wwPDB EM Validation Summary Report

Mar 20, 2026 – 04:35 PM UTC

PDB ID	:	8TEX / pdb_00008tex
EMDB ID	:	EMD-41208
Title	:	Avian Adeno-associated virus - empty capsid
Authors	:	Hsi, J.; Mietzsch, M.; Chipman, P.; Afione, S.; Zeher, A.; Huang, R.; Chiorini, J.; McKenna, R.
Deposited on	:	2023-07-07
Resolution	:	2.54 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:

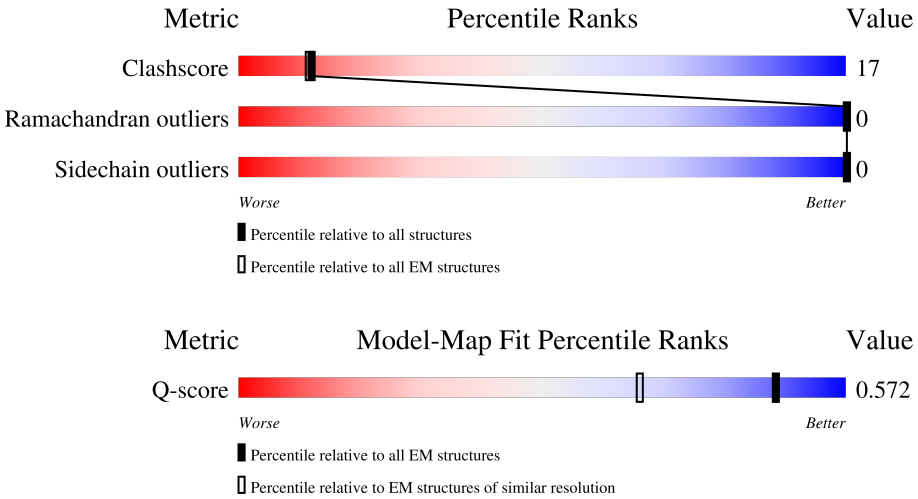
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & 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 2.54 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	7403 (2.04 - 3.04)

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	535	62% 33%
1	2	535	61% 34%
1	3	535	62% 34%
1	4	535	62% 34%

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Mol	Chain	Length	Quality of chain
1	5	535	63% 33%
1	6	535	61% 34%
1	7	535	62% 34%
1	8	535	62% 34%
1	A	535	61% 35%
1	B	535	62% 34%
1	C	535	62% 34%
1	D	535	62% 34%
1	E	535	63% 33%
1	F	535	62% 34%
1	G	535	62% 34%
1	H	535	63% 33%
1	I	535	62% 33%
1	J	535	62% 34%
1	K	535	62% 34%
1	L	535	61% 34%
1	M	535	61% 35%
1	N	535	63% 33%
1	O	535	61% 35%
1	P	535	62% 34%
1	Q	535	62% 34%
1	R	535	62% 34%
1	S	535	61% 35%
1	T	535	62% 34%
1	U	535	62% 34%

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Mol	Chain	Length	Quality of chain
1	V	535	61% 35%
1	W	535	62% 34%
1	X	535	62% 33%
1	Y	535	61% 34%
1	Z	535	62% 34%
1	a	535	62% 33%
1	b	535	62% 34%
1	c	535	62% 34%
1	d	535	62% 34%
1	e	535	62% 33%
1	f	535	62% 34%
1	g	535	62% 34%
1	h	535	61% 35%
1	i	535	62% 33%
1	j	535	62% 34%
1	k	535	62% 34%
1	l	535	61% 35%
1	m	535	62% 34%
1	n	535	62% 34%
1	o	535	62% 33%
1	p	535	62% 34%
1	q	535	62% 33%
1	r	535	61% 35%
1	s	535	62% 34%
1	t	535	62% 34%

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Mol	Chain	Length	Quality of chain
1	u	535	62% 33%
1	v	535	61% 35%
1	w	535	63% 33%
1	x	535	62% 34%
1	y	535	62% 34%
1	z	535	62% 34%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 247440 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	512	Total 4124	C 2619	N 717	O 774	S 14	0	0
1	B	512	Total 4124	C 2619	N 717	O 774	S 14	0	0
1	C	512	Total 4124	C 2619	N 717	O 774	S 14	0	0
1	D	512	Total 4124	C 2619	N 717	O 774	S 14	0	0
1	E	512	Total 4124	C 2619	N 717	O 774	S 14	0	0
1	F	512	Total 4124	C 2619	N 717	O 774	S 14	0	0
1	G	512	Total 4124	C 2619	N 717	O 774	S 14	0	0
1	H	512	Total 4124	C 2619	N 717	O 774	S 14	0	0
1	I	512	Total 4124	C 2619	N 717	O 774	S 14	0	0
1	J	512	Total 4124	C 2619	N 717	O 774	S 14	0	0
1	K	512	Total 4124	C 2619	N 717	O 774	S 14	0	0
1	L	512	Total 4124	C 2619	N 717	O 774	S 14	0	0
1	M	512	Total 4124	C 2619	N 717	O 774	S 14	0	0
1	N	512	Total 4124	C 2619	N 717	O 774	S 14	0	0
1	O	512	Total 4124	C 2619	N 717	O 774	S 14	0	0
1	P	512	Total 4124	C 2619	N 717	O 774	S 14	0	0
1	Q	512	Total 4124	C 2619	N 717	O 774	S 14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	S	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	T	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	U	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	V	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	W	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	X	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	Y	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	Z	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	a	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	b	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	c	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	d	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	e	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	f	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	g	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	h	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	i	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	j	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	k	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	l	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	n	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	o	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	p	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	q	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	r	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	s	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	t	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	u	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	v	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	w	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	x	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	y	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	z	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	1	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	2	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	3	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	4	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	5	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	6	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		
1	7	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	512	Total	C	N	O	S	0	0
			4124	2619	717	774	14		

There are 480 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	SER	PHE	conflict	UNP Q7TG43
A	339	ALA	GLY	conflict	UNP Q7TG43
A	621	LEU	PRO	conflict	UNP Q7TG43
A	622	GLN	THR	conflict	UNP Q7TG43
A	624	PRO	THR	conflict	UNP Q7TG43
A	625	ILE	HIS	conflict	UNP Q7TG43
A	626	TRP	LEU	conflict	UNP Q7TG43
A	644	GLY	ARG	conflict	UNP Q7TG43
B	334	SER	PHE	conflict	UNP Q7TG43
B	339	ALA	GLY	conflict	UNP Q7TG43
B	621	LEU	PRO	conflict	UNP Q7TG43
B	622	GLN	THR	conflict	UNP Q7TG43
B	624	PRO	THR	conflict	UNP Q7TG43
B	625	ILE	HIS	conflict	UNP Q7TG43
B	626	TRP	LEU	conflict	UNP Q7TG43
B	644	GLY	ARG	conflict	UNP Q7TG43
C	334	SER	PHE	conflict	UNP Q7TG43
C	339	ALA	GLY	conflict	UNP Q7TG43
C	621	LEU	PRO	conflict	UNP Q7TG43
C	622	GLN	THR	conflict	UNP Q7TG43
C	624	PRO	THR	conflict	UNP Q7TG43
C	625	ILE	HIS	conflict	UNP Q7TG43
C	626	TRP	LEU	conflict	UNP Q7TG43
C	644	GLY	ARG	conflict	UNP Q7TG43
D	334	SER	PHE	conflict	UNP Q7TG43
D	339	ALA	GLY	conflict	UNP Q7TG43
D	621	LEU	PRO	conflict	UNP Q7TG43
D	622	GLN	THR	conflict	UNP Q7TG43
D	624	PRO	THR	conflict	UNP Q7TG43
D	625	ILE	HIS	conflict	UNP Q7TG43
D	626	TRP	LEU	conflict	UNP Q7TG43
D	644	GLY	ARG	conflict	UNP Q7TG43
E	334	SER	PHE	conflict	UNP Q7TG43
E	339	ALA	GLY	conflict	UNP Q7TG43
E	621	LEU	PRO	conflict	UNP Q7TG43
E	622	GLN	THR	conflict	UNP Q7TG43

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Chain	Residue	Modelled	Actual	Comment	Reference
E	624	PRO	THR	conflict	UNP Q7TG43
E	625	ILE	HIS	conflict	UNP Q7TG43
E	626	TRP	LEU	conflict	UNP Q7TG43
E	644	GLY	ARG	conflict	UNP Q7TG43
F	334	SER	PHE	conflict	UNP Q7TG43
F	339	ALA	GLY	conflict	UNP Q7TG43
F	621	LEU	PRO	conflict	UNP Q7TG43
F	622	GLN	THR	conflict	UNP Q7TG43
F	624	PRO	THR	conflict	UNP Q7TG43
F	625	ILE	HIS	conflict	UNP Q7TG43
F	626	TRP	LEU	conflict	UNP Q7TG43
F	644	GLY	ARG	conflict	UNP Q7TG43
G	334	SER	PHE	conflict	UNP Q7TG43
G	339	ALA	GLY	conflict	UNP Q7TG43
G	621	LEU	PRO	conflict	UNP Q7TG43
G	622	GLN	THR	conflict	UNP Q7TG43
G	624	PRO	THR	conflict	UNP Q7TG43
G	625	ILE	HIS	conflict	UNP Q7TG43
G	626	TRP	LEU	conflict	UNP Q7TG43
G	644	GLY	ARG	conflict	UNP Q7TG43
H	334	SER	PHE	conflict	UNP Q7TG43
H	339	ALA	GLY	conflict	UNP Q7TG43
H	621	LEU	PRO	conflict	UNP Q7TG43
H	622	GLN	THR	conflict	UNP Q7TG43
H	624	PRO	THR	conflict	UNP Q7TG43
H	625	ILE	HIS	conflict	UNP Q7TG43
H	626	TRP	LEU	conflict	UNP Q7TG43
H	644	GLY	ARG	conflict	UNP Q7TG43
I	334	SER	PHE	conflict	UNP Q7TG43
I	339	ALA	GLY	conflict	UNP Q7TG43
I	621	LEU	PRO	conflict	UNP Q7TG43
I	622	GLN	THR	conflict	UNP Q7TG43
I	624	PRO	THR	conflict	UNP Q7TG43
I	625	ILE	HIS	conflict	UNP Q7TG43
I	626	TRP	LEU	conflict	UNP Q7TG43
I	644	GLY	ARG	conflict	UNP Q7TG43
J	334	SER	PHE	conflict	UNP Q7TG43
J	339	ALA	GLY	conflict	UNP Q7TG43
J	621	LEU	PRO	conflict	UNP Q7TG43
J	622	GLN	THR	conflict	UNP Q7TG43
J	624	PRO	THR	conflict	UNP Q7TG43
J	625	ILE	HIS	conflict	UNP Q7TG43

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Chain	Residue	Modelled	Actual	Comment	Reference
J	626	TRP	LEU	conflict	UNP Q7TG43
J	644	GLY	ARG	conflict	UNP Q7TG43
K	334	SER	PHE	conflict	UNP Q7TG43
K	339	ALA	GLY	conflict	UNP Q7TG43
K	621	LEU	PRO	conflict	UNP Q7TG43
K	622	GLN	THR	conflict	UNP Q7TG43
K	624	PRO	THR	conflict	UNP Q7TG43
K	625	ILE	HIS	conflict	UNP Q7TG43
K	626	TRP	LEU	conflict	UNP Q7TG43
K	644	GLY	ARG	conflict	UNP Q7TG43
L	334	SER	PHE	conflict	UNP Q7TG43
L	339	ALA	GLY	conflict	UNP Q7TG43
L	621	LEU	PRO	conflict	UNP Q7TG43
L	622	GLN	THR	conflict	UNP Q7TG43
L	624	PRO	THR	conflict	UNP Q7TG43
L	625	ILE	HIS	conflict	UNP Q7TG43
L	626	TRP	LEU	conflict	UNP Q7TG43
L	644	GLY	ARG	conflict	UNP Q7TG43
M	334	SER	PHE	conflict	UNP Q7TG43
M	339	ALA	GLY	conflict	UNP Q7TG43
M	621	LEU	PRO	conflict	UNP Q7TG43
M	622	GLN	THR	conflict	UNP Q7TG43
M	624	PRO	THR	conflict	UNP Q7TG43
M	625	ILE	HIS	conflict	UNP Q7TG43
M	626	TRP	LEU	conflict	UNP Q7TG43
M	644	GLY	ARG	conflict	UNP Q7TG43
N	334	SER	PHE	conflict	UNP Q7TG43
N	339	ALA	GLY	conflict	UNP Q7TG43
N	621	LEU	PRO	conflict	UNP Q7TG43
N	622	GLN	THR	conflict	UNP Q7TG43
N	624	PRO	THR	conflict	UNP Q7TG43
N	625	ILE	HIS	conflict	UNP Q7TG43
N	626	TRP	LEU	conflict	UNP Q7TG43
N	644	GLY	ARG	conflict	UNP Q7TG43
O	334	SER	PHE	conflict	UNP Q7TG43
O	339	ALA	GLY	conflict	UNP Q7TG43
O	621	LEU	PRO	conflict	UNP Q7TG43
O	622	GLN	THR	conflict	UNP Q7TG43
O	624	PRO	THR	conflict	UNP Q7TG43
O	625	ILE	HIS	conflict	UNP Q7TG43
O	626	TRP	LEU	conflict	UNP Q7TG43
O	644	GLY	ARG	conflict	UNP Q7TG43

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Chain	Residue	Modelled	Actual	Comment	Reference
P	334	SER	PHE	conflict	UNP Q7TG43
P	339	ALA	GLY	conflict	UNP Q7TG43
P	621	LEU	PRO	conflict	UNP Q7TG43
P	622	GLN	THR	conflict	UNP Q7TG43
P	624	PRO	THR	conflict	UNP Q7TG43
P	625	ILE	HIS	conflict	UNP Q7TG43
P	626	TRP	LEU	conflict	UNP Q7TG43
P	644	GLY	ARG	conflict	UNP Q7TG43
Q	334	SER	PHE	conflict	UNP Q7TG43
Q	339	ALA	GLY	conflict	UNP Q7TG43
Q	621	LEU	PRO	conflict	UNP Q7TG43
Q	622	GLN	THR	conflict	UNP Q7TG43
Q	624	PRO	THR	conflict	UNP Q7TG43
Q	625	ILE	HIS	conflict	UNP Q7TG43
Q	626	TRP	LEU	conflict	UNP Q7TG43
Q	644	GLY	ARG	conflict	UNP Q7TG43
R	334	SER	PHE	conflict	UNP Q7TG43
R	339	ALA	GLY	conflict	UNP Q7TG43
R	621	LEU	PRO	conflict	UNP Q7TG43
R	622	GLN	THR	conflict	UNP Q7TG43
R	624	PRO	THR	conflict	UNP Q7TG43
R	625	ILE	HIS	conflict	UNP Q7TG43
R	626	TRP	LEU	conflict	UNP Q7TG43
R	644	GLY	ARG	conflict	UNP Q7TG43
S	334	SER	PHE	conflict	UNP Q7TG43
S	339	ALA	GLY	conflict	UNP Q7TG43
S	621	LEU	PRO	conflict	UNP Q7TG43
S	622	GLN	THR	conflict	UNP Q7TG43
S	624	PRO	THR	conflict	UNP Q7TG43
S	625	ILE	HIS	conflict	UNP Q7TG43
S	626	TRP	LEU	conflict	UNP Q7TG43
S	644	GLY	ARG	conflict	UNP Q7TG43
T	334	SER	PHE	conflict	UNP Q7TG43
T	339	ALA	GLY	conflict	UNP Q7TG43
T	621	LEU	PRO	conflict	UNP Q7TG43
T	622	GLN	THR	conflict	UNP Q7TG43
T	624	PRO	THR	conflict	UNP Q7TG43
T	625	ILE	HIS	conflict	UNP Q7TG43
T	626	TRP	LEU	conflict	UNP Q7TG43
T	644	GLY	ARG	conflict	UNP Q7TG43
U	334	SER	PHE	conflict	UNP Q7TG43
U	339	ALA	GLY	conflict	UNP Q7TG43

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Chain	Residue	Modelled	Actual	Comment	Reference
U	621	LEU	PRO	conflict	UNP Q7TG43
U	622	GLN	THR	conflict	UNP Q7TG43
U	624	PRO	THR	conflict	UNP Q7TG43
U	625	ILE	HIS	conflict	UNP Q7TG43
U	626	TRP	LEU	conflict	UNP Q7TG43
U	644	GLY	ARG	conflict	UNP Q7TG43
V	334	SER	PHE	conflict	UNP Q7TG43
V	339	ALA	GLY	conflict	UNP Q7TG43
V	621	LEU	PRO	conflict	UNP Q7TG43
V	622	GLN	THR	conflict	UNP Q7TG43
V	624	PRO	THR	conflict	UNP Q7TG43
V	625	ILE	HIS	conflict	UNP Q7TG43
V	626	TRP	LEU	conflict	UNP Q7TG43
V	644	GLY	ARG	conflict	UNP Q7TG43
W	334	SER	PHE	conflict	UNP Q7TG43
W	339	ALA	GLY	conflict	UNP Q7TG43
W	621	LEU	PRO	conflict	UNP Q7TG43
W	622	GLN	THR	conflict	UNP Q7TG43
W	624	PRO	THR	conflict	UNP Q7TG43
W	625	ILE	HIS	conflict	UNP Q7TG43
W	626	TRP	LEU	conflict	UNP Q7TG43
W	644	GLY	ARG	conflict	UNP Q7TG43
X	334	SER	PHE	conflict	UNP Q7TG43
X	339	ALA	GLY	conflict	UNP Q7TG43
X	621	LEU	PRO	conflict	UNP Q7TG43
X	622	GLN	THR	conflict	UNP Q7TG43
X	624	PRO	THR	conflict	UNP Q7TG43
X	625	ILE	HIS	conflict	UNP Q7TG43
X	626	TRP	LEU	conflict	UNP Q7TG43
X	644	GLY	ARG	conflict	UNP Q7TG43
Y	334	SER	PHE	conflict	UNP Q7TG43
Y	339	ALA	GLY	conflict	UNP Q7TG43
Y	621	LEU	PRO	conflict	UNP Q7TG43
Y	622	GLN	THR	conflict	UNP Q7TG43
Y	624	PRO	THR	conflict	UNP Q7TG43
Y	625	ILE	HIS	conflict	UNP Q7TG43
Y	626	TRP	LEU	conflict	UNP Q7TG43
Y	644	GLY	ARG	conflict	UNP Q7TG43
Z	334	SER	PHE	conflict	UNP Q7TG43
Z	339	ALA	GLY	conflict	UNP Q7TG43
Z	621	LEU	PRO	conflict	UNP Q7TG43
Z	622	GLN	THR	conflict	UNP Q7TG43

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	624	PRO	THR	conflict	UNP Q7TG43
Z	625	ILE	HIS	conflict	UNP Q7TG43
Z	626	TRP	LEU	conflict	UNP Q7TG43
Z	644	GLY	ARG	conflict	UNP Q7TG43
a	334	SER	PHE	conflict	UNP Q7TG43
a	339	ALA	GLY	conflict	UNP Q7TG43
a	621	LEU	PRO	conflict	UNP Q7TG43
a	622	GLN	THR	conflict	UNP Q7TG43
a	624	PRO	THR	conflict	UNP Q7TG43
a	625	ILE	HIS	conflict	UNP Q7TG43
a	626	TRP	LEU	conflict	UNP Q7TG43
a	644	GLY	ARG	conflict	UNP Q7TG43
b	334	SER	PHE	conflict	UNP Q7TG43
b	339	ALA	GLY	conflict	UNP Q7TG43
b	621	LEU	PRO	conflict	UNP Q7TG43
b	622	GLN	THR	conflict	UNP Q7TG43
b	624	PRO	THR	conflict	UNP Q7TG43
b	625	ILE	HIS	conflict	UNP Q7TG43
b	626	TRP	LEU	conflict	UNP Q7TG43
b	644	GLY	ARG	conflict	UNP Q7TG43
c	334	SER	PHE	conflict	UNP Q7TG43
c	339	ALA	GLY	conflict	UNP Q7TG43
c	621	LEU	PRO	conflict	UNP Q7TG43
c	622	GLN	THR	conflict	UNP Q7TG43
c	624	PRO	THR	conflict	UNP Q7TG43
c	625	ILE	HIS	conflict	UNP Q7TG43
c	626	TRP	LEU	conflict	UNP Q7TG43
c	644	GLY	ARG	conflict	UNP Q7TG43
d	334	SER	PHE	conflict	UNP Q7TG43
d	339	ALA	GLY	conflict	UNP Q7TG43
d	621	LEU	PRO	conflict	UNP Q7TG43
d	622	GLN	THR	conflict	UNP Q7TG43
d	624	PRO	THR	conflict	UNP Q7TG43
d	625	ILE	HIS	conflict	UNP Q7TG43
d	626	TRP	LEU	conflict	UNP Q7TG43
d	644	GLY	ARG	conflict	UNP Q7TG43
e	334	SER	PHE	conflict	UNP Q7TG43
e	339	ALA	GLY	conflict	UNP Q7TG43
e	621	LEU	PRO	conflict	UNP Q7TG43
e	622	GLN	THR	conflict	UNP Q7TG43
e	624	PRO	THR	conflict	UNP Q7TG43
e	625	ILE	HIS	conflict	UNP Q7TG43

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Chain	Residue	Modelled	Actual	Comment	Reference
e	626	TRP	LEU	conflict	UNP Q7TG43
e	644	GLY	ARG	conflict	UNP Q7TG43
f	334	SER	PHE	conflict	UNP Q7TG43
f	339	ALA	GLY	conflict	UNP Q7TG43
f	621	LEU	PRO	conflict	UNP Q7TG43
f	622	GLN	THR	conflict	UNP Q7TG43
f	624	PRO	THR	conflict	UNP Q7TG43
f	625	ILE	HIS	conflict	UNP Q7TG43
f	626	TRP	LEU	conflict	UNP Q7TG43
f	644	GLY	ARG	conflict	UNP Q7TG43
g	334	SER	PHE	conflict	UNP Q7TG43
g	339	ALA	GLY	conflict	UNP Q7TG43
g	621	LEU	PRO	conflict	UNP Q7TG43
g	622	GLN	THR	conflict	UNP Q7TG43
g	624	PRO	THR	conflict	UNP Q7TG43
g	625	ILE	HIS	conflict	UNP Q7TG43
g	626	TRP	LEU	conflict	UNP Q7TG43
g	644	GLY	ARG	conflict	UNP Q7TG43
h	334	SER	PHE	conflict	UNP Q7TG43
h	339	ALA	GLY	conflict	UNP Q7TG43
h	621	LEU	PRO	conflict	UNP Q7TG43
h	622	GLN	THR	conflict	UNP Q7TG43
h	624	PRO	THR	conflict	UNP Q7TG43
h	625	ILE	HIS	conflict	UNP Q7TG43
h	626	TRP	LEU	conflict	UNP Q7TG43
h	644	GLY	ARG	conflict	UNP Q7TG43
i	334	SER	PHE	conflict	UNP Q7TG43
i	339	ALA	GLY	conflict	UNP Q7TG43
i	621	LEU	PRO	conflict	UNP Q7TG43
i	622	GLN	THR	conflict	UNP Q7TG43
i	624	PRO	THR	conflict	UNP Q7TG43
i	625	ILE	HIS	conflict	UNP Q7TG43
i	626	TRP	LEU	conflict	UNP Q7TG43
i	644	GLY	ARG	conflict	UNP Q7TG43
j	334	SER	PHE	conflict	UNP Q7TG43
j	339	ALA	GLY	conflict	UNP Q7TG43
j	621	LEU	PRO	conflict	UNP Q7TG43
j	622	GLN	THR	conflict	UNP Q7TG43
j	624	PRO	THR	conflict	UNP Q7TG43
j	625	ILE	HIS	conflict	UNP Q7TG43
j	626	TRP	LEU	conflict	UNP Q7TG43
j	644	GLY	ARG	conflict	UNP Q7TG43

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Chain	Residue	Modelled	Actual	Comment	Reference
k	334	SER	PHE	conflict	UNP Q7TG43
k	339	ALA	GLY	conflict	UNP Q7TG43
k	621	LEU	PRO	conflict	UNP Q7TG43
k	622	GLN	THR	conflict	UNP Q7TG43
k	624	PRO	THR	conflict	UNP Q7TG43
k	625	ILE	HIS	conflict	UNP Q7TG43
k	626	TRP	LEU	conflict	UNP Q7TG43
k	644	GLY	ARG	conflict	UNP Q7TG43
l	334	SER	PHE	conflict	UNP Q7TG43
l	339	ALA	GLY	conflict	UNP Q7TG43
l	621	LEU	PRO	conflict	UNP Q7TG43
l	622	GLN	THR	conflict	UNP Q7TG43
l	624	PRO	THR	conflict	UNP Q7TG43
l	625	ILE	HIS	conflict	UNP Q7TG43
l	626	TRP	LEU	conflict	UNP Q7TG43
l	644	GLY	ARG	conflict	UNP Q7TG43
m	334	SER	PHE	conflict	UNP Q7TG43
m	339	ALA	GLY	conflict	UNP Q7TG43
m	621	LEU	PRO	conflict	UNP Q7TG43
m	622	GLN	THR	conflict	UNP Q7TG43
m	624	PRO	THR	conflict	UNP Q7TG43
m	625	ILE	HIS	conflict	UNP Q7TG43
m	626	TRP	LEU	conflict	UNP Q7TG43
m	644	GLY	ARG	conflict	UNP Q7TG43
n	334	SER	PHE	conflict	UNP Q7TG43
n	339	ALA	GLY	conflict	UNP Q7TG43
n	621	LEU	PRO	conflict	UNP Q7TG43
n	622	GLN	THR	conflict	UNP Q7TG43
n	624	PRO	THR	conflict	UNP Q7TG43
n	625	ILE	HIS	conflict	UNP Q7TG43
n	626	TRP	LEU	conflict	UNP Q7TG43
n	644	GLY	ARG	conflict	UNP Q7TG43
o	334	SER	PHE	conflict	UNP Q7TG43
o	339	ALA	GLY	conflict	UNP Q7TG43
o	621	LEU	PRO	conflict	UNP Q7TG43
o	622	GLN	THR	conflict	UNP Q7TG43
o	624	PRO	THR	conflict	UNP Q7TG43
o	625	ILE	HIS	conflict	UNP Q7TG43
o	626	TRP	LEU	conflict	UNP Q7TG43
o	644	GLY	ARG	conflict	UNP Q7TG43
p	334	SER	PHE	conflict	UNP Q7TG43
p	339	ALA	GLY	conflict	UNP Q7TG43

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Chain	Residue	Modelled	Actual	Comment	Reference
p	621	LEU	PRO	conflict	UNP Q7TG43
p	622	GLN	THR	conflict	UNP Q7TG43
p	624	PRO	THR	conflict	UNP Q7TG43
p	625	ILE	HIS	conflict	UNP Q7TG43
p	626	TRP	LEU	conflict	UNP Q7TG43
p	644	GLY	ARG	conflict	UNP Q7TG43
q	334	SER	PHE	conflict	UNP Q7TG43
q	339	ALA	GLY	conflict	UNP Q7TG43
q	621	LEU	PRO	conflict	UNP Q7TG43
q	622	GLN	THR	conflict	UNP Q7TG43
q	624	PRO	THR	conflict	UNP Q7TG43
q	625	ILE	HIS	conflict	UNP Q7TG43
q	626	TRP	LEU	conflict	UNP Q7TG43
q	644	GLY	ARG	conflict	UNP Q7TG43
r	334	SER	PHE	conflict	UNP Q7TG43
r	339	ALA	GLY	conflict	UNP Q7TG43
r	621	LEU	PRO	conflict	UNP Q7TG43
r	622	GLN	THR	conflict	UNP Q7TG43
r	624	PRO	THR	conflict	UNP Q7TG43
r	625	ILE	HIS	conflict	UNP Q7TG43
r	626	TRP	LEU	conflict	UNP Q7TG43
r	644	GLY	ARG	conflict	UNP Q7TG43
s	334	SER	PHE	conflict	UNP Q7TG43
s	339	ALA	GLY	conflict	UNP Q7TG43
s	621	LEU	PRO	conflict	UNP Q7TG43
s	622	GLN	THR	conflict	UNP Q7TG43
s	624	PRO	THR	conflict	UNP Q7TG43
s	625	ILE	HIS	conflict	UNP Q7TG43
s	626	TRP	LEU	conflict	UNP Q7TG43
s	644	GLY	ARG	conflict	UNP Q7TG43
t	334	SER	PHE	conflict	UNP Q7TG43
t	339	ALA	GLY	conflict	UNP Q7TG43
t	621	LEU	PRO	conflict	UNP Q7TG43
t	622	GLN	THR	conflict	UNP Q7TG43
t	624	PRO	THR	conflict	UNP Q7TG43
t	625	ILE	HIS	conflict	UNP Q7TG43
t	626	TRP	LEU	conflict	UNP Q7TG43
t	644	GLY	ARG	conflict	UNP Q7TG43
u	334	SER	PHE	conflict	UNP Q7TG43
u	339	ALA	GLY	conflict	UNP Q7TG43
u	621	LEU	PRO	conflict	UNP Q7TG43
u	622	GLN	THR	conflict	UNP Q7TG43

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Chain	Residue	Modelled	Actual	Comment	Reference
u	624	PRO	THR	conflict	UNP Q7TG43
u	625	ILE	HIS	conflict	UNP Q7TG43
u	626	TRP	LEU	conflict	UNP Q7TG43
u	644	GLY	ARG	conflict	UNP Q7TG43
v	334	SER	PHE	conflict	UNP Q7TG43
v	339	ALA	GLY	conflict	UNP Q7TG43
v	621	LEU	PRO	conflict	UNP Q7TG43
v	622	GLN	THR	conflict	UNP Q7TG43
v	624	PRO	THR	conflict	UNP Q7TG43
v	625	ILE	HIS	conflict	UNP Q7TG43
v	626	TRP	LEU	conflict	UNP Q7TG43
v	644	GLY	ARG	conflict	UNP Q7TG43
w	334	SER	PHE	conflict	UNP Q7TG43
w	339	ALA	GLY	conflict	UNP Q7TG43
w	621	LEU	PRO	conflict	UNP Q7TG43
w	622	GLN	THR	conflict	UNP Q7TG43
w	624	PRO	THR	conflict	UNP Q7TG43
w	625	ILE	HIS	conflict	UNP Q7TG43
w	626	TRP	LEU	conflict	UNP Q7TG43
w	644	GLY	ARG	conflict	UNP Q7TG43
x	334	SER	PHE	conflict	UNP Q7TG43
x	339	ALA	GLY	conflict	UNP Q7TG43
x	621	LEU	PRO	conflict	UNP Q7TG43
x	622	GLN	THR	conflict	UNP Q7TG43
x	624	PRO	THR	conflict	UNP Q7TG43
x	625	ILE	HIS	conflict	UNP Q7TG43
x	626	TRP	LEU	conflict	UNP Q7TG43
x	644	GLY	ARG	conflict	UNP Q7TG43
y	334	SER	PHE	conflict	UNP Q7TG43
y	339	ALA	GLY	conflict	UNP Q7TG43
y	621	LEU	PRO	conflict	UNP Q7TG43
y	622	GLN	THR	conflict	UNP Q7TG43
y	624	PRO	THR	conflict	UNP Q7TG43
y	625	ILE	HIS	conflict	UNP Q7TG43
y	626	TRP	LEU	conflict	UNP Q7TG43
y	644	GLY	ARG	conflict	UNP Q7TG43
z	334	SER	PHE	conflict	UNP Q7TG43
z	339	ALA	GLY	conflict	UNP Q7TG43
z	621	LEU	PRO	conflict	UNP Q7TG43
z	622	GLN	THR	conflict	UNP Q7TG43
z	624	PRO	THR	conflict	UNP Q7TG43
z	625	ILE	HIS	conflict	UNP Q7TG43

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Chain	Residue	Modelled	Actual	Comment	Reference
z	626	TRP	LEU	conflict	UNP Q7TG43
z	644	GLY	ARG	conflict	UNP Q7TG43
1	334	SER	PHE	conflict	UNP Q7TG43
1	339	ALA	GLY	conflict	UNP Q7TG43
1	621	LEU	PRO	conflict	UNP Q7TG43
1	622	GLN	THR	conflict	UNP Q7TG43
1	624	PRO	THR	conflict	UNP Q7TG43
1	625	ILE	HIS	conflict	UNP Q7TG43
1	626	TRP	LEU	conflict	UNP Q7TG43
1	644	GLY	ARG	conflict	UNP Q7TG43
2	334	SER	PHE	conflict	UNP Q7TG43
2	339	ALA	GLY	conflict	UNP Q7TG43
2	621	LEU	PRO	conflict	UNP Q7TG43
2	622	GLN	THR	conflict	UNP Q7TG43
2	624	PRO	THR	conflict	UNP Q7TG43
2	625	ILE	HIS	conflict	UNP Q7TG43
2	626	TRP	LEU	conflict	UNP Q7TG43
2	644	GLY	ARG	conflict	UNP Q7TG43
3	334	SER	PHE	conflict	UNP Q7TG43
3	339	ALA	GLY	conflict	UNP Q7TG43
3	621	LEU	PRO	conflict	UNP Q7TG43
3	622	GLN	THR	conflict	UNP Q7TG43
3	624	PRO	THR	conflict	UNP Q7TG43
3	625	ILE	HIS	conflict	UNP Q7TG43
3	626	TRP	LEU	conflict	UNP Q7TG43
3	644	GLY	ARG	conflict	UNP Q7TG43
4	334	SER	PHE	conflict	UNP Q7TG43
4	339	ALA	GLY	conflict	UNP Q7TG43
4	621	LEU	PRO	conflict	UNP Q7TG43
4	622	GLN	THR	conflict	UNP Q7TG43
4	624	PRO	THR	conflict	UNP Q7TG43
4	625	ILE	HIS	conflict	UNP Q7TG43
4	626	TRP	LEU	conflict	UNP Q7TG43
4	644	GLY	ARG	conflict	UNP Q7TG43
5	334	SER	PHE	conflict	UNP Q7TG43
5	339	ALA	GLY	conflict	UNP Q7TG43
5	621	LEU	PRO	conflict	UNP Q7TG43
5	622	GLN	THR	conflict	UNP Q7TG43
5	624	PRO	THR	conflict	UNP Q7TG43
5	625	ILE	HIS	conflict	UNP Q7TG43
5	626	TRP	LEU	conflict	UNP Q7TG43
5	644	GLY	ARG	conflict	UNP Q7TG43

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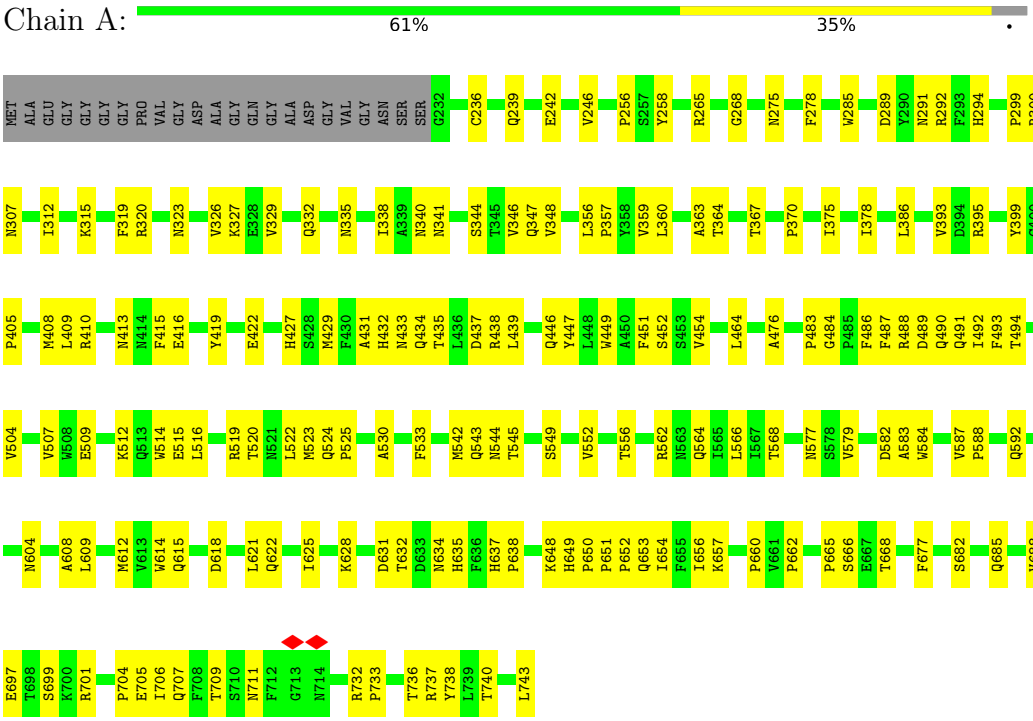
Chain	Residue	Modelled	Actual	Comment	Reference
6	334	SER	PHE	conflict	UNP Q7TG43
6	339	ALA	GLY	conflict	UNP Q7TG43
6	621	LEU	PRO	conflict	UNP Q7TG43
6	622	GLN	THR	conflict	UNP Q7TG43
6	624	PRO	THR	conflict	UNP Q7TG43
6	625	ILE	HIS	conflict	UNP Q7TG43
6	626	TRP	LEU	conflict	UNP Q7TG43
6	644	GLY	ARG	conflict	UNP Q7TG43
7	334	SER	PHE	conflict	UNP Q7TG43
7	339	ALA	GLY	conflict	UNP Q7TG43
7	621	LEU	PRO	conflict	UNP Q7TG43
7	622	GLN	THR	conflict	UNP Q7TG43
7	624	PRO	THR	conflict	UNP Q7TG43
7	625	ILE	HIS	conflict	UNP Q7TG43
7	626	TRP	LEU	conflict	UNP Q7TG43
7	644	GLY	ARG	conflict	UNP Q7TG43
8	334	SER	PHE	conflict	UNP Q7TG43
8	339	ALA	GLY	conflict	UNP Q7TG43
8	621	LEU	PRO	conflict	UNP Q7TG43
8	622	GLN	THR	conflict	UNP Q7TG43
8	624	PRO	THR	conflict	UNP Q7TG43
8	625	ILE	HIS	conflict	UNP Q7TG43
8	626	TRP	LEU	conflict	UNP Q7TG43
8	644	GLY	ARG	conflict	UNP Q7TG43

3 Residue-property plots (i)

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.

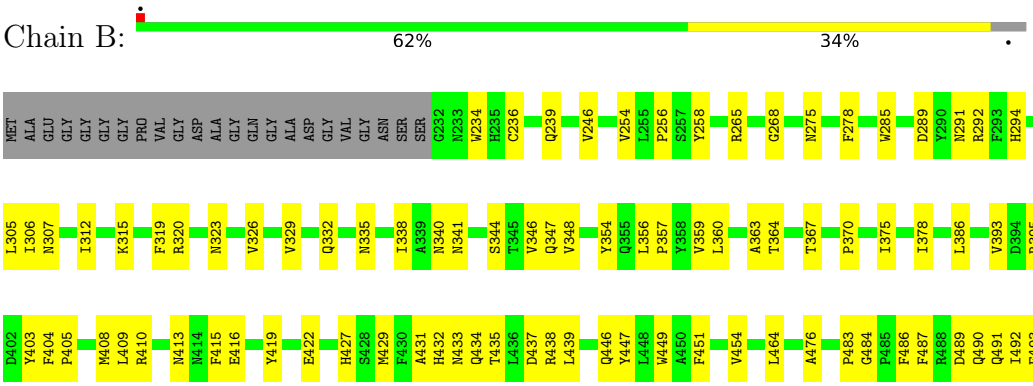
- Molecule 1: Capsid protein

Chain A:



- Molecule 1: Capsid protein

Chain B:





• Molecule 1: Capsid protein

Chain C:

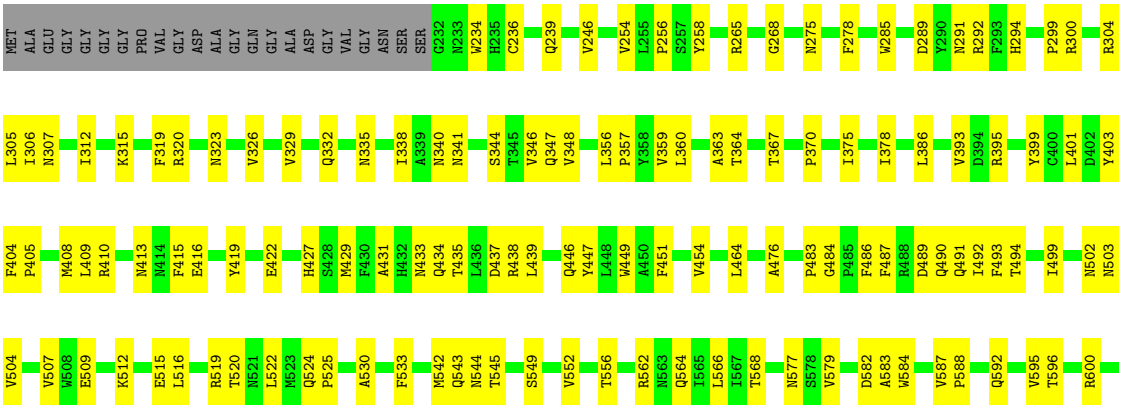


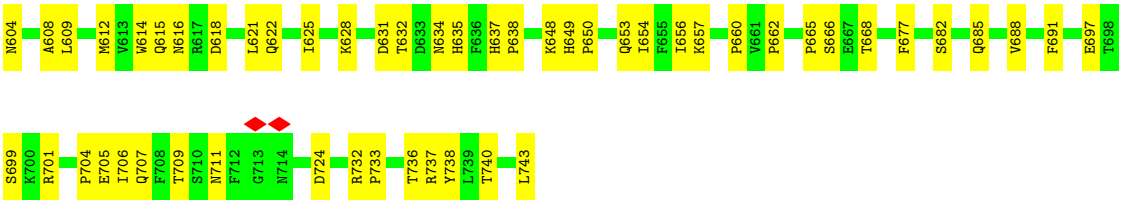


• Molecule 1: Capsid protein

Chain D:



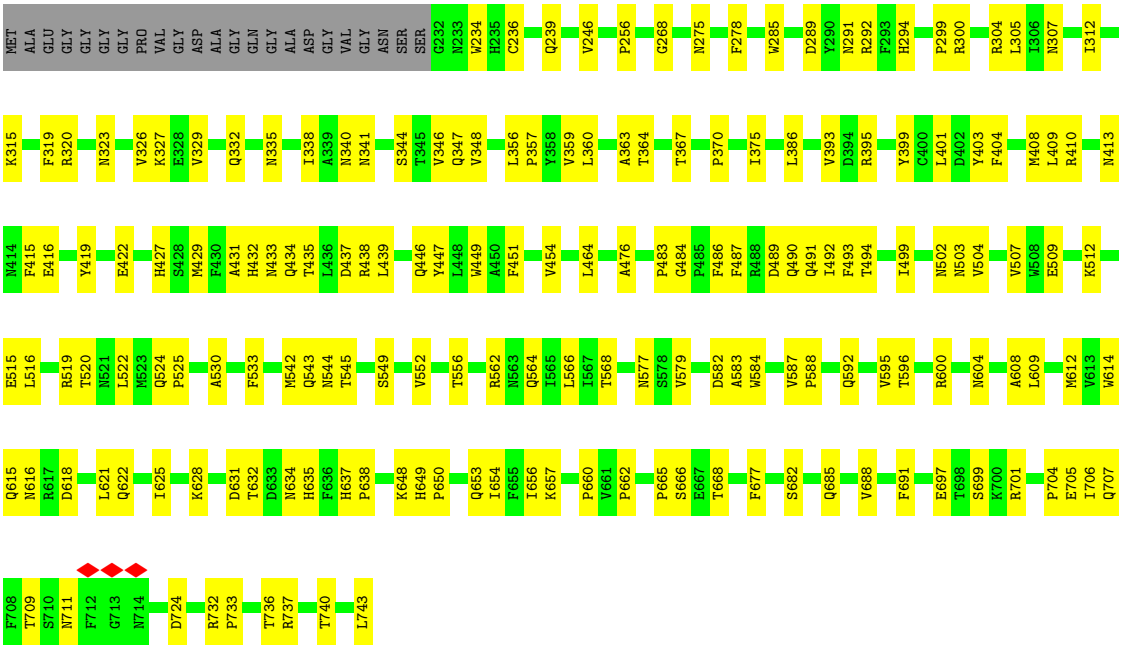




• Molecule 1: Capsid protein

Chain E:

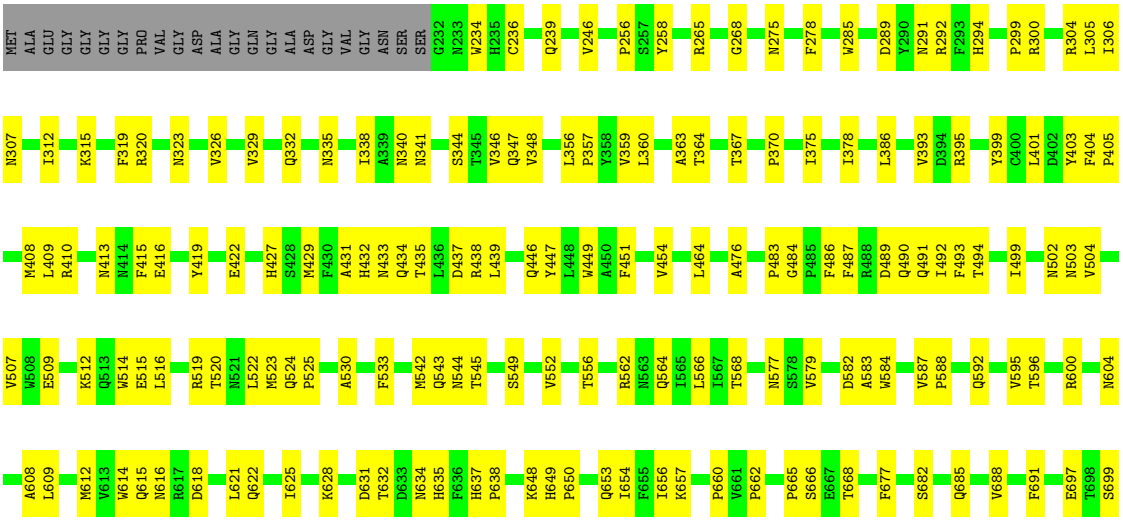


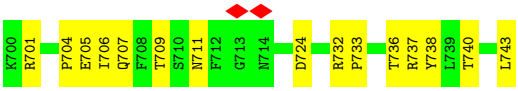


• Molecule 1: Capsid protein

Chain F:



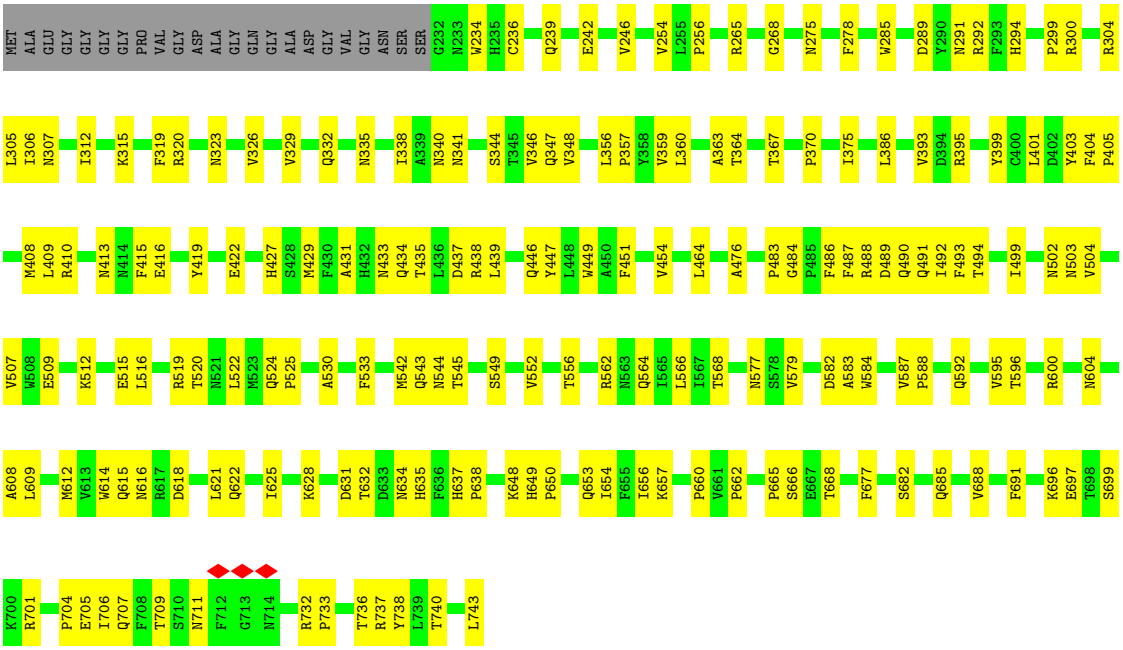




• Molecule 1: Capsid protein

Chain G:

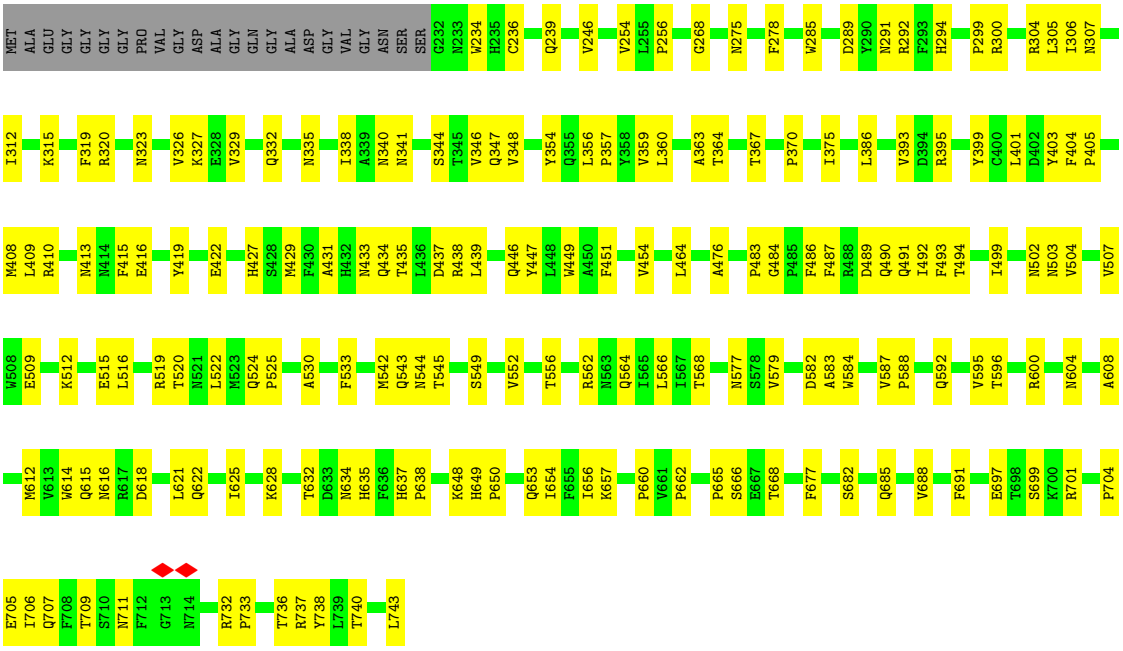




• Molecule 1: Capsid protein

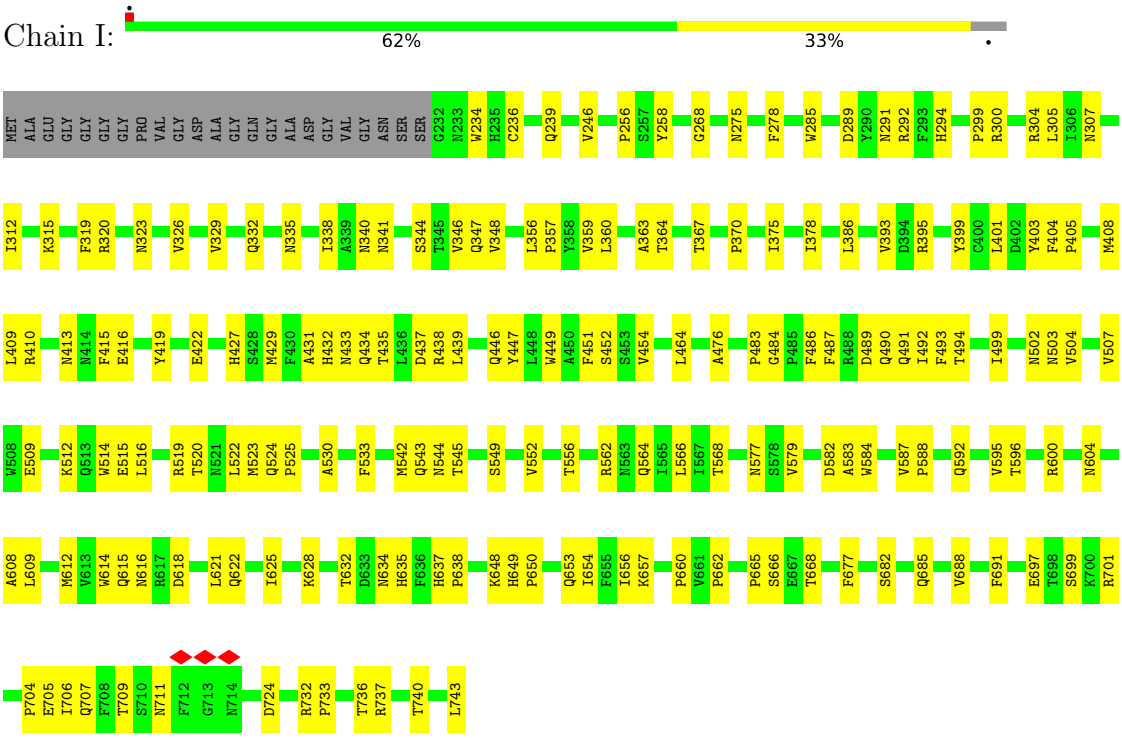
Chain H:





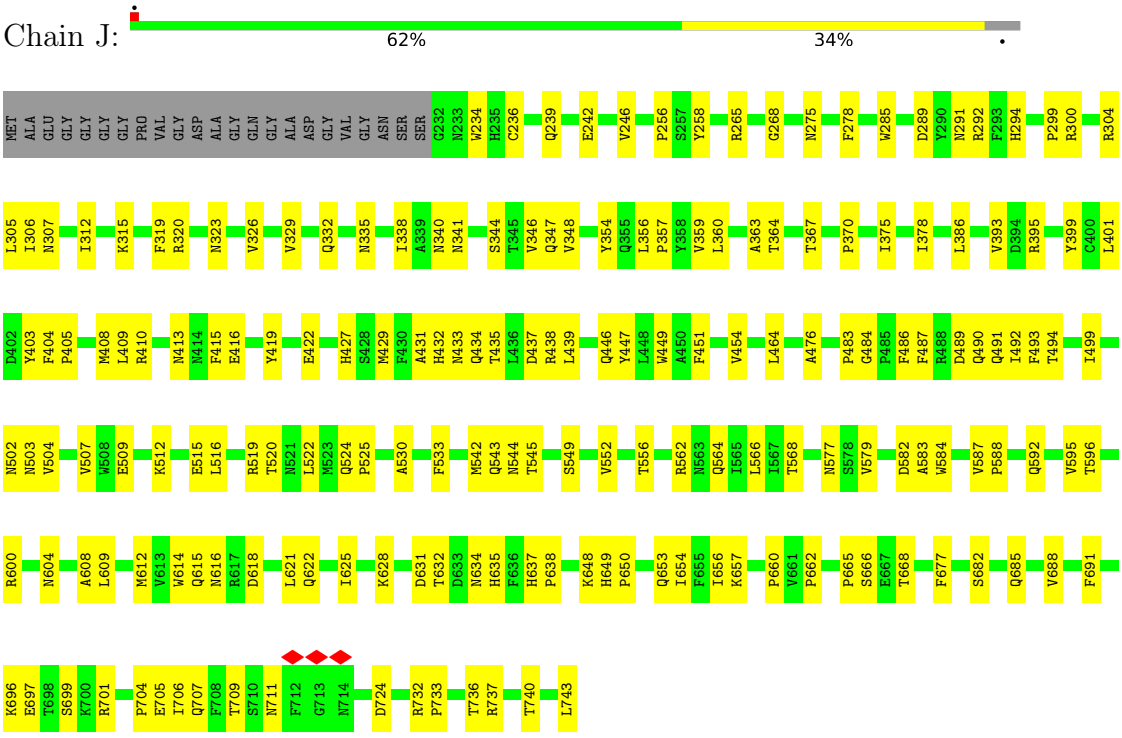
• Molecule 1: Capsid protein

Chain I:



• Molecule 1: Capsid protein

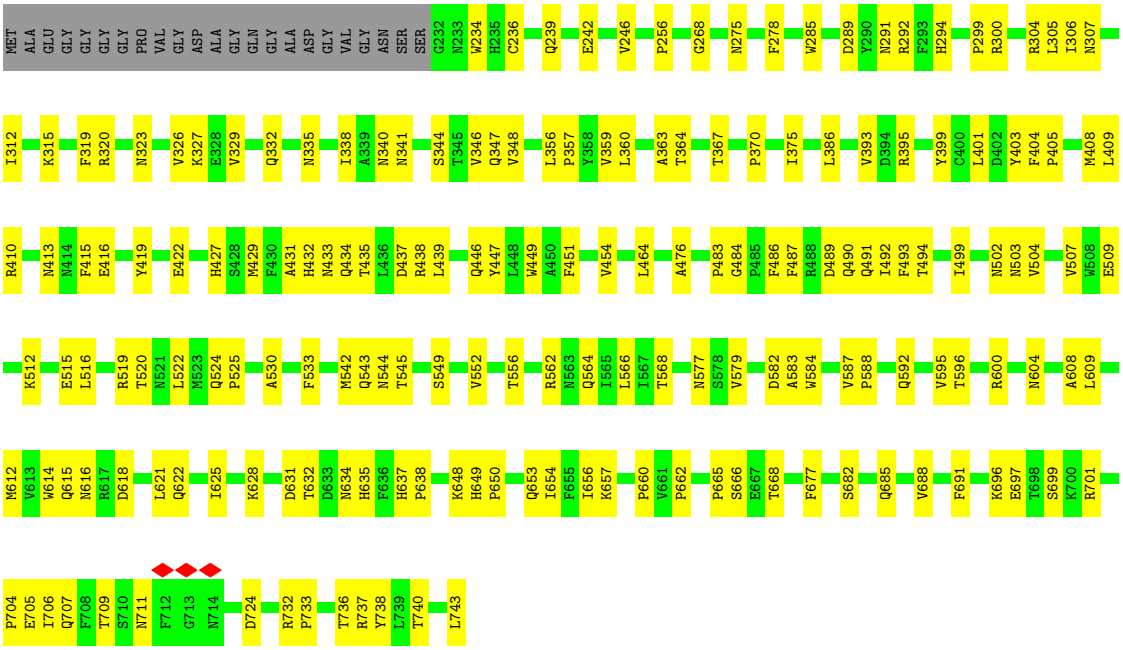
Chain J:



• Molecule 1: Capsid protein

Chain K:

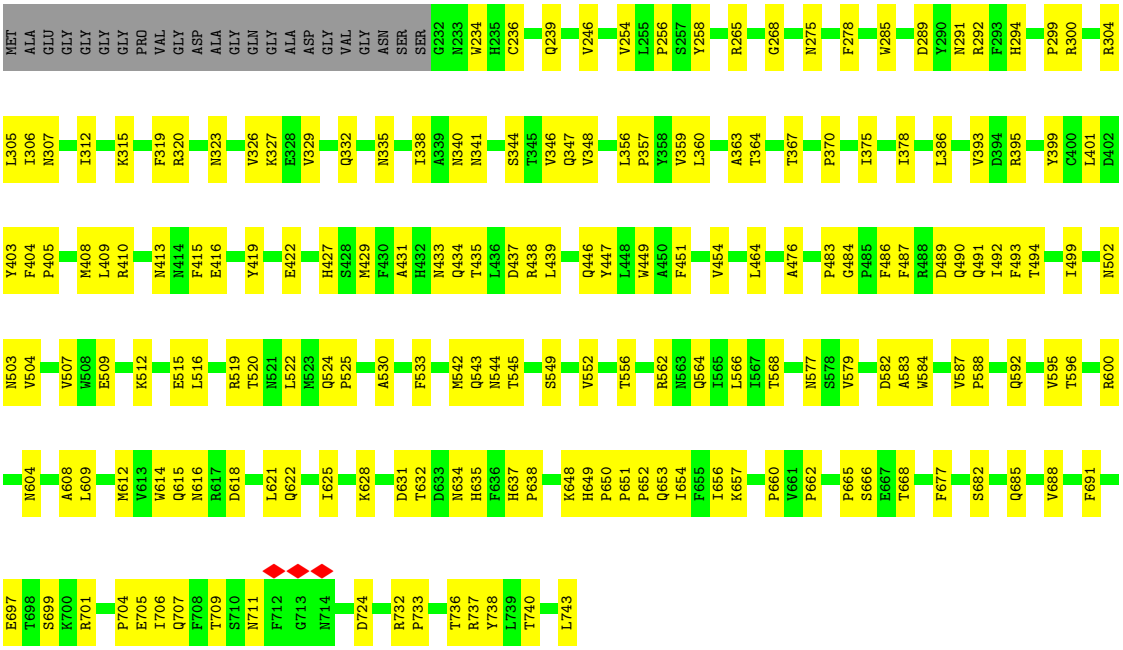




• Molecule 1: Capsid protein

Chain L:



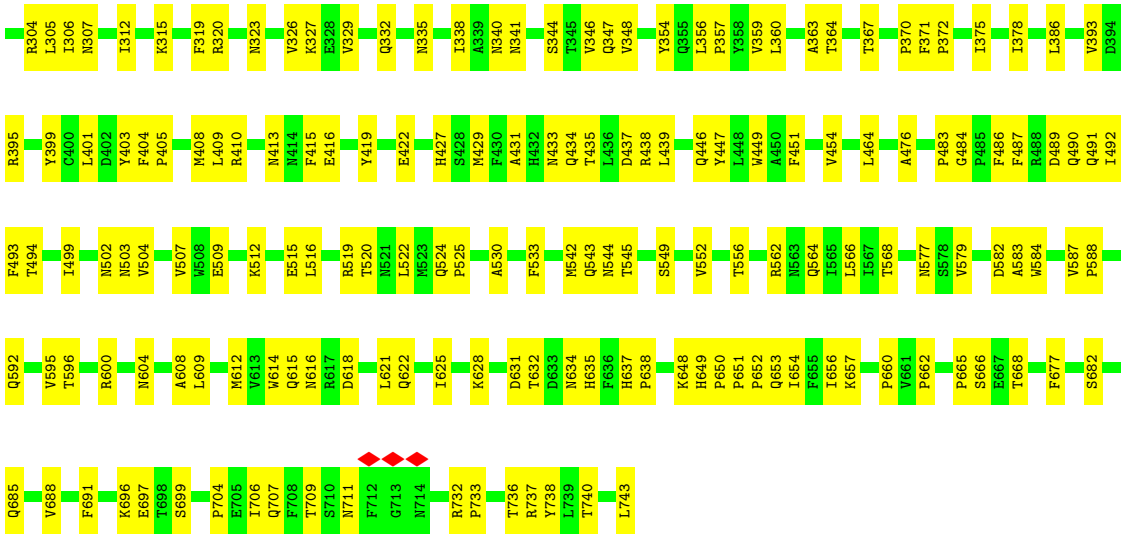


• Molecule 1: Capsid protein

Chain M:



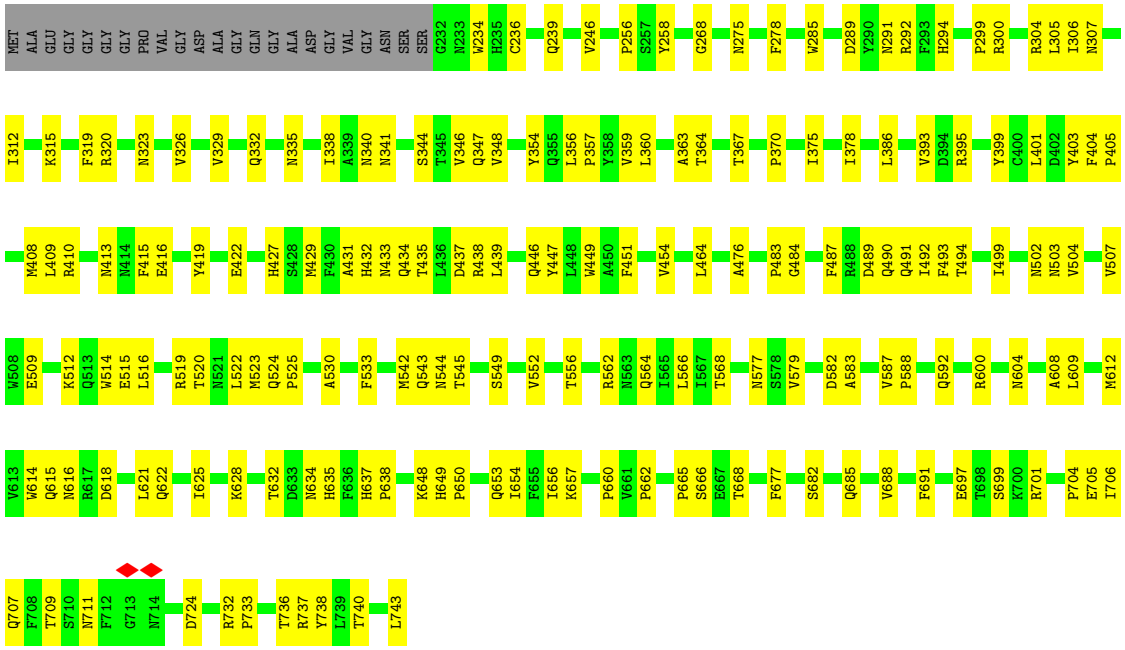




- Molecule 1: Capsid protein

Chain N:

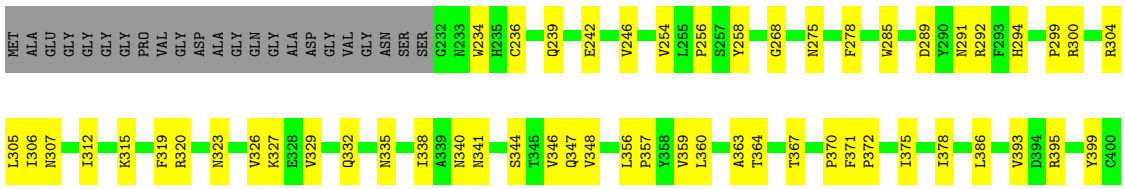


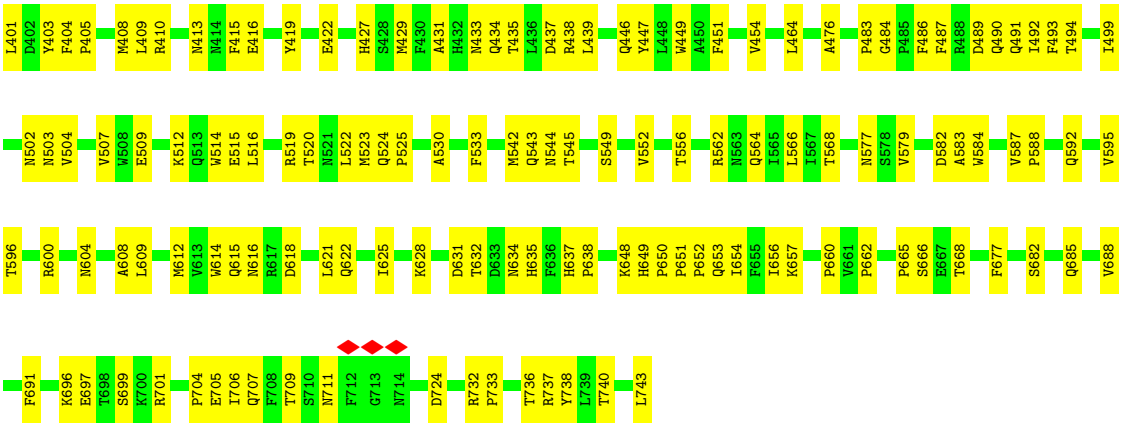


- Molecule 1: Capsid protein

Chain O:



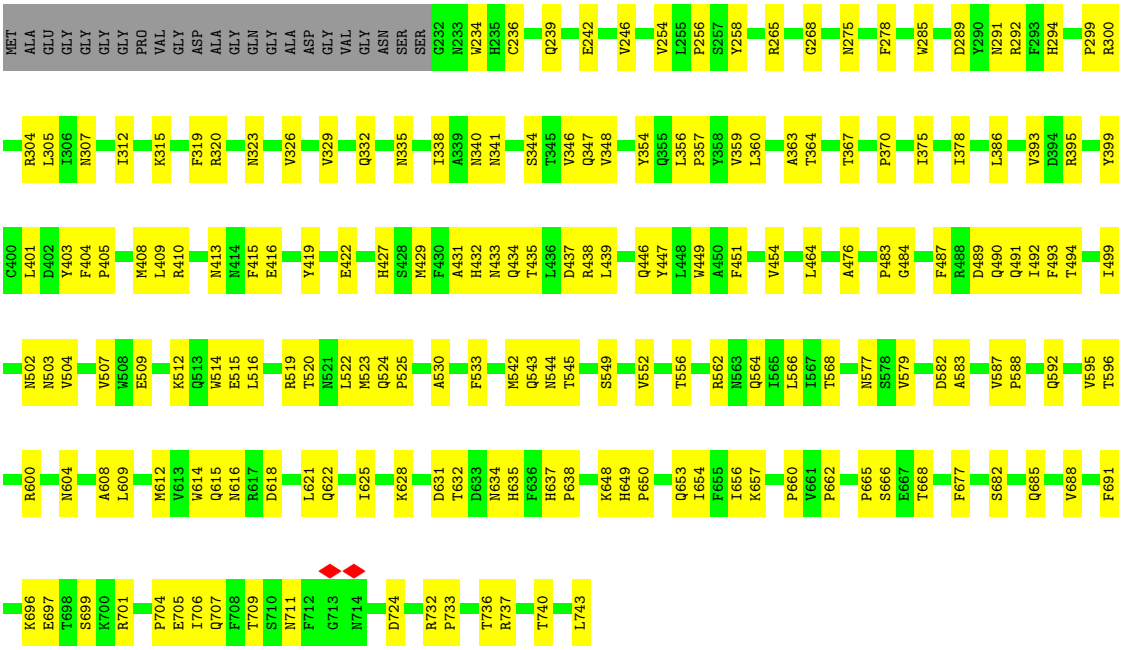




• Molecule 1: Capsid protein

Chain P:

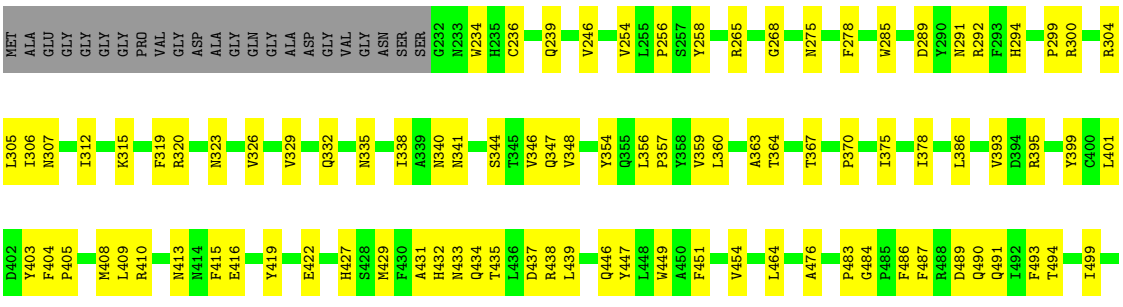


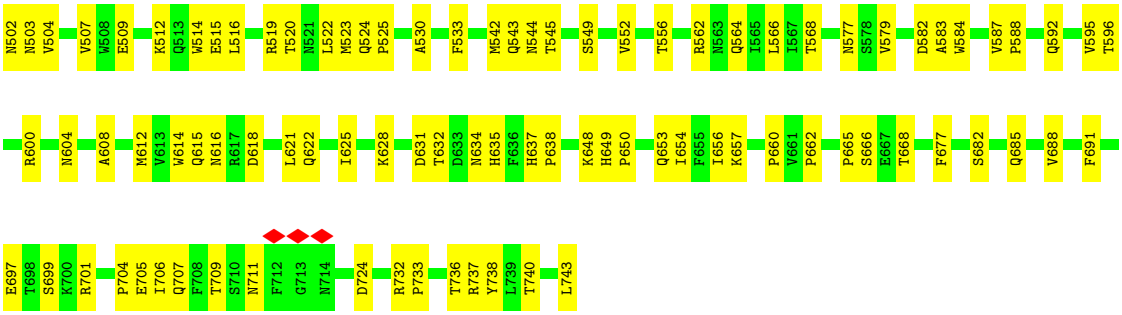


• Molecule 1: Capsid protein

Chain Q:



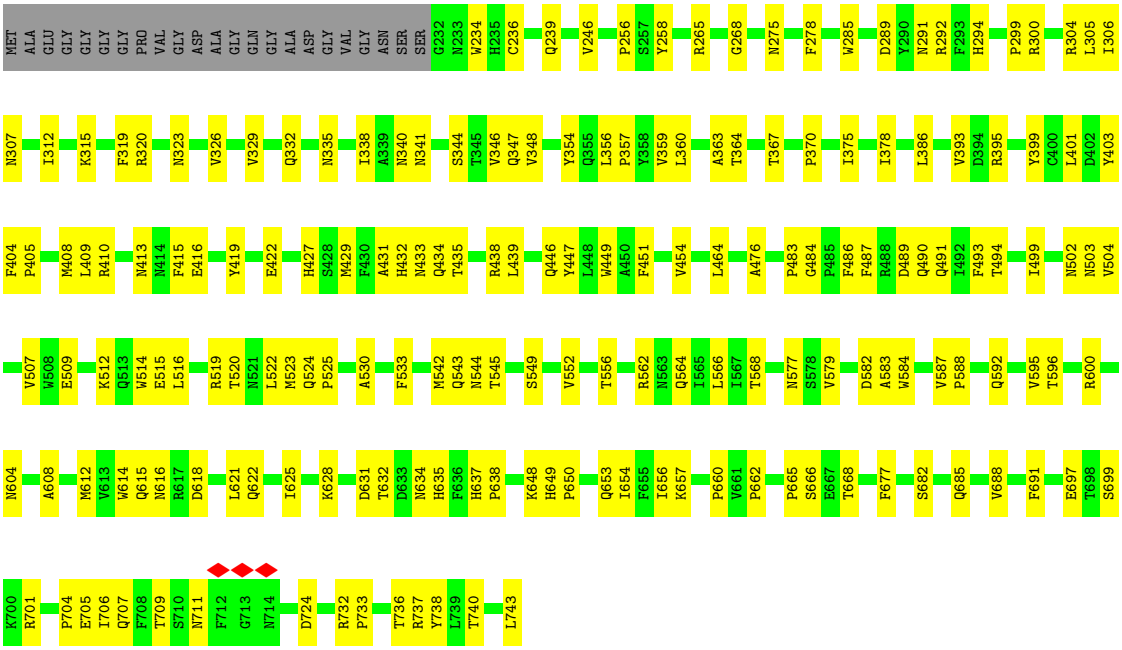




• Molecule 1: Capsid protein

Chain R:

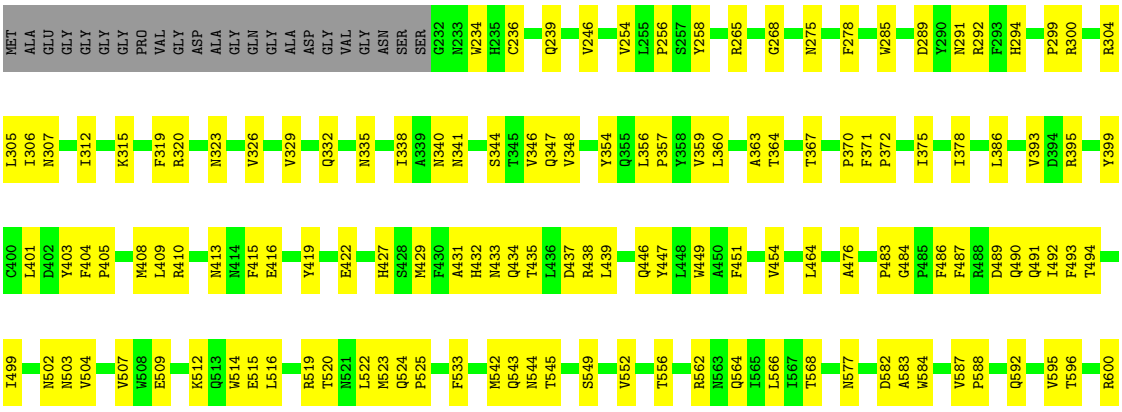


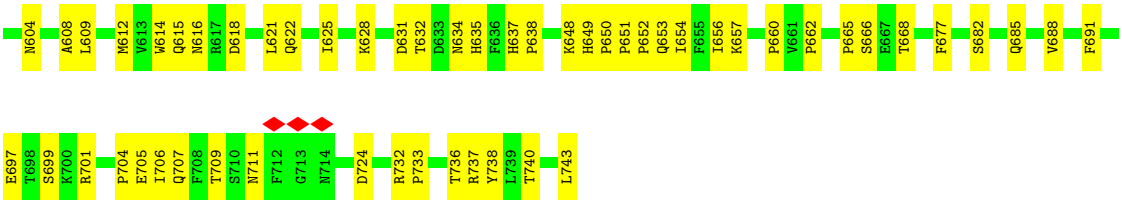


• Molecule 1: Capsid protein

Chain S:



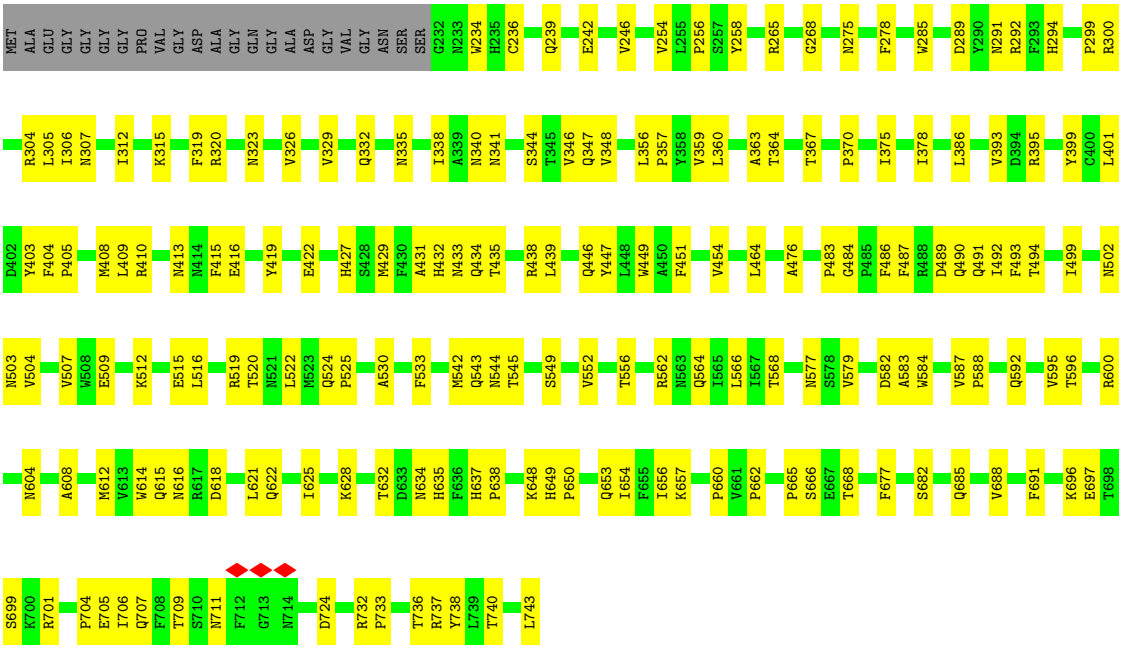




• Molecule 1: Capsid protein

Chain T:

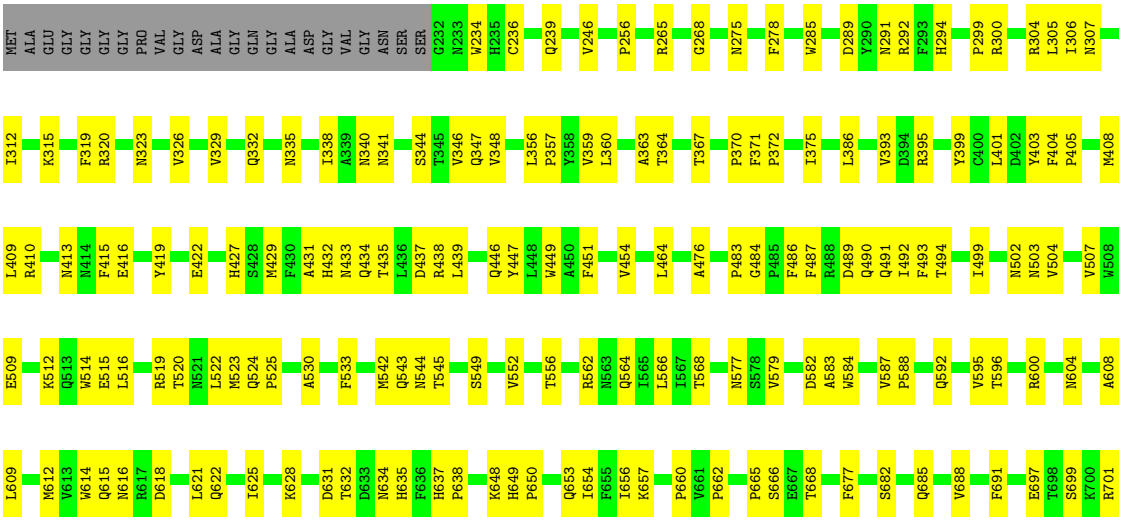


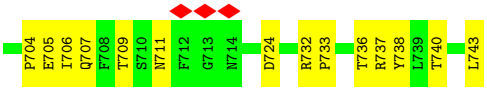


• Molecule 1: Capsid protein

Chain U:



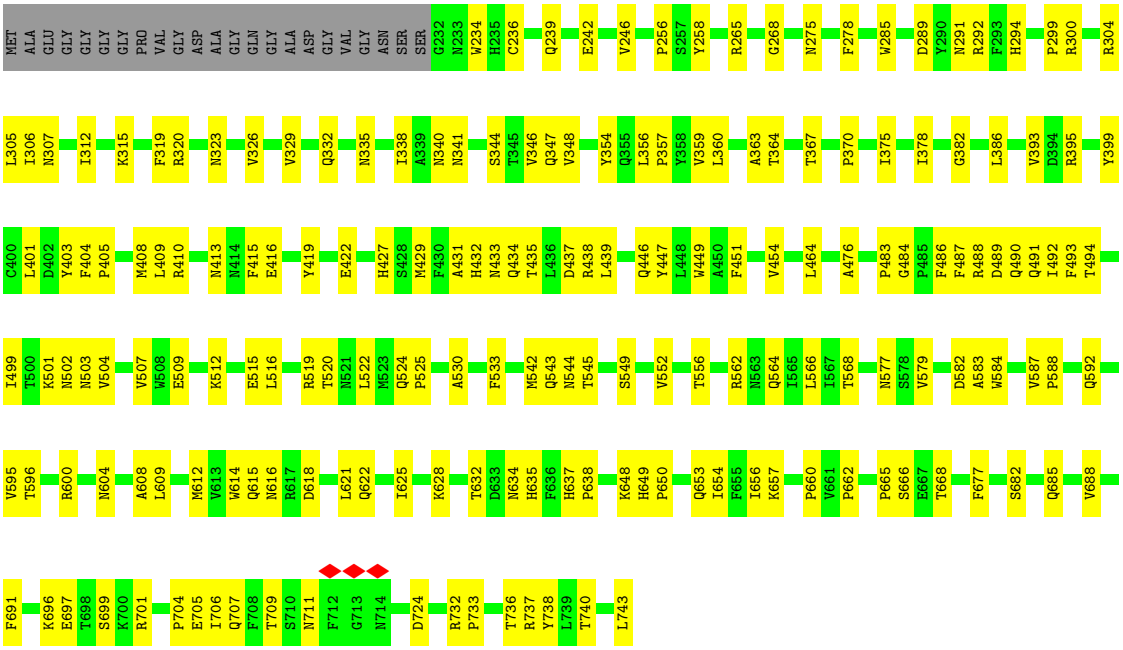




• Molecule 1: Capsid protein

Chain V:

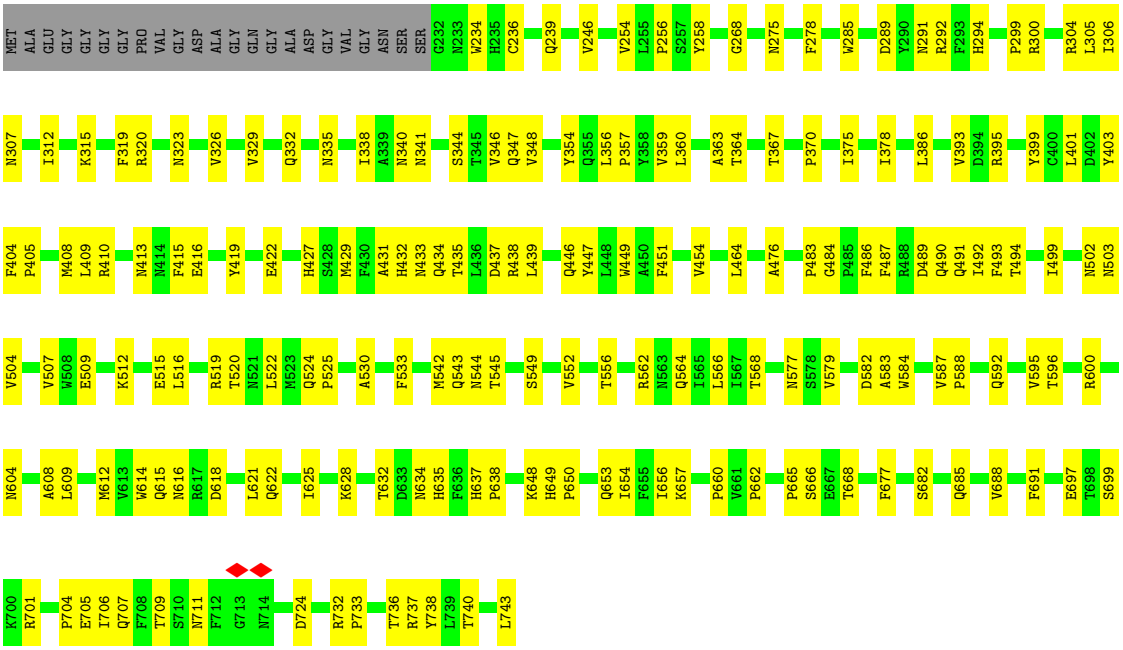




• Molecule 1: Capsid protein

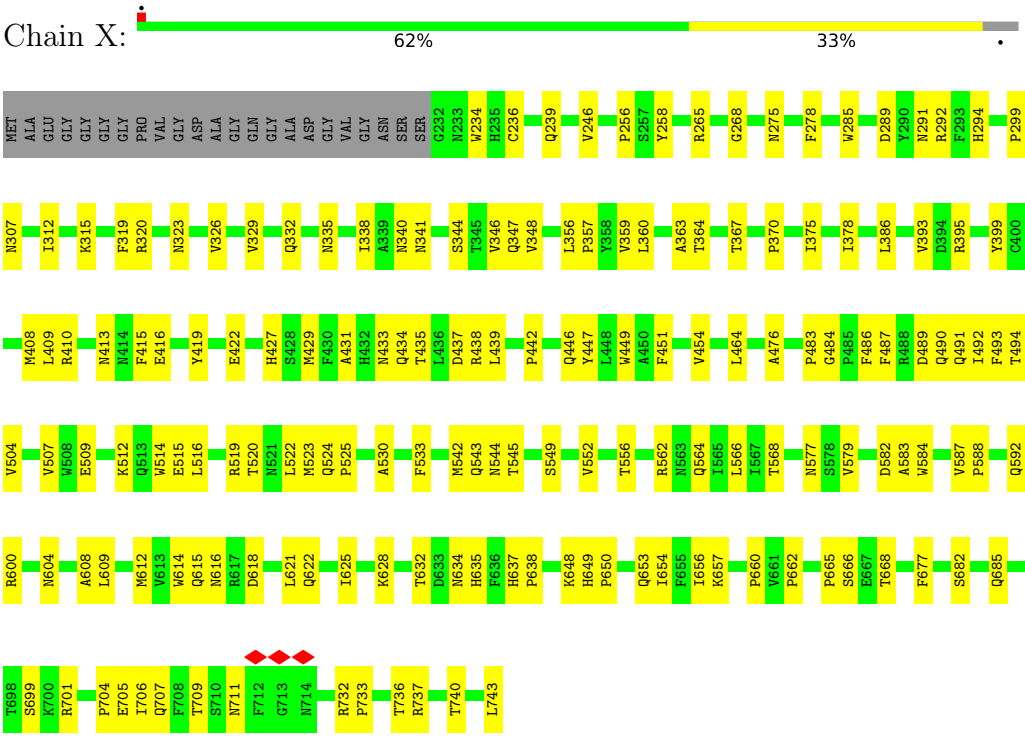
Chain W:





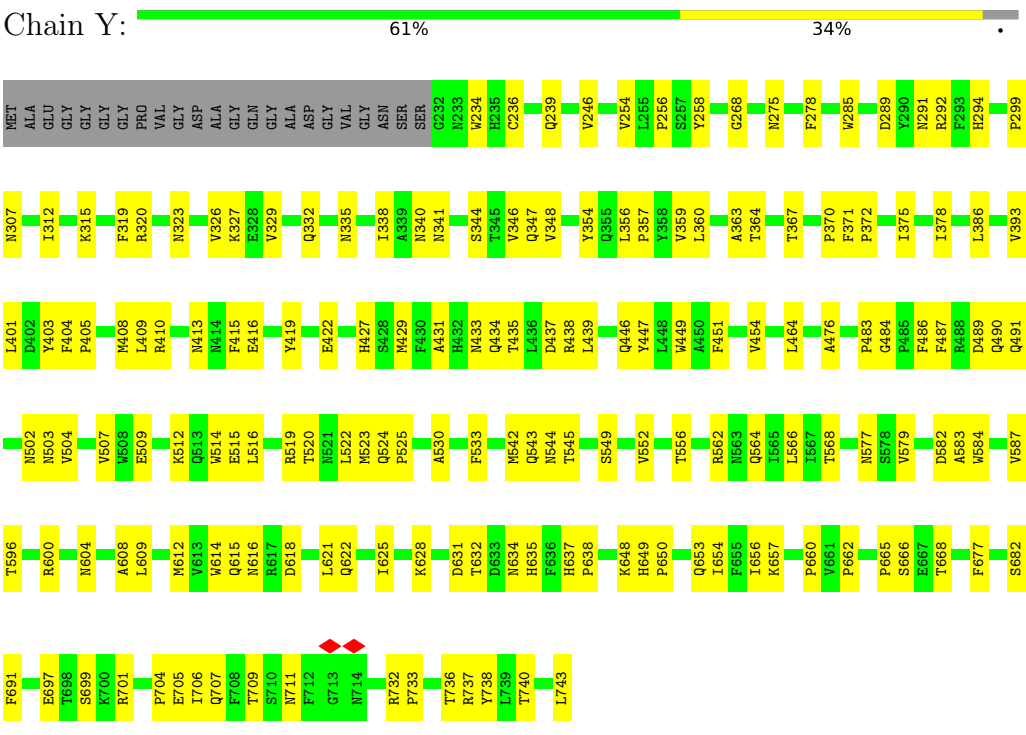
• Molecule 1: Capsid protein

Chain X:



• Molecule 1: Capsid protein

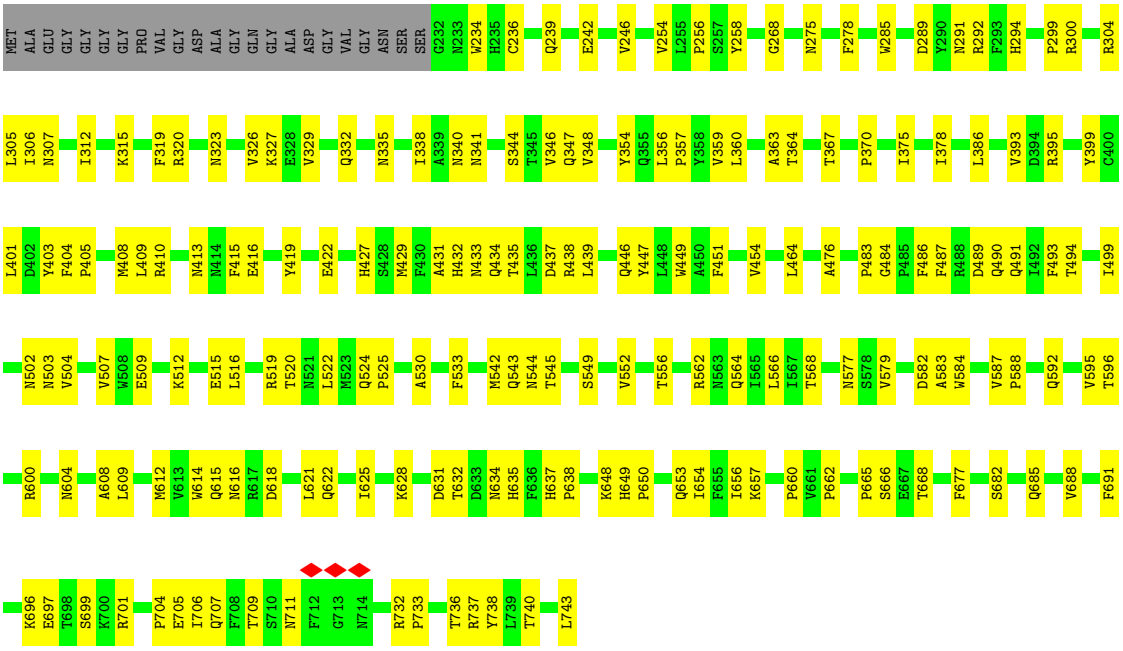
Chain Y:



• Molecule 1: Capsid protein

Chain Z:

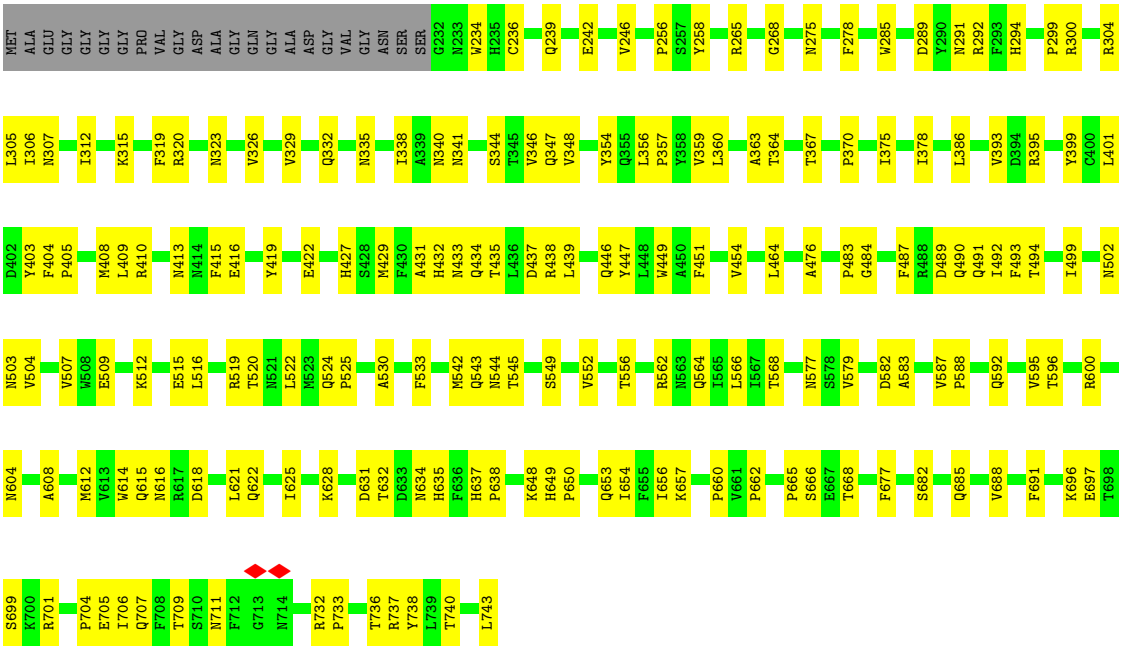




• Molecule 1: Capsid protein

Chain a:



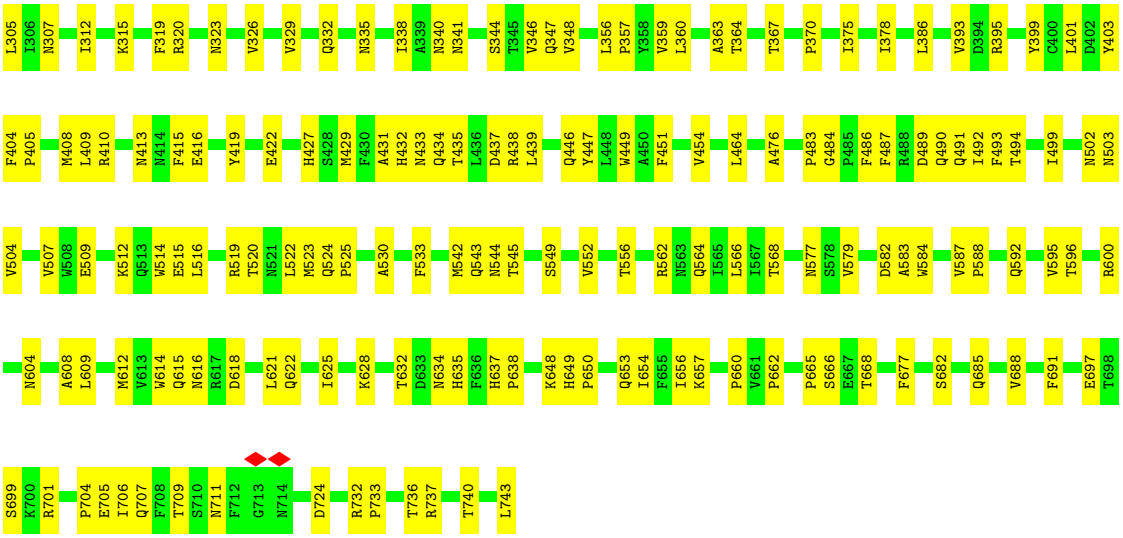


• Molecule 1: Capsid protein

Chain b:



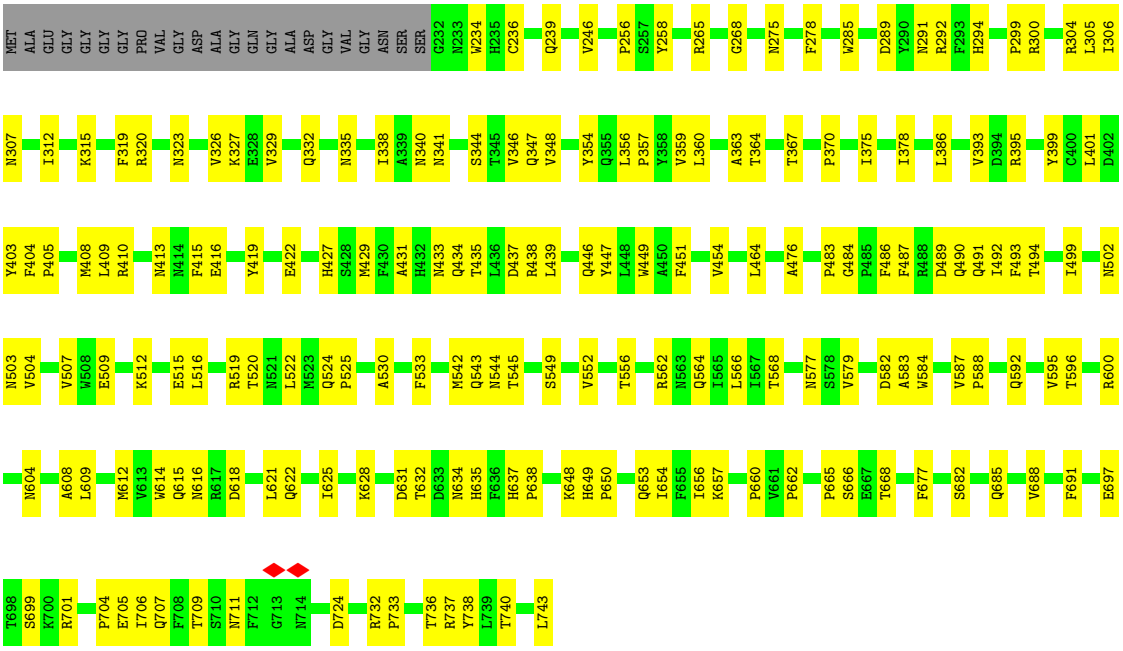




• Molecule 1: Capsid protein

Chain c:

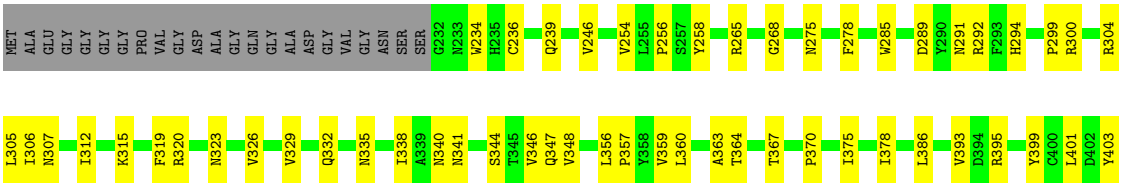


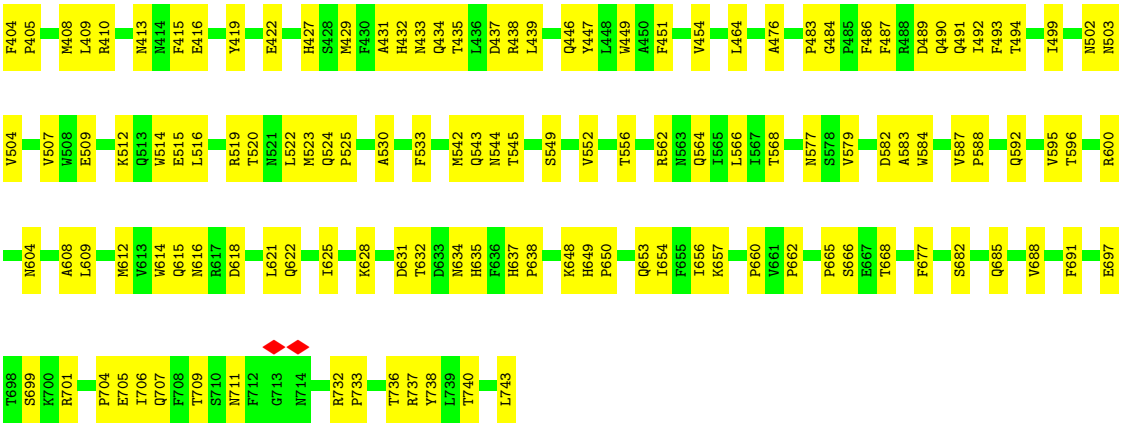


• Molecule 1: Capsid protein

Chain d:



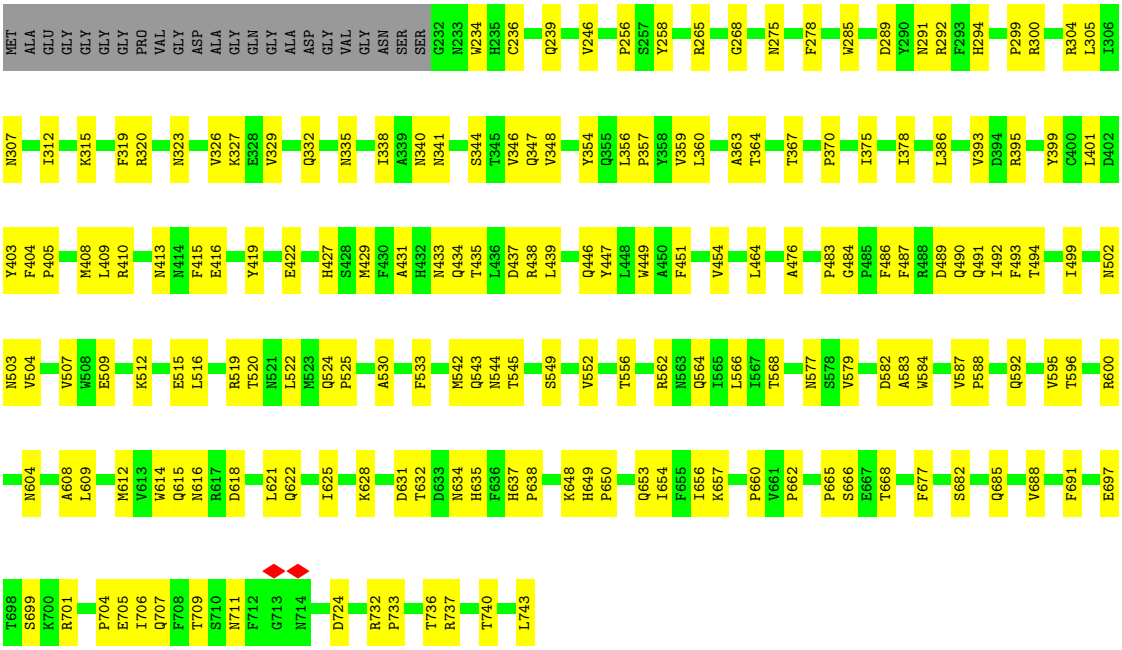




• Molecule 1: Capsid protein

Chain e:

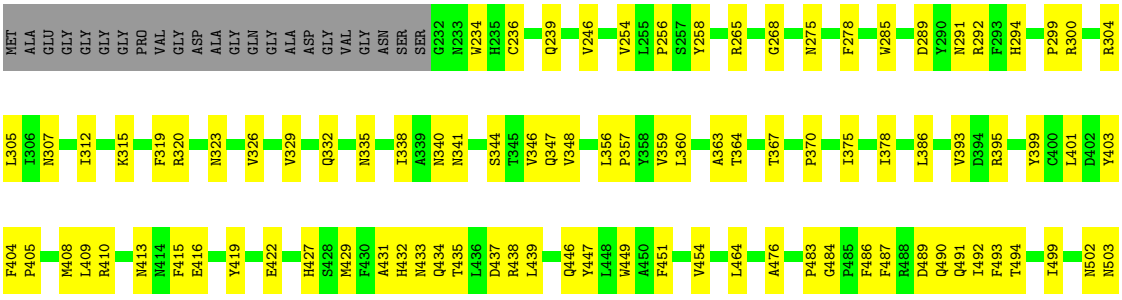


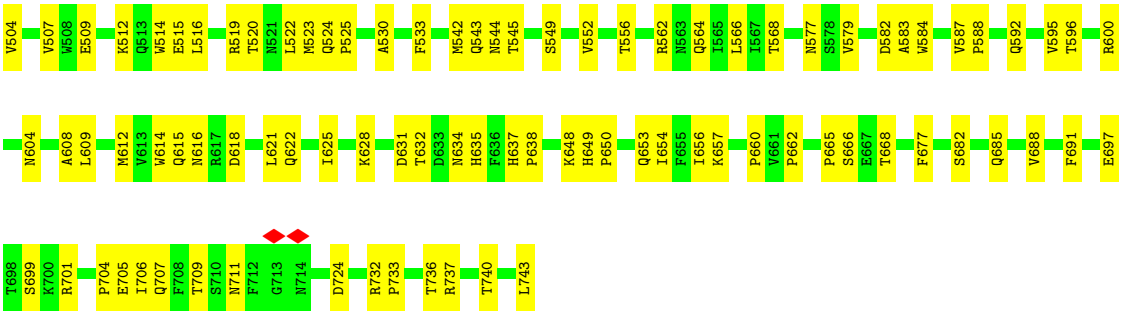


• Molecule 1: Capsid protein

Chain f:



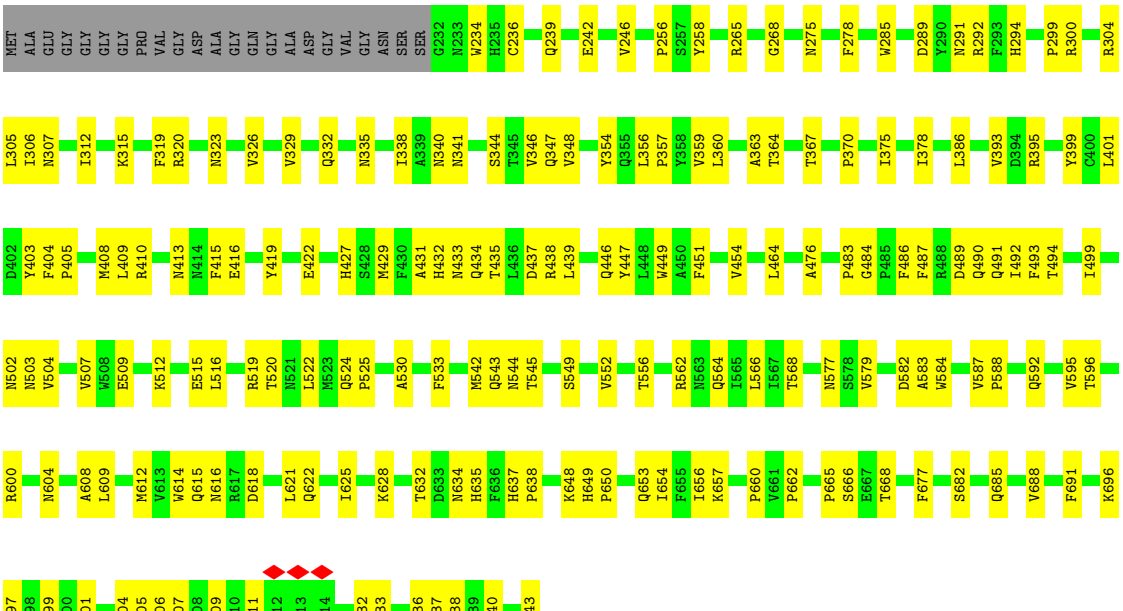




• Molecule 1: Capsid protein

Chain g:

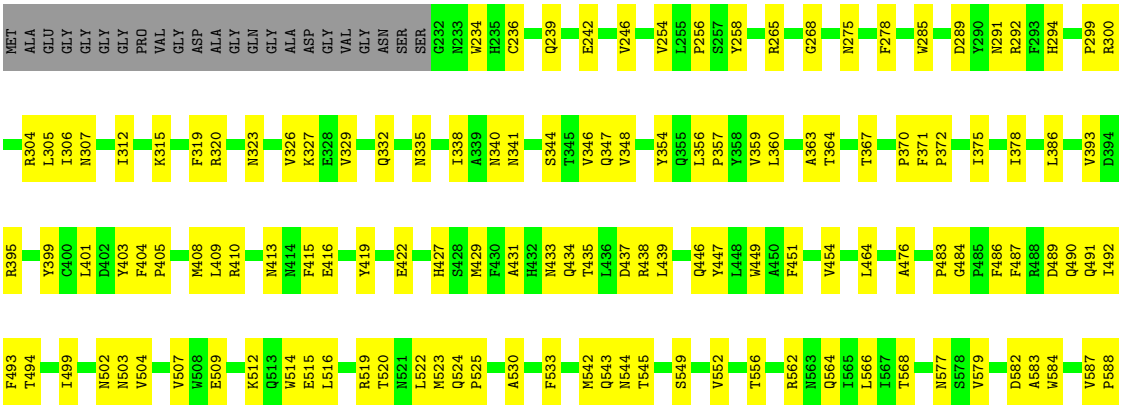




• Molecule 1: Capsid protein

Chain h:

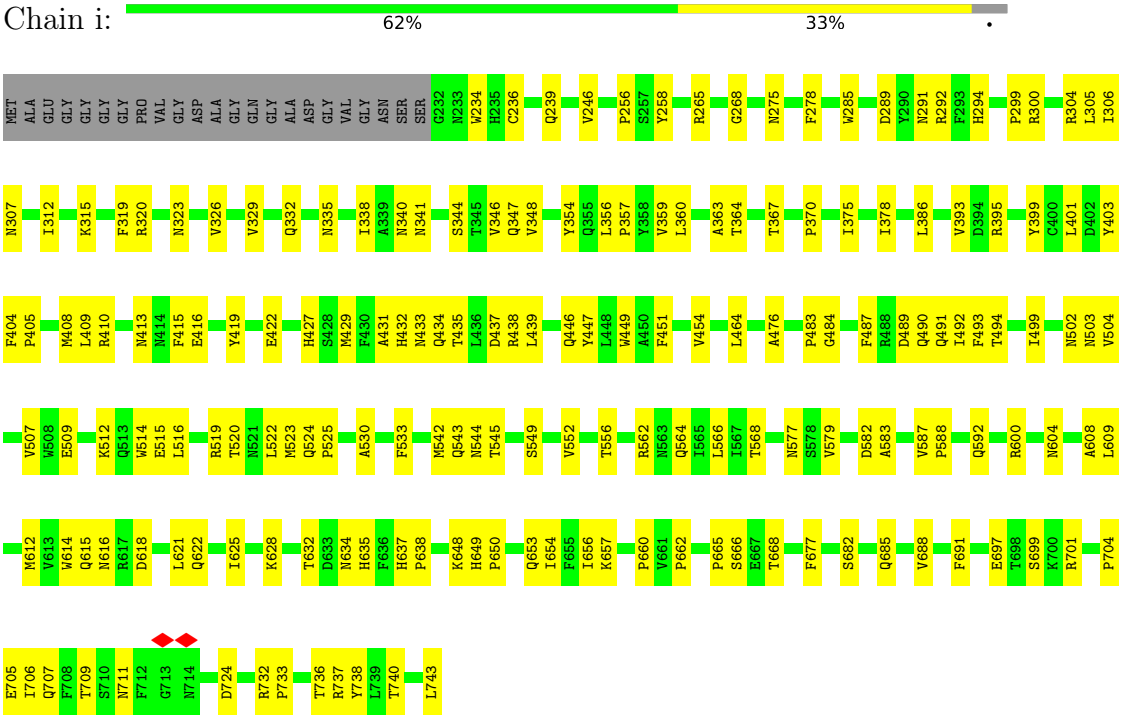






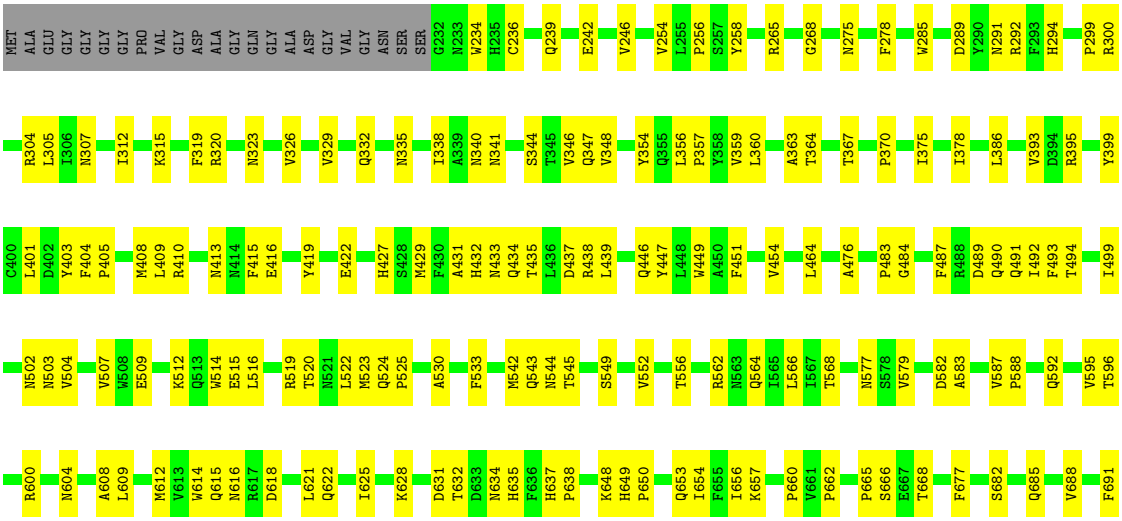
• Molecule 1: Capsid protein

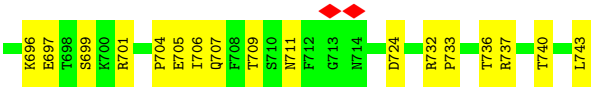
Chain i:



• Molecule 1: Capsid protein

Chain j:

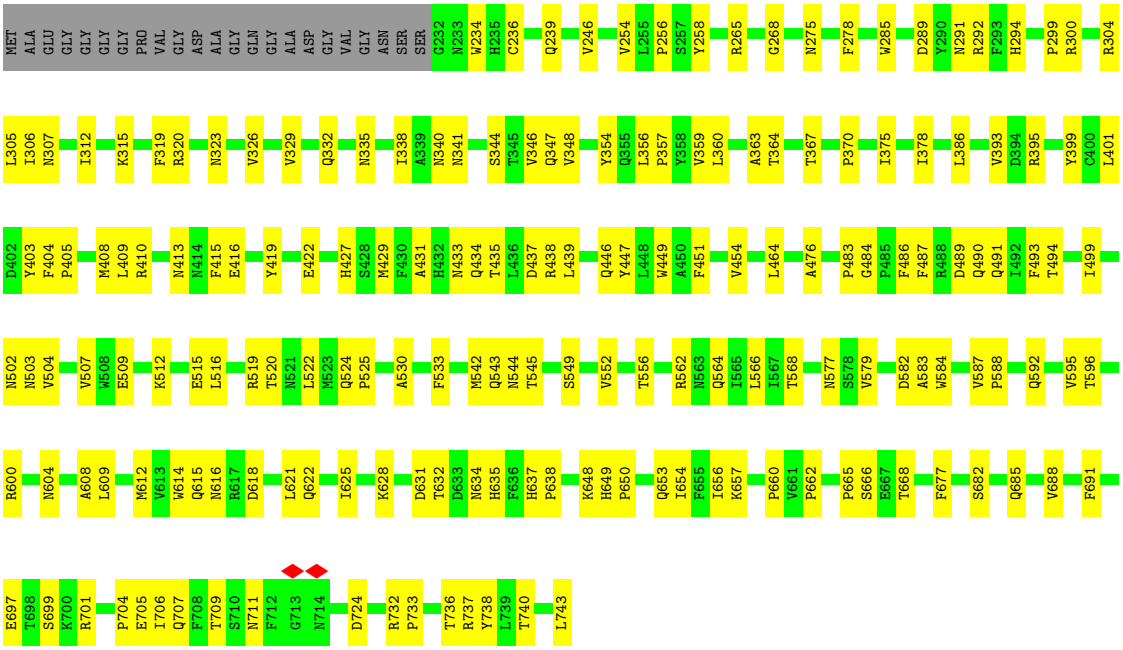




• Molecule 1: Capsid protein

Chain k:

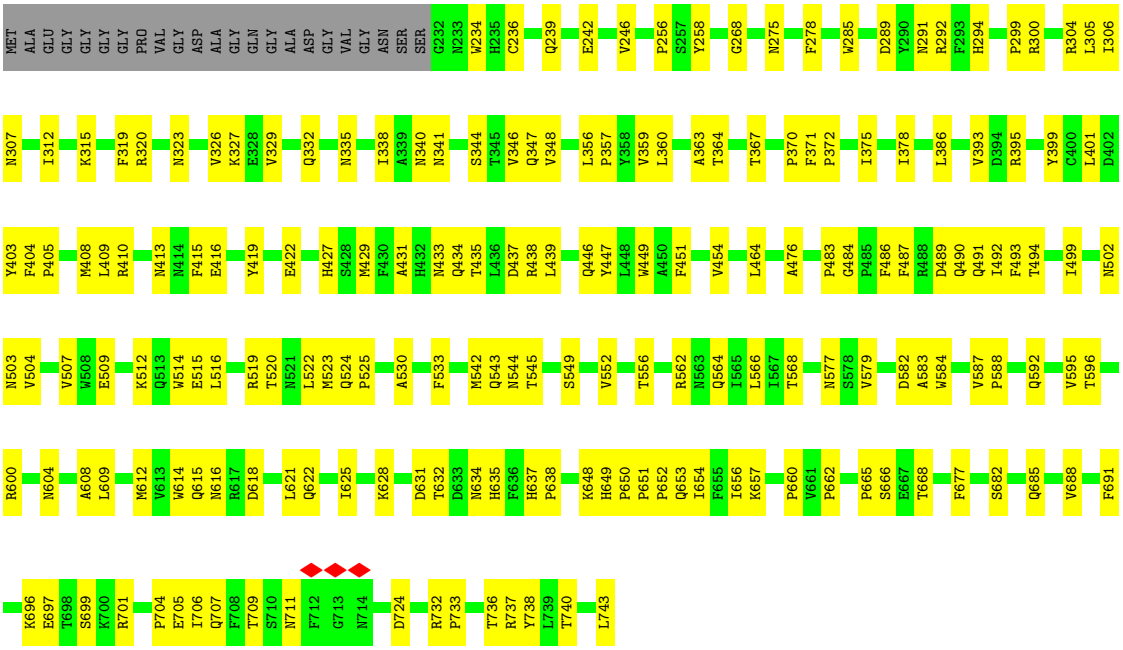




• Molecule 1: Capsid protein

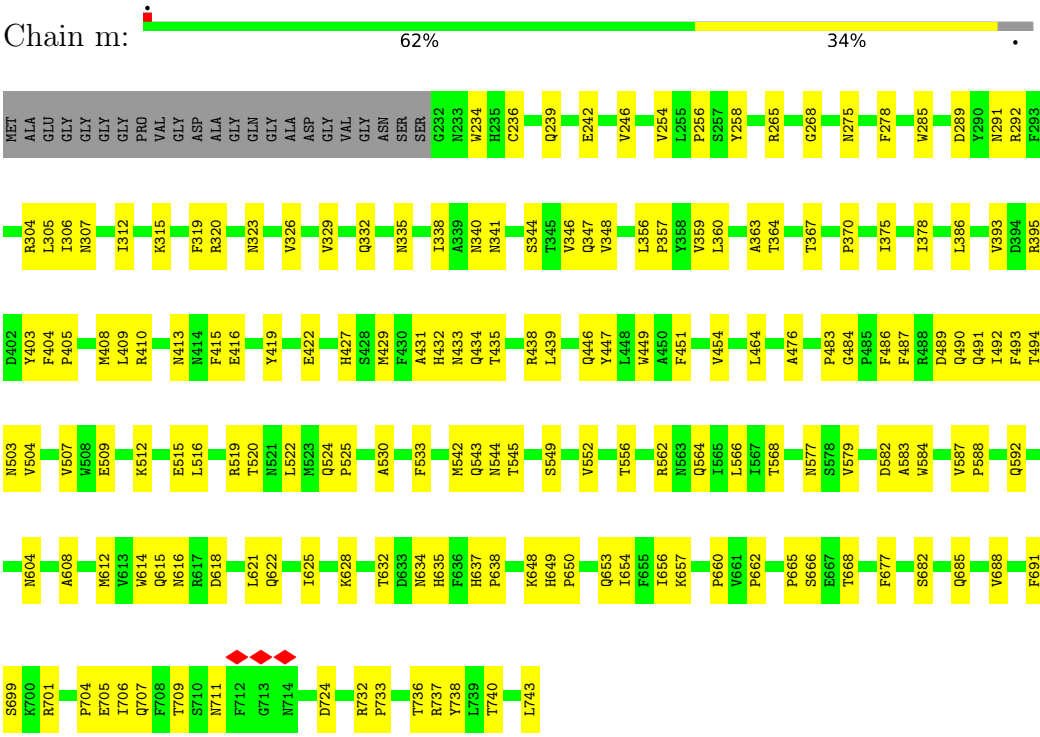
Chain l:





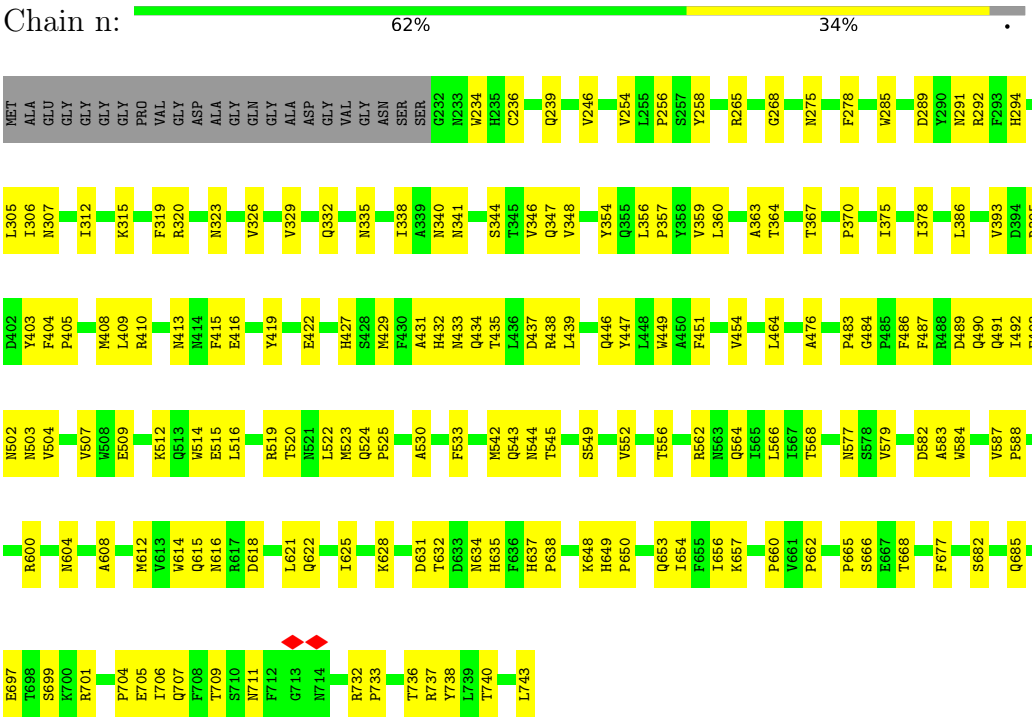
• Molecule 1: Capsid protein

Chain m:



• Molecule 1: Capsid protein

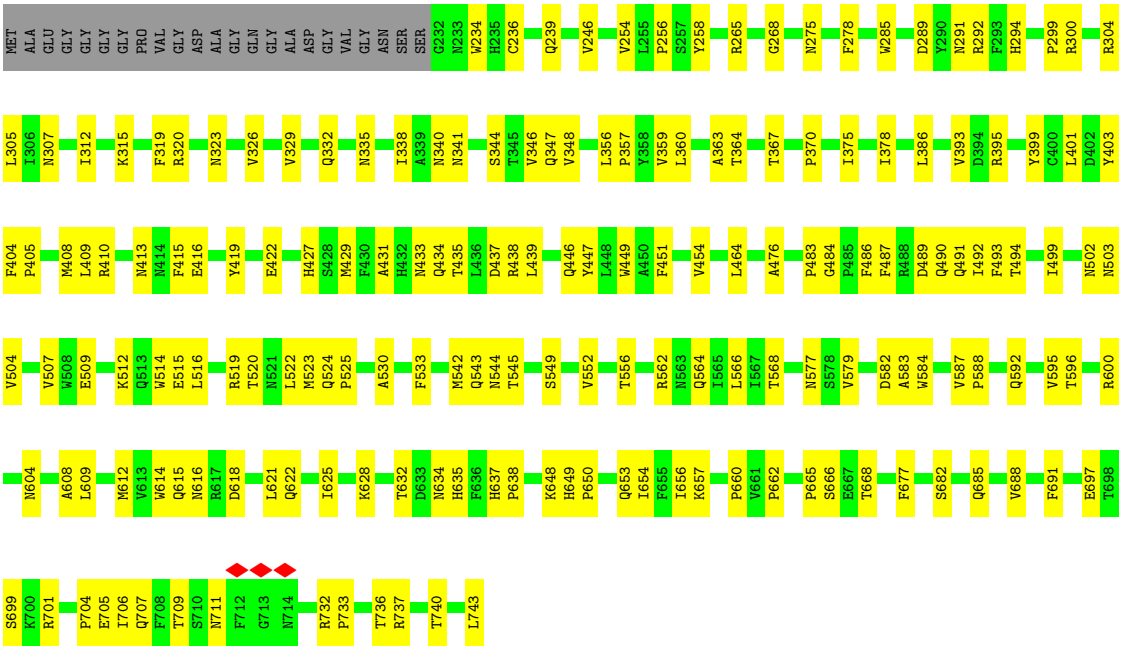
Chain n:



• Molecule 1: Capsid protein

Chain o:

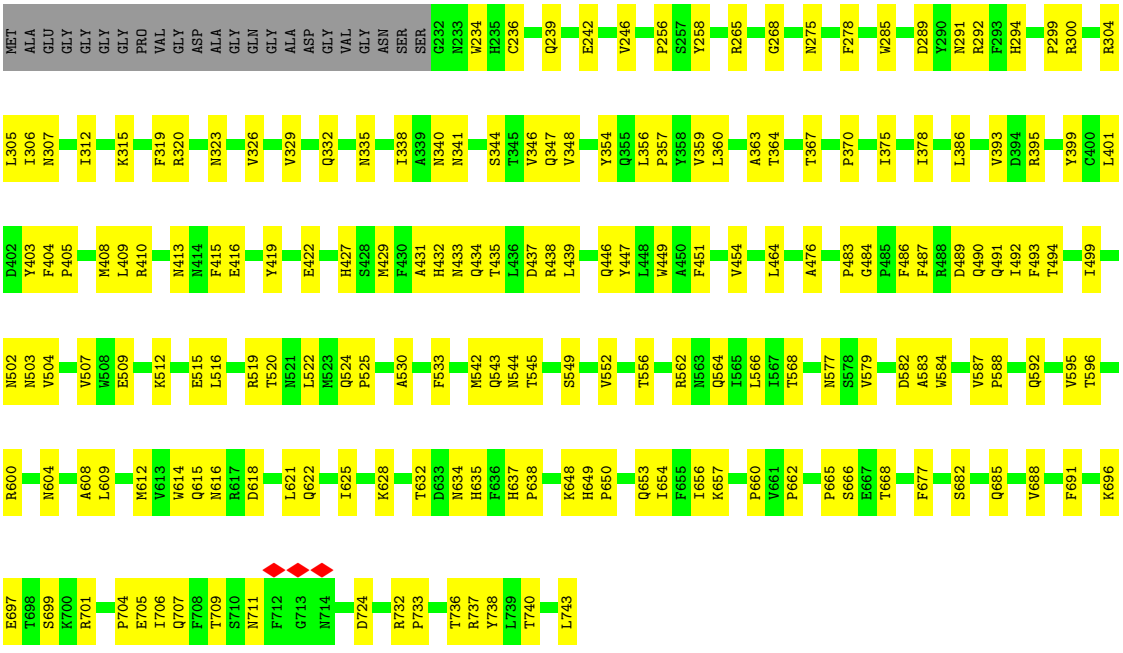




• Molecule 1: Capsid protein

Chain p:



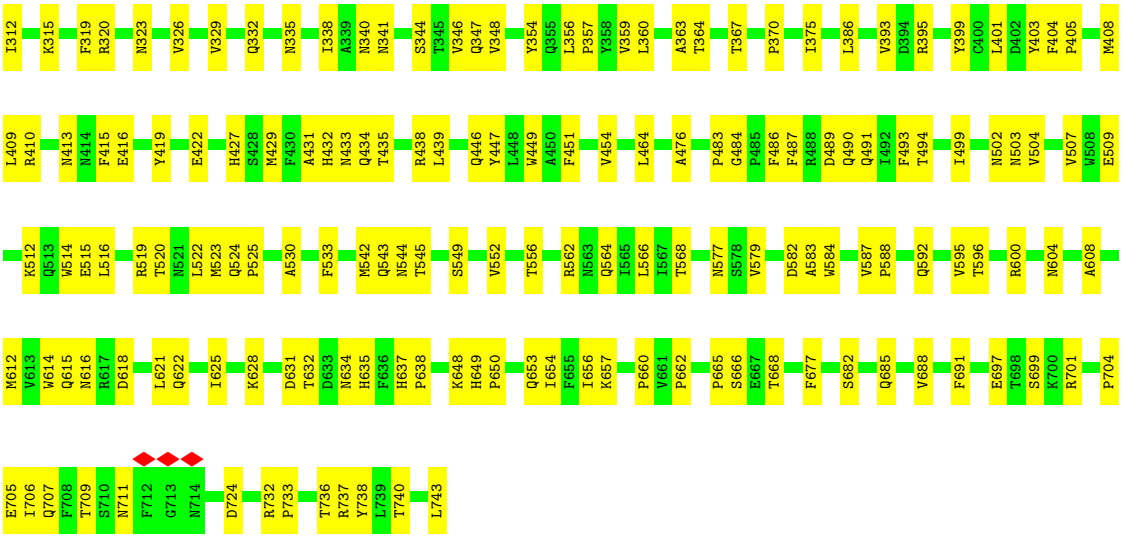


• Molecule 1: Capsid protein

Chain q:



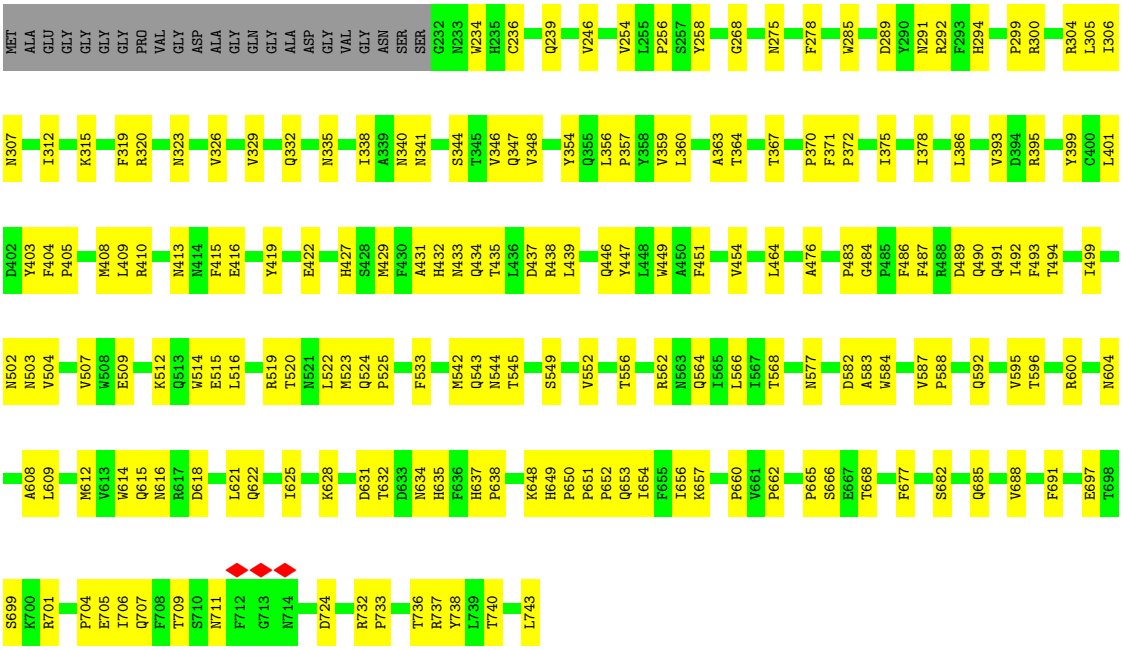




• Molecule 1: Capsid protein

Chain r:

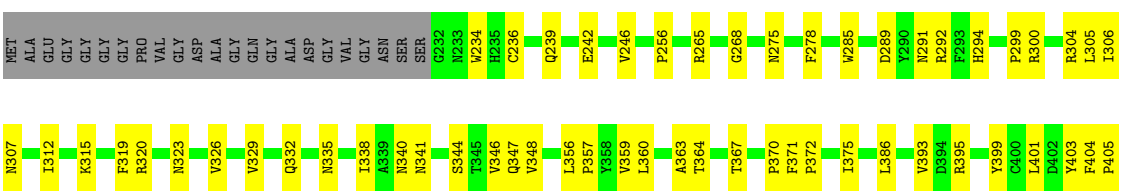


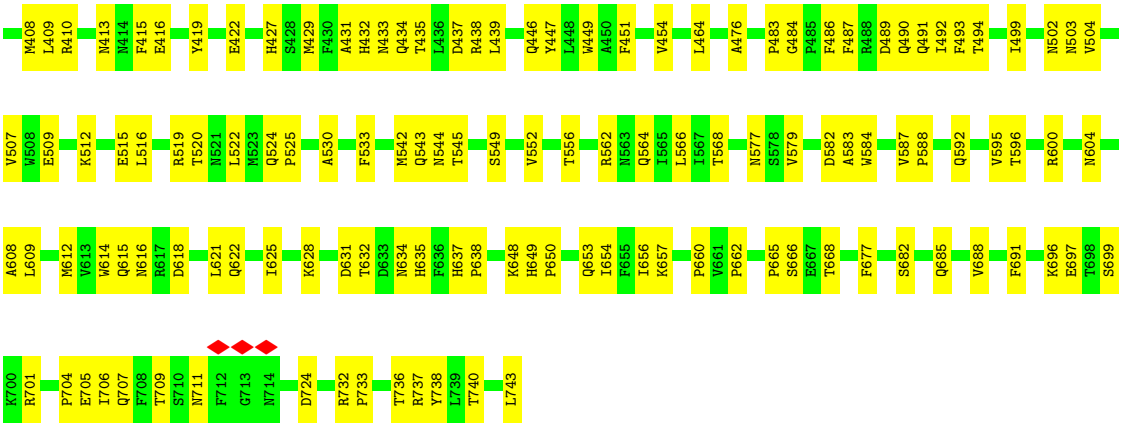


• Molecule 1: Capsid protein

Chain s:



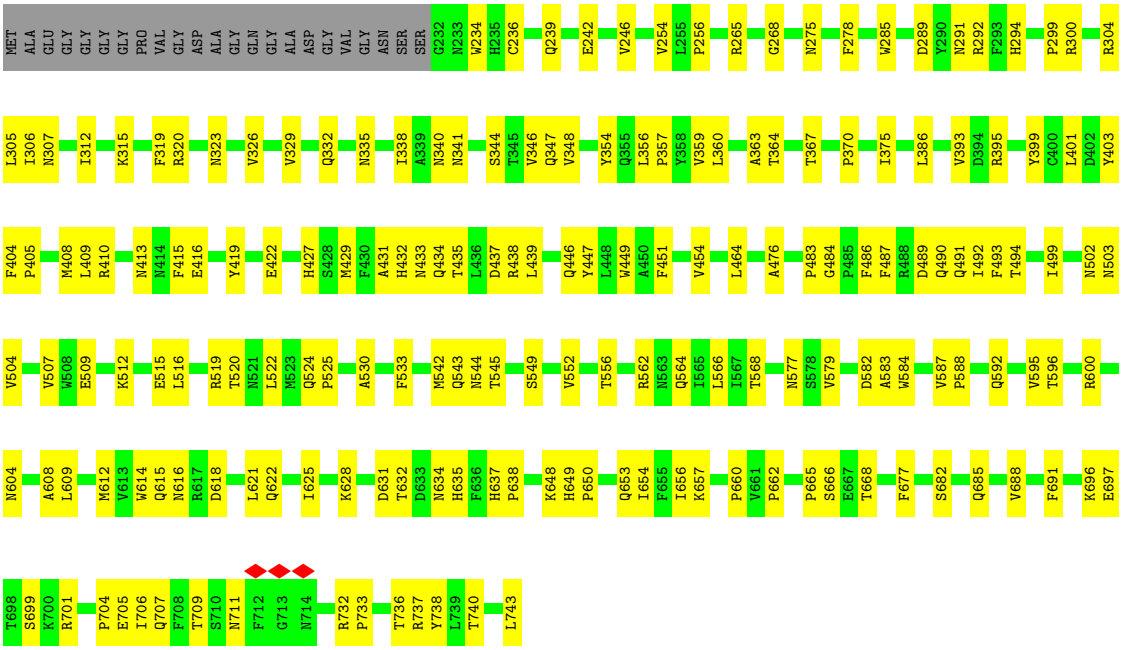




• Molecule 1: Capsid protein

Chain t:

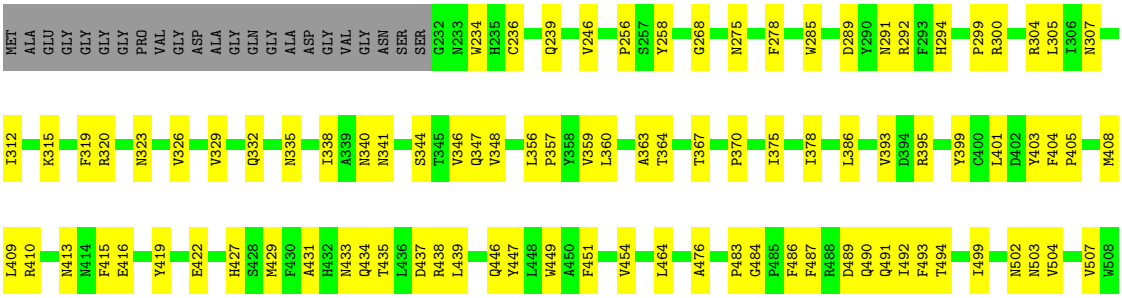


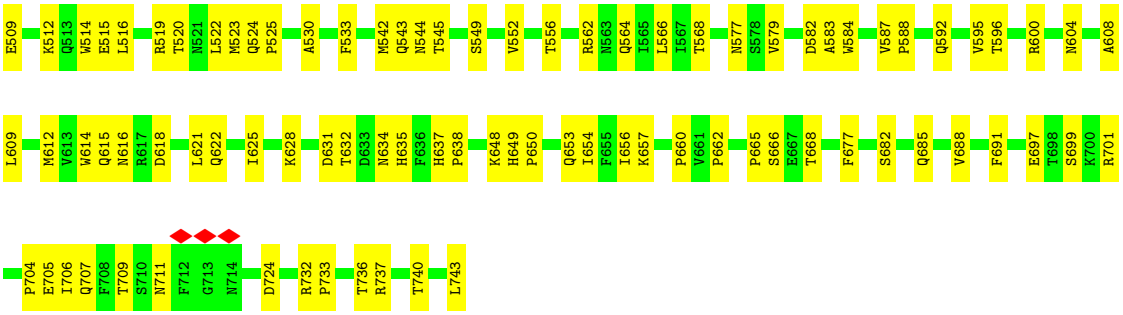


• Molecule 1: Capsid protein

Chain u:



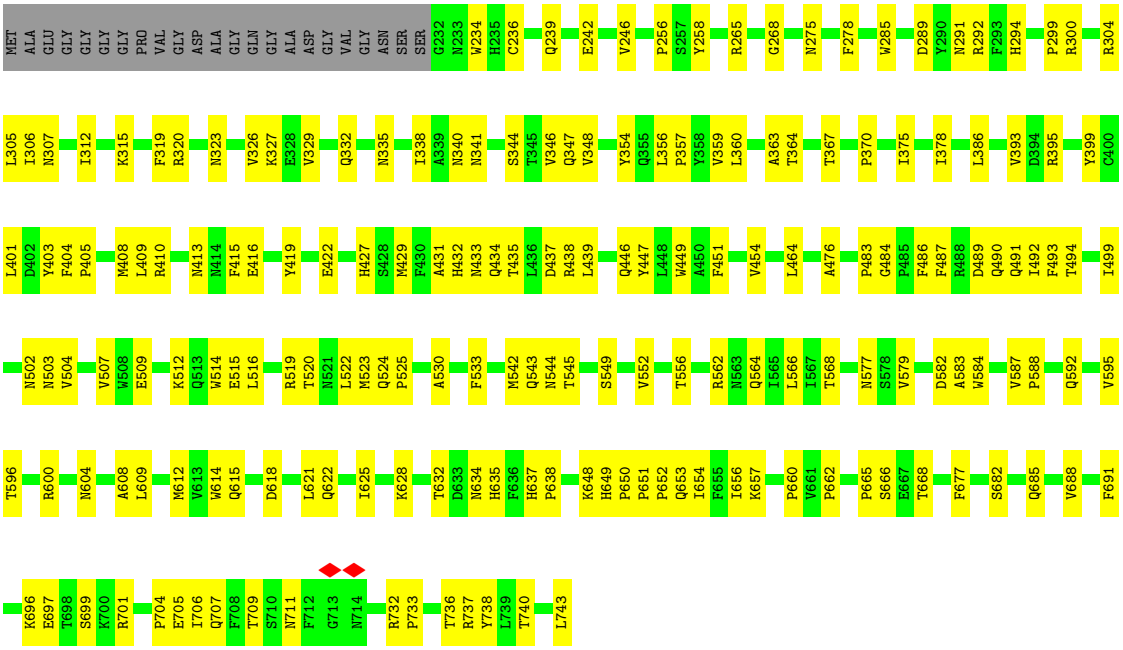




• Molecule 1: Capsid protein

Chain v:

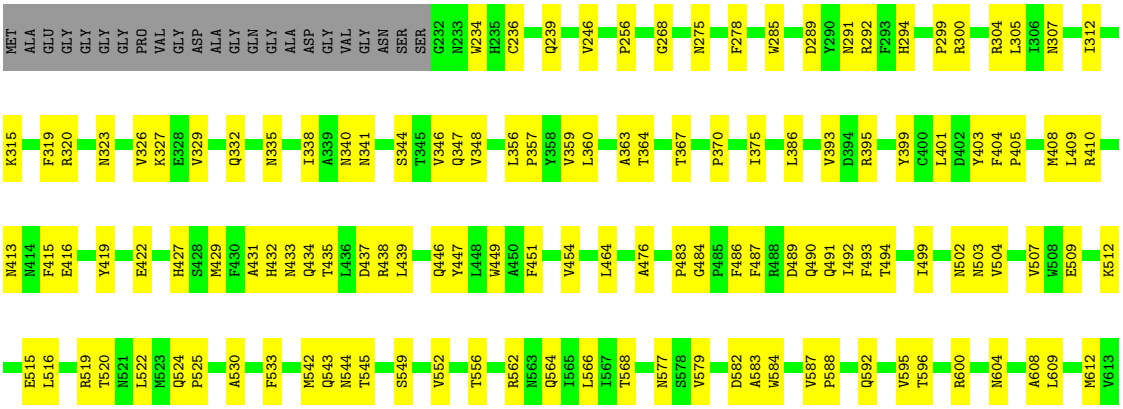




• Molecule 1: Capsid protein

Chain w:



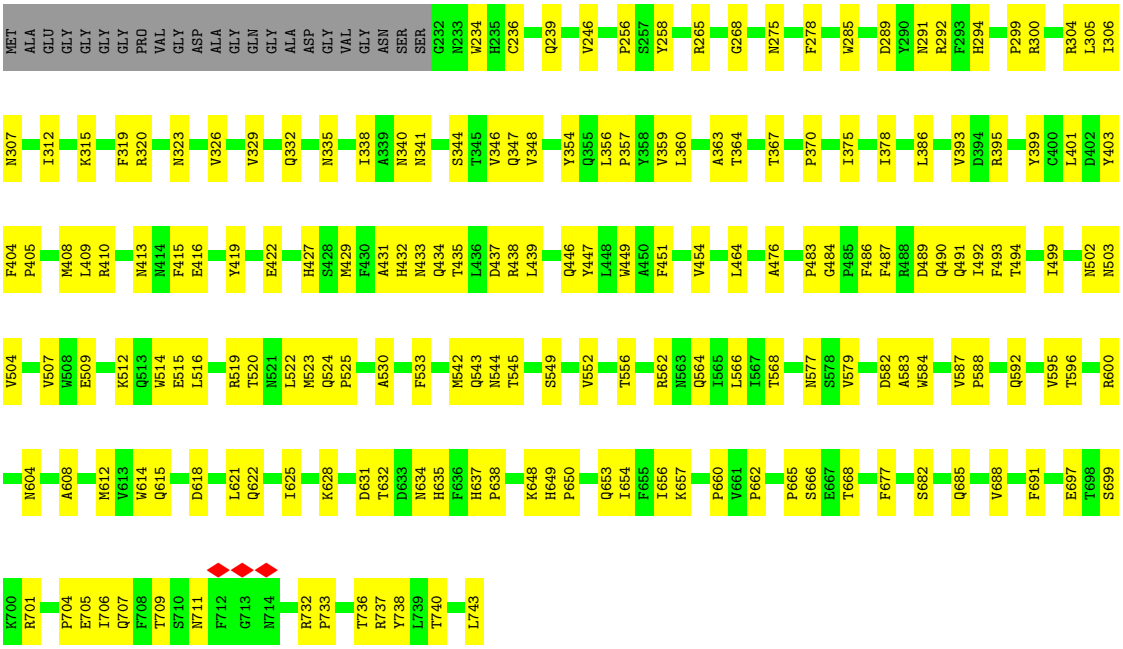




• Molecule 1: Capsid protein

Chain x:

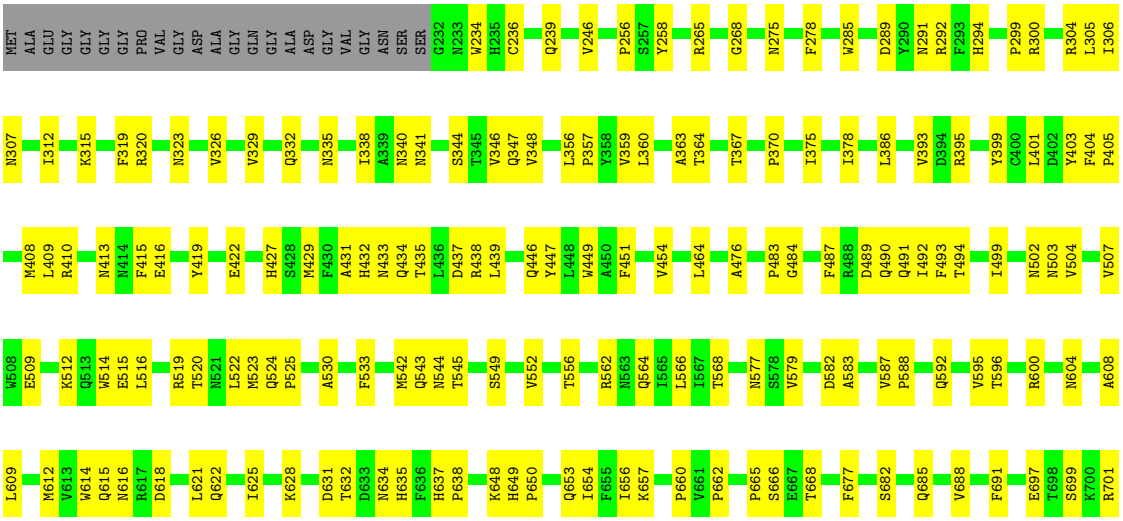


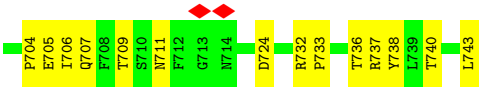


• Molecule 1: Capsid protein

Chain y:



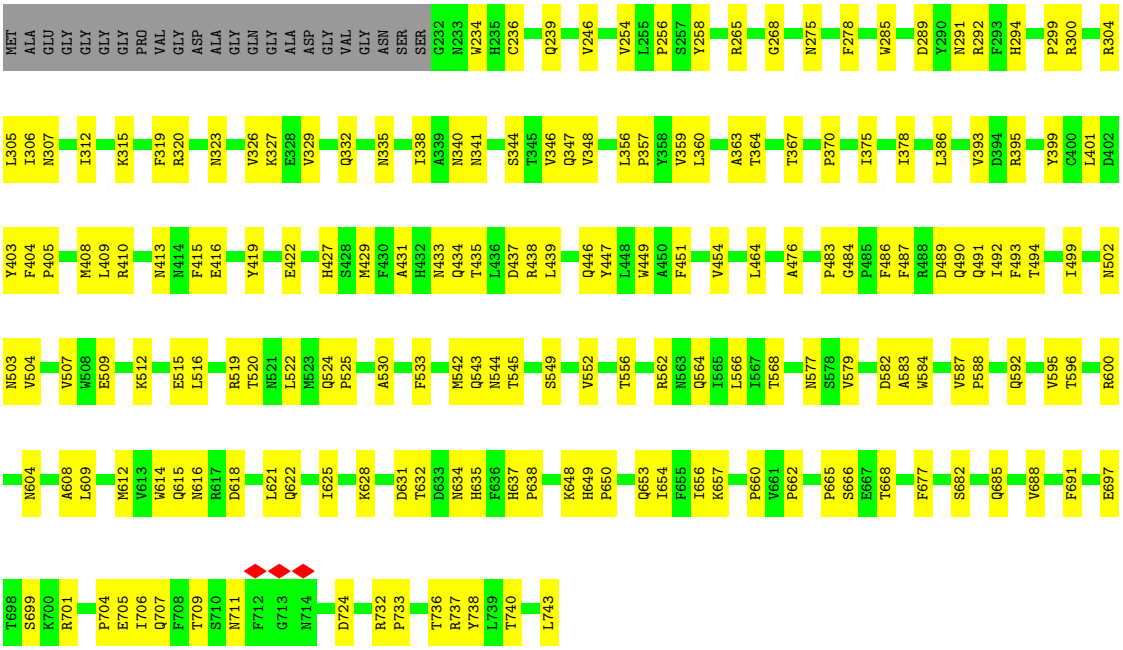




• Molecule 1: Capsid protein

Chain z:

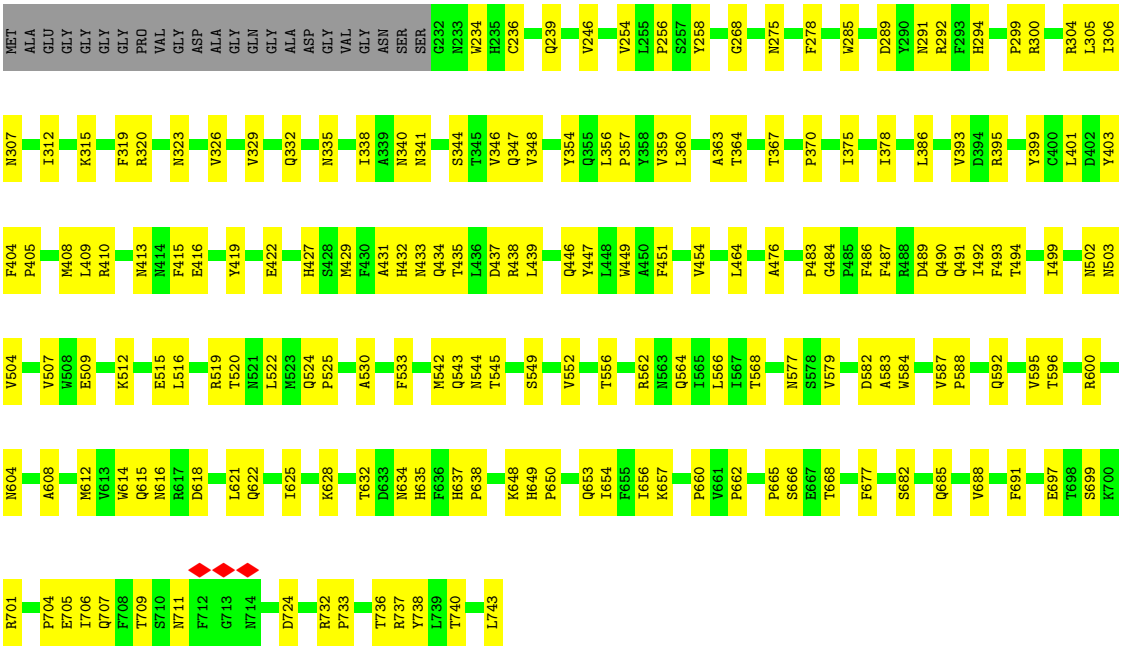




• Molecule 1: Capsid protein

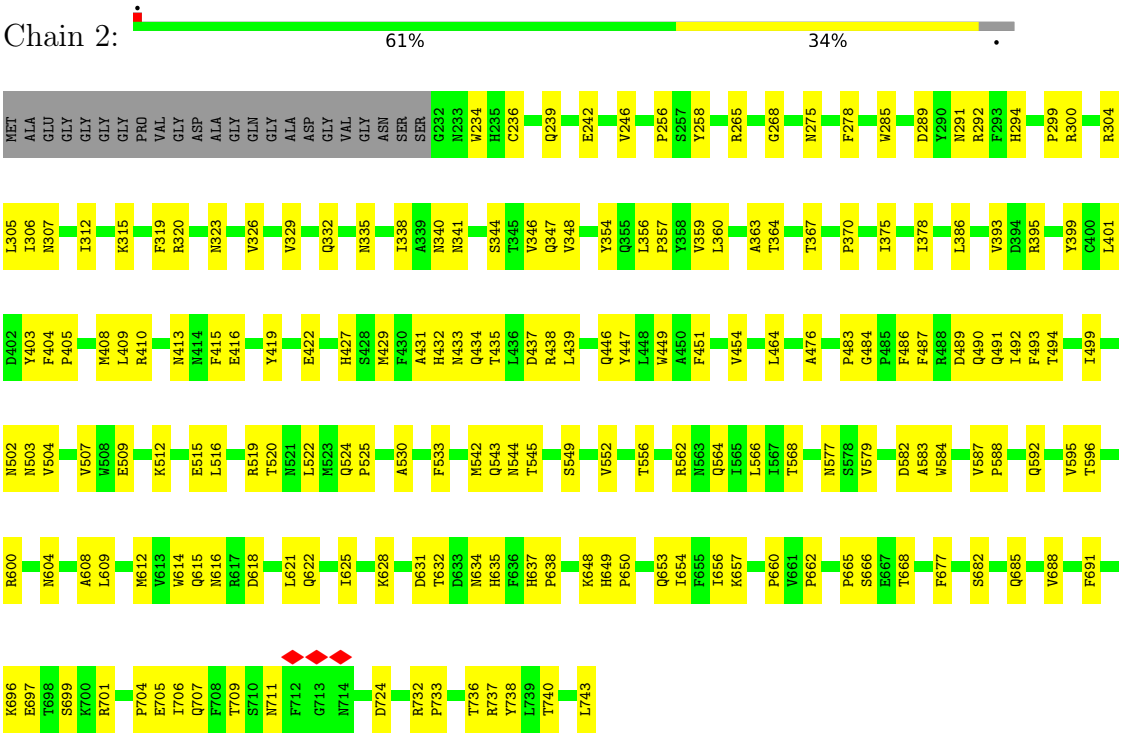
Chain 1:





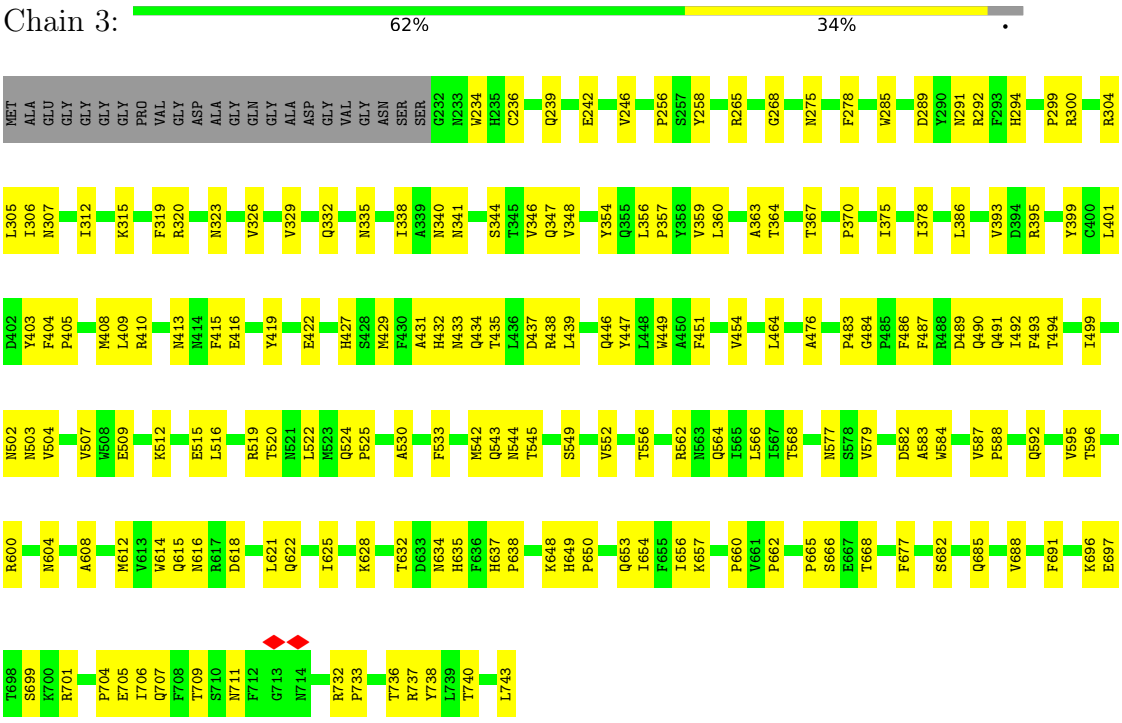
• Molecule 1: Capsid protein

Chain 2:



• Molecule 1: Capsid protein

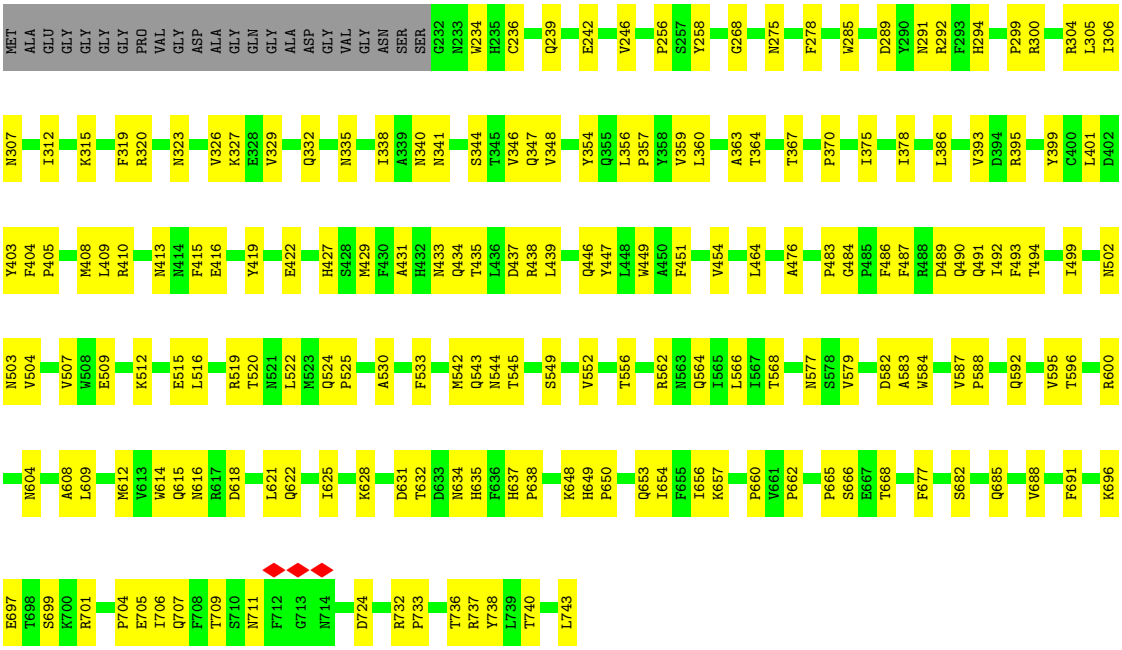
Chain 3:



• Molecule 1: Capsid protein

Chain 4:

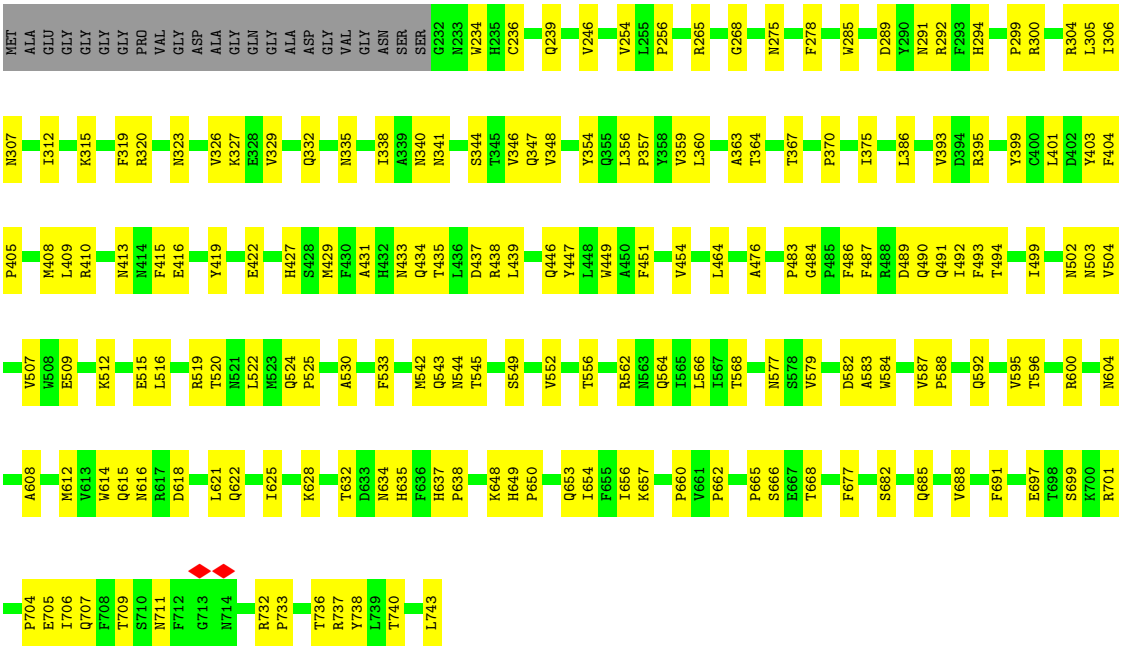




• Molecule 1: Capsid protein

Chain 5:



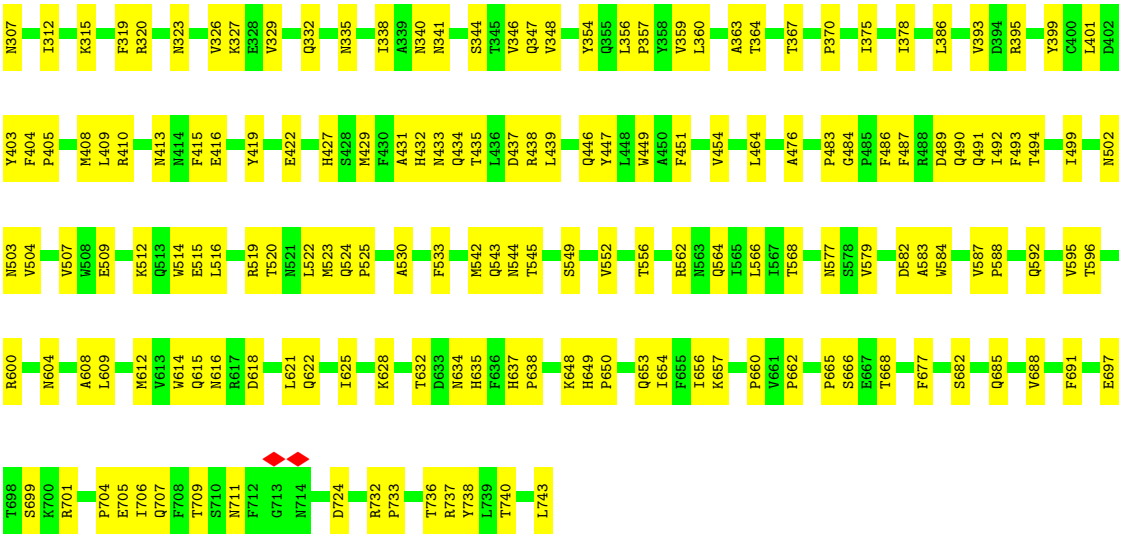


• Molecule 1: Capsid protein

Chain 6:



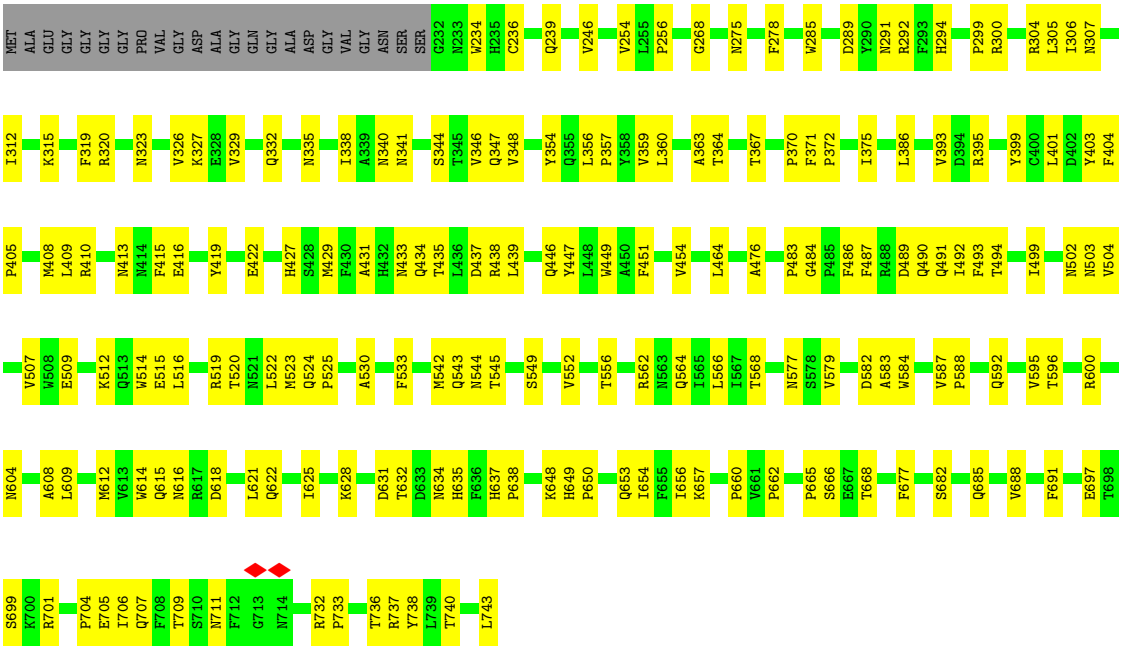




• Molecule 1: Capsid protein

Chain 7:

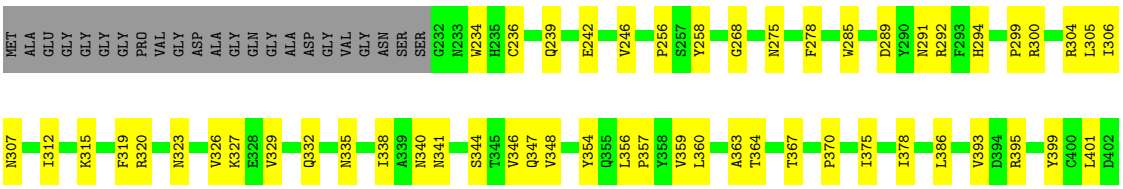


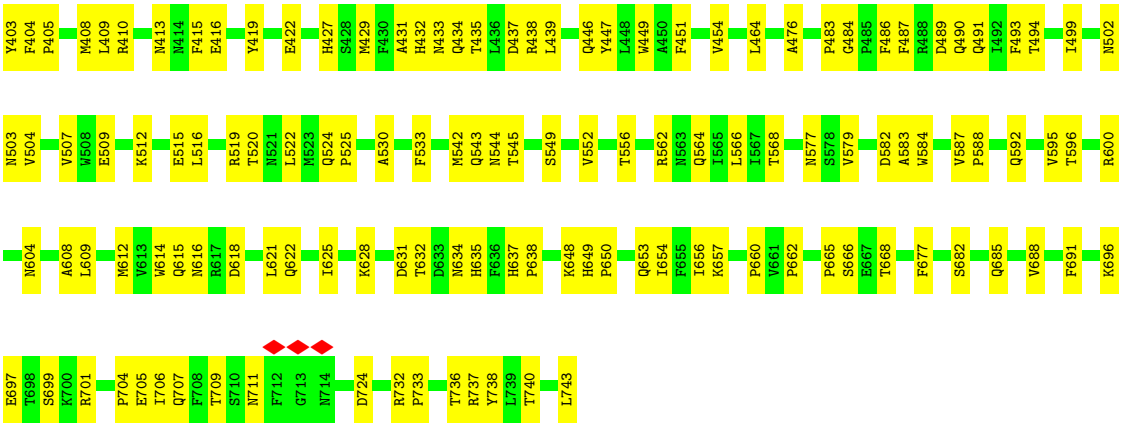


• Molecule 1: Capsid protein

Chain 8:






Y403 F404 P405 M408 L409 R410 N413 N414 F415 E416 Y419 E422 H427 S428 M429 F430 A431 H432 N433 Q434 T435 L436 D437 R438 L439 Q446 Y447 L448 W449 A450 F451 V454 L464 A476 P483 G484 P485 F486 F487 R488 D489 Q490 Q491 I492 F493 T494 I499 N502
N503 V504 V507 W508 E509 K512 E515 L516 R519 T520 N521 L522 M523 Q524 P525 A530 F533 M542 Q543 N544 T545 S549 V552 T556 R562 N563 Q564 I565 L566 I567 T568 N577 S578 V579 D582 A583 W584 V587 P588 Q592 V595 T596 R600
N604 A608 L609 M612 V613 W614 Q615 N616 R617 D618 L621 Q622 I625 K628 D631 T632 D633 N634 H635 F636 H637 P638 K648 H649 P650 Q653 I654 F655 I656 K657 P660 V661 P662 P665 S666 E667 T668 F677 S682 Q685 V688 F691 K696
E697 T698 S699 K700 R701 P704 E705 I706 Q707 F708 T709 S710 N711 F712 G713 N714 D724 R732 P733 T736 R737 Y738 L739 T740 L743

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38672	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 ($e^-/Å^2$)	61	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	16.383	Depositor
Minimum map value	-10.851	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2	Depositor
Map size (Å)	441.84003, 441.84003, 441.84003	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	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	0.45	1/4254 (0.0%)	0.49	0/5809
1	2	0.45	1/4254 (0.0%)	0.49	0/5809
1	3	0.45	1/4254 (0.0%)	0.49	0/5809
1	4	0.45	1/4254 (0.0%)	0.49	0/5809
1	5	0.45	1/4254 (0.0%)	0.49	0/5809
1	6	0.45	1/4254 (0.0%)	0.49	0/5809
1	7	0.45	1/4254 (0.0%)	0.49	0/5809
1	8	0.45	1/4254 (0.0%)	0.49	0/5809
1	A	0.45	1/4254 (0.0%)	0.49	0/5809
1	B	0.45	1/4254 (0.0%)	0.49	0/5809
1	C	0.45	1/4254 (0.0%)	0.49	0/5809
1	D	0.45	1/4254 (0.0%)	0.49	0/5809
1	E	0.45	1/4254 (0.0%)	0.49	0/5809
1	F	0.45	1/4254 (0.0%)	0.49	0/5809
1	G	0.45	1/4254 (0.0%)	0.49	0/5809
1	H	0.45	1/4254 (0.0%)	0.49	0/5809
1	I	0.45	1/4254 (0.0%)	0.49	0/5809
1	J	0.45	1/4254 (0.0%)	0.49	0/5809
1	K	0.45	1/4254 (0.0%)	0.49	0/5809
1	L	0.45	1/4254 (0.0%)	0.49	0/5809
1	M	0.45	1/4254 (0.0%)	0.49	0/5809
1	N	0.45	1/4254 (0.0%)	0.49	0/5809
1	O	0.45	1/4254 (0.0%)	0.49	0/5809
1	P	0.45	1/4254 (0.0%)	0.49	0/5809
1	Q	0.45	1/4254 (0.0%)	0.49	0/5809
1	R	0.45	1/4254 (0.0%)	0.49	0/5809
1	S	0.45	1/4254 (0.0%)	0.49	0/5809
1	T	0.45	1/4254 (0.0%)	0.49	0/5809
1	U	0.45	1/4254 (0.0%)	0.49	0/5809
1	V	0.45	1/4254 (0.0%)	0.49	0/5809
1	W	0.45	1/4254 (0.0%)	0.49	0/5809
1	X	0.45	1/4254 (0.0%)	0.49	0/5809
1	Y	0.45	1/4254 (0.0%)	0.49	0/5809
1	Z	0.45	1/4254 (0.0%)	0.49	0/5809

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	a	0.45	1/4254 (0.0%)	0.49	0/5809
1	b	0.45	1/4254 (0.0%)	0.49	0/5809
1	c	0.45	1/4254 (0.0%)	0.49	0/5809
1	d	0.45	1/4254 (0.0%)	0.49	0/5809
1	e	0.45	1/4254 (0.0%)	0.49	0/5809
1	f	0.45	1/4254 (0.0%)	0.49	0/5809
1	g	0.45	1/4254 (0.0%)	0.49	0/5809
1	h	0.45	1/4254 (0.0%)	0.49	0/5809
1	i	0.45	1/4254 (0.0%)	0.49	0/5809
1	j	0.45	1/4254 (0.0%)	0.49	0/5809
1	k	0.45	1/4254 (0.0%)	0.49	0/5809
1	l	0.45	1/4254 (0.0%)	0.49	0/5809
1	m	0.45	1/4254 (0.0%)	0.49	0/5809
1	n	0.45	1/4254 (0.0%)	0.49	0/5809
1	o	0.45	1/4254 (0.0%)	0.49	0/5809
1	p	0.45	1/4254 (0.0%)	0.49	0/5809
1	q	0.45	1/4254 (0.0%)	0.49	0/5809
1	r	0.45	1/4254 (0.0%)	0.49	0/5809
1	s	0.45	1/4254 (0.0%)	0.49	0/5809
1	t	0.45	1/4254 (0.0%)	0.49	0/5809
1	u	0.45	1/4254 (0.0%)	0.49	0/5809
1	v	0.45	1/4254 (0.0%)	0.49	0/5809
1	w	0.45	1/4254 (0.0%)	0.49	0/5809
1	x	0.45	1/4254 (0.0%)	0.49	0/5809
1	y	0.45	1/4254 (0.0%)	0.49	0/5809
1	z	0.45	1/4254 (0.0%)	0.49	0/5809
All	All	0.45	60/255240 (0.0%)	0.49	0/348540

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	638	PRO	C-N	-5.10	1.23	1.33
1	L	638	PRO	C-N	-5.10	1.23	1.33
1	r	638	PRO	C-N	-5.10	1.23	1.33
1	Z	638	PRO	C-N	-5.09	1.23	1.33
1	l	638	PRO	C-N	-5.09	1.23	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	4124	0	3890	183	0
1	2	4124	0	3890	185	0
1	3	4124	0	3890	182	0
1	4	4124	0	3890	185	0
1	5	4124	0	3890	182	0
1	6	4124	0	3890	186	0
1	7	4124	0	3890	187	0
1	8	4124	0	3890	183	0
1	A	4124	0	3890	192	0
1	B	4124	0	3890	183	0
1	C	4124	0	3890	184	0
1	D	4124	0	3890	182	0
1	E	4124	0	3890	183	0
1	F	4124	0	3890	186	0
1	G	4124	0	3890	184	0
1	H	4124	0	3890	182	0
1	I	4124	0	3890	189	0
1	J	4124	0	3890	185	0
1	K	4124	0	3890	184	0
1	L	4124	0	3890	186	0
1	M	4124	0	3890	183	0
1	N	4124	0	3890	182	0
1	O	4124	0	3890	191	0
1	P	4124	0	3890	184	0
1	Q	4124	0	3890	186	0
1	R	4124	0	3890	185	0
1	S	4124	0	3890	188	0
1	T	4124	0	3890	186	0
1	U	4124	0	3890	190	0
1	V	4124	0	3890	190	0
1	W	4124	0	3890	185	0
1	X	4124	0	3890	186	0
1	Y	4124	0	3890	187	0
1	Z	4124	0	3890	183	0
1	a	4124	0	3890	182	0
1	b	4124	0	3890	185	0
1	c	4124	0	3890	184	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	d	4124	0	3890	183	0
1	e	4124	0	3890	182	0
1	f	4124	0	3890	184	0
1	g	4124	0	3890	183	0
1	h	4124	0	3890	187	0
1	i	4124	0	3890	185	0
1	j	4124	0	3890	183	0
1	k	4124	0	3890	181	0
1	l	4124	0	3890	189	0
1	m	4124	0	3890	185	0
1	n	4124	0	3890	184	0
1	o	4124	0	3890	186	0
1	p	4124	0	3890	185	0
1	q	4124	0	3890	184	0
1	r	4124	0	3890	185	0
1	s	4124	0	3890	189	0
1	t	4124	0	3890	184	0
1	u	4124	0	3890	188	0
1	v	4124	0	3890	192	0
1	w	4124	0	3890	183	0
1	x	4124	0	3890	185	0
1	y	4124	0	3890	185	0
1	z	4124	0	3890	184	0
All	All	247440	0	233400	8325	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 17.

The worst 5 of 8325 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:q:493:PHE:H	1:q:502:ASN:HD21	1.16	0.94
1:Q:493:PHE:H	1:Q:502:ASN:HD21	1.16	0.94
1:R:493:PHE:H	1:R:502:ASN:HD21	1.16	0.94
1:n:493:PHE:H	1:n:502:ASN:HD21	1.15	0.94
1:H:493:PHE:H	1:H:502:ASN:HD21	1.16	0.94

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	510/535 (95%)	497 (98%)	13 (2%)	0	100	100
1	2	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	3	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	4	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	5	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	6	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	7	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	8	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	A	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	B	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	C	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	D	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	E	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	F	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	G	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	H	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	I	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	J	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	K	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	L	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	M	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	N	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	O	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	P	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	Q	510/535 (95%)	496 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	S	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	T	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	U	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	V	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	W	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	X	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	Y	510/535 (95%)	497 (98%)	13 (2%)	0	100	100
1	Z	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	a	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	b	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	c	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	d	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	e	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	f	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	g	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	h	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	i	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	j	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	k	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	l	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	m	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	n	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	o	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	p	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	q	510/535 (95%)	497 (98%)	13 (2%)	0	100	100
1	r	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	s	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	t	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	u	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	v	510/535 (95%)	496 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	x	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	y	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
1	z	510/535 (95%)	496 (97%)	14 (3%)	0	100	100
All	All	30600/32100 (95%)	29763 (97%)	837 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	447/458 (98%)	447 (100%)	0	100	100
1	2	447/458 (98%)	447 (100%)	0	100	100
1	3	447/458 (98%)	447 (100%)	0	100	100
1	4	447/458 (98%)	447 (100%)	0	100	100
1	5	447/458 (98%)	447 (100%)	0	100	100
1	6	447/458 (98%)	447 (100%)	0	100	100
1	7	447/458 (98%)	447 (100%)	0	100	100
1	8	447/458 (98%)	447 (100%)	0	100	100
1	A	447/458 (98%)	447 (100%)	0	100	100
1	B	447/458 (98%)	447 (100%)	0	100	100
1	C	447/458 (98%)	447 (100%)	0	100	100
1	D	447/458 (98%)	447 (100%)	0	100	100
1	E	447/458 (98%)	447 (100%)	0	100	100
1	F	447/458 (98%)	447 (100%)	0	100	100
1	G	447/458 (98%)	447 (100%)	0	100	100
1	H	447/458 (98%)	447 (100%)	0	100	100
1	I	447/458 (98%)	447 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	447/458 (98%)	447 (100%)	0	100	100
1	K	447/458 (98%)	447 (100%)	0	100	100
1	L	447/458 (98%)	447 (100%)	0	100	100
1	M	447/458 (98%)	447 (100%)	0	100	100
1	N	447/458 (98%)	447 (100%)	0	100	100
1	O	447/458 (98%)	447 (100%)	0	100	100
1	P	447/458 (98%)	447 (100%)	0	100	100
1	Q	447/458 (98%)	447 (100%)	0	100	100
1	R	447/458 (98%)	447 (100%)	0	100	100
1	S	447/458 (98%)	447 (100%)	0	100	100
1	T	447/458 (98%)	447 (100%)	0	100	100
1	U	447/458 (98%)	447 (100%)	0	100	100
1	V	447/458 (98%)	447 (100%)	0	100	100
1	W	447/458 (98%)	447 (100%)	0	100	100
1	X	447/458 (98%)	447 (100%)	0	100	100
1	Y	447/458 (98%)	447 (100%)	0	100	100
1	Z	447/458 (98%)	447 (100%)	0	100	100
1	a	447/458 (98%)	447 (100%)	0	100	100
1	b	447/458 (98%)	447 (100%)	0	100	100
1	c	447/458 (98%)	447 (100%)	0	100	100
1	d	447/458 (98%)	447 (100%)	0	100	100
1	e	447/458 (98%)	447 (100%)	0	100	100
1	f	447/458 (98%)	447 (100%)	0	100	100
1	g	447/458 (98%)	447 (100%)	0	100	100
1	h	447/458 (98%)	447 (100%)	0	100	100
1	i	447/458 (98%)	447 (100%)	0	100	100
1	j	447/458 (98%)	447 (100%)	0	100	100
1	k	447/458 (98%)	447 (100%)	0	100	100
1	l	447/458 (98%)	447 (100%)	0	100	100
1	m	447/458 (98%)	447 (100%)	0	100	100
1	n	447/458 (98%)	447 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	447/458 (98%)	447 (100%)	0	100	100
1	p	447/458 (98%)	447 (100%)	0	100	100
1	q	447/458 (98%)	447 (100%)	0	100	100
1	r	447/458 (98%)	447 (100%)	0	100	100
1	s	447/458 (98%)	447 (100%)	0	100	100
1	t	447/458 (98%)	447 (100%)	0	100	100
1	u	447/458 (98%)	447 (100%)	0	100	100
1	v	447/458 (98%)	447 (100%)	0	100	100
1	w	447/458 (98%)	447 (100%)	0	100	100
1	x	447/458 (98%)	447 (100%)	0	100	100
1	y	447/458 (98%)	447 (100%)	0	100	100
1	z	447/458 (98%)	447 (100%)	0	100	100
All	All	26820/27480 (98%)	26820 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1055 such sidechains are listed below:

Mol	Chain	Res	Type
1	1	521	ASN
1	3	323	ASN
1	1	502	ASN
1	8	335	ASN
1	V	653	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

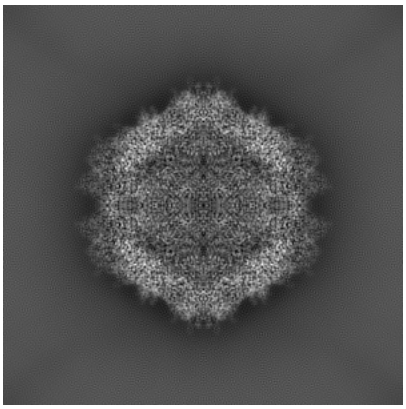
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41208. These allow visual inspection of the internal detail of the map and identification of artifacts.

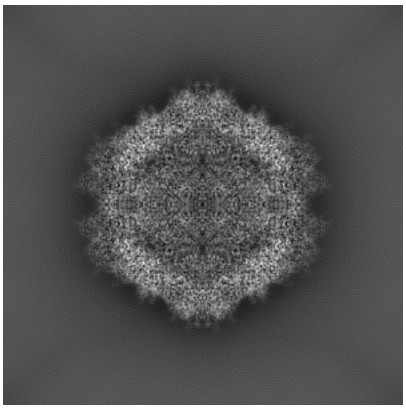
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

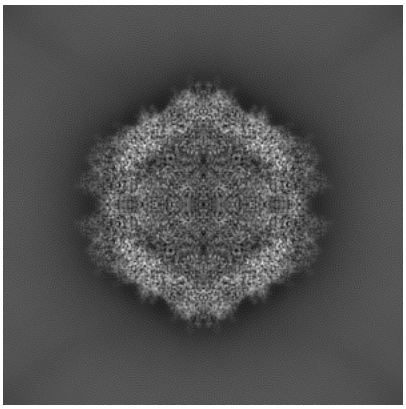
6.1.1 Primary map



X

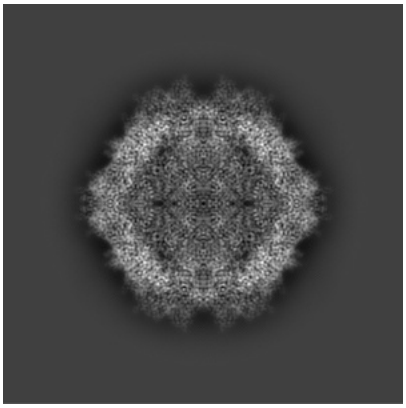


Y

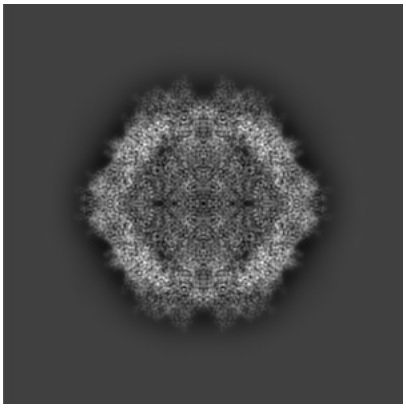


Z

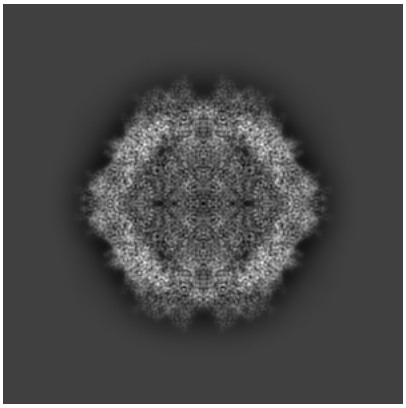
6.1.2 Raw map



X



Y

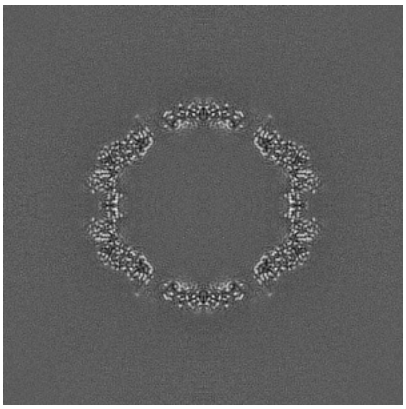


Z

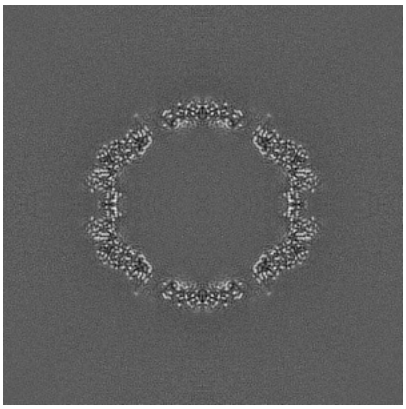
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

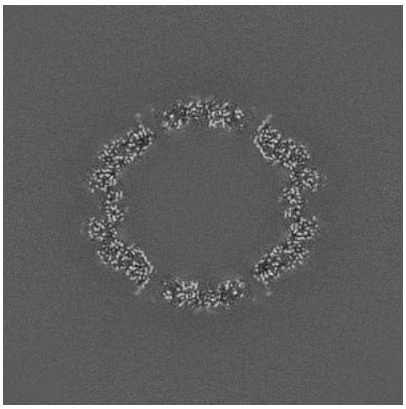
6.2.1 Primary map



X Index: 210

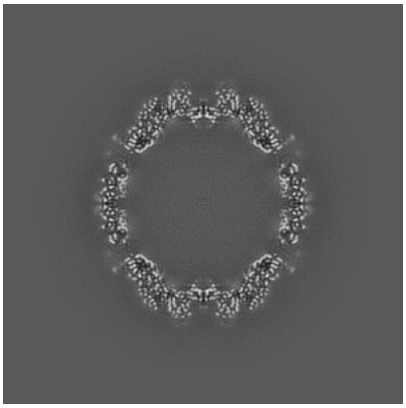


Y Index: 210

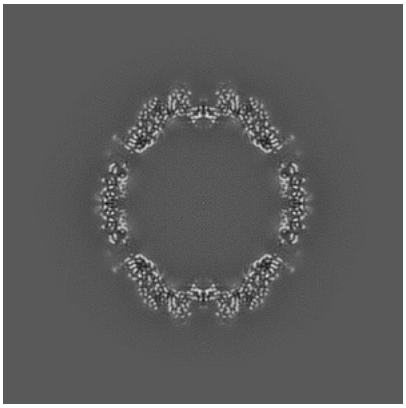


Z Index: 210

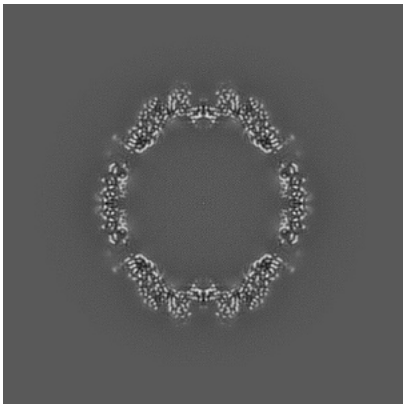
6.2.2 Raw map



X Index: 210



Y Index: 210

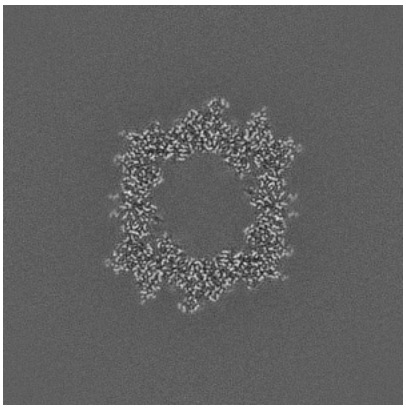


Z Index: 210

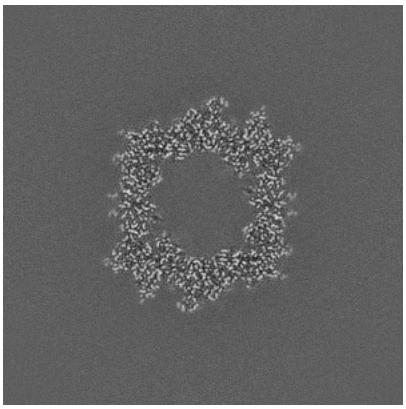
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

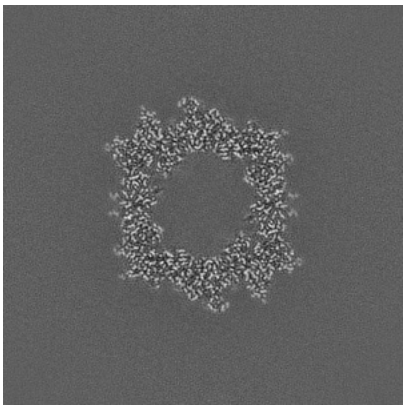
6.3.1 Primary map



X Index: 273

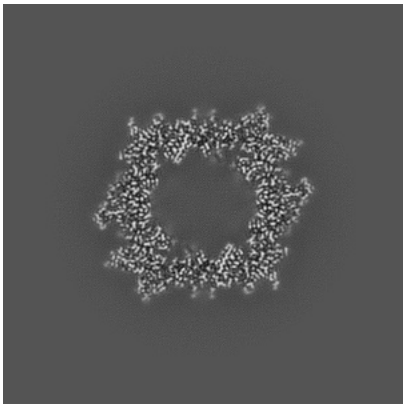


Y Index: 273

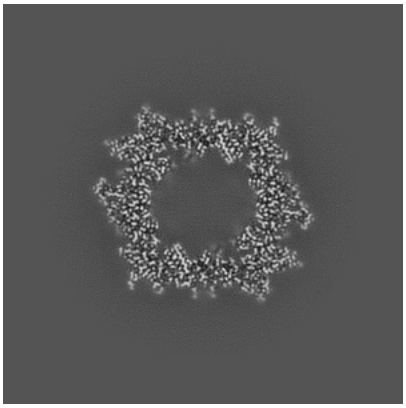


Z Index: 146

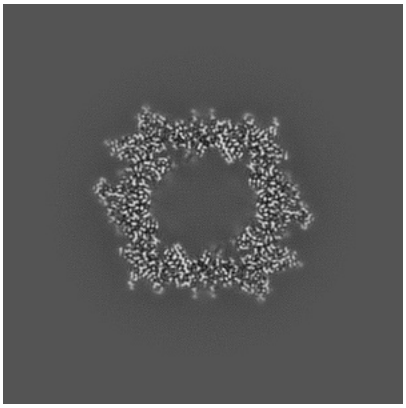
6.3.2 Raw map



X Index: 272



Y Index: 148

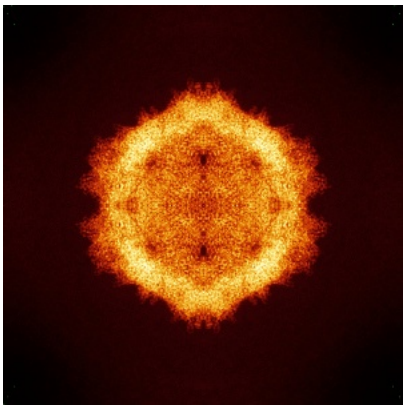


Z Index: 148

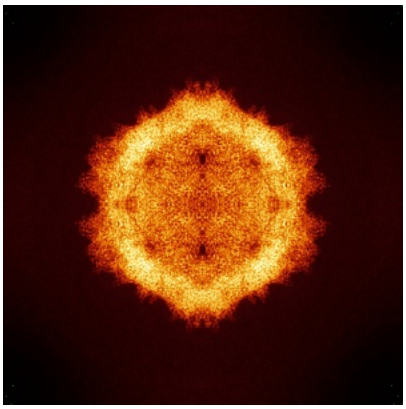
The images above show the largest variance slices of the map in three orthogonal directions.

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

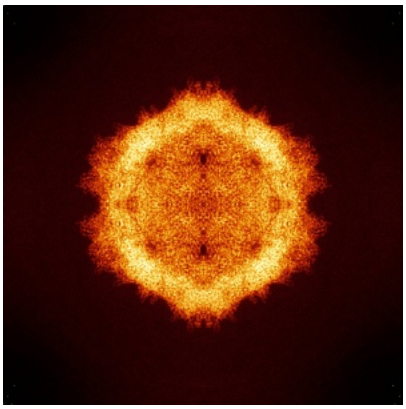
6.4.1 Primary map



X

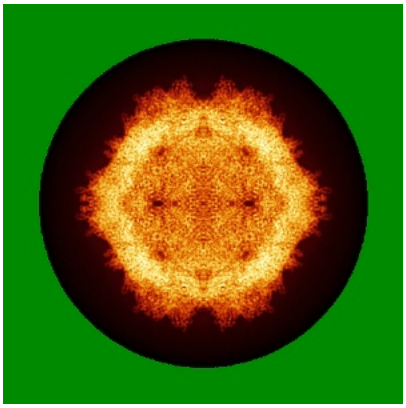


Y

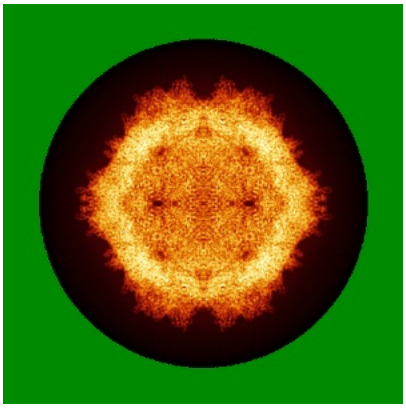


Z

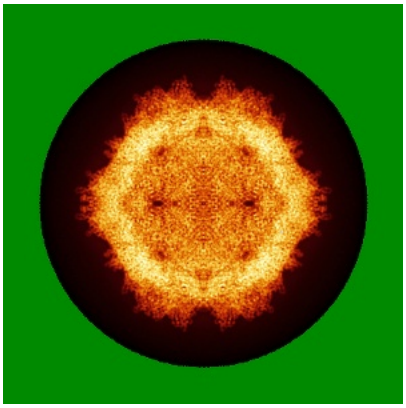
6.4.2 Raw map



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



X Y Z

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.

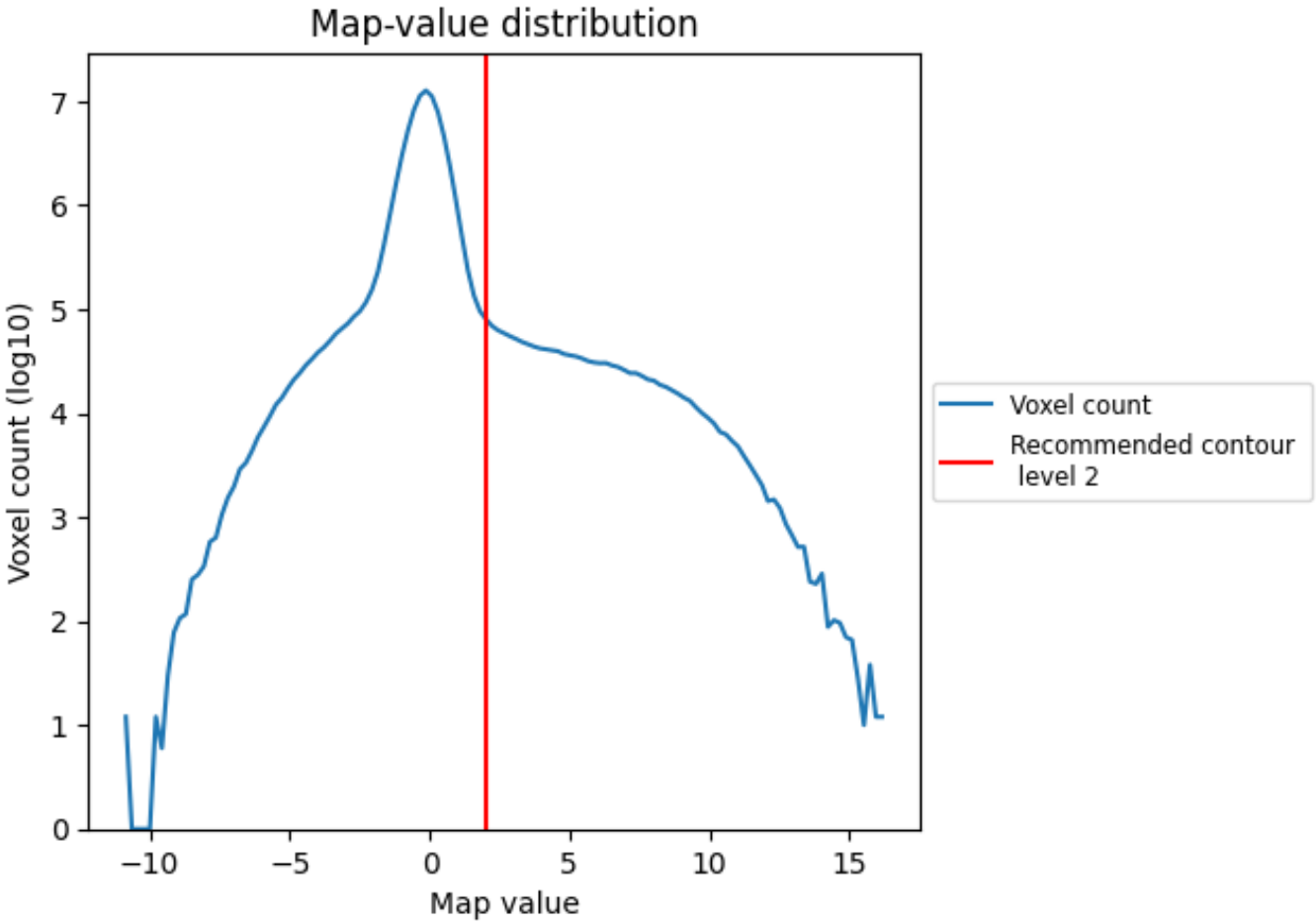
6.6 Mask visualisation (i)

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

7 Map analysis

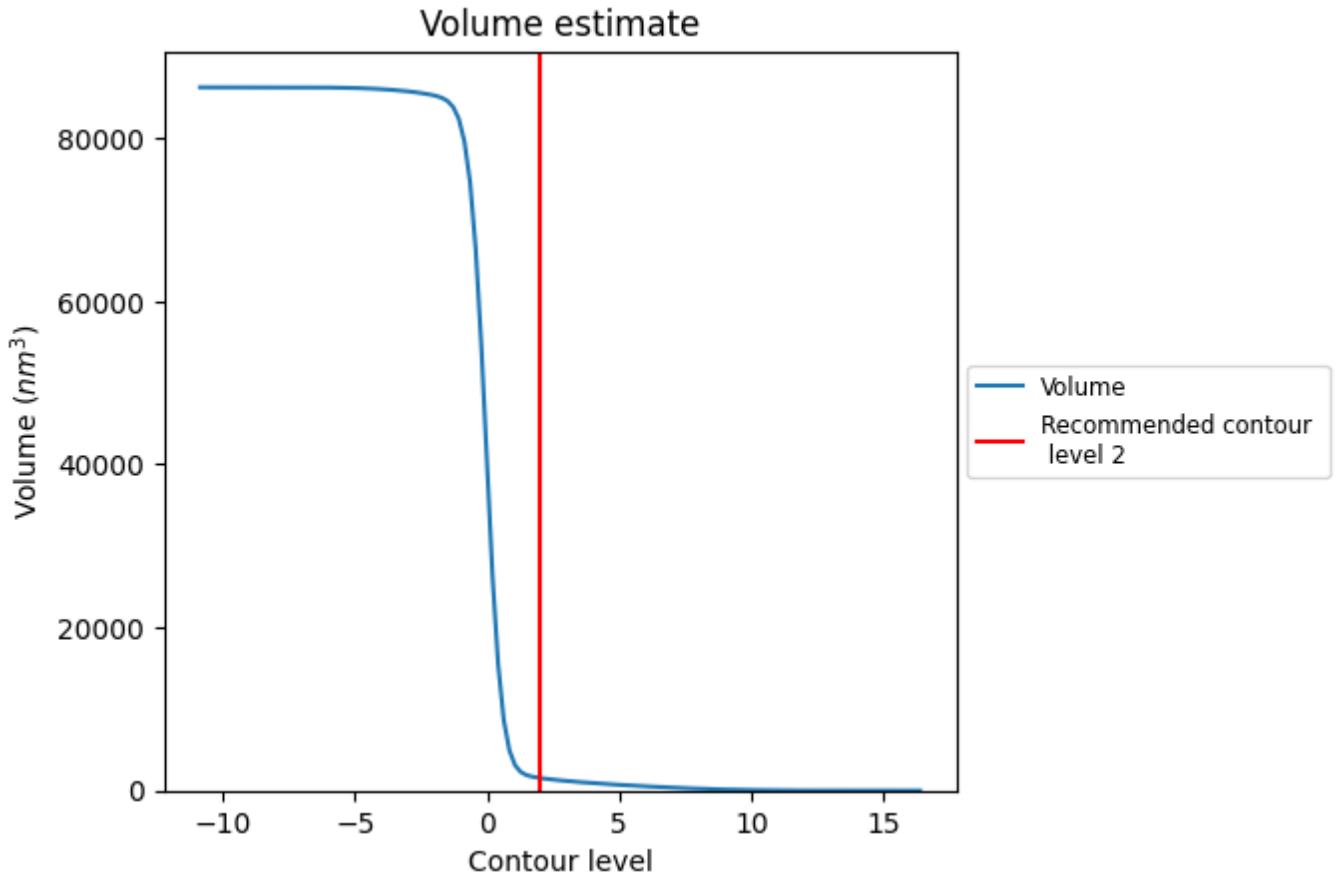
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

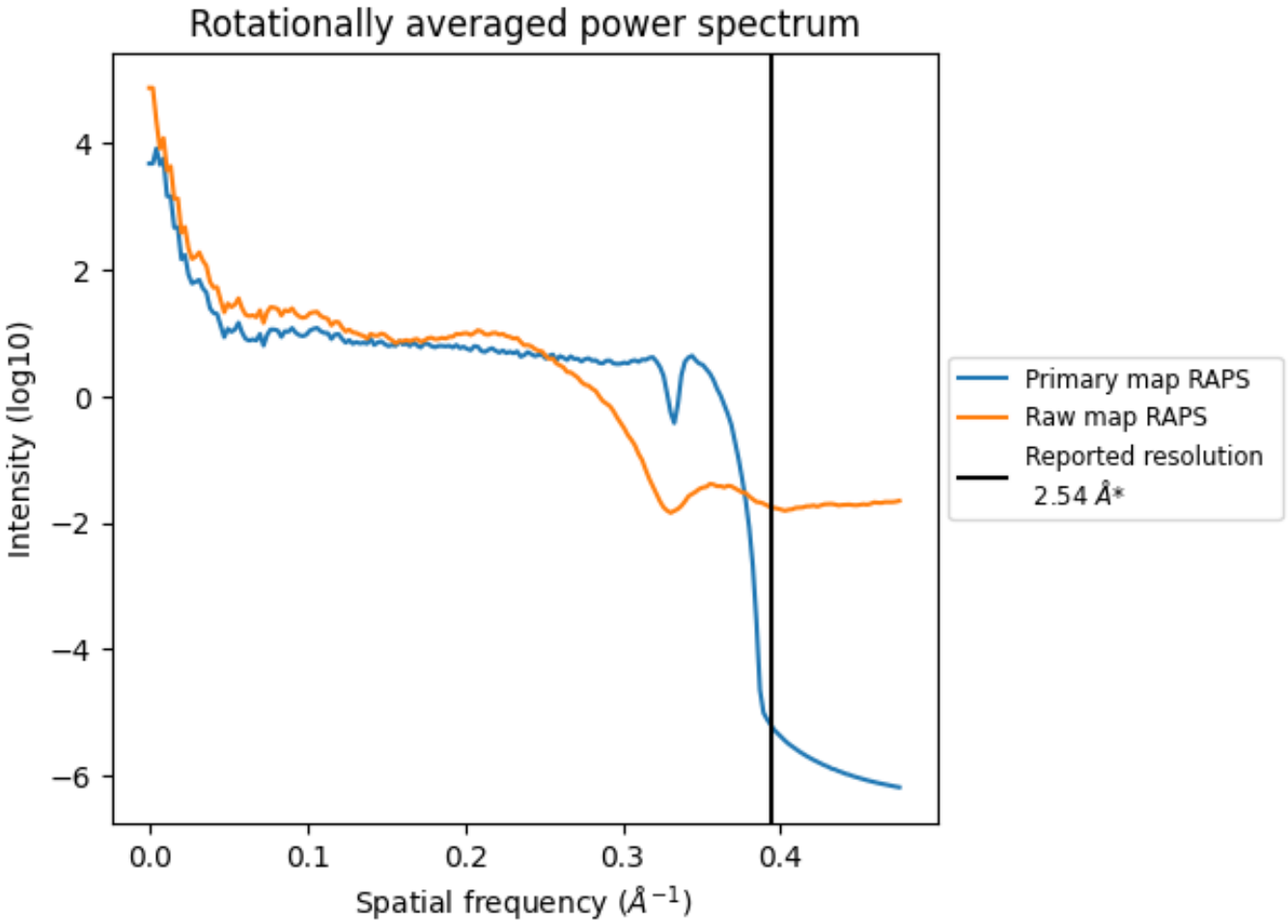
7.2 Volume estimate (i)



The volume at the recommended contour level is 1543 nm^3; this corresponds to an approximate mass of 1394 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

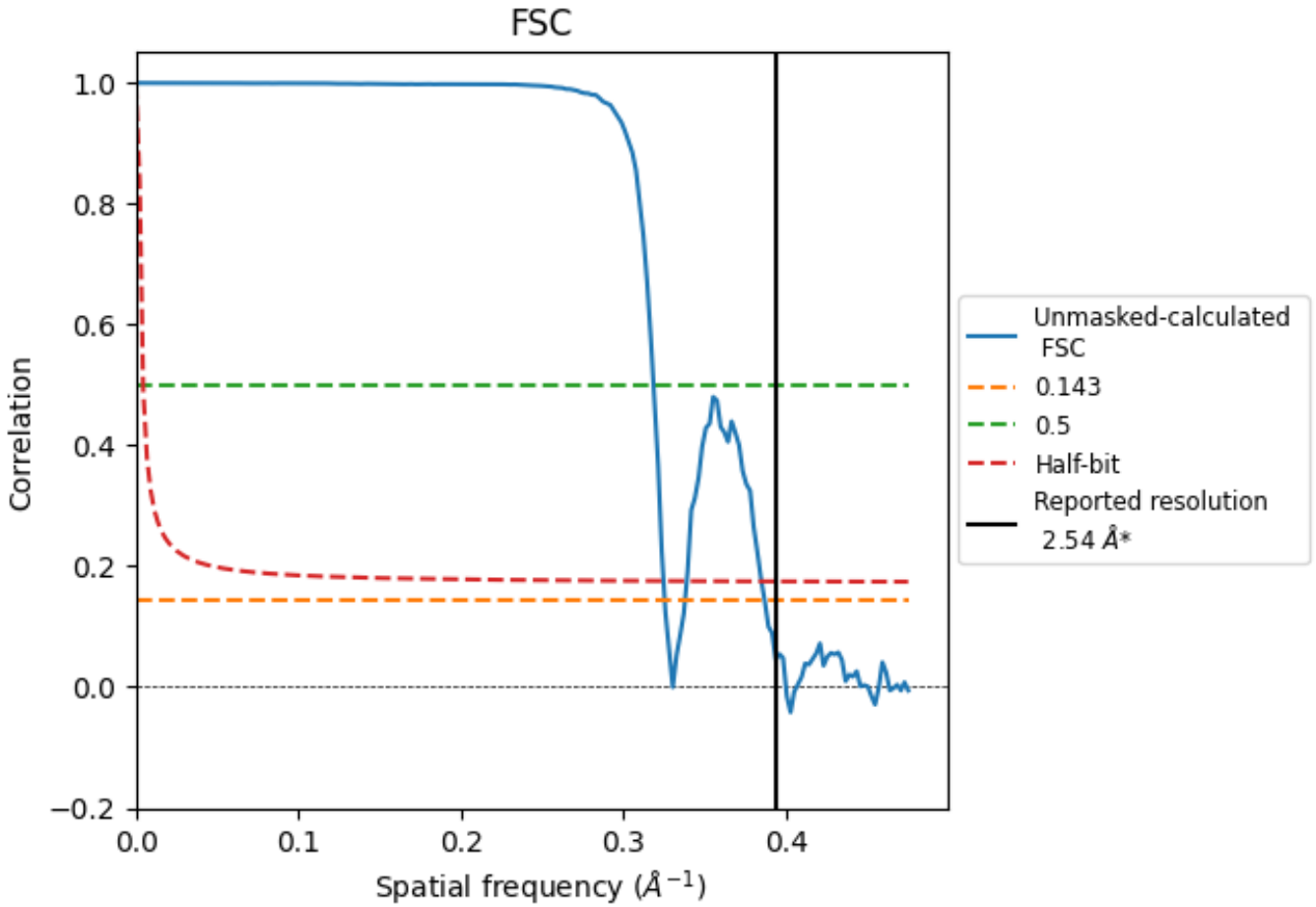


*Reported resolution corresponds to spatial frequency of 0.394 Å^{-1}

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 0.394 Å^{-1}

8.2 Resolution estimates (i)

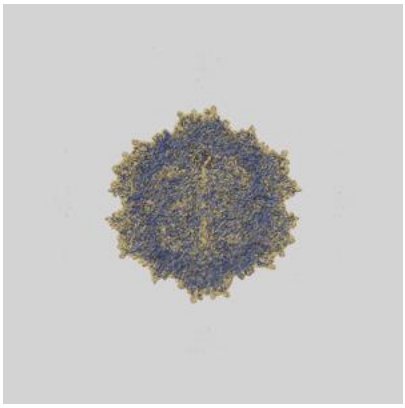
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.54	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.07	3.14	3.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.07 differs from the reported value 2.54 by more than 10 %

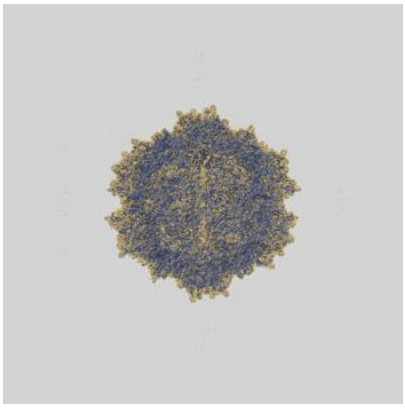
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41208 and PDB model 8TEX. Per-residue inclusion information can be found in section 3 on page 21.

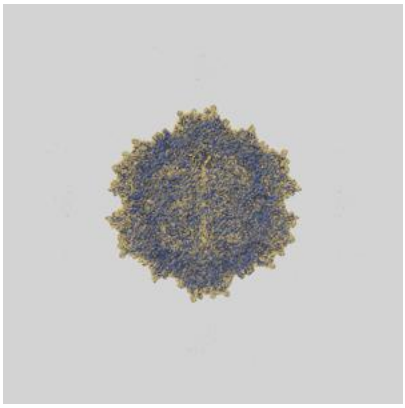
9.1 Map-model overlay



X



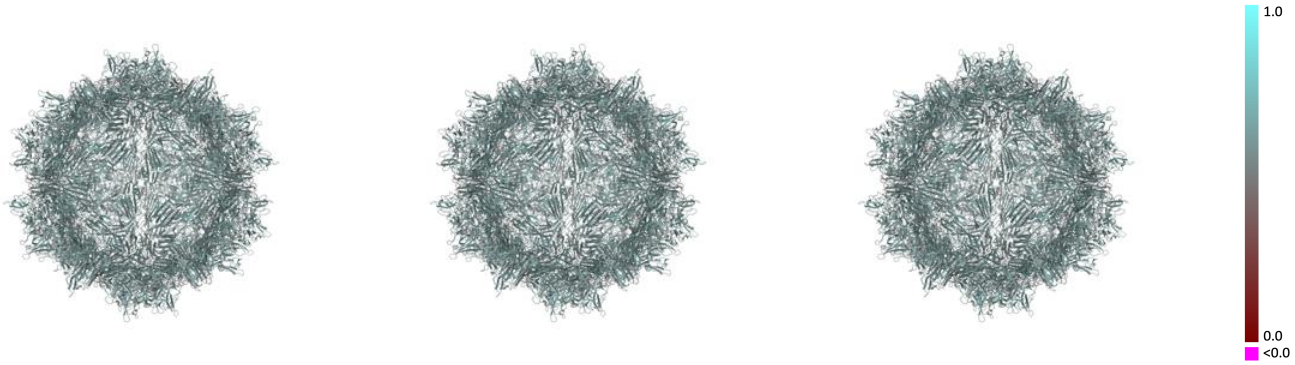
Y



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.

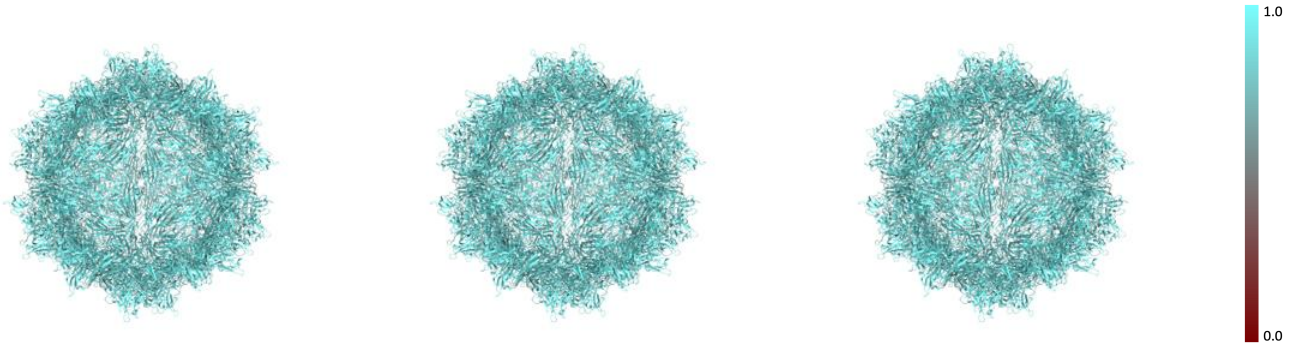
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

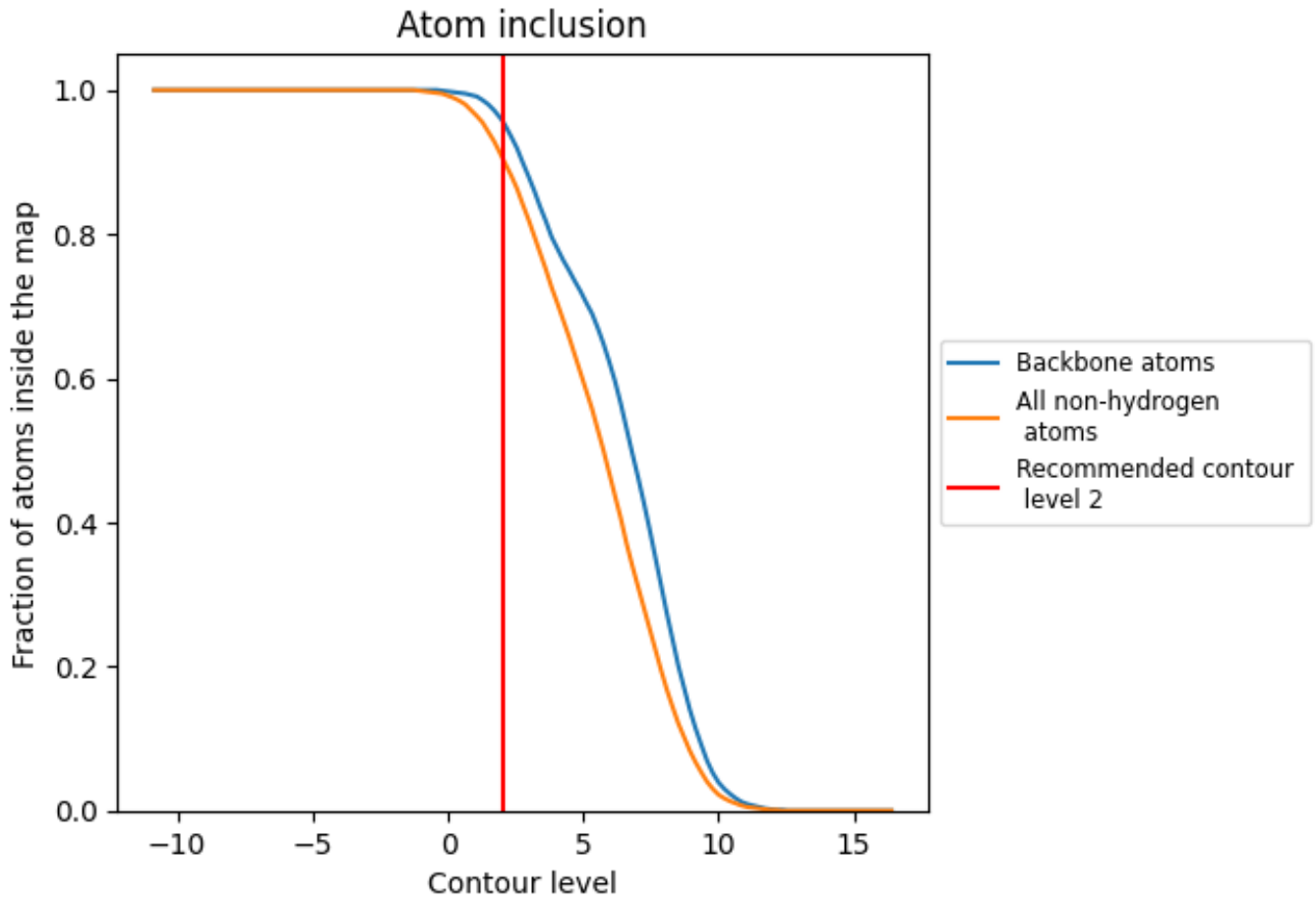
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.9070	0.5720
1	0.9080	0.5730
2	0.9080	0.5730
3	0.9070	0.5720
4	0.9080	0.5720
5	0.9090	0.5730
6	0.9100	0.5730
7	0.9100	0.5730
8	0.9070	0.5730
A	0.9040	0.5720
B	0.9080	0.5730
C	0.9070	0.5720
D	0.9090	0.5730
E	0.9060	0.5720
F	0.9050	0.5720
G	0.9060	0.5720
H	0.9090	0.5730
I	0.9070	0.5720
J	0.9080	0.5730
K	0.9080	0.5730
L	0.9080	0.5730
M	0.9060	0.5720
N	0.9090	0.5720
O	0.9070	0.5720
P	0.9090	0.5730
Q	0.9070	0.5720
R	0.9080	0.5730
S	0.9080	0.5730
T	0.9080	0.5730
U	0.9080	0.5730
V	0.9070	0.5720
W	0.9090	0.5720
X	0.9080	0.5720
Y	0.9100	0.5730
Z	0.9060	0.5720



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Continued from previous page...

Chain	Atom inclusion	Q-score
a	0.9060	0.5710
b	0.9070	0.5730
c	0.9070	0.5720
d	0.9060	0.5730
e	0.9070	0.5720
f	0.9070	0.5730
g	0.9080	0.5720
h	0.9070	0.5720
i	0.9100	0.5730
j	0.9090	0.5740
k	0.9100	0.5730
l	0.9060	0.5710
m	0.9070	0.5730
n	0.9060	0.5730
o	0.9070	0.5720
p	0.9080	0.5720
q	0.9080	0.5730
r	0.9080	0.5730
s	0.9080	0.5730
t	0.9070	0.5720
u	0.9080	0.5720
v	0.9070	0.5720
w	0.9070	0.5710
x	0.9080	0.5720
y	0.9070	0.5720
z	0.9080	0.5720