Full wwPDB EM Validation Report ⓘ

Apr 7, 2025 – 10:45 PM JST

PDB ID	:	9LW6 / pdb_00009lw6
EMDB ID	:	EMD-63432
Title	:	Top cap of bacteriophage Mycofy1 mature head (C5 symmetry)
Authors	:	Li, X.; Shao, Q.; Li, L.; Xie, L.; Ruan, Z.; Fang, Q.
Deposited on	:	2025-02-13
Resolution	:	3.42 Å(reported)

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

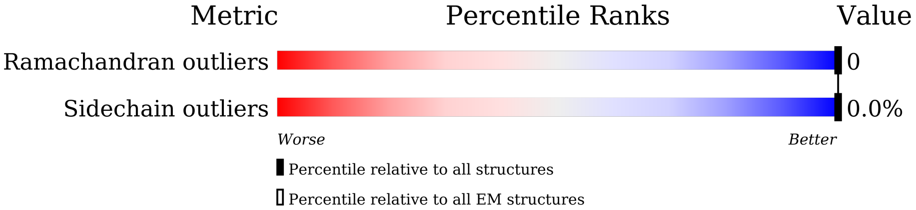
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.42 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	207382	16835
Sidechain outliers	206894	16415

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	1	543	 53% 47%
1	2	543	 53% 47%
1	3	543	 53% 47%
1	4	543	 53% 47%
1	5	543	 53% 47%
1	A	543	 54% 46%
1	B	543	 54% 46%
1	C	543	 54% 46%
1	D	543	 54% 46%

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Mol	Chain	Length	Quality of chain
1	E	543	
1	F	543	
1	G	543	
1	H	543	
1	I	543	
1	J	543	
1	K	543	
1	L	543	
1	M	543	
1	N	543	
1	O	543	
1	P	543	
1	Q	543	
1	R	543	
1	S	543	
1	T	543	
1	U	543	
1	V	543	
1	W	543	
1	X	543	
1	Y	543	
1	Z	543	
1	a	543	
1	b	543	
1	c	543	

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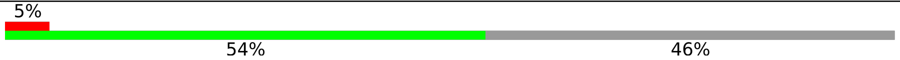
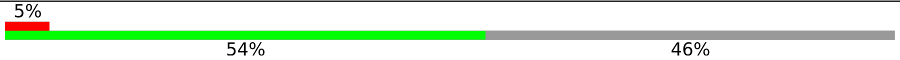
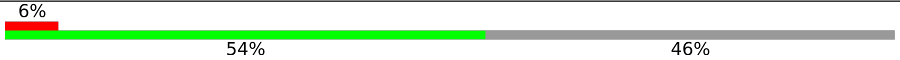
Mol	Chain	Length	Quality of chain
1	d	543	
1	e	543	
1	f	543	
1	g	543	
1	h	543	
1	i	543	
1	j	543	
1	k	543	
1	l	543	
1	m	543	
1	n	543	
1	o	543	
1	p	543	
1	q	543	
1	r	543	
1	s	543	
1	t	543	
1	u	543	
1	v	543	
1	w	543	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 120816 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 Phage capsid-like C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	293	Total C N O S 2241 1416 385 436 4	0	0
1	B	293	Total C N O S 2241 1416 385 436 4	0	0
1	C	293	Total C N O S 2241 1416 385 436 4	0	0
1	D	293	Total C N O S 2241 1416 385 436 4	0	0
1	E	293	Total C N O S 2241 1416 385 436 4	0	0
1	F	293	Total C N O S 2241 1416 385 436 4	0	0
1	G	293	Total C N O S 2241 1416 385 436 4	0	0
1	H	293	Total C N O S 2241 1416 385 436 4	0	0
1	I	293	Total C N O S 2241 1416 385 436 4	0	0
1	J	293	Total C N O S 2241 1416 385 436 4	0	0
1	K	293	Total C N O S 2241 1416 385 436 4	0	0
1	L	293	Total C N O S 2241 1416 385 436 4	0	0
1	M	293	Total C N O S 2241 1416 385 436 4	0	0
1	N	293	Total C N O S 2241 1416 385 436 4	0	0
1	O	293	Total C N O S 2241 1416 385 436 4	0	0
1	P	293	Total C N O S 2241 1416 385 436 4	0	0
1	Q	293	Total C N O S 2241 1416 385 436 4	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
1	R	293	Total C N O S 2241 1416 385 436 4	0	0
1	S	293	Total C N O S 2241 1416 385 436 4	0	0
1	T	293	Total C N O S 2241 1416 385 436 4	0	0
1	U	293	Total C N O S 2241 1416 385 436 4	0	0
1	V	293	Total C N O S 2241 1416 385 436 4	0	0
1	W	293	Total C N O S 2241 1416 385 436 4	0	0
1	X	293	Total C N O S 2241 1416 385 436 4	0	0
1	Y	293	Total C N O S 2241 1416 385 436 4	0	0
1	Z	293	Total C N O S 2241 1416 385 436 4	0	0
1	a	293	Total C N O S 2241 1416 385 436 4	0	0
1	b	293	Total C N O S 2241 1416 385 436 4	0	0
1	c	293	Total C N O S 2241 1416 385 436 4	0	0
1	d	293	Total C N O S 2241 1416 385 436 4	0	0
1	e	293	Total C N O S 2241 1416 385 436 4	0	0
1	f	293	Total C N O S 2241 1416 385 436 4	0	0
1	g	293	Total C N O S 2241 1416 385 436 4	0	0
1	h	293	Total C N O S 2241 1416 385 436 4	0	0
1	i	293	Total C N O S 2241 1416 385 436 4	0	0
1	j	293	Total C N O S 2241 1416 385 436 4	0	0
1	k	293	Total C N O S 2241 1416 385 436 4	0	0
1	l	293	Total C N O S 2241 1416 385 436 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	n	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	o	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	p	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	q	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	r	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	s	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	t	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	u	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	v	293	Total 2241	C 1416	N 385	O 436	S 4	0	0
1	w	288	Total 2208	C 1397	N 379	O 428	S 4	0	0
1	1	288	Total 2208	C 1397	N 379	O 428	S 4	0	0
1	2	288	Total 2208	C 1397	N 379	O 428	S 4	0	0
1	3	288	Total 2208	C 1397	N 379	O 428	S 4	0	0
1	4	288	Total 2208	C 1397	N 379	O 428	S 4	0	0
1	5	288	Total 2208	C 1397	N 379	O 428	S 4	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	HIS	LYS	conflict	UNP Q854Z2
B	197	HIS	LYS	conflict	UNP Q854Z2
C	197	HIS	LYS	conflict	UNP Q854Z2
D	197	HIS	LYS	conflict	UNP Q854Z2
E	197	HIS	LYS	conflict	UNP Q854Z2
F	197	HIS	LYS	conflict	UNP Q854Z2
G	197	HIS	LYS	conflict	UNP Q854Z2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	197	HIS	LYS	conflict	UNP Q854Z2
I	197	HIS	LYS	conflict	UNP Q854Z2
J	197	HIS	LYS	conflict	UNP Q854Z2
K	197	HIS	LYS	conflict	UNP Q854Z2
L	197	HIS	LYS	conflict	UNP Q854Z2
M	197	HIS	LYS	conflict	UNP Q854Z2
N	197	HIS	LYS	conflict	UNP Q854Z2
O	197	HIS	LYS	conflict	UNP Q854Z2
P	197	HIS	LYS	conflict	UNP Q854Z2
Q	197	HIS	LYS	conflict	UNP Q854Z2
R	197	HIS	LYS	conflict	UNP Q854Z2
S	197	HIS	LYS	conflict	UNP Q854Z2
T	197	HIS	LYS	conflict	UNP Q854Z2
U	197	HIS	LYS	conflict	UNP Q854Z2
V	197	HIS	LYS	conflict	UNP Q854Z2
W	197	HIS	LYS	conflict	UNP Q854Z2
X	197	HIS	LYS	conflict	UNP Q854Z2
Y	197	HIS	LYS	conflict	UNP Q854Z2
Z	197	HIS	LYS	conflict	UNP Q854Z2
a	197	HIS	LYS	conflict	UNP Q854Z2
b	197	HIS	LYS	conflict	UNP Q854Z2
c	197	HIS	LYS	conflict	UNP Q854Z2
d	197	HIS	LYS	conflict	UNP Q854Z2
e	197	HIS	LYS	conflict	UNP Q854Z2
f	197	HIS	LYS	conflict	UNP Q854Z2
g	197	HIS	LYS	conflict	UNP Q854Z2
h	197	HIS	LYS	conflict	UNP Q854Z2
i	197	HIS	LYS	conflict	UNP Q854Z2
j	197	HIS	LYS	conflict	UNP Q854Z2
k	197	HIS	LYS	conflict	UNP Q854Z2
l	197	HIS	LYS	conflict	UNP Q854Z2
m	197	HIS	LYS	conflict	UNP Q854Z2
n	197	HIS	LYS	conflict	UNP Q854Z2
o	197	HIS	LYS	conflict	UNP Q854Z2
p	197	HIS	LYS	conflict	UNP Q854Z2
q	197	HIS	LYS	conflict	UNP Q854Z2
r	197	HIS	LYS	conflict	UNP Q854Z2
s	197	HIS	LYS	conflict	UNP Q854Z2
t	197	HIS	LYS	conflict	UNP Q854Z2
u	197	HIS	LYS	conflict	UNP Q854Z2
v	197	HIS	LYS	conflict	UNP Q854Z2
w	197	HIS	LYS	conflict	UNP Q854Z2

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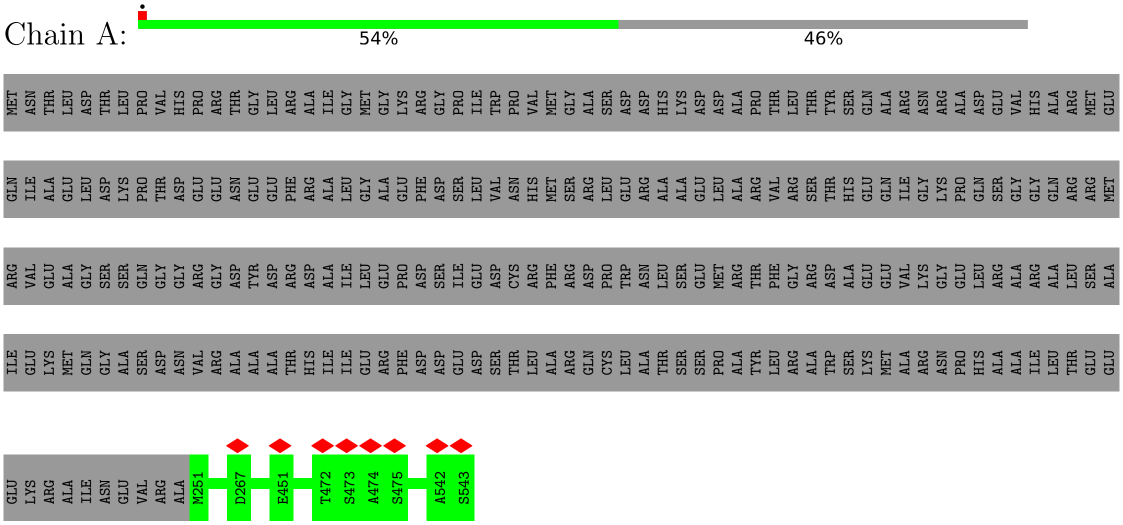
Chain	Residue	Modelled	Actual	Comment	Reference
1	197	HIS	LYS	conflict	UNP Q854Z2
2	197	HIS	LYS	conflict	UNP Q854Z2
3	197	HIS	LYS	conflict	UNP Q854Z2
4	197	HIS	LYS	conflict	UNP Q854Z2
5	197	HIS	LYS	conflict	UNP Q854Z2

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.

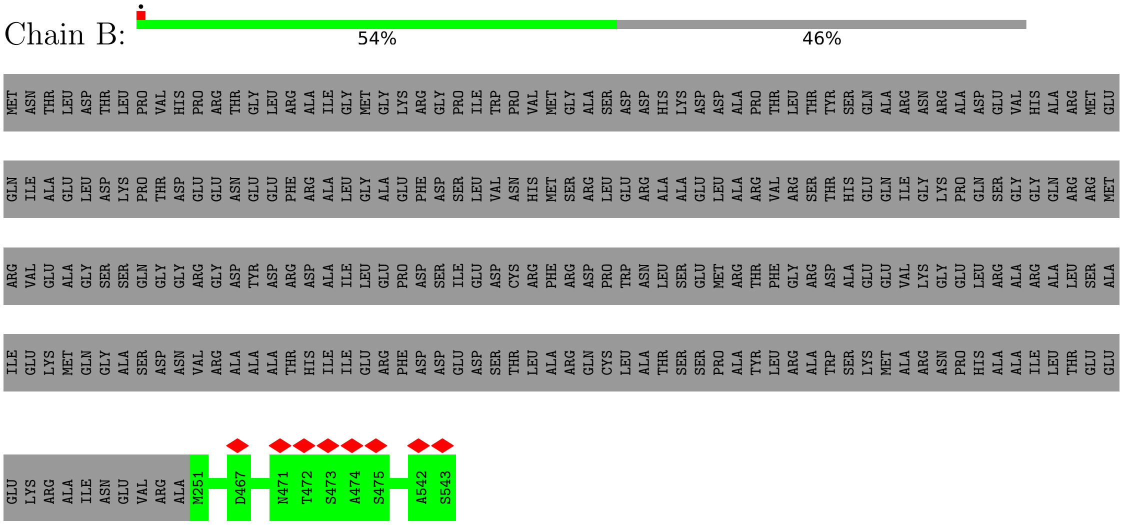
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain A:

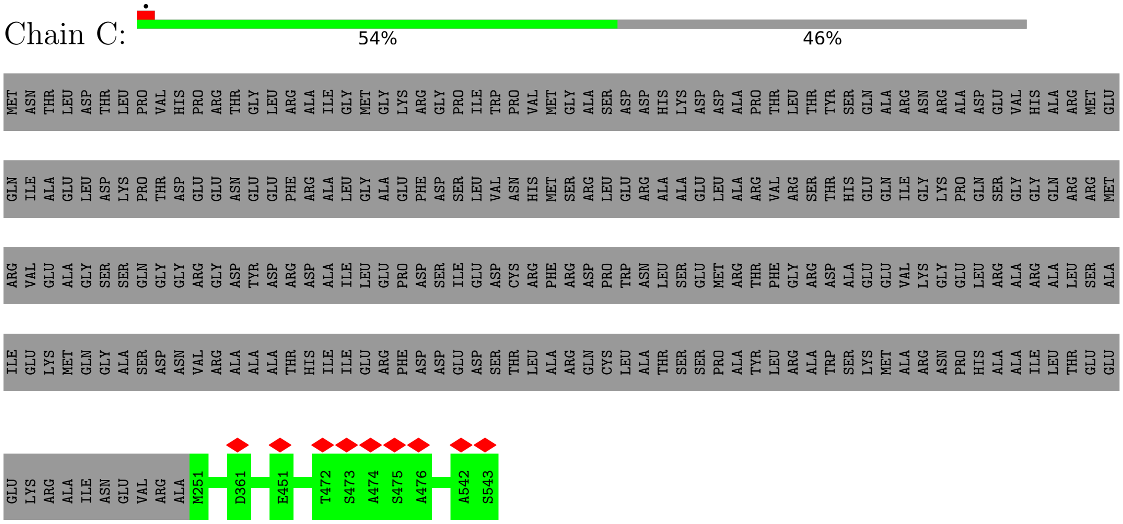


- Molecule 1: Phage capsid-like C-terminal domain-containing protein

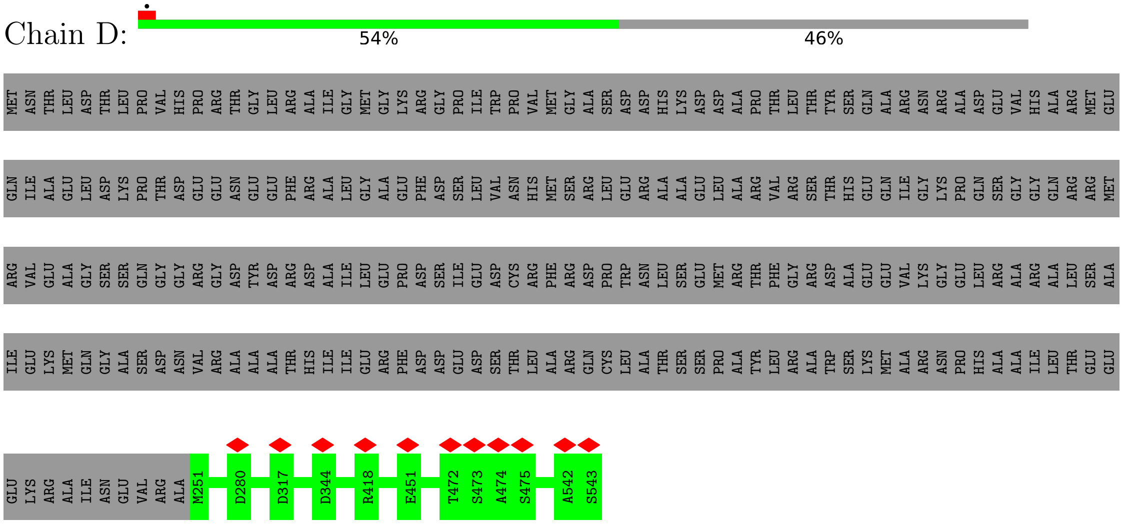
Chain B:



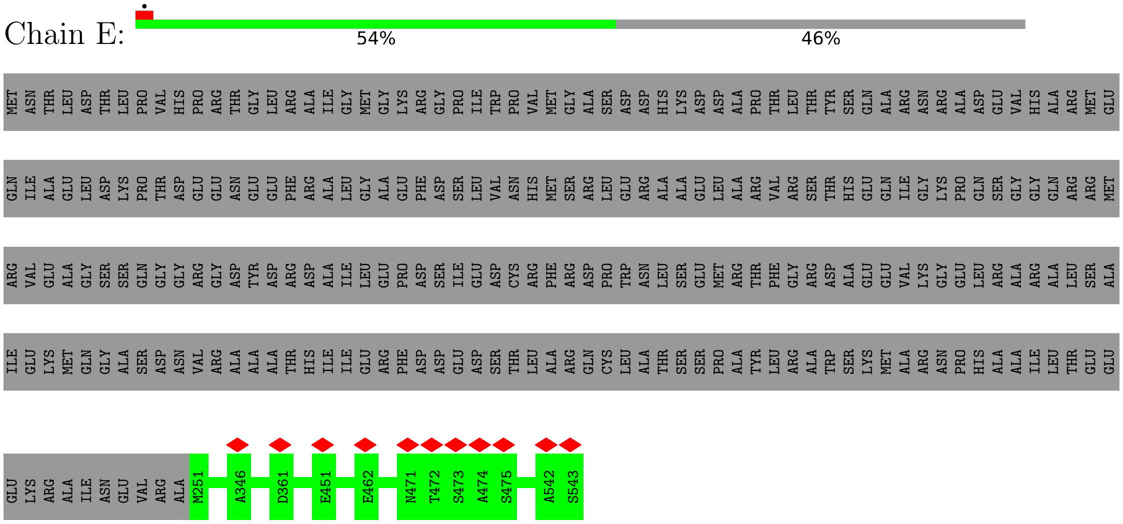
- Molecule 1: Phage capsid-like C-terminal domain-containing protein



- Molecule 1: Phage capsid-like C-terminal domain-containing protein

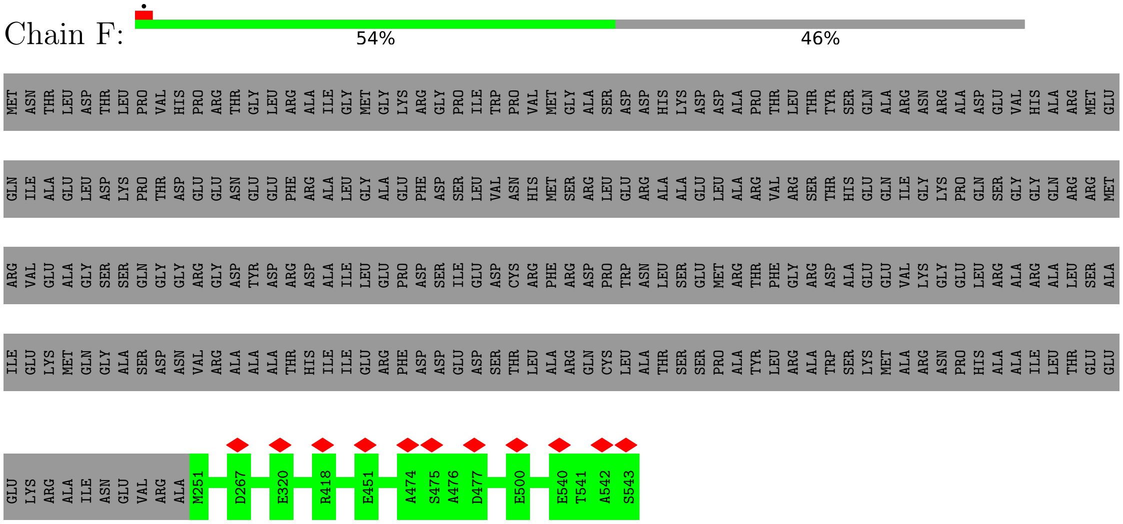


- Molecule 1: Phage capsid-like C-terminal domain-containing protein



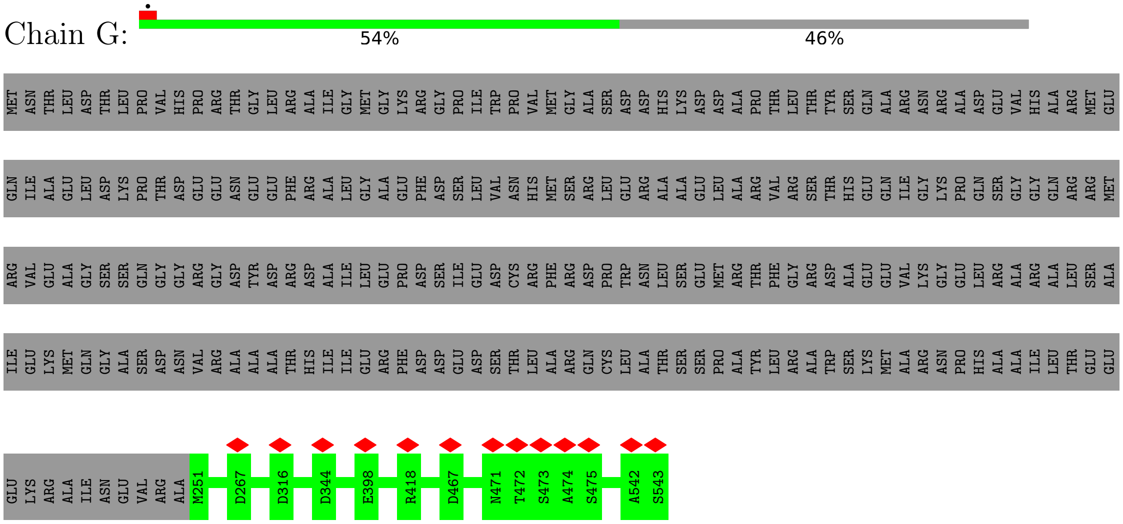
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain F:



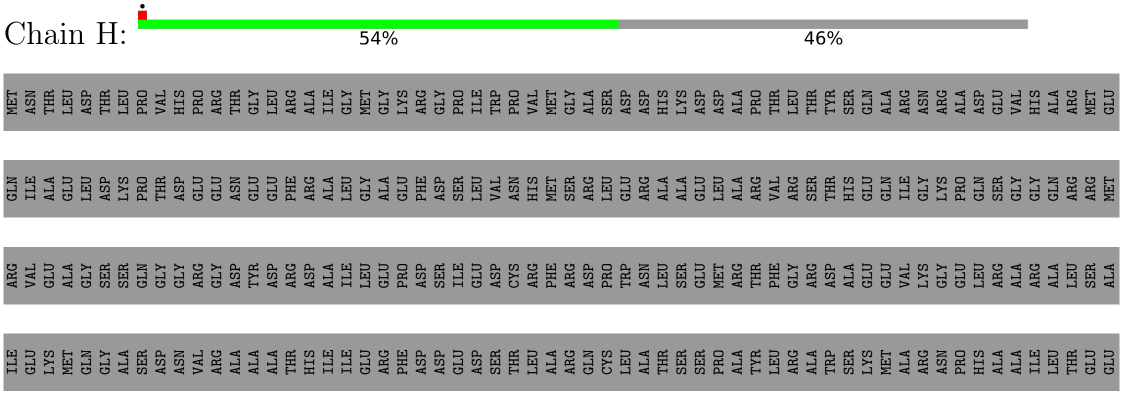
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

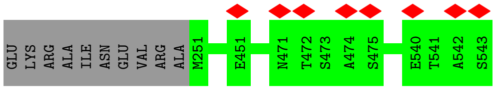
Chain G:



- Molecule 1: Phage capsid-like C-terminal domain-containing protein

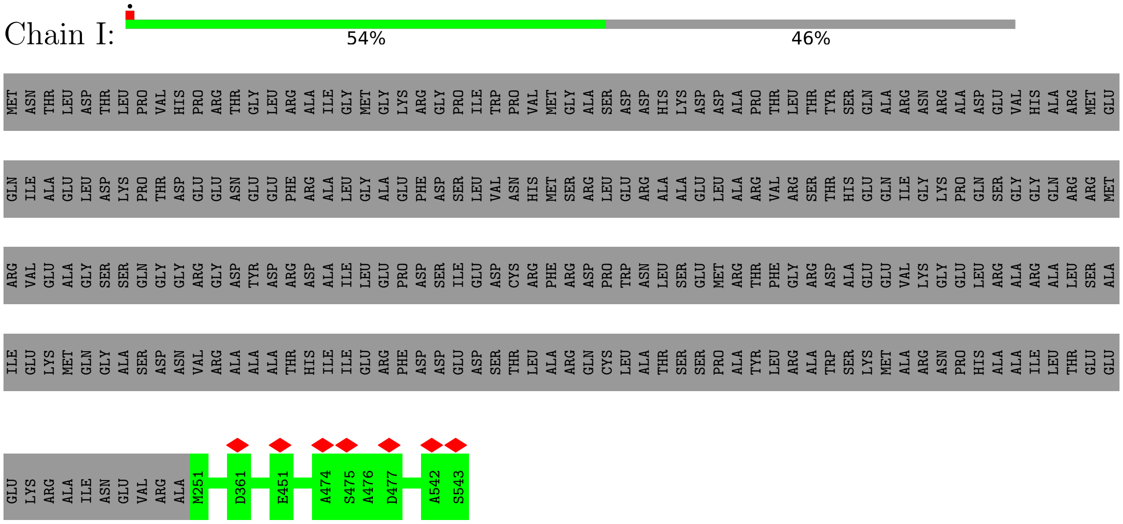
Chain H:





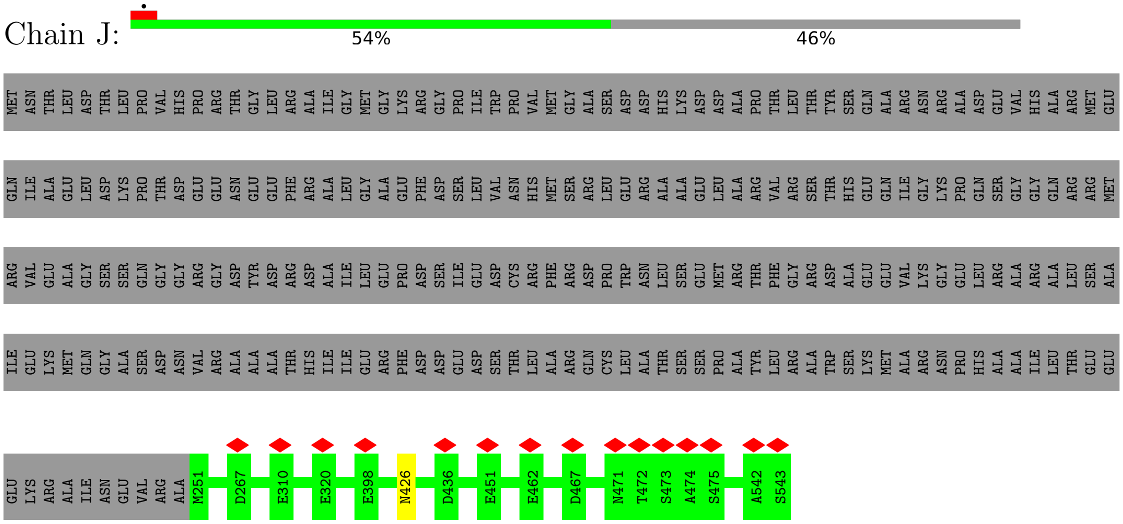
• Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain I:



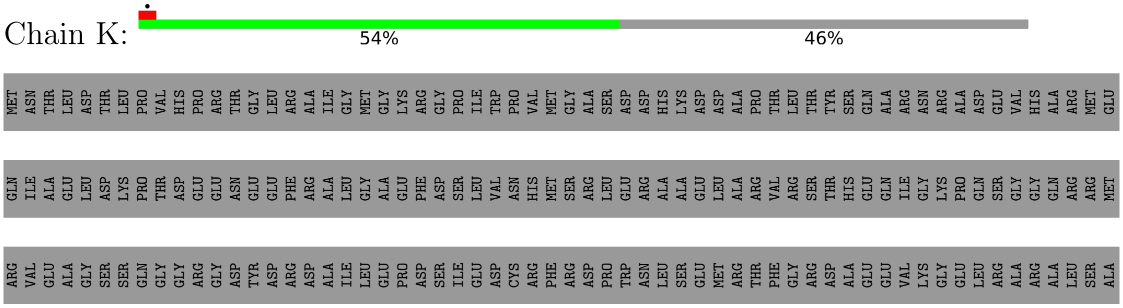
• Molecule 1: Phage capsid-like C-terminal domain-containing protein

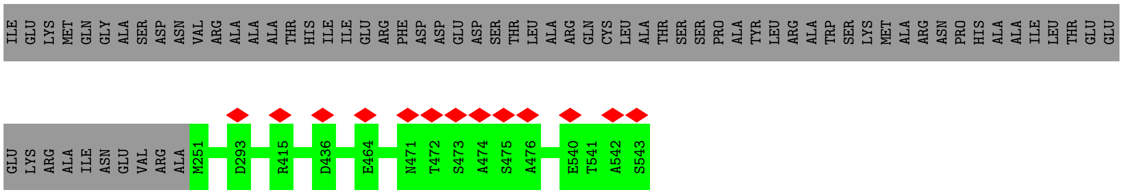
Chain J:



• Molecule 1: Phage capsid-like C-terminal domain-containing protein

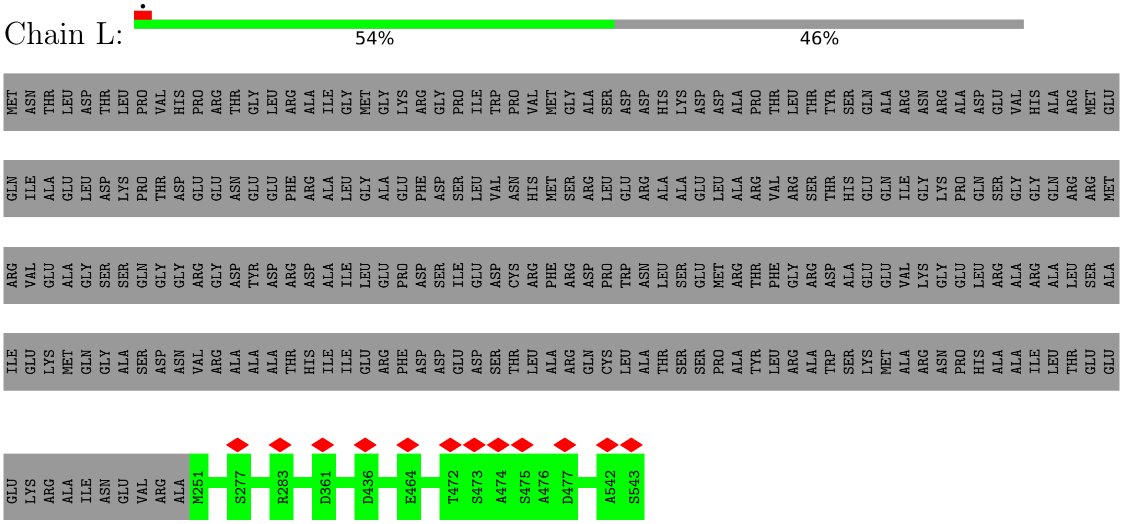
Chain K:





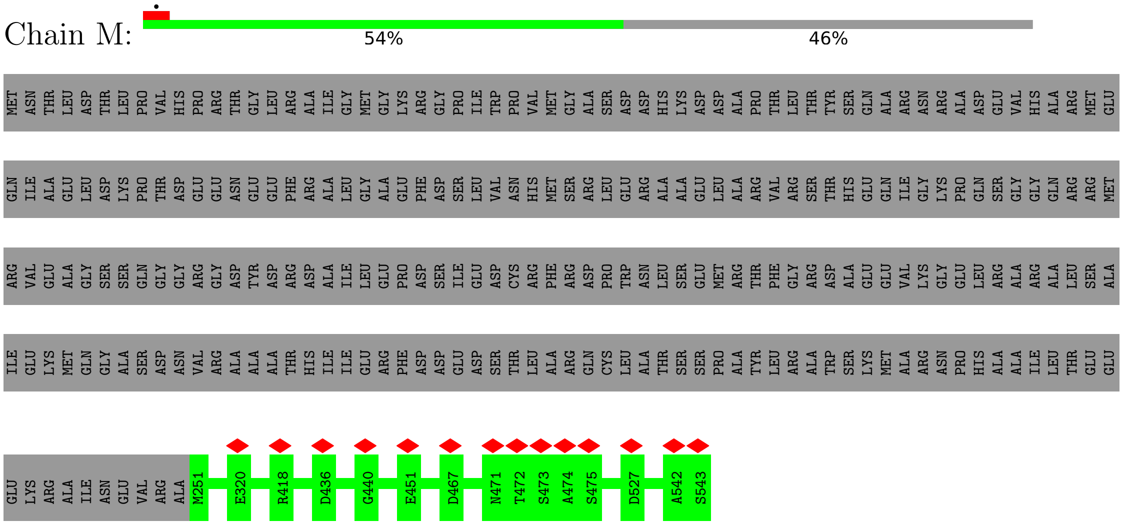
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain L:



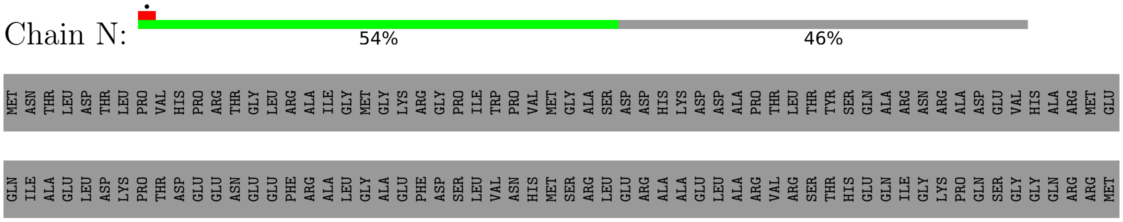
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

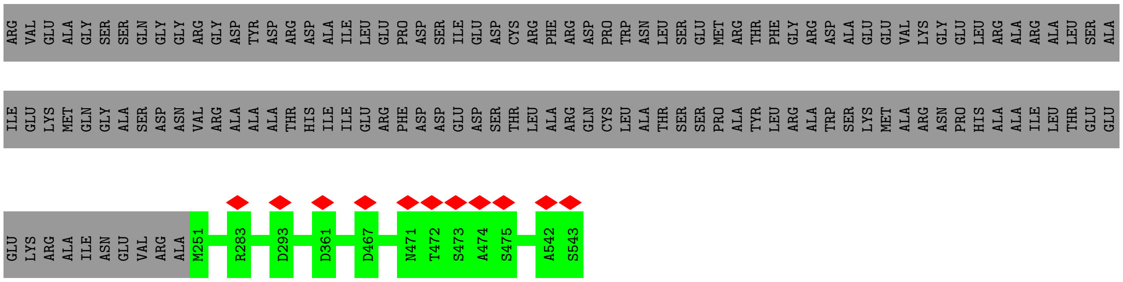
Chain M:



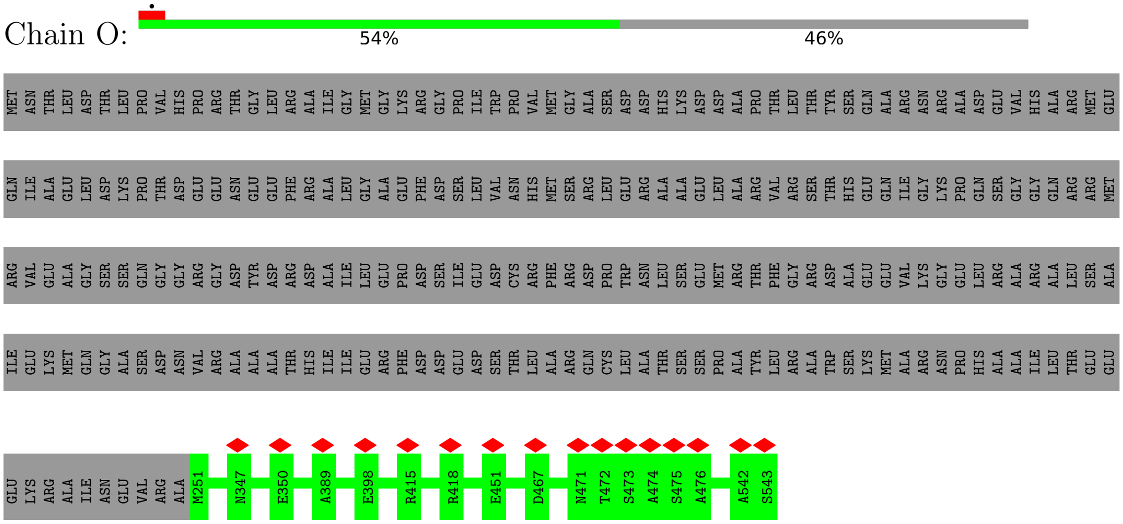
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain N:

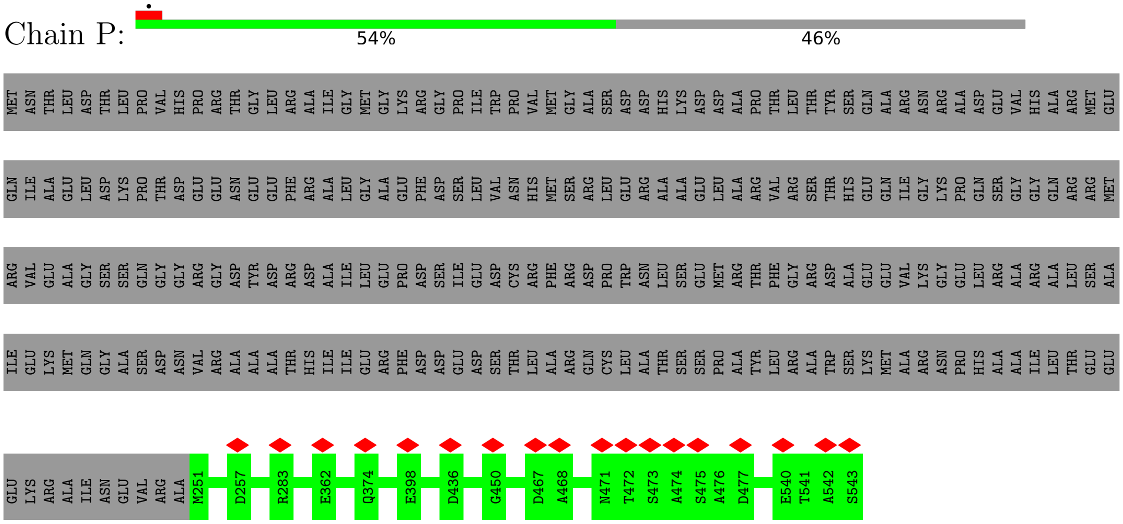




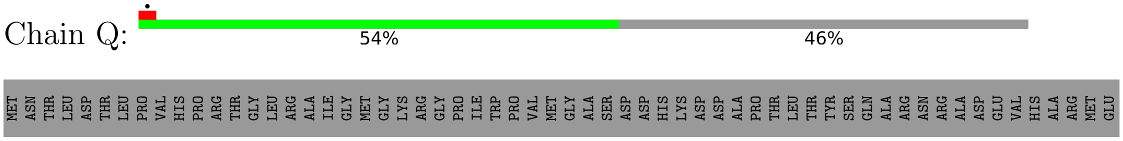
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

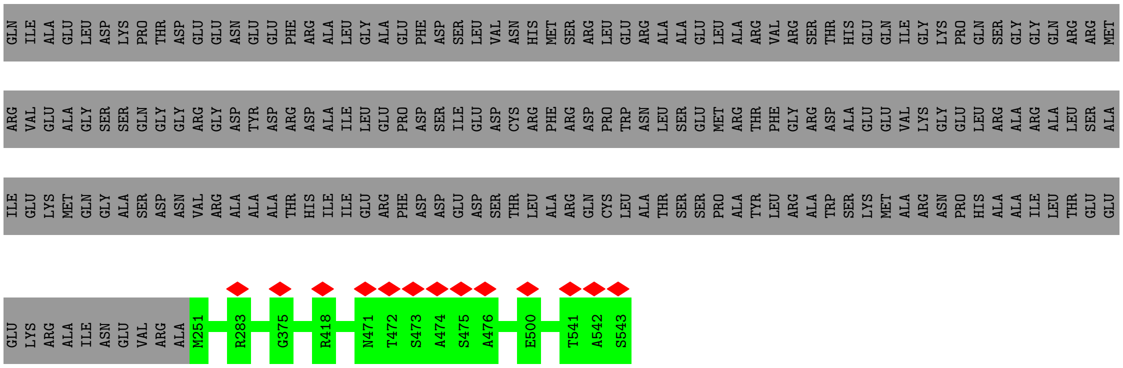


- Molecule 1: Phage capsid-like C-terminal domain-containing protein



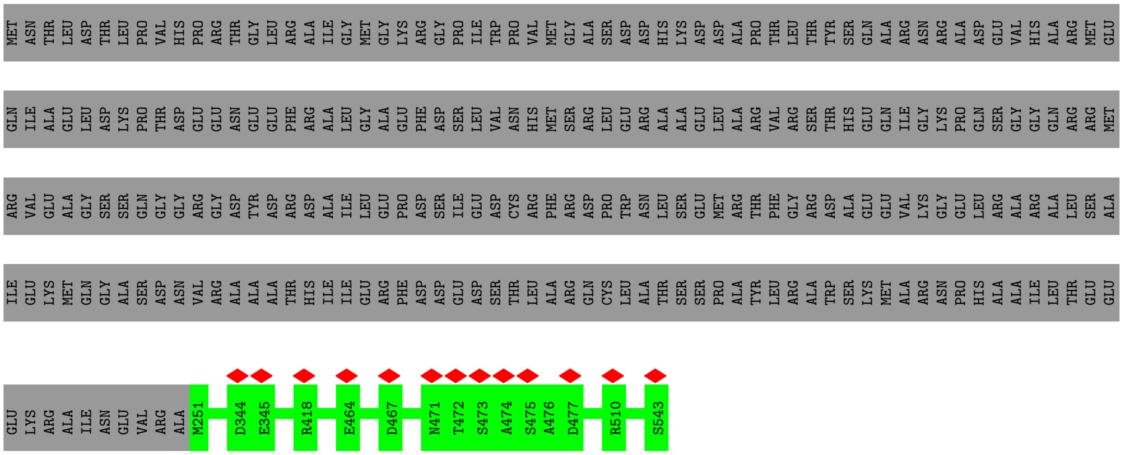
- Molecule 1: Phage capsid-like C-terminal domain-containing protein





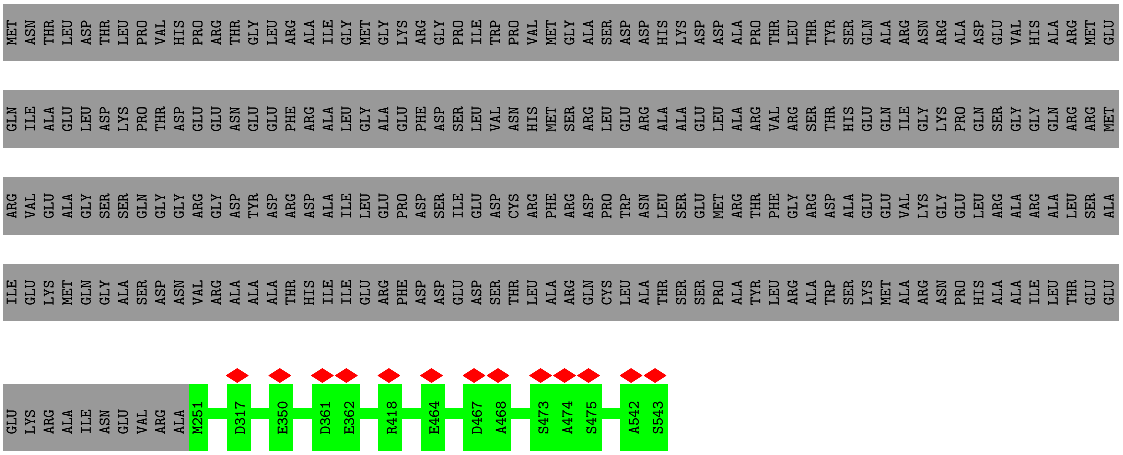
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain R:



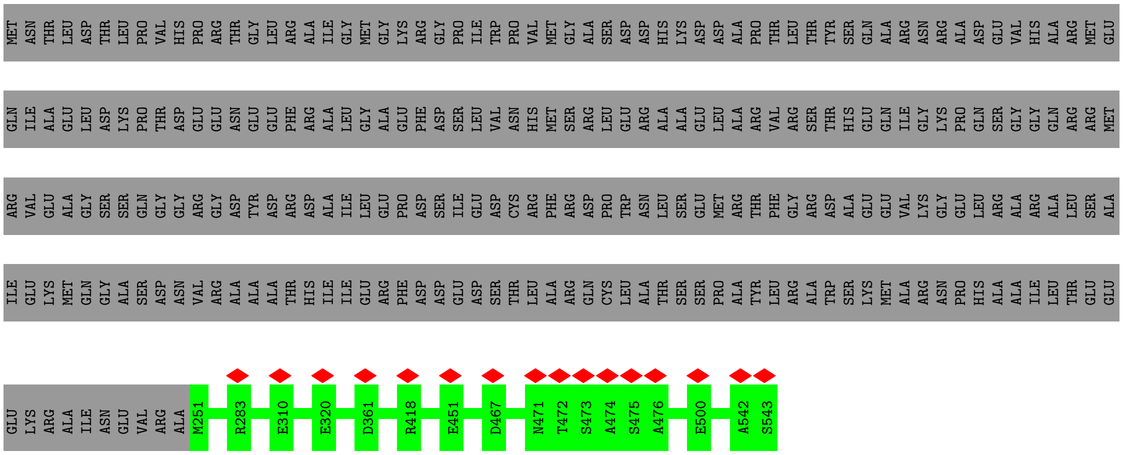
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain S:



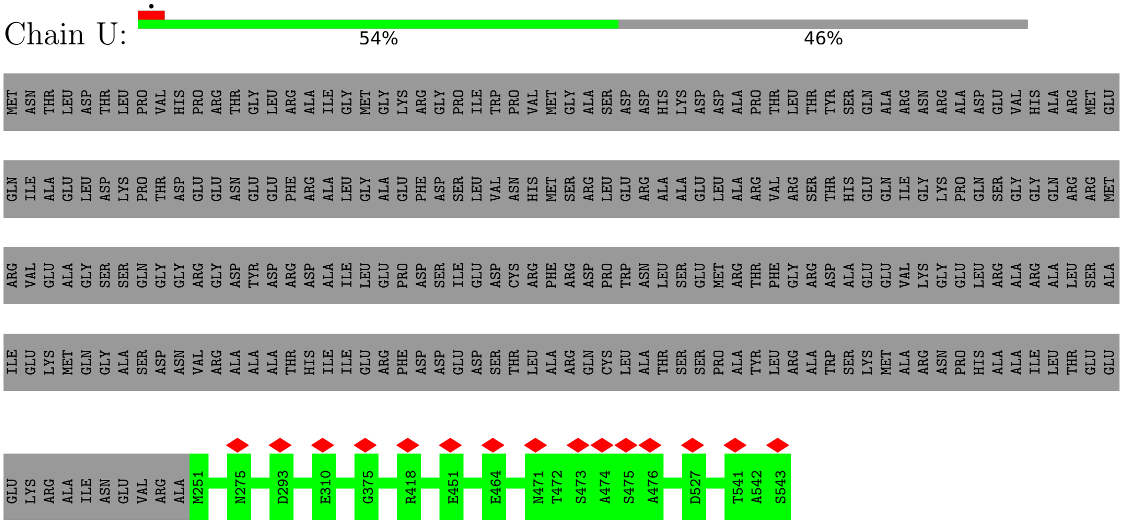
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain T:



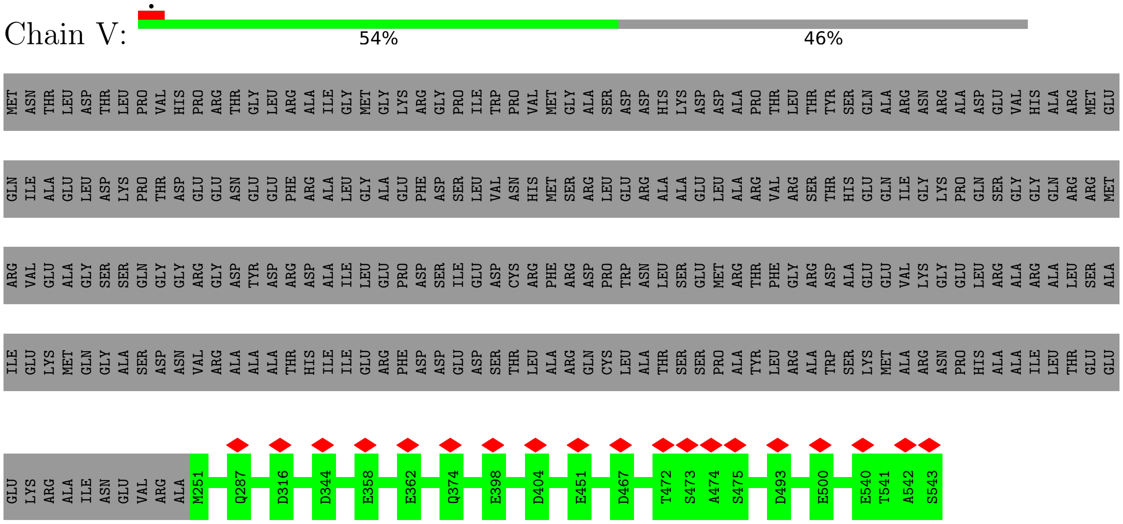
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain U:

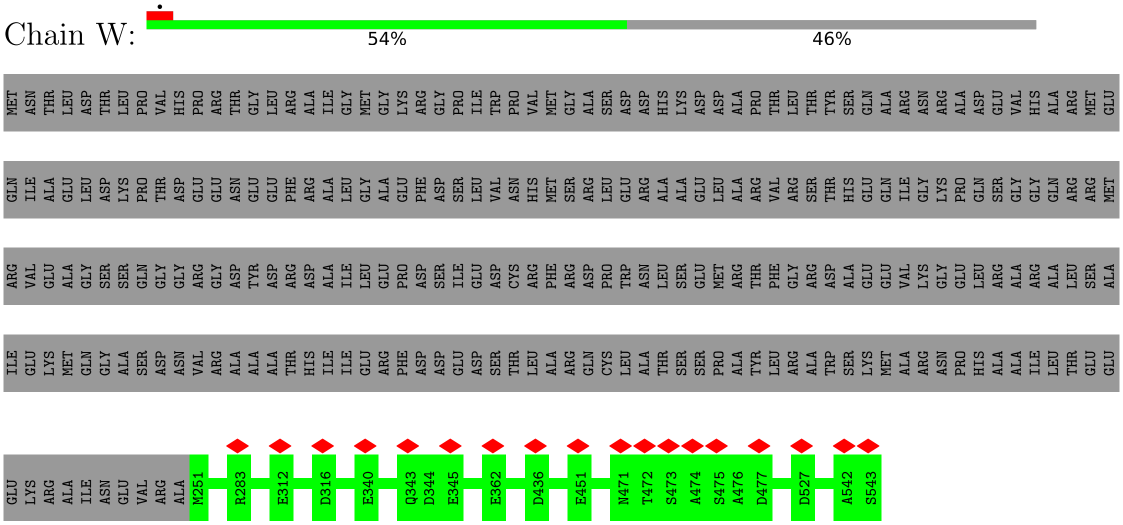


- Molecule 1: Phage capsid-like C-terminal domain-containing protein

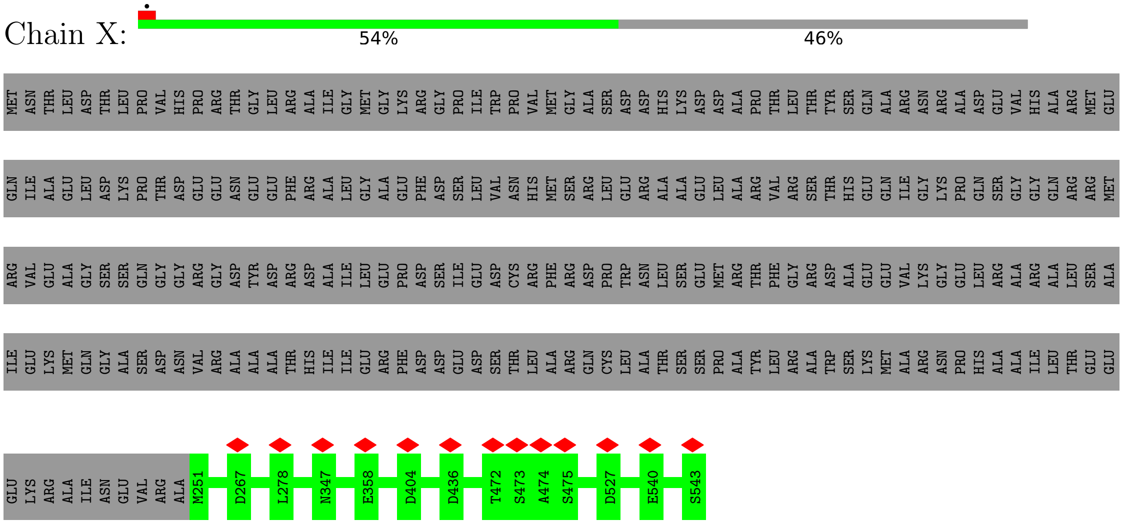
Chain V:



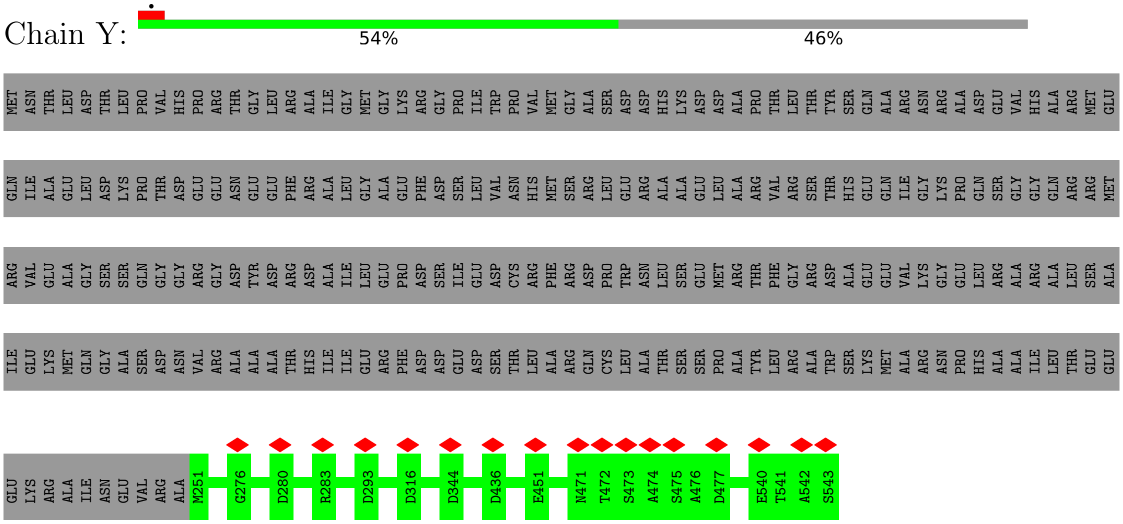
- Molecule 1: Phage capsid-like C-terminal domain-containing protein



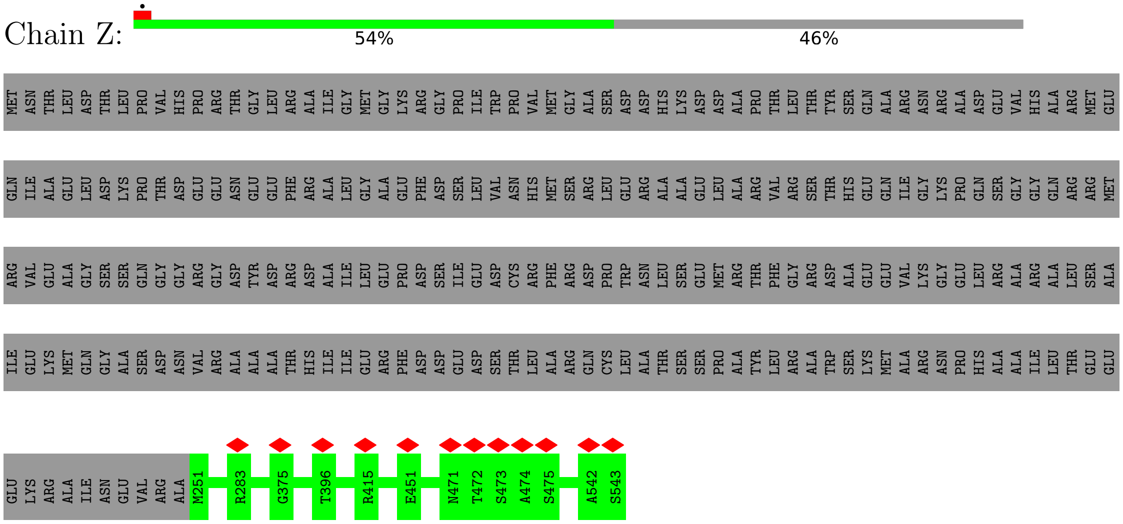
• Molecule 1: Phage capsid-like C-terminal domain-containing protein



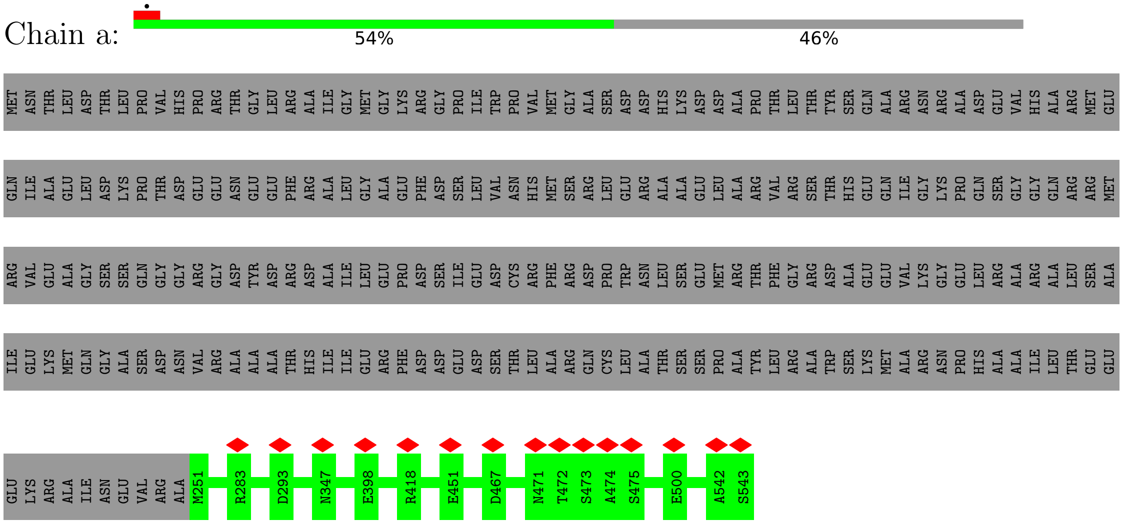
• Molecule 1: Phage capsid-like C-terminal domain-containing protein



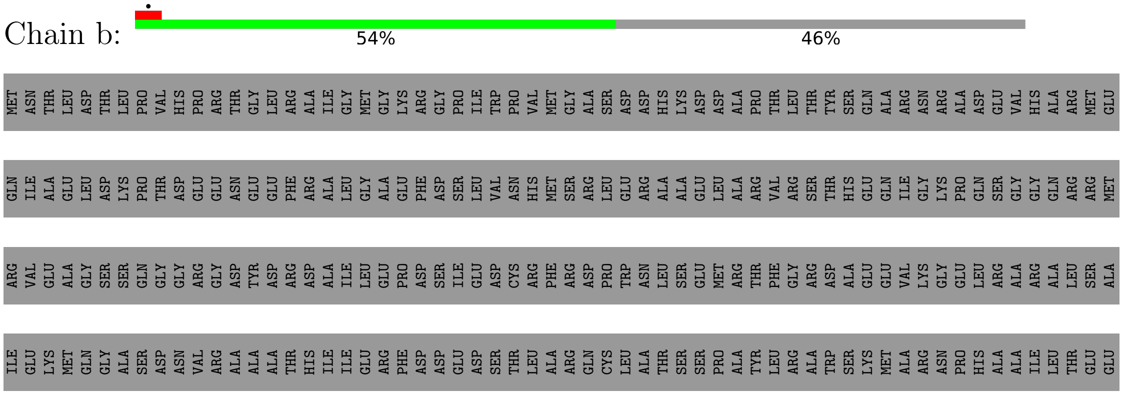
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

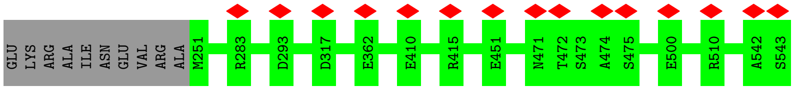


- Molecule 1: Phage capsid-like C-terminal domain-containing protein



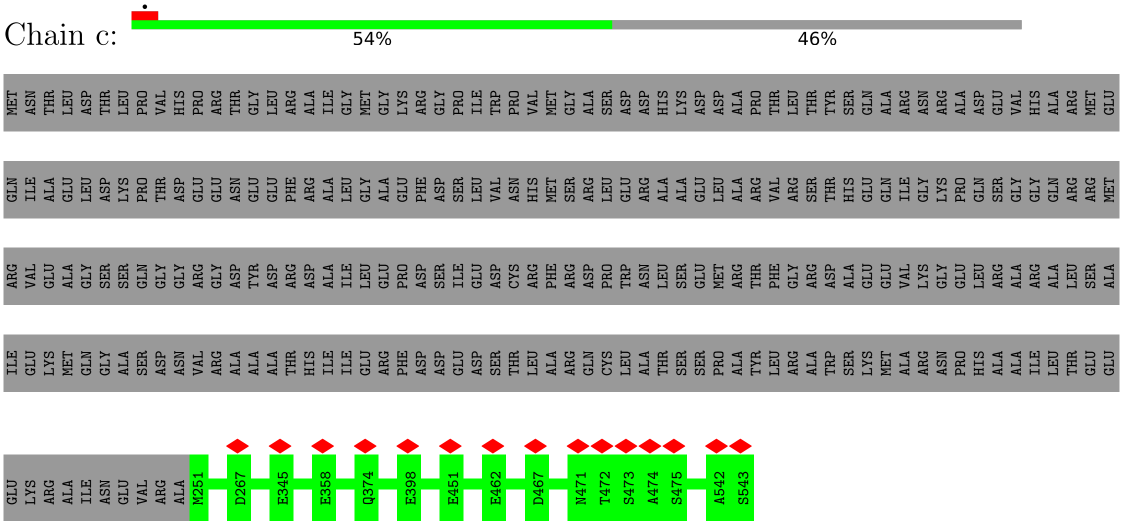
- Molecule 1: Phage capsid-like C-terminal domain-containing protein





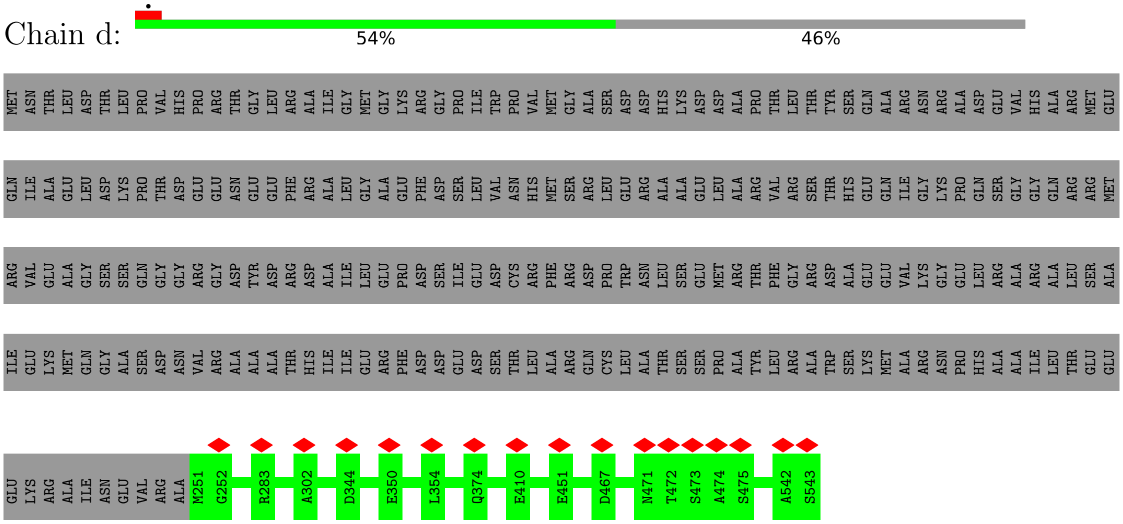
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain c:



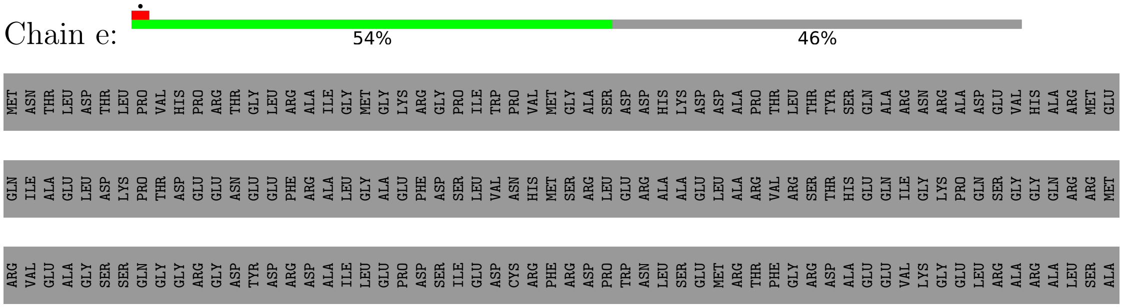
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

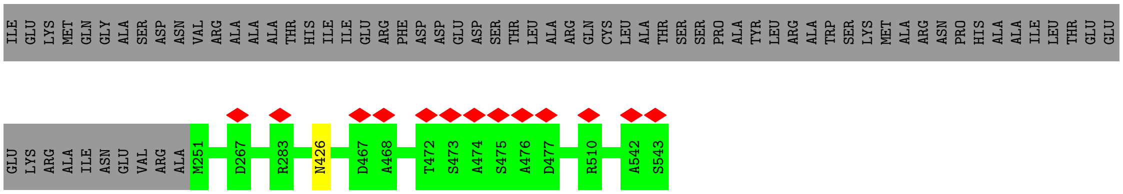
Chain d:



- Molecule 1: Phage capsid-like C-terminal domain-containing protein

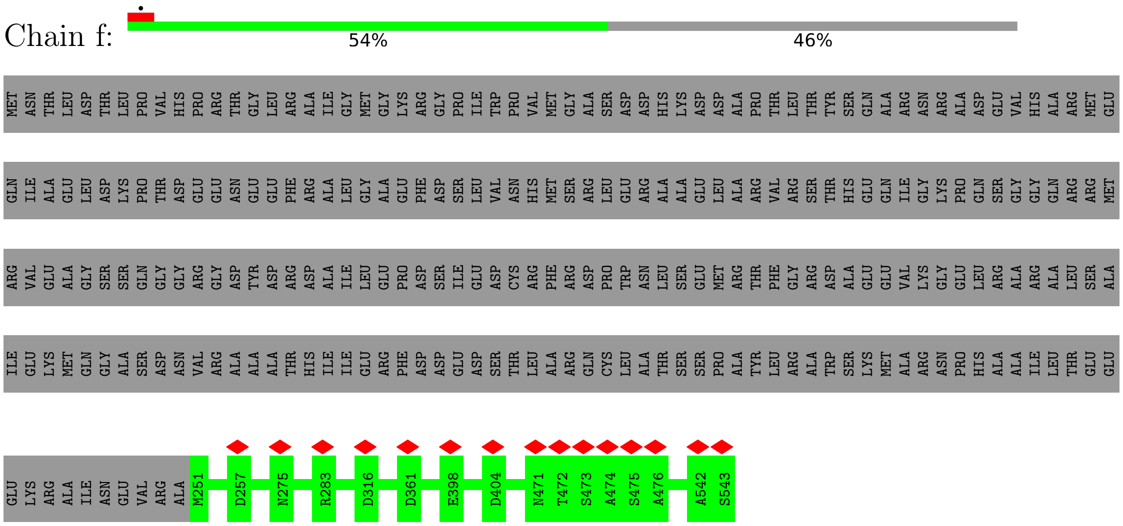
Chain e:





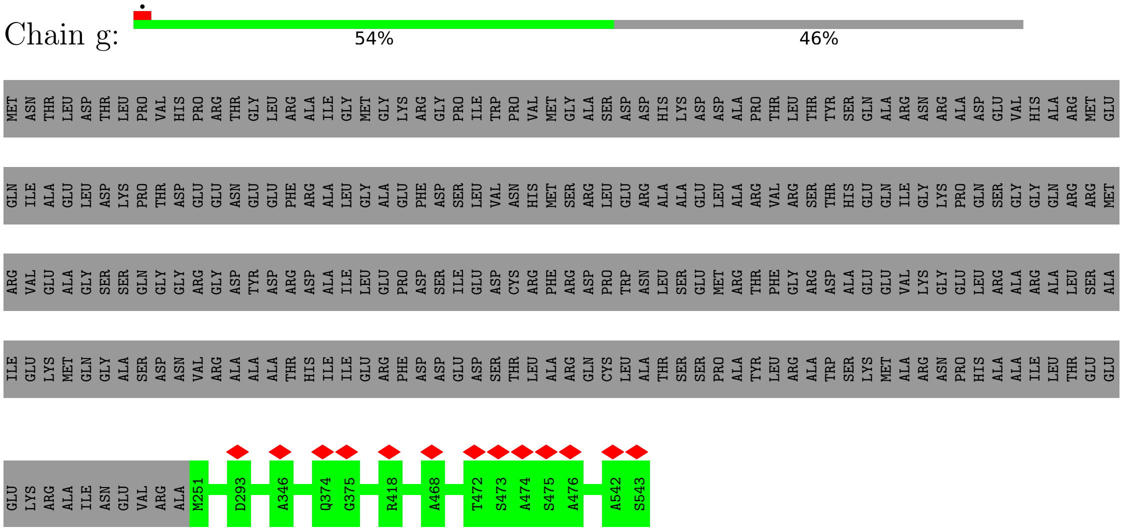
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain f:



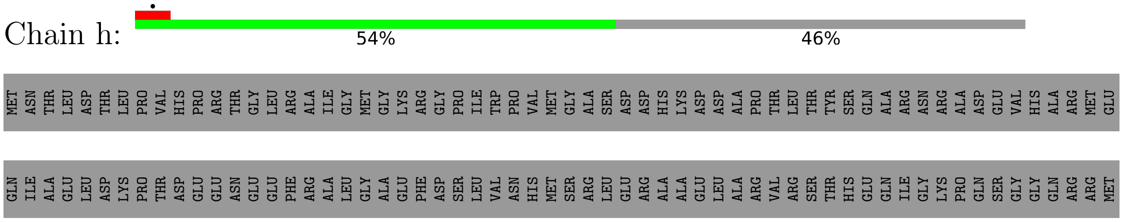
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

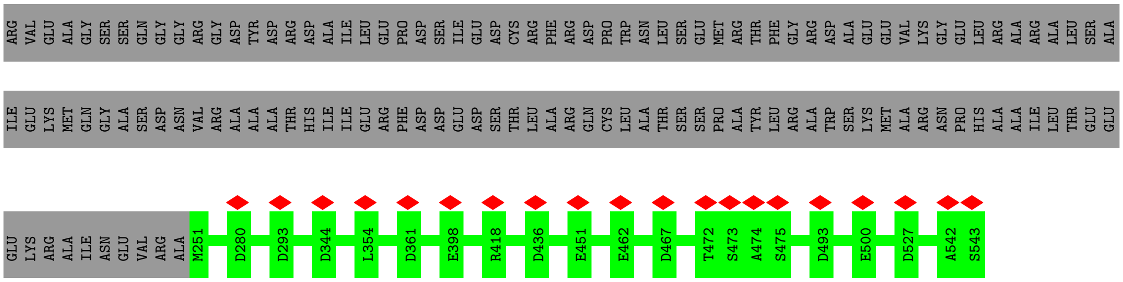
Chain g:



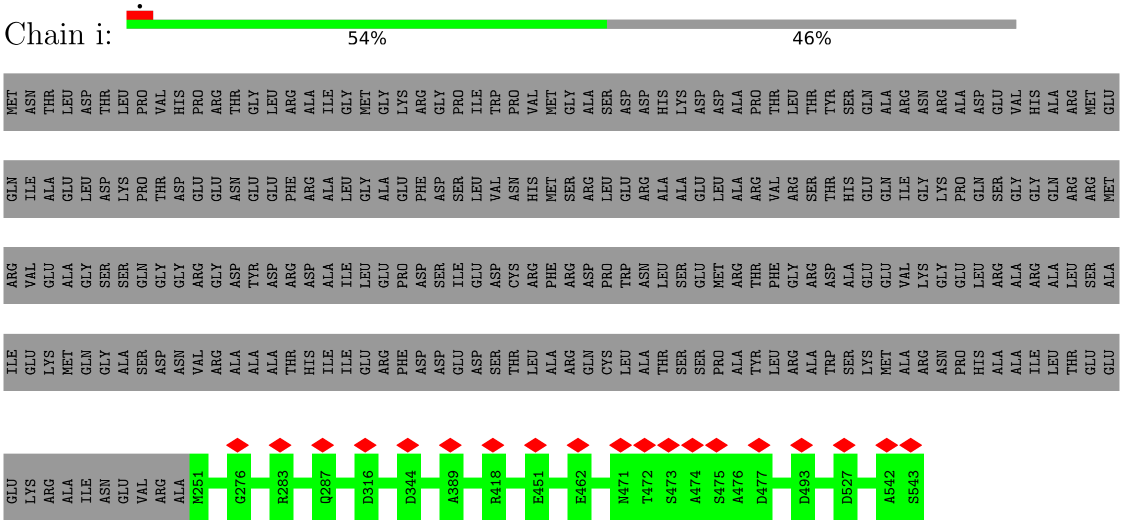
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain h:

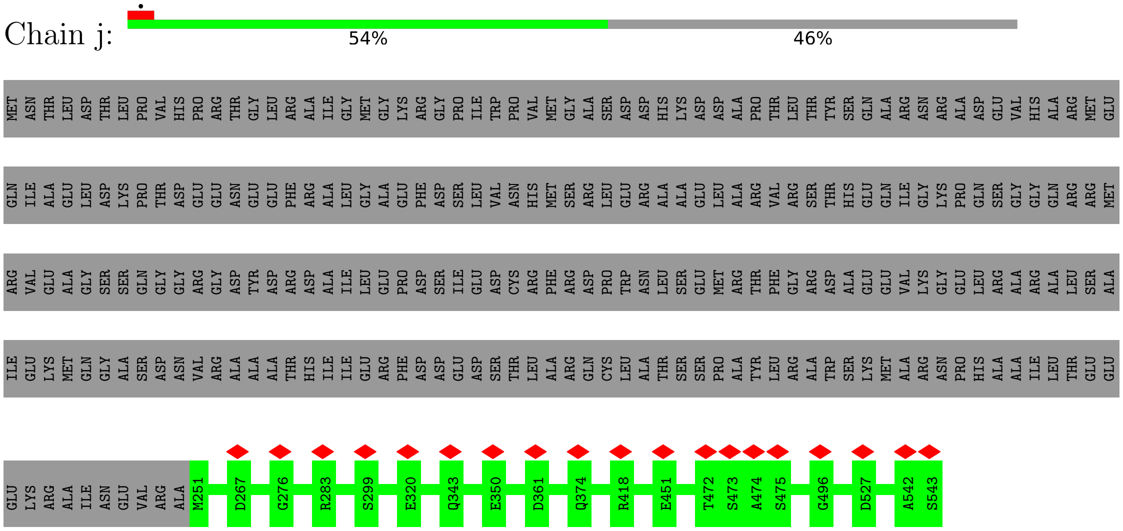




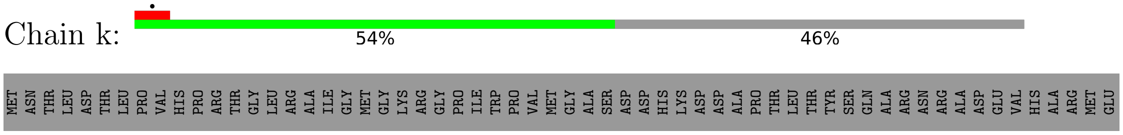
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

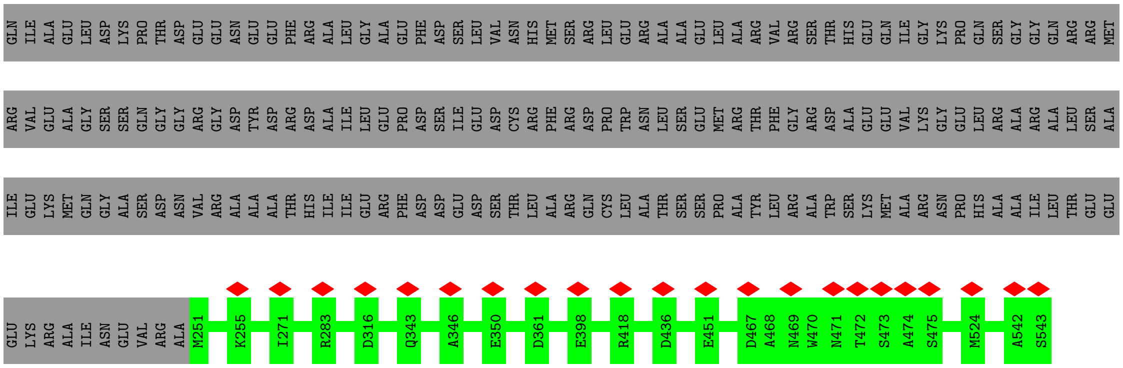


- Molecule 1: Phage capsid-like C-terminal domain-containing protein



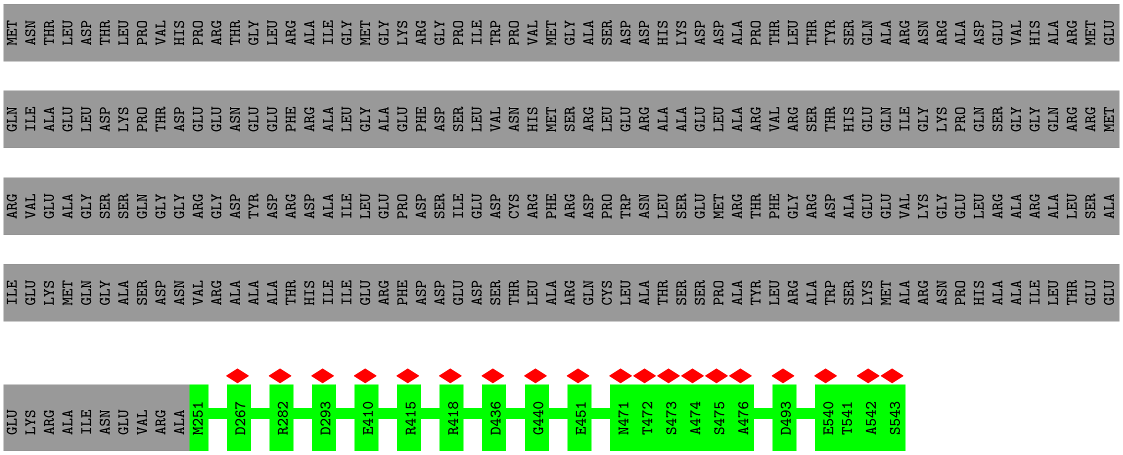
- Molecule 1: Phage capsid-like C-terminal domain-containing protein





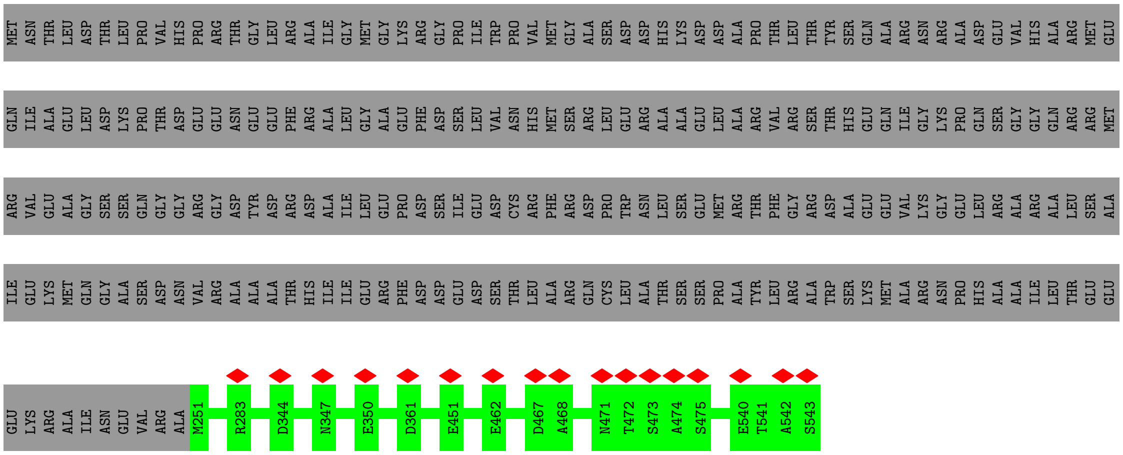
• Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain l:



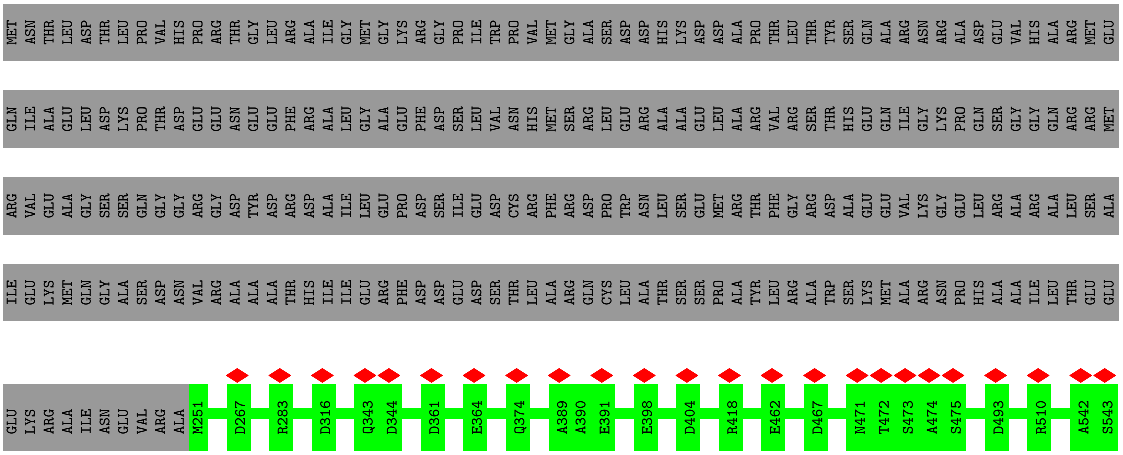
• Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain m:



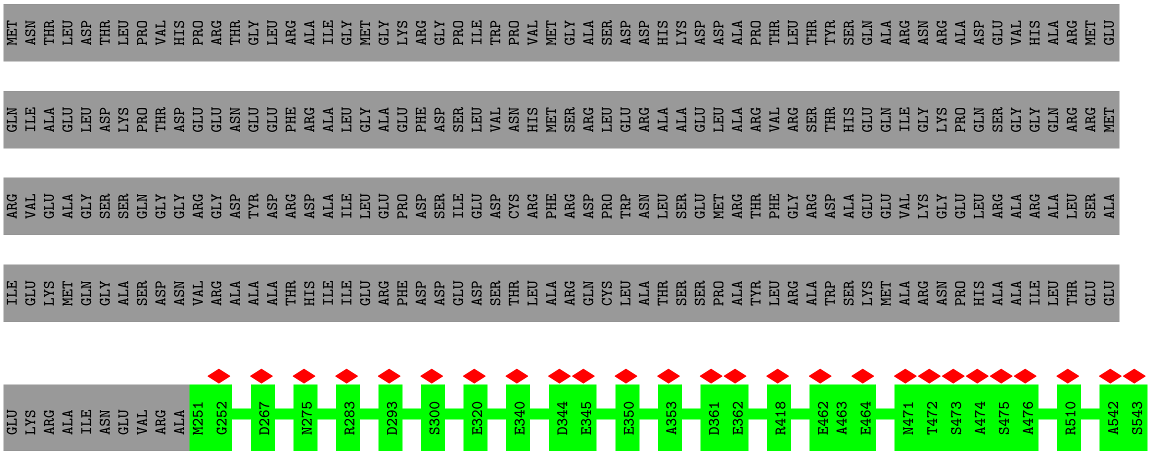
• Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain n:



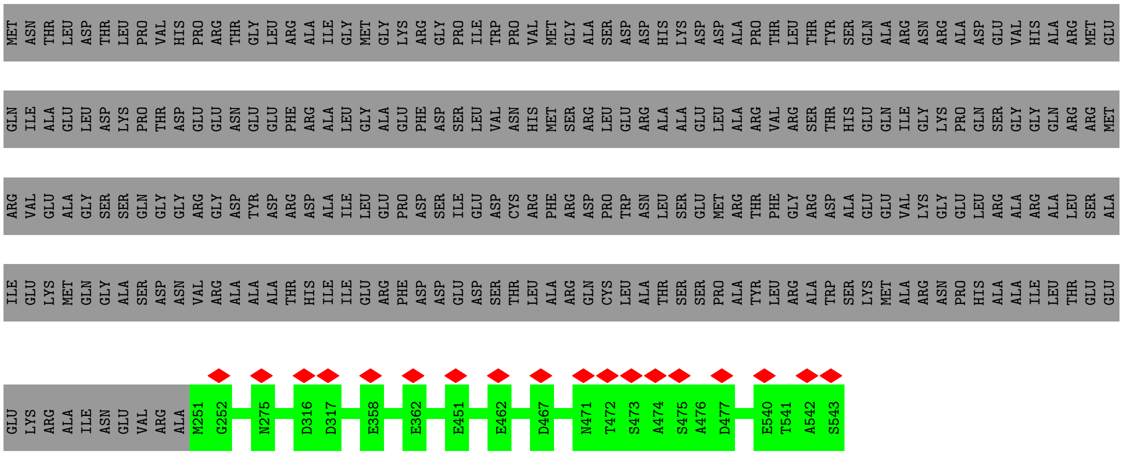
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain o:

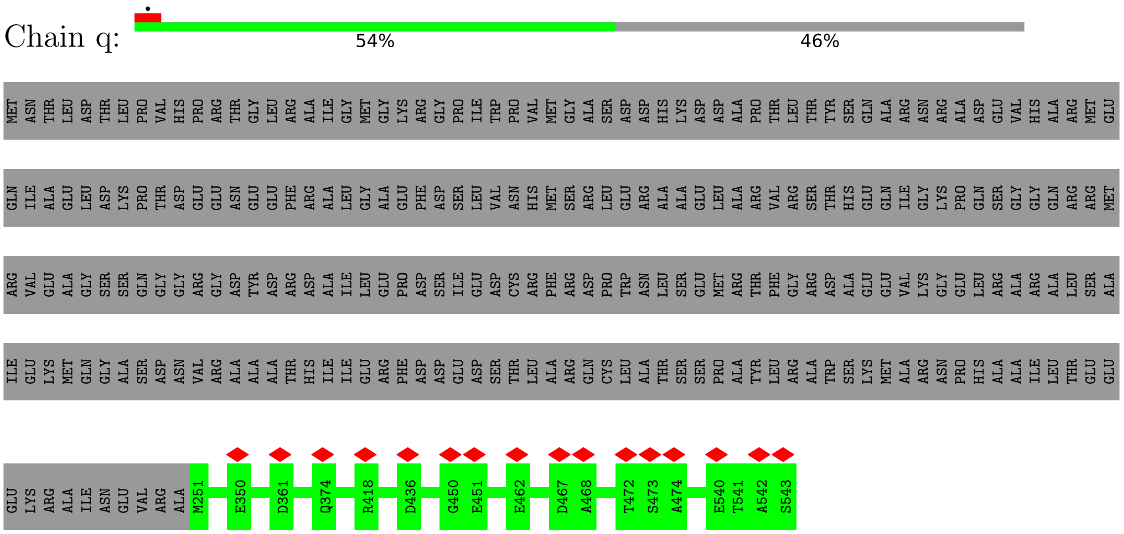


- Molecule 1: Phage capsid-like C-terminal domain-containing protein

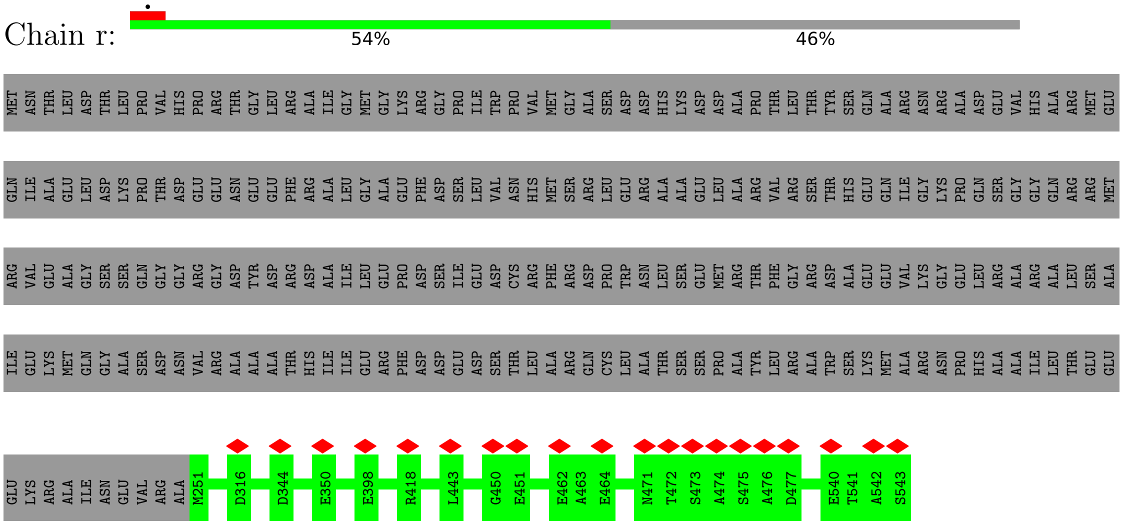
Chain p:



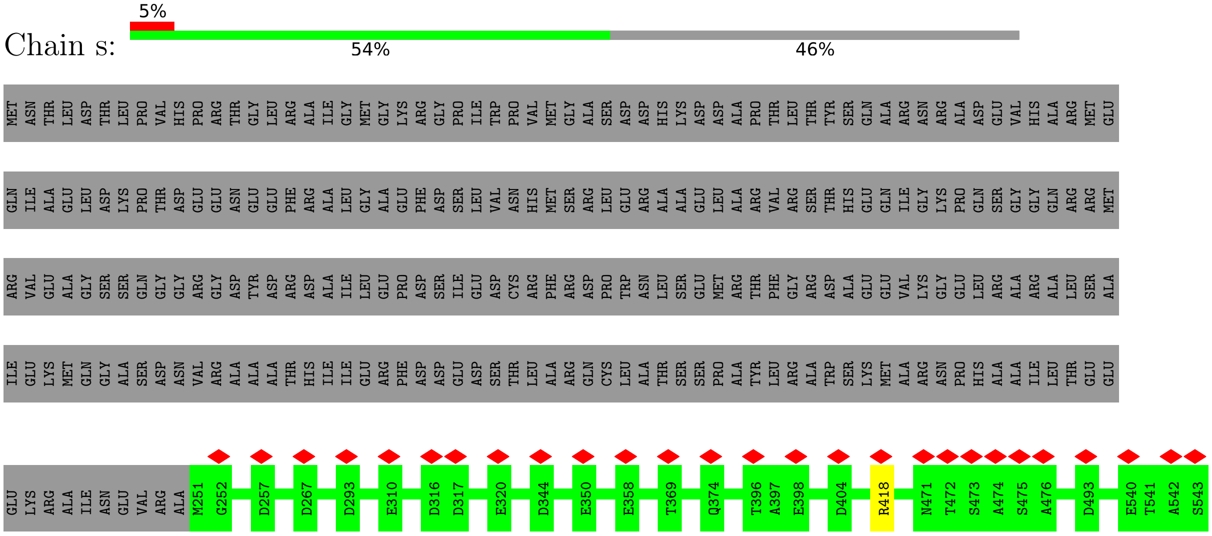
- Molecule 1: Phage capsid-like C-terminal domain-containing protein



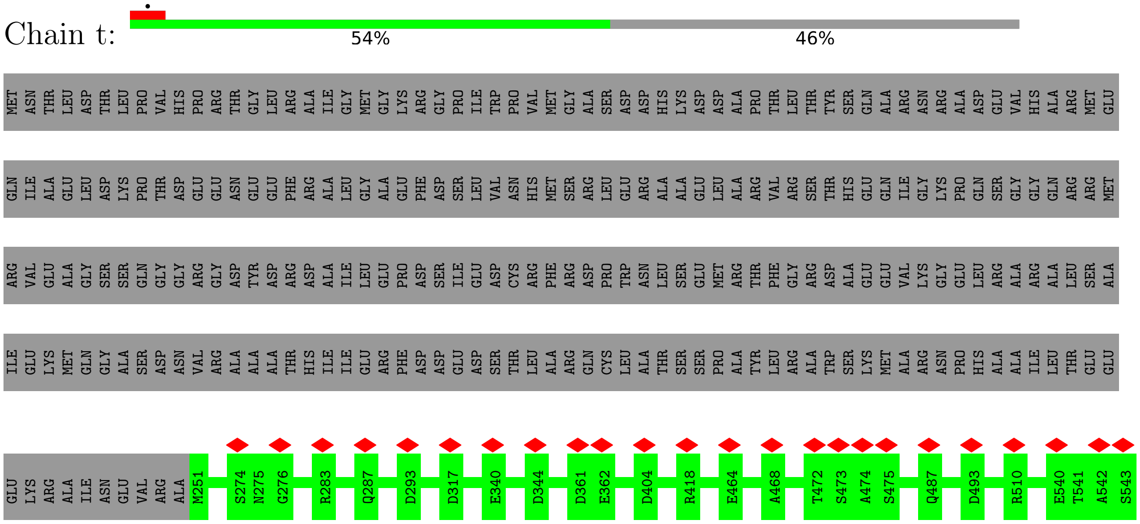
• Molecule 1: Phage capsid-like C-terminal domain-containing protein



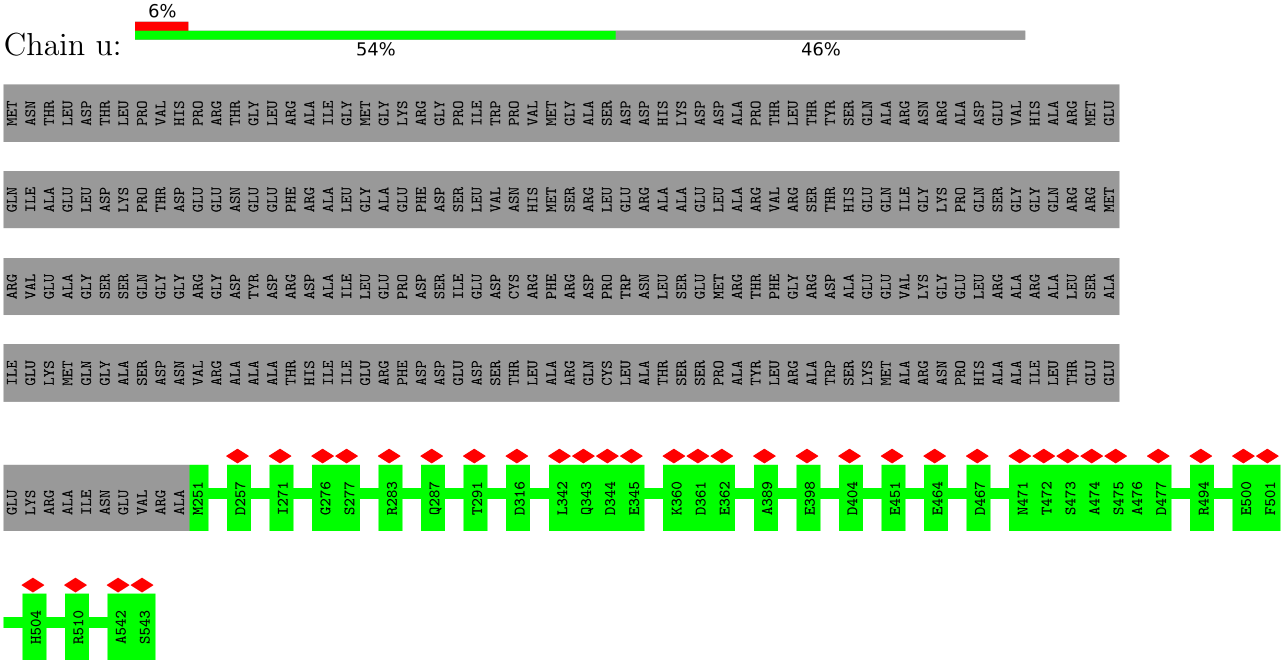
• Molecule 1: Phage capsid-like C-terminal domain-containing protein



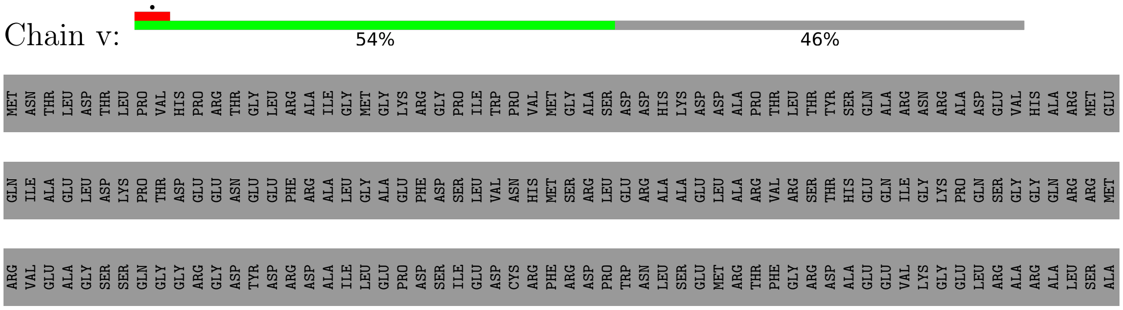
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

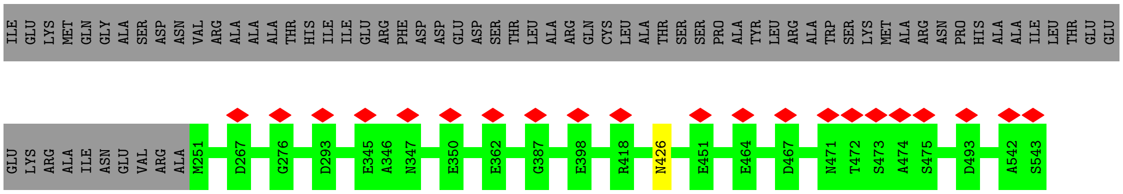


- Molecule 1: Phage capsid-like C-terminal domain-containing protein



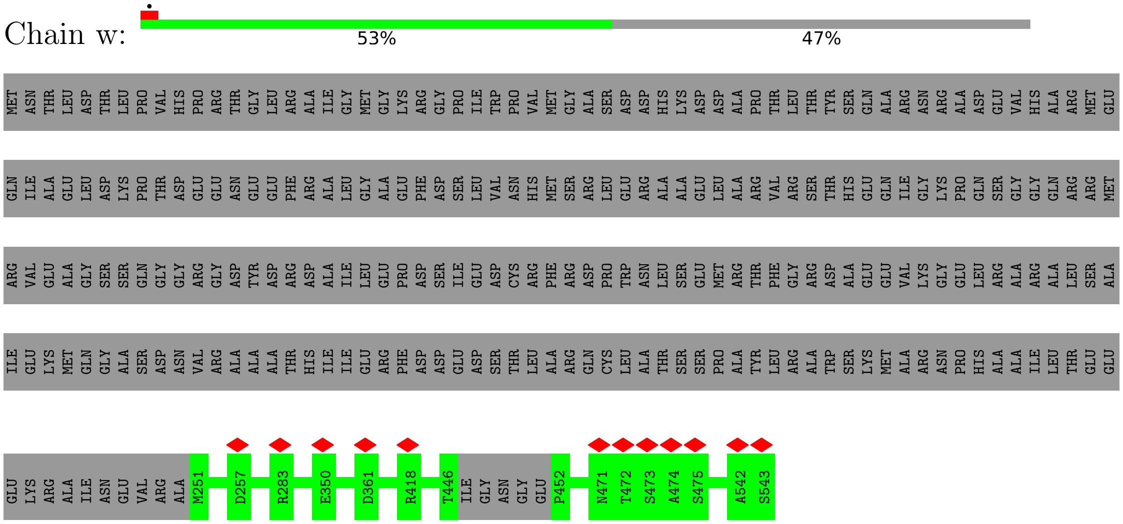
- Molecule 1: Phage capsid-like C-terminal domain-containing protein





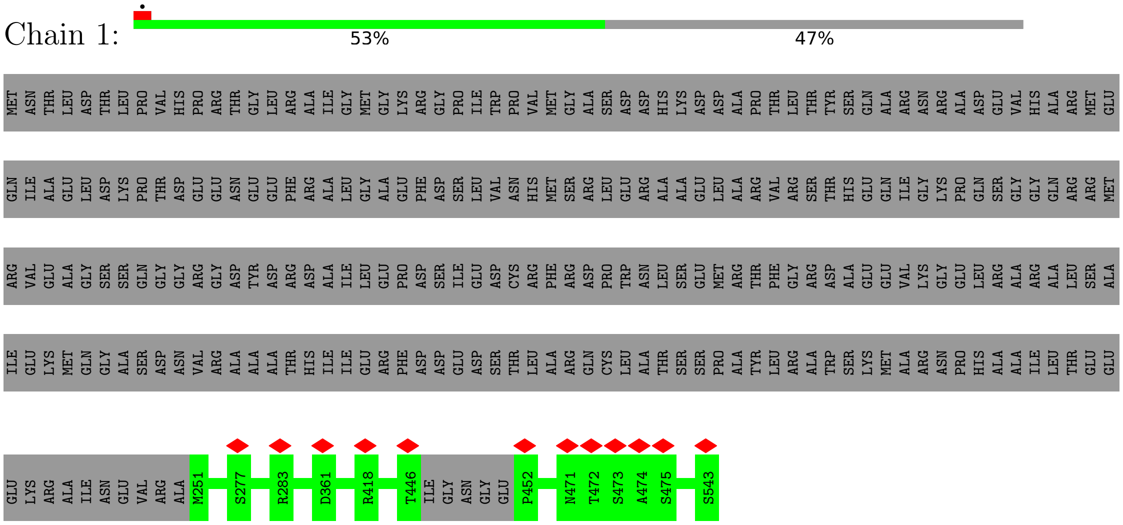
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain w:



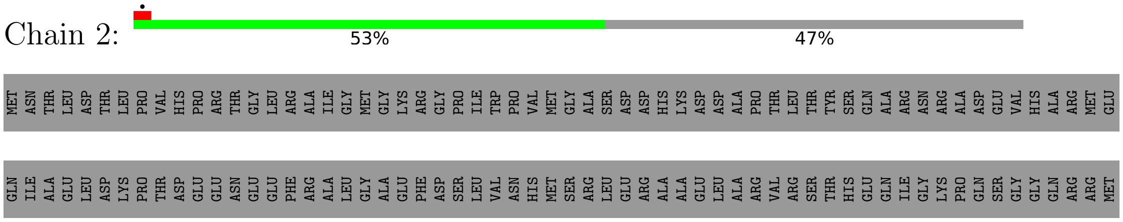
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

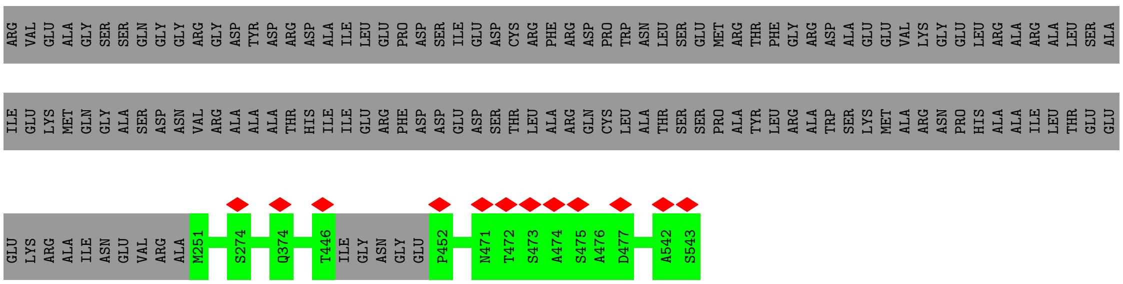
Chain 1:



- Molecule 1: Phage capsid-like C-terminal domain-containing protein

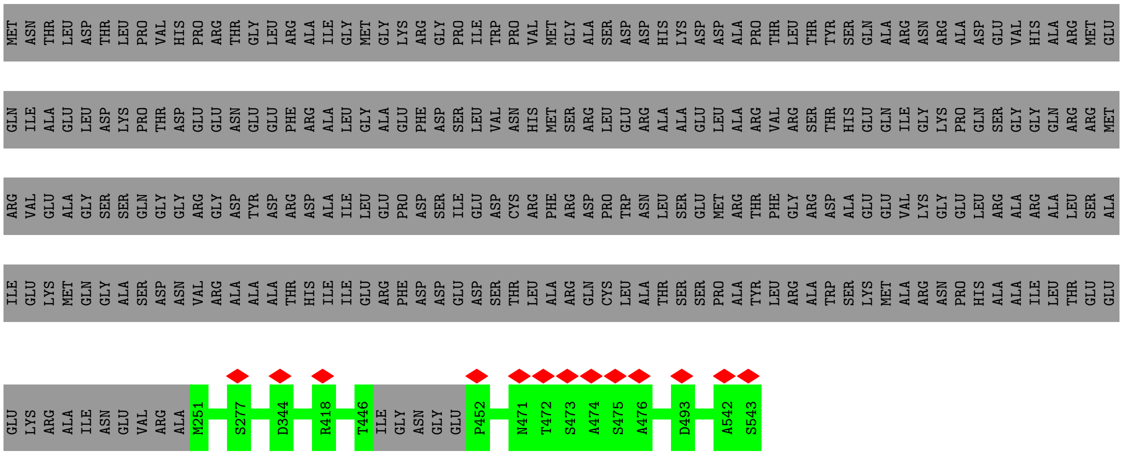
Chain 2:





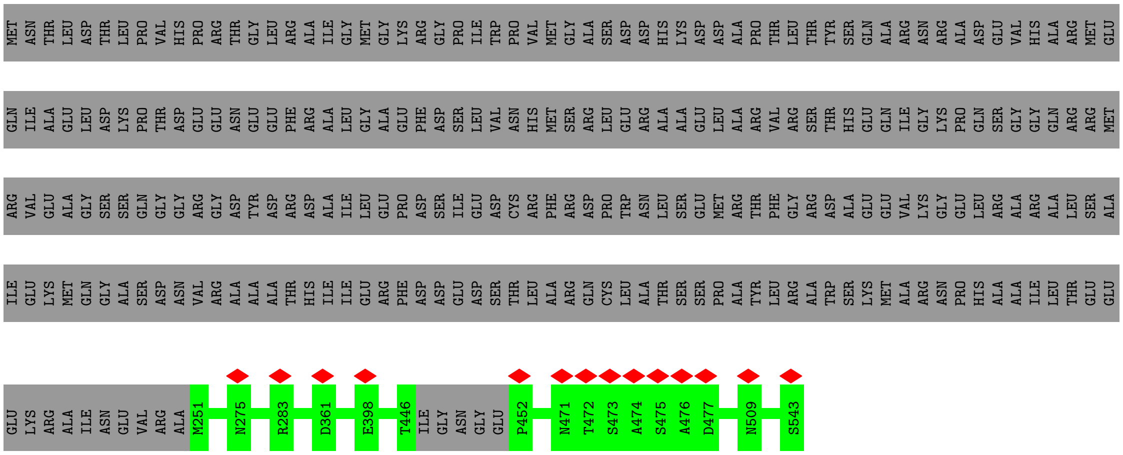
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain 3:



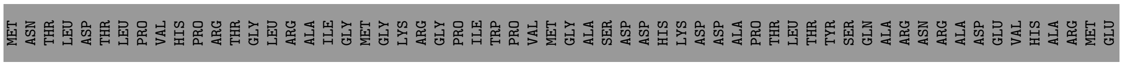
- Molecule 1: Phage capsid-like C-terminal domain-containing protein

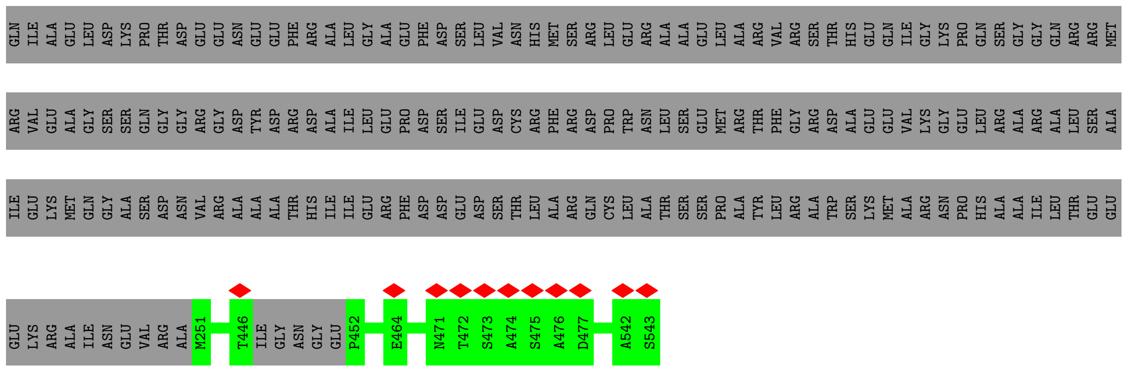
Chain 4:



- Molecule 1: Phage capsid-like C-terminal domain-containing protein

Chain 5:




GLN ILE ALA GLU LEU ASP LYS PRO THR ASP GLU GLU ASN GLU GLU PHE ARG ALA LEU GLY ALA GLU PHE ASP SER LEU VAL ASN HIS MET SER ARG LEU GLU ARG ALA ALA GLU LEU ALA ARG VAL ARG SER THR HIS GLU GLN ILE GLY LYS PRO GLN SER GLY GLY GLN ARG ARG MET
ARG VAL GLU ALA GLY SER SER GLN GLY GLY ARG GLY ASP TYR ASP ARG ASP ALA ILE LEU GLU PRO ASP SER ILE GLU ASP CYS ARG PHE ARG ASP PRO TRP ASN LEU SER GLU MET ARG THR PHE GLY ARG ASP ALA GLU GLU VAL LYS GLY GLU LEU ARG ALA ARG ALA LEU SER ALA
ILE GLU LYS MET GLN GLY ALA SER ASP ASN VAL ARG ALA ALA ALA THR HIS ILE ILE GLU ARG PHE ASP ASP GLU ASP SER THR LEU ALA ARG GLN CYS LEU ALA THR SER SER PRO ALA TYR LEU ARG ALA TRP SER LYS MET ALA ARG ASN PRO HIS ALA ALA ILE LEU THR GLU GLU
GLU LYS ARG ALA ILE ASN GLU VAL ARG ALA M251 T446 ILE GLY ASN GLY GLU P452 E464 N471 T472 S473 A474 S475 A476 D477 A542 S543

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	19765	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 ($e^-/\text{Å}^2$)	25.7	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.098	Depositor
Minimum map value	-0.051	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0203	Depositor
Map size (Å)	823.2, 823.2, 823.2	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.6464, 1.6464, 1.6464	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	1	0.28	0/2258	0.49	0/3081
1	2	0.28	0/2258	0.50	0/3081
1	3	0.28	0/2258	0.49	0/3081
1	4	0.28	0/2258	0.50	0/3081
1	5	0.28	0/2258	0.49	0/3081
1	A	0.29	0/2292	0.49	0/3129
1	B	0.28	0/2292	0.50	0/3129
1	C	0.29	0/2292	0.48	0/3129
1	D	0.29	0/2292	0.50	0/3129
1	E	0.29	0/2292	0.50	0/3129
1	F	0.29	0/2292	0.51	0/3129
1	G	0.28	0/2292	0.50	0/3129
1	H	0.29	0/2292	0.50	0/3129
1	I	0.29	0/2292	0.51	0/3129
1	J	0.29	0/2292	0.50	0/3129
1	K	0.28	0/2292	0.49	0/3129
1	L	0.28	0/2292	0.49	0/3129
1	M	0.29	0/2292	0.50	0/3129
1	N	0.28	0/2292	0.50	0/3129
1	O	0.28	0/2292	0.50	0/3129
1	P	0.28	0/2292	0.49	0/3129
1	Q	0.28	0/2292	0.49	0/3129
1	R	0.28	0/2292	0.49	0/3129
1	S	0.28	0/2292	0.49	0/3129
1	T	0.29	0/2292	0.51	0/3129
1	U	0.28	0/2292	0.48	0/3129
1	V	0.29	0/2292	0.50	0/3129
1	W	0.27	0/2292	0.49	0/3129
1	X	0.28	0/2292	0.50	0/3129
1	Y	0.29	0/2292	0.50	0/3129
1	Z	0.28	0/2292	0.50	0/3129
1	a	0.28	0/2292	0.50	0/3129
1	b	0.28	0/2292	0.50	0/3129
1	c	0.27	0/2292	0.49	0/3129

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	d	0.27	0/2292	0.50	0/3129
1	e	0.28	0/2292	0.51	0/3129
1	f	0.28	0/2292	0.49	0/3129
1	g	0.28	0/2292	0.49	0/3129
1	h	0.28	0/2292	0.50	0/3129
1	i	0.28	0/2292	0.50	0/3129
1	j	0.28	0/2292	0.49	0/3129
1	k	0.28	0/2292	0.50	0/3129
1	l	0.28	0/2292	0.50	0/3129
1	m	0.28	0/2292	0.50	0/3129
1	n	0.27	0/2292	0.48	0/3129
1	o	0.27	0/2292	0.49	0/3129
1	p	0.28	0/2292	0.49	0/3129
1	q	0.28	0/2292	0.49	0/3129
1	r	0.27	0/2292	0.48	0/3129
1	s	0.27	0/2292	0.49	0/3129
1	t	0.27	0/2292	0.49	0/3129
1	u	0.27	0/2292	0.48	0/3129
1	v	0.27	0/2292	0.47	0/3129
1	w	0.28	0/2258	0.49	0/3081
All	All	0.28	0/123564	0.49	0/168678

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1	284/543 (52%)	278 (98%)	6 (2%)	0	100	100
1	2	284/543 (52%)	274 (96%)	10 (4%)	0	100	100
1	3	284/543 (52%)	277 (98%)	7 (2%)	0	100	100
1	4	284/543 (52%)	278 (98%)	6 (2%)	0	100	100
1	5	284/543 (52%)	278 (98%)	6 (2%)	0	100	100
1	A	291/543 (54%)	282 (97%)	9 (3%)	0	100	100
1	B	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	C	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	D	291/543 (54%)	285 (98%)	6 (2%)	0	100	100
1	E	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	F	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	G	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	H	291/543 (54%)	289 (99%)	2 (1%)	0	100	100
1	I	291/543 (54%)	289 (99%)	2 (1%)	0	100	100
1	J	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	K	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	L	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	M	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	N	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	O	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	P	291/543 (54%)	286 (98%)	5 (2%)	0	100	100
1	Q	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	R	291/543 (54%)	284 (98%)	7 (2%)	0	100	100
1	S	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	T	291/543 (54%)	289 (99%)	2 (1%)	0	100	100
1	U	291/543 (54%)	286 (98%)	5 (2%)	0	100	100
1	V	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	W	291/543 (54%)	284 (98%)	7 (2%)	0	100	100
1	X	291/543 (54%)	286 (98%)	5 (2%)	0	100	100
1	Y	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	Z	291/543 (54%)	285 (98%)	6 (2%)	0	100	100
1	a	291/543 (54%)	289 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	291/543 (54%)	285 (98%)	6 (2%)	0	100	100
1	c	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	d	291/543 (54%)	283 (97%)	8 (3%)	0	100	100
1	e	291/543 (54%)	282 (97%)	9 (3%)	0	100	100
1	f	291/543 (54%)	290 (100%)	1 (0%)	0	100	100
1	g	291/543 (54%)	283 (97%)	8 (3%)	0	100	100
1	h	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	i	291/543 (54%)	282 (97%)	9 (3%)	0	100	100
1	j	291/543 (54%)	286 (98%)	5 (2%)	0	100	100
1	k	291/543 (54%)	289 (99%)	2 (1%)	0	100	100
1	l	291/543 (54%)	288 (99%)	3 (1%)	0	100	100
1	m	291/543 (54%)	290 (100%)	1 (0%)	0	100	100
1	n	291/543 (54%)	289 (99%)	2 (1%)	0	100	100
1	o	291/543 (54%)	287 (99%)	4 (1%)	0	100	100
1	p	291/543 (54%)	284 (98%)	7 (2%)	0	100	100
1	q	291/543 (54%)	285 (98%)	6 (2%)	0	100	100
1	r	291/543 (54%)	286 (98%)	5 (2%)	0	100	100
1	s	291/543 (54%)	281 (97%)	10 (3%)	0	100	100
1	t	291/543 (54%)	290 (100%)	1 (0%)	0	100	100
1	u	291/543 (54%)	281 (97%)	10 (3%)	0	100	100
1	v	291/543 (54%)	289 (99%)	2 (1%)	0	100	100
1	w	284/543 (52%)	278 (98%)	6 (2%)	0	100	100
All	All	15672/29322 (53%)	15415 (98%)	257 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	226/432 (52%)	226 (100%)	0	100	100
1	2	226/432 (52%)	226 (100%)	0	100	100
1	3	226/432 (52%)	226 (100%)	0	100	100
1	4	226/432 (52%)	226 (100%)	0	100	100
1	5	226/432 (52%)	226 (100%)	0	100	100
1	A	229/432 (53%)	229 (100%)	0	100	100
1	B	229/432 (53%)	229 (100%)	0	100	100
1	C	229/432 (53%)	229 (100%)	0	100	100
1	D	229/432 (53%)	229 (100%)	0	100	100
1	E	229/432 (53%)	229 (100%)	0	100	100
1	F	229/432 (53%)	229 (100%)	0	100	100
1	G	229/432 (53%)	229 (100%)	0	100	100
1	H	229/432 (53%)	229 (100%)	0	100	100
1	I	229/432 (53%)	229 (100%)	0	100	100
1	J	229/432 (53%)	228 (100%)	1 (0%)	89	93
1	K	229/432 (53%)	229 (100%)	0	100	100
1	L	229/432 (53%)	229 (100%)	0	100	100
1	M	229/432 (53%)	229 (100%)	0	100	100
1	N	229/432 (53%)	229 (100%)	0	100	100
1	O	229/432 (53%)	229 (100%)	0	100	100
1	P	229/432 (53%)	229 (100%)	0	100	100
1	Q	229/432 (53%)	229 (100%)	0	100	100
1	R	229/432 (53%)	229 (100%)	0	100	100
1	S	229/432 (53%)	229 (100%)	0	100	100
1	T	229/432 (53%)	229 (100%)	0	100	100
1	U	229/432 (53%)	229 (100%)	0	100	100
1	V	229/432 (53%)	229 (100%)	0	100	100
1	W	229/432 (53%)	229 (100%)	0	100	100
1	X	229/432 (53%)	229 (100%)	0	100	100
1	Y	229/432 (53%)	229 (100%)	0	100	100
1	Z	229/432 (53%)	229 (100%)	0	100	100
1	a	229/432 (53%)	229 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	229/432 (53%)	229 (100%)	0	100	100
1	c	229/432 (53%)	229 (100%)	0	100	100
1	d	229/432 (53%)	229 (100%)	0	100	100
1	e	229/432 (53%)	228 (100%)	1 (0%)	89	93
1	f	229/432 (53%)	229 (100%)	0	100	100
1	g	229/432 (53%)	229 (100%)	0	100	100
1	h	229/432 (53%)	229 (100%)	0	100	100
1	i	229/432 (53%)	229 (100%)	0	100	100
1	j	229/432 (53%)	229 (100%)	0	100	100
1	k	229/432 (53%)	229 (100%)	0	100	100
1	l	229/432 (53%)	229 (100%)	0	100	100
1	m	229/432 (53%)	229 (100%)	0	100	100
1	n	229/432 (53%)	229 (100%)	0	100	100
1	o	229/432 (53%)	229 (100%)	0	100	100
1	p	229/432 (53%)	229 (100%)	0	100	100
1	q	229/432 (53%)	229 (100%)	0	100	100
1	r	229/432 (53%)	229 (100%)	0	100	100
1	s	229/432 (53%)	228 (100%)	1 (0%)	89	93
1	t	229/432 (53%)	229 (100%)	0	100	100
1	u	229/432 (53%)	229 (100%)	0	100	100
1	v	229/432 (53%)	228 (100%)	1 (0%)	89	93
1	w	226/432 (52%)	226 (100%)	0	100	100
All	All	12348/23328 (53%)	12344 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	426	ASN
1	e	426	ASN
1	s	418	ARG
1	v	426	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	487	GLN
1	I	438	GLN
1	M	343	GLN
1	O	532	ASN
1	P	275	ASN
1	Q	471	ASN
1	T	430	ASN
1	U	296	HIS
1	U	376	ASN
1	Y	504	HIS
1	e	426	ASN
1	f	426	ASN
1	g	376	ASN
1	q	275	ASN
1	t	279	ASN
1	4	323	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

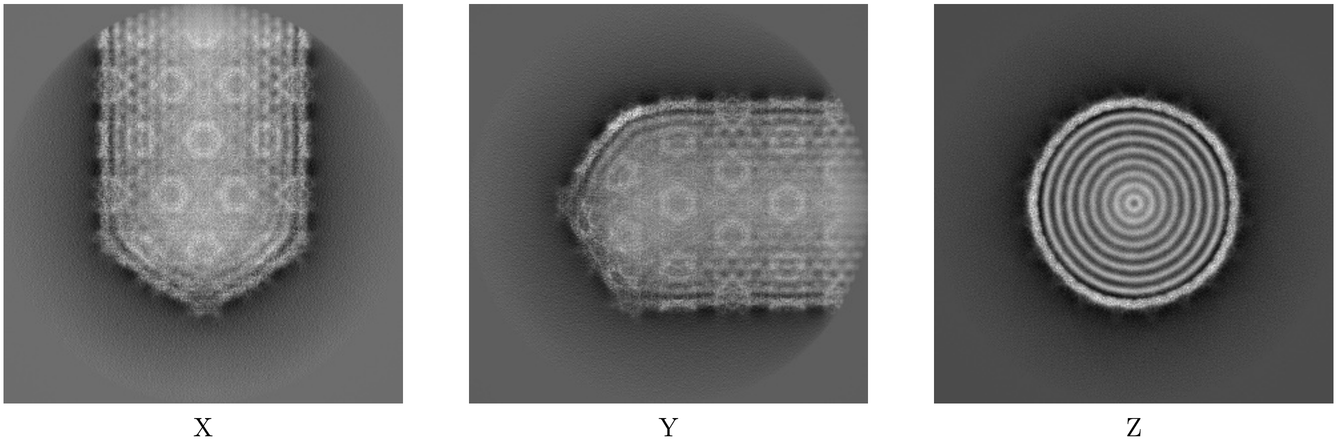
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-63432. These allow visual inspection of the internal detail of the map and identification of artifacts.

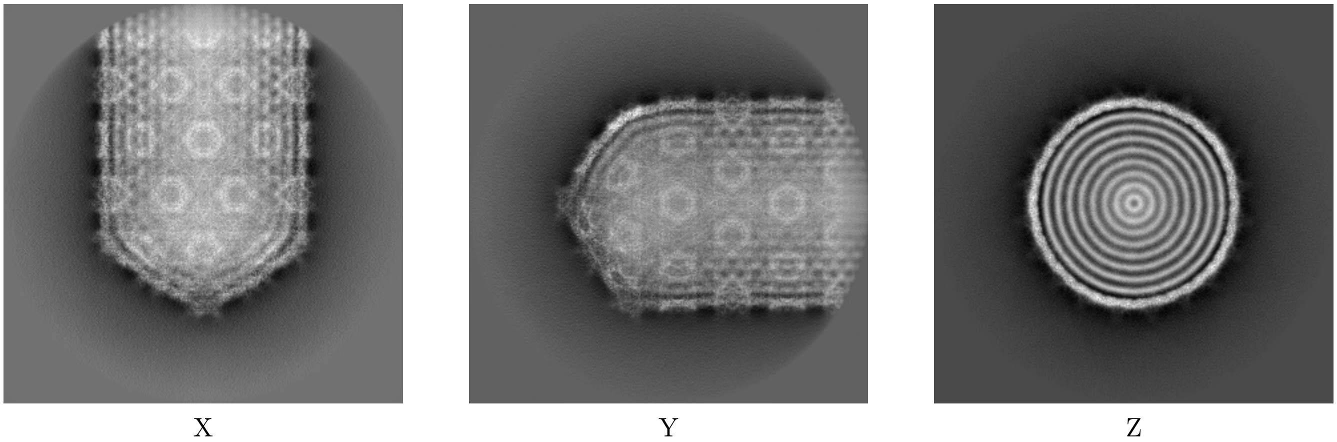
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ

6.1.1 Primary map



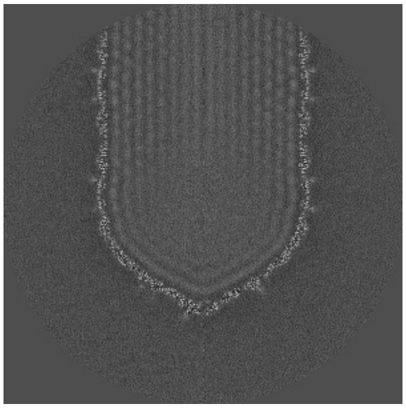
6.1.2 Raw map



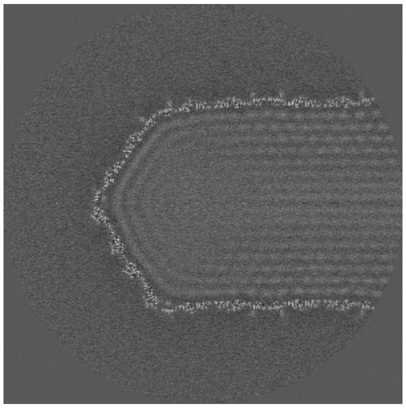
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

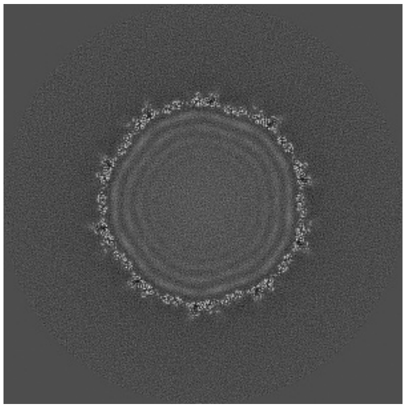
6.2.1 Primary map



X Index: 250

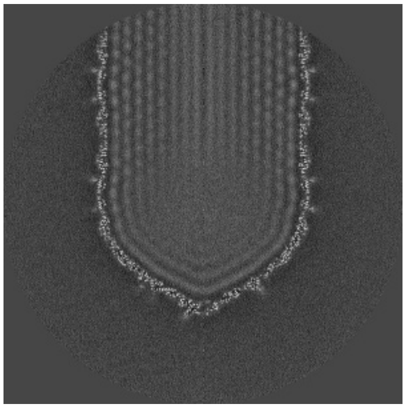


Y Index: 250

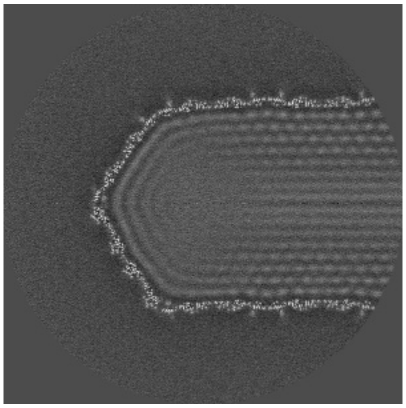


Z Index: 250

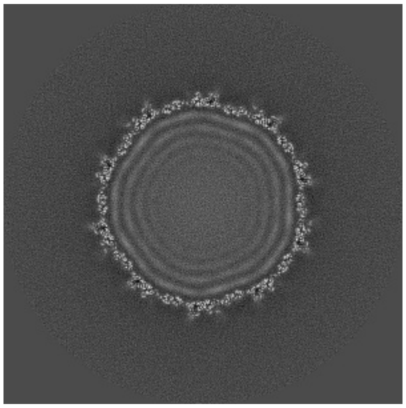
6.2.2 Raw map



X Index: 250



Y Index: 250

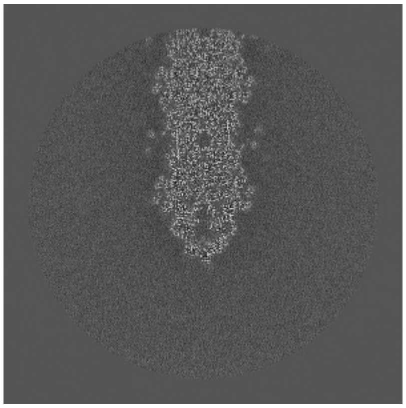


Z Index: 250

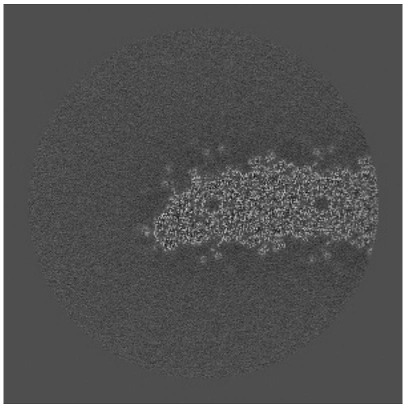
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

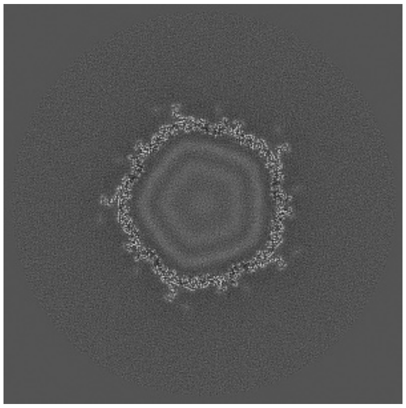
6.3.1 Primary map



X Index: 127

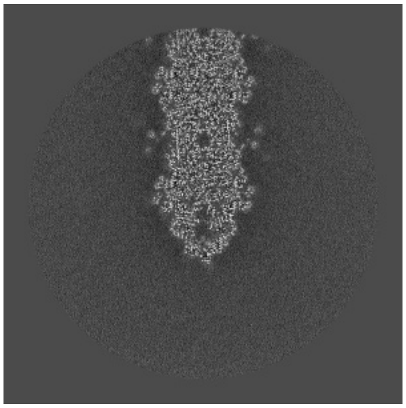


Y Index: 373

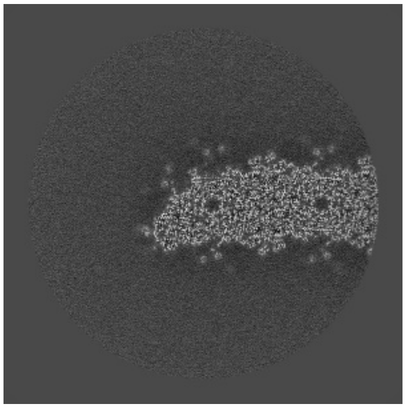


Z Index: 178

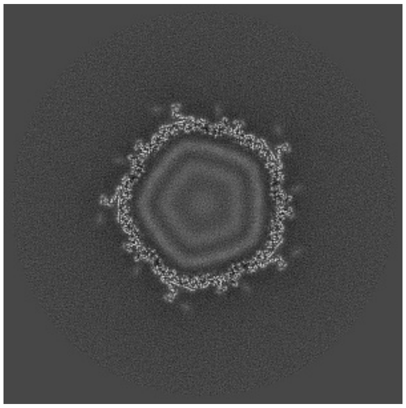
6.3.2 Raw map



X Index: 127



Y Index: 373

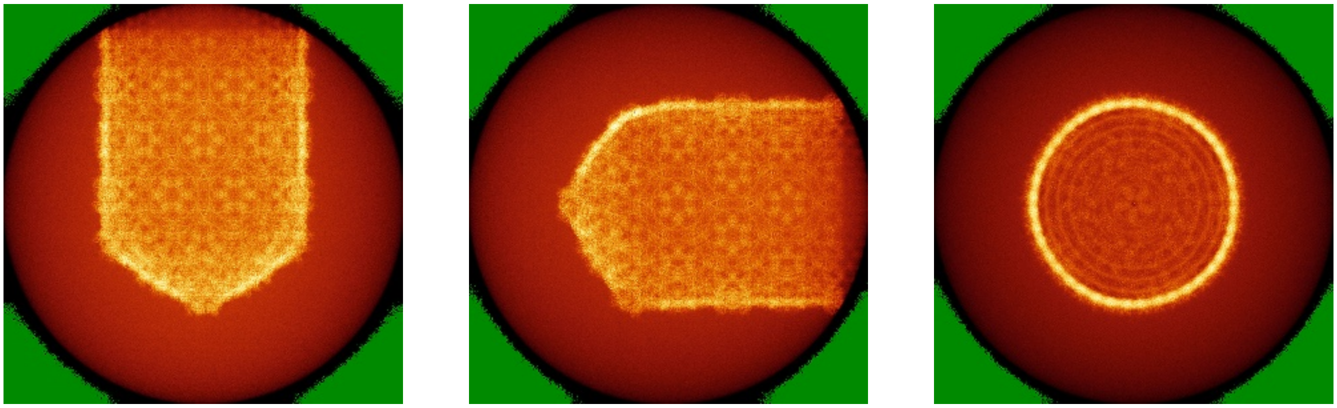


Z Index: 178

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

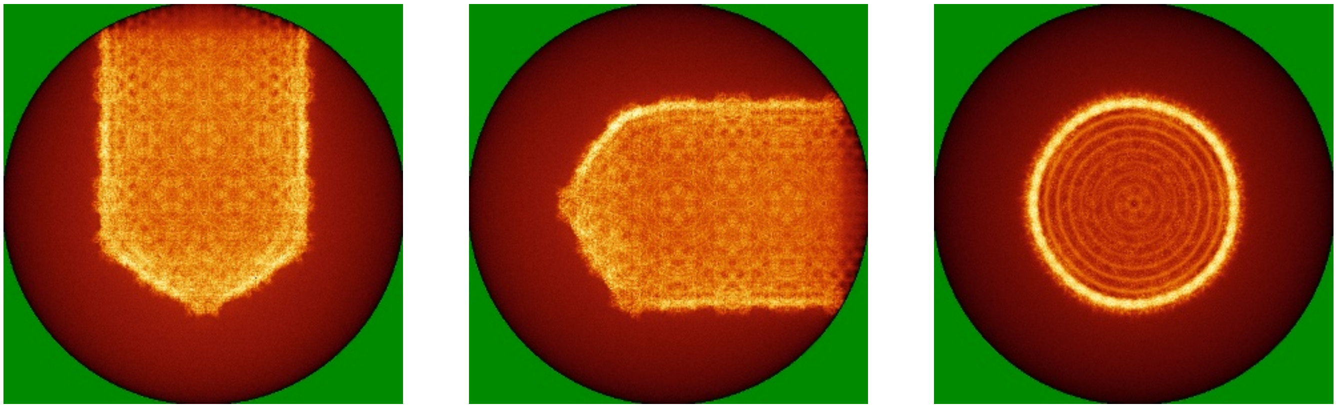
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



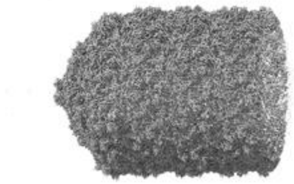
X Y Z

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.

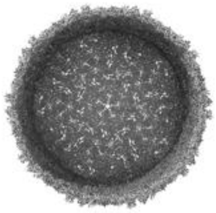
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X



Y

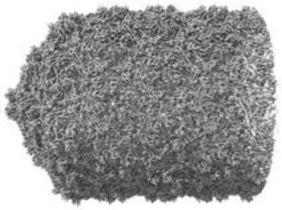


Z

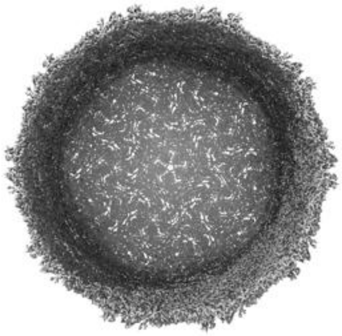
The images above show the 3D surface view of the map at the recommended contour level 0.0203. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X



Y



Z

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.

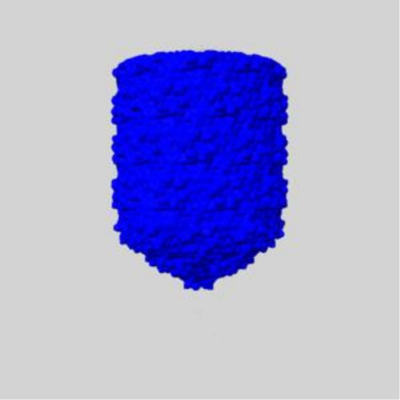
6.6 Mask visualisation ⓘ

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

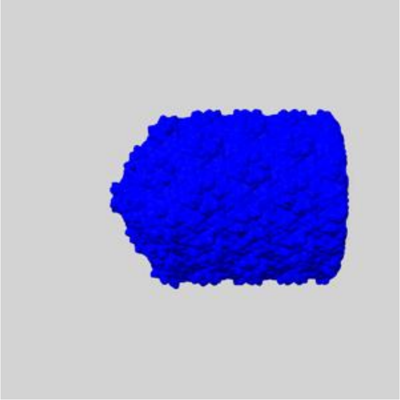
A mask typically either:

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

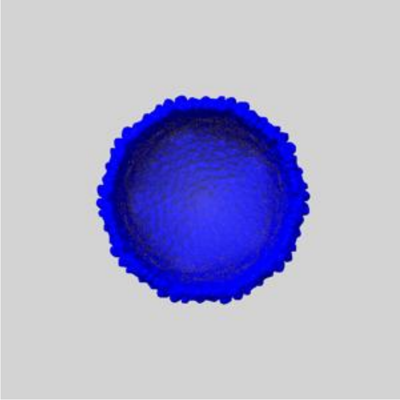
6.6.1 emd_63432_msk_1.map ⓘ



X



Y

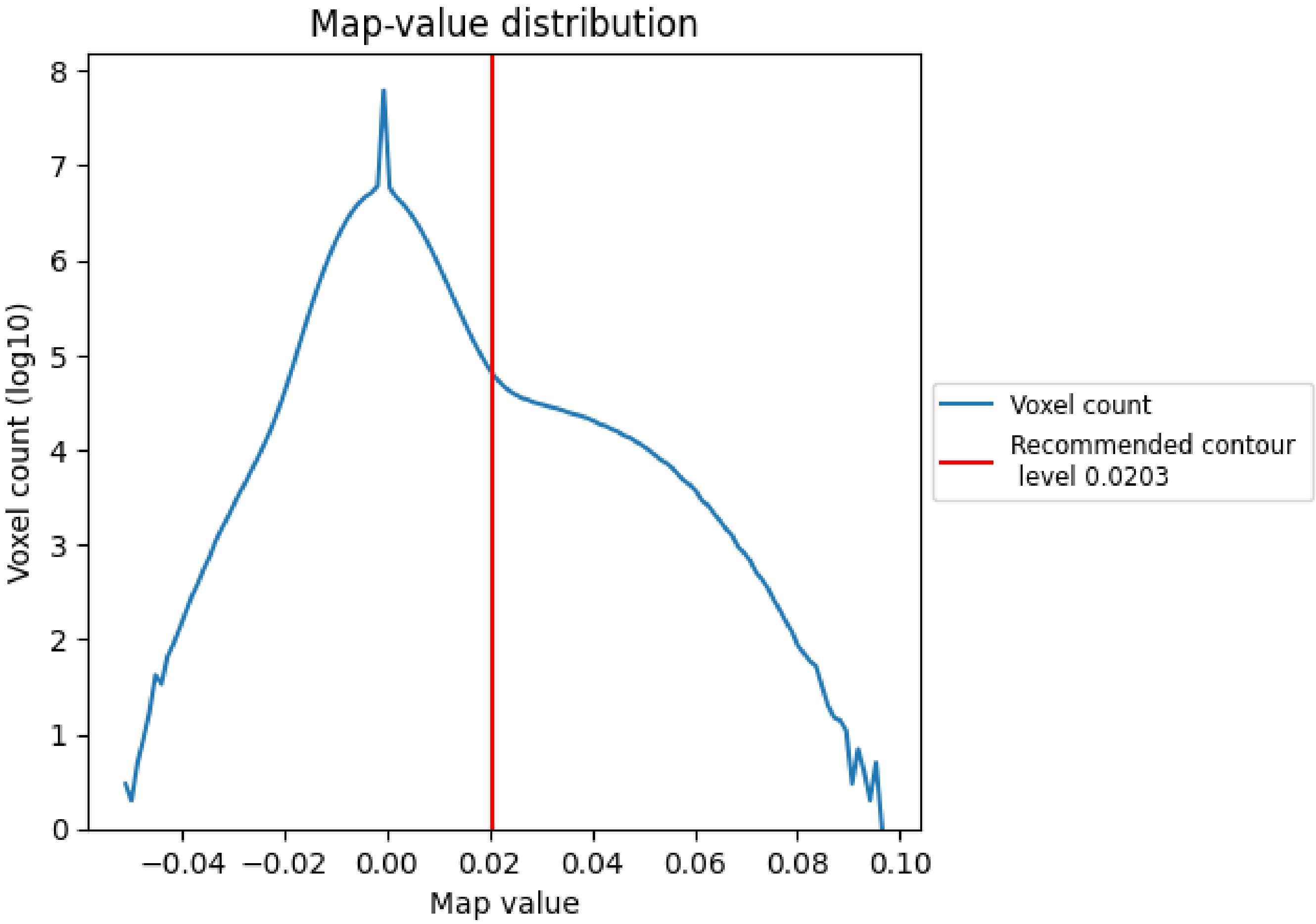


Z

7 Map analysis ⓘ

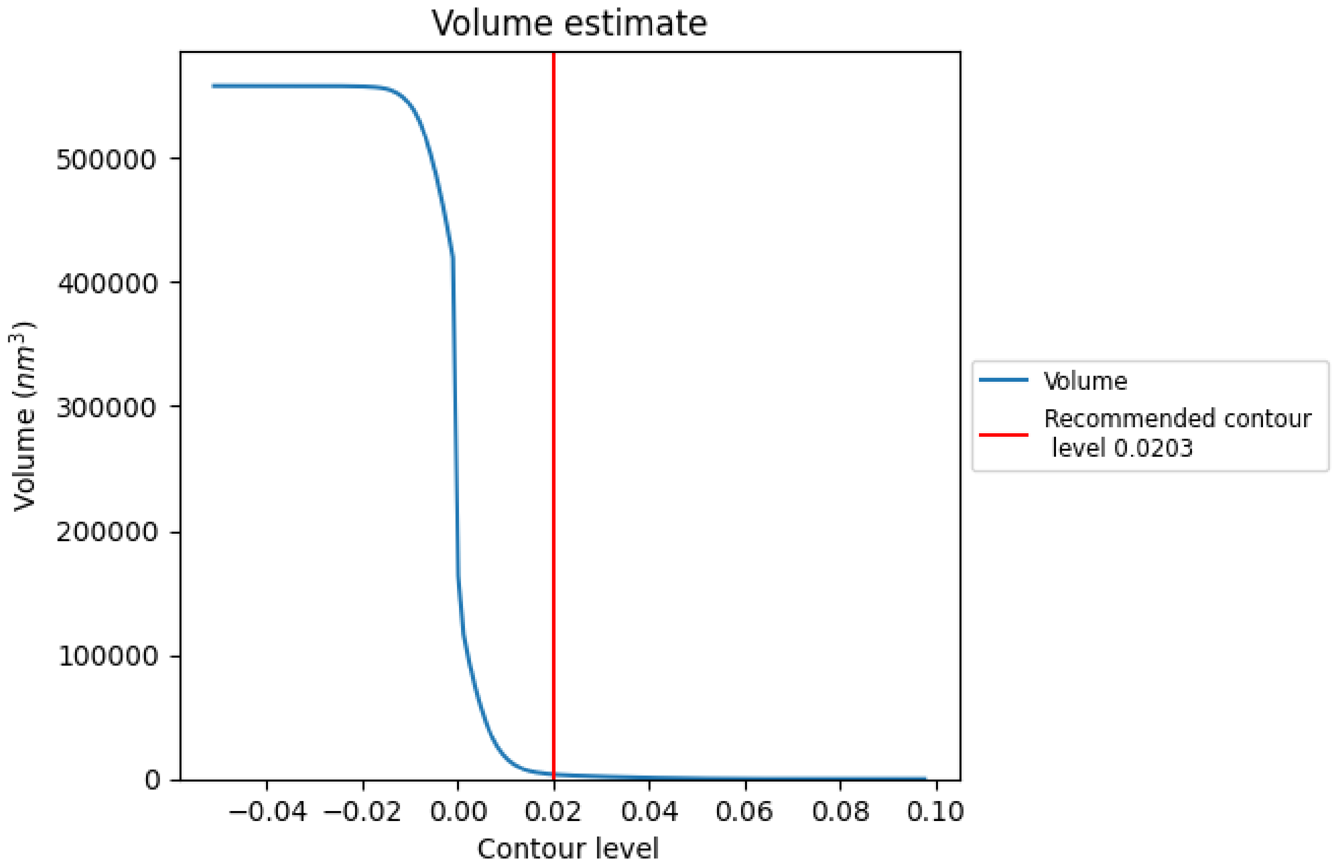
This section contains the results of statistical analysis of the map.

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.

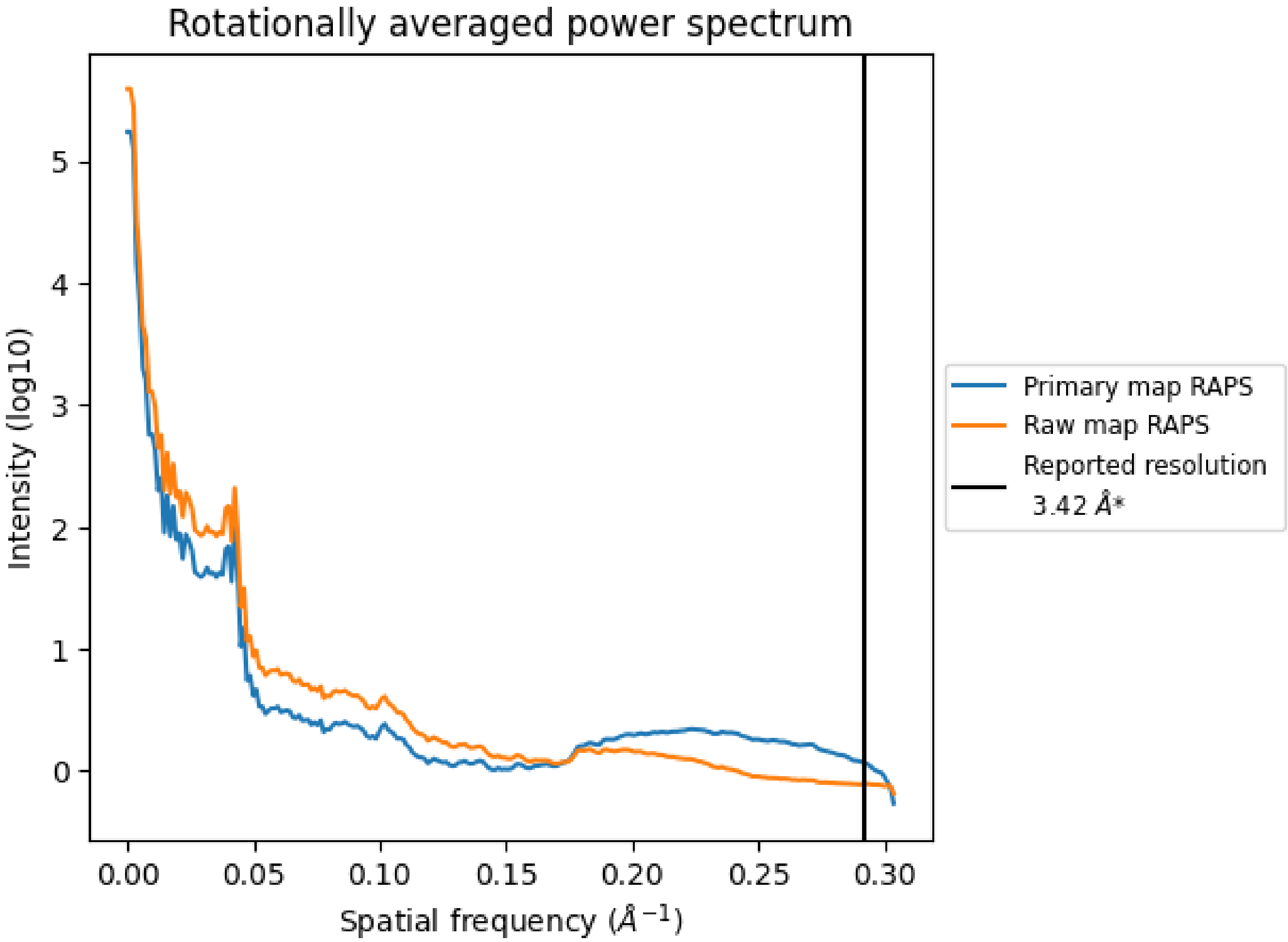
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 3591 nm^3; this corresponds to an approximate mass of 3244 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 ⓘ

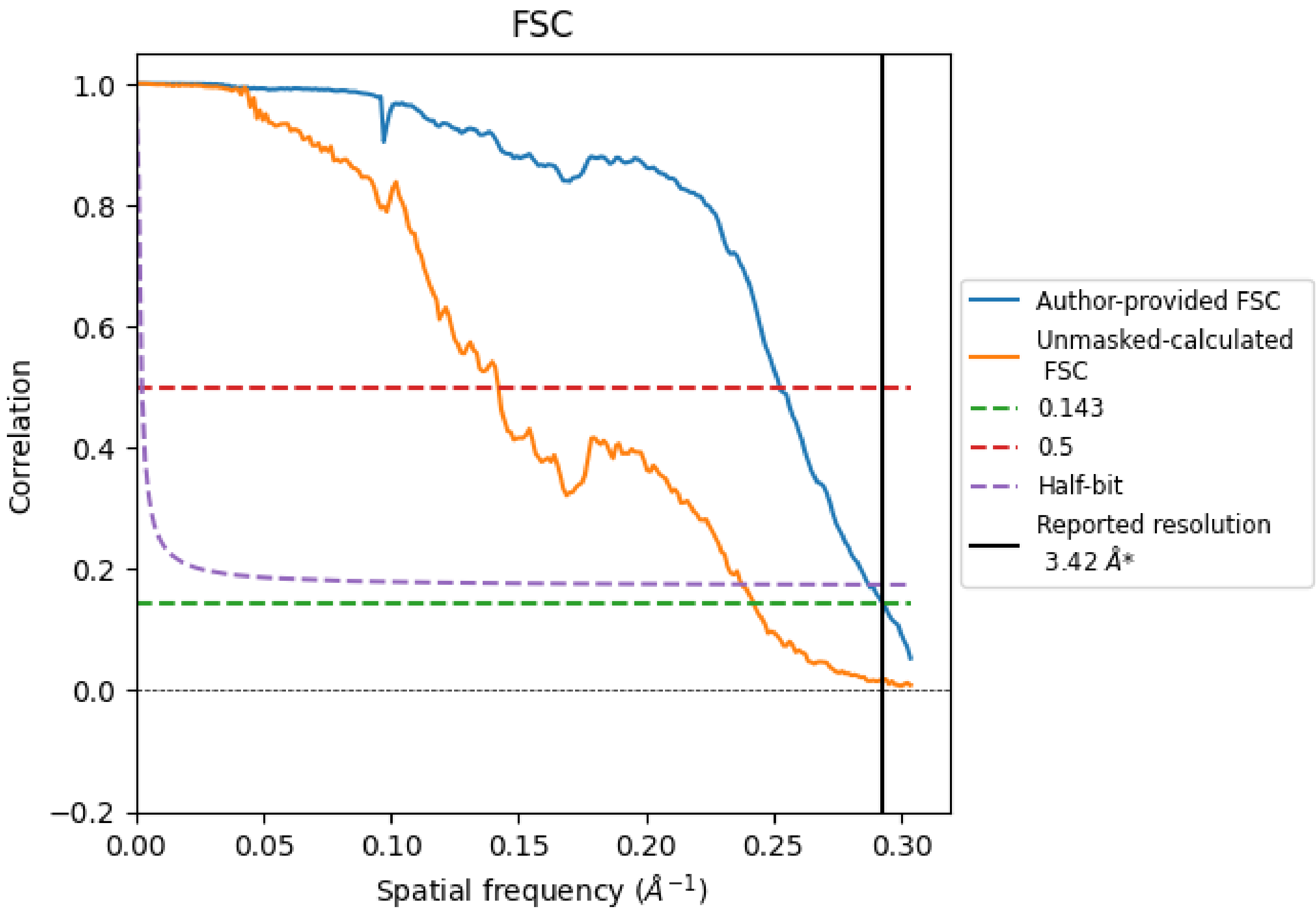


*Reported resolution corresponds to spatial frequency of 0.292 $Å^{-1}$

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.292 Å^{-1}

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.42	3.96	3.48
Unmasked-calculated*	4.13	7.03	4.21

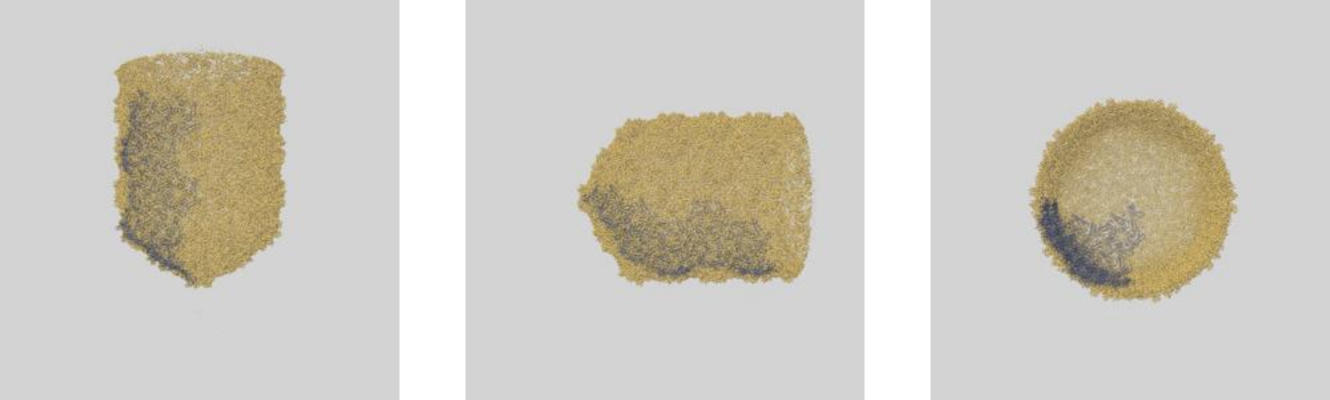
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.13 differs from the reported value 3.42 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-63432 and PDB model 9LW6. Per-residue inclusion information can be found in section 3 on page 10.

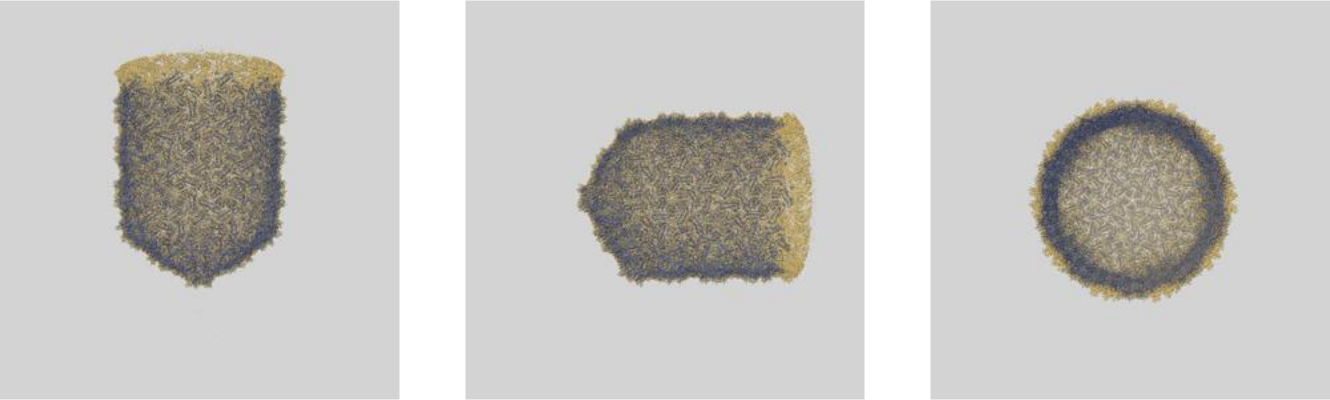
9.1 Map-model overlays

9.1.1 Map-model overlay



X Y Z

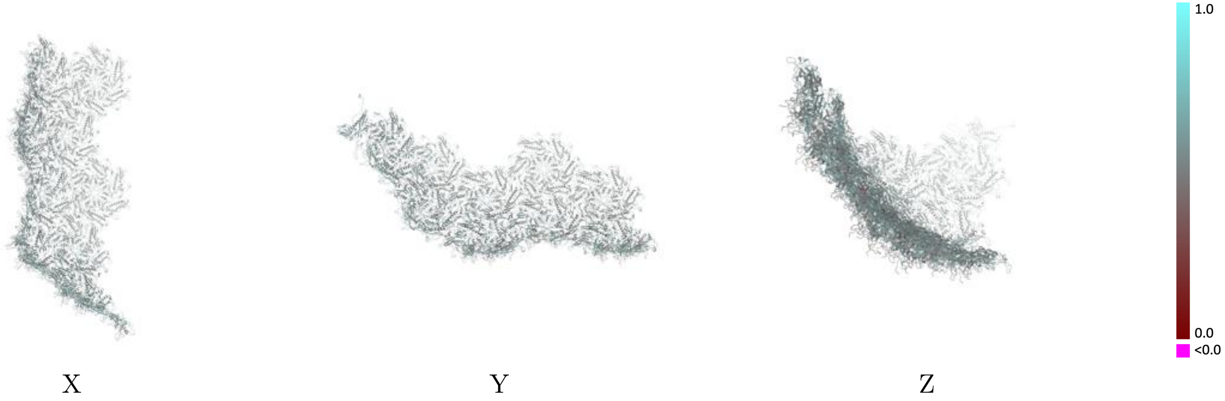
9.1.2 Map-model assembly overlay



X Y Z

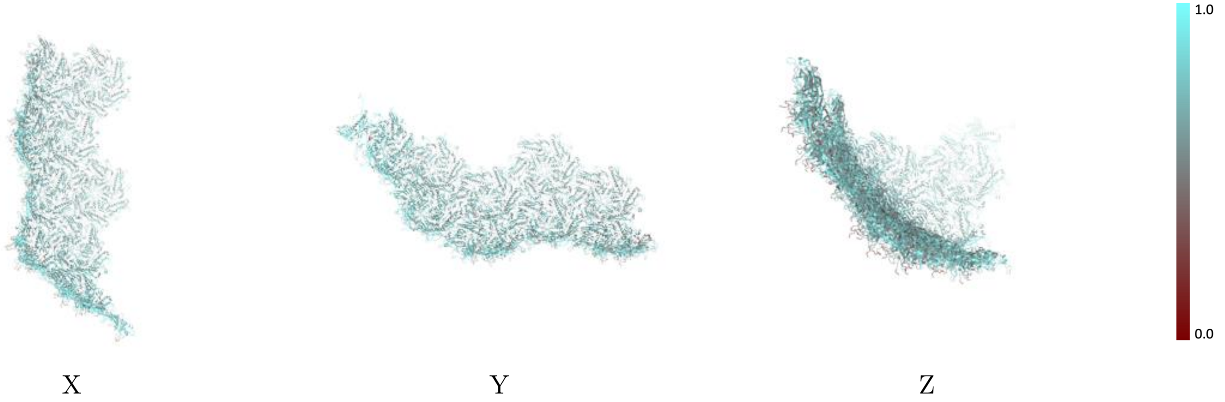
The images above show the 3D surface view of the map at the recommended contour level 0.0203 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



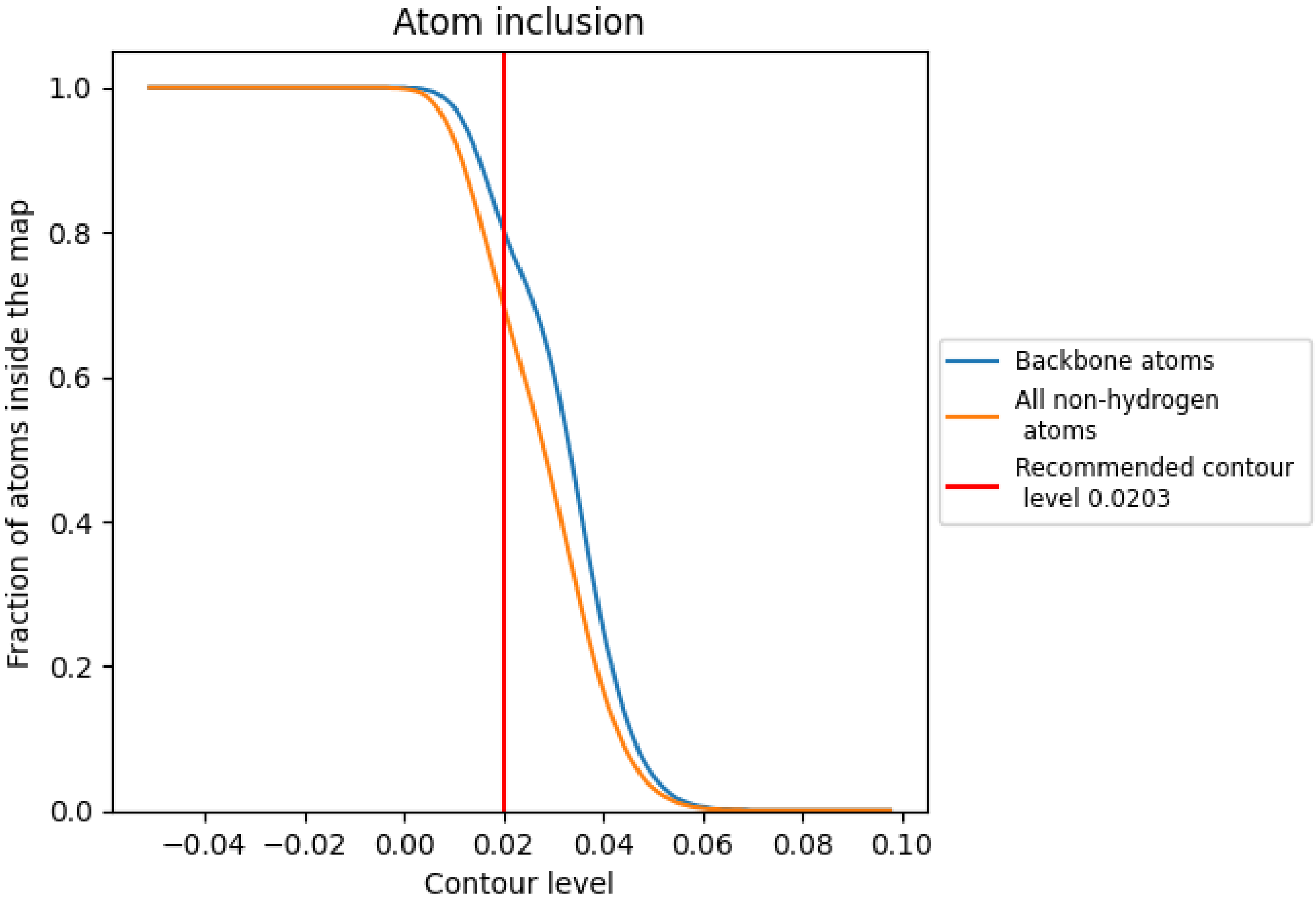
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.0203).

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 69% 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 (0.0203) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6940	0.5300
1	0.7180	0.5340
2	0.7100	0.5310
3	0.7090	0.5290
4	0.7000	0.5270
5	0.6990	0.5260
A	0.7480	0.5470
B	0.7450	0.5410
C	0.7410	0.5480
D	0.7370	0.5370
E	0.7380	0.5440
F	0.7360	0.5430
G	0.7330	0.5370
H	0.7300	0.5370
I	0.7250	0.5330
J	0.7140	0.5350
K	0.6900	0.5340
L	0.7100	0.5320
M	0.6950	0.5330
N	0.7100	0.5340
O	0.7040	0.5320
P	0.6910	0.5350
Q	0.6870	0.5260
R	0.7000	0.5360
S	0.7060	0.5340
T	0.7050	0.5340
U	0.6900	0.5320
V	0.6930	0.5350
W	0.6830	0.5310
X	0.6930	0.5290
Y	0.6940	0.5300
Z	0.6880	0.5290
a	0.6880	0.5230
b	0.6840	0.5230
c	0.6840	0.5240

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Chain	Atom inclusion	Q-score
d	0.6760	0.5280
e	0.6840	0.5280
f	0.6880	0.5320
g	0.6890	0.5280
h	0.6830	0.5300
i	0.6940	0.5250
j	0.6860	0.5300
k	0.6710	0.5280
l	0.6700	0.5210
m	0.6590	0.5160
n	0.6440	0.5190
o	0.6310	0.5110
p	0.6500	0.5190
q	0.6710	0.5270
r	0.6700	0.5200
s	0.6560	0.5200
t	0.6430	0.5230
u	0.6140	0.5120
v	0.6540	0.5190
w	0.7520	0.5470