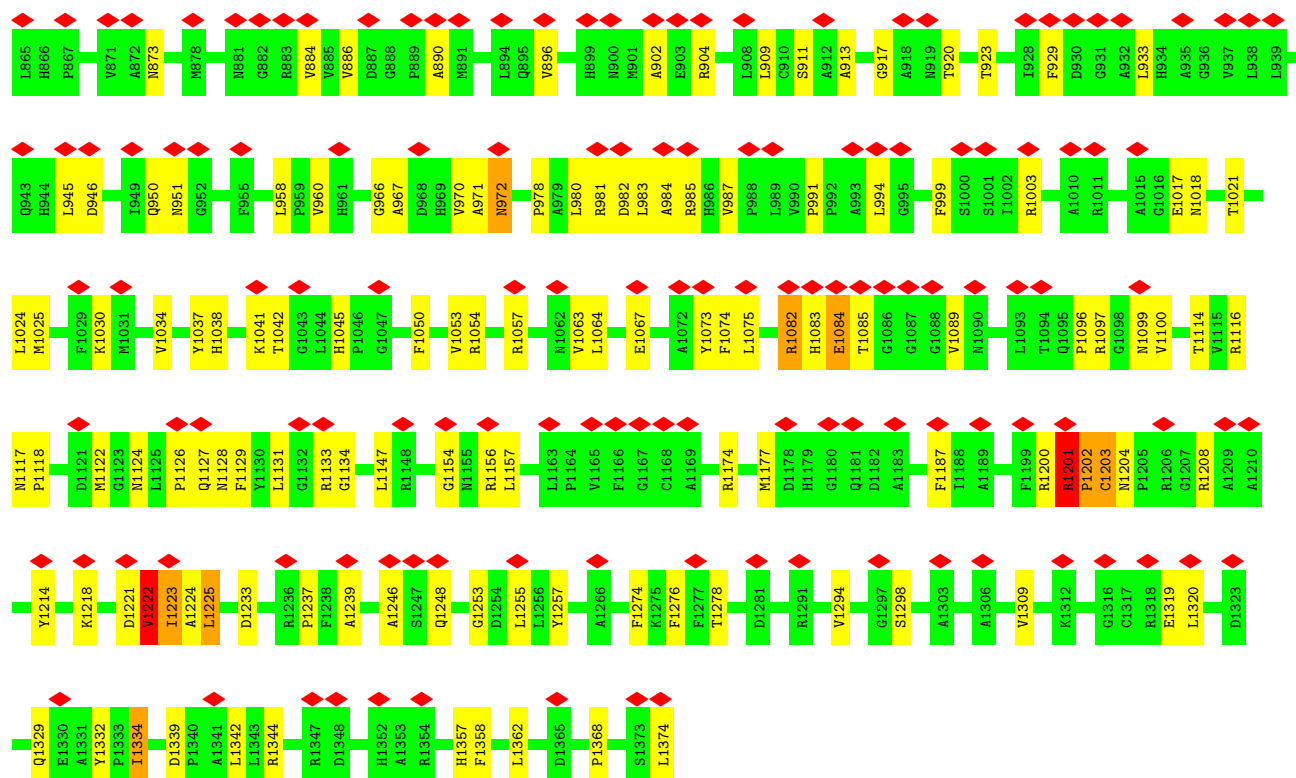
Mol	Chain	Residues	Atoms					AltConf	Trace
9	n	47	Total	C	N	O	S	0	0
			383	234	87	60	2		
9	o	47	Total	C	N	O	S	0	0
			383	234	87	60	2		

3 Residue-property plots

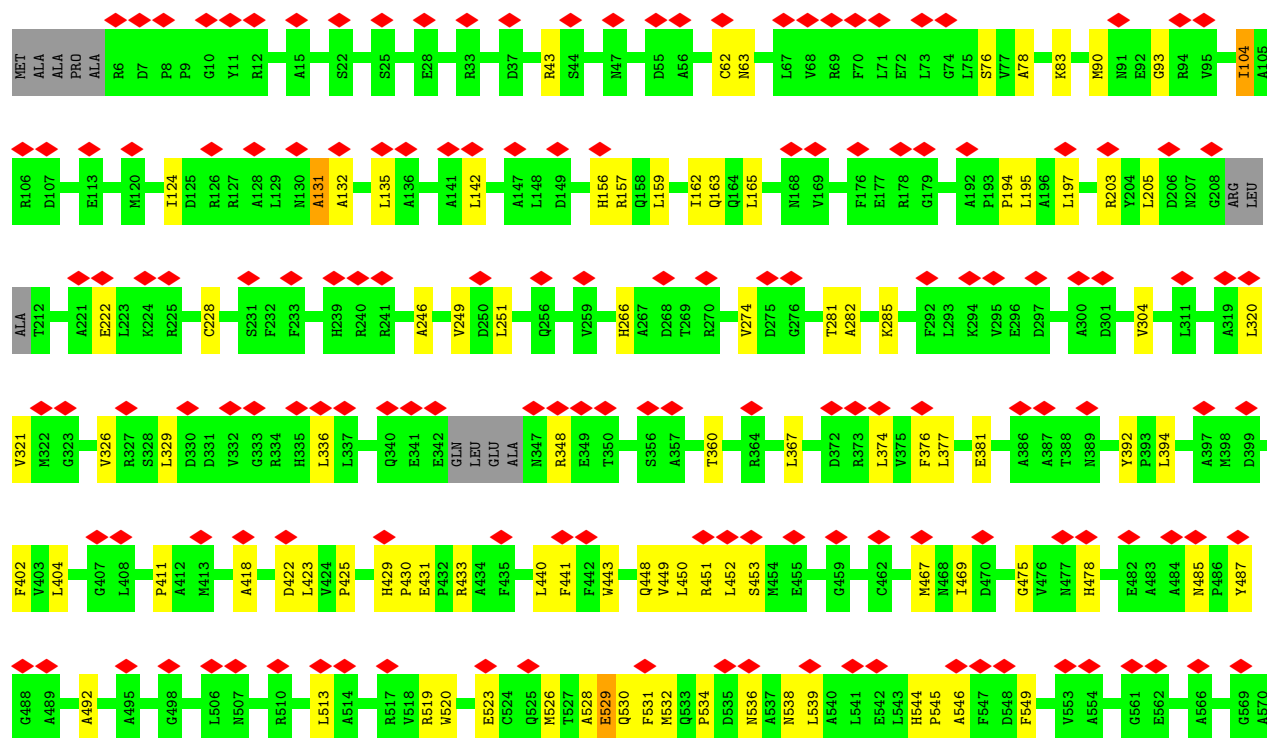
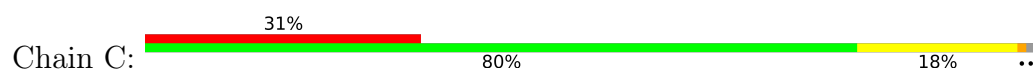
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

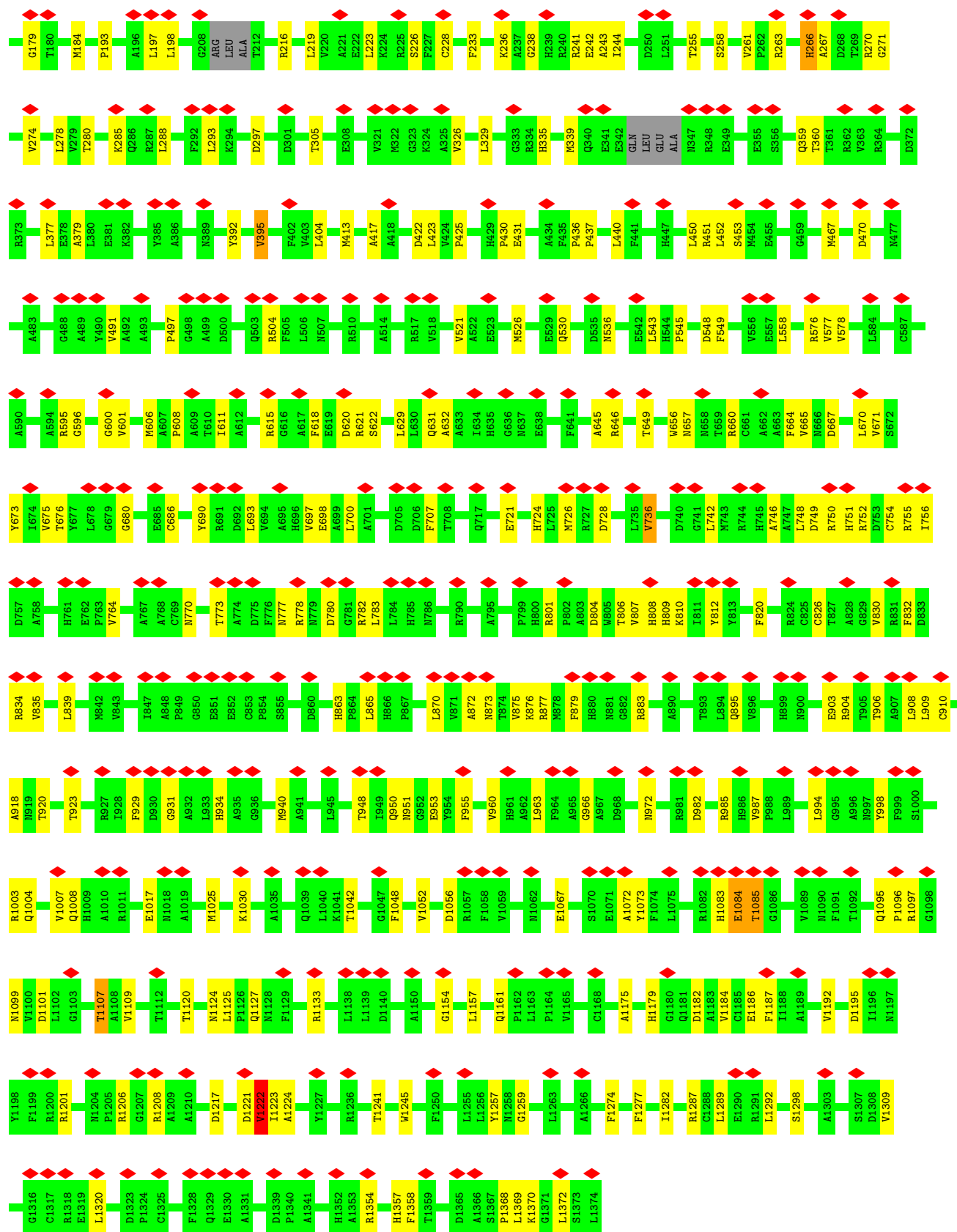
• Molecule 1: Major capsid protein



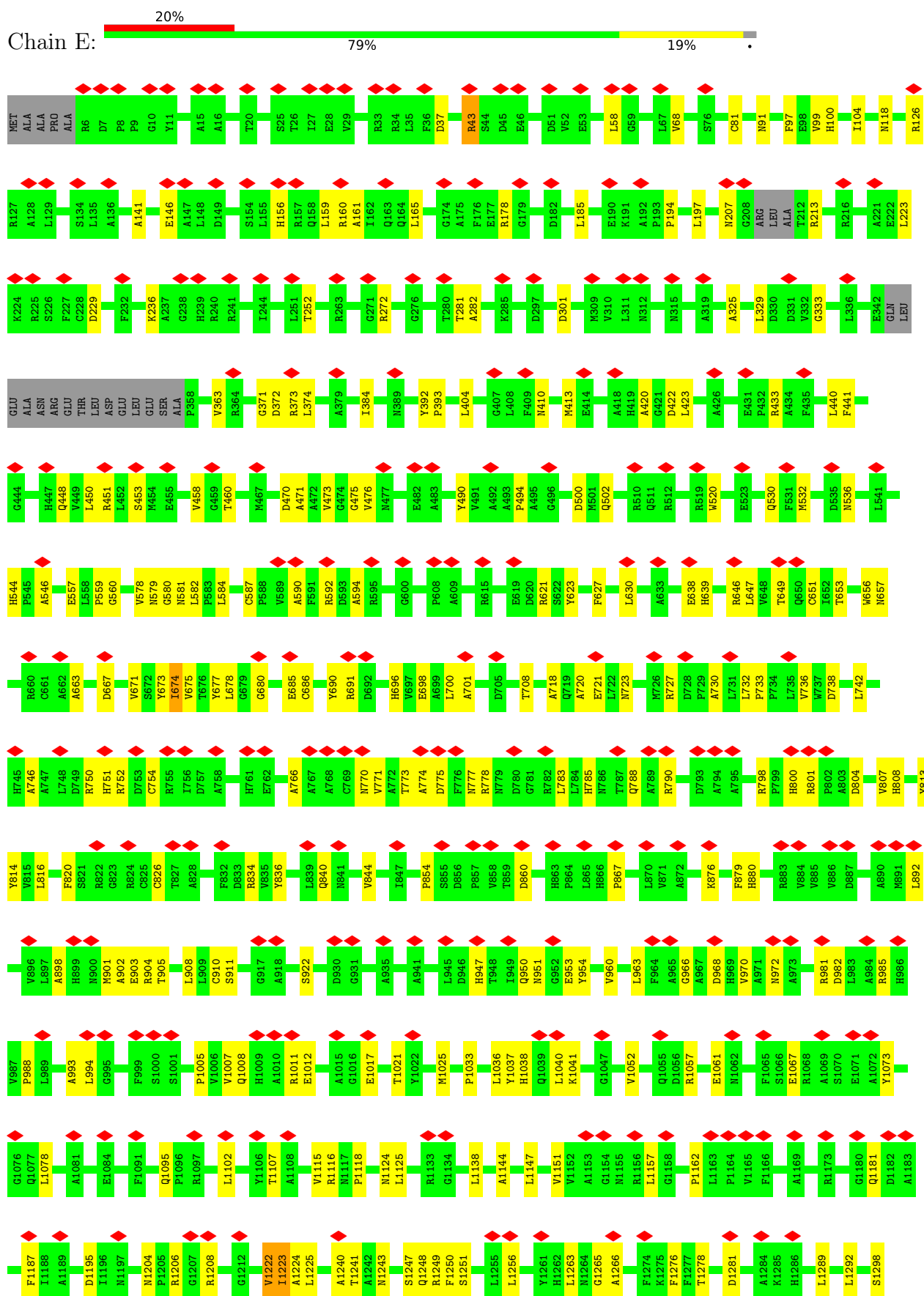


• Molecule 1: Major capsid protein

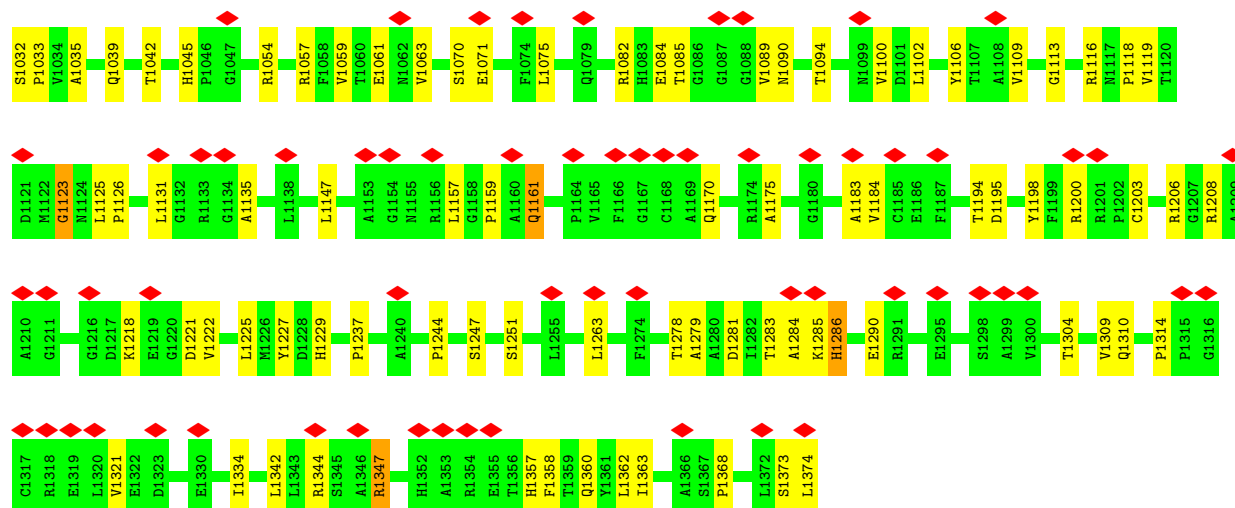




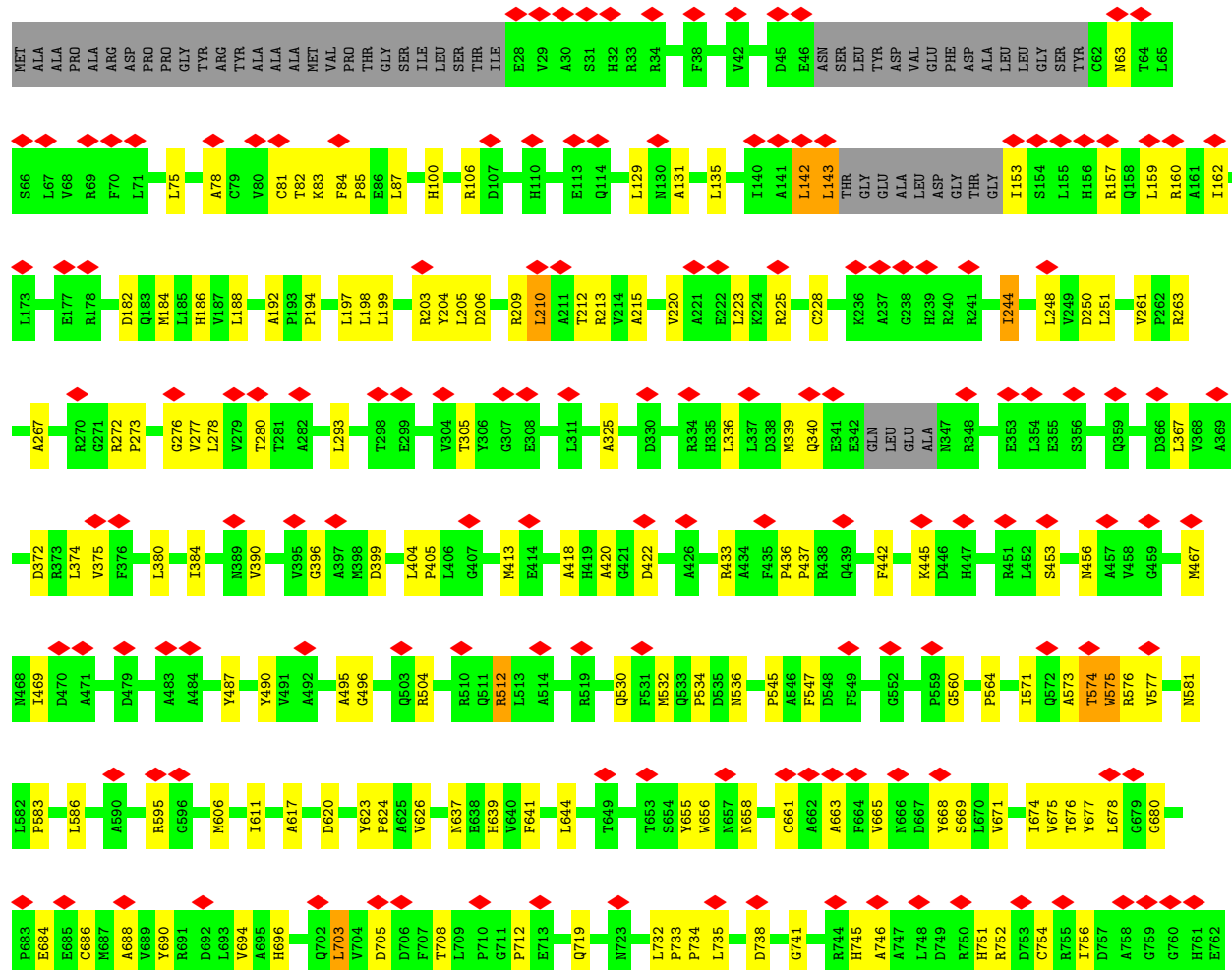
- Molecule 1: Major capsid protein

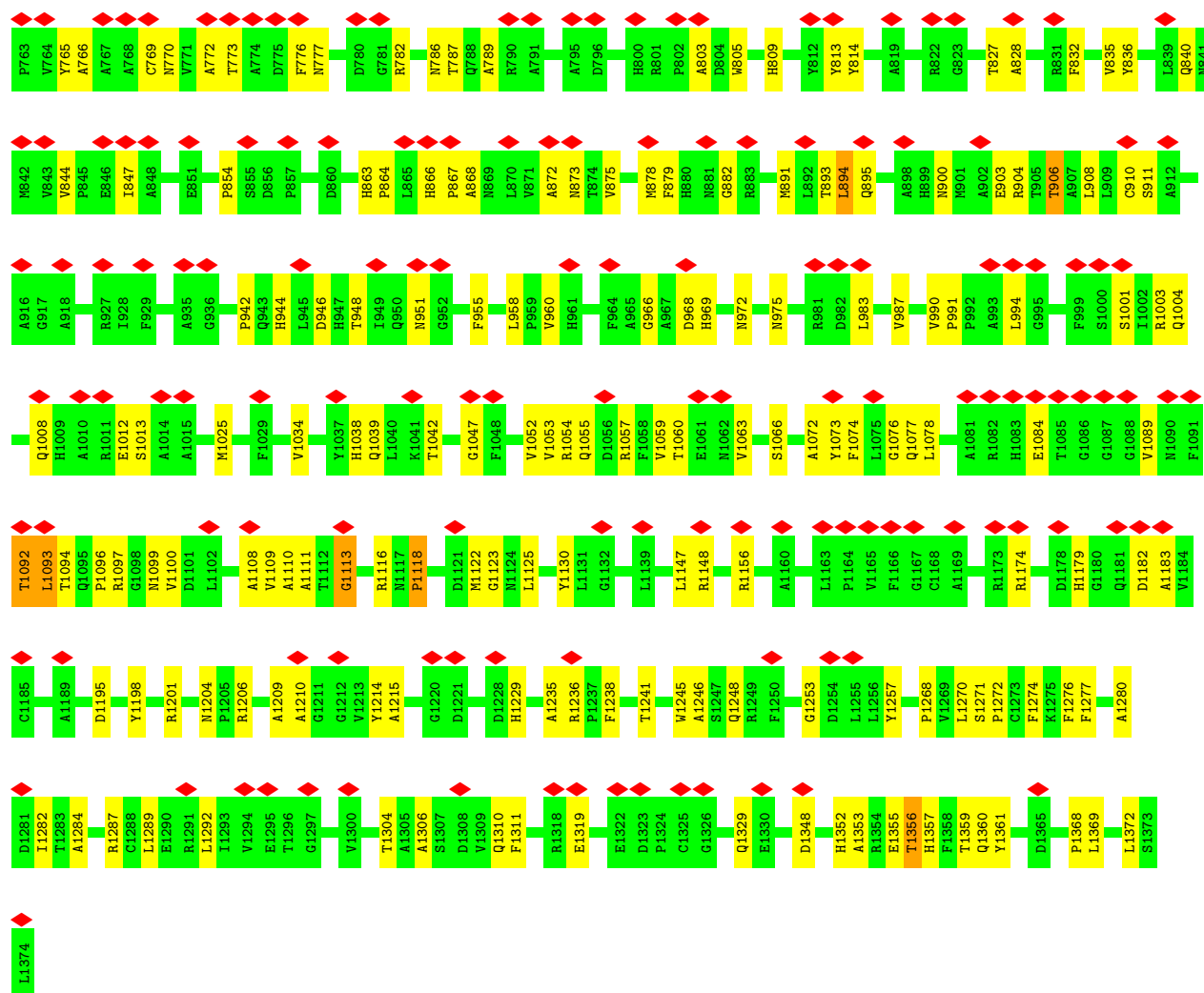




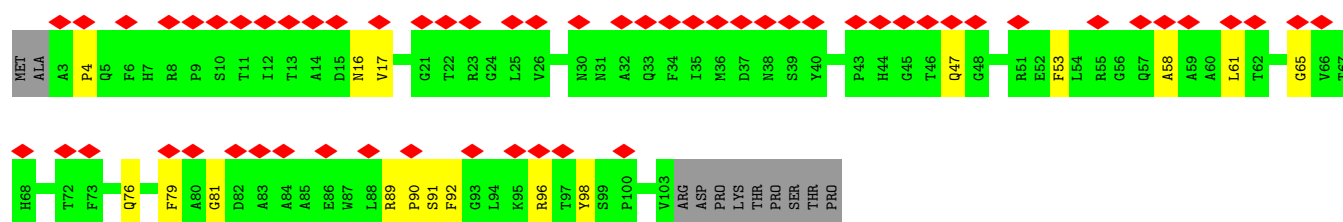
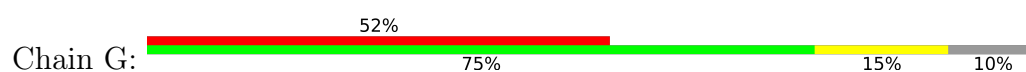


• Molecule 1: Major capsid protein

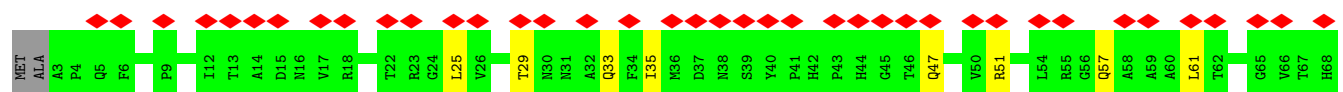
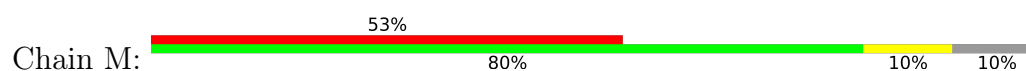


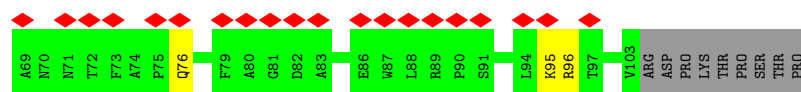


• Molecule 2: Small capsomere-interacting protein

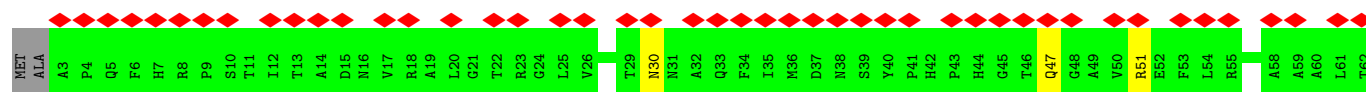
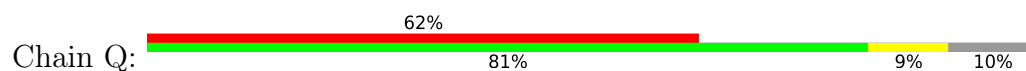


• Molecule 2: Small capsomere-interacting protein

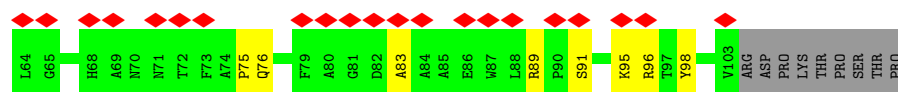
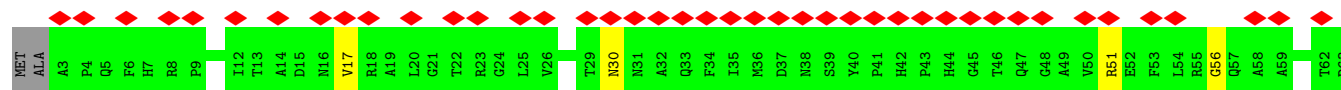
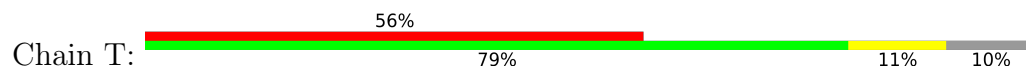




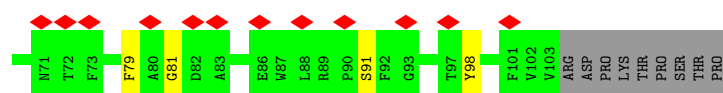
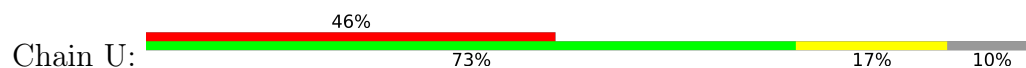
- Molecule 2: Small capsomere-interacting protein



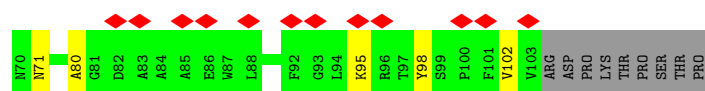
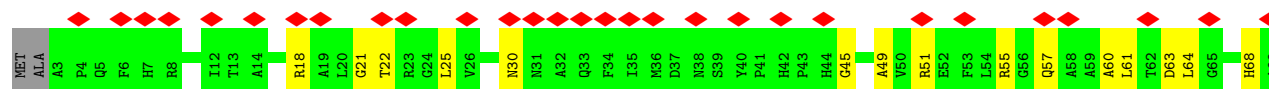
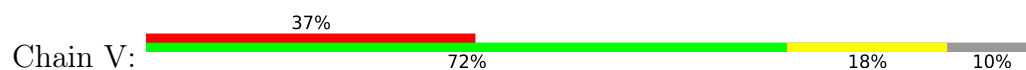
- Molecule 2: Small capsomere-interacting protein



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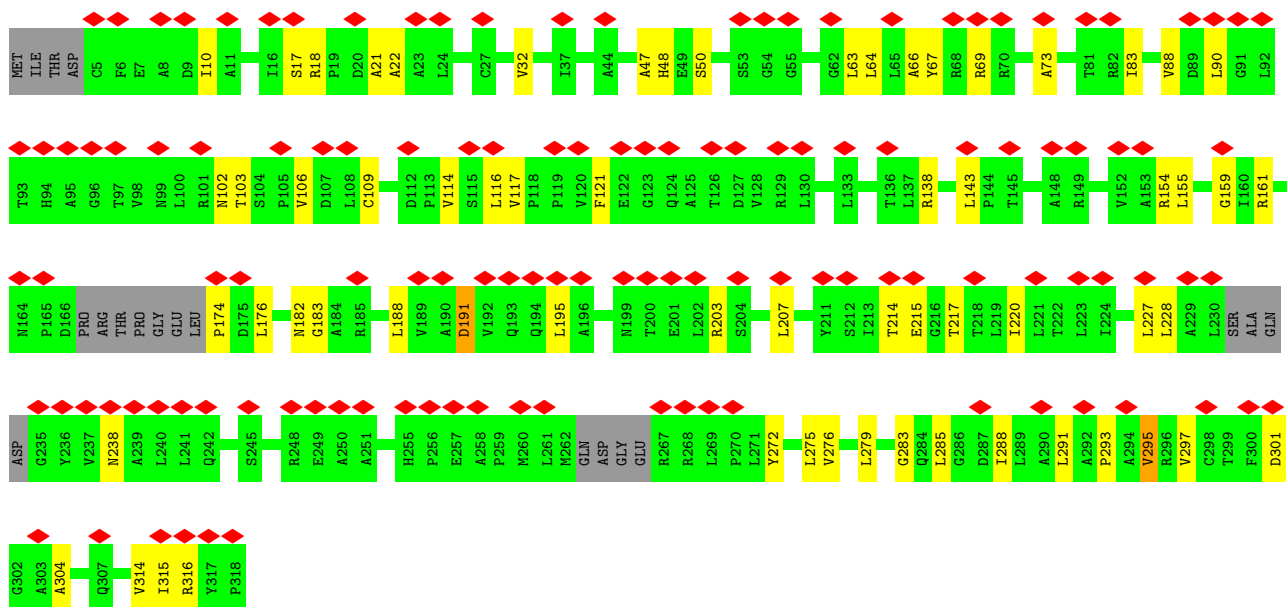


- Molecule 2: Small capsomere-interacting protein



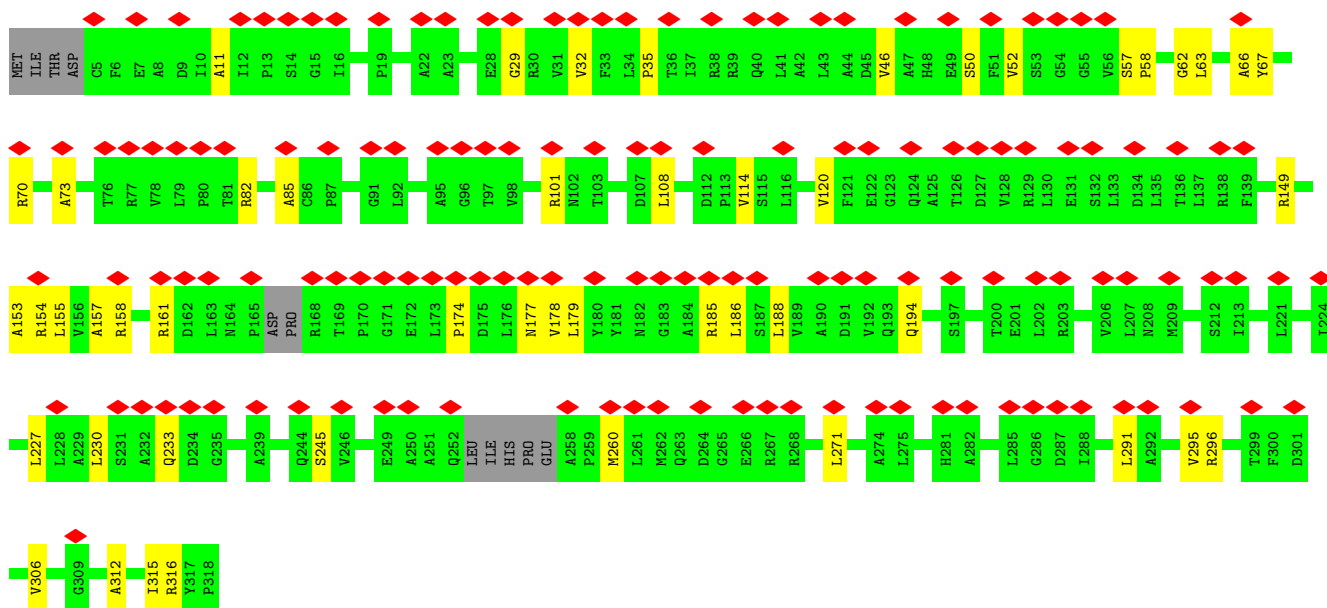
- Molecule 3: Triplex capsid protein 2

Chain K: 

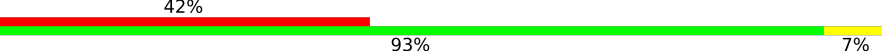


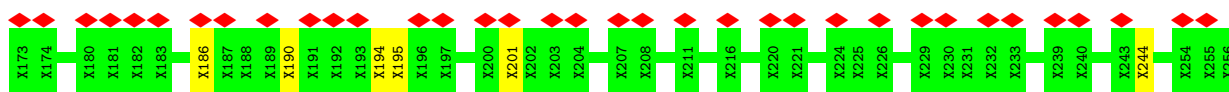
• Molecule 3: Triplex capsid protein 2

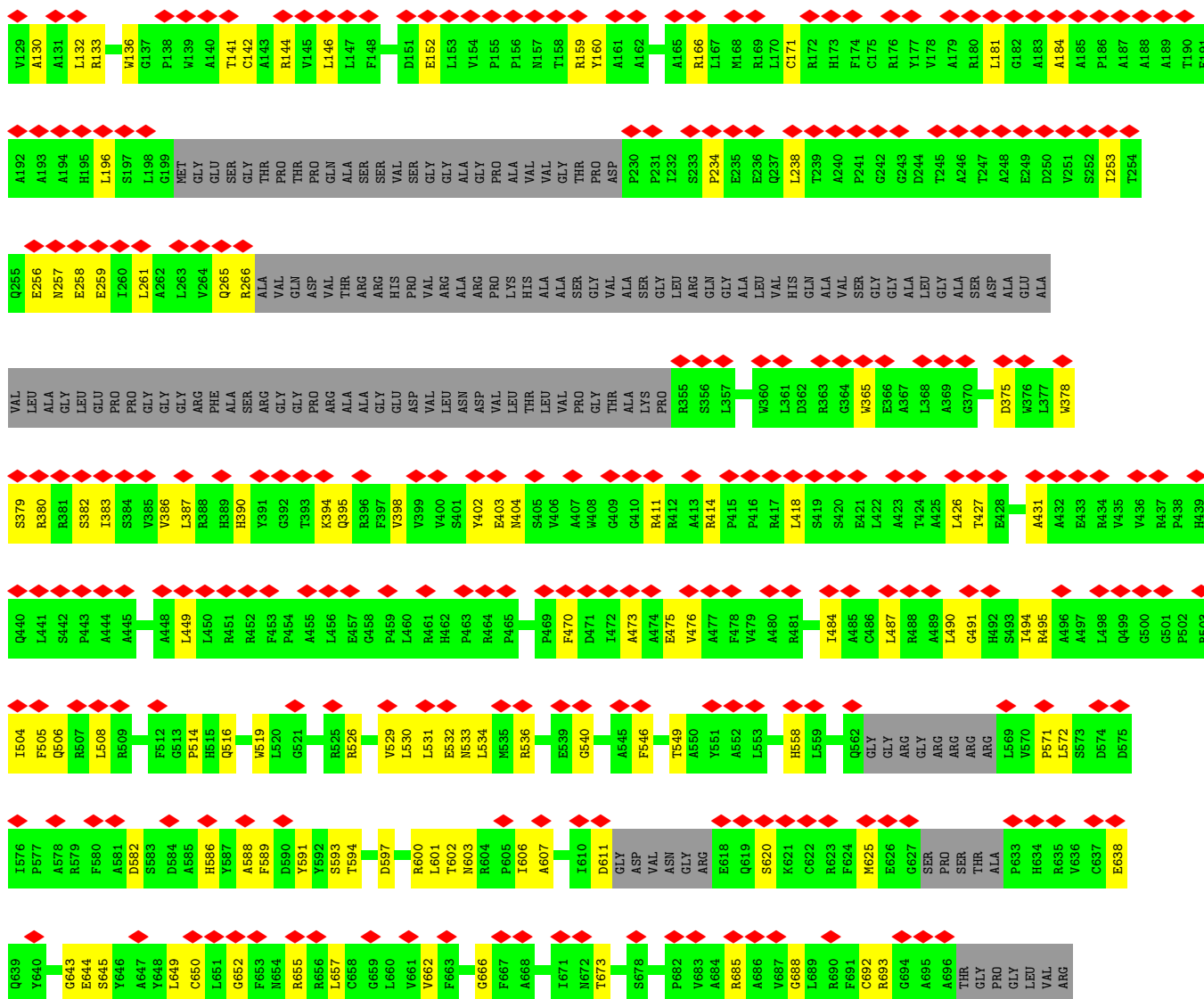
Chain O: 



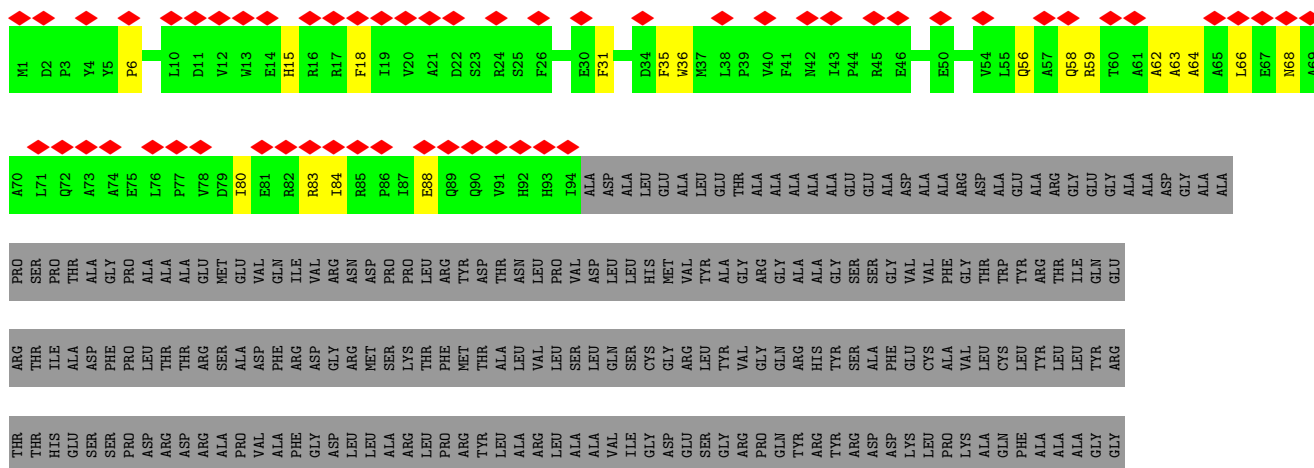
• Molecule 4: coiled coils

Chain L: 





• Molecule 8: Capsid vertex component 2







◆
L3121
GLY

Chain 0: 98%

ASP	THR	PRO	GLY	SER	MET
ARG	TYR	ALA	GLU	ALA	ILE
PRO	LEU	PHE	PRO	GLU	PRO
PRO	GLN	ILE	THR	ALA	ALA
GLU	ASP	ALA	GLY	ILE	ALA
ALA	GLU	LYS	GLY	GLU	LEU
PRO	PRO	VAL	LEU	GLY	PRO
ARG	PHE	ARG	LEU	CYS	HIS
GLY	VAL	ALA	GLU	LEU	PRO
ALA	GLU	GLY	THR	VAL	THR
SER	ARG	ASP	GLN	GLU	MET
GLY	ARG	VAL	CYS	GLY	LYS
PRO	VAL	TYR	PRO	GLY	ARG
ASP	ILE	PRO	HIS	GLN	GLY
THR	ILE	TYR	ASP	THR	ASP
PRO	HIS	LEU	PHE	ARG	ARG
PRO	THR	THR	PHE	ALA	ASP
GLN	LEU	TYR	ALA	ALA	ILE
ALA	PRO	TYR	GLY	ALA	VAL
GLY	ARG	ALA	PRO	GLY	VAL
HIS	GLY	HIS	TRP	GLY	VAL
PRO	ILE	ASP	ALA	GLY	GLY
ASN	ILE	ARG	ALA	PRO	VAL
ARG	GLY	PRO	MET	PRO	ARG
PRO	GLY	LYS	ARG	PRO	ASN
ASP	GLY	VAL	LEU	MET	GLN
ASP	GLY	ARG	LEU	GLY	PHE
ALA	LEU	ALA	TRP	CYS	ALA
VAL	LEU	ALA	TYR	SER	ALA
VAL	PHE	GLY	THR	ILE	THR
TRP	VAL	GLY	LEU	ILE	ASP
ALA	VAL	ALA	LEU	ILE	LEU
ALA	GLY	MET	LEU	GLU	GLU
ALA	VAL	VAL	THR	LEU	PRO
LEU	VAL	PHE	ILE	PRO	PRO
GLU	PRO	PHE	GLY	ASN	GLY
GLY	ARG	VAL	PRO	PHE	GLY
THR	GLY	PRO	LEU	LEU	SER
PRO	ASP	SER	GLY	LEU	VAL
PRO	GLY	GLY	MET	TYR	SER
ALA	GLU	PRO	GLY	PRO	CYS
LYS	GLY	GLY	LEU	ALA	MET
PRO	SER	ALA	TYR	ALA	ARG
SER	GLY	VAL	ARG	ALA	ARG
ALA	PRO	ALA	ASP	GLY	SER
PRO	VAL	PRO	GLY	GLY	LEU
ASP	VAL	ALA	ASP	LEU	PHE
ALA	PRO	ASP	THR	CYS	LEU
ALA	ALA	LEU	ALA	ARG	LEU
ALA	LEU	THR	TYR	VAL	SER
SER	PRO	ALA	PHE	PHE	LEU
GLY	ALA	ALA	LEU	SER	LEU
PRO	PRO	ALA	ASP	ARG	PHE
PRO	PRO	PRO	PRO	VAL	ASP
HIS	THR	HIS	PRO	VAL	VAL
ALA	VAL	HIS	HIS	TYR	VAL
ALA	GLN	VAL	GLY	GLY	GLY
PRO	THR	THR	PRO	VAL	ARG
PRO	PRO	GLY	ALA	GLY	ASP
PRO	ALA	SER	THR	PHE	VAL
TYR	ALA	GLU	THR	THR	THR





LEU	THR	PRO	GLN	THR	ALA	GLY
PRO	LEU	THR	GLN	ARG	ALA	ASP
VAL	PRO	THR	PRO	ALA	ALA	ARG
GLN	ILE	PRO	PRO	ALA	ALA	ARG
ALA	ILE	PRO	LEU	VAL	VAL	GLY
ASN	SER	SER	PRO	ARG	PRO	ARG
ALA	ASP	PRO	PRO	ALA	PRO	ARG
VAL	ASP	VAL	VAL	ARG	SER	ARG
LEU	GLU	THR	THR	VAL	PRO	GLN
SER	HIS	ARG	THR	ARG	LEU	THR
ARG	SER	SER	THR	THR	ALA	GLY
TYR	ALA	THR	LEU	GLN	PRO	GLY
VAL	ASP	PRO	PRO	PRO	PRO	PRO
R3075	SER	ASP	GLN	LEU	THR	SER
S3076	LEU	SER	SER	ARG	THR	SER
T3077	PHE	LEU	ARG	GLN	ALA	THR
G3078	SER	SER	ASP	PRO	VAL	PRO
R3079	SER	VAL	SER	PRO	GLN	PRO
S3080	ASP	ASP	PRO	LEU	SER	ARG
A3081	ASP	THR	PRO	PRO	PRO	THR
L3082	THR	GLU	SER	PRO	ALA	ALA
A3083	ALA	PRO	GLU	LEU	LEU	GLY
V3084	LEU	PRO	ALA	PRO	ALA	PRO
L3085	ASP	THR	THR	GLN	PRO	PRO
I3086	LEU	THR	ASN	LEU	VAL	ARG
R3087	LEU	THR	THR	PRO	ALA	THR
A3088	PRO	PRO	HIS	GLN	PRO	ARG
C3089	GLU	LEU	LEU	PRO	SER	PRO
R3090	PRO	PRO	PRO	GLU	ALA	ALA
R3091	HIS	VAL	VAL	PRO	PRO	VAL
I3092	LEU	SER	LEU	PRO	LEU	ALA
Q3093	PRO	ALA	ALA	GLN	CYS	SER
Q3094	PRO	VAL	VAL	PRO	GLY	LEU
Q3095	ALA	THR	SER	PRO	TRP	SER
L3096	ASP	ALA	THR	LEU	VAL	ALA
Q3097	GLU	TRP	TRP	PRO	VAL	ALA
R3098	PRO	ALA	ALA	GLN	PRO	LEU
T3099	GLY	SER	SER	PRO	GLY	ASN
R3100	PRO	PRO	SER	LEU	PRO	LEU
R3101	ALA	ALA	LEU	ALA	PRO	PRO
A3102	ASP	HIS	HIS	VAL	ARG	PRO
L3103	HIS	ASP	ASP	LEU	PRO	ASP
F3104	LEU	SER	SER	PRO	PRO	PRO
Q3105	GLN	ALA	ALA	GLN	PRO	ALA
R3106	SER	SER	PRO	PRO	GLN	ASP
S3107	PRO	PRO	PRO	PRO	SER	HIS
N3108	HIS	PRO	PRO	LEU	PRO	ALA
A3109	SER	ALA	ALA	PRO	ALA	ALA
V3110	GLN	SER	SER	GLN	THR	ALA
L3111	PHE	LEU	LEU	GLY	LYS	VAL
L3114	GLY	PRO	PRO	GLN	PRO	SER
H3115					ALA	
H3116					PRO	
V3117					GLN	
R3118					THR	
L3121					VAL	
GLY					ALA	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12001	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 ($e^-/\text{\AA}^2$)	30.0, 30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k), FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.035	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.007	Depositor
Map size ($\text{\AA}$)	472.5, 472.5, 472.5	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.35, 1.35, 1.35	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	B	0.37	0/10453	0.75	4/14290 (0.0%)
1	C	0.32	0/10464	0.70	6/14305 (0.0%)
1	D	0.34	0/10475	0.73	8/14317 (0.1%)
1	E	0.36	0/10416	0.72	3/14233 (0.0%)
1	F	0.37	0/10227	0.79	14/13995 (0.1%)
1	I	0.38	0/10071	0.82	13/13769 (0.1%)
2	G	0.25	0/794	0.53	0/1084
2	M	0.15	0/794	0.43	0/1084
2	Q	0.17	0/794	0.45	0/1084
2	T	0.25	0/794	0.57	2/1084 (0.2%)
2	U	0.23	0/794	0.56	0/1084
2	V	0.24	0/794	0.57	0/1084
3	K	0.30	0/2114	0.80	1/2909 (0.0%)
3	O	0.28	0/2215	0.74	5/3047 (0.2%)
6	S	0.32	0/2020	0.82	0/2768
7	k	0.31	0/4342	0.64	0/5924
8	l	0.26	0/792	0.64	0/1081
8	m	0.27	0/664	0.69	0/905
9	n	0.22	0/385	0.60	0/514
9	o	0.24	0/385	0.61	0/514
All	All	0.34	0/79787	0.74	56/109075 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	5
1	C	0	8
1	D	0	6
1	E	0	6
1	F	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	7
3	K	0	2
3	O	0	1
5	P	0	1
6	S	0	1
7	k	0	1
All	All	0	45

There are no bond length outliers.

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1123	GLY	N-CA-C	10.90	122.57	111.56
1	E	1266	ALA	N-CA-C	-8.46	100.97	114.09
1	F	1285	LYS	CA-C-N	8.28	137.35	121.54
1	F	1285	LYS	C-N-CA	8.28	137.35	121.54
1	D	1084	GLU	CA-C-N	7.79	136.43	121.54

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1201	ARG	Peptide
1	B	1222	VAL	Peptide
1	B	534	PRO	Peptide
1	B	764	VAL	Peptide
1	B	972	ASN	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	10198	0	9937	193	0
1	C	10209	0	9940	154	0
1	D	10221	0	9963	168	0
1	E	10162	0	9939	165	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	9978	0	9630	191	0
1	I	9831	0	9549	209	0
2	G	772	0	746	15	0
2	M	772	0	746	8	0
2	Q	772	0	746	9	0
2	T	772	0	746	10	0
2	U	772	0	746	18	0
2	V	772	0	746	19	0
3	K	2078	0	2053	40	0
3	O	2175	0	2213	31	0
4	L	420	0	88	6	0
5	P	435	0	89	2	0
6	S	1975	0	1858	31	0
7	k	4233	0	4180	122	0
8	l	770	0	751	16	0
8	m	648	0	636	49	0
9	n	383	0	418	7	0
9	o	383	0	418	12	0
All	All	78731	0	76138	1301	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 1301 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:k:495:ARG:HA	8:m:36:TRP:CH2	1.52	1.45
7:k:495:ARG:HB2	8:m:36:TRP:CZ3	1.59	1.38
7:k:495:ARG:CA	8:m:36:TRP:CH2	2.10	1.33
7:k:495:ARG:CB	8:m:36:TRP:CZ3	2.32	1.11
7:k:495:ARG:HA	8:m:36:TRP:CZ2	1.89	1.06

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1356/1374 (99%)	1200 (88%)	150 (11%)	6 (0%)	30	67
1	C	1356/1374 (99%)	1223 (90%)	130 (10%)	3 (0%)	43	77
1	D	1356/1374 (99%)	1205 (89%)	146 (11%)	5 (0%)	30	67
1	E	1345/1374 (98%)	1193 (89%)	151 (11%)	1 (0%)	48	82
1	F	1347/1374 (98%)	1162 (86%)	183 (14%)	2 (0%)	48	82
1	I	1311/1374 (95%)	1114 (85%)	193 (15%)	4 (0%)	36	71
2	G	99/112 (88%)	91 (92%)	8 (8%)	0	100	100
2	M	99/112 (88%)	93 (94%)	6 (6%)	0	100	100
2	Q	99/112 (88%)	96 (97%)	3 (3%)	0	100	100
2	T	99/112 (88%)	92 (93%)	7 (7%)	0	100	100
2	U	99/112 (88%)	89 (90%)	10 (10%)	0	100	100
2	V	99/112 (88%)	90 (91%)	9 (9%)	0	100	100
3	K	291/318 (92%)	253 (87%)	38 (13%)	0	100	100
3	O	301/318 (95%)	274 (91%)	27 (9%)	0	100	100
6	S	267/466 (57%)	216 (81%)	50 (19%)	1 (0%)	30	67
7	k	539/702 (77%)	506 (94%)	32 (6%)	1 (0%)	43	77
8	l	92/585 (16%)	84 (91%)	8 (9%)	0	100	100
8	m	78/585 (13%)	72 (92%)	6 (8%)	0	100	100
9	n	45/3122 (1%)	44 (98%)	1 (2%)	0	100	100
9	o	45/3122 (1%)	45 (100%)	0	0	100	100
All	All	10323/18134 (57%)	9142 (89%)	1158 (11%)	23 (0%)	44	77

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1223	ILE
1	C	1223	ILE
1	D	1085	THR
1	D	1223	ILE
1	E	1223	ILE

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	B	1014/1080 (94%)	998 (98%)	16 (2%)	55	69
1	C	1018/1080 (94%)	1010 (99%)	8 (1%)	73	78
1	D	1020/1080 (94%)	1012 (99%)	8 (1%)	73	78
1	E	1018/1080 (94%)	1017 (100%)	1 (0%)	88	88
1	F	968/1080 (90%)	961 (99%)	7 (1%)	76	80
1	I	970/1080 (90%)	952 (98%)	18 (2%)	50	66
2	G	78/88 (89%)	78 (100%)	0	100	100
2	M	78/88 (89%)	78 (100%)	0	100	100
2	Q	78/88 (89%)	78 (100%)	0	100	100
2	T	78/88 (89%)	78 (100%)	0	100	100
2	U	78/88 (89%)	78 (100%)	0	100	100
2	V	78/88 (89%)	78 (100%)	0	100	100
3	K	195/264 (74%)	193 (99%)	2 (1%)	68	76
3	O	214/264 (81%)	214 (100%)	0	100	100
6	S	181/365 (50%)	179 (99%)	2 (1%)	65	74
7	k	426/529 (80%)	419 (98%)	7 (2%)	55	69
8	l	78/451 (17%)	78 (100%)	0	100	100
8	m	64/451 (14%)	64 (100%)	0	100	100
9	n	41/2370 (2%)	41 (100%)	0	100	100
9	o	41/2370 (2%)	41 (100%)	0	100	100
All	All	7716/14072 (55%)	7647 (99%)	69 (1%)	68	77

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	1356	THR
3	K	295	VAL
7	k	261	LEU

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Mol	Chain	Res	Type
1	D	99	VAL
1	C	1334	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 187 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	1062	ASN
1	I	972	ASN
1	F	1310	GLN
1	I	502	GLN
1	I	1310	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.

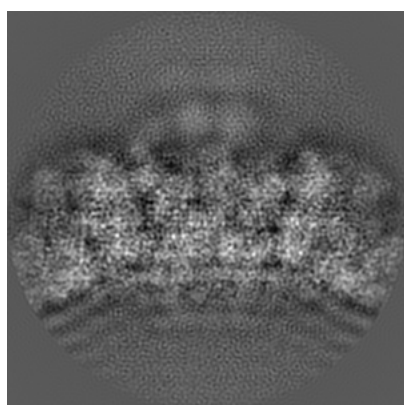
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30123. These allow visual inspection of the internal detail of the map and identification of artifacts.

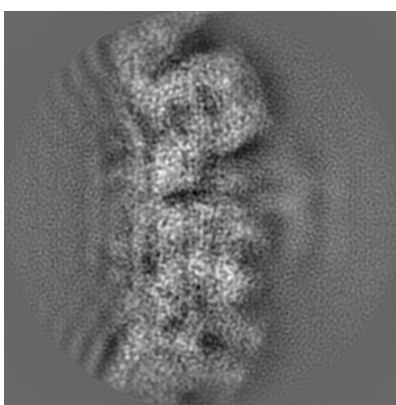
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

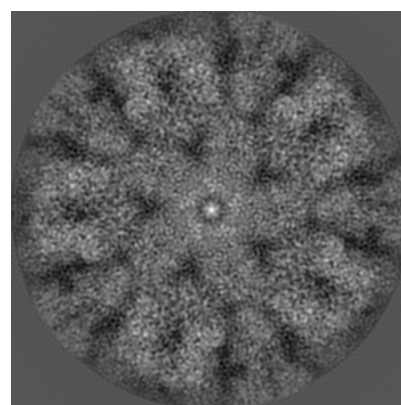
6.1.1 Primary map



X



Y

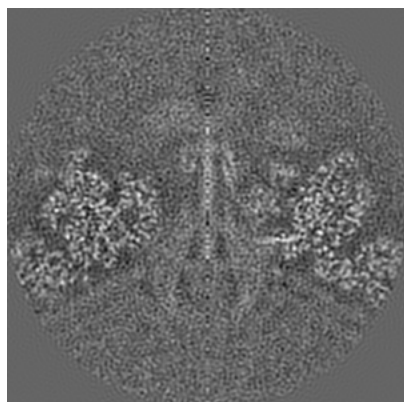


Z

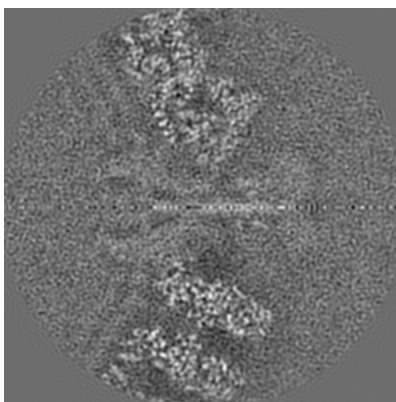
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

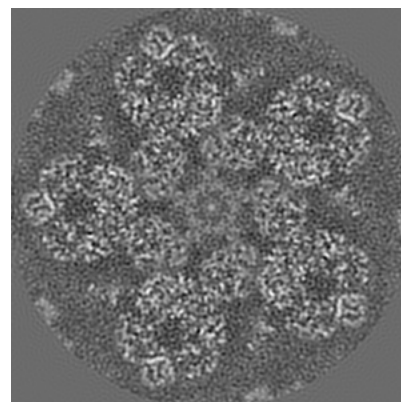
6.2.1 Primary map



X Index: 175



Y Index: 175

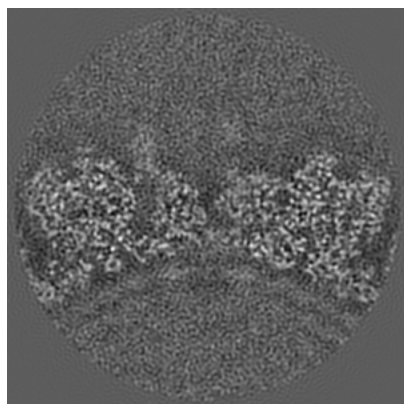


Z Index: 175

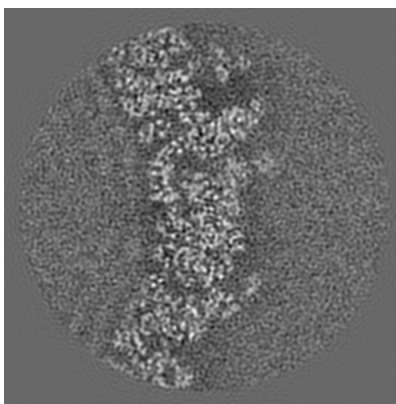
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

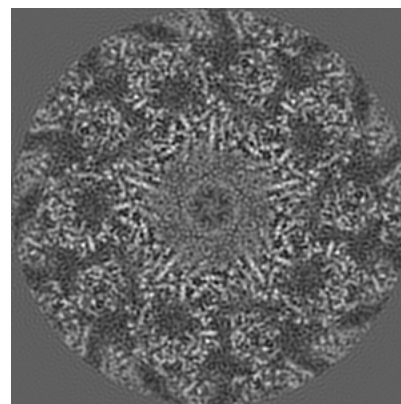
6.3.1 Primary map



X Index: 123



Y Index: 103

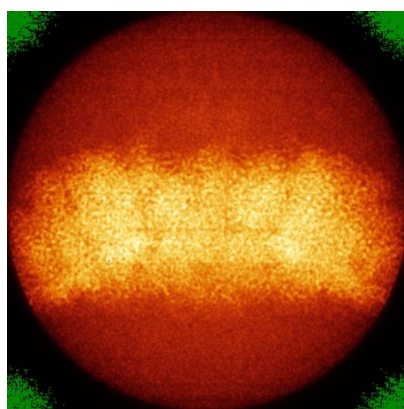


Z Index: 147

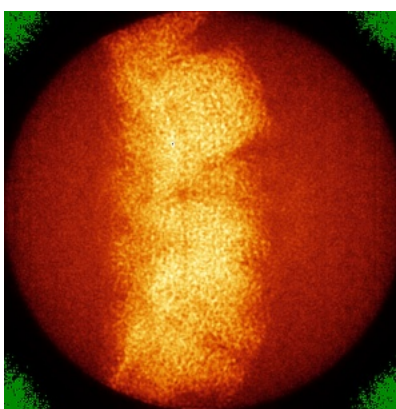
The images above show the largest variance slices of the map in three orthogonal directions.

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

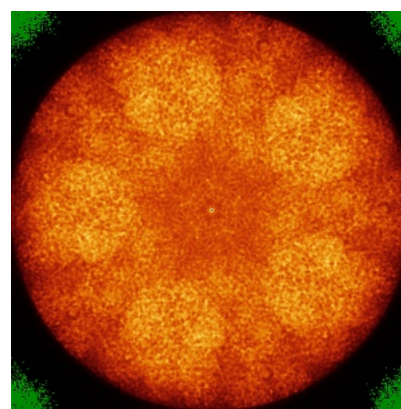
6.4.1 Primary map



X



Y

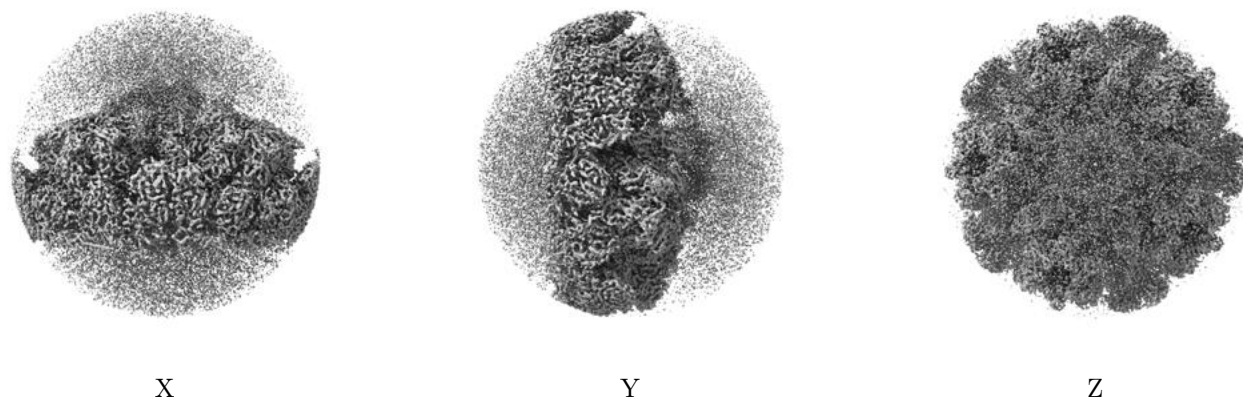


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

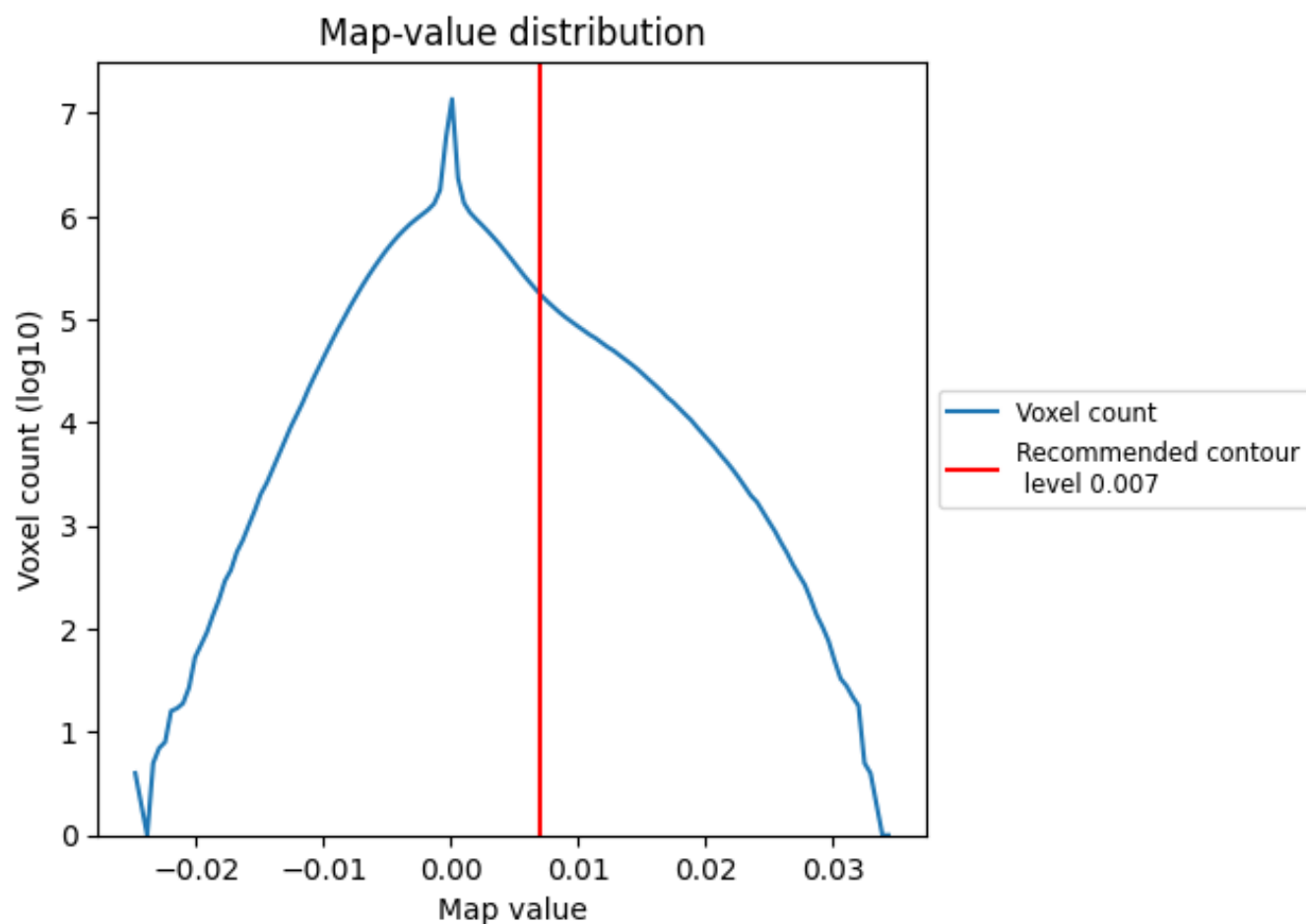
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

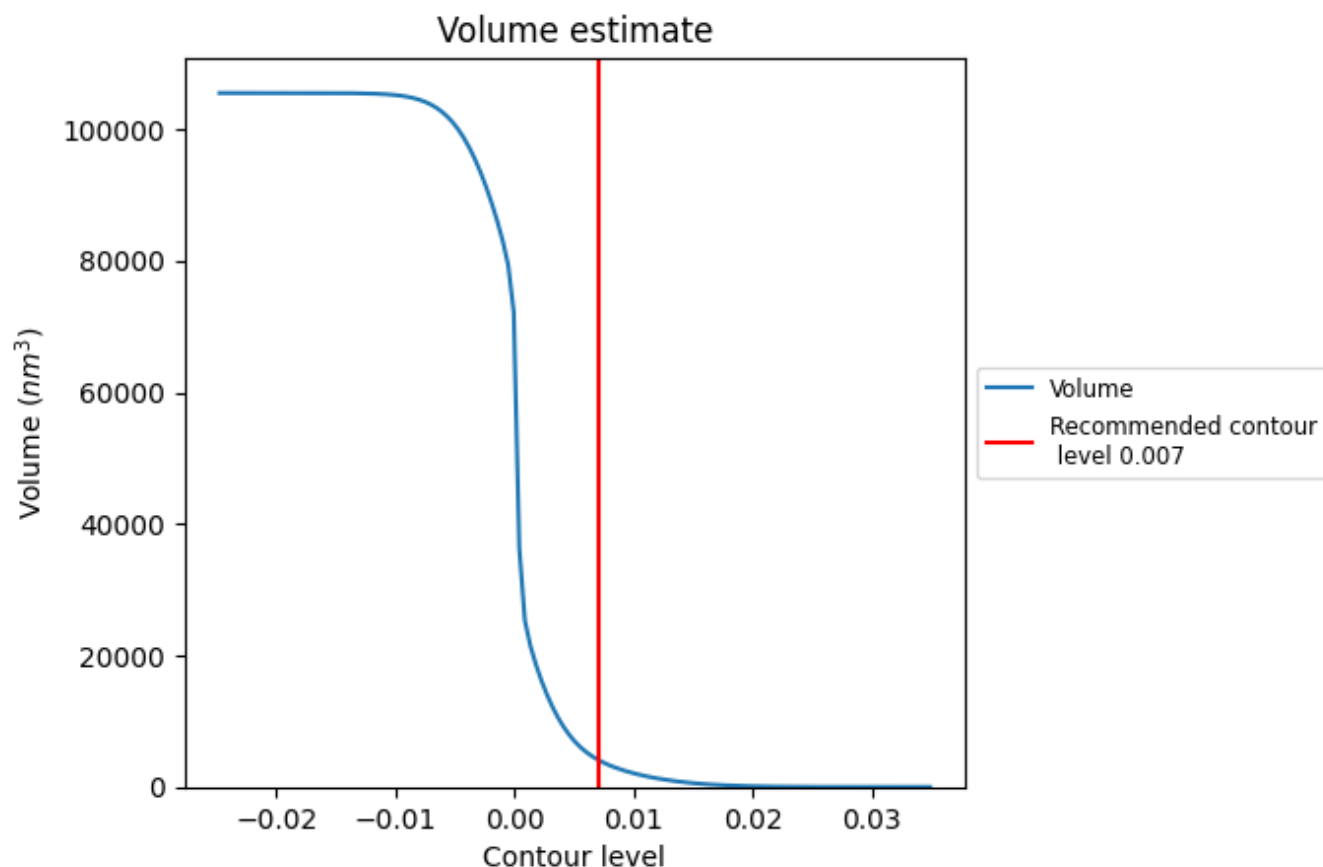
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

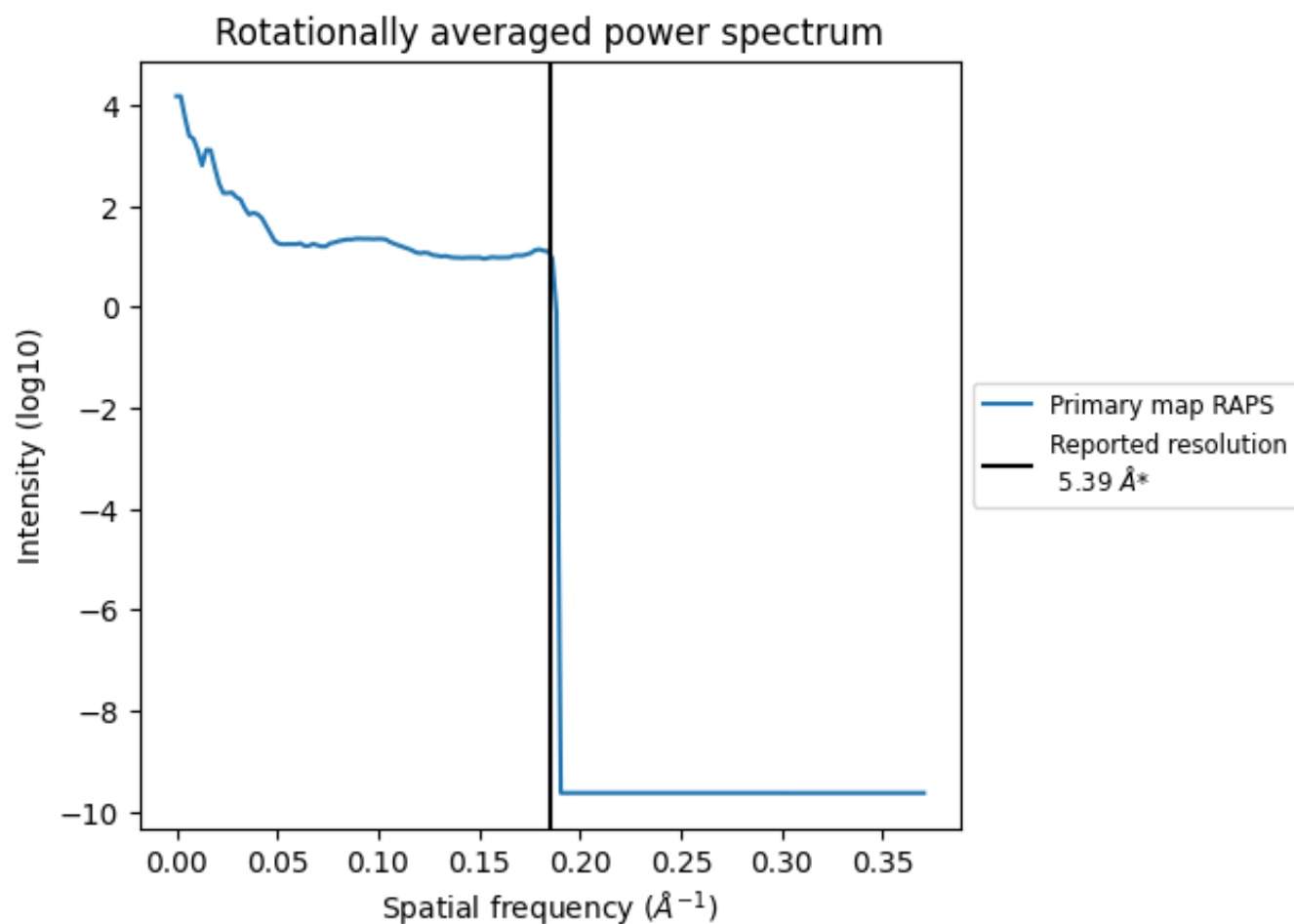
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4131 nm³; this corresponds to an approximate mass of 3731 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 0.186 $\text{\AA}^{-1}$

8 Fourier-Shell correlation

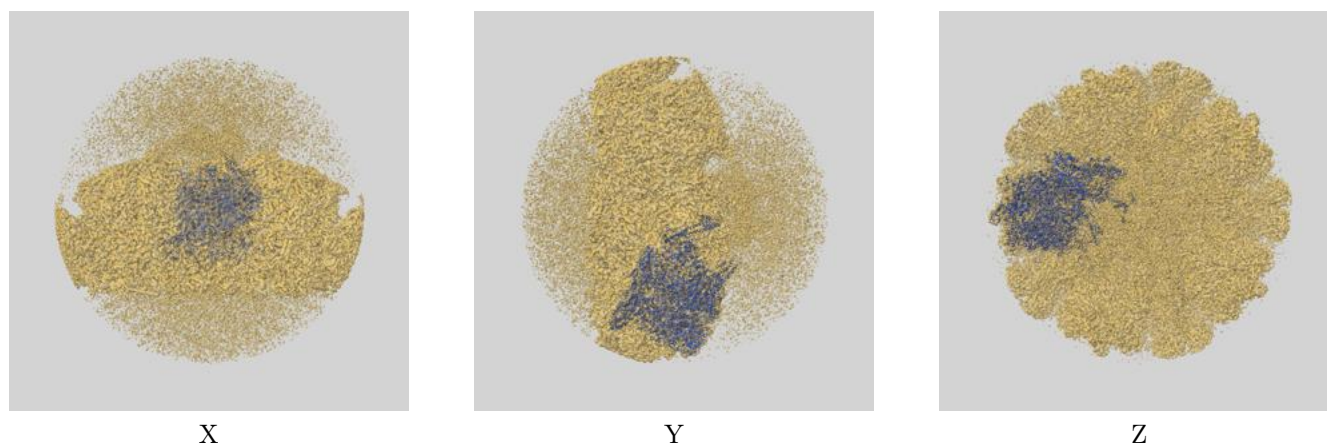
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

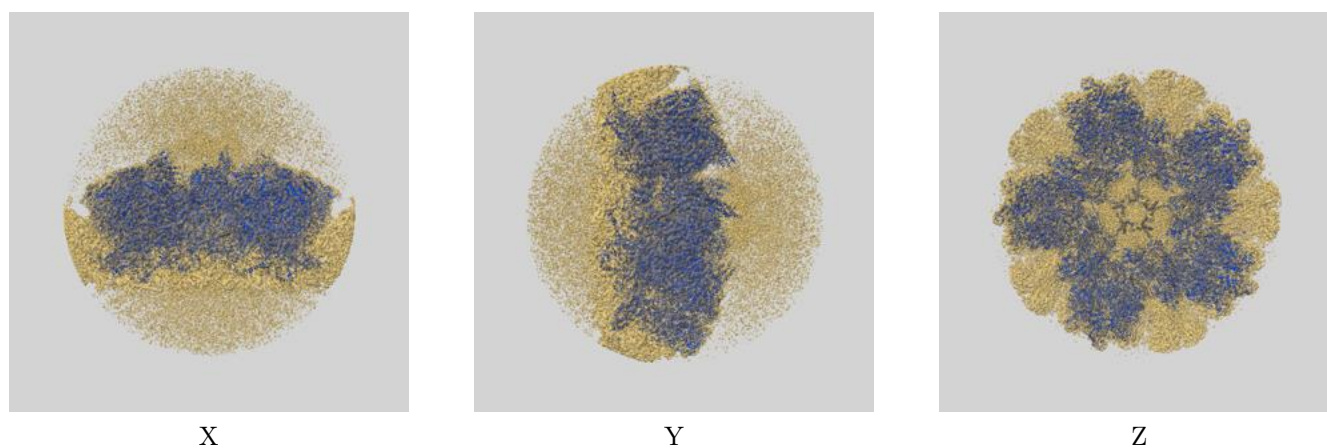
This section contains information regarding the fit between EMDB map EMD-30123 and PDB model 6M6G. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

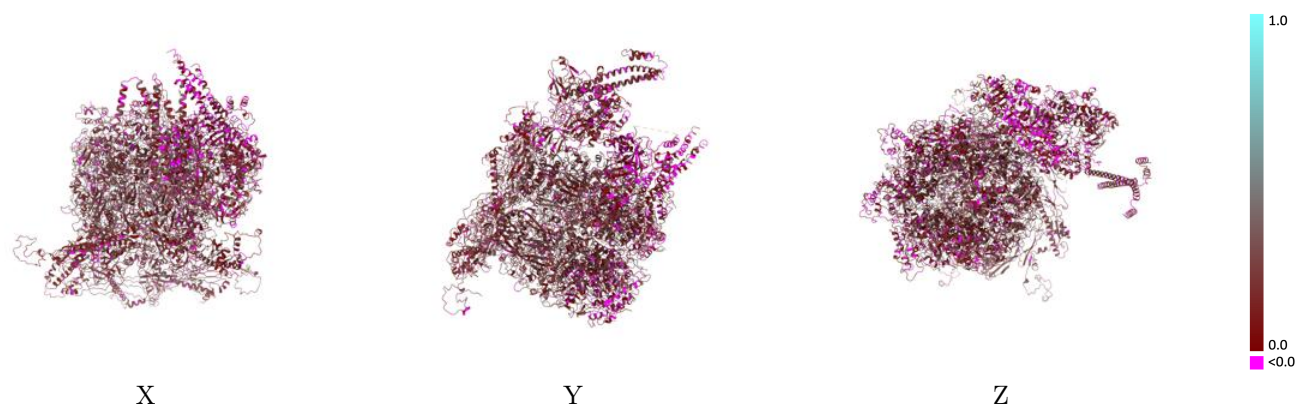


9.1.2 Map-model assembly overlay [i](#)



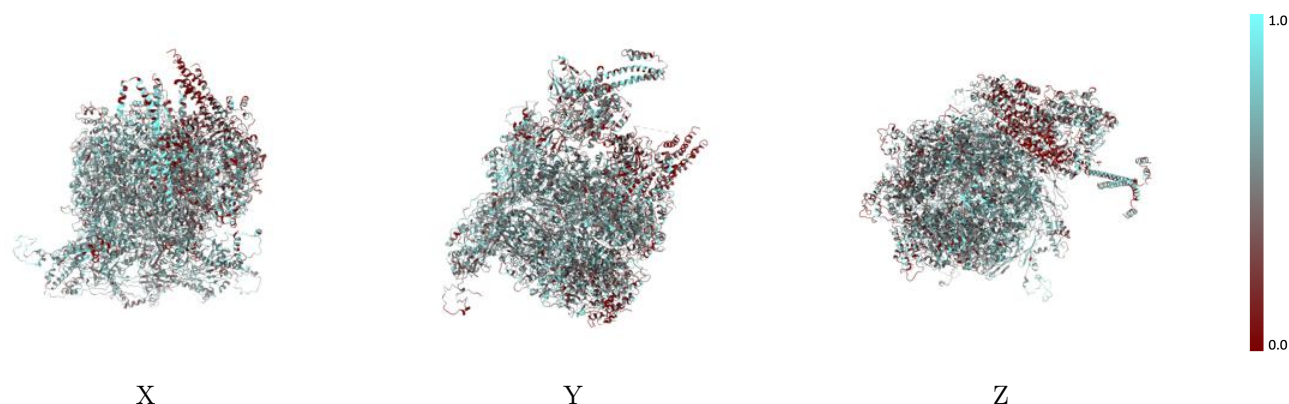
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



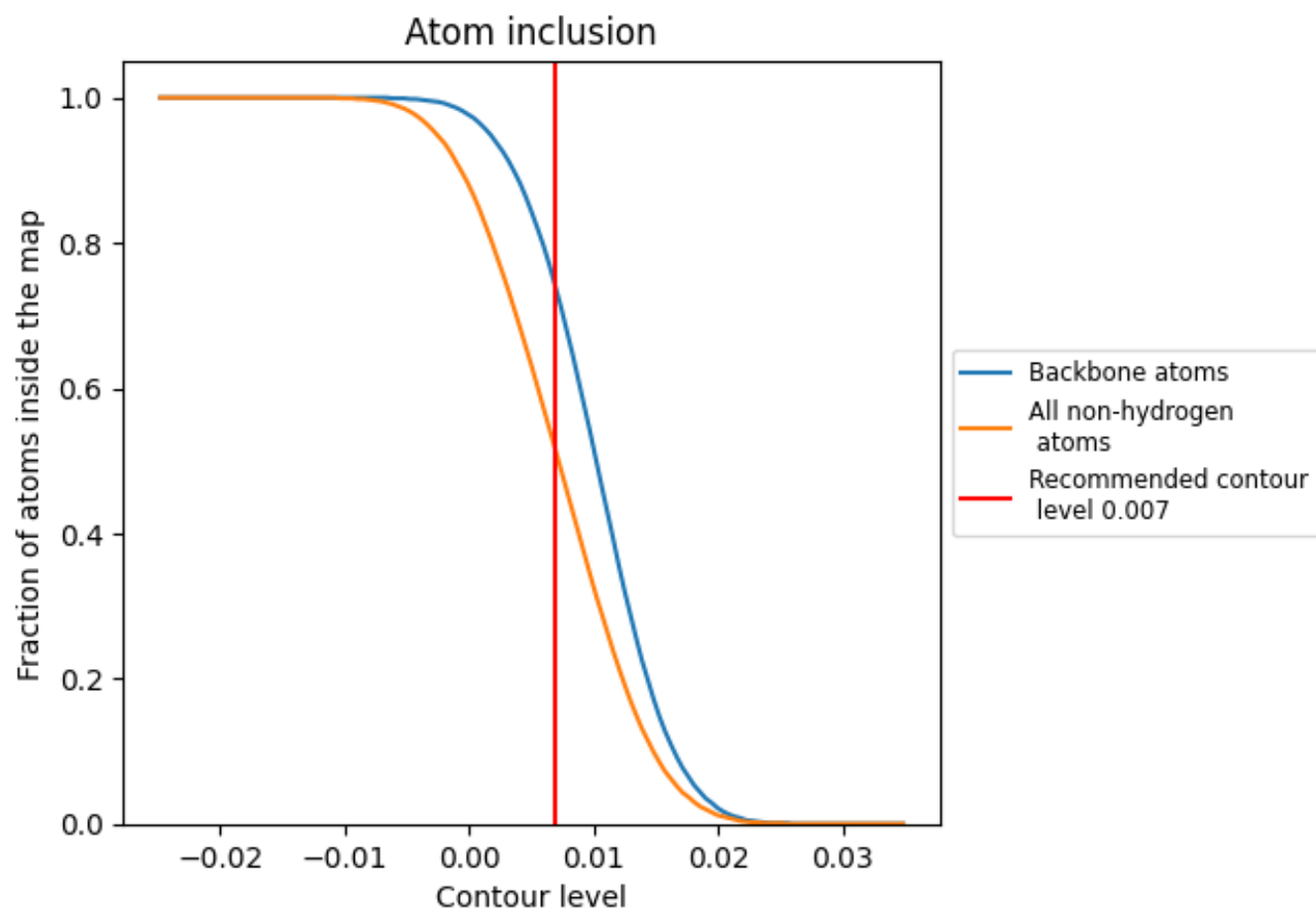
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 51% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5120	 0.1880
B	 0.5500	 0.2060
C	 0.5180	 0.2010
D	 0.5360	 0.2040
E	 0.5700	 0.2130
F	 0.5680	 0.2140
G	 0.3720	 0.1420
I	 0.5580	 0.2110
K	 0.4620	 0.1560
L	 0.5480	 0.1710
M	 0.3460	 0.1140
O	 0.4340	 0.1720
P	 0.5380	 0.1790
Q	 0.2810	 0.0660
S	 0.3840	 0.1140
T	 0.3210	 0.0940
U	 0.3780	 0.1160
V	 0.4520	 0.1580
k	 0.3670	 0.0930
l	 0.3540	 0.1190
m	 0.3510	 0.1150
n	 0.1300	 0.0470
o	 0.2070	 0.0270

