



wwPDB EM Validation Summary Report ⓘ

Apr 15, 2026 – 11:40 AM UTC

PDB ID : 8U11 / pdb_00008u11
EMDB ID : EMD-41792
Title : In situ cryo-EM structure of bacteriophage P22 gp1:gp5:gp4: gp10: gp9 N-term complex in conformation 2 at 3.1Å resolution
Authors : Iglesias, S.; Feng-Hou, C.; Cingolani, G.
Deposited on : 2023-08-30
Resolution : 3.10 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

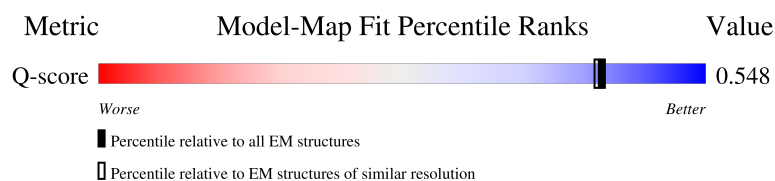
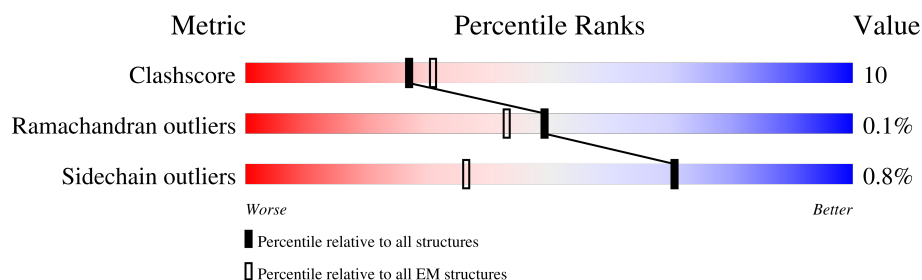
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	1	472	
1	2	472	
1	3	472	
1	4	472	

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Mol	Chain	Length	Quality of chain
1	5	472	
1	6	472	
2	10	667	
2	11	667	
2	12	667	
2	13	667	
2	14	667	
2	15	667	
2	16	667	
2	17	667	
2	18	667	
2	19	667	
2	20	667	
2	21	667	
2	22	667	
2	23	667	
2	24	667	
2	7	667	
2	8	667	
2	9	667	
3	a	725	
3	b	725	
3	c	725	
3	d	725	
3	e	725	

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Mol	Chain	Length	Quality of chain
3	f	725	
3	g	725	
3	h	725	
3	i	725	
3	j	725	
3	k	725	
3	l	725	
4	m	166	
4	n	166	
4	o	166	
4	p	166	
4	q	166	
4	r	166	
4	s	166	
4	t	166	
4	u	166	
4	v	166	
4	x	166	
4	y	166	
5	A	430	
5	B	430	
5	C	430	
5	D	430	
5	E	430	
5	F	430	

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Mol	Chain	Length	Quality of chain
5	G	430	
5	H	430	
5	I	430	
5	J	430	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 138386 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 Packaged DNA stabilization protein gp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
1	2	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
1	3	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
1	4	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
1	5	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
1	6	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		

- Molecule 2 is a protein called Tail spike protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	120	Total	C	N	O	S	0	0
			934	595	156	182	1		
2	8	120	Total	C	N	O	S	0	0
			934	595	156	182	1		
2	9	120	Total	C	N	O	S	0	0
			934	595	156	182	1		
2	10	120	Total	C	N	O	S	0	0
			934	595	156	182	1		
2	11	120	Total	C	N	O	S	0	0
			934	595	156	182	1		
2	12	120	Total	C	N	O	S	0	0
			934	595	156	182	1		
2	13	120	Total	C	N	O	S	0	0
			934	595	156	182	1		
2	14	120	Total	C	N	O	S	0	0
			934	595	156	182	1		
2	15	120	Total	C	N	O	S	0	0
			934	595	156	182	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	16	120	Total 934	C 595	N 156	O 182	S 1	0	0
2	17	120	Total 934	C 595	N 156	O 182	S 1	0	0
2	18	120	Total 934	C 595	N 156	O 182	S 1	0	0
2	19	120	Total 934	C 595	N 156	O 182	S 1	0	0
2	20	120	Total 934	C 595	N 156	O 182	S 1	0	0
2	21	120	Total 934	C 595	N 156	O 182	S 1	0	0
2	22	120	Total 934	C 595	N 156	O 182	S 1	0	0
2	23	120	Total 934	C 595	N 156	O 182	S 1	0	0
2	24	120	Total 934	C 595	N 156	O 182	S 1	0	0

- Molecule 3 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
3	b	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
3	c	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
3	d	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
3	e	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
3	l	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
3	f	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
3	k	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
3	i	544	Total 4417	C 2791	N 756	O 850	S 20	0	0
3	j	544	Total 4417	C 2791	N 756	O 850	S 20	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	h	544	Total	C	N	O	S	0	0
			4417	2791	756	850	20		
3	g	544	Total	C	N	O	S	0	0
			4417	2791	756	850	20		

- Molecule 4 is a protein called Peptidoglycan hydrolase gp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	y	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	m	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	n	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	o	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	p	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	q	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	r	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	s	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	t	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	u	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	v	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		
4	x	152	Total	C	N	O	S	0	0
			1166	731	200	229	6		

- Molecule 5 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	429	Total	C	N	O	S	0	0
			3277	2053	568	643	13		
5	C	429	Total	C	N	O	S	0	0
			3277	2053	568	643	13		
5	A	429	Total	C	N	O	S	0	0
			3277	2053	568	643	13		

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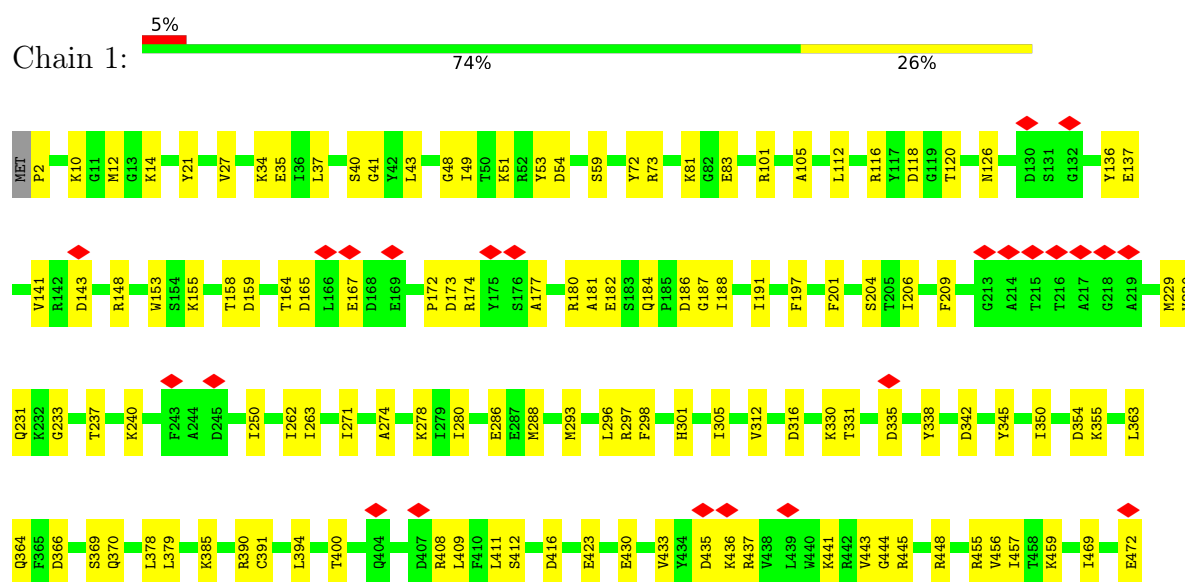
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Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	429	Total	C	N	O	S	0	0
			3277	2053	568	643	13		
5	I	429	Total	C	N	O	S	0	0
			3277	2053	568	643	13		
5	D	421	Total	C	N	O	S	0	0
			3219	2017	558	631	13		
5	B	421	Total	C	N	O	S	0	0
			3219	2017	558	631	13		
5	F	421	Total	C	N	O	S	0	0
			3219	2017	558	631	13		
5	H	421	Total	C	N	O	S	0	0
			3219	2017	558	631	13		
5	J	421	Total	C	N	O	S	0	0
			3219	2017	558	631	13		

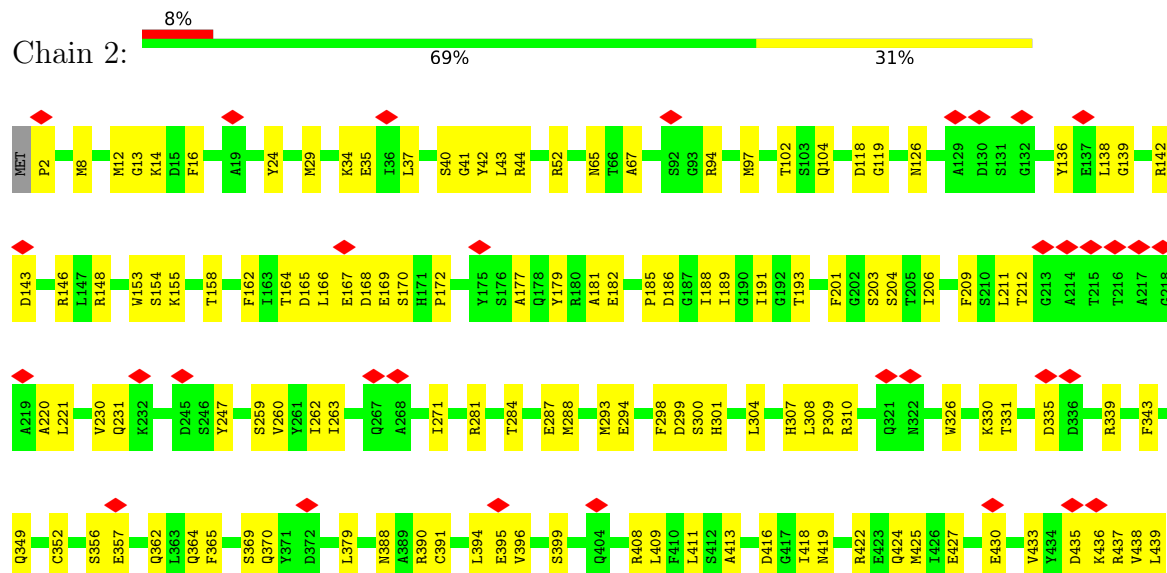
3 Residue-property plots

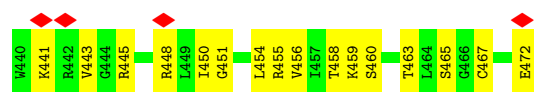
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Packaged DNA stabilization protein gp10

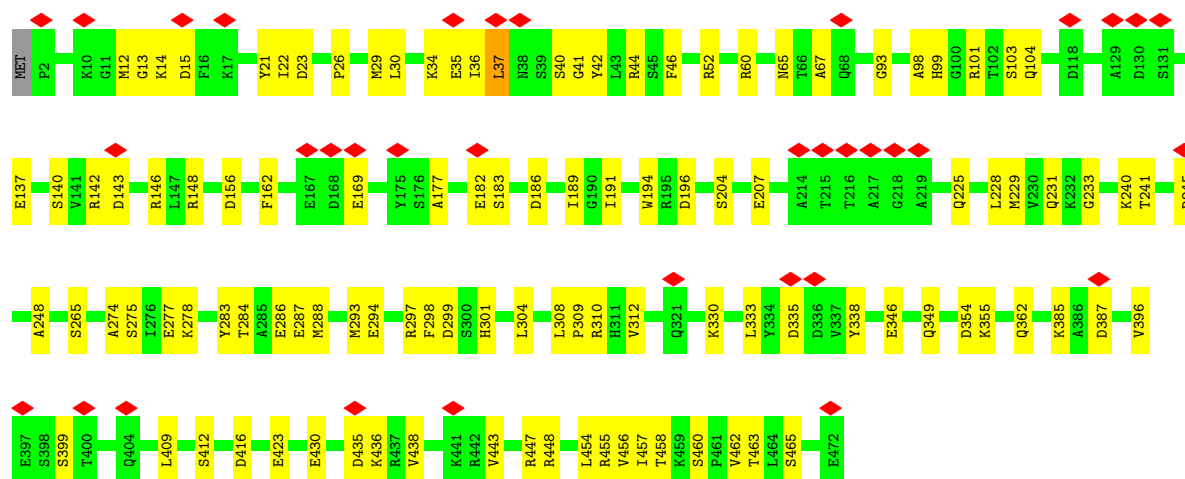
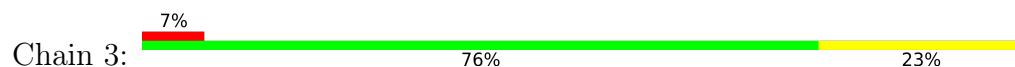


• Molecule 1: Packaged DNA stabilization protein gp10

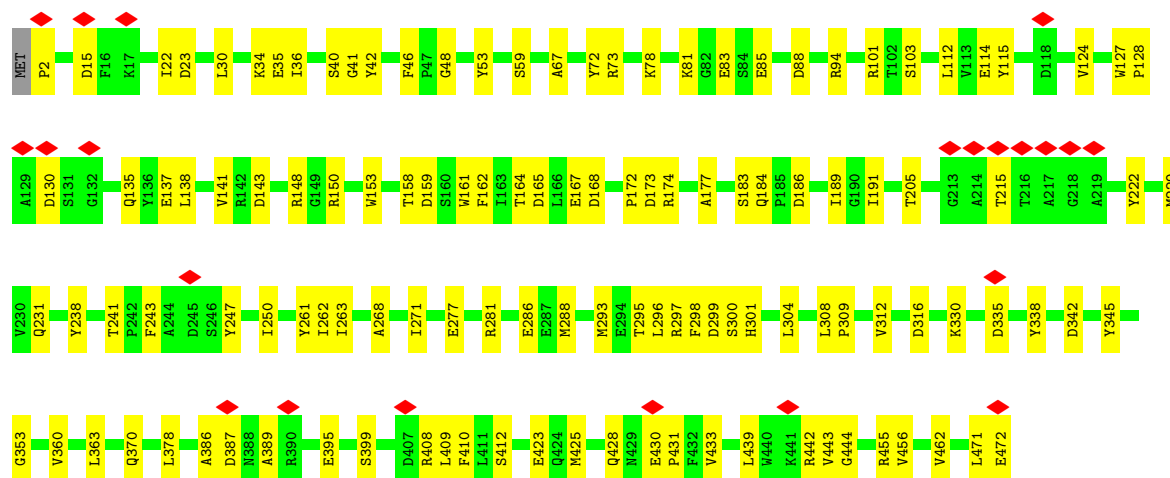
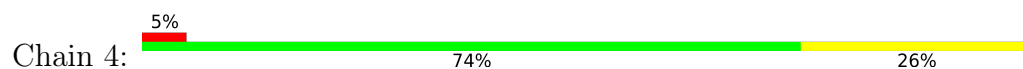




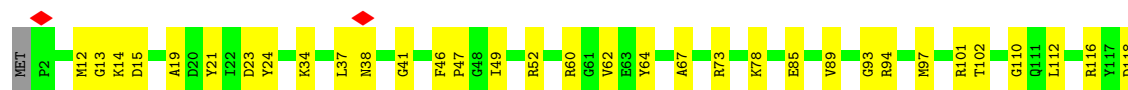
• Molecule 1: Packaged DNA stabilization protein gp10



• Molecule 1: Packaged DNA stabilization protein gp10



• Molecule 1: Packaged DNA stabilization protein gp10





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

- Molecule 2: Tail spike protein

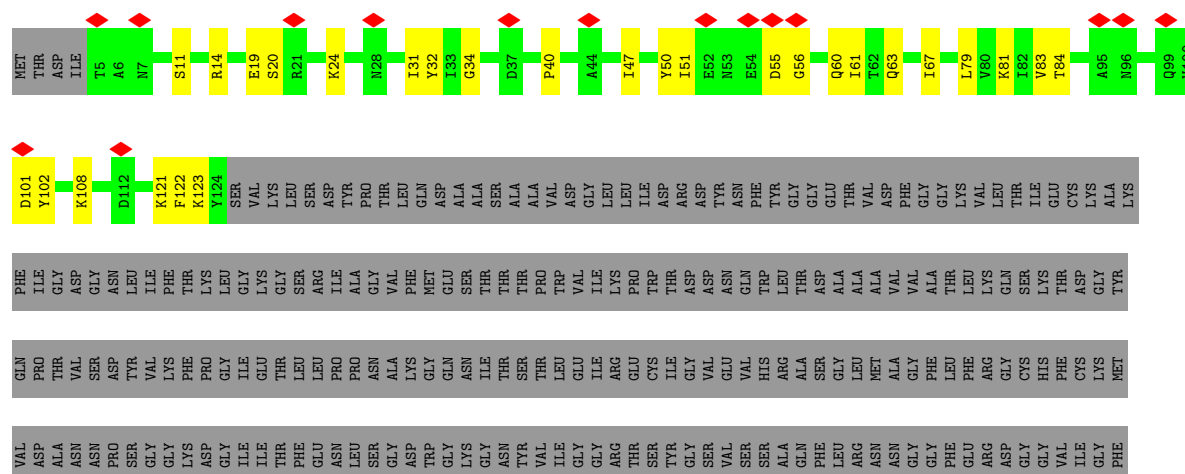
Chain 11: 13% 82%

[illegible]

Chain 12: 14% 82%

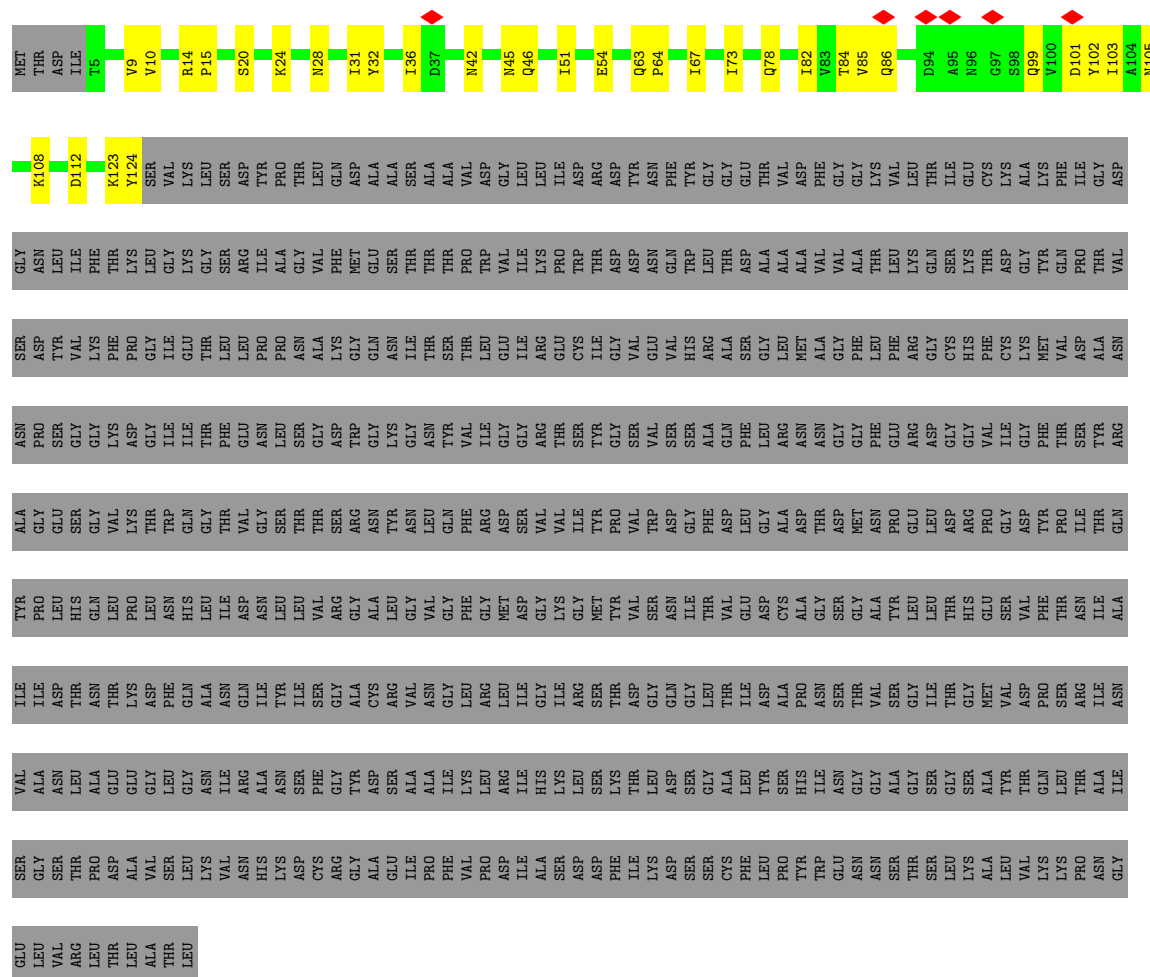


Chain 13: 14% 82%





- Molecule 2: Tail spike protein

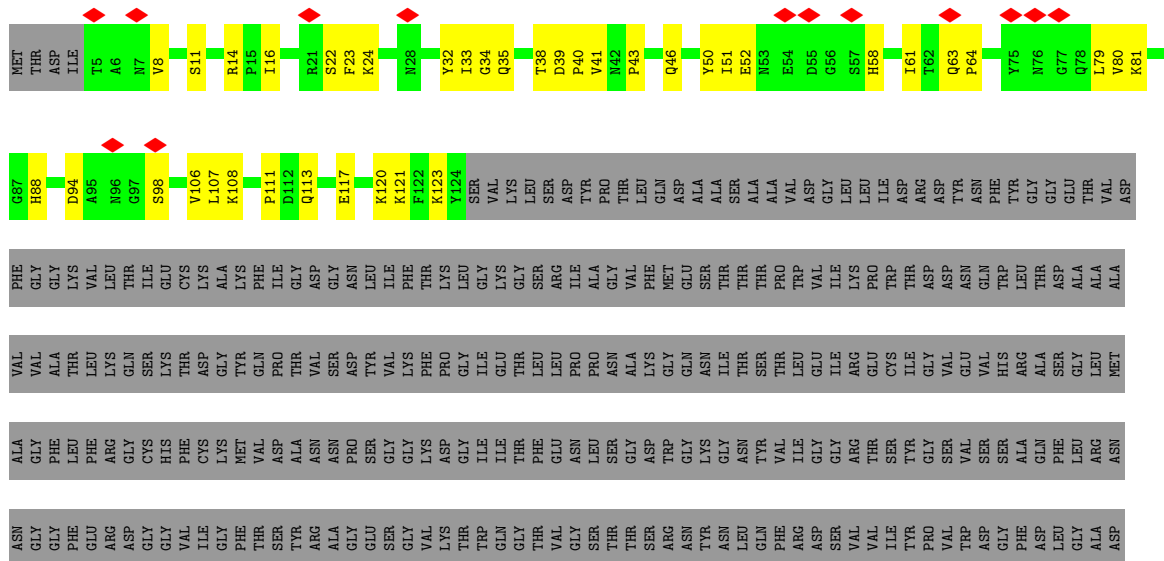


- Molecule 2: Tail spike protein





- Molecule 2: Tail spike protein



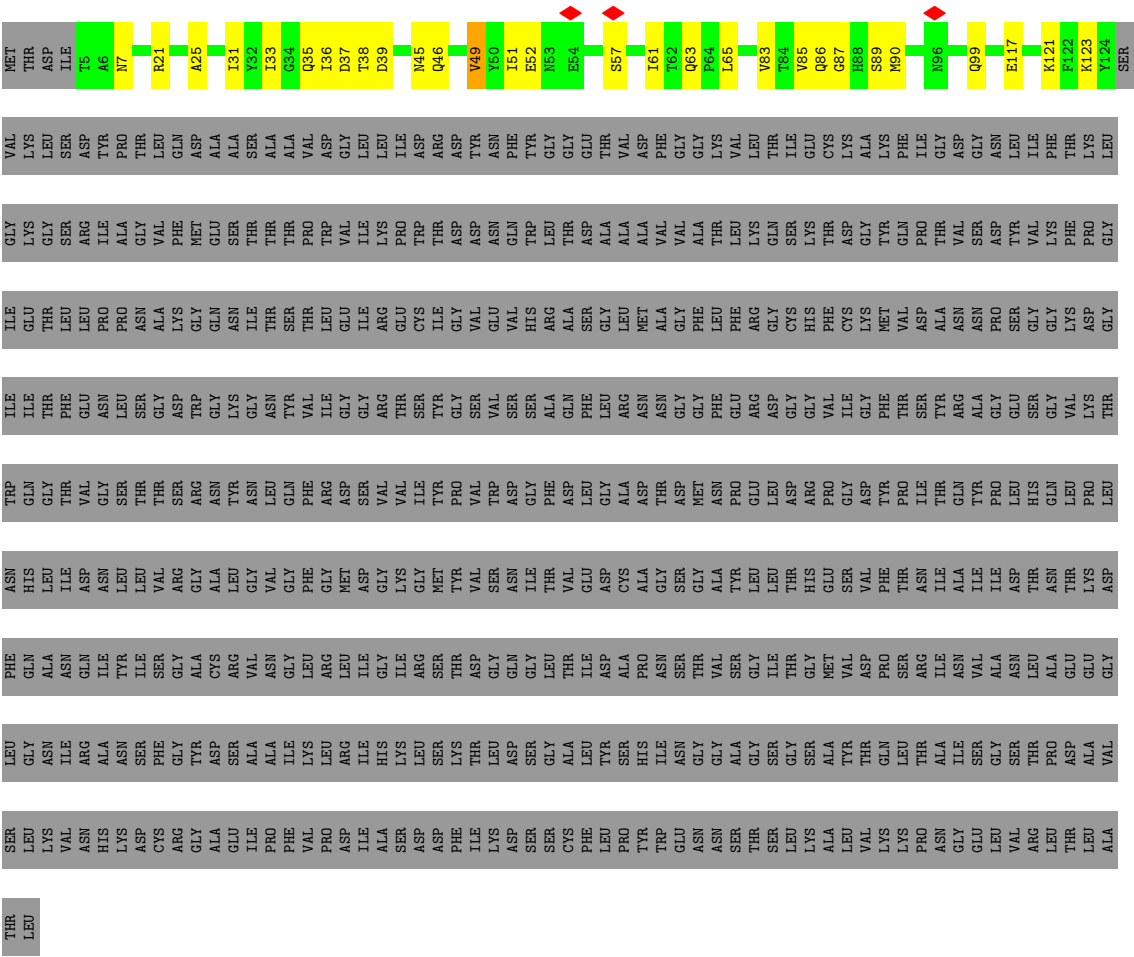
- Molecule 2: Tail spike protein



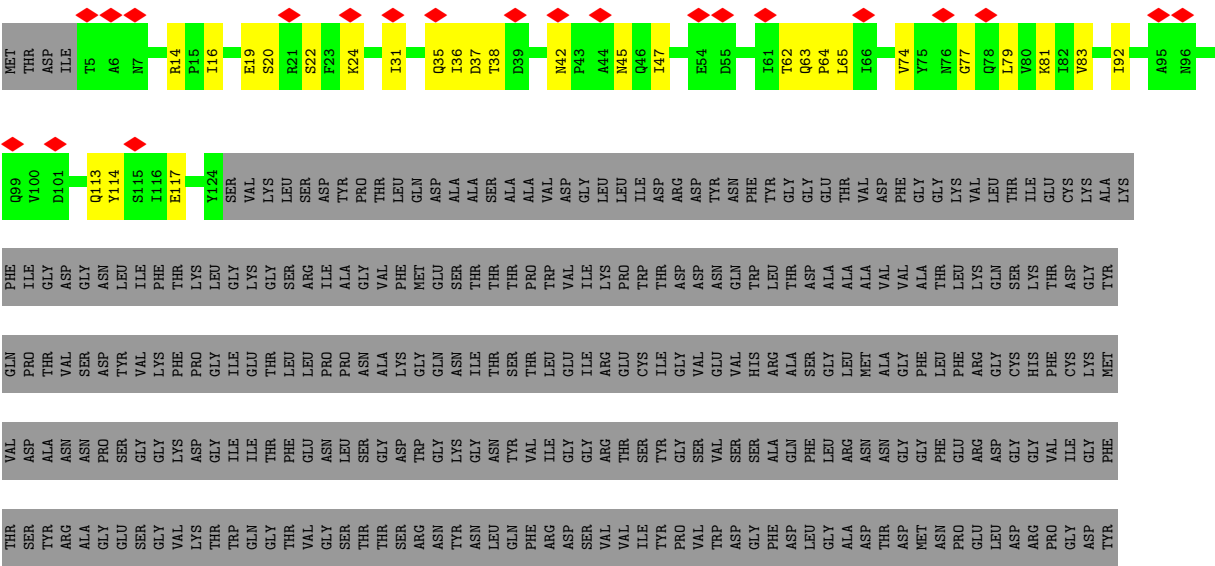
LEU	THR	LEU	ALA	PRO	THR	ASP	GLU	ALA	ASN	GLN	GLY	GLY	LYS	PHE	K123	Y124	MET
THR	LEU	ALA	GLU	ASP	THR	ASP	GLU	LYS	LYS	PRO	LYS	PRO	PRO	THR	THR	ASP	THR
THR	LEU	ALA	GLY	VAL	PHE	ASP	GLY	THR	THR	ASN	THR	ILE	ILE	GLY	VAL	SER	ILE
LEU			GLY	LEU	GLN		ASN	GLN	HIS	ASN	THR	ILE	GLU	LYS	LYS	A6	
LYS			ASN	LYS	GLN	ASN	LEU	GLY	LEU	THR	THR	THR	THR	GLY	LEU	N7	
VAL			ILE	ASN	ASN	ASN	ILE	ILE	ILE	ILE	THR	THR	THR	SER	ASP	V8	
ASN			ARG	ASN	GLN	GLY	ASN	VAL	GLN	ASP	GLY	GLY	GLY	ARG	VAL	Y9	
HIS			ALA	ILE	ALA	ILE	ASN	THR	THR	GLY	ASN	PRO	PRO	ILE	TYR		
LYS			ASN	TYR	THR	LEU	LEU	SER	LEU	SER	ASN	PRO	ASN	GLY	THR	P15	
ASP			SER	ILE	THR	ILE	THR	THR	THR	THR	GLY	THR	THR	GLY	THR		
CYS			PHE	THR	THR	THR	VAL	SER	VAL	VAL	GLY	ALA	ALA	VAL	LEU	S20	
ARG			GLY	GLY	GLY	GLY	ARG	ASP	GLY	THR	LYS	LYS	THR	PHE	GLN	K21	
GLY			TYR	ALA	ALA	ALA	GLY	ARG	TRP	GLY	GLY	GLY	GLY	MET	ASP	S22	
ALA			ASP	CYS	CYS	VAL	ASN	ASN	GLY	GLN	GLN	ASN	GLU	GLU	ALA	F23	
SER			SER	ARG	ARG	ARG	LEU	THR	LYS	THR	LYS	ASN	SER	SER	SER	K24	
ILE			ALA	VAL	VAL	VAL	GLY	ASN	GLY	GLY	GLY	ILE	THR	THR	ALA	A27	
PRO			ALA	ASN	ASN	GLY	VAL	ASN	VAL	ASN	THR	THR	THR	THR	ALA	N28	
PHE			ILE	GLY	GLY	GLY	PHE	GLN	VAL	THR	THR	THR	PRO	VAL	VAL		
VAL			LYS	LEU	LEU	ARG	GLY	ILE	ILE	THR	THR	THR	TRP	ASP	GLY	Y32	
ASP			ARG	LEU	LEU	LEU	MET	ASP	GLY	GLY	GLU	GLU	VAL	VAL	ILE		
ILE			ILE	ILE	ILE	ILE	ASP	THR	GLY	ILE	ILE	ILE	THR	THR	THR	D37	
ALA			HIS	GLY	GLY	GLY	GLY	VAL	ARG	GLY	ARG	ARG	PRO	ILE	ILE	T38	
SER			LYS	ILE	ILE	ILE	LYS	THR	THR	GLU	THR	GLU	THR	ASP	ASP	D39	
ASP			LEU	ARG	ARG	ARG	MET	ILE	SER	THR	TYR	ILE	THR	THR	ARG	P40	
ASP			SER	SER	THR	THR	TYR	PRO	GLY	GLY	GLY	GLY	ASP	ASP	ASP	V41	
PHE			LYS	THR	ASP	THR	THR	VAL	SER	VAL	VAL	VAL	VAL	ASP	TYR	N42	
ILE			THR	ASP	GLY	GLY	VAL	TRP	VAL	GLN	GLY	GLU	ASN	ASN	ASN		
LYS			LEU	GLN	GLN	ASP	ASN	THR	SER	ASN	THR	THR	GLN	PHE	PHE	Q46	
ASP			ASP	GLY	GLY	GLY	ILE	GLY	SER	ILE	ALA	ARG	THR	TRP	TYR		
SER			GLY	LEU	LEU	LEU	THR	PHE	ALA	THR	ALA	ALA	LEU	LEU	GLY		
CYS			ALA	THR	THR	THR	VAL	ASP	GLN	VAL	ALA	ALA	ALA	THR	GLY	LEU	
PHE			LEU	ILE	ILE	ILE	GLU	LEU	PHE	GLY	THR	THR	THR	ASP	GLU	E52	
LEU			TYR	ASP	ASP	ASP	ASP	GLY	LEU	GLY	GLY	GLY	GLY	ALA	THR		
PRO			SER	ALA	ALA	ALA	CYS	ALA	ASN	THR	THR	THR	THR	ALA	VAL		
TYR			HIS	PRO	PRO	PRO	ALA	ALA	ASN	GLY	ASN	ASN	ASN	ALA	ASP		
THR			SER	ILE	ASN	ASN	GLY	THR	ASN	GLY	THR	THR	THR	VAL	PHE	Q63	
GLU			ASN	SER	SER	SER	SER							VAL	GLY	P64	
THR			ASN	THR	THR	THR	GLY	THR	GLY	GLY	PHE	THR	THR	ALA	GLY	L65	
SER			ALA	SER	ALA	ALA	VAL	ASN	PHE	GLY	LEU	LEU	THR	LYS	LYS	L66	
THR			ALA	ALA	GLY	GLY	THR	GLY	GLU	ARG	ARG	ARG	LYS	VAL	VAL	L67	
SER			SER	ILE	ILE	ILE	LEU	LEU	GLY	ASP	GLY	GLY	GLN	THR	THR	L73	
LEU			GLY	THR	THR	THR	THR	THR	GLY	ARG	CYS	CYS	SER	ILE	ILE		
ALA			SER	GLY	GLY	GLY	HIS	ARG	GLY	GLY	PHE	HIS	LYS	GLY	GLU	K81	
ALA			ALA	MET	ALA	ALA	GLU	PRO	VAL	VAL	THR	THR	THR	CYS	CYS	T82	
LEU			TYR	VAL	VAL	VAL	SER	GLY	ILE	ILE	CYS	CYS	ASP	ASP	ALA		
VAL			THR	ASP	ASP	ASP	PHE	THR	GLY	GLY	LYS	LYS	GLY	TYR	LYS	Q86	
LYS			GLN	PRO	PRO	PRO	THR	TYR	PHE	THR	THR	THR	TYR	THR	LYS		
LYS			LEU	SER	THR	THR	THR	PRO	THR	VAL	VAL	VAL	GLN	GLN	PHE	K108	
PRO			THR	ARG	ARG	ARG	ASN	ILE	SER	THR	THR	THR	THR	GLY	ILE	Y109	
ASN			ALA	ILE	ILE	ILE	ILE	THR	TYR	THR	ALA	ALA	VAL	ASP	GLY		
GLY			ILE	ASN	ASN	ASN	ALA	GLN	ARG	ALA	ASN	ASN	SER	GLY	GLY	D112	
GLU			SER	VAL	VAL	VAL	ILE	THR	ALA	ILE	ASN	ASN	THR	THR	ASN		
LEU			GLY	SER	GLY	GLY	GLY	THR	ALA	THR	GLY	PRO	ASP	ASP	ASN	S115	
VAL			SER	ASN	ASN	ASN	ILE	PRO	GLY	GLY	GLU	GLU	TYR	THR	LEU	I116	
ARG			THR	ASN	ASN	ASN	ASP	THR	GLY	GLY	GLY	GLY	LEU	VAL	ILE	E117	
																A118	
																P319	

- Molecule 2: Tail spike protein





• Molecule 2: Tail spike protein



[illegible]

- Molecule 2: Tail spike protein

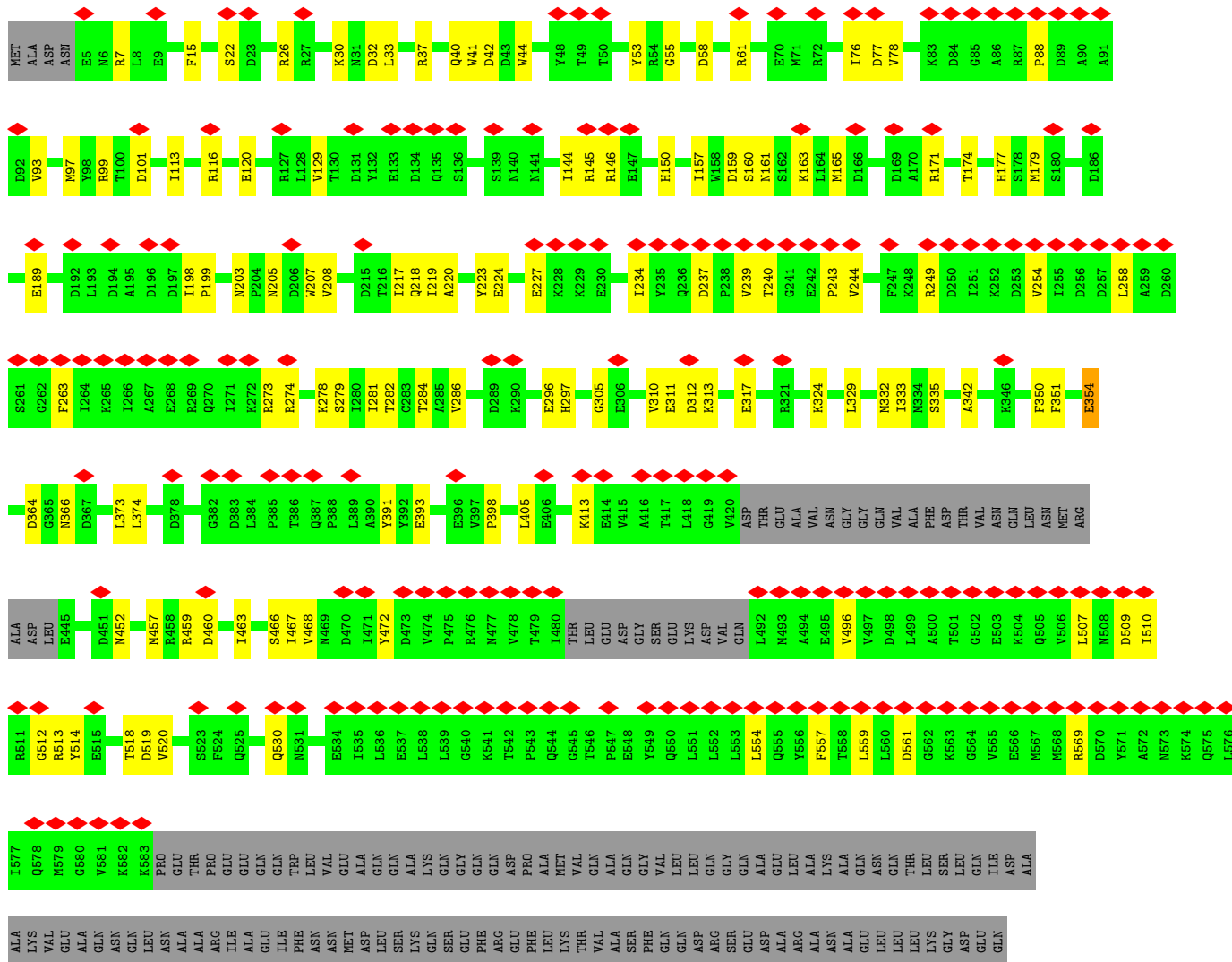


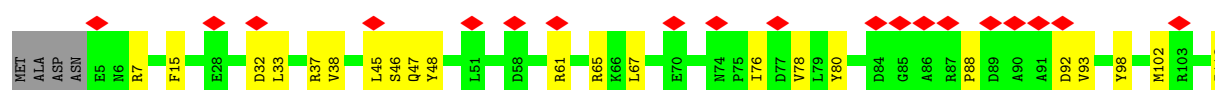
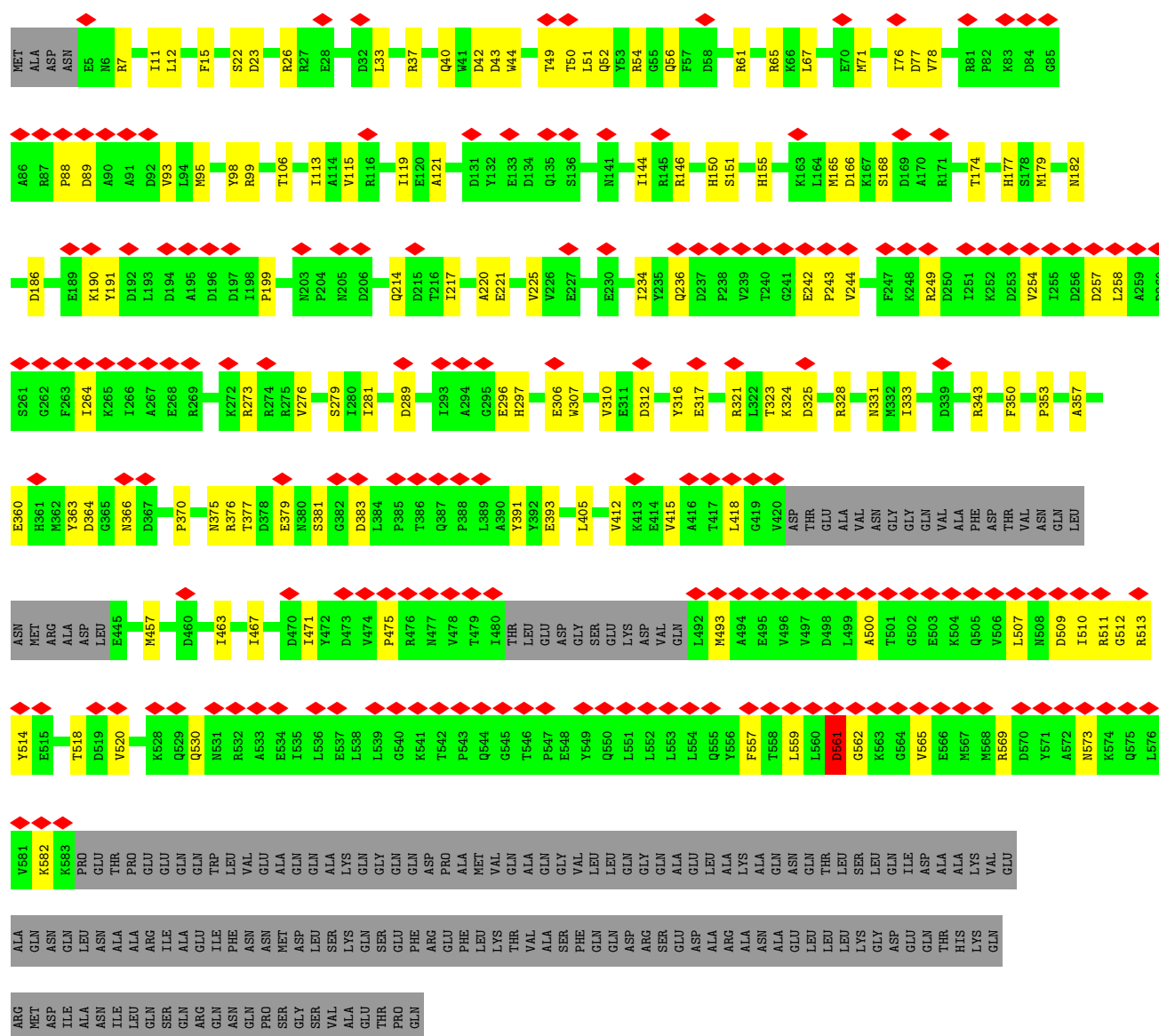
- Molecule 2: Tail spike protein

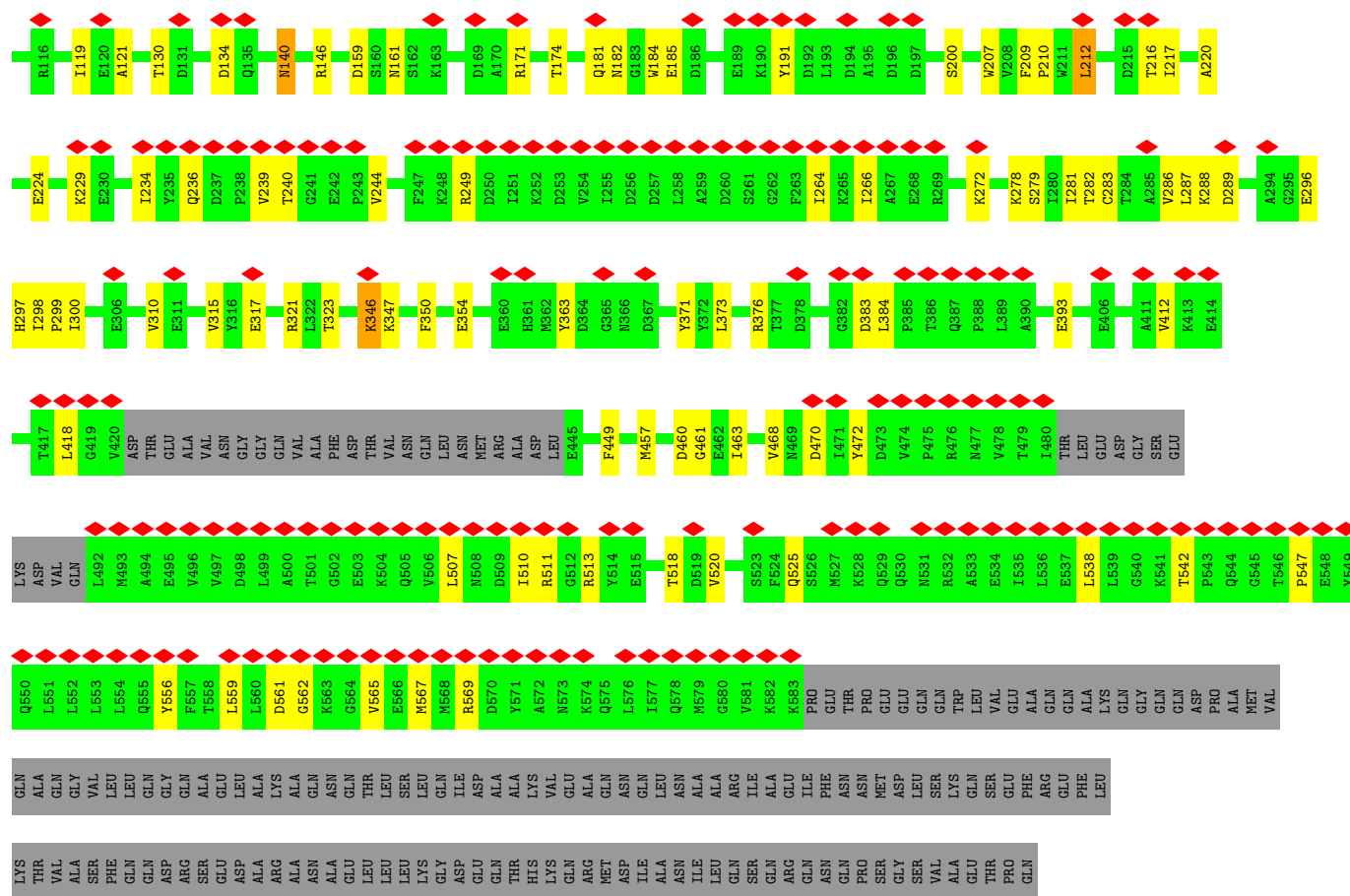




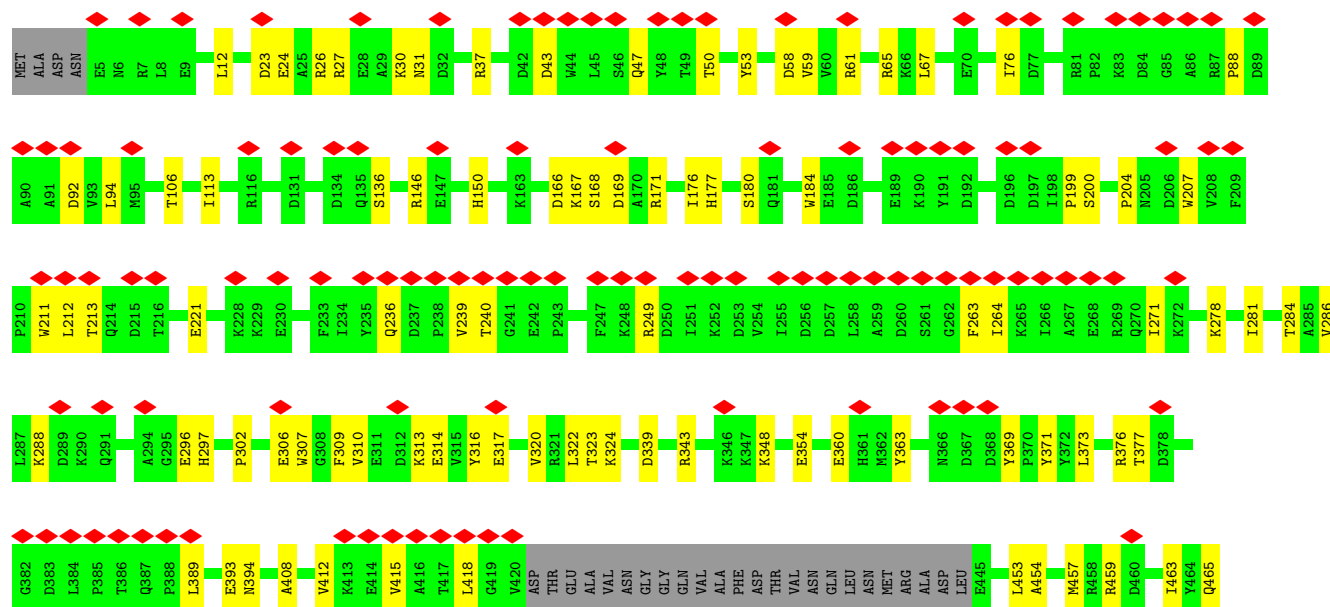
- Molecule 3: Portal protein







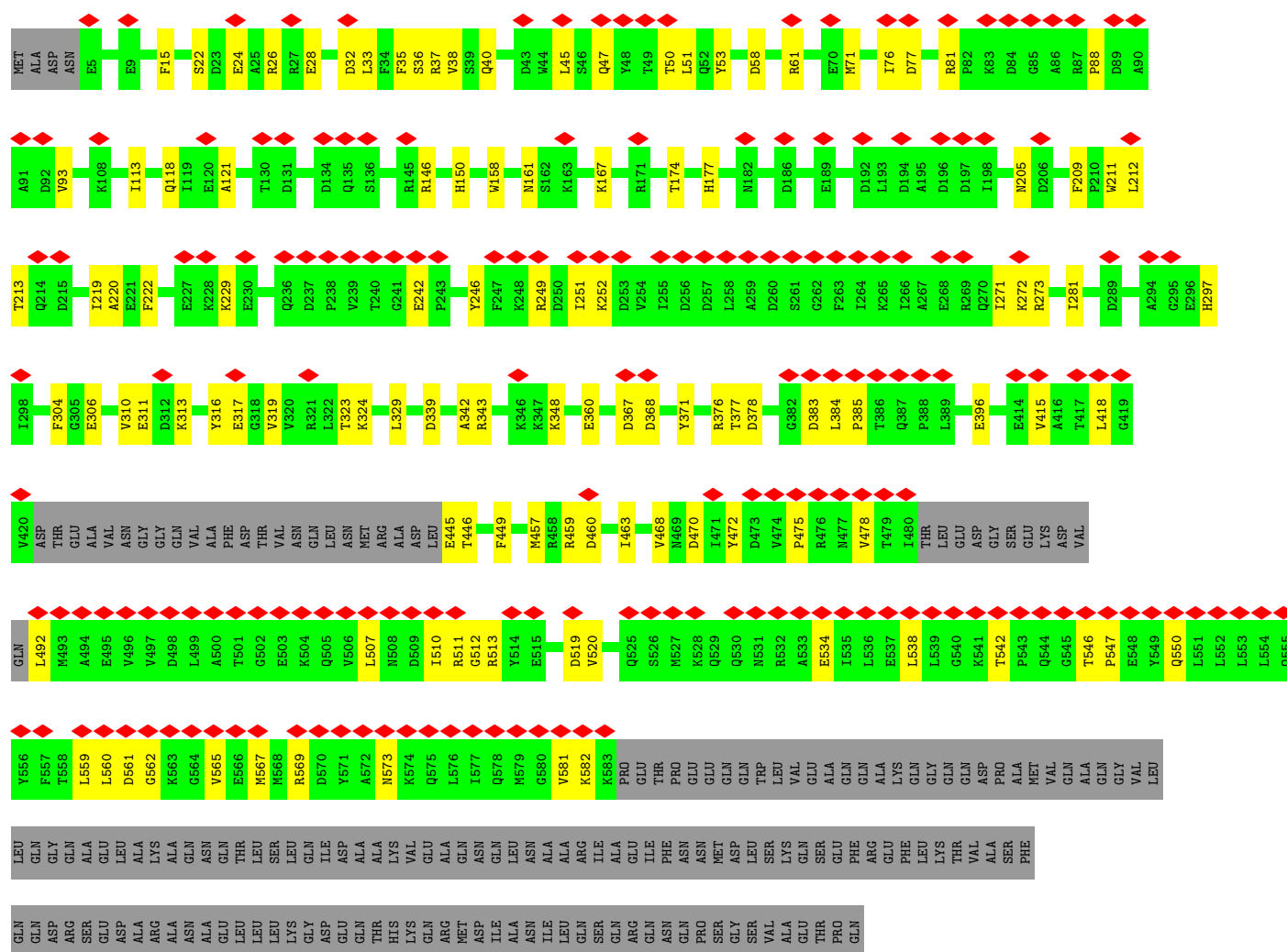
• Molecule 3: Portal protein



MET ASP
TLE ASP
ALA ASN
TLE LEU
LEU GLN
SER GLN
ARG GLN
GLN GLN
ASN GLN
PRO GLN
SER GLY
SER GLY
VAL VAL
ALA ALA
GLU GLU
THR THR
PRO PRO
GLN GLN

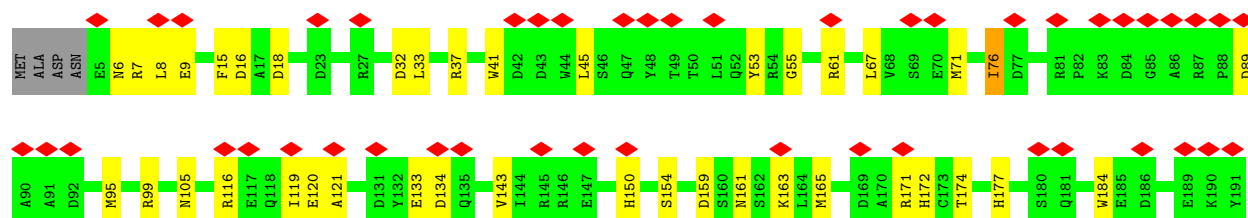
• Molecule 3: Portal protein

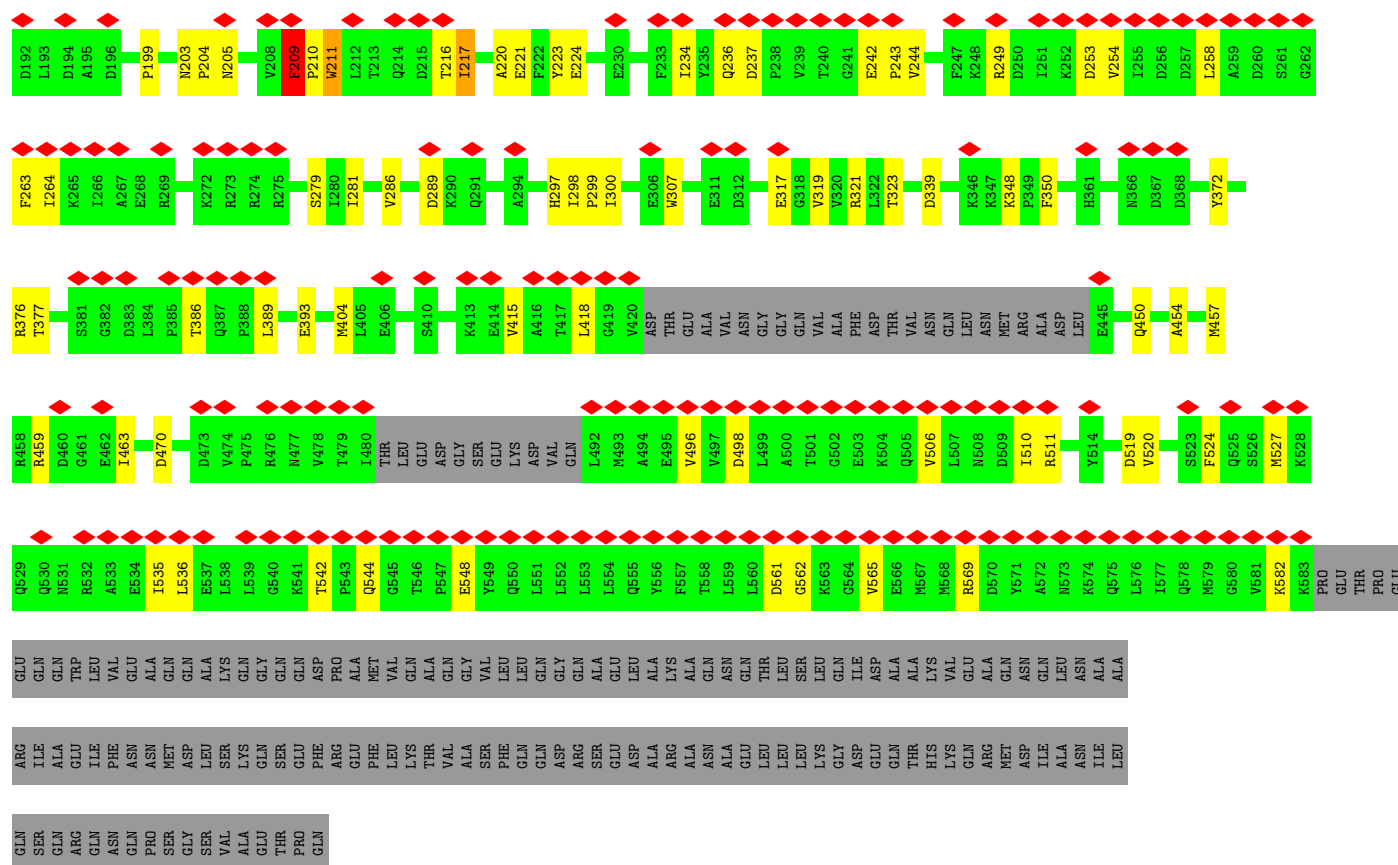
Chain f: 26% 59% 16% 25%



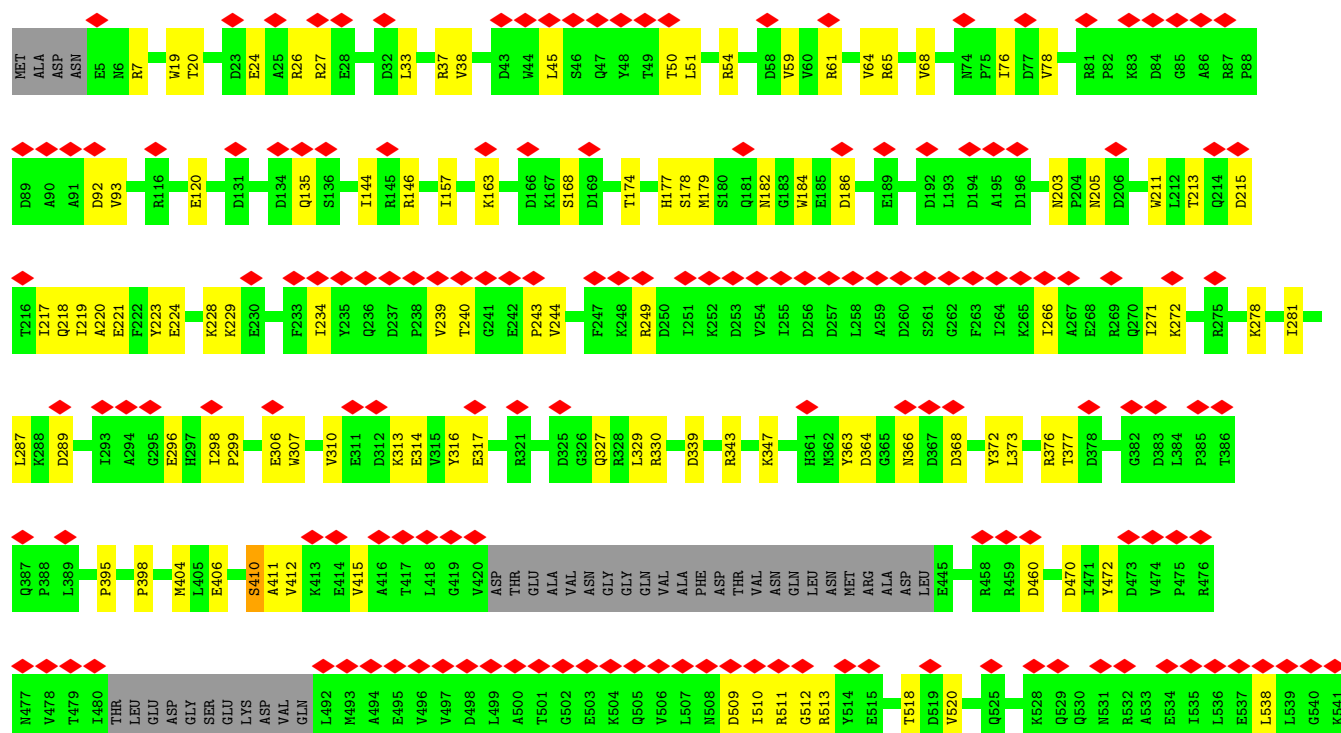
• Molecule 3: Portal protein

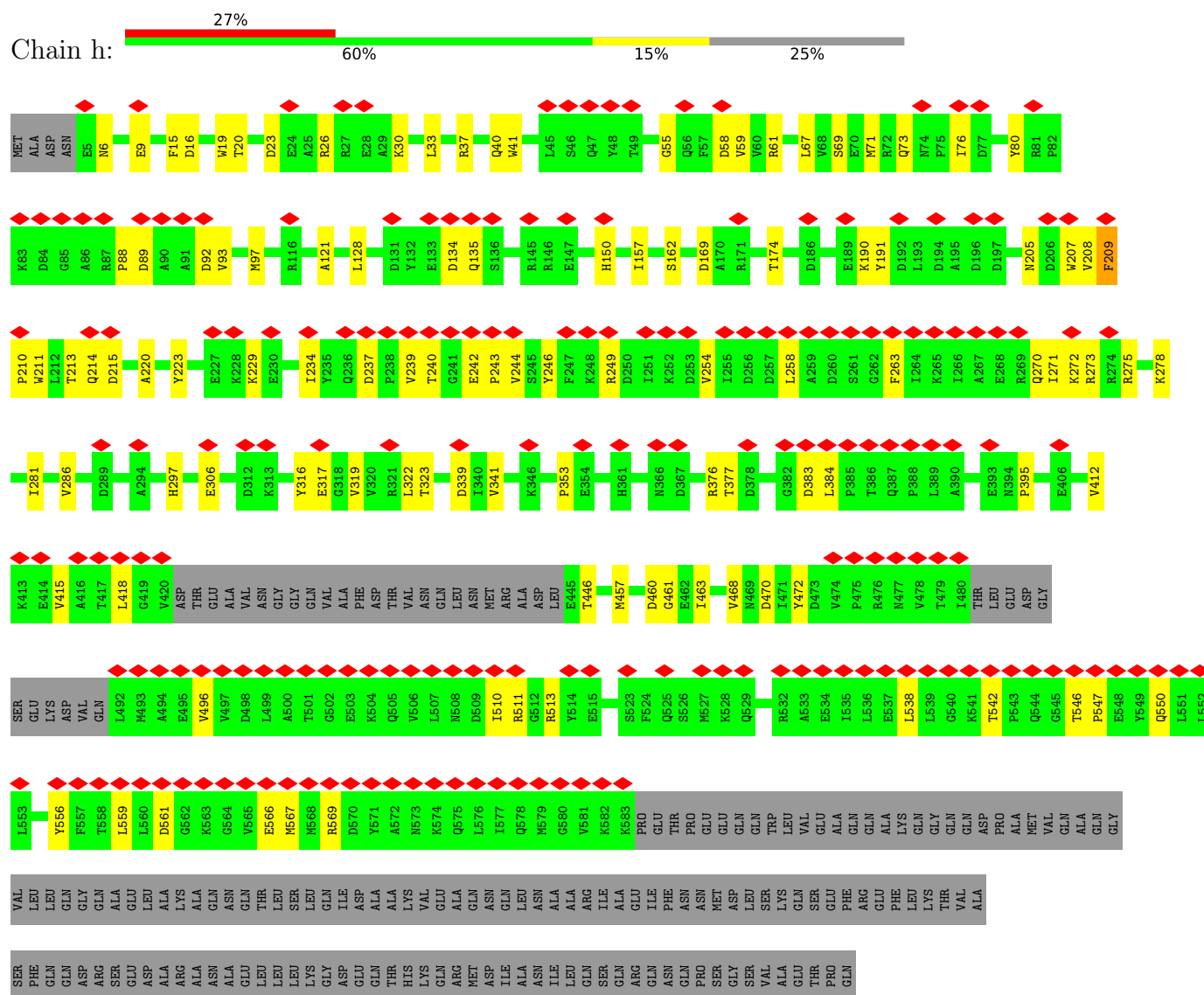
Chain k: 29% 59% 15% 25%



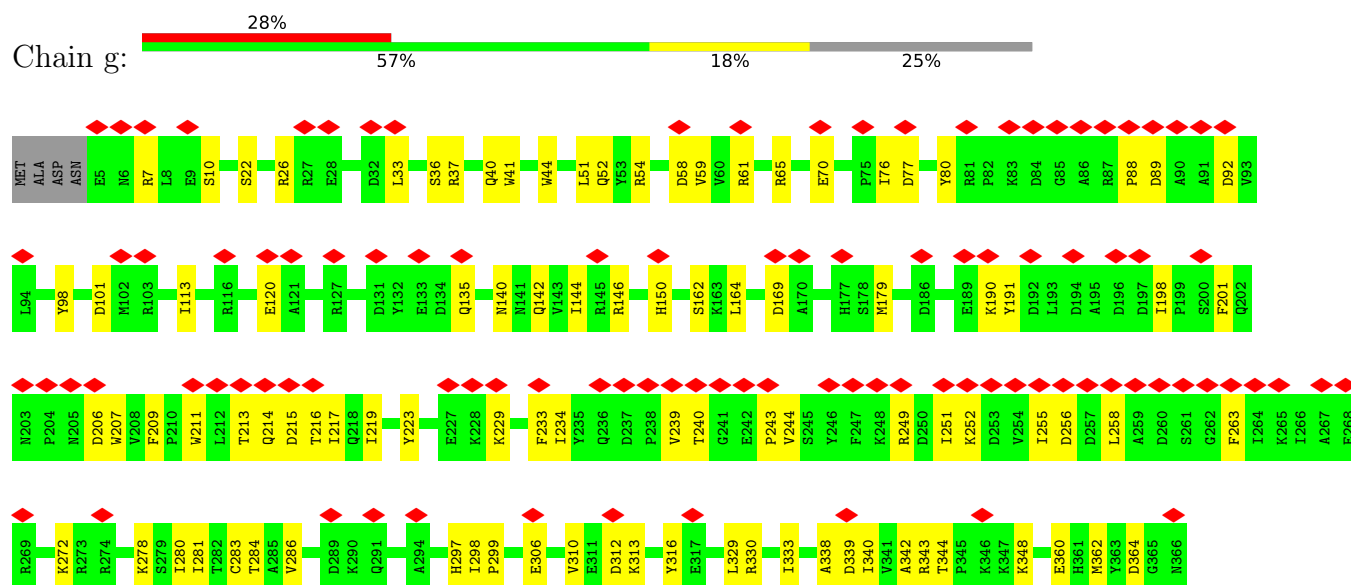


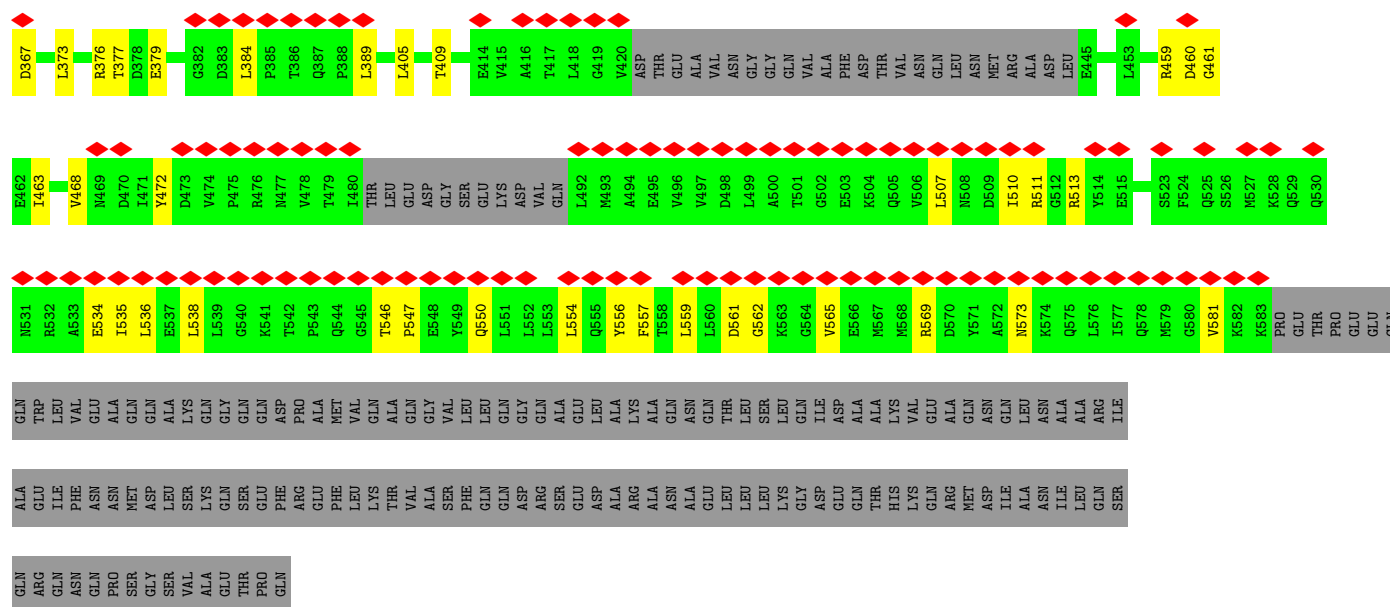
• Molecule 3: Portal protein



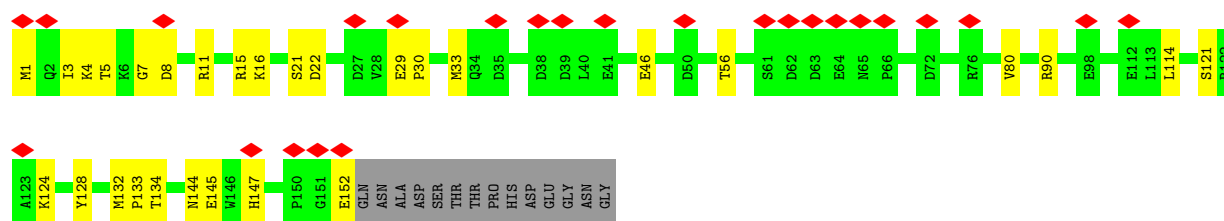
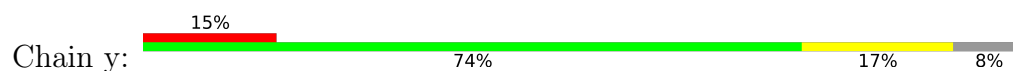


• Molecule 3: Portal protein

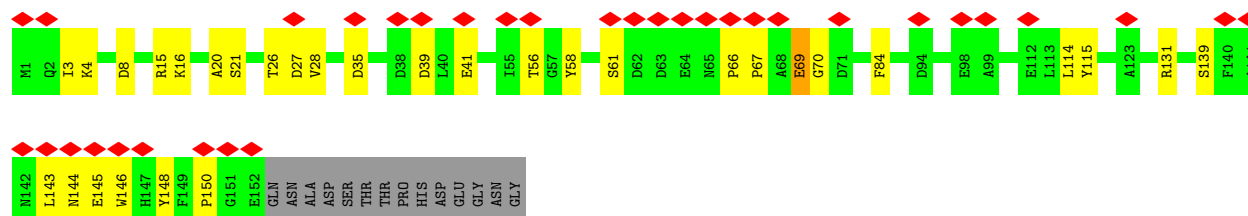
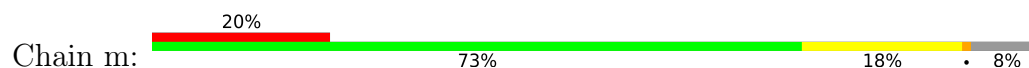




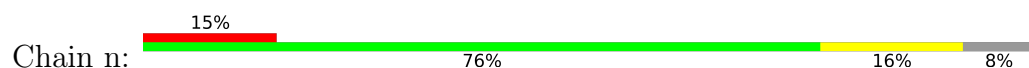
- Molecule 4: Peptidoglycan hydrolase gp4

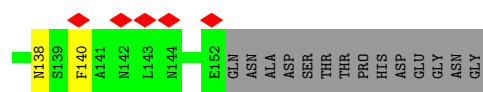


- Molecule 4: Peptidoglycan hydrolase gp4

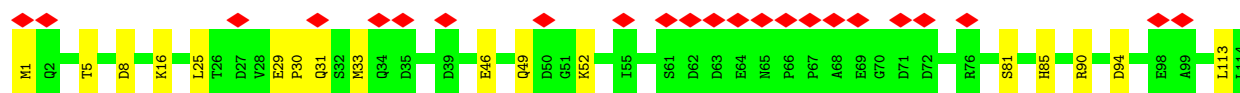
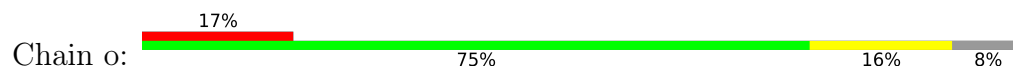


- Molecule 4: Peptidoglycan hydrolase gp4

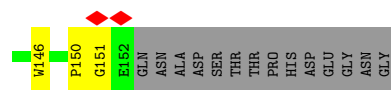
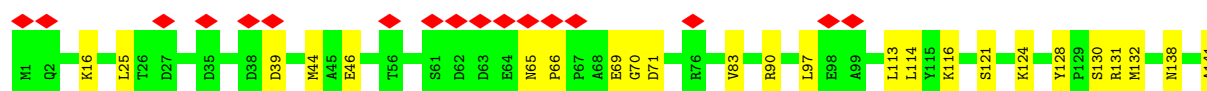
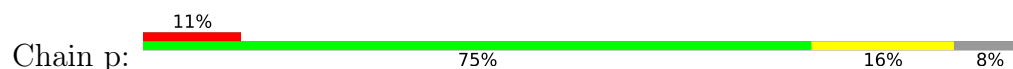




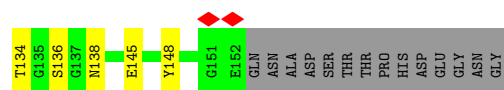
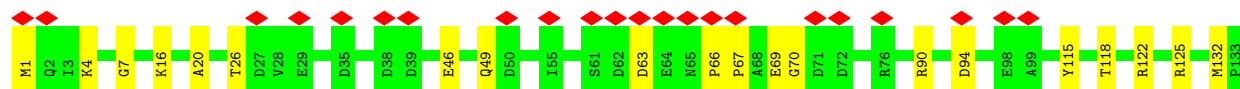
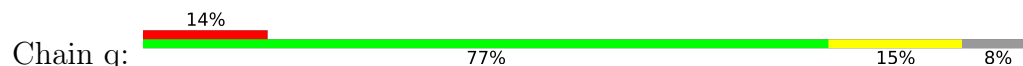
- Molecule 4: Peptidoglycan hydrolase gp4



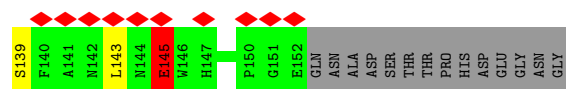
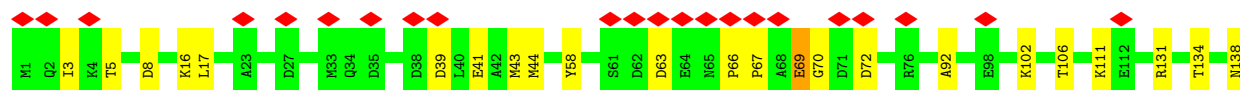
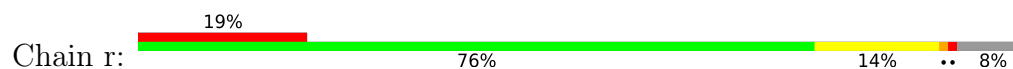
- Molecule 4: Peptidoglycan hydrolase gp4



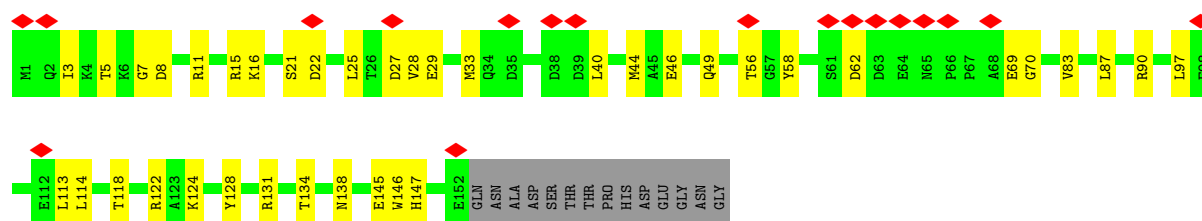
- Molecule 4: Peptidoglycan hydrolase gp4



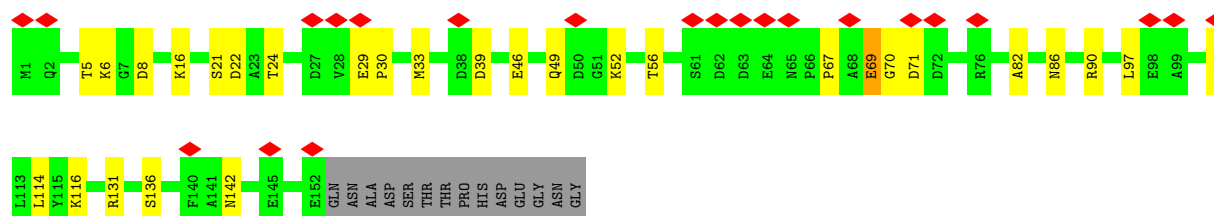
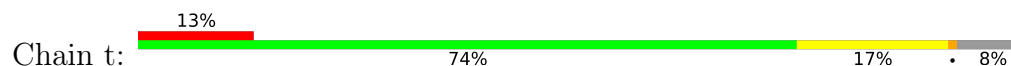
- Molecule 4: Peptidoglycan hydrolase gp4



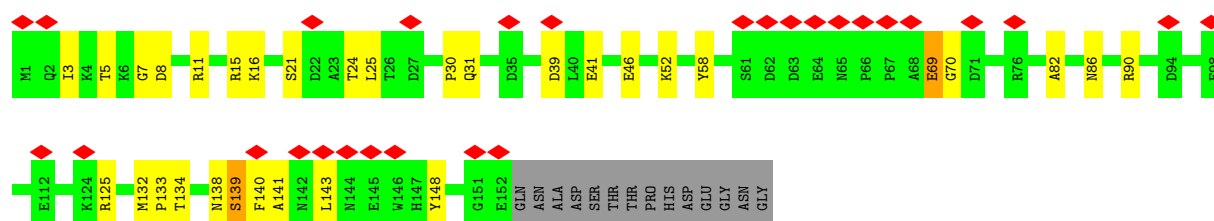
- Molecule 4: Peptidoglycan hydrolase gp4



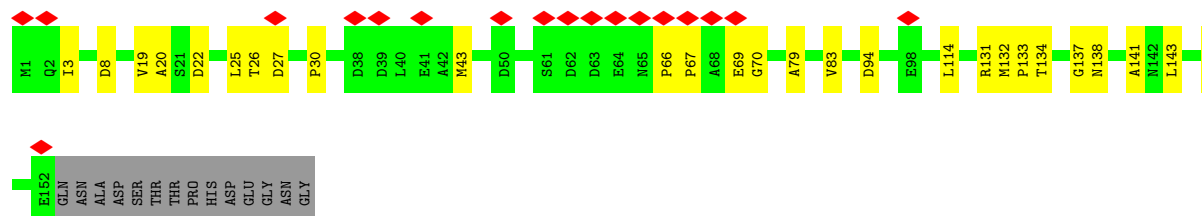
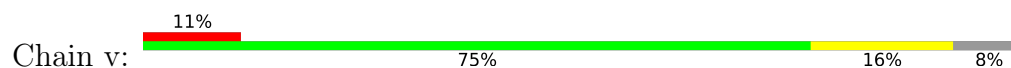
• Molecule 4: Peptidoglycan hydrolase gp4



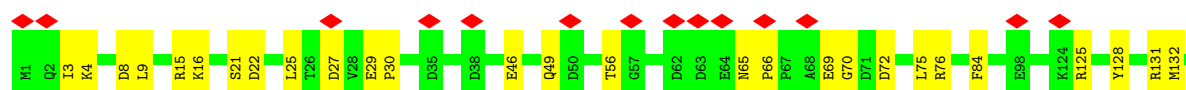
• Molecule 4: Peptidoglycan hydrolase gp4

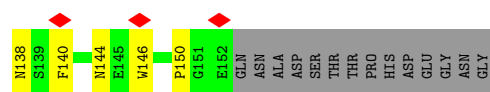


• Molecule 4: Peptidoglycan hydrolase gp4

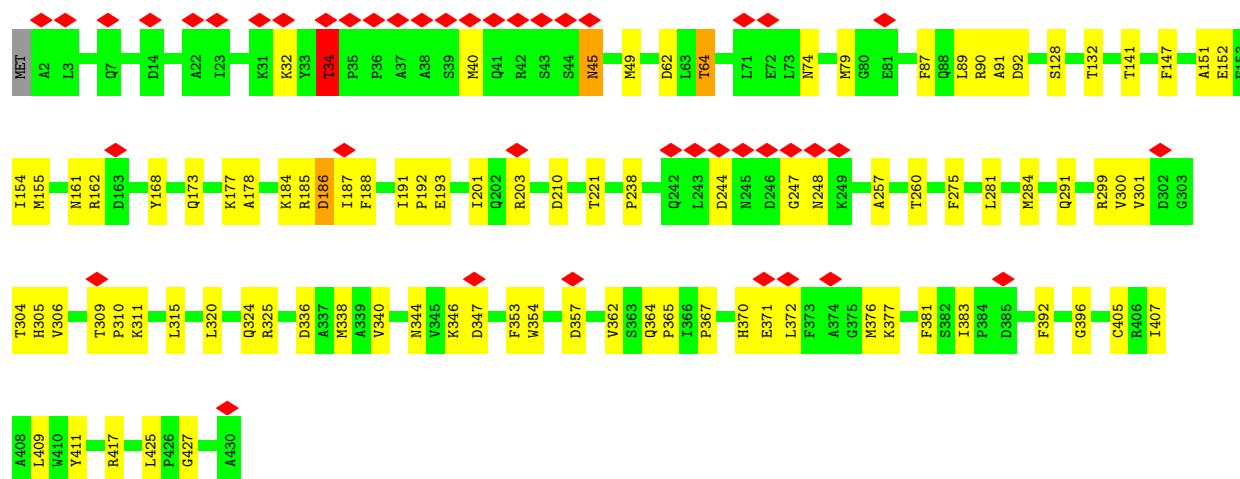
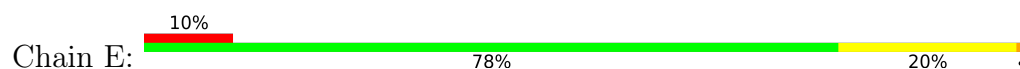


• Molecule 4: Peptidoglycan hydrolase gp4

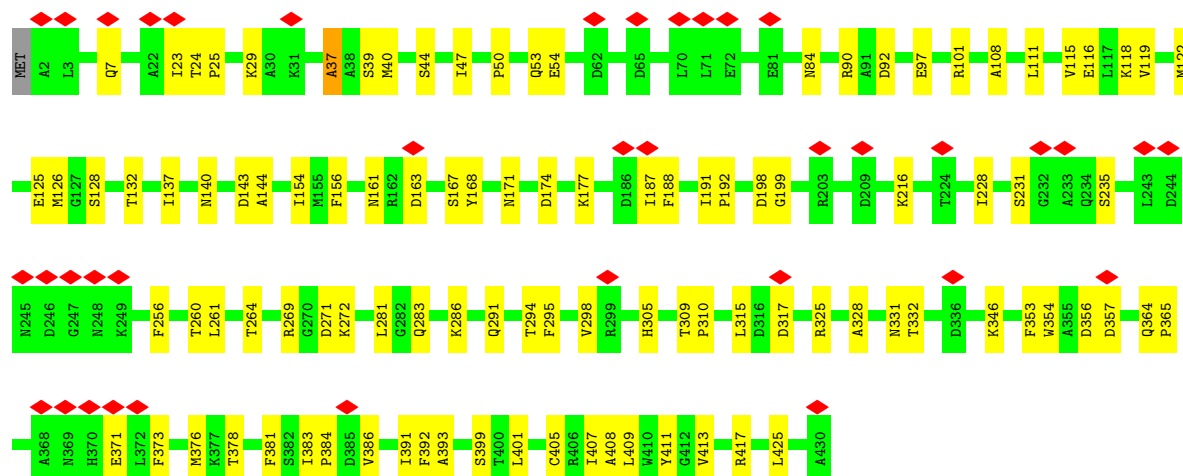
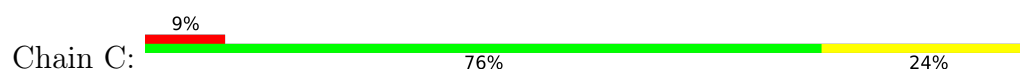




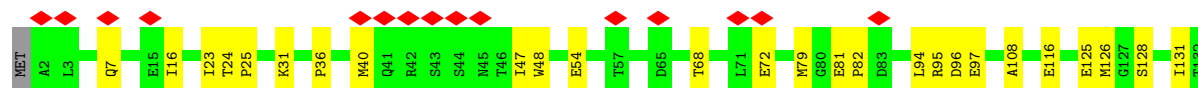
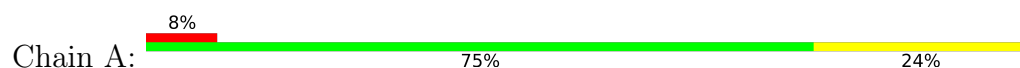
• Molecule 5: Major capsid protein

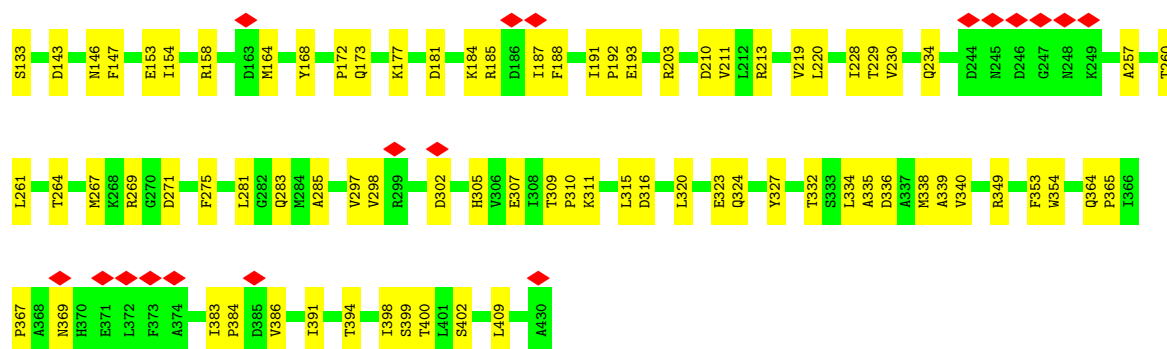


• Molecule 5: Major capsid protein

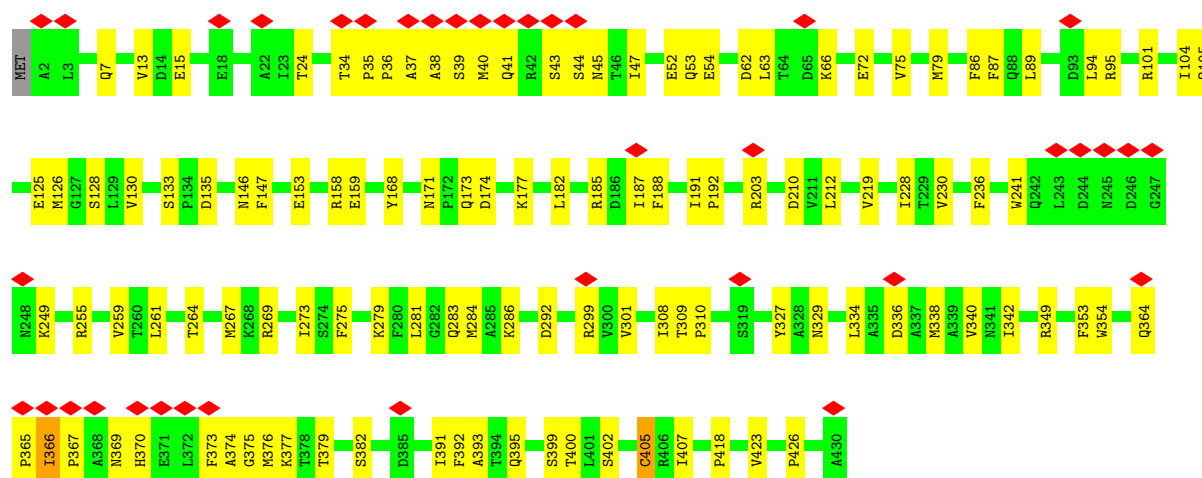
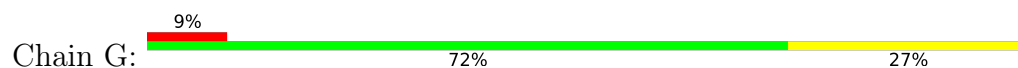


• Molecule 5: Major capsid protein

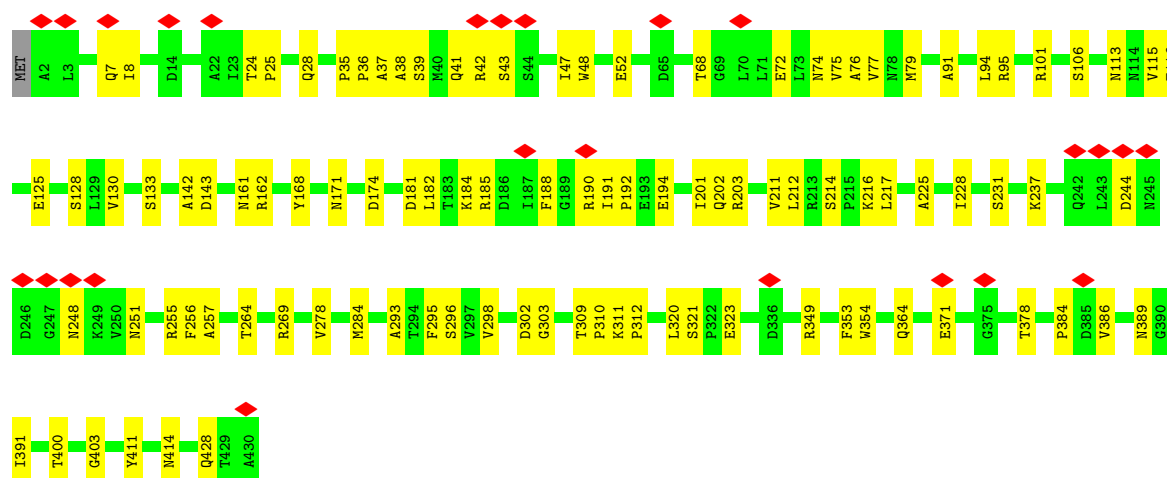
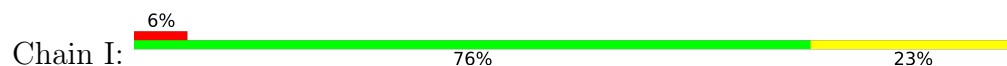




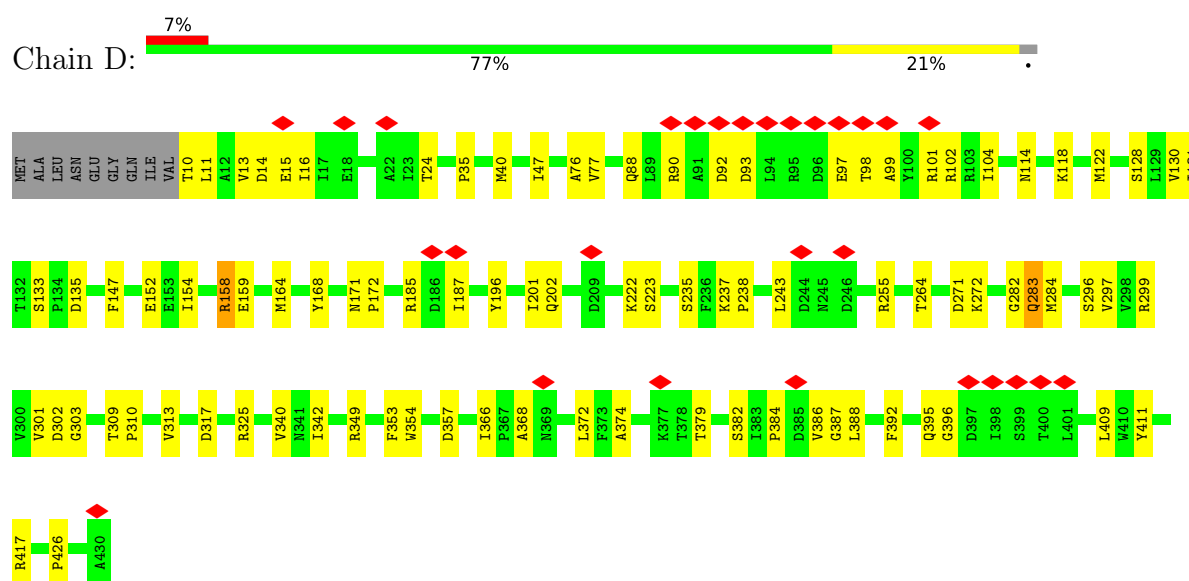
• Molecule 5: Major capsid protein



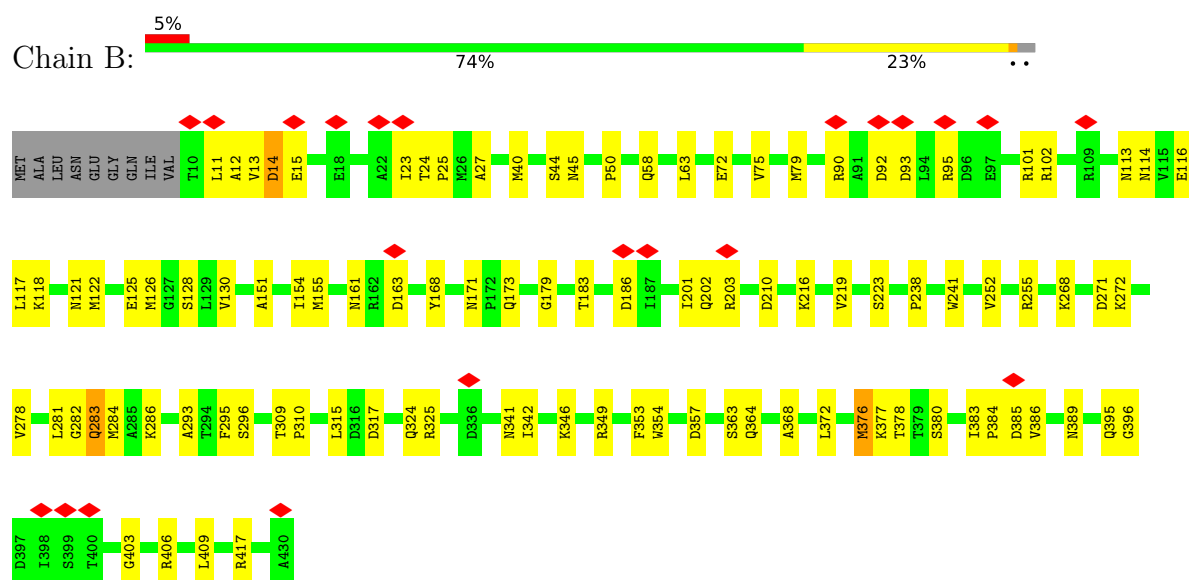
• Molecule 5: Major capsid protein



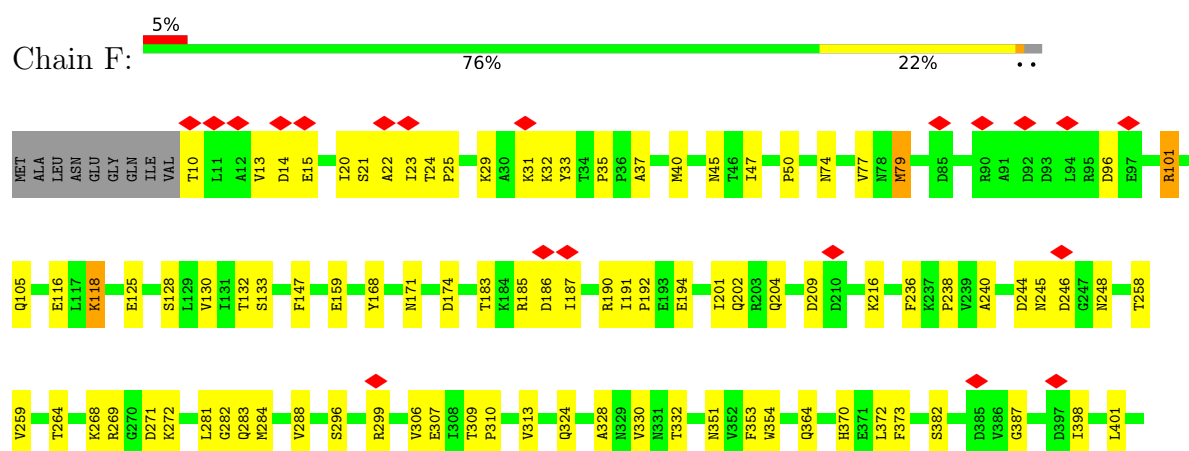
• Molecule 5: Major capsid protein



• Molecule 5: Major capsid protein

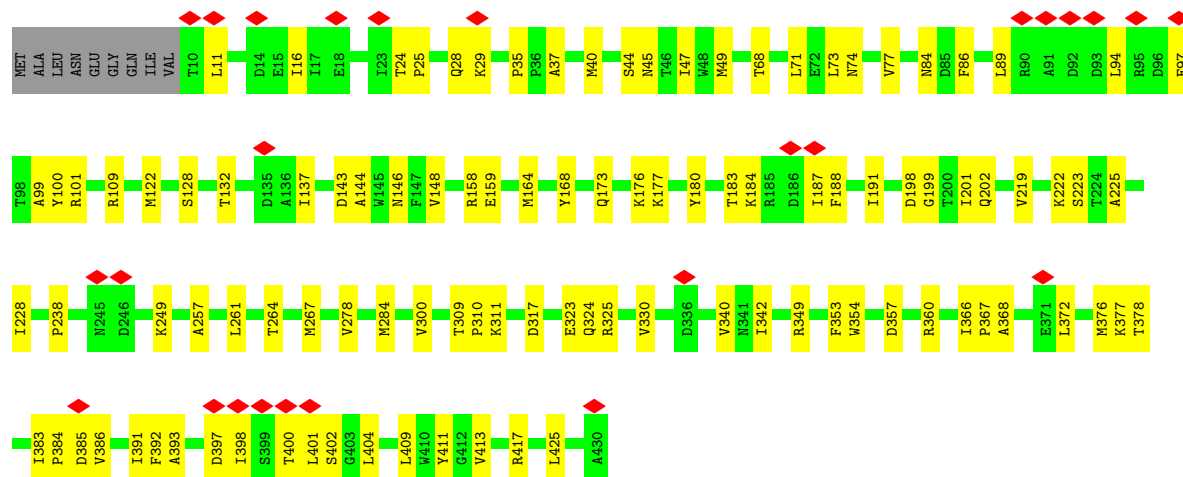
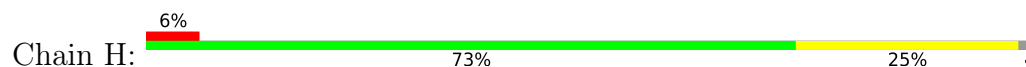


• Molecule 5: Major capsid protein

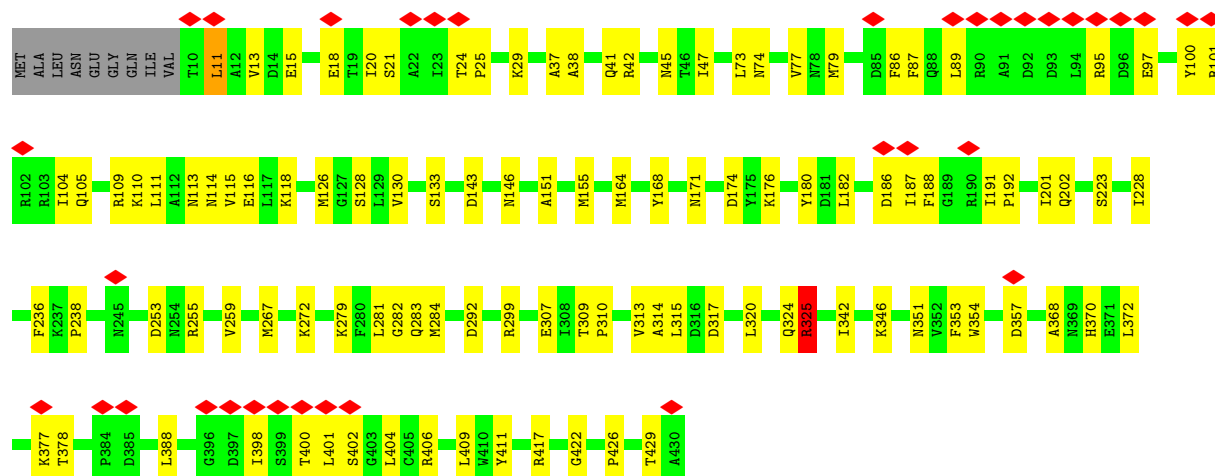
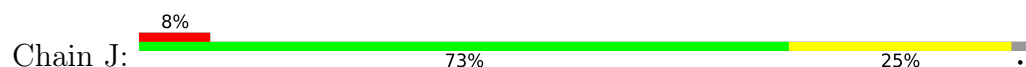




• Molecule 5: Major capsid protein



• Molecule 5: Major capsid protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17944	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.08	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	23.428	Depositor
Minimum map value	-16.095	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	512.9599, 512.9599, 512.9599	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.165818, 1.165818, 1.165818	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.25	0/3764	0.38	0/5097
1	2	0.26	0/3764	0.41	0/5097
1	3	0.24	0/3764	0.39	0/5097
1	4	0.25	0/3764	0.41	0/5097
1	5	0.24	0/3764	0.39	0/5097
1	6	0.25	0/3764	0.39	0/5097
2	10	0.24	0/953	0.40	0/1299
2	11	0.27	0/953	0.39	0/1299
2	12	0.24	0/953	0.36	0/1299
2	13	0.21	0/953	0.37	0/1299
2	14	0.29	0/953	0.46	0/1299
2	15	0.31	0/953	0.47	0/1299
2	16	0.22	0/953	0.38	0/1299
2	17	0.27	0/953	0.40	0/1299
2	18	0.24	0/953	0.36	0/1299
2	19	0.24	0/953	0.41	0/1299
2	20	0.29	0/953	0.39	0/1299
2	21	0.29	0/953	0.41	0/1299
2	22	0.21	0/953	0.34	0/1299
2	23	0.26	0/953	0.38	0/1299
2	24	0.26	0/953	0.37	0/1299
2	7	0.22	0/953	0.41	0/1299
2	8	0.31	0/953	0.53	0/1299
2	9	0.32	0/953	0.47	0/1299
3	a	0.25	0/4512	0.38	0/6117
3	b	0.26	0/4512	0.36	0/6117
3	c	0.26	0/4512	0.44	3/6117 (0.0%)
3	d	0.26	0/4512	0.38	0/6117
3	e	0.24	0/4512	0.35	0/6117
3	f	0.24	0/4512	0.34	0/6117
3	g	0.25	0/4512	0.36	1/6117 (0.0%)
3	h	0.25	0/4512	0.36	0/6117
3	i	0.25	0/4512	0.35	0/6117
3	j	0.25	0/4512	0.37	0/6117

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	k	0.24	0/4512	0.35	0/6117
3	l	0.25	0/4512	0.36	0/6117
4	m	0.26	0/1191	0.39	0/1614
4	n	0.27	0/1191	0.35	0/1614
4	o	0.26	0/1191	0.37	0/1614
4	p	0.29	0/1191	0.39	0/1614
4	q	0.26	0/1191	0.38	0/1614
4	r	0.26	0/1191	0.39	0/1614
4	s	0.28	0/1191	0.38	0/1614
4	t	0.27	0/1191	0.38	0/1614
4	u	0.28	0/1191	0.42	0/1614
4	v	0.27	0/1191	0.37	0/1614
4	x	0.27	0/1191	0.38	0/1614
4	y	0.25	0/1191	0.36	0/1614
5	A	0.29	0/3335	0.39	0/4535
5	B	0.31	0/3277	0.43	0/4456
5	C	0.28	0/3335	0.41	0/4535
5	D	0.29	0/3277	0.41	0/4456
5	E	0.29	0/3335	0.45	2/4535 (0.0%)
5	F	0.32	0/3277	0.42	0/4456
5	G	0.31	0/3335	0.40	0/4535
5	H	0.31	0/3277	0.41	0/4456
5	I	0.29	0/3335	0.41	0/4535
5	J	0.31	0/3277	0.46	0/4456
All	All	0.27	0/141234	0.39	6/191691 (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	1	0	1
1	6	0	1
3	a	0	1
3	e	0	1
3	f	0	1
3	k	0	2
3	l	0	2
4	r	0	1
4	u	0	1
5	C	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
5	D	0	1
5	G	0	1
5	H	0	1
5	J	0	1
All	All	0	16

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	561	ASP	CB-CA-C	-16.17	89.51	111.82
3	c	561	ASP	N-CA-C	7.74	123.40	107.37
5	E	34	THR	CB-CA-C	-6.12	99.72	109.82
5	E	34	THR	N-CA-C	5.73	119.81	109.44
3	c	561	ASP	N-CA-CB	-5.36	101.03	111.11

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	437	ARG	Sidechain
1	6	408	ARG	Sidechain
3	a	376	ARG	Sidechain
3	e	37	ARG	Sidechain
3	l	61	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3683	0	3590	95	0
1	2	3683	0	3590	104	0
1	3	3683	0	3590	80	0
1	4	3683	0	3590	88	0
1	5	3683	0	3590	101	0
1	6	3683	0	3590	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	10	934	0	925	33	0
2	11	934	0	925	22	0
2	12	934	0	925	22	0
2	13	934	0	925	25	0
2	14	934	0	925	26	0
2	15	934	0	925	27	0
2	16	934	0	925	37	0
2	17	934	0	925	26	0
2	18	934	0	925	31	0
2	19	934	0	925	34	0
2	20	934	0	925	21	0
2	21	934	0	925	21	0
2	22	934	0	925	21	0
2	23	934	0	925	26	0
2	24	934	0	925	19	0
2	7	934	0	925	33	0
2	8	934	0	925	44	0
2	9	934	0	925	28	0
3	a	4417	0	4295	103	0
3	b	4417	0	4295	101	0
3	c	4417	0	4295	105	0
3	d	4417	0	4295	89	0
3	e	4417	0	4295	101	0
3	f	4417	0	4295	88	0
3	g	4417	0	4295	104	0
3	h	4417	0	4295	89	0
3	i	4417	0	4295	93	0
3	j	4417	0	4295	95	0
3	k	4417	0	4295	93	0
3	l	4417	0	4295	91	0
4	m	1166	0	1133	28	0
4	n	1166	0	1133	22	0
4	o	1166	0	1133	24	0
4	p	1166	0	1133	23	0
4	q	1166	0	1133	20	0
4	r	1166	0	1133	22	0
4	s	1166	0	1133	30	0
4	t	1166	0	1133	21	0
4	u	1166	0	1133	24	0
4	v	1166	0	1133	21	0
4	x	1166	0	1133	26	0
4	y	1166	0	1133	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	3277	0	3247	76	0
5	B	3219	0	3188	72	0
5	C	3277	0	3247	67	0
5	D	3219	0	3188	65	0
5	E	3277	0	3247	58	0
5	F	3219	0	3188	74	0
5	G	3277	0	3247	100	0
5	H	3219	0	3188	79	0
5	I	3277	0	3247	78	0
5	J	3219	0	3188	80	0
All	All	138386	0	135501	2716	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 10.

The worst 5 of 2716 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:367:PRO:HD2	5:G:391:ILE:HD12	1.26	1.08
5:G:366:ILE:HB	5:G:391:ILE:HD11	1.15	1.08
5:G:367:PRO:HD2	5:G:391:ILE:CD1	2.01	0.90
3:I:44:TRP:HB2	5:J:97:GLU:HG2	1.53	0.88
5:A:94:LEU:HD11	5:J:372:LEU:HD23	1.58	0.86

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	1	469/472 (99%)	427 (91%)	42 (9%)	0	100	100
1	2	469/472 (99%)	435 (93%)	34 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	469/472 (99%)	428 (91%)	41 (9%)	0	100	100
1	4	469/472 (99%)	425 (91%)	44 (9%)	0	100	100
1	5	469/472 (99%)	425 (91%)	44 (9%)	0	100	100
1	6	469/472 (99%)	437 (93%)	32 (7%)	0	100	100
2	10	118/667 (18%)	108 (92%)	10 (8%)	0	100	100
2	11	118/667 (18%)	112 (95%)	6 (5%)	0	100	100
2	12	118/667 (18%)	114 (97%)	4 (3%)	0	100	100
2	13	118/667 (18%)	113 (96%)	5 (4%)	0	100	100
2	14	118/667 (18%)	112 (95%)	6 (5%)	0	100	100
2	15	118/667 (18%)	111 (94%)	7 (6%)	0	100	100
2	16	118/667 (18%)	111 (94%)	7 (6%)	0	100	100
2	17	118/667 (18%)	110 (93%)	8 (7%)	0	100	100
2	18	118/667 (18%)	108 (92%)	10 (8%)	0	100	100
2	19	118/667 (18%)	112 (95%)	6 (5%)	0	100	100
2	20	118/667 (18%)	111 (94%)	7 (6%)	0	100	100
2	21	118/667 (18%)	111 (94%)	7 (6%)	0	100	100
2	22	118/667 (18%)	110 (93%)	8 (7%)	0	100	100
2	23	118/667 (18%)	110 (93%)	8 (7%)	0	100	100
2	24	118/667 (18%)	114 (97%)	4 (3%)	0	100	100
2	7	118/667 (18%)	111 (94%)	7 (6%)	0	100	100
2	8	118/667 (18%)	110 (93%)	8 (7%)	0	100	100
2	9	118/667 (18%)	113 (96%)	5 (4%)	0	100	100
3	a	538/725 (74%)	511 (95%)	27 (5%)	0	100	100
3	b	538/725 (74%)	512 (95%)	26 (5%)	0	100	100
3	c	538/725 (74%)	508 (94%)	28 (5%)	2 (0%)	30	61
3	d	538/725 (74%)	508 (94%)	30 (6%)	0	100	100
3	e	538/725 (74%)	511 (95%)	26 (5%)	1 (0%)	43	73
3	f	538/725 (74%)	507 (94%)	31 (6%)	0	100	100
3	g	538/725 (74%)	505 (94%)	33 (6%)	0	100	100
3	h	538/725 (74%)	510 (95%)	27 (5%)	1 (0%)	43	73
3	i	538/725 (74%)	513 (95%)	25 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	j	538/725 (74%)	513 (95%)	25 (5%)	0	100	100
3	k	538/725 (74%)	507 (94%)	29 (5%)	2 (0%)	30	61
3	l	538/725 (74%)	508 (94%)	30 (6%)	0	100	100
4	m	150/166 (90%)	143 (95%)	7 (5%)	0	100	100
4	n	150/166 (90%)	147 (98%)	3 (2%)	0	100	100
4	o	150/166 (90%)	141 (94%)	9 (6%)	0	100	100
4	p	150/166 (90%)	147 (98%)	3 (2%)	0	100	100
4	q	150/166 (90%)	142 (95%)	8 (5%)	0	100	100
4	r	150/166 (90%)	142 (95%)	7 (5%)	1 (1%)	18	49
4	s	150/166 (90%)	147 (98%)	3 (2%)	0	100	100
4	t	150/166 (90%)	149 (99%)	1 (1%)	0	100	100
4	u	150/166 (90%)	141 (94%)	8 (5%)	1 (1%)	18	49
4	v	150/166 (90%)	145 (97%)	5 (3%)	0	100	100
4	x	150/166 (90%)	144 (96%)	5 (3%)	1 (1%)	18	49
4	y	150/166 (90%)	143 (95%)	7 (5%)	0	100	100
5	A	427/430 (99%)	392 (92%)	35 (8%)	0	100	100
5	B	419/430 (97%)	396 (94%)	22 (5%)	1 (0%)	43	73
5	C	427/430 (99%)	400 (94%)	25 (6%)	2 (0%)	24	57
5	D	419/430 (97%)	405 (97%)	13 (3%)	1 (0%)	43	73
5	E	427/430 (99%)	396 (93%)	31 (7%)	0	100	100
5	F	419/430 (97%)	397 (95%)	21 (5%)	1 (0%)	43	73
5	G	427/430 (99%)	387 (91%)	39 (9%)	1 (0%)	43	73
5	H	419/430 (97%)	398 (95%)	20 (5%)	1 (0%)	43	73
5	I	427/430 (99%)	396 (93%)	31 (7%)	0	100	100
5	J	419/430 (97%)	397 (95%)	21 (5%)	1 (0%)	43	73
All	All	17424/29830 (58%)	16386 (94%)	1021 (6%)	17 (0%)	49	78

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	r	145	GLU
3	k	209	PHE
3	h	209	PHE

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Mol	Chain	Res	Type
5	C	37	ALA
5	F	283	GLN

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	1	394/395 (100%)	394 (100%)	0	100	100
1	2	394/395 (100%)	391 (99%)	3 (1%)	73	81
1	3	394/395 (100%)	392 (100%)	2 (0%)	81	85
1	4	394/395 (100%)	389 (99%)	5 (1%)	61	77
1	5	394/395 (100%)	391 (99%)	3 (1%)	73	81
1	6	394/395 (100%)	389 (99%)	5 (1%)	61	77
2	10	103/548 (19%)	102 (99%)	1 (1%)	68	79
2	11	103/548 (19%)	102 (99%)	1 (1%)	68	79
2	12	103/548 (19%)	103 (100%)	0	100	100
2	13	103/548 (19%)	103 (100%)	0	100	100
2	14	103/548 (19%)	101 (98%)	2 (2%)	50	73
2	15	103/548 (19%)	102 (99%)	1 (1%)	68	79
2	16	103/548 (19%)	103 (100%)	0	100	100
2	17	103/548 (19%)	102 (99%)	1 (1%)	68	79
2	18	103/548 (19%)	102 (99%)	1 (1%)	68	79
2	19	103/548 (19%)	103 (100%)	0	100	100
2	20	103/548 (19%)	102 (99%)	1 (1%)	68	79
2	21	103/548 (19%)	101 (98%)	2 (2%)	50	73
2	22	103/548 (19%)	103 (100%)	0	100	100
2	23	103/548 (19%)	103 (100%)	0	100	100
2	24	103/548 (19%)	103 (100%)	0	100	100
2	7	103/548 (19%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	8	103/548 (19%)	100 (97%)	3 (3%)	37	66
2	9	103/548 (19%)	102 (99%)	1 (1%)	68	79
3	a	480/630 (76%)	477 (99%)	3 (1%)	78	83
3	b	480/630 (76%)	475 (99%)	5 (1%)	68	79
3	c	480/630 (76%)	477 (99%)	3 (1%)	78	83
3	d	480/630 (76%)	475 (99%)	5 (1%)	68	79
3	e	480/630 (76%)	479 (100%)	1 (0%)	87	89
3	f	480/630 (76%)	478 (100%)	2 (0%)	84	86
3	g	480/630 (76%)	475 (99%)	5 (1%)	68	79
3	h	480/630 (76%)	478 (100%)	2 (0%)	84	86
3	i	480/630 (76%)	475 (99%)	5 (1%)	68	79
3	j	480/630 (76%)	476 (99%)	4 (1%)	73	81
3	k	480/630 (76%)	477 (99%)	3 (1%)	78	83
3	l	480/630 (76%)	478 (100%)	2 (0%)	84	86
4	m	120/131 (92%)	119 (99%)	1 (1%)	73	81
4	n	120/131 (92%)	119 (99%)	1 (1%)	73	81
4	o	120/131 (92%)	120 (100%)	0	100	100
4	p	120/131 (92%)	120 (100%)	0	100	100
4	q	120/131 (92%)	120 (100%)	0	100	100
4	r	120/131 (92%)	119 (99%)	1 (1%)	73	81
4	s	120/131 (92%)	120 (100%)	0	100	100
4	t	120/131 (92%)	119 (99%)	1 (1%)	73	81
4	u	120/131 (92%)	119 (99%)	1 (1%)	73	81
4	v	120/131 (92%)	119 (99%)	1 (1%)	73	81
4	x	120/131 (92%)	119 (99%)	1 (1%)	73	81
4	y	120/131 (92%)	120 (100%)	0	100	100
5	A	351/352 (100%)	350 (100%)	1 (0%)	86	87
5	B	345/352 (98%)	341 (99%)	4 (1%)	63	78
5	C	351/352 (100%)	350 (100%)	1 (0%)	86	87
5	D	345/352 (98%)	338 (98%)	7 (2%)	48	72
5	E	351/352 (100%)	343 (98%)	8 (2%)	44	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	345/352 (98%)	338 (98%)	7 (2%)	48	72
5	G	351/352 (100%)	348 (99%)	3 (1%)	70	80
5	H	345/352 (98%)	343 (99%)	2 (1%)	78	83
5	I	351/352 (100%)	349 (99%)	2 (1%)	78	83
5	J	345/352 (98%)	342 (99%)	3 (1%)	70	80
All	All	14898/24886 (60%)	14781 (99%)	117 (1%)	70	81

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	k	498	ASP
5	F	101	ARG
3	h	550	GLN
5	F	79	MET
5	D	283	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 178 such sidechains are listed below:

Mol	Chain	Res	Type
3	g	74	ASN
5	G	248	ASN
3	g	575	GLN
5	C	41	GLN
5	I	389	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

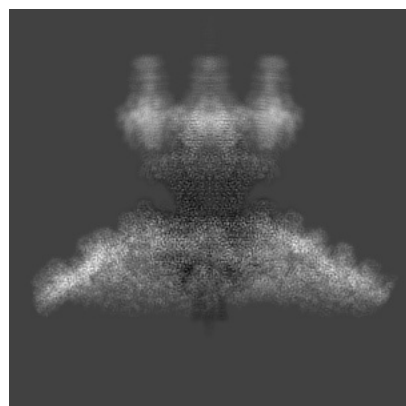
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41792. These allow visual inspection of the internal detail of the map and identification of artifacts.

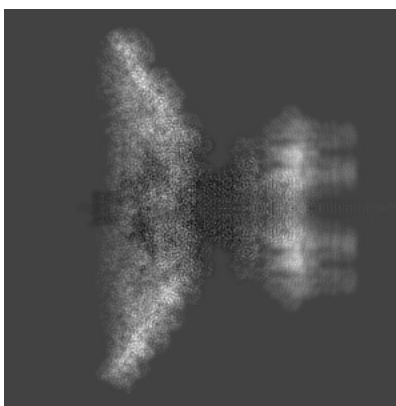
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

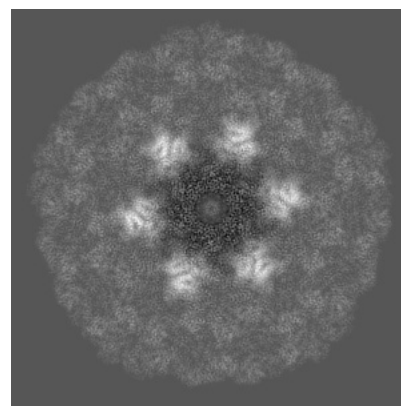
6.1.1 Primary map



X

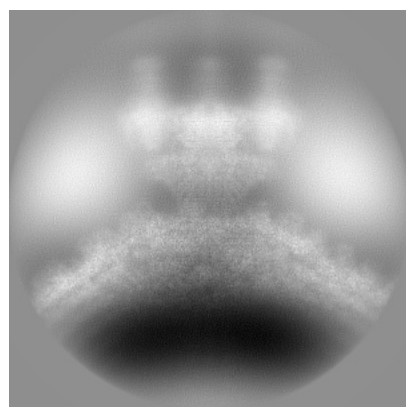


Y

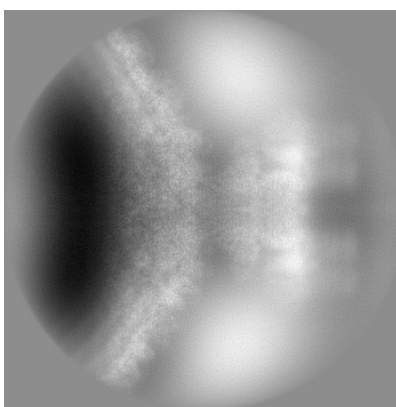


Z

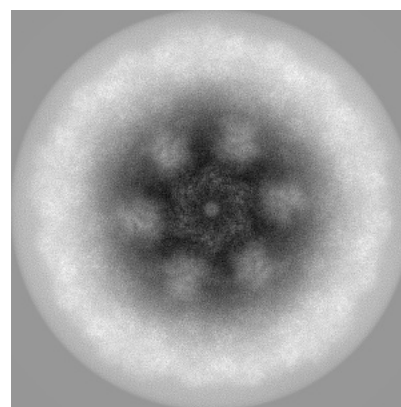
6.1.2 Raw map



X



Y

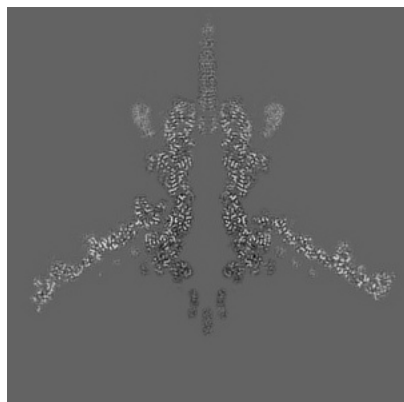


Z

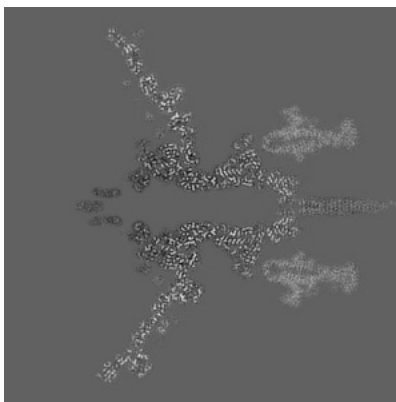
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

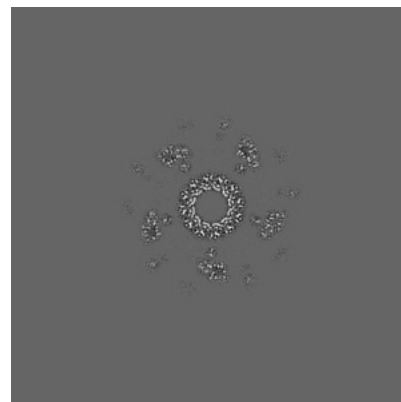
6.2.1 Primary map



X Index: 220

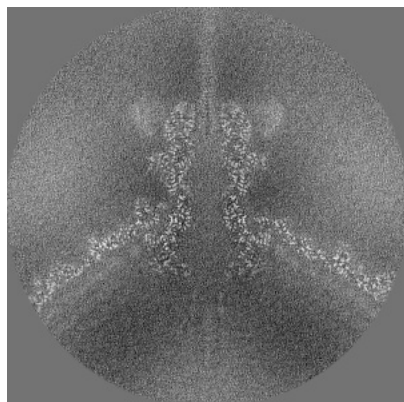


Y Index: 220

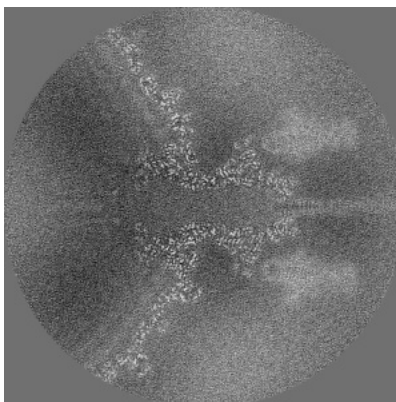


Z Index: 220

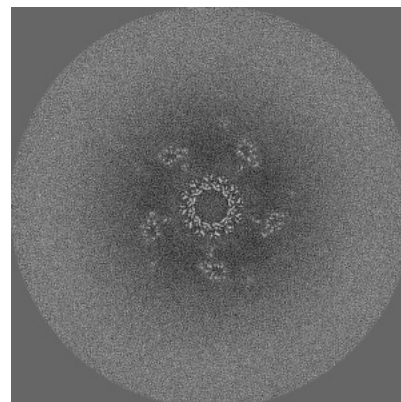
6.2.2 Raw map



X Index: 220



Y Index: 220

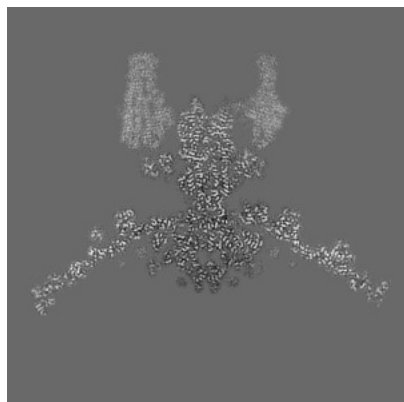


Z Index: 220

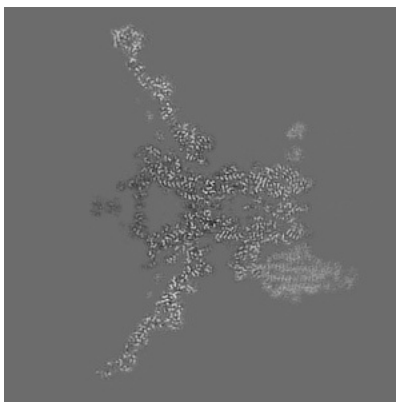
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

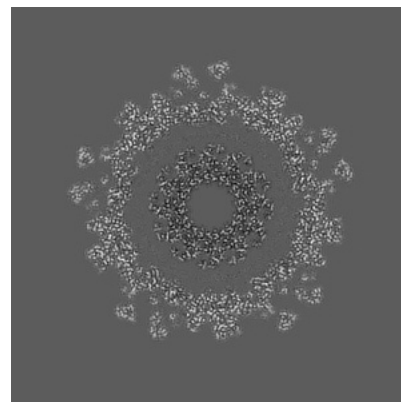
6.3.1 Primary map



X Index: 188

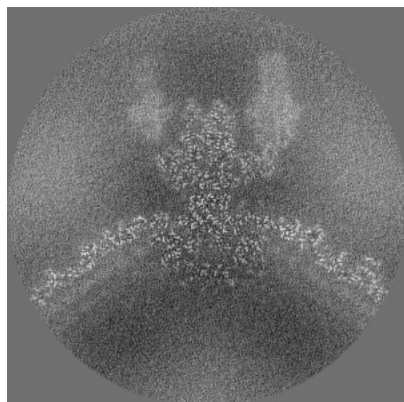


Y Index: 202

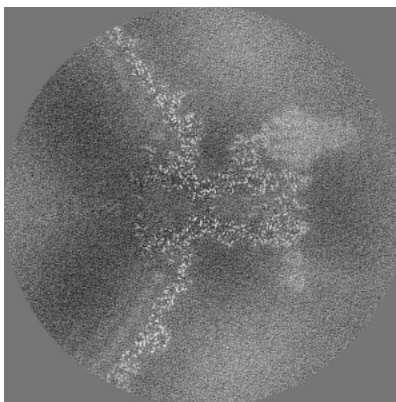


Z Index: 177

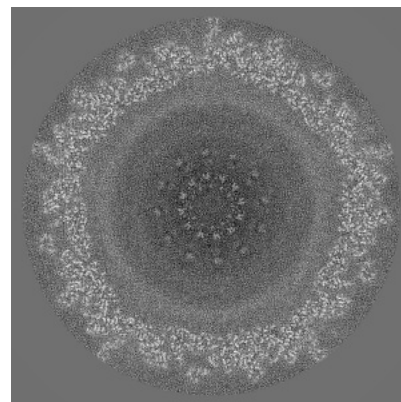
6.3.2 Raw map



X Index: 247



Y Index: 236

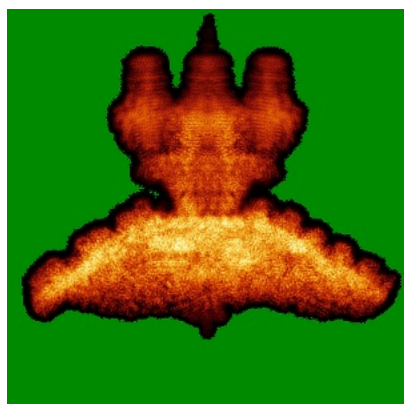


Z Index: 144

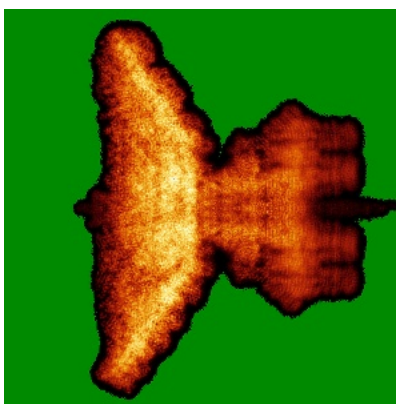
The images above show the largest variance slices of the map in three orthogonal directions.

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

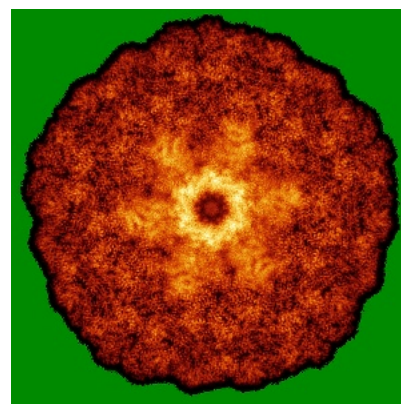
6.4.1 Primary map



X

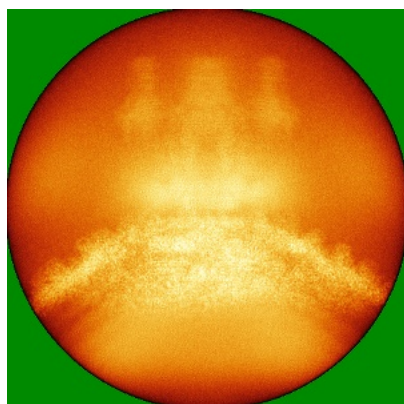


Y

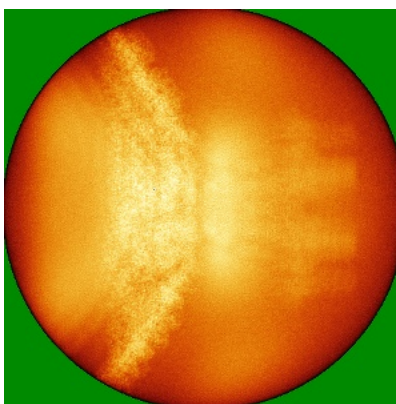


Z

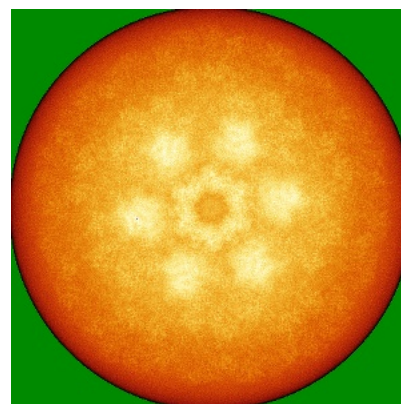
6.4.2 Raw map



X



Y

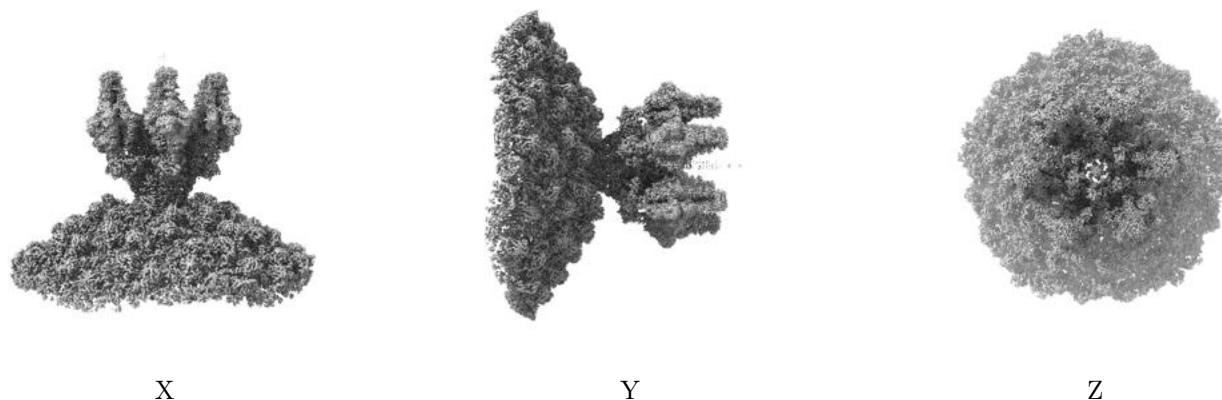


Z

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.

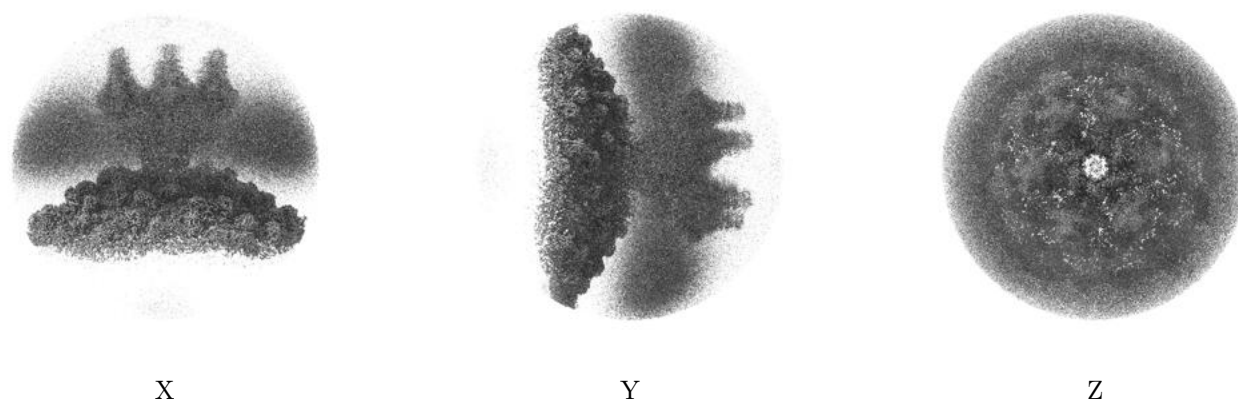
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

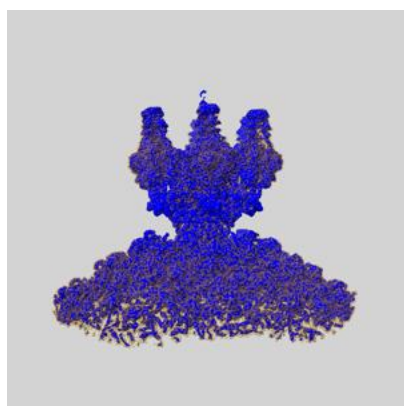
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

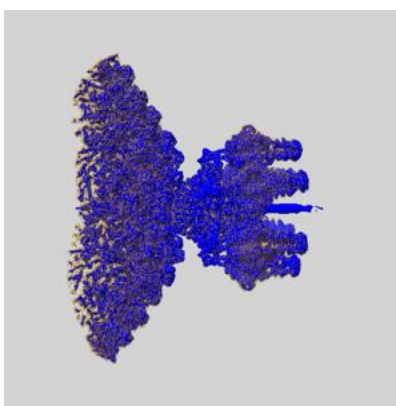
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

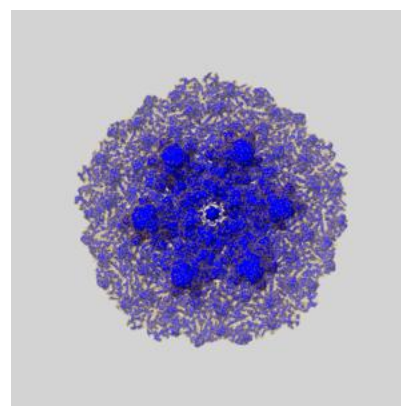
6.6.1 emd_41792_msk_1.map [i](#)



X



Y

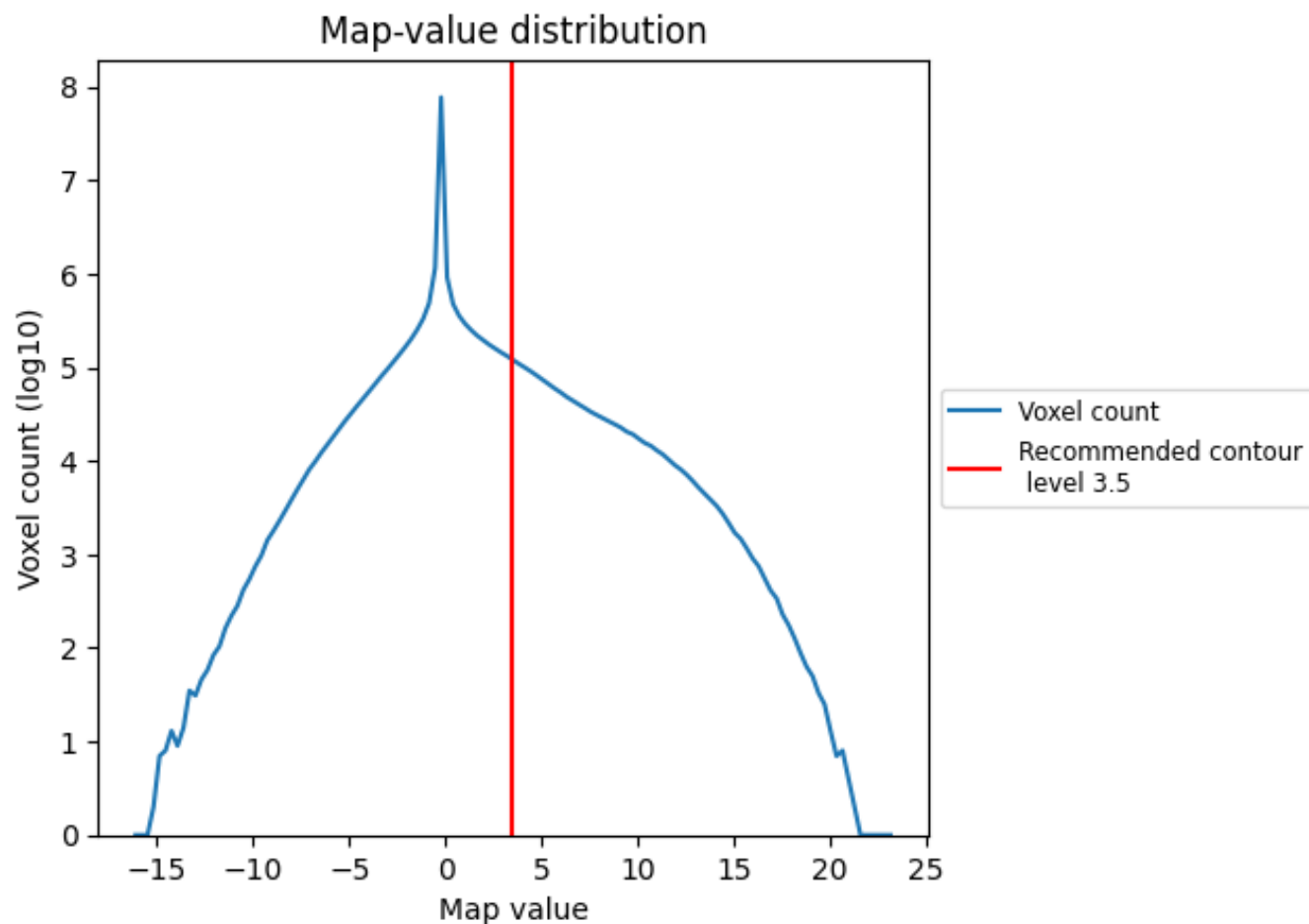


Z

7 Map analysis [i](#)

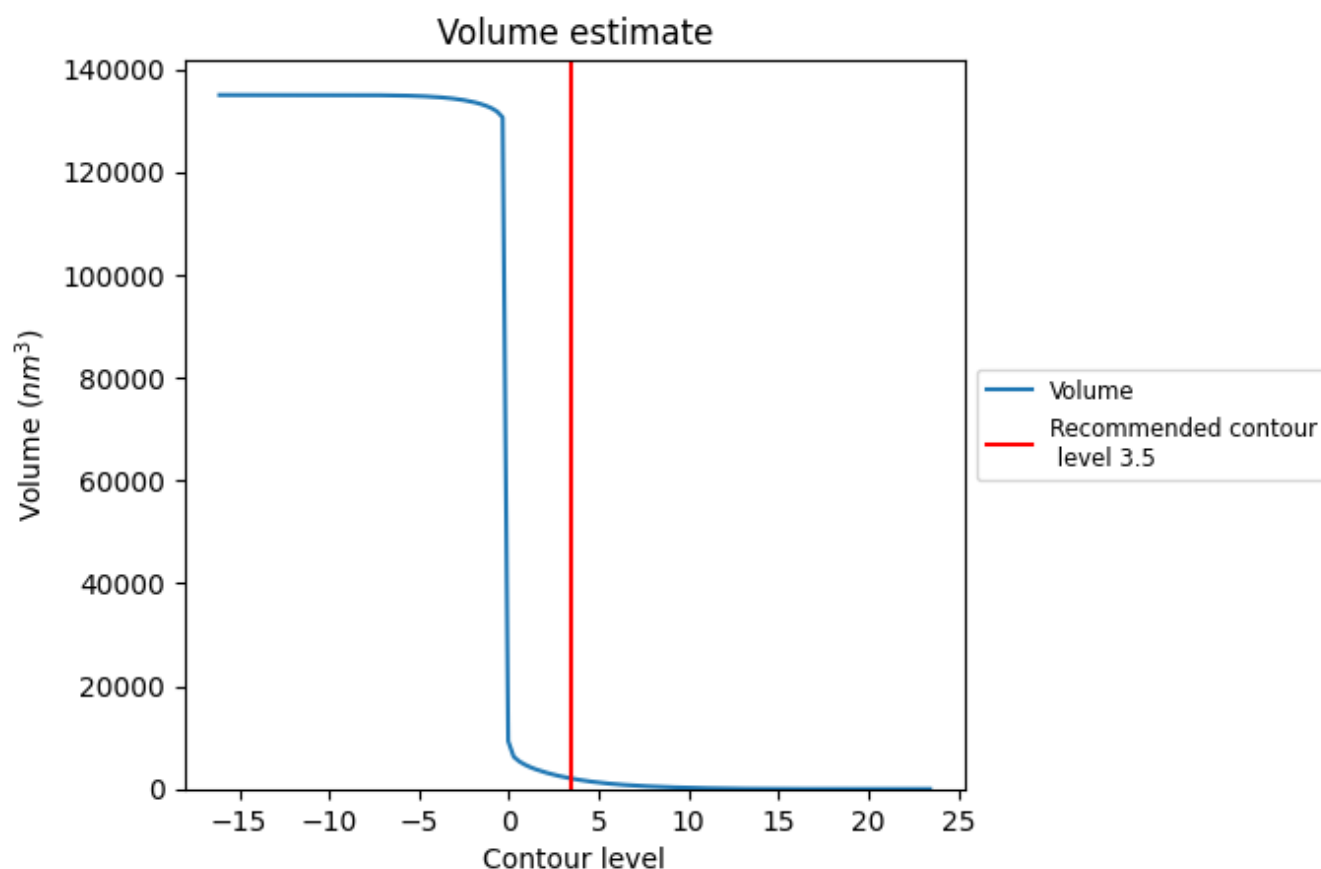
This section contains the results of statistical analysis of the map.

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.

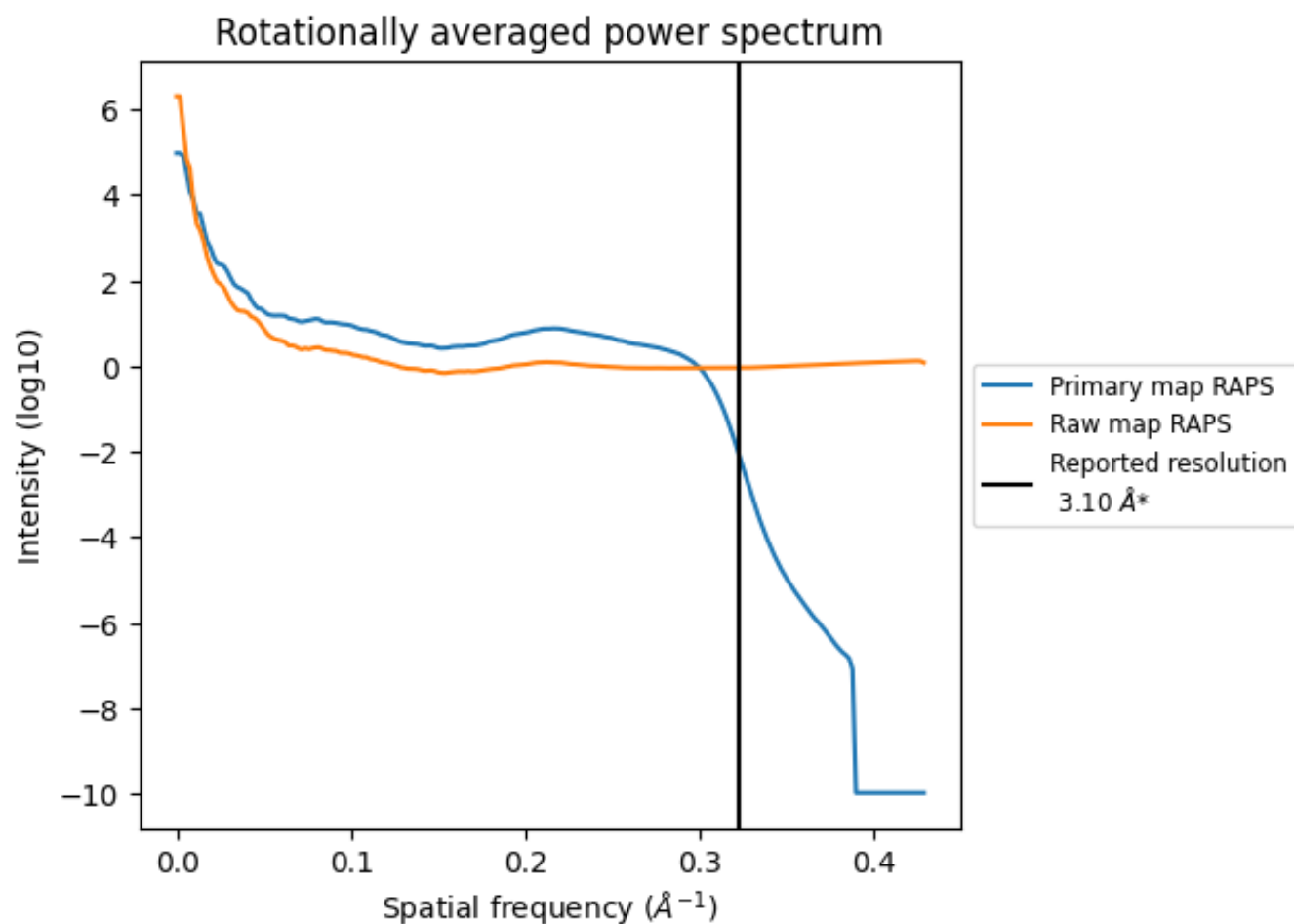
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2023 nm^3 ; this corresponds to an approximate mass of 1827 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 ⓘ

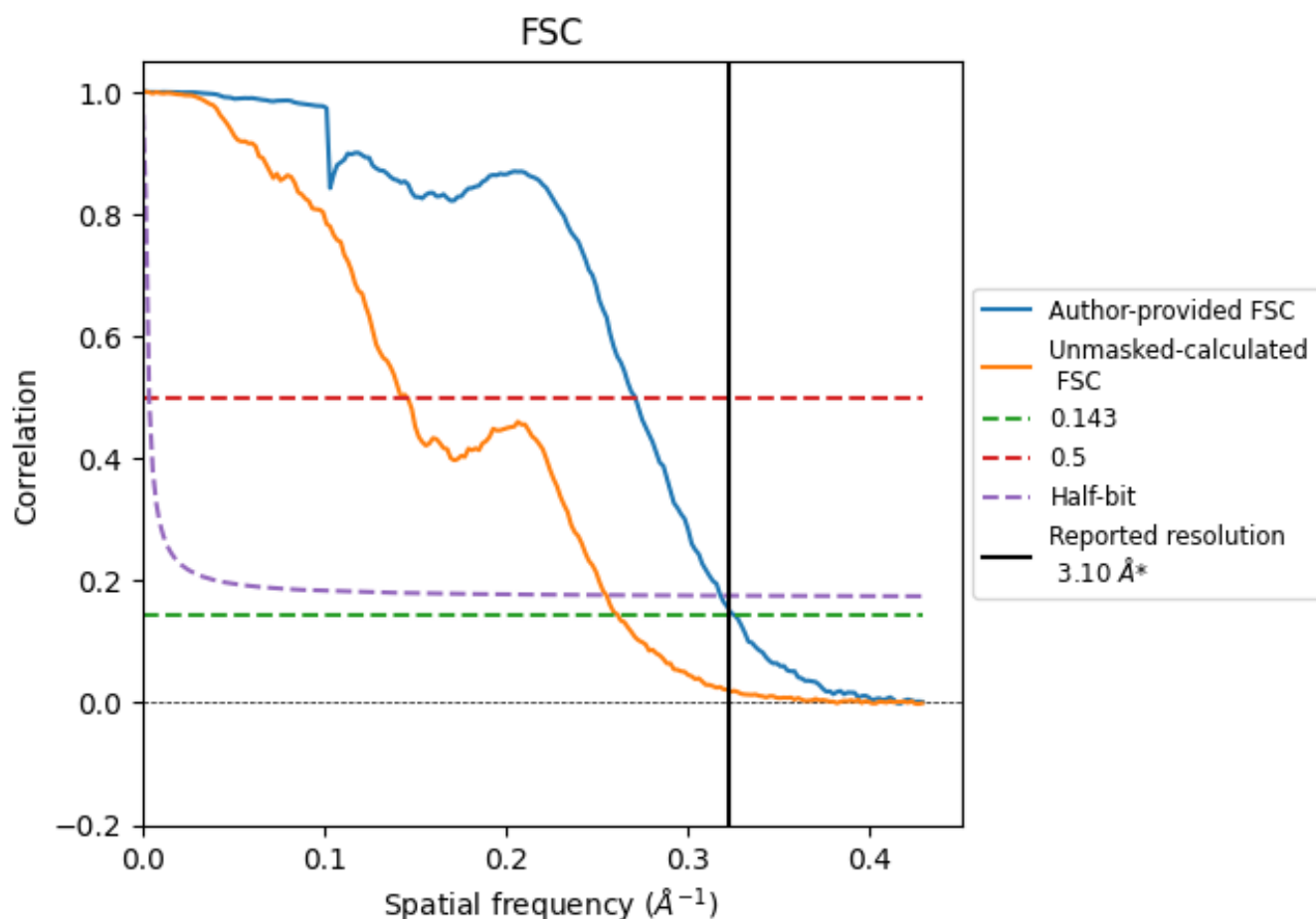


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

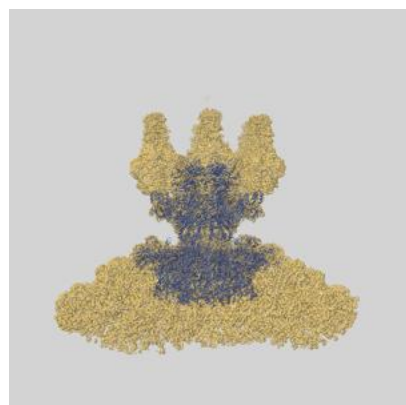
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.69	3.14
Unmasked-calculated*	3.82	7.03	3.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.82 differs from the reported value 3.1 by more than 10 %

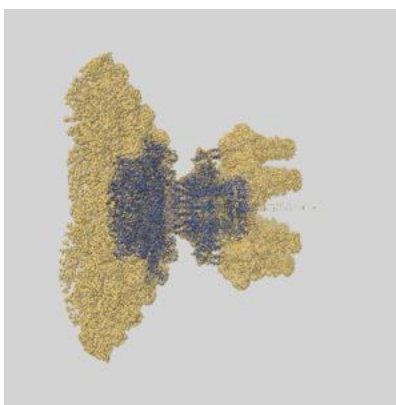
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41792 and PDB model 8U11. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

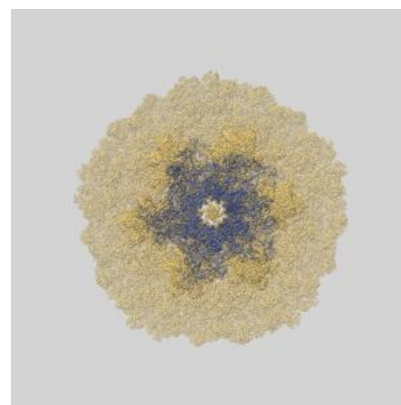
9.1 Map-model overlay [i](#)



X



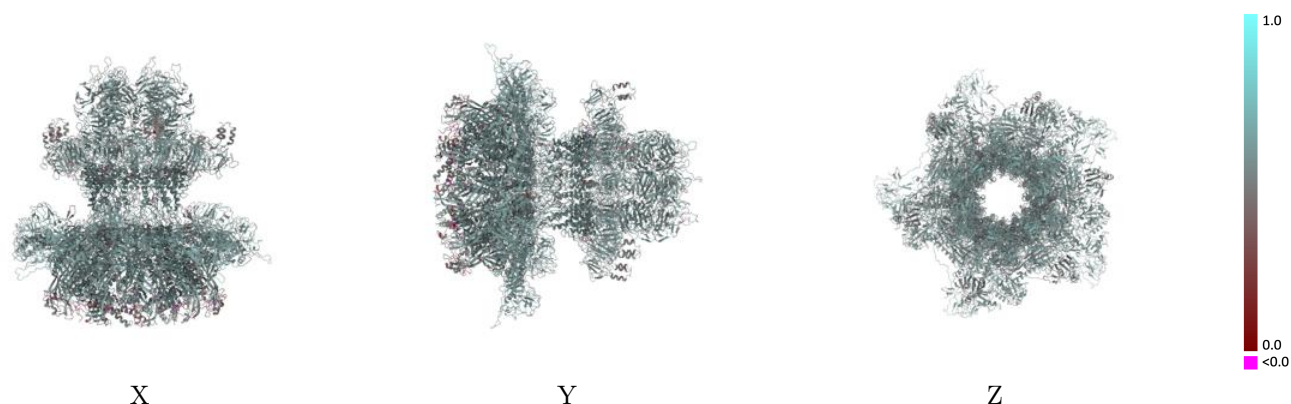
Y



Z

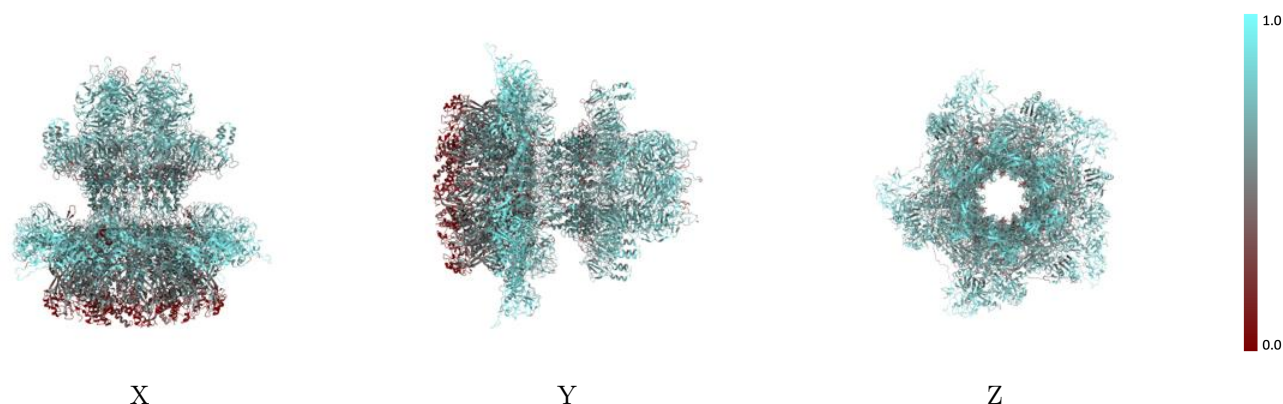
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



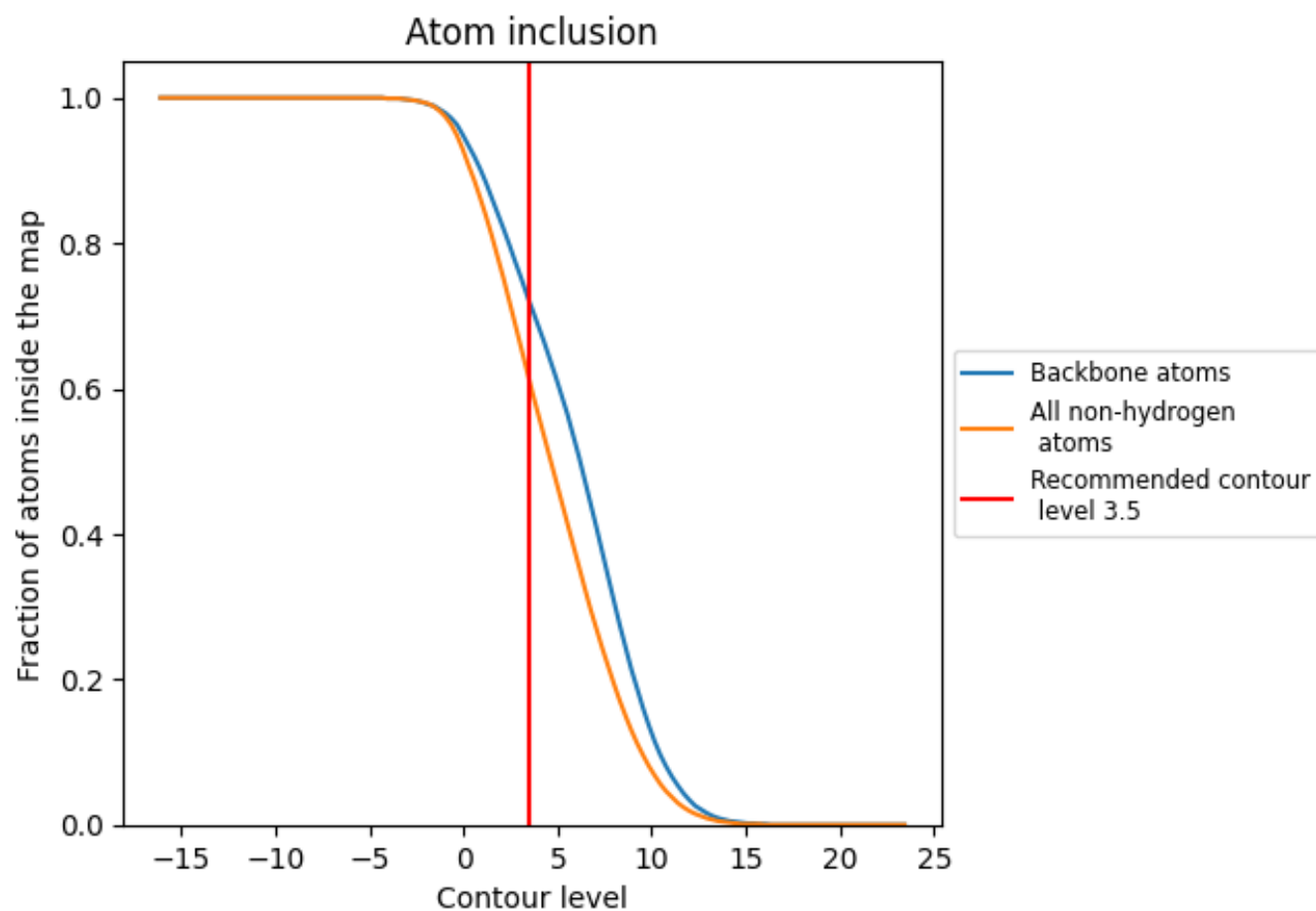
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 61% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6110	 0.5480
1	 0.7130	 0.5540
10	 0.6170	 0.5120
11	 0.6600	 0.5390
12	 0.6840	 0.5530
13	 0.6150	 0.5050
14	 0.6530	 0.5390
15	 0.6830	 0.5480
16	 0.6110	 0.5040
17	 0.6710	 0.5410
18	 0.6670	 0.5480
19	 0.6320	 0.5150
2	 0.6970	 0.5500
20	 0.6600	 0.5440
21	 0.7070	 0.5460
22	 0.6040	 0.5120
23	 0.6540	 0.5450
24	 0.6910	 0.5450
3	 0.7000	 0.5540
4	 0.7100	 0.5550
5	 0.7080	 0.5540
6	 0.7110	 0.5540
7	 0.6230	 0.5120
8	 0.6570	 0.5440
9	 0.6820	 0.5420
A	 0.7100	 0.5650
B	 0.7790	 0.5690
C	 0.7020	 0.5700
D	 0.7470	 0.5630
E	 0.6770	 0.5630
F	 0.7730	 0.5680
G	 0.6870	 0.5570
H	 0.7680	 0.5690
I	 0.7040	 0.5670
J	 0.7510	 0.5580



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Chain	Atom inclusion	Q-score
a	 0.4830	 0.5380
b	 0.4930	 0.5390
c	 0.5000	 0.5390
d	 0.4880	 0.5410
e	 0.4710	 0.5410
f	 0.4900	 0.5370
g	 0.4780	 0.5390
h	 0.4800	 0.5330
i	 0.4930	 0.5430
j	 0.4770	 0.5360
k	 0.4750	 0.5320
l	 0.4620	 0.5270
m	 0.5620	 0.5350
n	 0.6170	 0.5610
o	 0.6010	 0.5520
p	 0.6320	 0.5650
q	 0.6240	 0.5550
r	 0.5800	 0.5380
s	 0.6340	 0.5740
t	 0.6250	 0.5650
u	 0.6030	 0.5490
v	 0.6120	 0.5550
x	 0.6450	 0.5650
y	 0.6320	 0.5640