



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 11:05 AM UTC

PDB ID : 9UMB / pdb_00009umb
EMDB ID : EMD-64272
Title : Structure of Modified adeno-associated viral vector, AAV5-BCD
Authors : Zhang, H.; Burtseva, A.D.; Strelkova, A.N.; Perepelkina, M.P.; Iurlova, E.V.; Gershovich, P.M.; Prokof'ev, A.V.; Kolesnichenko, A.S.; Gulnova, A.R.; Nurt-dinov, R.F.; Vasilev, A.A.; Yakovlev, P.A.; Popov, V.O.; Boyko, K.M.
Deposited on : 2025-04-21
Resolution : 2.55 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:

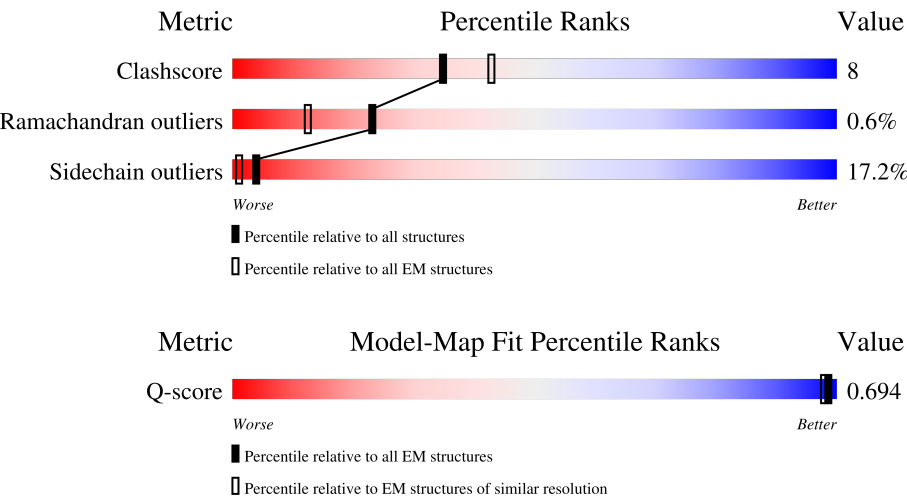
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.55 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	7475 (2.05 - 3.05)

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	724	
1	2	724	
1	3	724	
1	4	724	

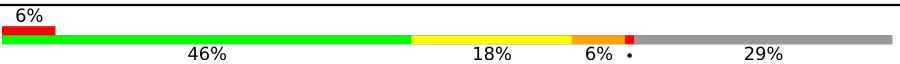
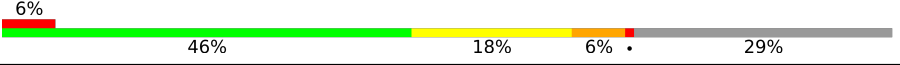
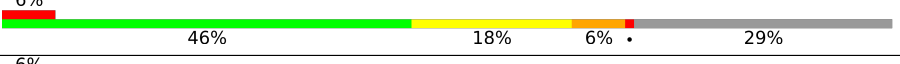
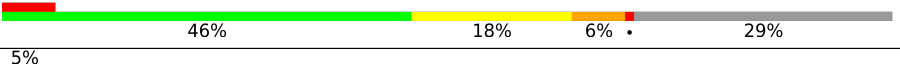
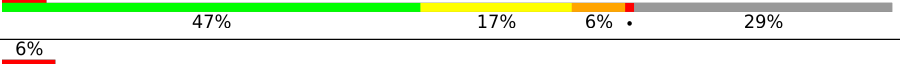
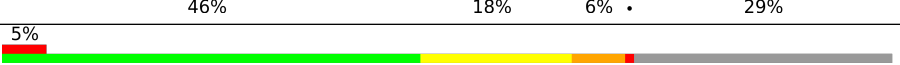
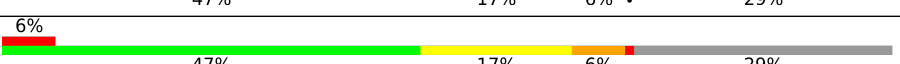
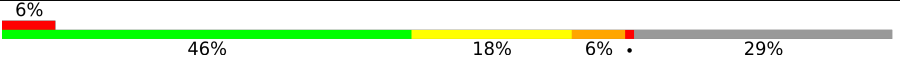
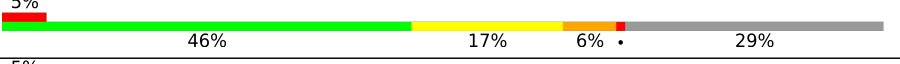
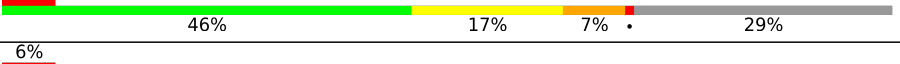
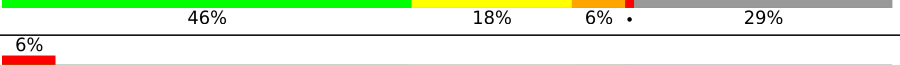
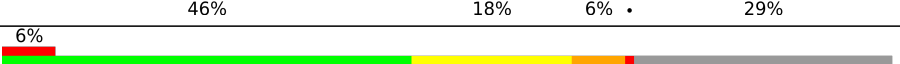
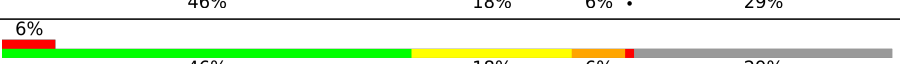
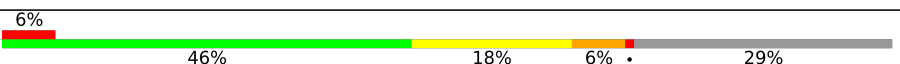
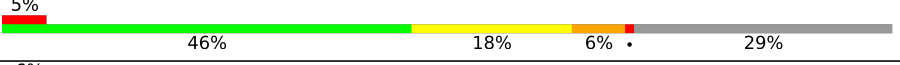
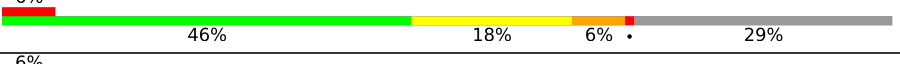
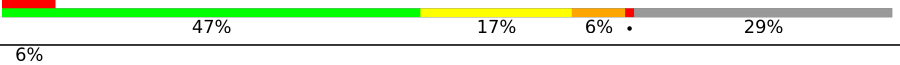
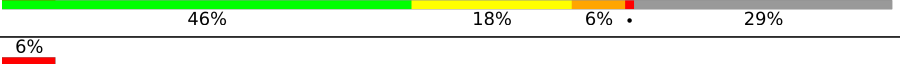
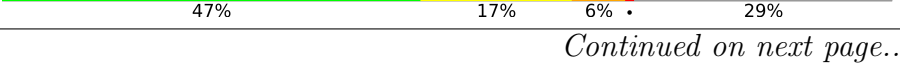
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Mol	Chain	Length	Quality of chain
1	5	724	
1	6	724	
1	7	724	
1	8	724	
1	A	724	
1	B	724	
1	C	724	
1	D	724	
1	E	724	
1	F	724	
1	G	724	
1	H	724	
1	I	724	
1	J	724	
1	K	724	
1	L	724	
1	M	724	
1	N	724	
1	O	724	
1	P	724	
1	Q	724	
1	R	724	
1	S	724	
1	T	724	
1	U	724	

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Mol	Chain	Length	Quality of chain
1	V	724	
1	W	724	
1	X	724	
1	Y	724	
1	Z	724	
1	a	724	
1	b	724	
1	c	724	
1	d	724	
1	e	724	
1	f	724	
1	g	724	
1	h	724	
1	i	724	
1	j	724	
1	k	724	
1	l	724	
1	m	724	
1	n	724	
1	o	724	
1	p	724	
1	q	724	
1	r	724	
1	s	724	
1	t	724	

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Mol	Chain	Length	Quality of chain
1	u	724	
1	v	724	
1	w	724	
1	x	724	
1	y	724	
1	z	724	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 246600 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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	516	Total	C	N	O	S	0	0
			4110	2599	705	790	16		
1	B	516	Total	C	N	O	S	0	0
			4110	2599	705	790	16		
1	C	516	Total	C	N	O	S	0	0
			4110	2599	705	790	16		
1	D	516	Total	C	N	O	S	0	0
			4110	2599	705	790	16		
1	E	516	Total	C	N	O	S	0	0
			4110	2599	705	790	16		
1	F	516	Total	C	N	O	S	0	0
			4110	2599	705	790	16		
1	G	516	Total	C	N	O	S	0	0
			4110	2599	705	790	16		
1	H	516	Total	C	N	O	S	0	0
			4110	2599	705	790	16		
1	I	516	Total	C	N	O	S	0	0
			4110	2599	705	790	16		
1	J	516	Total	C	N	O	S	0	0
			4110	2599	705	790	16		
1	K	516	Total	C	N	O	S	0	0
			4110	2599	705	790	16		
1	L	516	Total	C	N	O	S	0	0
			4110	2599	705	790	16		
1	M	516	Total	C	N	O	S	0	0
			4110	2599	705	790	16		
1	N	516	Total	C	N	O	S	0	0
			4110	2599	705	790	16		
1	O	516	Total	C	N	O	S	0	0
			4110	2599	705	790	16		
1	P	516	Total	C	N	O	S	0	0
			4110	2599	705	790	16		
1	Q	516	Total	C	N	O	S	0	0
			4110	2599	705	790	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	S	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	T	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	U	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	V	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	W	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	X	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	Y	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	Z	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	a	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	b	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	c	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	d	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	e	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	f	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	g	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	h	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	i	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	j	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	k	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	l	516	Total 4110	C 2599	N 705	O 790	S 16	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	n	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	o	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	p	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	q	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	r	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	s	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	t	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	u	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	v	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	w	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	x	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	y	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	z	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	1	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	2	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	3	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	4	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	5	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	6	516	Total 4110	C 2599	N 705	O 790	S 16	0	0
1	7	516	Total 4110	C 2599	N 705	O 790	S 16	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	516	Total	C	N	O	S	0	0
			4110	2599	705	790	16		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	conflict	UNP Q9YIJ1
A	711	SER	THR	conflict	UNP Q9YIJ1
B	2	ALA	SER	conflict	UNP Q9YIJ1
B	711	SER	THR	conflict	UNP Q9YIJ1
C	2	ALA	SER	conflict	UNP Q9YIJ1
C	711	SER	THR	conflict	UNP Q9YIJ1
D	2	ALA	SER	conflict	UNP Q9YIJ1
D	711	SER	THR	conflict	UNP Q9YIJ1
E	2	ALA	SER	conflict	UNP Q9YIJ1
E	711	SER	THR	conflict	UNP Q9YIJ1
F	2	ALA	SER	conflict	UNP Q9YIJ1
F	711	SER	THR	conflict	UNP Q9YIJ1
G	2	ALA	SER	conflict	UNP Q9YIJ1
G	711	SER	THR	conflict	UNP Q9YIJ1
H	2	ALA	SER	conflict	UNP Q9YIJ1
H	711	SER	THR	conflict	UNP Q9YIJ1
I	2	ALA	SER	conflict	UNP Q9YIJ1
I	711	SER	THR	conflict	UNP Q9YIJ1
J	2	ALA	SER	conflict	UNP Q9YIJ1
J	711	SER	THR	conflict	UNP Q9YIJ1
K	2	ALA	SER	conflict	UNP Q9YIJ1
K	711	SER	THR	conflict	UNP Q9YIJ1
L	2	ALA	SER	conflict	UNP Q9YIJ1
L	711	SER	THR	conflict	UNP Q9YIJ1
M	2	ALA	SER	conflict	UNP Q9YIJ1
M	711	SER	THR	conflict	UNP Q9YIJ1
N	2	ALA	SER	conflict	UNP Q9YIJ1
N	711	SER	THR	conflict	UNP Q9YIJ1
O	2	ALA	SER	conflict	UNP Q9YIJ1
O	711	SER	THR	conflict	UNP Q9YIJ1
P	2	ALA	SER	conflict	UNP Q9YIJ1
P	711	SER	THR	conflict	UNP Q9YIJ1
Q	2	ALA	SER	conflict	UNP Q9YIJ1
Q	711	SER	THR	conflict	UNP Q9YIJ1
R	2	ALA	SER	conflict	UNP Q9YIJ1
R	711	SER	THR	conflict	UNP Q9YIJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
S	2	ALA	SER	conflict	UNP Q9YIJ1
S	711	SER	THR	conflict	UNP Q9YIJ1
T	2	ALA	SER	conflict	UNP Q9YIJ1
T	711	SER	THR	conflict	UNP Q9YIJ1
U	2	ALA	SER	conflict	UNP Q9YIJ1
U	711	SER	THR	conflict	UNP Q9YIJ1
V	2	ALA	SER	conflict	UNP Q9YIJ1
V	711	SER	THR	conflict	UNP Q9YIJ1
W	2	ALA	SER	conflict	UNP Q9YIJ1
W	711	SER	THR	conflict	UNP Q9YIJ1
X	2	ALA	SER	conflict	UNP Q9YIJ1
X	711	SER	THR	conflict	UNP Q9YIJ1
Y	2	ALA	SER	conflict	UNP Q9YIJ1
Y	711	SER	THR	conflict	UNP Q9YIJ1
Z	2	ALA	SER	conflict	UNP Q9YIJ1
Z	711	SER	THR	conflict	UNP Q9YIJ1
a	2	ALA	SER	conflict	UNP Q9YIJ1
a	711	SER	THR	conflict	UNP Q9YIJ1
b	2	ALA	SER	conflict	UNP Q9YIJ1
b	711	SER	THR	conflict	UNP Q9YIJ1
c	2	ALA	SER	conflict	UNP Q9YIJ1
c	711	SER	THR	conflict	UNP Q9YIJ1
d	2	ALA	SER	conflict	UNP Q9YIJ1
d	711	SER	THR	conflict	UNP Q9YIJ1
e	2	ALA	SER	conflict	UNP Q9YIJ1
e	711	SER	THR	conflict	UNP Q9YIJ1
f	2	ALA	SER	conflict	UNP Q9YIJ1
f	711	SER	THR	conflict	UNP Q9YIJ1
g	2	ALA	SER	conflict	UNP Q9YIJ1
g	711	SER	THR	conflict	UNP Q9YIJ1
h	2	ALA	SER	conflict	UNP Q9YIJ1
h	711	SER	THR	conflict	UNP Q9YIJ1
i	2	ALA	SER	conflict	UNP Q9YIJ1
i	711	SER	THR	conflict	UNP Q9YIJ1
j	2	ALA	SER	conflict	UNP Q9YIJ1
j	711	SER	THR	conflict	UNP Q9YIJ1
k	2	ALA	SER	conflict	UNP Q9YIJ1
k	711	SER	THR	conflict	UNP Q9YIJ1
l	2	ALA	SER	conflict	UNP Q9YIJ1
l	711	SER	THR	conflict	UNP Q9YIJ1
m	2	ALA	SER	conflict	UNP Q9YIJ1
m	711	SER	THR	conflict	UNP Q9YIJ1

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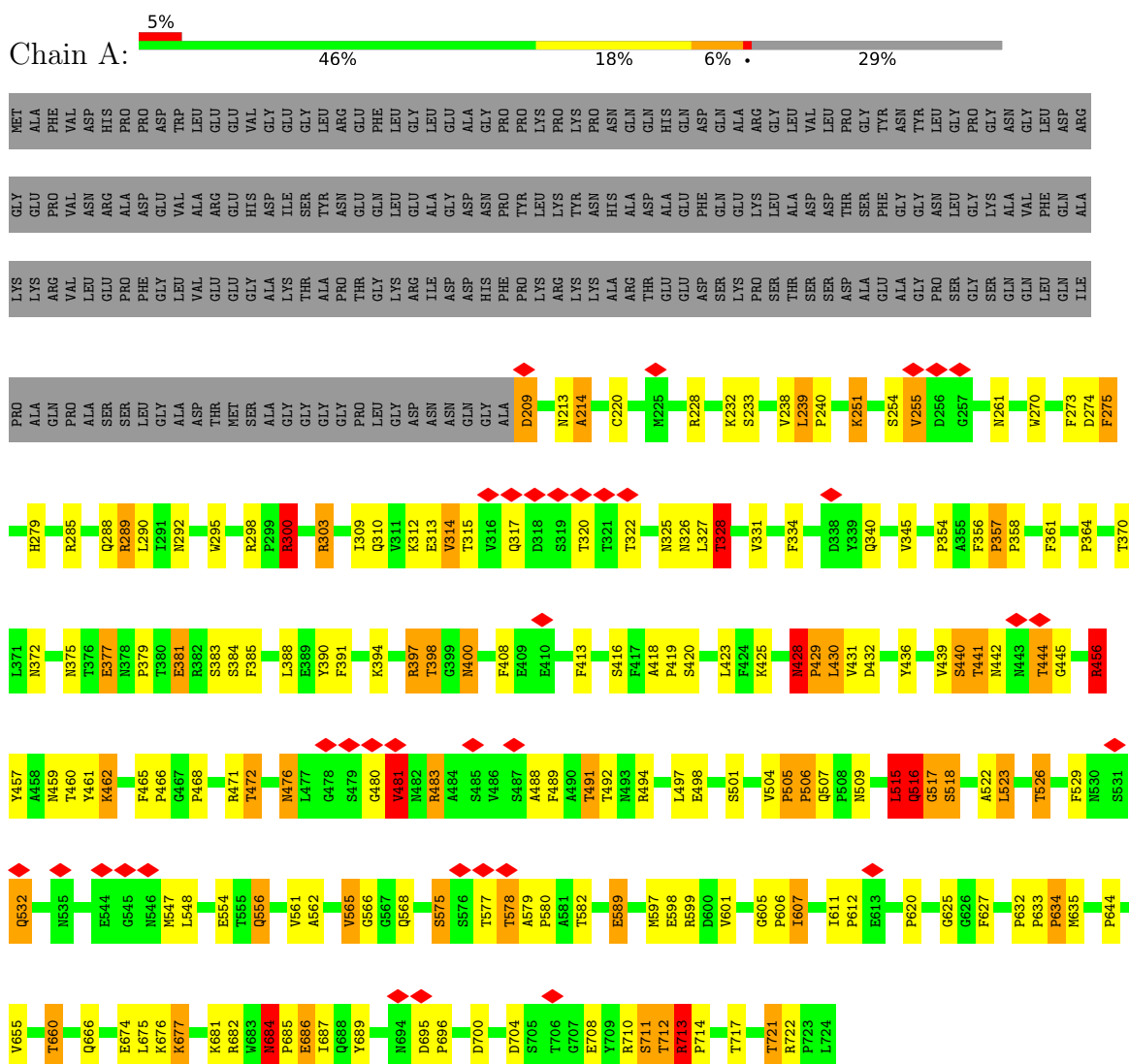
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Chain	Residue	Modelled	Actual	Comment	Reference
n	2	ALA	SER	conflict	UNP Q9YIJ1
n	711	SER	THR	conflict	UNP Q9YIJ1
o	2	ALA	SER	conflict	UNP Q9YIJ1
o	711	SER	THR	conflict	UNP Q9YIJ1
p	2	ALA	SER	conflict	UNP Q9YIJ1
p	711	SER	THR	conflict	UNP Q9YIJ1
q	2	ALA	SER	conflict	UNP Q9YIJ1
q	711	SER	THR	conflict	UNP Q9YIJ1
r	2	ALA	SER	conflict	UNP Q9YIJ1
r	711	SER	THR	conflict	UNP Q9YIJ1
s	2	ALA	SER	conflict	UNP Q9YIJ1
s	711	SER	THR	conflict	UNP Q9YIJ1
t	2	ALA	SER	conflict	UNP Q9YIJ1
t	711	SER	THR	conflict	UNP Q9YIJ1
u	2	ALA	SER	conflict	UNP Q9YIJ1
u	711	SER	THR	conflict	UNP Q9YIJ1
v	2	ALA	SER	conflict	UNP Q9YIJ1
v	711	SER	THR	conflict	UNP Q9YIJ1
w	2	ALA	SER	conflict	UNP Q9YIJ1
w	711	SER	THR	conflict	UNP Q9YIJ1
x	2	ALA	SER	conflict	UNP Q9YIJ1
x	711	SER	THR	conflict	UNP Q9YIJ1
y	2	ALA	SER	conflict	UNP Q9YIJ1
y	711	SER	THR	conflict	UNP Q9YIJ1
z	2	ALA	SER	conflict	UNP Q9YIJ1
z	711	SER	THR	conflict	UNP Q9YIJ1
1	2	ALA	SER	conflict	UNP Q9YIJ1
1	711	SER	THR	conflict	UNP Q9YIJ1
2	2	ALA	SER	conflict	UNP Q9YIJ1
2	711	SER	THR	conflict	UNP Q9YIJ1
3	2	ALA	SER	conflict	UNP Q9YIJ1
3	711	SER	THR	conflict	UNP Q9YIJ1
4	2	ALA	SER	conflict	UNP Q9YIJ1
4	711	SER	THR	conflict	UNP Q9YIJ1
5	2	ALA	SER	conflict	UNP Q9YIJ1
5	711	SER	THR	conflict	UNP Q9YIJ1
6	2	ALA	SER	conflict	UNP Q9YIJ1
6	711	SER	THR	conflict	UNP Q9YIJ1
7	2	ALA	SER	conflict	UNP Q9YIJ1
7	711	SER	THR	conflict	UNP Q9YIJ1
8	2	ALA	SER	conflict	UNP Q9YIJ1
8	711	SER	THR	conflict	UNP Q9YIJ1

3 Residue-property plots

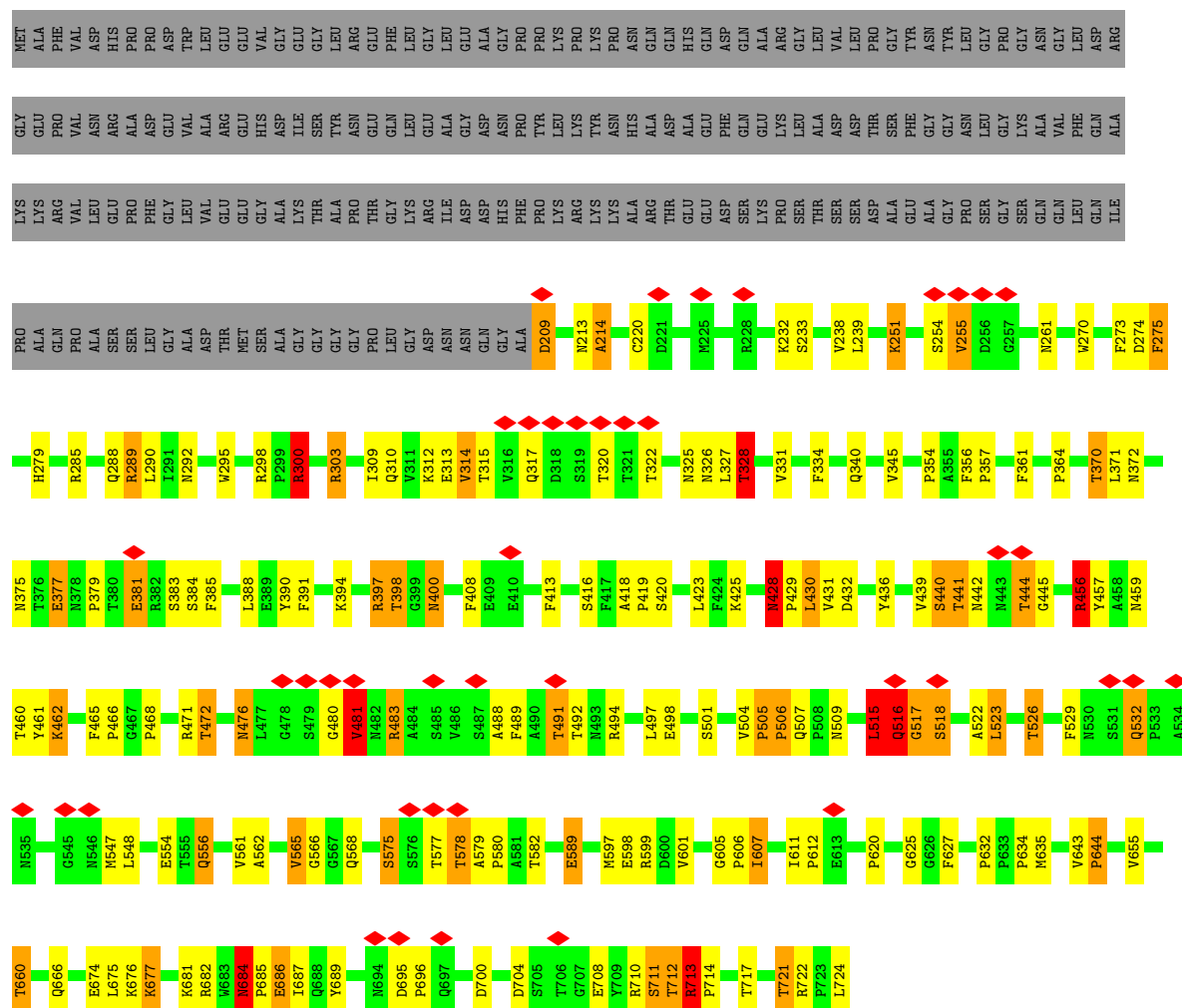
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

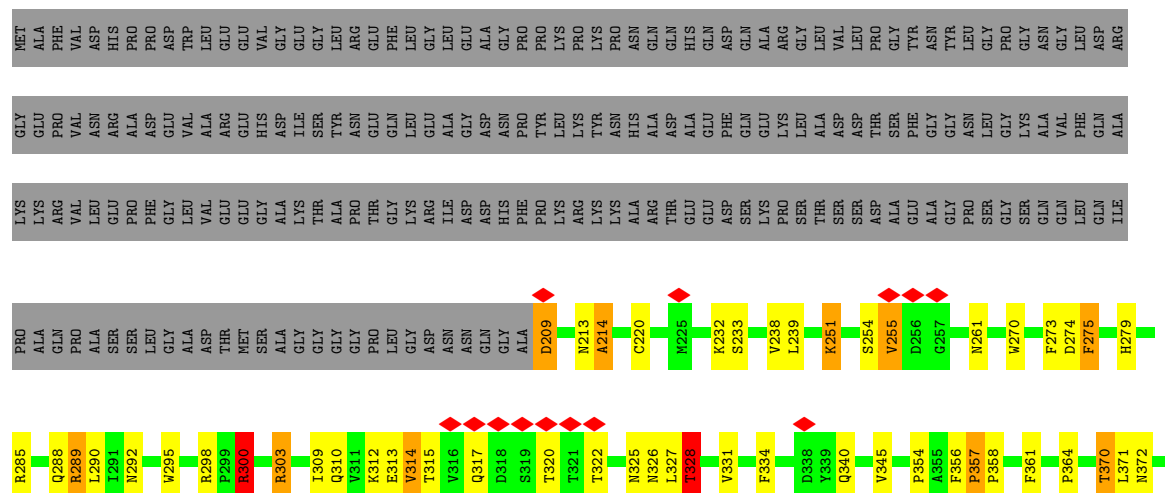


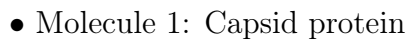
• Molecule 1: Capsid protein

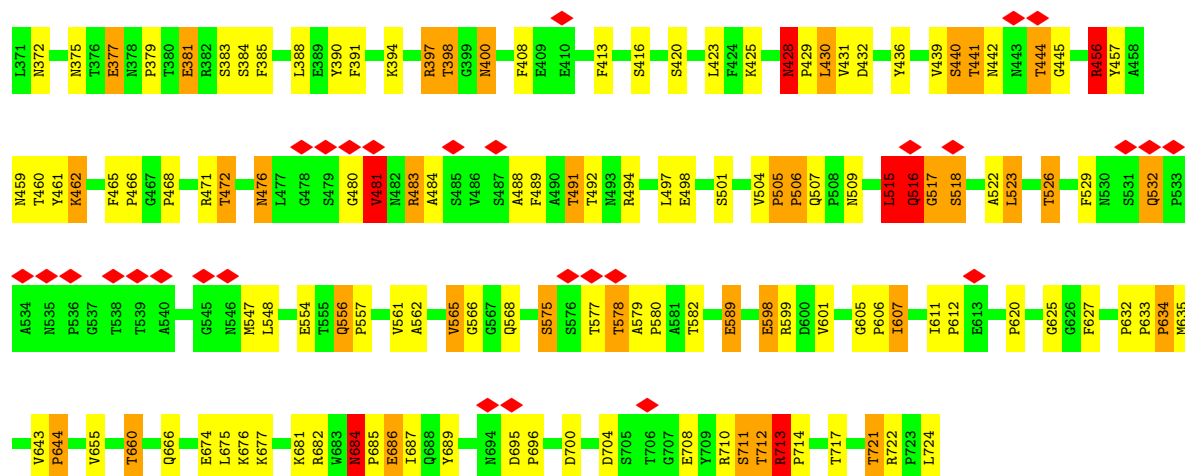




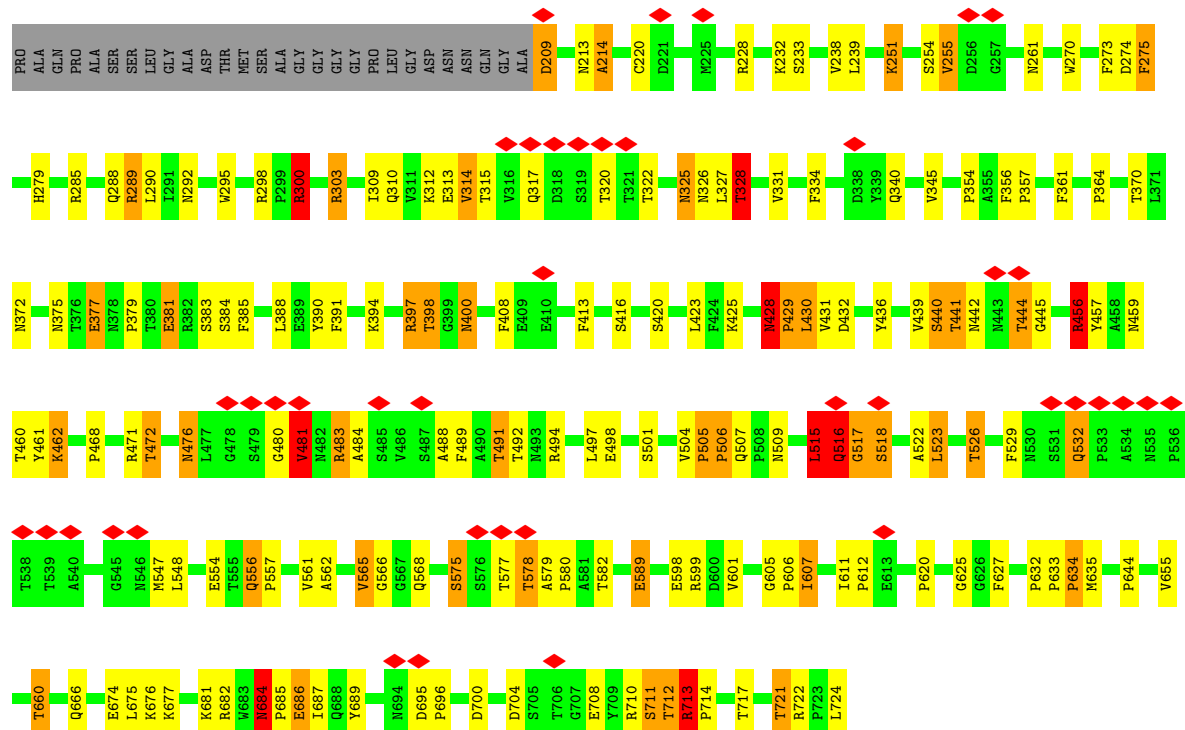
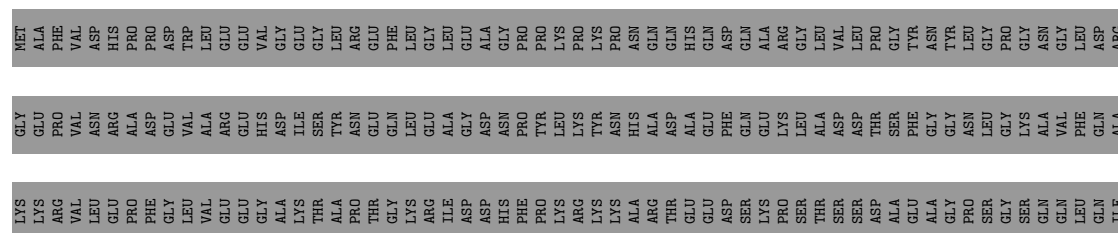
• Molecule 1: Capsid protein



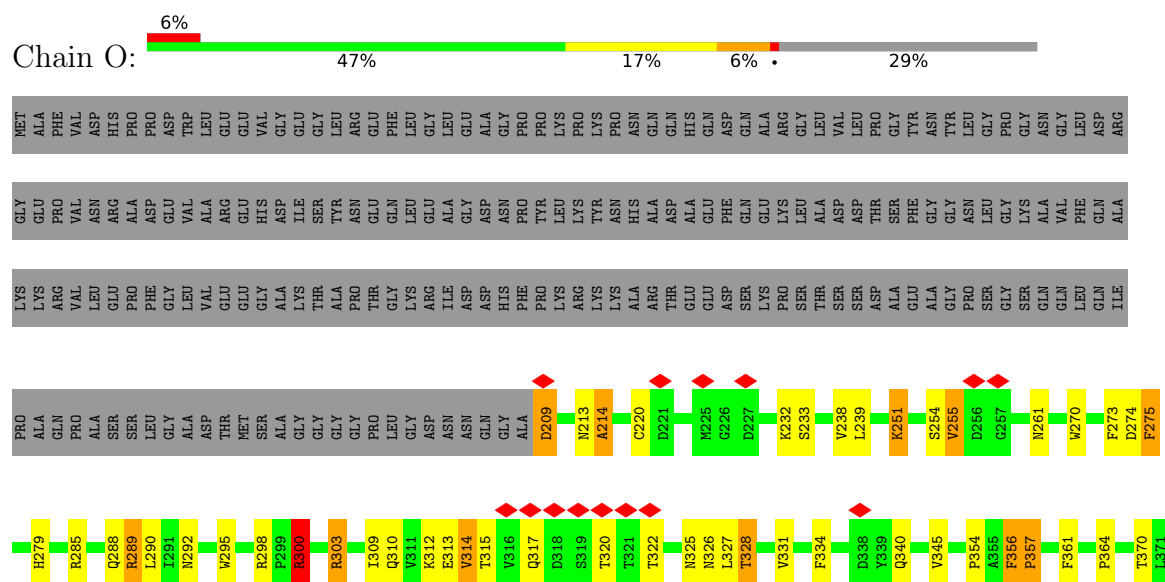


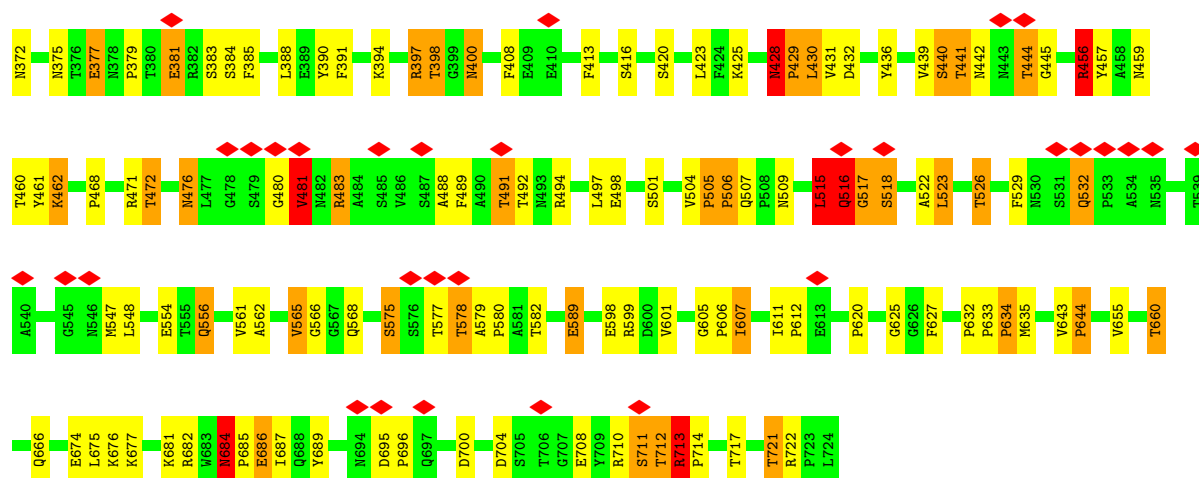


• Molecule 1: Capsid protein

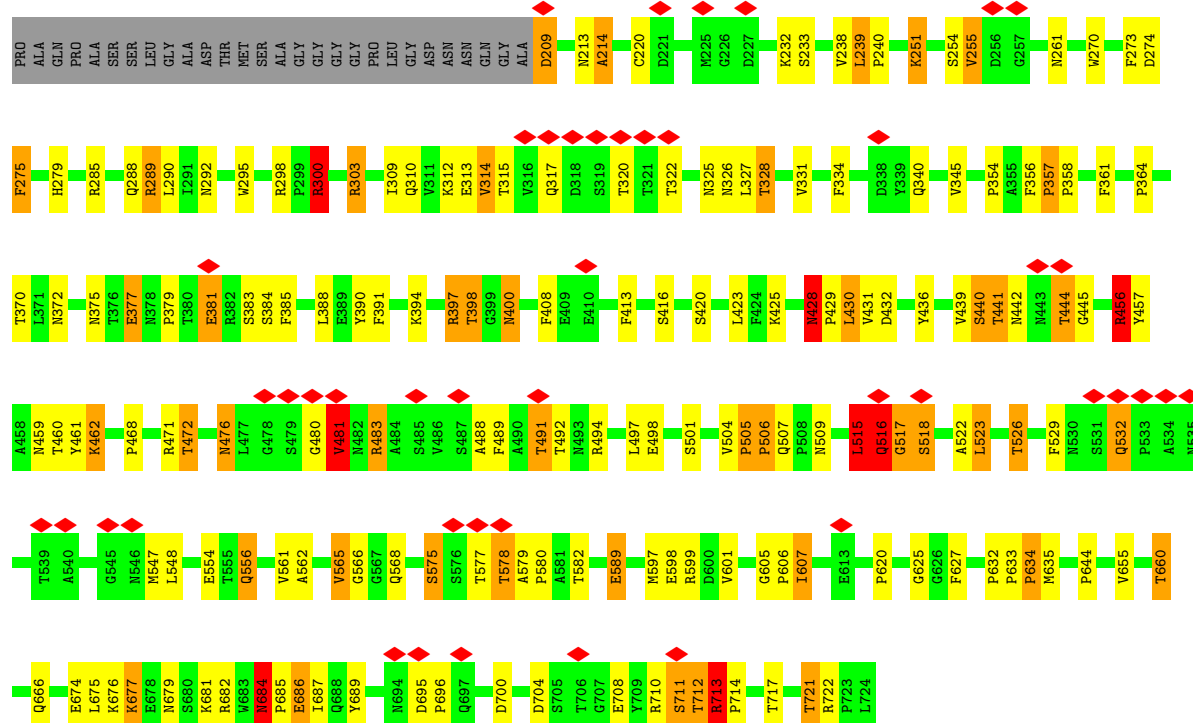
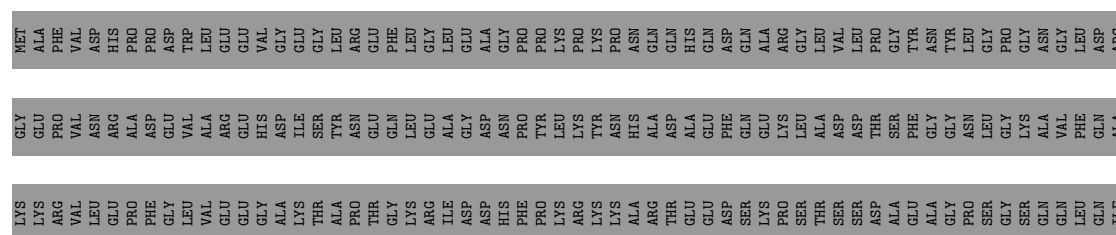


• Molecule 1: Capsid protein

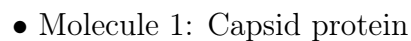




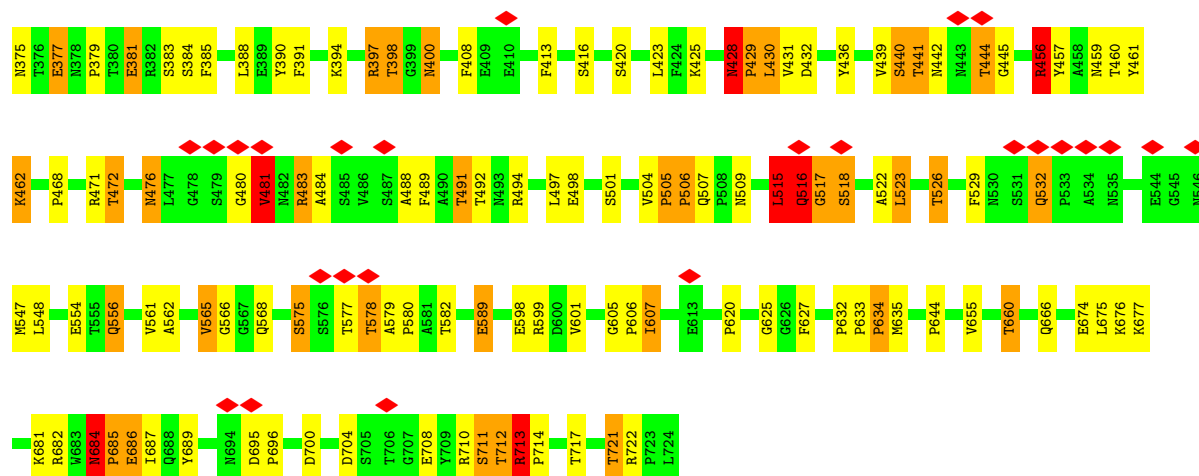
• Molecule 1: Capsid protein



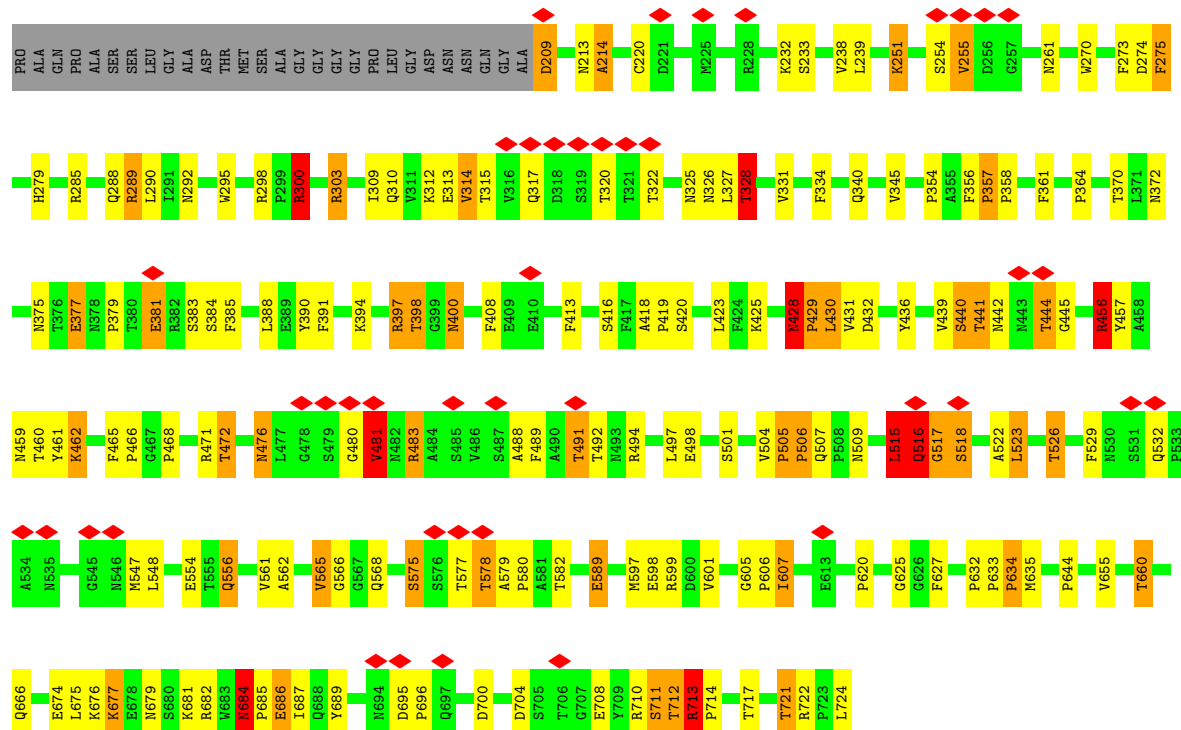
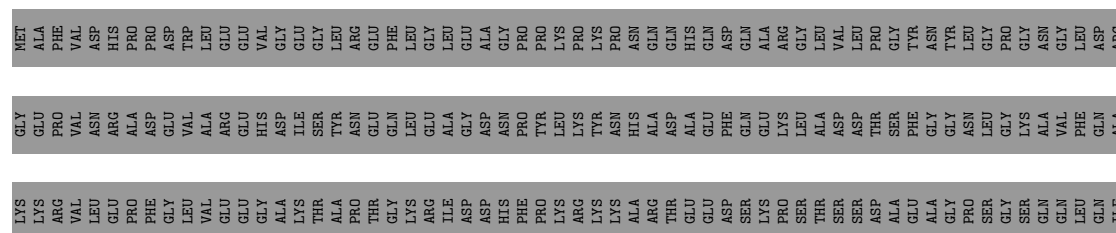
• Molecule 1: Capsid protein



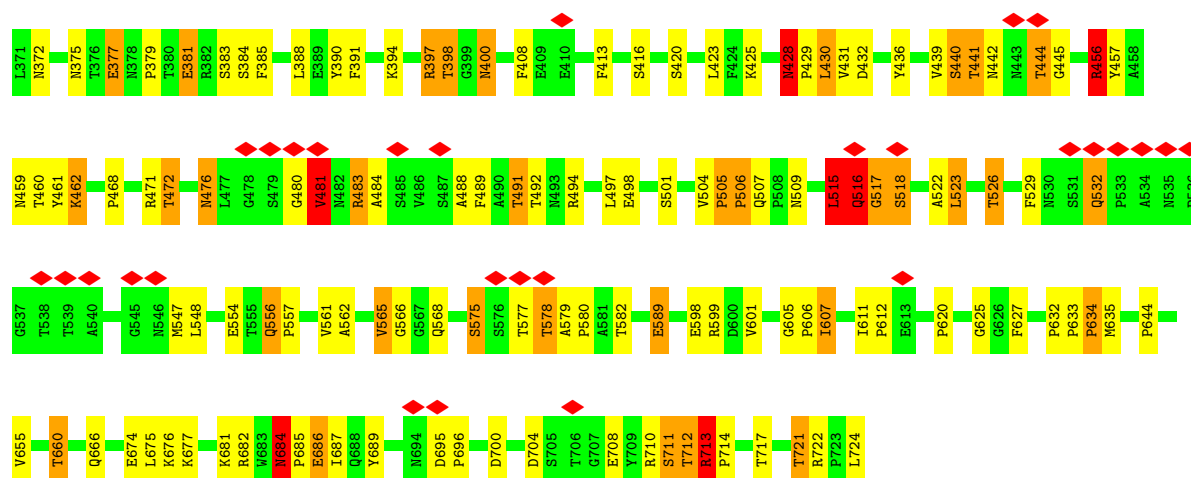




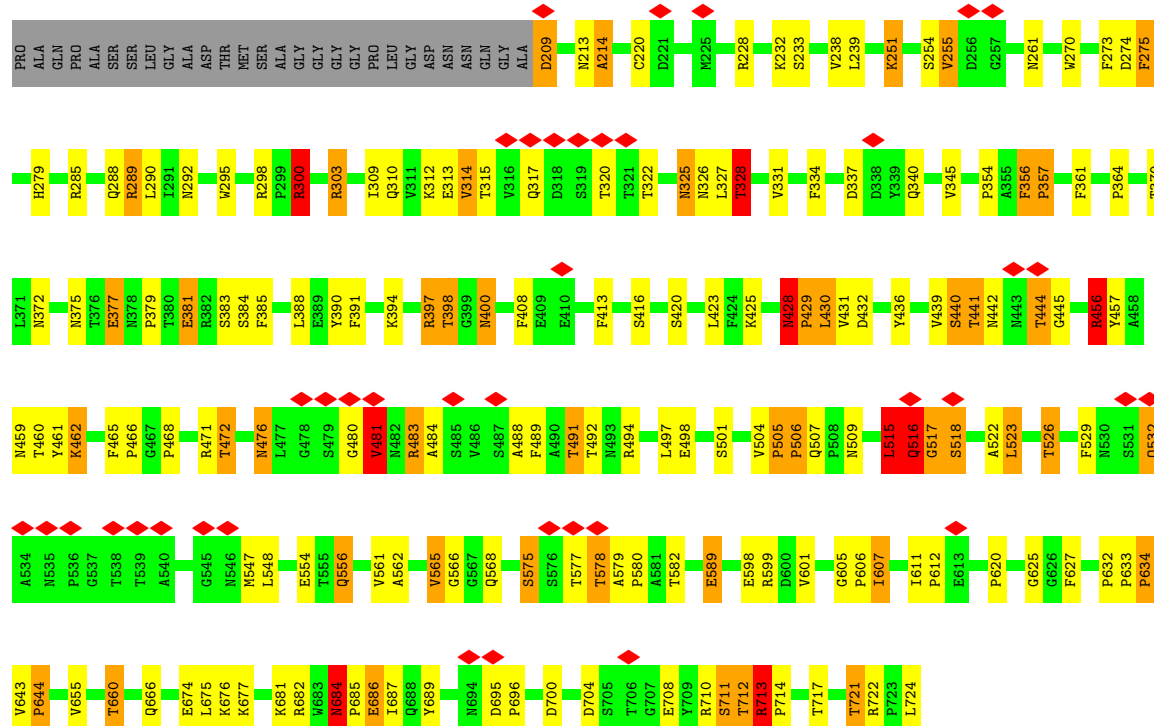
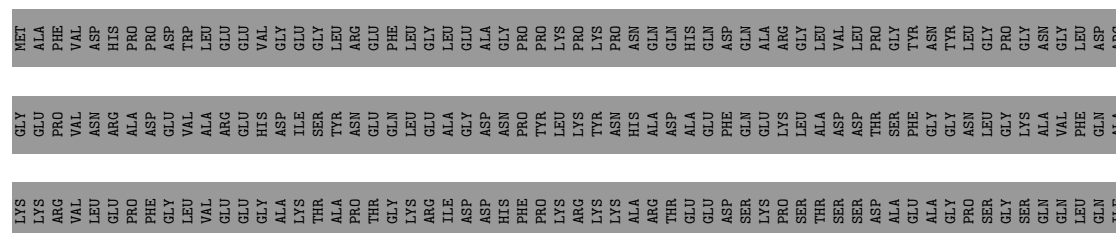
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein

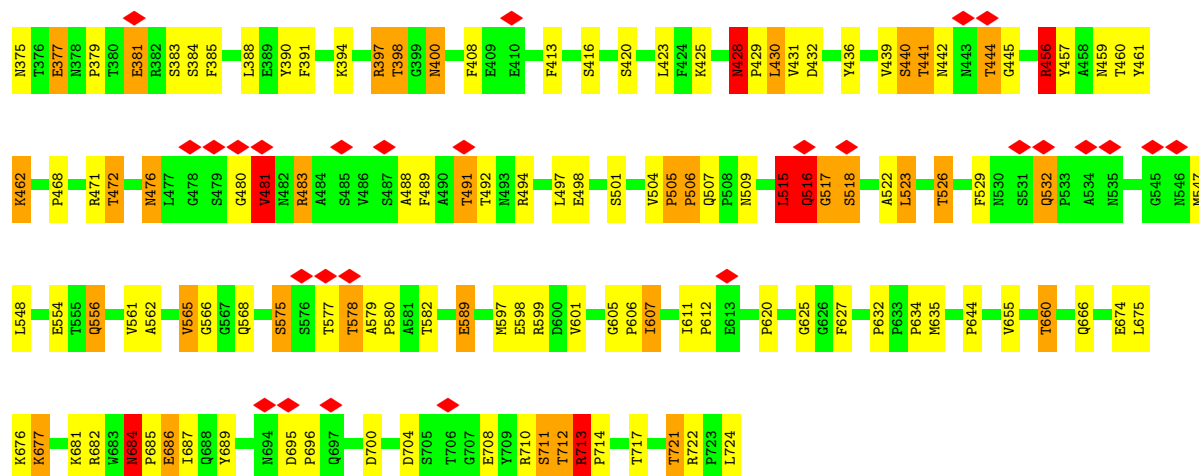


• Molecule 1: Capsid protein

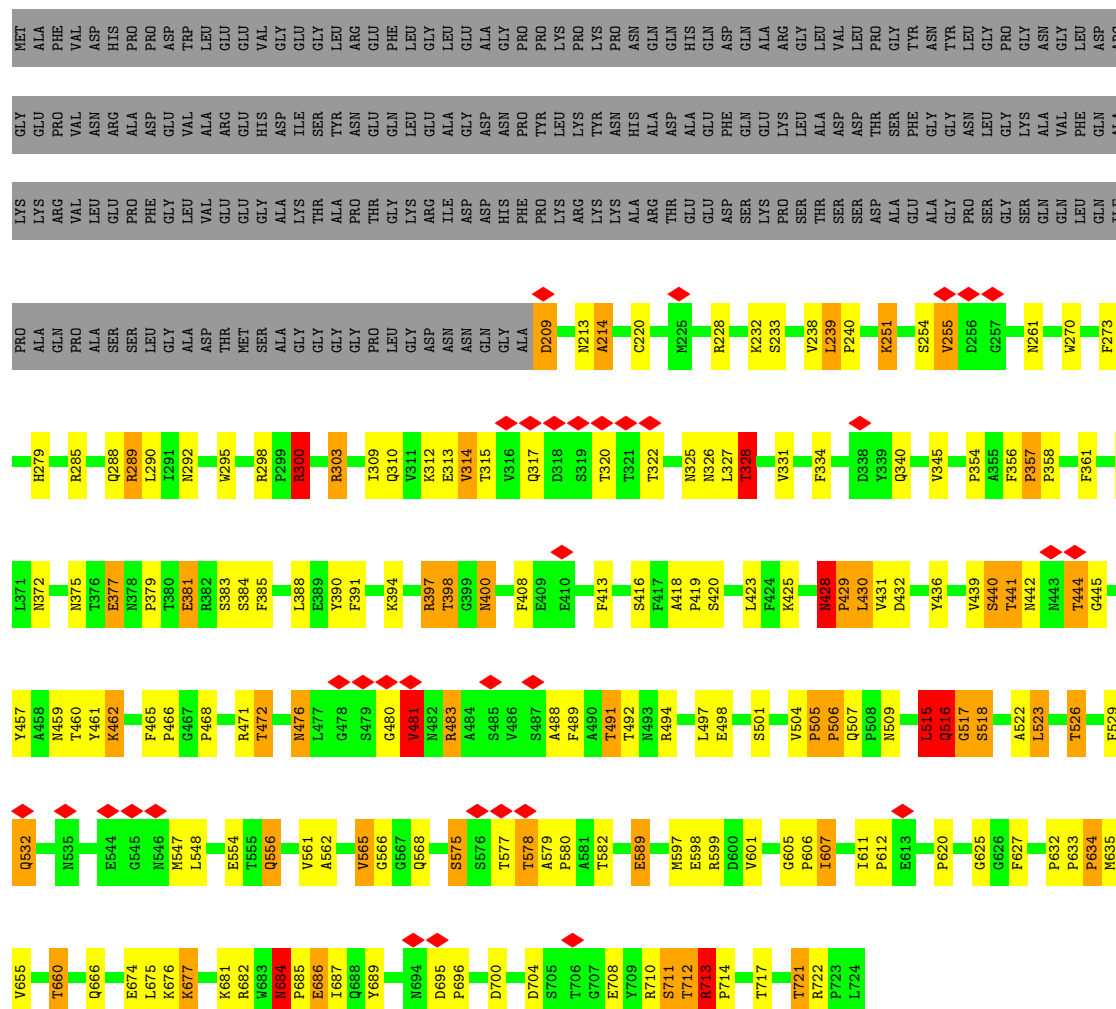


• Molecule 1: Capsid protein

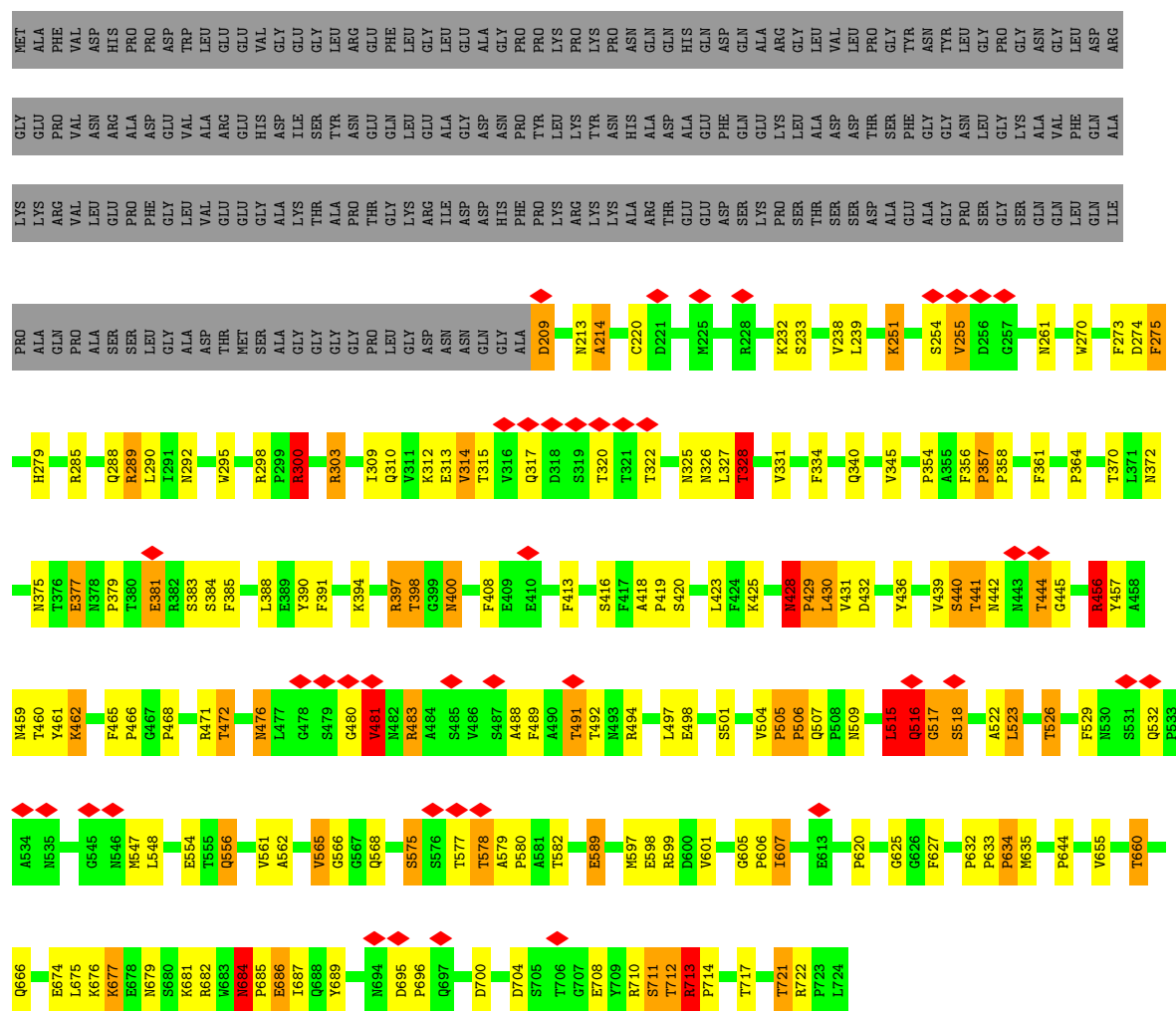




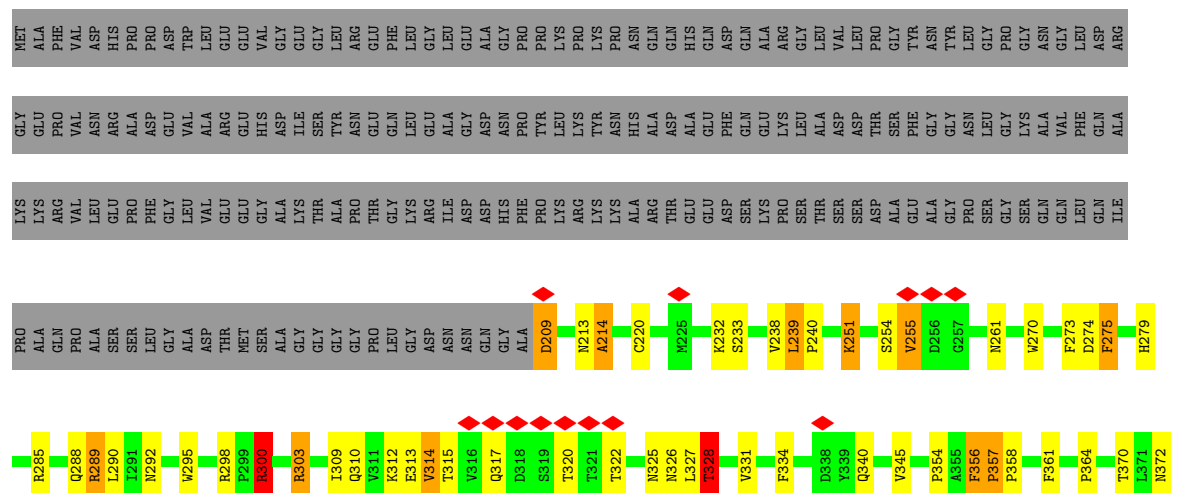
• Molecule 1: Capsid protein

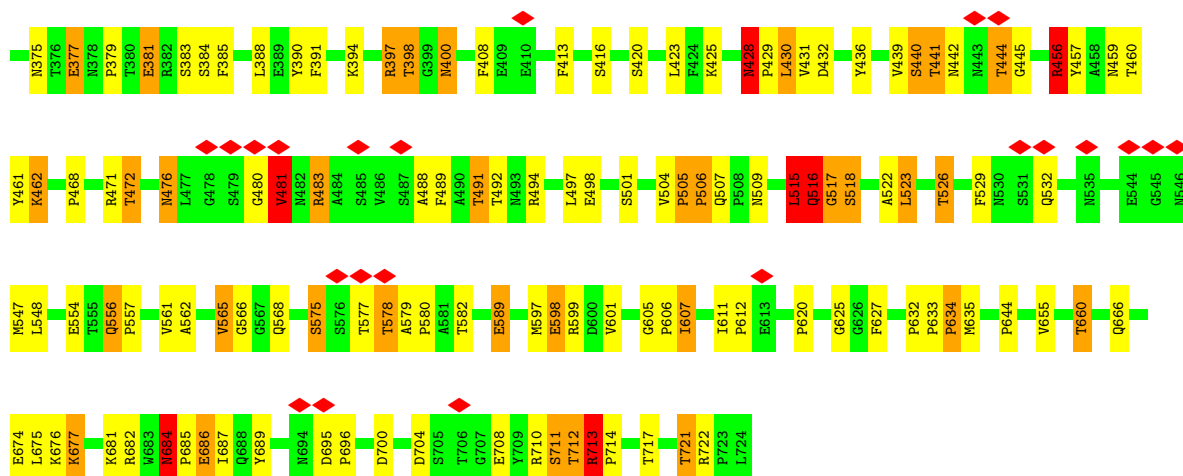


• Molecule 1: Capsid protein

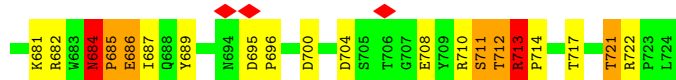
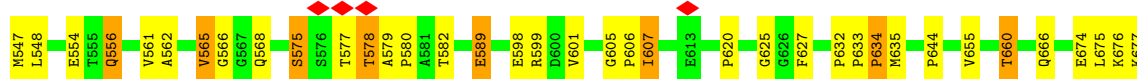
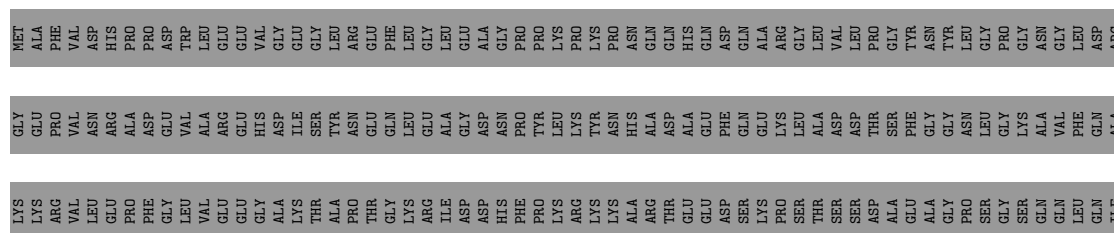


• Molecule 1: Capsid protein

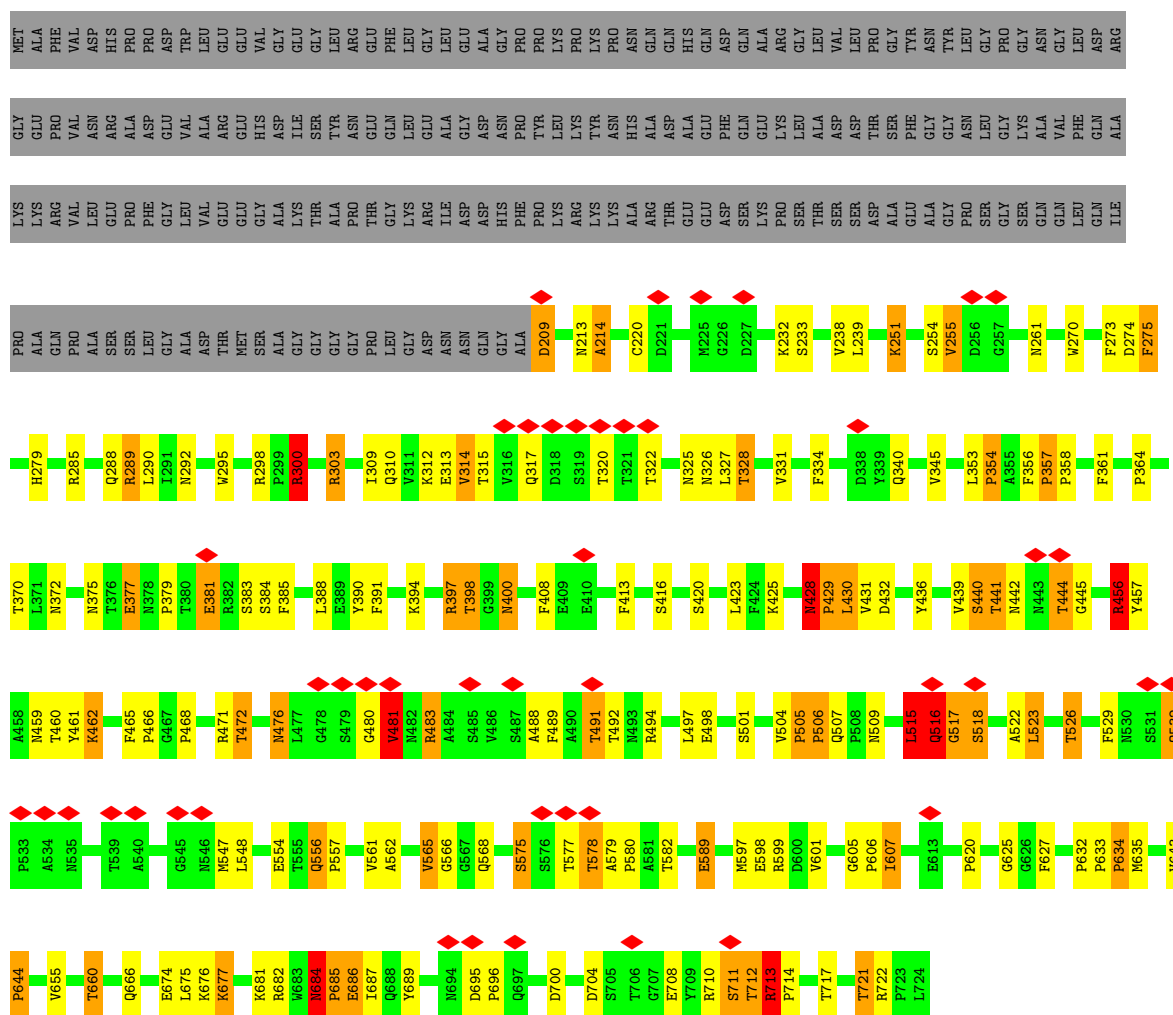
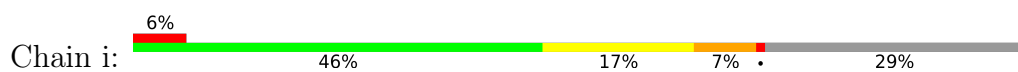




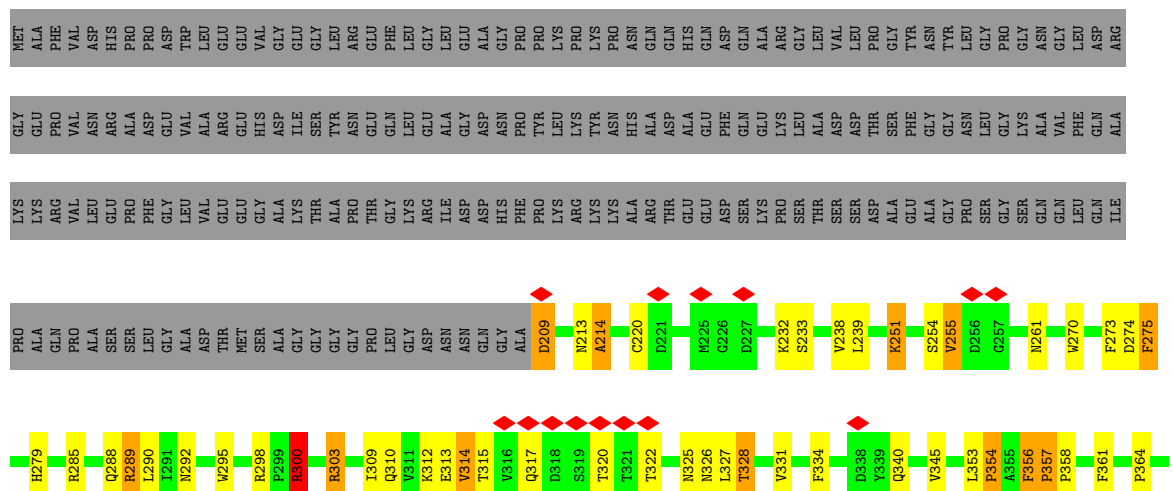
• Molecule 1: Capsid protein

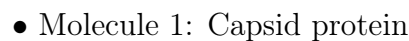


• Molecule 1: Capsid protein



• Molecule 1: Capsid protein







MET ALA PHE VAL ASP HIS PRO PRO GLU LEU TRP ALA LEU GLU VAL GLY ILE GLY THR ARG GLU PHE LEU GLY LEU ASP ALA GLU LEU ASP MET HIS VAL

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

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

PRO ALA GLN PRO VAL ALA SER SER LEU GLY ASP MET SER MET THR ASP VAL ALA LEU GLY LEU THR SER THR SER ASP THR ASP GLU TYR ALA GLY TYR PRO GLY SER GLN GLN LEU ASP ILE

R285 Q288 R289 R290 L291 N292 W295 R298 R299 R300 R303 I309 Q310 V311 K312 E313 V314 T315 V316 Q317 D318 S319 T320 T321 T322 N325 N326 L327 T328 V331 F334 D338 Y339 Q340 V345 P354 A355 F356 P357 F361 P364 T370 T371 N372 N375

T376 E377 N378 R379 T380 E381 R382 S383 S384 F385 L388 R389 F390 Y391 F394 R397 T398 G399 N400 F408 F409 E410 F413 S416 S420 L423 F424 K425 N428 P429 L430 V431 D432 Y436 V439 S440 T441 N442 N443 T444 G445 R456 Y457 A458 N459 T460 L461 K462

P468 R471 T472 R476 L477 G478 S479 G480 Y481 Y482 R483 A484 S485 S486 S487 A488 F489 A490 T491 T492 N493 R494 L497 E498 S501 V504 P505 P506 Q507 P508 N509 L515 Q516 G517 S518 A522 L523 T526 F529 N530 S531 Q532 N535 E544 G545 N546 L548

E554 T555 Q556 V561 A562 V565 G566 G567 Q568 S575 S576 T577 T578 A579 P580 A581 T582 T589 E589 N597 E598 R599 T600 L601 G605 P606 I611 R612 P613 P620 G625 G626 F627 P632 P633 P634 N635 V643 P644 V655 T660 Q666 E674 L675

K676 K677 K681 R682 R683 R684 P685 E686 I687 Q688 Y689 N694 D695 P696 D700 D704 S705 T706 T707 E708 Y709 R710 S711 T712 R713 P714 T717 T721 R722 P723 L724

• Molecule 1: Capsid protein



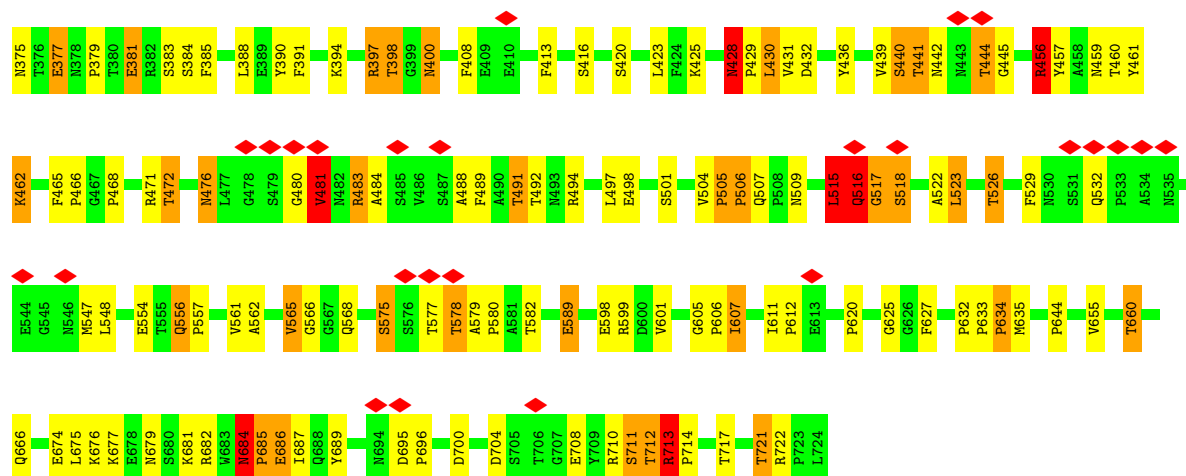
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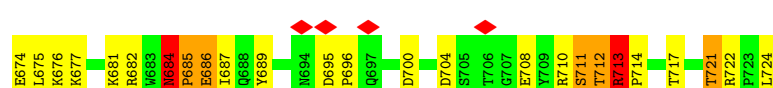
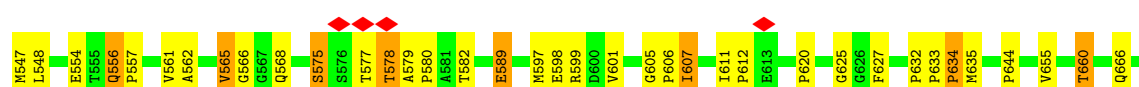
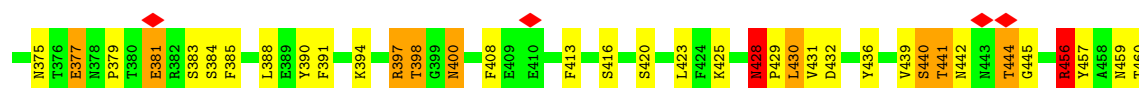
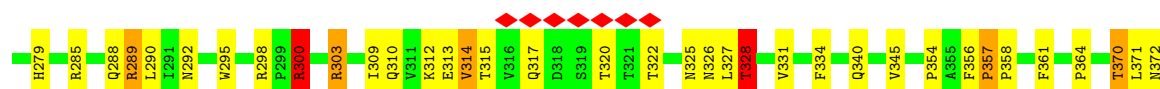
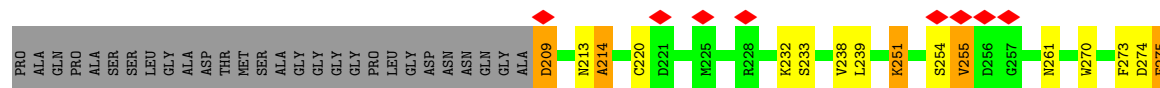
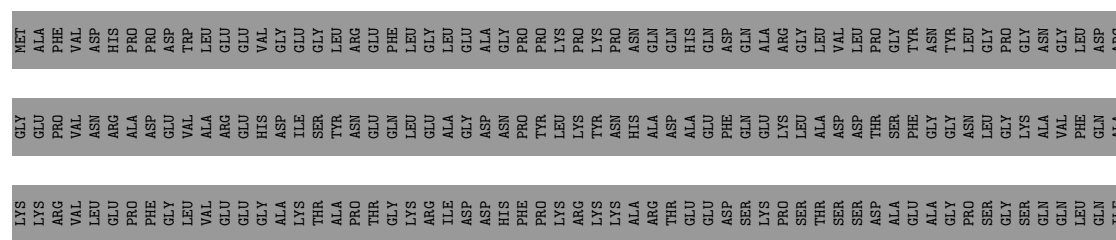
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PRO ALA GLN PRO VAL SER SER LEU GLY ASP MET SER MET THR ASP VAL ALA LEU GLY LEU THR SER THR SER ASP THR ASP GLU TYR ALA GLY TYR PRO GLY SER GLN GLN LEU ASP ILE

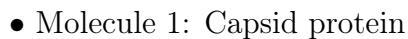
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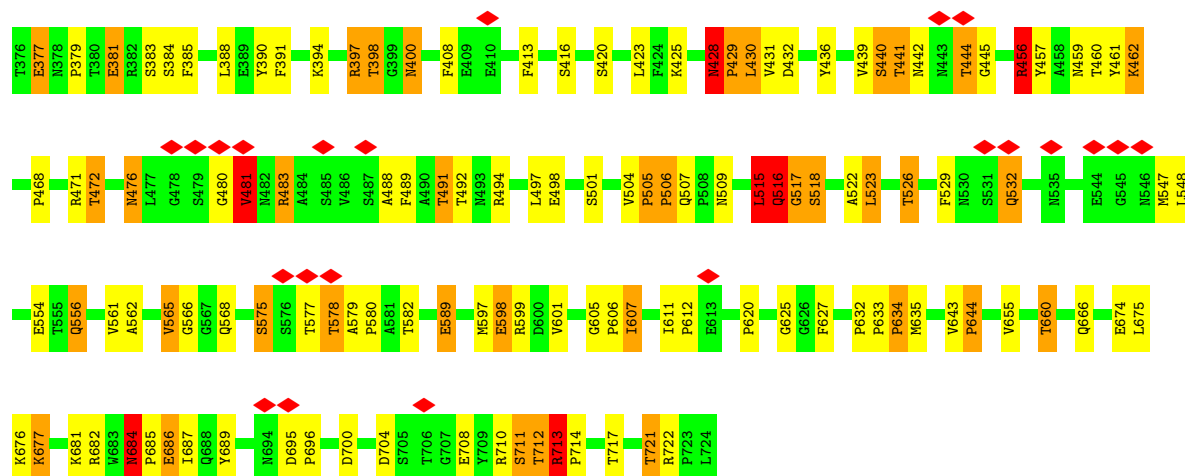


• Molecule 1: Capsid protein

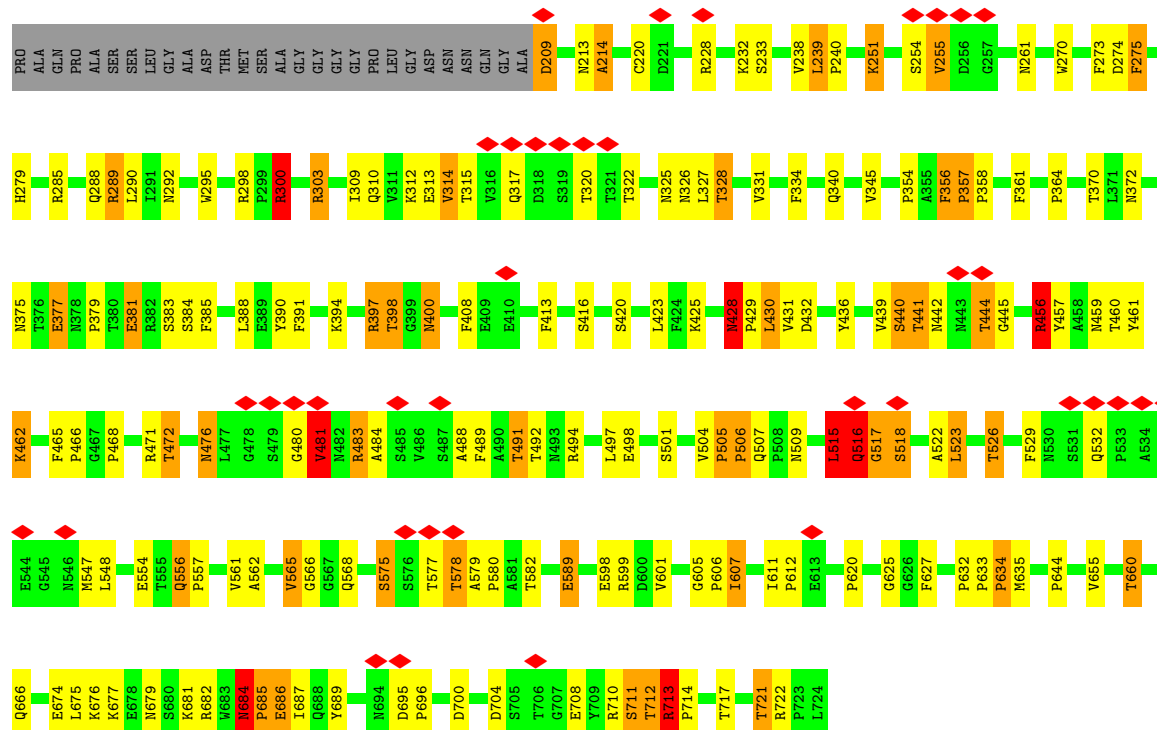
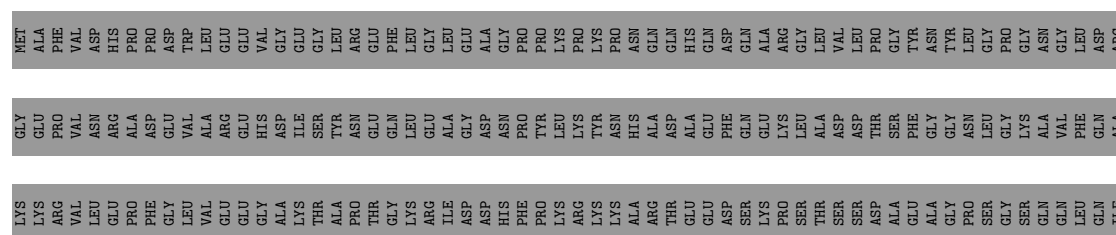


• Molecule 1: Capsid protein

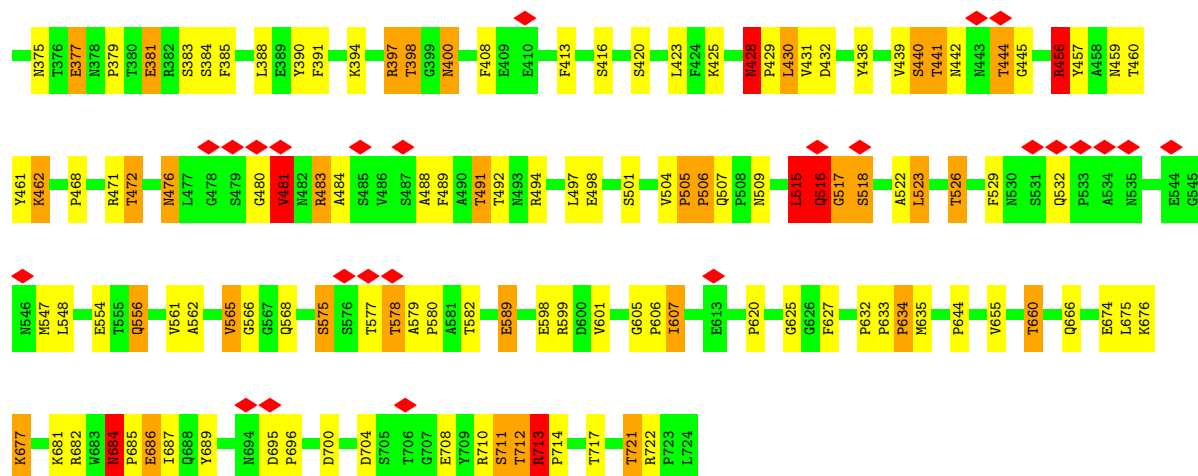




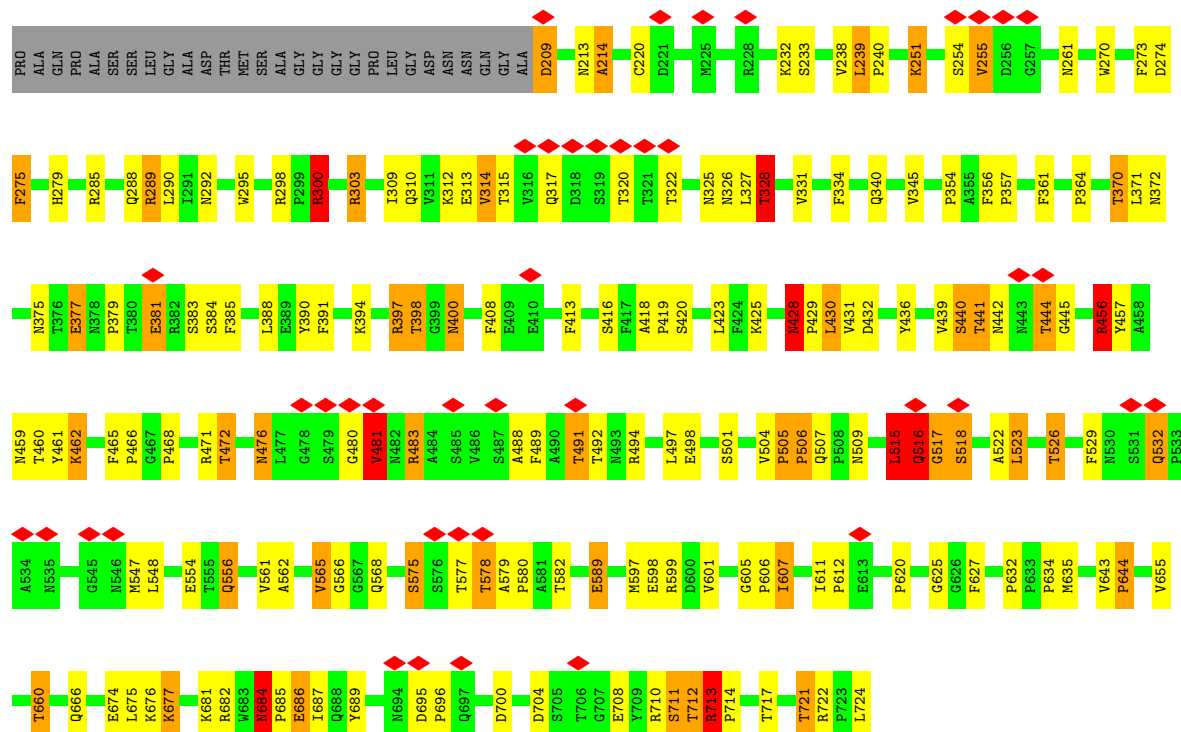
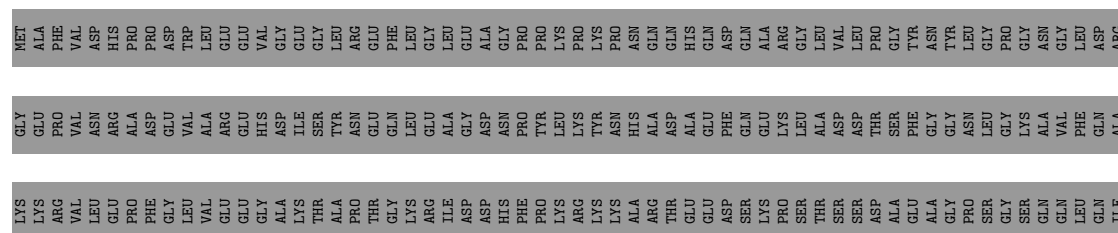
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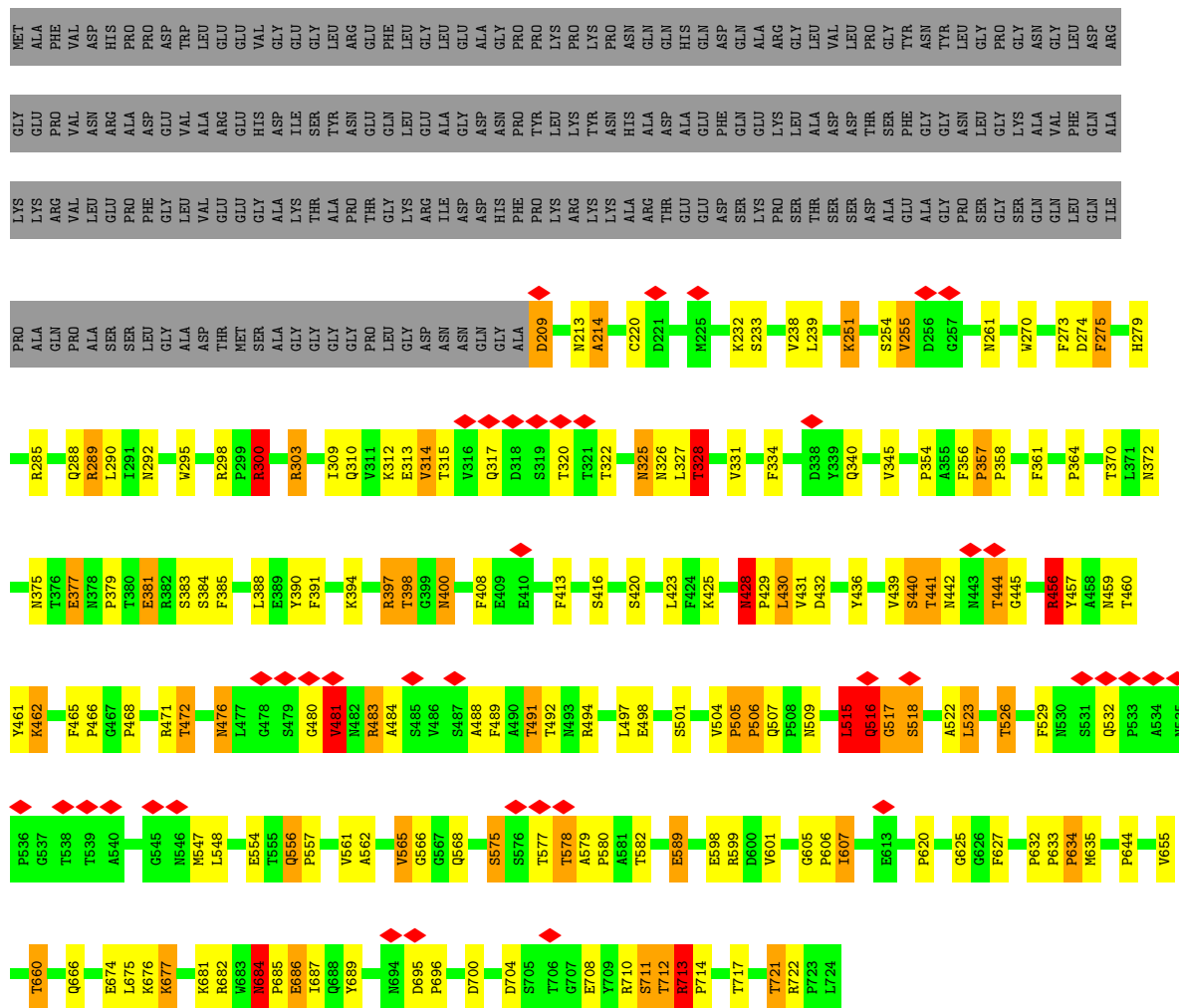
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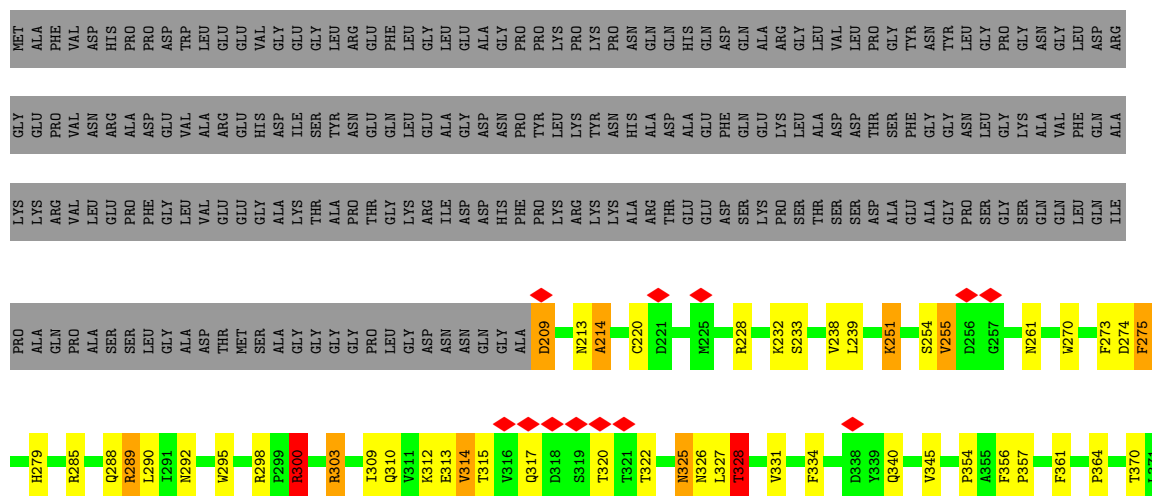
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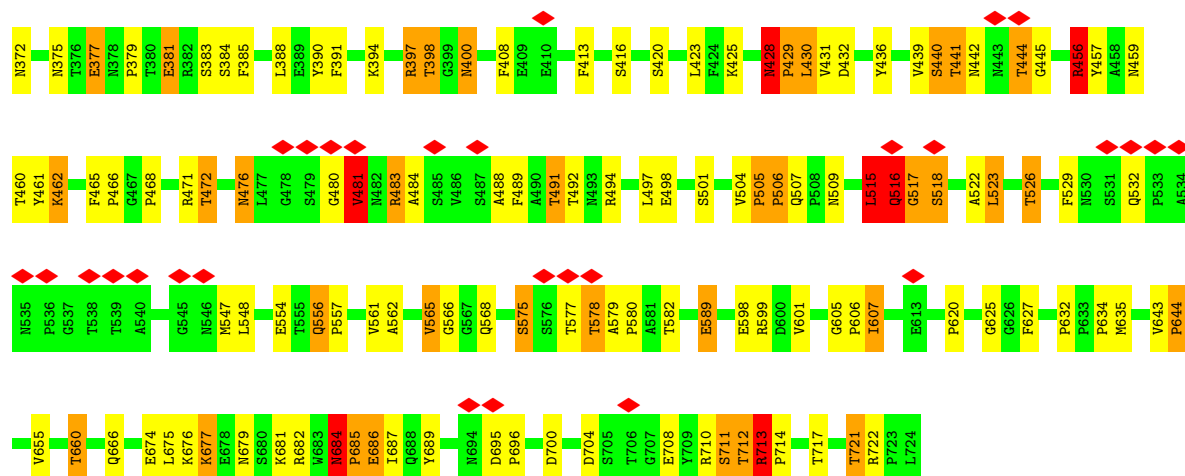


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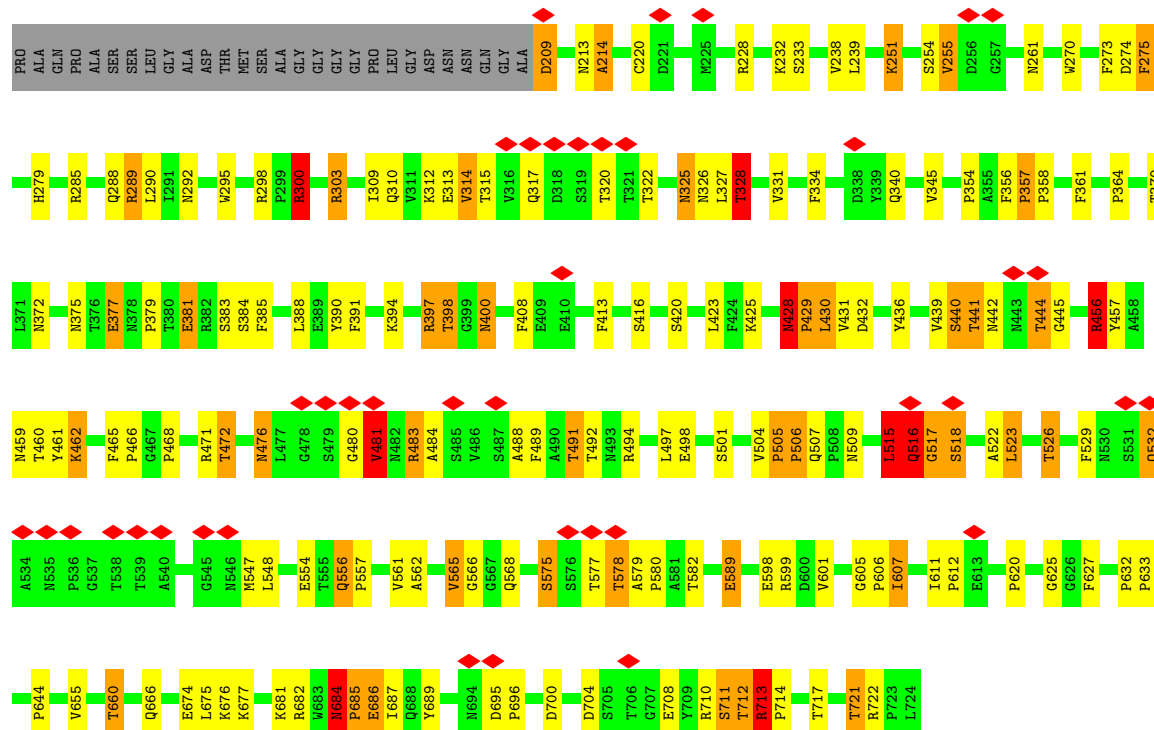
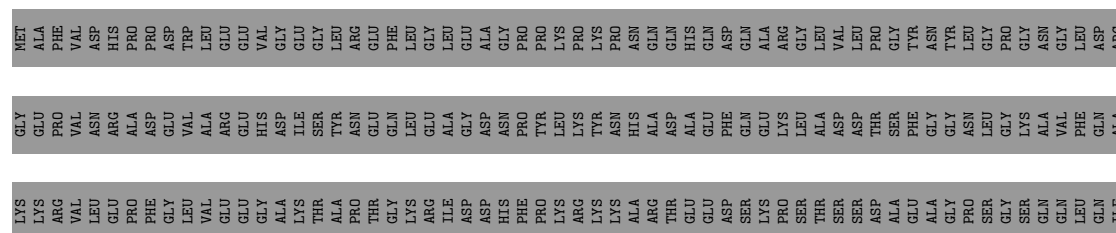


• Molecule 1: Capsid protein

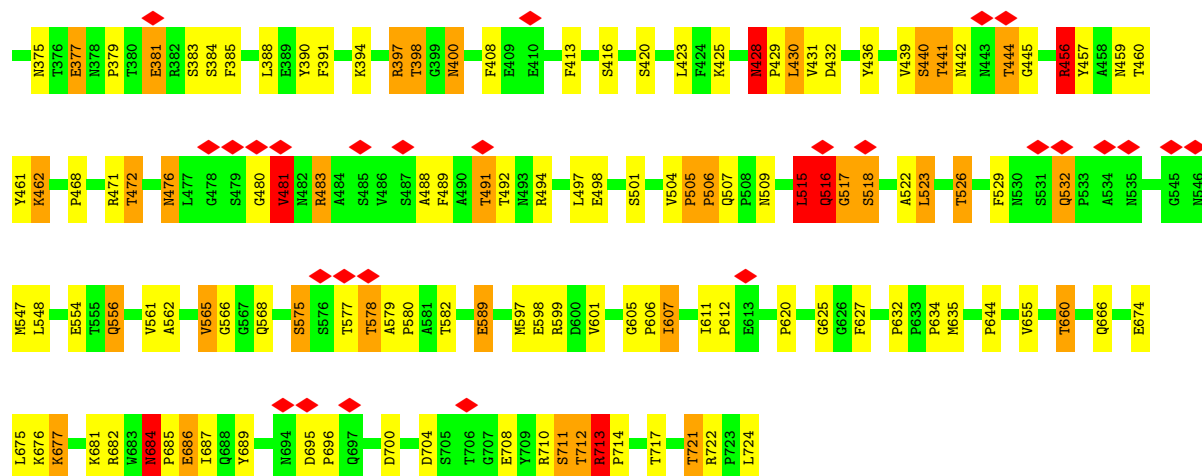




• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	285362	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	8.157	Depositor
Minimum map value	-5.436	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.452	Depositor
Recommended contour level	2	Depositor
Map size (Å)	410.40002, 410.40002, 410.40002	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8550001, 0.8550001, 0.8550001	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	1.16	1/4238 (0.0%)	1.76	86/5791 (1.5%)
1	2	1.16	1/4238 (0.0%)	1.76	86/5791 (1.5%)
1	3	1.16	1/4238 (0.0%)	1.76	86/5791 (1.5%)
1	4	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	5	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	6	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	7	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	8	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	A	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	B	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	C	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	D	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	E	1.16	1/4238 (0.0%)	1.76	83/5791 (1.4%)
1	F	1.16	1/4238 (0.0%)	1.76	83/5791 (1.4%)
1	G	1.16	1/4238 (0.0%)	1.76	83/5791 (1.4%)
1	H	1.16	1/4238 (0.0%)	1.76	87/5791 (1.5%)
1	I	1.16	1/4238 (0.0%)	1.76	87/5791 (1.5%)
1	J	1.16	1/4238 (0.0%)	1.76	86/5791 (1.5%)
1	K	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	L	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	M	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	N	1.16	1/4238 (0.0%)	1.76	83/5791 (1.4%)
1	O	1.16	1/4238 (0.0%)	1.76	83/5791 (1.4%)
1	P	1.16	1/4238 (0.0%)	1.76	83/5791 (1.4%)
1	Q	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	R	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	S	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	T	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	U	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	V	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	W	1.16	1/4238 (0.0%)	1.76	86/5791 (1.5%)
1	X	1.16	1/4238 (0.0%)	1.76	87/5791 (1.5%)
1	Y	1.16	1/4238 (0.0%)	1.76	87/5791 (1.5%)
1	Z	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	b	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	c	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	d	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	e	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	f	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	g	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	h	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	i	1.16	1/4238 (0.0%)	1.76	83/5791 (1.4%)
1	j	1.16	1/4238 (0.0%)	1.76	83/5791 (1.4%)
1	k	1.16	1/4238 (0.0%)	1.76	83/5791 (1.4%)
1	l	1.16	1/4238 (0.0%)	1.76	86/5791 (1.5%)
1	m	1.16	1/4238 (0.0%)	1.76	87/5791 (1.5%)
1	n	1.16	1/4238 (0.0%)	1.76	87/5791 (1.5%)
1	o	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	p	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	q	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	r	1.16	1/4238 (0.0%)	1.76	83/5791 (1.4%)
1	s	1.16	1/4238 (0.0%)	1.76	83/5791 (1.4%)
1	t	1.16	1/4238 (0.0%)	1.76	83/5791 (1.4%)
1	u	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	v	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	w	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	x	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	y	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
1	z	1.16	1/4238 (0.0%)	1.76	84/5791 (1.5%)
All	All	1.16	60/254280 (0.0%)	1.76	5058/347460 (1.5%)

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	12
1	2	0	12
1	3	0	12
1	4	0	12
1	5	0	12
1	6	0	12
1	7	0	12
1	8	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	12
1	B	0	12
1	C	0	12
1	D	0	12
1	E	0	12
1	F	0	12
1	G	0	12
1	H	0	12
1	I	0	12
1	J	0	12
1	K	0	12
1	L	0	12
1	M	0	12
1	N	0	12
1	O	0	12
1	P	0	12
1	Q	0	12
1	R	0	12
1	S	0	12
1	T	0	12
1	U	0	12
1	V	0	12
1	W	0	12
1	X	0	12
1	Y	0	12
1	Z	0	12
1	a	0	12
1	b	0	12
1	c	0	12
1	d	0	12
1	e	0	12
1	f	0	12
1	g	0	12
1	h	0	12
1	i	0	12
1	j	0	12
1	k	0	12
1	l	0	12
1	m	0	12
1	n	0	12
1	o	0	12
1	p	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	q	0	12
1	r	0	12
1	s	0	12
1	t	0	12
1	u	0	12
1	v	0	12
1	w	0	12
1	x	0	12
1	y	0	12
1	z	0	12
All	All	0	720

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	695	ASP	N-CA	5.12	1.50	1.46
1	I	695	ASP	N-CA	5.12	1.50	1.46
1	J	695	ASP	N-CA	5.12	1.50	1.46
1	W	695	ASP	N-CA	5.12	1.50	1.46
1	X	695	ASP	N-CA	5.12	1.50	1.46

The worst 5 of 5058 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	605	GLY	N-CA-C	9.29	123.53	112.10
1	M	605	GLY	N-CA-C	9.29	123.53	112.10
1	Q	605	GLY	N-CA-C	9.29	123.53	112.10
1	V	605	GLY	N-CA-C	9.29	123.53	112.10
1	a	605	GLY	N-CA-C	9.29	123.53	112.10

There are no chirality outliers.

5 of 720 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289	ARG	Sidechain
1	A	298	ARG	Sidechain
1	A	300	ARG	Sidechain
1	A	303	ARG	Sidechain
1	A	397	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	4110	0	3856	93	0
1	2	4110	0	3856	96	0
1	3	4110	0	3856	95	0
1	4	4110	0	3856	94	0
1	5	4110	0	3856	92	0
1	6	4110	0	3856	93	0
1	7	4110	0	3856	95	0
1	8	4110	0	3856	93	0
1	A	4110	0	3856	98	0
1	B	4110	0	3856	95	0
1	C	4110	0	3856	94	0
1	D	4110	0	3856	94	0
1	E	4110	0	3856	94	0
1	F	4110	0	3856	98	0
1	G	4110	0	3856	92	0
1	H	4110	0	3856	99	0
1	I	4110	0	3856	98	0
1	J	4110	0	3856	95	0
1	K	4110	0	3856	98	0
1	L	4110	0	3856	92	0
1	M	4110	0	3856	95	0
1	N	4110	0	3856	97	0
1	O	4110	0	3856	93	0
1	P	4110	0	3856	93	0
1	Q	4110	0	3856	95	0
1	R	4110	0	3856	97	0
1	S	4110	0	3856	93	0
1	T	4110	0	3856	95	0
1	U	4110	0	3856	92	0
1	V	4110	0	3856	95	0
1	W	4110	0	3856	97	0
1	X	4110	0	3856	92	0
1	Y	4110	0	3856	96	0
1	Z	4110	0	3856	93	0
1	a	4110	0	3856	93	0
1	b	4110	0	3856	98	0
1	c	4110	0	3856	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	d	4110	0	3856	93	0
1	e	4110	0	3856	92	0
1	f	4110	0	3856	95	0
1	g	4110	0	3856	95	0
1	h	4110	0	3856	93	0
1	i	4110	0	3856	97	0
1	j	4110	0	3856	95	0
1	k	4110	0	3856	97	0
1	l	4110	0	3856	96	0
1	m	4110	0	3856	94	0
1	n	4110	0	3856	97	0
1	o	4110	0	3856	95	0
1	p	4110	0	3856	98	0
1	q	4110	0	3856	97	0
1	r	4110	0	3856	95	0
1	s	4110	0	3856	97	0
1	t	4110	0	3856	96	0
1	u	4110	0	3856	96	0
1	v	4110	0	3856	95	0
1	w	4110	0	3856	98	0
1	x	4110	0	3856	97	0
1	y	4110	0	3856	92	0
1	z	4110	0	3856	95	0
All	All	246600	0	231360	3831	0

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

The worst 5 of 3831 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)
1:B:310:GLN:HG2	1:g:328:THR:CG2	1.84	1.08
1:I:328:THR:CG2	1:4:310:GLN:HG2	1.84	1.08
1:T:328:THR:CG2	1:z:310:GLN:HG2	1.84	1.08
1:V:328:THR:CG2	1:X:310:GLN:HG2	1.84	1.08
1:W:328:THR:CG2	1:c:310:GLN:HG2	1.84	1.08

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	2	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	3	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	4	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	5	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	6	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	7	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	8	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	A	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	B	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	C	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	D	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	E	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	F	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	G	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	H	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	I	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	J	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	K	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	L	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	M	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	N	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	O	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	P	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	Q	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	S	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	T	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	U	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	V	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	W	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	X	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	Y	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	Z	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	a	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	b	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	c	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	d	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	e	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	f	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	g	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	h	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	i	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	j	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	k	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	l	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	m	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	n	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	o	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	p	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	q	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	r	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	s	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	t	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	u	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	v	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	x	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	y	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
1	z	514/724 (71%)	502 (98%)	9 (2%)	3 (1%)	21	29
All	All	30840/43440 (71%)	30120 (98%)	540 (2%)	180 (1%)	23	29

5 of 180 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	481	VAL
1	A	516	GLN
1	A	518	SER
1	B	481	VAL
1	B	516	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	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	2	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	3	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	4	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	5	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	6	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	7	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	8	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	A	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	B	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	C	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	D	451/612 (74%)	374 (83%)	77 (17%)	2	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	F	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	G	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	H	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	I	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	J	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	K	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	L	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	M	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	N	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	O	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	P	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	Q	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	R	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	S	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	T	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	U	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	V	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	W	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	X	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	Y	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	Z	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	a	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	b	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	c	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	d	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	e	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	f	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	g	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	h	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	i	451/612 (74%)	373 (83%)	78 (17%)	2	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	j	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	k	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	l	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	m	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	n	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	o	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	p	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	q	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	r	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	s	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	t	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	u	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	v	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	w	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	x	451/612 (74%)	373 (83%)	78 (17%)	2	1
1	y	451/612 (74%)	374 (83%)	77 (17%)	2	1
1	z	451/612 (74%)	373 (83%)	78 (17%)	2	1
All	All	27060/36720 (74%)	22410 (83%)	4650 (17%)	4	1

5 of 4650 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	v	598	GLU
1	8	300	ARG
1	x	312	LYS
1	v	577	THR
1	2	532	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1305 such sidechains are listed below:

Mol	Chain	Res	Type
1	q	619	HIS
1	l	661	GLN
1	r	684	ASN
1	q	564	ASN

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Mol	Chain	Res	Type
1	v	679	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.

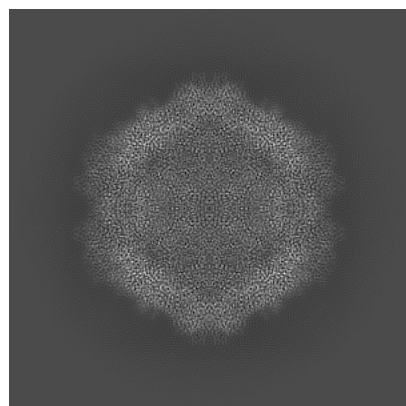
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64272. These allow visual inspection of the internal detail of the map and identification of artifacts.

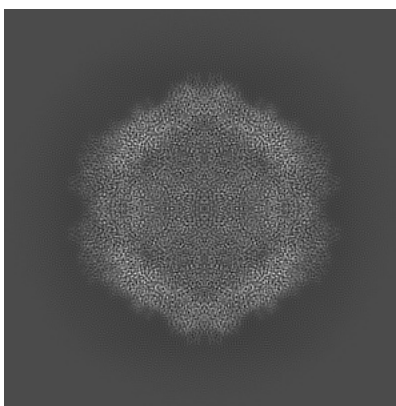
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

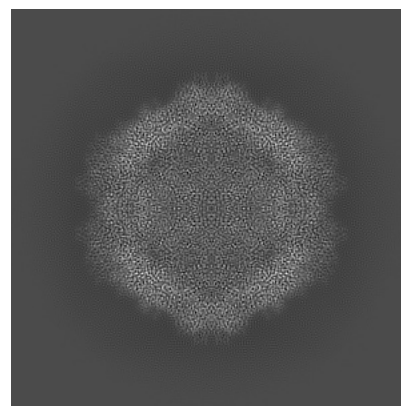
6.1.1 Primary map



X

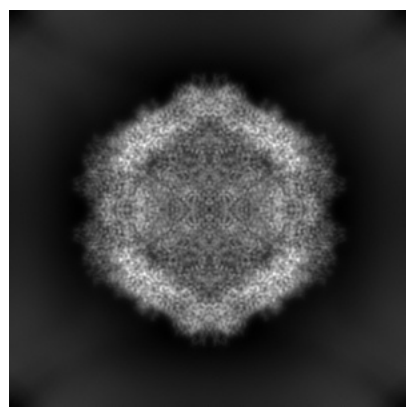


Y

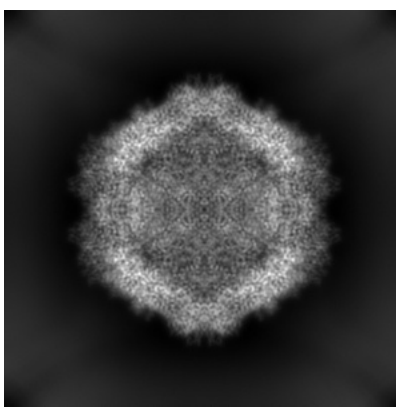


Z

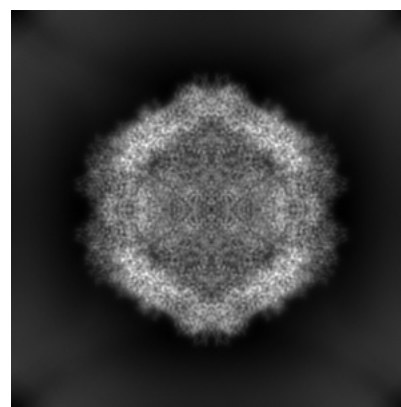
6.1.2 Raw map



X



Y

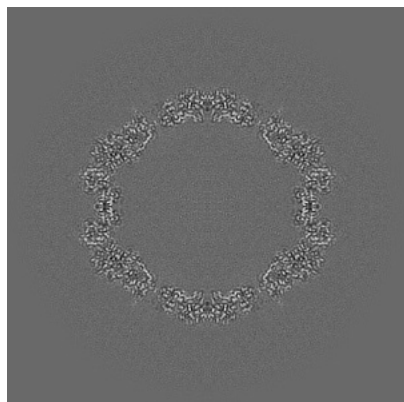


Z

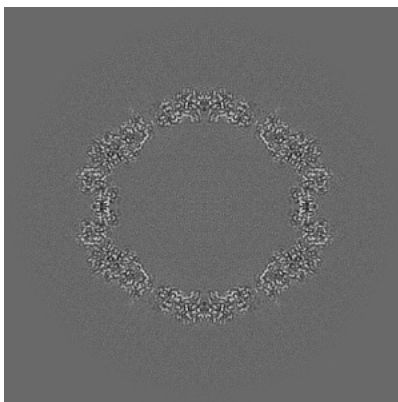
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

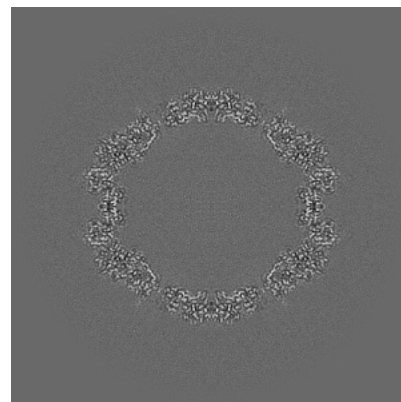
6.2.1 Primary map



X Index: 240

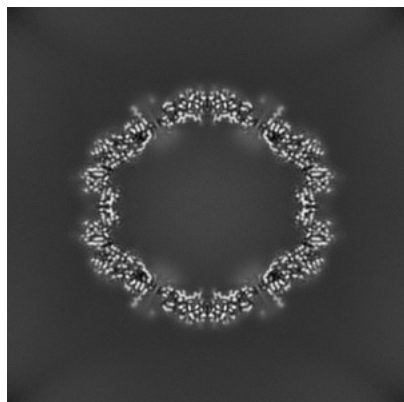


Y Index: 240

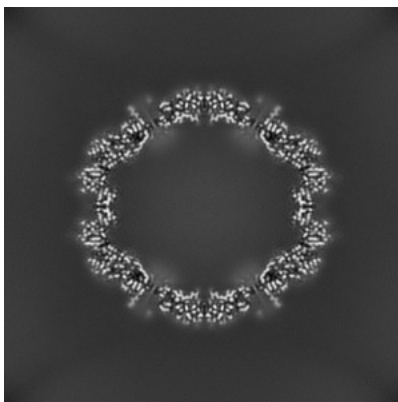


Z Index: 240

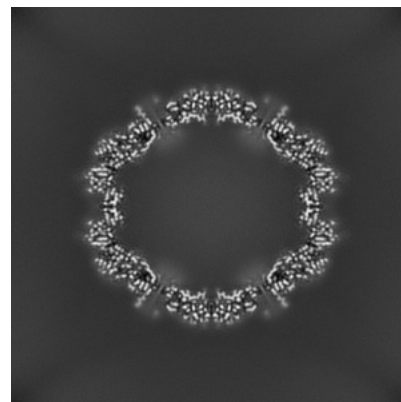
6.2.2 Raw map



X Index: 240



Y Index: 240

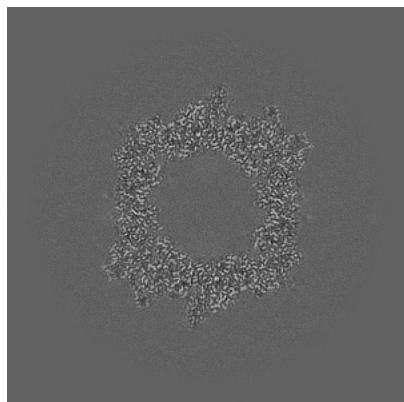


Z Index: 240

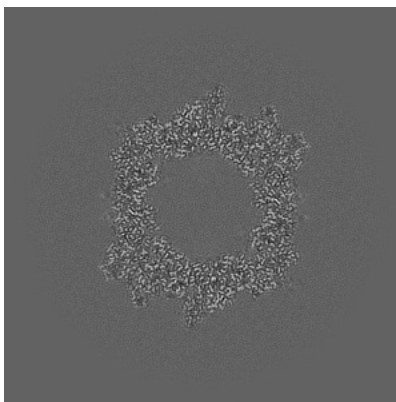
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

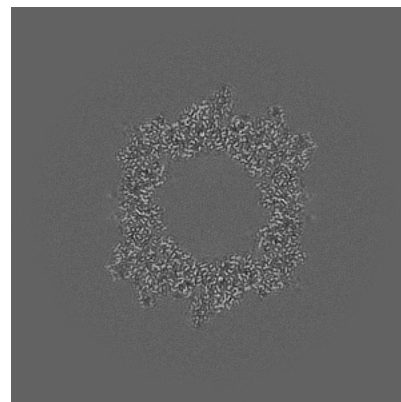
6.3.1 Primary map



X Index: 321

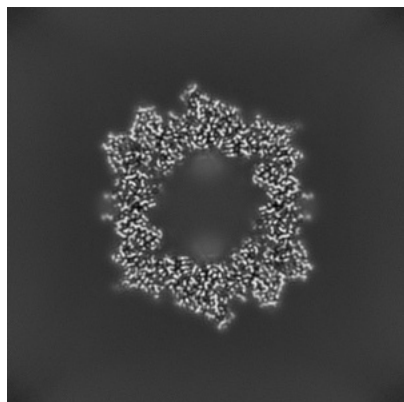


Y Index: 321

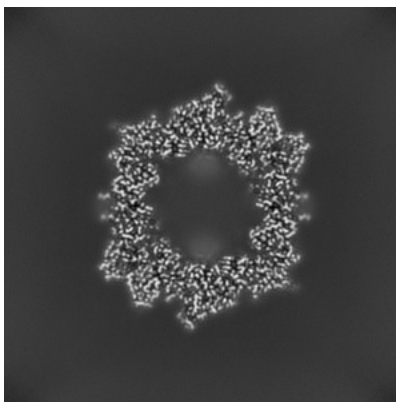


Z Index: 321

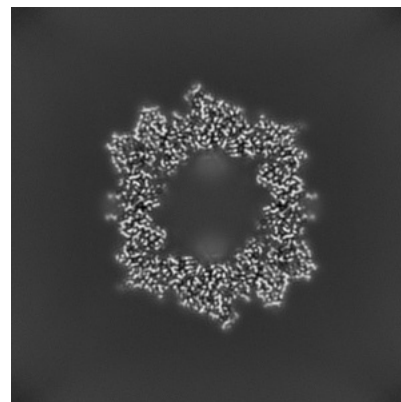
6.3.2 Raw map



X Index: 161



Y Index: 319

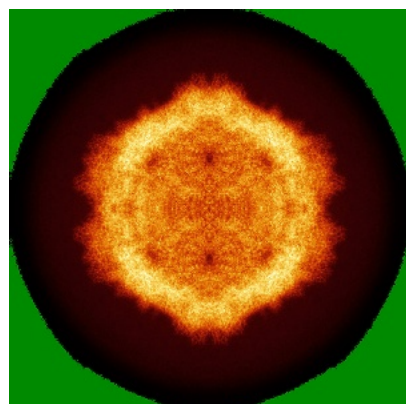


Z Index: 161

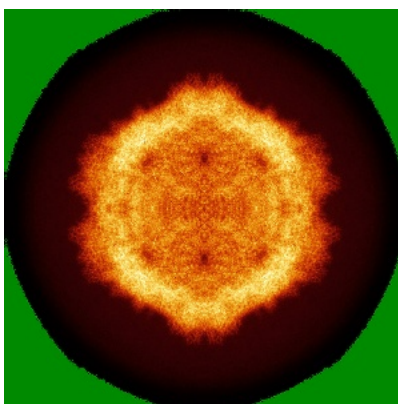
The images above show the largest variance slices of the map in three orthogonal directions.

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

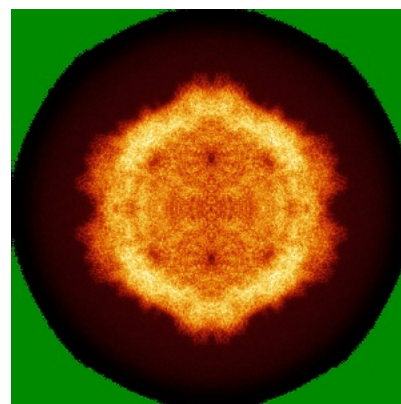
6.4.1 Primary map



X

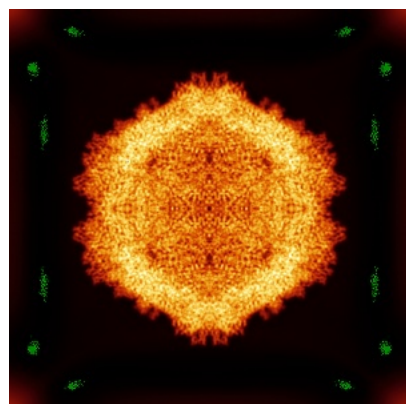


Y

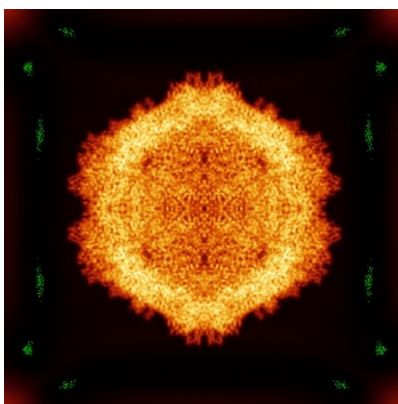


Z

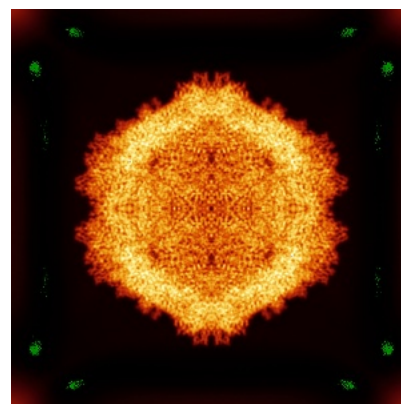
6.4.2 Raw map



X



Y

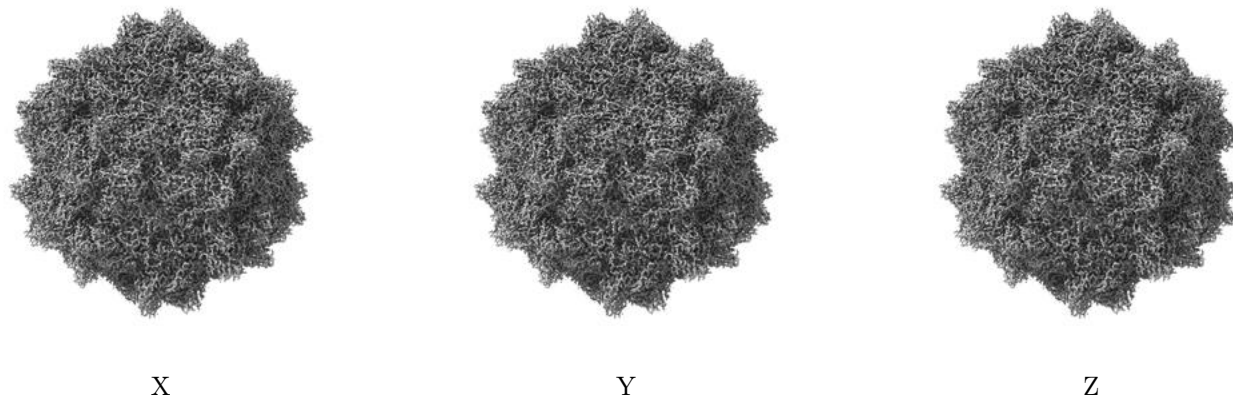


Z

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.

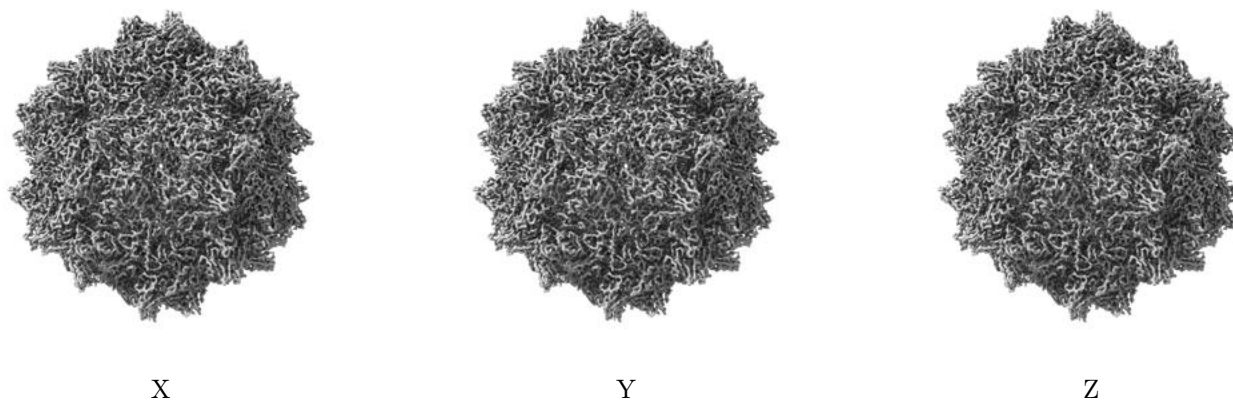
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.0. 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.

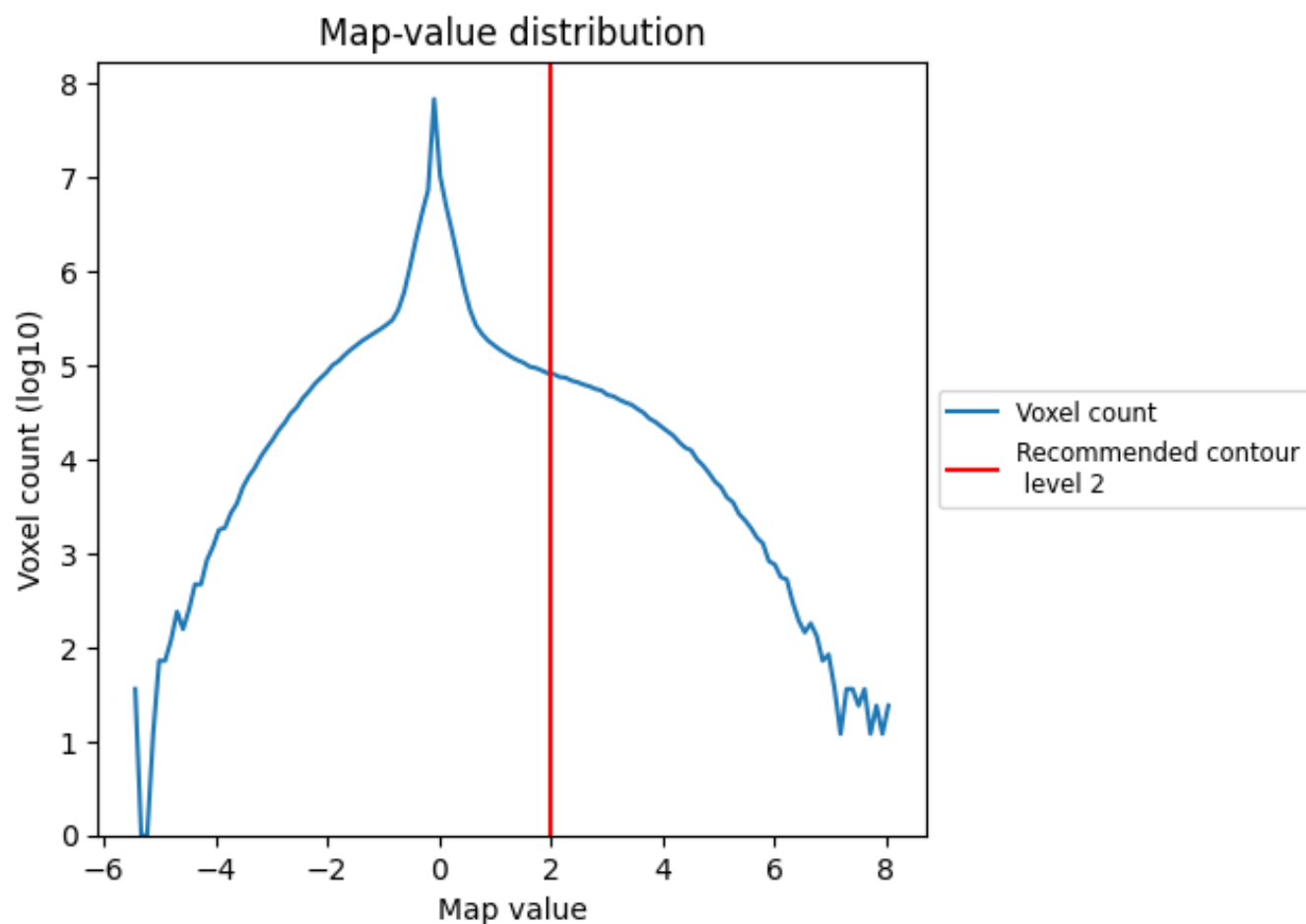
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

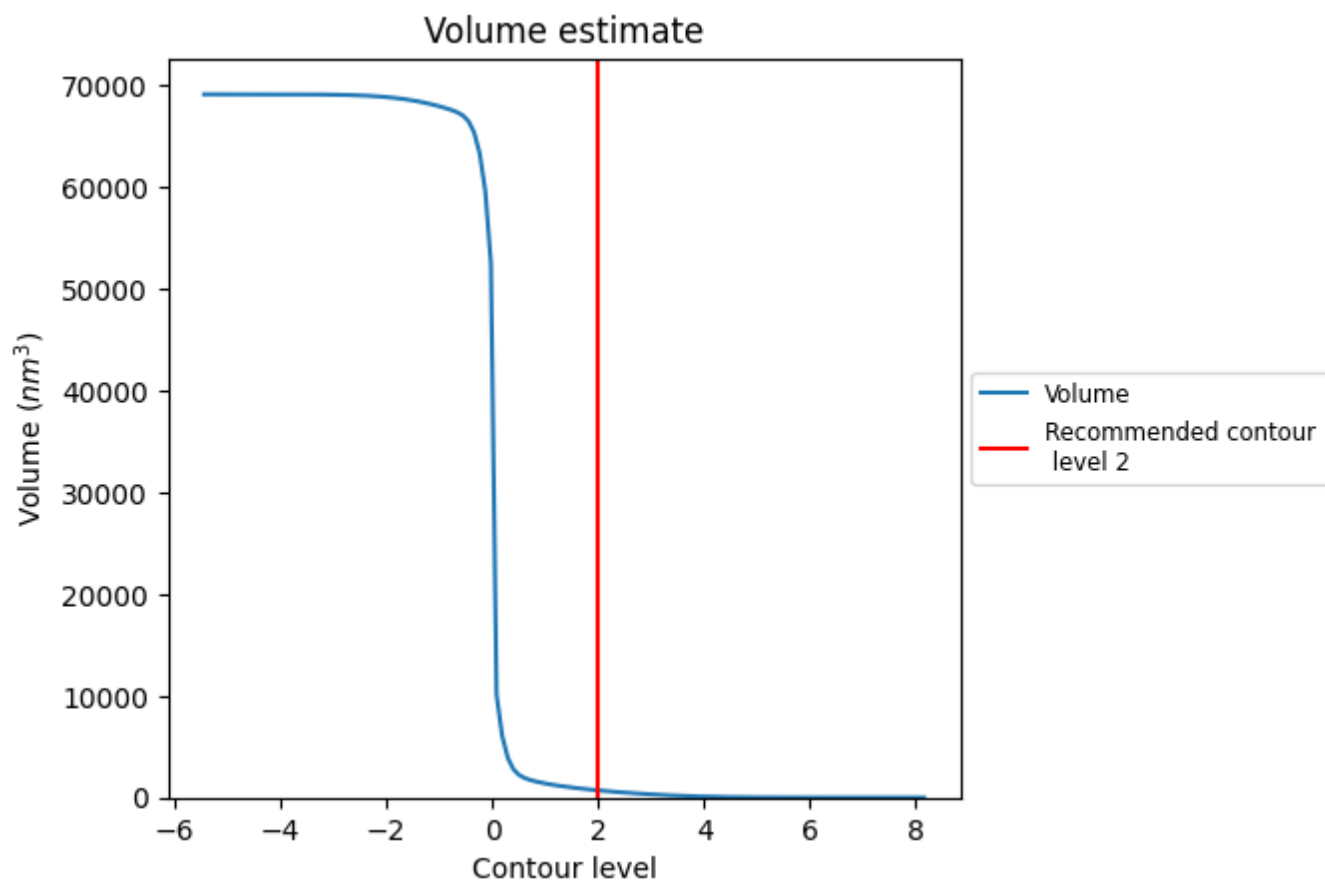
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

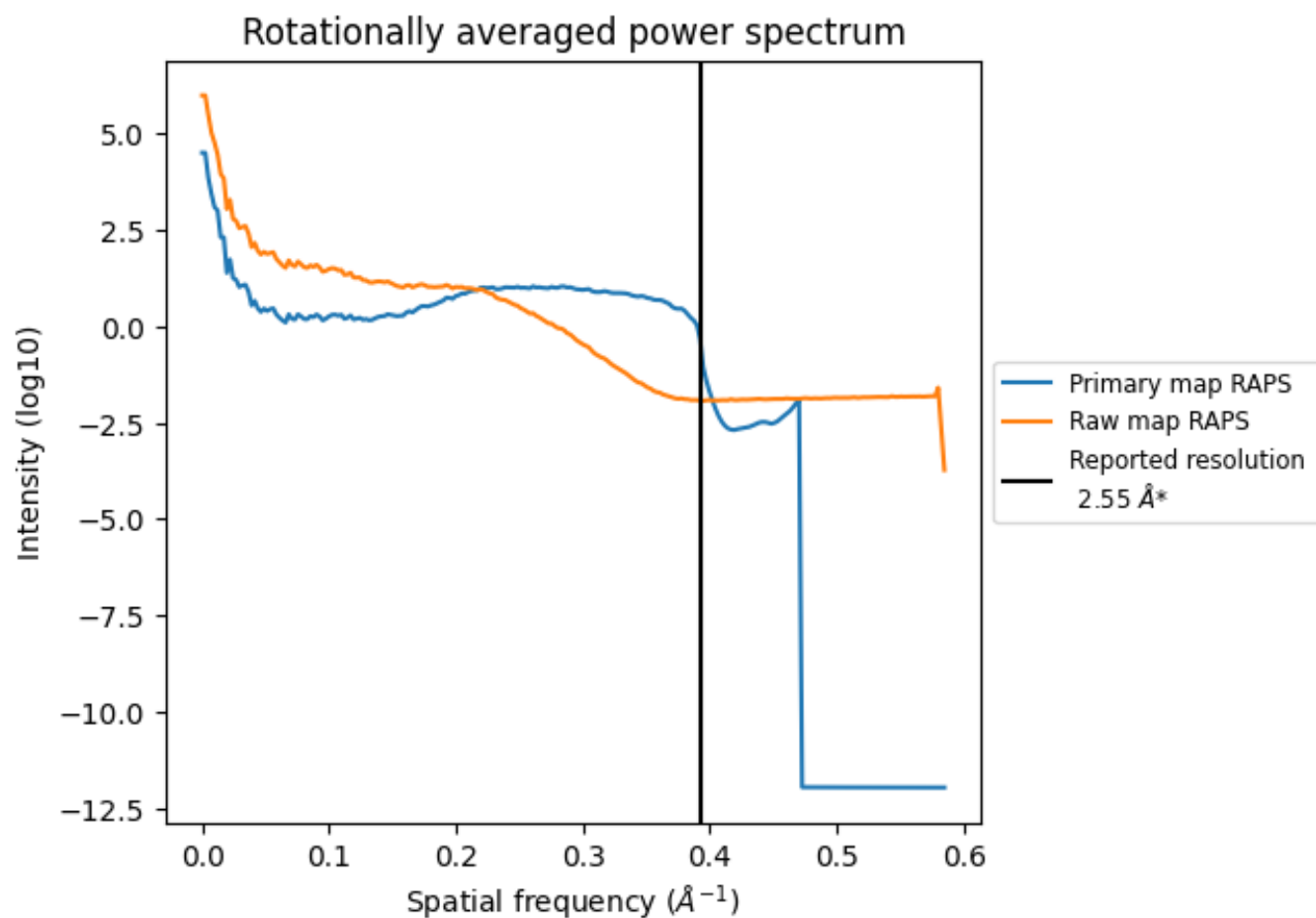
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 711 nm³; this corresponds to an approximate mass of 642 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 ⓘ

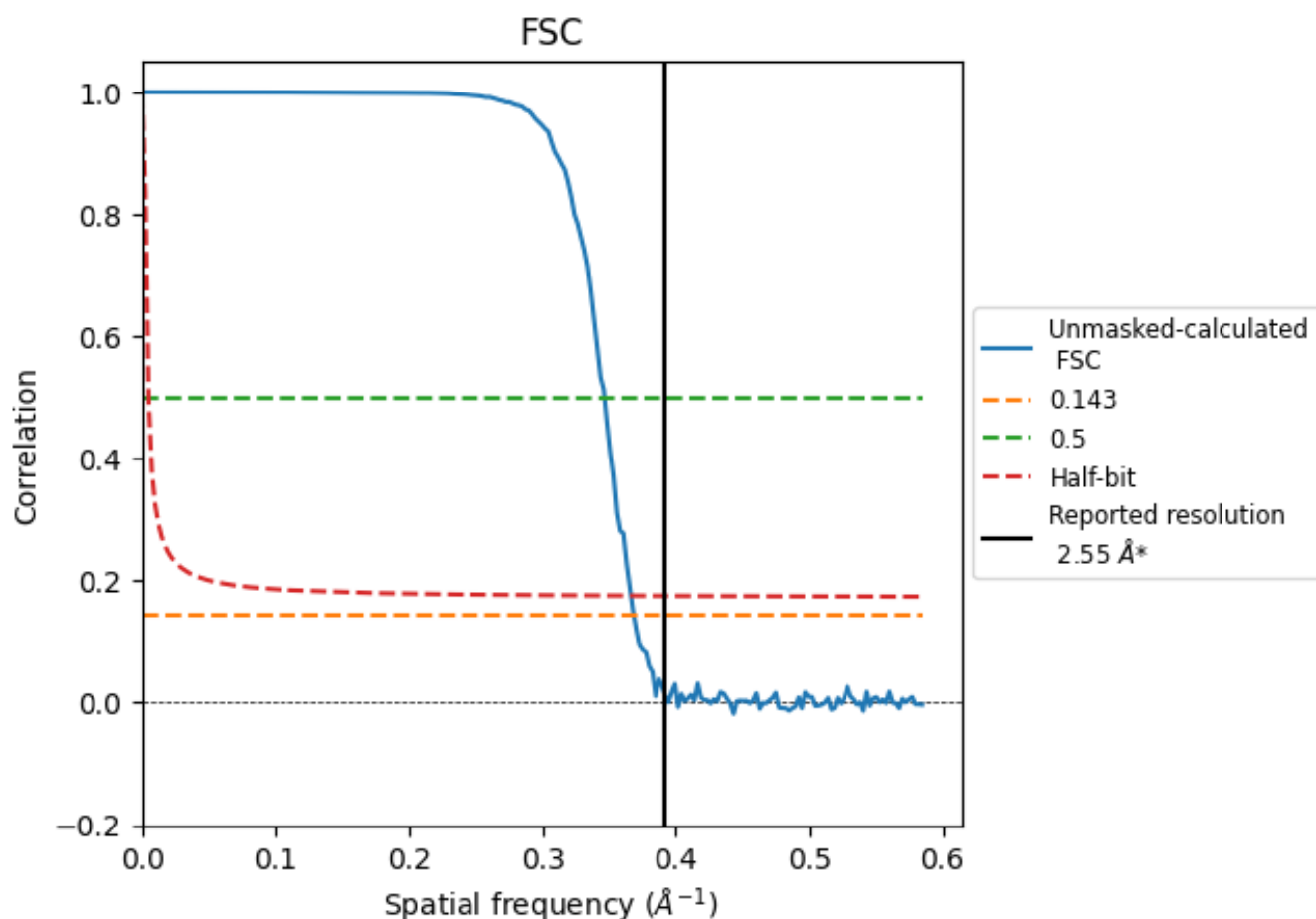


*Reported resolution corresponds to spatial frequency of $0.392 \text{ \AA}^{-1}$

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 0.392 Å⁻¹

8.2 Resolution estimates [i](#)

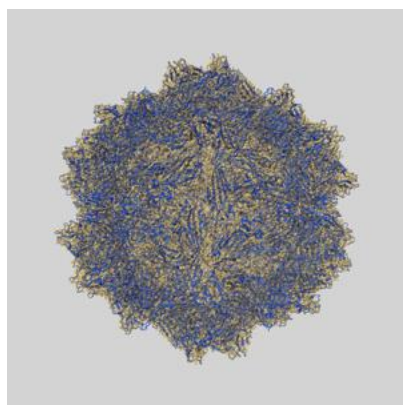
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.55	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.71	2.89	2.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

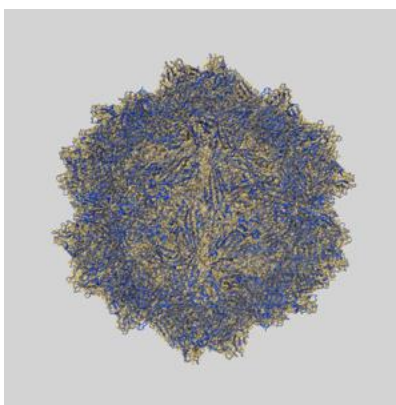
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64272 and PDB model 9UMB. Per-residue inclusion information can be found in section [3](#) on page [12](#).

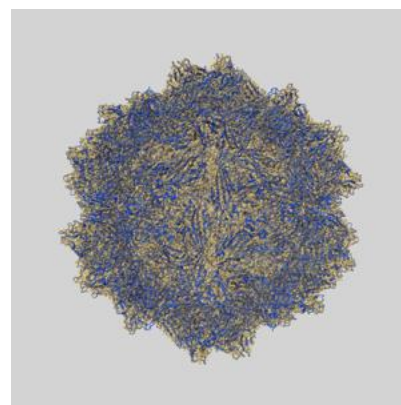
9.1 Map-model overlay [i](#)



X



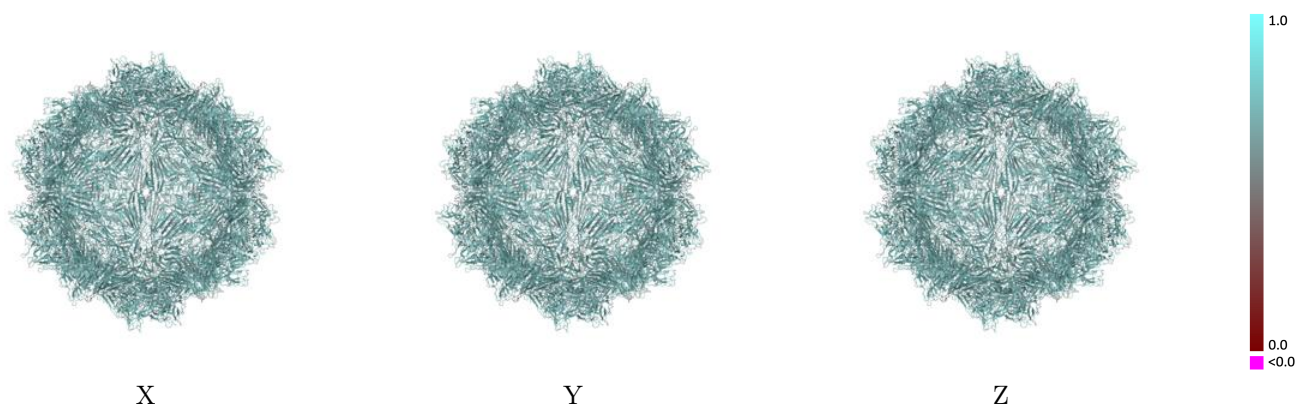
Y



Z

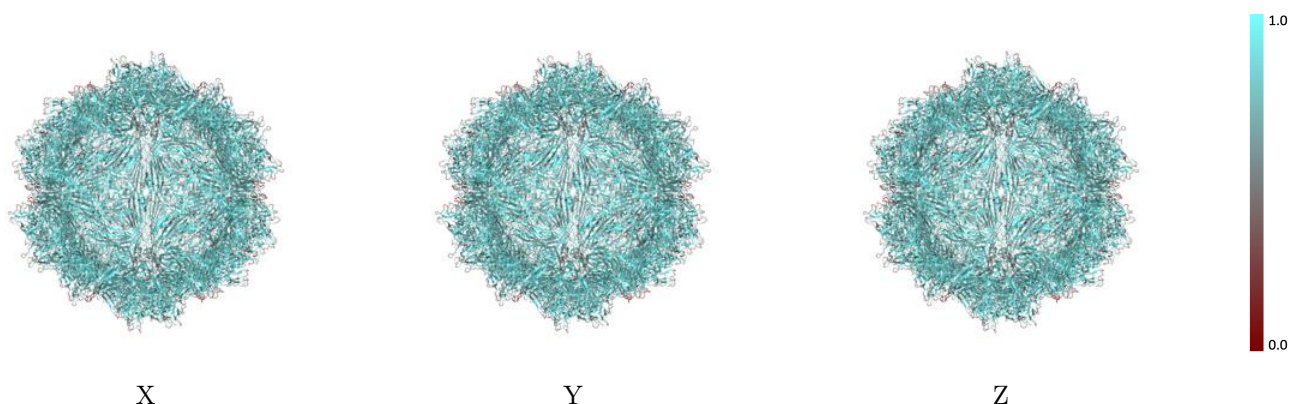
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



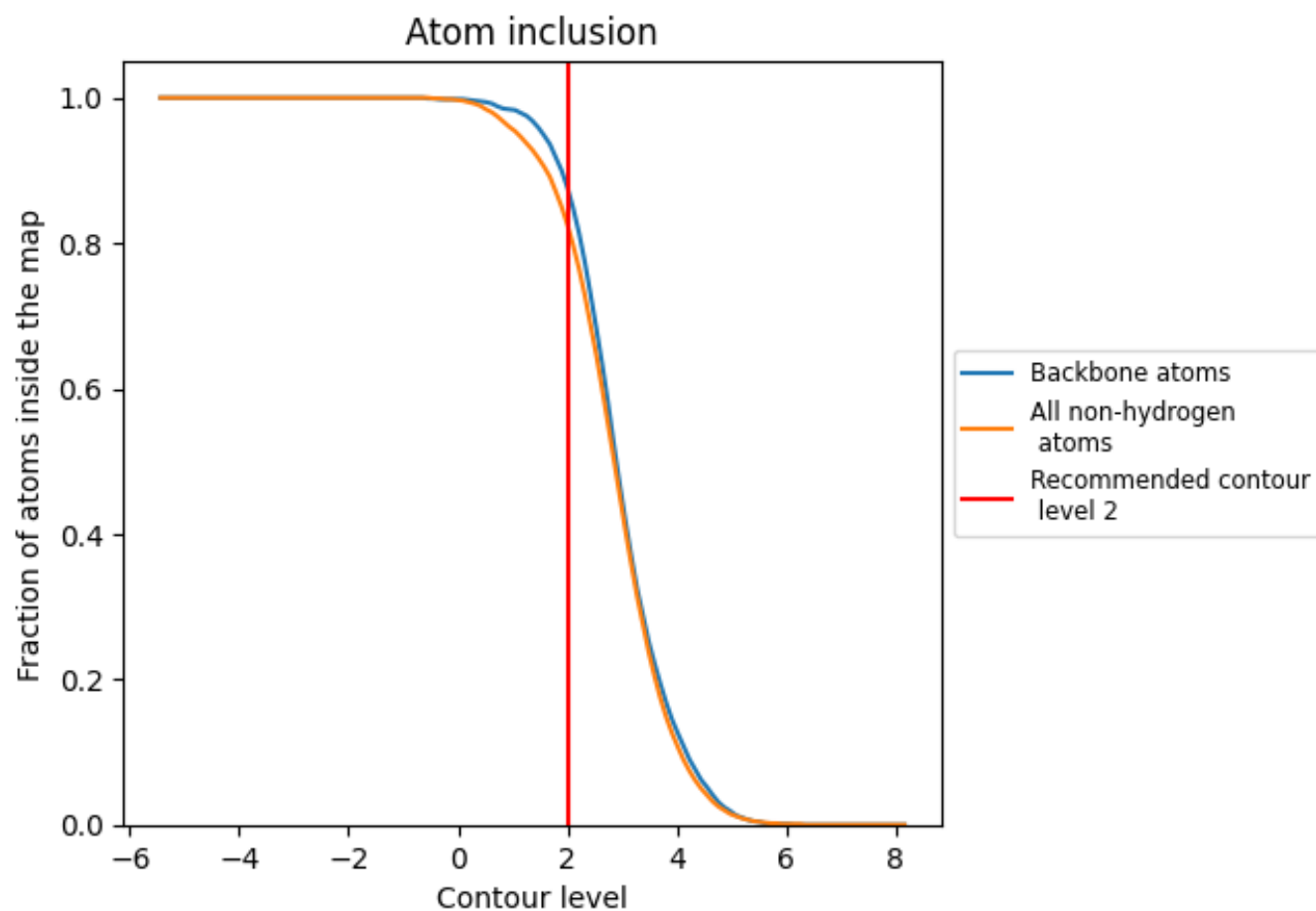
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 82% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8250	 0.6940
1	 0.8240	 0.6940
2	 0.8240	 0.6940
3	 0.8240	 0.6930
4	 0.8250	 0.6930
5	 0.8240	 0.6930
6	 0.8310	 0.6970
7	 0.8250	 0.6930
8	 0.8240	 0.6930
A	 0.8310	 0.6950
B	 0.8240	 0.6930
C	 0.8310	 0.6960
D	 0.8250	 0.6930
E	 0.8230	 0.6930
F	 0.8230	 0.6940
G	 0.8230	 0.6940
H	 0.8230	 0.6940
I	 0.8240	 0.6940
J	 0.8240	 0.6940
K	 0.8310	 0.6980
L	 0.8250	 0.6940
M	 0.8240	 0.6940
N	 0.8230	 0.6930
O	 0.8230	 0.6940
P	 0.8230	 0.6930
Q	 0.8240	 0.6940
R	 0.8310	 0.6980
S	 0.8250	 0.6940
T	 0.8310	 0.6970
U	 0.8250	 0.6930
V	 0.8240	 0.6940
W	 0.8240	 0.6940
X	 0.8240	 0.6940
Y	 0.8240	 0.6930
Z	 0.8250	 0.6930



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Chain	Atom inclusion	Q-score
a	 0.8240	 0.6930
b	 0.8310	 0.6960
c	 0.8250	 0.6920
d	 0.8240	 0.6930
e	 0.8310	 0.6960
f	 0.8240	 0.6930
g	 0.8310	 0.6960
h	 0.8250	 0.6930
i	 0.8230	 0.6930
j	 0.8230	 0.6930
k	 0.8230	 0.6930
l	 0.8230	 0.6940
m	 0.8240	 0.6940
n	 0.8240	 0.6940
o	 0.8310	 0.6970
p	 0.8250	 0.6950
q	 0.8240	 0.6940
r	 0.8230	 0.6930
s	 0.8230	 0.6940
t	 0.8230	 0.6930
u	 0.8240	 0.6940
v	 0.8310	 0.6980
w	 0.8250	 0.6940
x	 0.8310	 0.6970
y	 0.8250	 0.6930
z	 0.8240	 0.6940