wwPDB EM Validation Summary Report

May 25, 2024 – 03:58 PM EDT

PDB ID	:	7RK9
EMDB ID	:	EMD-24495
Title	:	Cryo-EM Structure of Adeno-Associated Virus Serotype 1 with Engineered Peptide Domain PHP.B (AAV1-PHP.B)
Authors	:	Fluck, E.C.; Pumroy, R.A.; Moiseenkova-Bell, V.Y.
Deposited on	:	2021-07-22
Resolution	:	2.32 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:

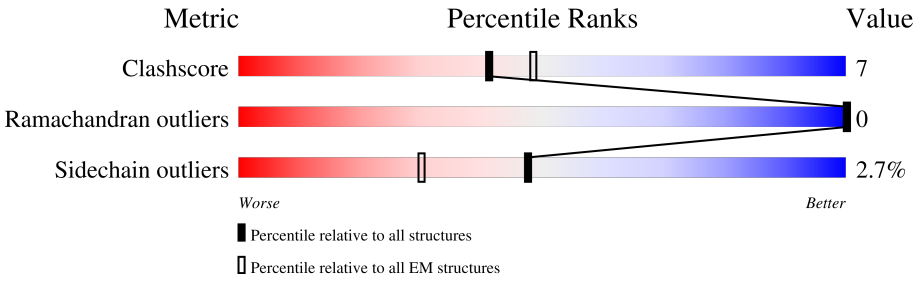
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.32 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	743	6% 56% 13% • 30%
1	AA	743	6% 56% 14% • 30%
1	AB	743	6% 56% 14% • 30%
1	B	743	6% 56% 14% • 30%
1	BA	743	6% 56% 14% • 30%
1	BB	743	6% 56% 14% • 30%
1	C	743	6% 56% 14% • 30%
1	CA	743	6% 56% 14% • 30%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	CB	743	6% 56% 14% 30%
1	D	743	6% 56% 14% 30%
1	DA	743	6% 56% 14% 30%
1	DB	743	6% 56% 14% 30%
1	E	743	6% 56% 14% 30%
1	EA	743	6% 56% 13% 30%
1	EB	743	6% 56% 14% 30%
1	F	743	6% 56% 14% 30%
1	FA	743	6% 56% 14% 30%
1	FB	743	6% 56% 14% 30%
1	G	743	6% 56% 14% 30%
1	GA	743	6% 56% 14% 30%
1	GB	743	6% 56% 14% 30%
1	H	743	6% 56% 14% 30%
1	HA	743	6% 56% 14% 30%
1	HB	743	6% 56% 13% 30%
1	I	743	6% 56% 14% 30%
1	IA	743	6% 56% 13% 30%
1	IB	743	6% 56% 14% 30%
1	J	743	6% 56% 13% 30%
1	JA	743	6% 57% 13% 30%
1	K	743	6% 56% 14% 30%
1	KA	743	6% 56% 14% 30%
1	L	743	6% 56% 14% 30%
1	LA	743	6% 56% 14% 30%

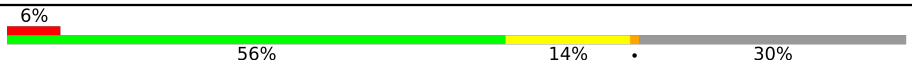
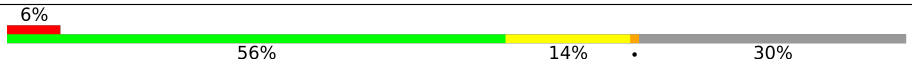
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	M	743	6% 56% 14% 30%
1	MA	743	6% 56% 13% 30%
1	N	743	6% 56% 13% 30%
1	NA	743	6% 56% 14% 30%
1	O	743	6% 56% 14% 30%
1	OA	743	6% 57% 13% 30%
1	P	743	6% 56% 14% 30%
1	PA	743	6% 56% 13% 30%
1	Q	743	6% 56% 14% 30%
1	QA	743	6% 56% 14% 30%
1	R	743	6% 56% 14% 30%
1	RA	743	6% 56% 14% 30%
1	S	743	6% 56% 14% 30%
1	SA	743	6% 56% 14% 30%
1	T	743	6% 56% 13% 30%
1	TA	743	6% 56% 13% 30%
1	UA	743	6% 56% 13% 30%
1	V	743	6% 56% 14% 30%
1	VA	743	6% 56% 14% 30%
1	W	743	6% 56% 14% 30%
1	WA	743	6% 56% 14% 30%
1	X	743	6% 56% 13% 30%
1	XA	743	6% 56% 14% 30%
1	Y	743	6% 56% 14% 30%
1	YA	743	6% 56% 14% 30%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Z	743	
1	ZA	743	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 247500 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	523	Total 4125	C 2615	N 712	O 782	S 16	0	0
1	B	523	Total 4125	C 2615	N 712	O 782	S 16	0	0
1	C	523	Total 4125	C 2615	N 712	O 782	S 16	0	0
1	D	523	Total 4125	C 2615	N 712	O 782	S 16	0	0
1	E	523	Total 4125	C 2615	N 712	O 782	S 16	0	0
1	F	523	Total 4125	C 2615	N 712	O 782	S 16	0	0
1	G	523	Total 4125	C 2615	N 712	O 782	S 16	0	0
1	H	523	Total 4125	C 2615	N 712	O 782	S 16	0	0
1	I	523	Total 4125	C 2615	N 712	O 782	S 16	0	0
1	J	523	Total 4125	C 2615	N 712	O 782	S 16	0	0
1	K	523	Total 4125	C 2615	N 712	O 782	S 16	0	0
1	L	523	Total 4125	C 2615	N 712	O 782	S 16	0	0
1	M	523	Total 4125	C 2615	N 712	O 782	S 16	0	0
1	N	523	Total 4125	C 2615	N 712	O 782	S 16	0	0
1	O	523	Total 4125	C 2615	N 712	O 782	S 16	0	0
1	P	523	Total 4125	C 2615	N 712	O 782	S 16	0	0
1	Q	523	Total 4125	C 2615	N 712	O 782	S 16	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	S	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	T	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	V	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	W	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	X	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	Y	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	Z	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	AA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	BA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	CA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	DA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	EA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	FA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	GA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	HA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	IA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	JA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	KA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	LA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	MA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	NA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	OA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	PA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	QA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	RA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	SA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	TA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	UA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	VA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	WA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	XA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	YA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	ZA	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	AB	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	BB	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	CB	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	DB	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	EB	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	FB	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	GB	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		
1	HB	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	IB	523	Total	C	N	O	S	0	0
			4125	2615	712	782	16		

There are 420 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	589	THR	-	insertion	UNP Q9WBP8
A	590	LEU	-	insertion	UNP Q9WBP8
A	591	ALA	-	insertion	UNP Q9WBP8
A	592	VAL	-	insertion	UNP Q9WBP8
A	593	PRO	-	insertion	UNP Q9WBP8
A	594	PHE	-	insertion	UNP Q9WBP8
A	595	LYS	-	insertion	UNP Q9WBP8
B	589	THR	-	insertion	UNP Q9WBP8
B	590	LEU	-	insertion	UNP Q9WBP8
B	591	ALA	-	insertion	UNP Q9WBP8
B	592	VAL	-	insertion	UNP Q9WBP8
B	593	PRO	-	insertion	UNP Q9WBP8
B	594	PHE	-	insertion	UNP Q9WBP8
B	595	LYS	-	insertion	UNP Q9WBP8
C	589	THR	-	insertion	UNP Q9WBP8
C	590	LEU	-	insertion	UNP Q9WBP8
C	591	ALA	-	insertion	UNP Q9WBP8
C	592	VAL	-	insertion	UNP Q9WBP8
C	593	PRO	-	insertion	UNP Q9WBP8
C	594	PHE	-	insertion	UNP Q9WBP8
C	595	LYS	-	insertion	UNP Q9WBP8
D	589	THR	-	insertion	UNP Q9WBP8
D	590	LEU	-	insertion	UNP Q9WBP8
D	591	ALA	-	insertion	UNP Q9WBP8
D	592	VAL	-	insertion	UNP Q9WBP8
D	593	PRO	-	insertion	UNP Q9WBP8
D	594	PHE	-	insertion	UNP Q9WBP8
D	595	LYS	-	insertion	UNP Q9WBP8
E	589	THR	-	insertion	UNP Q9WBP8
E	590	LEU	-	insertion	UNP Q9WBP8
E	591	ALA	-	insertion	UNP Q9WBP8
E	592	VAL	-	insertion	UNP Q9WBP8
E	593	PRO	-	insertion	UNP Q9WBP8
E	594	PHE	-	insertion	UNP Q9WBP8
E	595	LYS	-	insertion	UNP Q9WBP8
F	589	THR	-	insertion	UNP Q9WBP8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	590	LEU	-	insertion	UNP Q9WBP8
F	591	ALA	-	insertion	UNP Q9WBP8
F	592	VAL	-	insertion	UNP Q9WBP8
F	593	PRO	-	insertion	UNP Q9WBP8
F	594	PHE	-	insertion	UNP Q9WBP8
F	595	LYS	-	insertion	UNP Q9WBP8
G	589	THR	-	insertion	UNP Q9WBP8
G	590	LEU	-	insertion	UNP Q9WBP8
G	591	ALA	-	insertion	UNP Q9WBP8
G	592	VAL	-	insertion	UNP Q9WBP8
G	593	PRO	-	insertion	UNP Q9WBP8
G	594	PHE	-	insertion	UNP Q9WBP8
G	595	LYS	-	insertion	UNP Q9WBP8
H	589	THR	-	insertion	UNP Q9WBP8
H	590	LEU	-	insertion	UNP Q9WBP8
H	591	ALA	-	insertion	UNP Q9WBP8
H	592	VAL	-	insertion	UNP Q9WBP8
H	593	PRO	-	insertion	UNP Q9WBP8
H	594	PHE	-	insertion	UNP Q9WBP8
H	595	LYS	-	insertion	UNP Q9WBP8
I	589	THR	-	insertion	UNP Q9WBP8
I	590	LEU	-	insertion	UNP Q9WBP8
I	591	ALA	-	insertion	UNP Q9WBP8
I	592	VAL	-	insertion	UNP Q9WBP8
I	593	PRO	-	insertion	UNP Q9WBP8
I	594	PHE	-	insertion	UNP Q9WBP8
I	595	LYS	-	insertion	UNP Q9WBP8
J	589	THR	-	insertion	UNP Q9WBP8
J	590	LEU	-	insertion	UNP Q9WBP8
J	591	ALA	-	insertion	UNP Q9WBP8
J	592	VAL	-	insertion	UNP Q9WBP8
J	593	PRO	-	insertion	UNP Q9WBP8
J	594	PHE	-	insertion	UNP Q9WBP8
J	595	LYS	-	insertion	UNP Q9WBP8
K	589	THR	-	insertion	UNP Q9WBP8
K	590	LEU	-	insertion	UNP Q9WBP8
K	591	ALA	-	insertion	UNP Q9WBP8
K	592	VAL	-	insertion	UNP Q9WBP8
K	593	PRO	-	insertion	UNP Q9WBP8
K	594	PHE	-	insertion	UNP Q9WBP8
K	595	LYS	-	insertion	UNP Q9WBP8
L	589	THR	-	insertion	UNP Q9WBP8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	590	LEU	-	insertion	UNP Q9WBP8
L	591	ALA	-	insertion	UNP Q9WBP8
L	592	VAL	-	insertion	UNP Q9WBP8
L	593	PRO	-	insertion	UNP Q9WBP8
L	594	PHE	-	insertion	UNP Q9WBP8
L	595	LYS	-	insertion	UNP Q9WBP8
M	589	THR	-	insertion	UNP Q9WBP8
M	590	LEU	-	insertion	UNP Q9WBP8
M	591	ALA	-	insertion	UNP Q9WBP8
M	592	VAL	-	insertion	UNP Q9WBP8
M	593	PRO	-	insertion	UNP Q9WBP8
M	594	PHE	-	insertion	UNP Q9WBP8
M	595	LYS	-	insertion	UNP Q9WBP8
N	589	THR	-	insertion	UNP Q9WBP8
N	590	LEU	-	insertion	UNP Q9WBP8
N	591	ALA	-	insertion	UNP Q9WBP8
N	592	VAL	-	insertion	UNP Q9WBP8
N	593	PRO	-	insertion	UNP Q9WBP8
N	594	PHE	-	insertion	UNP Q9WBP8
N	595	LYS	-	insertion	UNP Q9WBP8
O	589	THR	-	insertion	UNP Q9WBP8
O	590	LEU	-	insertion	UNP Q9WBP8
O	591	ALA	-	insertion	UNP Q9WBP8
O	592	VAL	-	insertion	UNP Q9WBP8
O	593	PRO	-	insertion	UNP Q9WBP8
O	594	PHE	-	insertion	UNP Q9WBP8
O	595	LYS	-	insertion	UNP Q9WBP8
P	589	THR	-	insertion	UNP Q9WBP8
P	590	LEU	-	insertion	UNP Q9WBP8
P	591	ALA	-	insertion	UNP Q9WBP8
P	592	VAL	-	insertion	UNP Q9WBP8
P	593	PRO	-	insertion	UNP Q9WBP8
P	594	PHE	-	insertion	UNP Q9WBP8
P	595	LYS	-	insertion	UNP Q9WBP8
Q	589	THR	-	insertion	UNP Q9WBP8
Q	590	LEU	-	insertion	UNP Q9WBP8
Q	591	ALA	-	insertion	UNP Q9WBP8
Q	592	VAL	-	insertion	UNP Q9WBP8
Q	593	PRO	-	insertion	UNP Q9WBP8
Q	594	PHE	-	insertion	UNP Q9WBP8
Q	595	LYS	-	insertion	UNP Q9WBP8
R	589	THR	-	insertion	UNP Q9WBP8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	590	LEU	-	insertion	UNP Q9WBP8
R	591	ALA	-	insertion	UNP Q9WBP8
R	592	VAL	-	insertion	UNP Q9WBP8
R	593	PRO	-	insertion	UNP Q9WBP8
R	594	PHE	-	insertion	UNP Q9WBP8
R	595	LYS	-	insertion	UNP Q9WBP8
S	589	THR	-	insertion	UNP Q9WBP8
S	590	LEU	-	insertion	UNP Q9WBP8
S	591	ALA	-	insertion	UNP Q9WBP8
S	592	VAL	-	insertion	UNP Q9WBP8
S	593	PRO	-	insertion	UNP Q9WBP8
S	594	PHE	-	insertion	UNP Q9WBP8
S	595	LYS	-	insertion	UNP Q9WBP8
T	589	THR	-	insertion	UNP Q9WBP8
T	590	LEU	-	insertion	UNP Q9WBP8
T	591	ALA	-	insertion	UNP Q9WBP8
T	592	VAL	-	insertion	UNP Q9WBP8
T	593	PRO	-	insertion	UNP Q9WBP8
T	594	PHE	-	insertion	UNP Q9WBP8
T	595	LYS	-	insertion	UNP Q9WBP8
V	589	THR	-	insertion	UNP Q9WBP8
V	590	LEU	-	insertion	UNP Q9WBP8
V	591	ALA	-	insertion	UNP Q9WBP8
V	592	VAL	-	insertion	UNP Q9WBP8
V	593	PRO	-	insertion	UNP Q9WBP8
V	594	PHE	-	insertion	UNP Q9WBP8
V	595	LYS	-	insertion	UNP Q9WBP8
W	589	THR	-	insertion	UNP Q9WBP8
W	590	LEU	-	insertion	UNP Q9WBP8
W	591	ALA	-	insertion	UNP Q9WBP8
W	592	VAL	-	insertion	UNP Q9WBP8
W	593	PRO	-	insertion	UNP Q9WBP8
W	594	PHE	-	insertion	UNP Q9WBP8
W	595	LYS	-	insertion	UNP Q9WBP8
X	589	THR	-	insertion	UNP Q9WBP8
X	590	LEU	-	insertion	UNP Q9WBP8
X	591	ALA	-	insertion	UNP Q9WBP8
X	592	VAL	-	insertion	UNP Q9WBP8
X	593	PRO	-	insertion	UNP Q9WBP8
X	594	PHE	-	insertion	UNP Q9WBP8
X	595	LYS	-	insertion	UNP Q9WBP8
Y	589	THR	-	insertion	UNP Q9WBP8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Y	590	LEU	-	insertion	UNP Q9WBP8
Y	591	ALA	-	insertion	UNP Q9WBP8
Y	592	VAL	-	insertion	UNP Q9WBP8
Y	593	PRO	-	insertion	UNP Q9WBP8
Y	594	PHE	-	insertion	UNP Q9WBP8
Y	595	LYS	-	insertion	UNP Q9WBP8
Z	589	THR	-	insertion	UNP Q9WBP8
Z	590	LEU	-	insertion	UNP Q9WBP8
Z	591	ALA	-	insertion	UNP Q9WBP8
Z	592	VAL	-	insertion	UNP Q9WBP8
Z	593	PRO	-	insertion	UNP Q9WBP8
Z	594	PHE	-	insertion	UNP Q9WBP8
Z	595	LYS	-	insertion	UNP Q9WBP8
AA	589	THR	-	insertion	UNP Q9WBP8
AA	590	LEU	-	insertion	UNP Q9WBP8
AA	591	ALA	-	insertion	UNP Q9WBP8
AA	592	VAL	-	insertion	UNP Q9WBP8
AA	593	PRO	-	insertion	UNP Q9WBP8
AA	594	PHE	-	insertion	UNP Q9WBP8
AA	595	LYS	-	insertion	UNP Q9WBP8
BA	589	THR	-	insertion	UNP Q9WBP8
BA	590	LEU	-	insertion	UNP Q9WBP8
BA	591	ALA	-	insertion	UNP Q9WBP8
BA	592	VAL	-	insertion	UNP Q9WBP8
BA	593	PRO	-	insertion	UNP Q9WBP8
BA	594	PHE	-	insertion	UNP Q9WBP8
BA	595	LYS	-	insertion	UNP Q9WBP8
CA	589	THR	-	insertion	UNP Q9WBP8
CA	590	LEU	-	insertion	UNP Q9WBP8
CA	591	ALA	-	insertion	UNP Q9WBP8
CA	592	VAL	-	insertion	UNP Q9WBP8
CA	593	PRO	-	insertion	UNP Q9WBP8
CA	594	PHE	-	insertion	UNP Q9WBP8
CA	595	LYS	-	insertion	UNP Q9WBP8
DA	589	THR	-	insertion	UNP Q9WBP8
DA	590	LEU	-	insertion	UNP Q9WBP8
DA	591	ALA	-	insertion	UNP Q9WBP8
DA	592	VAL	-	insertion	UNP Q9WBP8
DA	593	PRO	-	insertion	UNP Q9WBP8
DA	594	PHE	-	insertion	UNP Q9WBP8
DA	595	LYS	-	insertion	UNP Q9WBP8
EA	589	THR	-	insertion	UNP Q9WBP8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
EA	590	LEU	-	insertion	UNP Q9WBP8
EA	591	ALA	-	insertion	UNP Q9WBP8
EA	592	VAL	-	insertion	UNP Q9WBP8
EA	593	PRO	-	insertion	UNP Q9WBP8
EA	594	PHE	-	insertion	UNP Q9WBP8
EA	595	LYS	-	insertion	UNP Q9WBP8
FA	589	THR	-	insertion	UNP Q9WBP8
FA	590	LEU	-	insertion	UNP Q9WBP8
FA	591	ALA	-	insertion	UNP Q9WBP8
FA	592	VAL	-	insertion	UNP Q9WBP8
FA	593	PRO	-	insertion	UNP Q9WBP8
FA	594	PHE	-	insertion	UNP Q9WBP8
FA	595	LYS	-	insertion	UNP Q9WBP8
GA	589	THR	-	insertion	UNP Q9WBP8
GA	590	LEU	-	insertion	UNP Q9WBP8
GA	591	ALA	-	insertion	UNP Q9WBP8
GA	592	VAL	-	insertion	UNP Q9WBP8
GA	593	PRO	-	insertion	UNP Q9WBP8
GA	594	PHE	-	insertion	UNP Q9WBP8
GA	595	LYS	-	insertion	UNP Q9WBP8
HA	589	THR	-	insertion	UNP Q9WBP8
HA	590	LEU	-	insertion	UNP Q9WBP8
HA	591	ALA	-	insertion	UNP Q9WBP8
HA	592	VAL	-	insertion	UNP Q9WBP8
HA	593	PRO	-	insertion	UNP Q9WBP8
HA	594	PHE	-	insertion	UNP Q9WBP8
HA	595	LYS	-	insertion	UNP Q9WBP8
IA	589	THR	-	insertion	UNP Q9WBP8
IA	590	LEU	-	insertion	UNP Q9WBP8
IA	591	ALA	-	insertion	UNP Q9WBP8
IA	592	VAL	-	insertion	UNP Q9WBP8
IA	593	PRO	-	insertion	UNP Q9WBP8
IA	594	PHE	-	insertion	UNP Q9WBP8
IA	595	LYS	-	insertion	UNP Q9WBP8
JA	589	THR	-	insertion	UNP Q9WBP8
JA	590	LEU	-	insertion	UNP Q9WBP8
JA	591	ALA	-	insertion	UNP Q9WBP8
JA	592	VAL	-	insertion	UNP Q9WBP8
JA	593	PRO	-	insertion	UNP Q9WBP8
JA	594	PHE	-	insertion	UNP Q9WBP8
JA	595	LYS	-	insertion	UNP Q9WBP8
KA	589	THR	-	insertion	UNP Q9WBP8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
KA	590	LEU	-	insertion	UNP Q9WBP8
KA	591	ALA	-	insertion	UNP Q9WBP8
KA	592	VAL	-	insertion	UNP Q9WBP8
KA	593	PRO	-	insertion	UNP Q9WBP8
KA	594	PHE	-	insertion	UNP Q9WBP8
KA	595	LYS	-	insertion	UNP Q9WBP8
LA	589	THR	-	insertion	UNP Q9WBP8
LA	590	LEU	-	insertion	UNP Q9WBP8
LA	591	ALA	-	insertion	UNP Q9WBP8
LA	592	VAL	-	insertion	UNP Q9WBP8
LA	593	PRO	-	insertion	UNP Q9WBP8
LA	594	PHE	-	insertion	UNP Q9WBP8
LA	595	LYS	-	insertion	UNP Q9WBP8
MA	589	THR	-	insertion	UNP Q9WBP8
MA	590	LEU	-	insertion	UNP Q9WBP8
MA	591	ALA	-	insertion	UNP Q9WBP8
MA	592	VAL	-	insertion	UNP Q9WBP8
MA	593	PRO	-	insertion	UNP Q9WBP8
MA	594	PHE	-	insertion	UNP Q9WBP8
MA	595	LYS	-	insertion	UNP Q9WBP8
NA	589	THR	-	insertion	UNP Q9WBP8
NA	590	LEU	-	insertion	UNP Q9WBP8
NA	591	ALA	-	insertion	UNP Q9WBP8
NA	592	VAL	-	insertion	UNP Q9WBP8
NA	593	PRO	-	insertion	UNP Q9WBP8
NA	594	PHE	-	insertion	UNP Q9WBP8
NA	595	LYS	-	insertion	UNP Q9WBP8
OA	589	THR	-	insertion	UNP Q9WBP8
OA	590	LEU	-	insertion	UNP Q9WBP8
OA	591	ALA	-	insertion	UNP Q9WBP8
OA	592	VAL	-	insertion	UNP Q9WBP8
OA	593	PRO	-	insertion	UNP Q9WBP8
OA	594	PHE	-	insertion	UNP Q9WBP8
OA	595	LYS	-	insertion	UNP Q9WBP8
PA	589	THR	-	insertion	UNP Q9WBP8
PA	590	LEU	-	insertion	UNP Q9WBP8
PA	591	ALA	-	insertion	UNP Q9WBP8
PA	592	VAL	-	insertion	UNP Q9WBP8
PA	593	PRO	-	insertion	UNP Q9WBP8
PA	594	PHE	-	insertion	UNP Q9WBP8
PA	595	LYS	-	insertion	UNP Q9WBP8
QA	589	THR	-	insertion	UNP Q9WBP8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
QA	590	LEU	-	insertion	UNP Q9WBP8
QA	591	ALA	-	insertion	UNP Q9WBP8
QA	592	VAL	-	insertion	UNP Q9WBP8
QA	593	PRO	-	insertion	UNP Q9WBP8
QA	594	PHE	-	insertion	UNP Q9WBP8
QA	595	LYS	-	insertion	UNP Q9WBP8
RA	589	THR	-	insertion	UNP Q9WBP8
RA	590	LEU	-	insertion	UNP Q9WBP8
RA	591	ALA	-	insertion	UNP Q9WBP8
RA	592	VAL	-	insertion	UNP Q9WBP8
RA	593	PRO	-	insertion	UNP Q9WBP8
RA	594	PHE	-	insertion	UNP Q9WBP8
RA	595	LYS	-	insertion	UNP Q9WBP8
SA	589	THR	-	insertion	UNP Q9WBP8
SA	590	LEU	-	insertion	UNP Q9WBP8
SA	591	ALA	-	insertion	UNP Q9WBP8
SA	592	VAL	-	insertion	UNP Q9WBP8
SA	593	PRO	-	insertion	UNP Q9WBP8
SA	594	PHE	-	insertion	UNP Q9WBP8
SA	595	LYS	-	insertion	UNP Q9WBP8
TA	589	THR	-	insertion	UNP Q9WBP8
TA	590	LEU	-	insertion	UNP Q9WBP8
TA	591	ALA	-	insertion	UNP Q9WBP8
TA	592	VAL	-	insertion	UNP Q9WBP8
TA	593	PRO	-	insertion	UNP Q9WBP8
TA	594	PHE	-	insertion	UNP Q9WBP8
TA	595	LYS	-	insertion	UNP Q9WBP8
UA	589	THR	-	insertion	UNP Q9WBP8
UA	590	LEU	-	insertion	UNP Q9WBP8
UA	591	ALA	-	insertion	UNP Q9WBP8
UA	592	VAL	-	insertion	UNP Q9WBP8
UA	593	PRO	-	insertion	UNP Q9WBP8
UA	594	PHE	-	insertion	UNP Q9WBP8
UA	595	LYS	-	insertion	UNP Q9WBP8
VA	589	THR	-	insertion	UNP Q9WBP8
VA	590	LEU	-	insertion	UNP Q9WBP8
VA	591	ALA	-	insertion	UNP Q9WBP8
VA	592	VAL	-	insertion	UNP Q9WBP8
VA	593	PRO	-	insertion	UNP Q9WBP8
VA	594	PHE	-	insertion	UNP Q9WBP8
VA	595	LYS	-	insertion	UNP Q9WBP8
WA	589	THR	-	insertion	UNP Q9WBP8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
WA	590	LEU	-	insertion	UNP Q9WBP8
WA	591	ALA	-	insertion	UNP Q9WBP8
WA	592	VAL	-	insertion	UNP Q9WBP8
WA	593	PRO	-	insertion	UNP Q9WBP8
WA	594	PHE	-	insertion	UNP Q9WBP8
WA	595	LYS	-	insertion	UNP Q9WBP8
XA	589	THR	-	insertion	UNP Q9WBP8
XA	590	LEU	-	insertion	UNP Q9WBP8
XA	591	ALA	-	insertion	UNP Q9WBP8
XA	592	VAL	-	insertion	UNP Q9WBP8
XA	593	PRO	-	insertion	UNP Q9WBP8
XA	594	PHE	-	insertion	UNP Q9WBP8
XA	595	LYS	-	insertion	UNP Q9WBP8
YA	589	THR	-	insertion	UNP Q9WBP8
YA	590	LEU	-	insertion	UNP Q9WBP8
YA	591	ALA	-	insertion	UNP Q9WBP8
YA	592	VAL	-	insertion	UNP Q9WBP8
YA	593	PRO	-	insertion	UNP Q9WBP8
YA	594	PHE	-	insertion	UNP Q9WBP8
YA	595	LYS	-	insertion	UNP Q9WBP8
ZA	589	THR	-	insertion	UNP Q9WBP8
ZA	590	LEU	-	insertion	UNP Q9WBP8
ZA	591	ALA	-	insertion	UNP Q9WBP8
ZA	592	VAL	-	insertion	UNP Q9WBP8
ZA	593	PRO	-	insertion	UNP Q9WBP8
ZA	594	PHE	-	insertion	UNP Q9WBP8
ZA	595	LYS	-	insertion	UNP Q9WBP8
AB	589	THR	-	insertion	UNP Q9WBP8
AB	590	LEU	-	insertion	UNP Q9WBP8
AB	591	ALA	-	insertion	UNP Q9WBP8
AB	592	VAL	-	insertion	UNP Q9WBP8
AB	593	PRO	-	insertion	UNP Q9WBP8
AB	594	PHE	-	insertion	UNP Q9WBP8
AB	595	LYS	-	insertion	UNP Q9WBP8
BB	589	THR	-	insertion	UNP Q9WBP8
BB	590	LEU	-	insertion	UNP Q9WBP8
BB	591	ALA	-	insertion	UNP Q9WBP8
BB	592	VAL	-	insertion	UNP Q9WBP8
BB	593	PRO	-	insertion	UNP Q9WBP8
BB	594	PHE	-	insertion	UNP Q9WBP8
BB	595	LYS	-	insertion	UNP Q9WBP8
CB	589	THR	-	insertion	UNP Q9WBP8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
CB	590	LEU	-	insertion	UNP Q9WBP8
CB	591	ALA	-	insertion	UNP Q9WBP8
CB	592	VAL	-	insertion	UNP Q9WBP8
CB	593	PRO	-	insertion	UNP Q9WBP8
CB	594	PHE	-	insertion	UNP Q9WBP8
CB	595	LYS	-	insertion	UNP Q9WBP8
DB	589	THR	-	insertion	UNP Q9WBP8
DB	590	LEU	-	insertion	UNP Q9WBP8
DB	591	ALA	-	insertion	UNP Q9WBP8
DB	592	VAL	-	insertion	UNP Q9WBP8
DB	593	PRO	-	insertion	UNP Q9WBP8
DB	594	PHE	-	insertion	UNP Q9WBP8
DB	595	LYS	-	insertion	UNP Q9WBP8
EB	589	THR	-	insertion	UNP Q9WBP8
EB	590	LEU	-	insertion	UNP Q9WBP8
EB	591	ALA	-	insertion	UNP Q9WBP8
EB	592	VAL	-	insertion	UNP Q9WBP8
EB	593	PRO	-	insertion	UNP Q9WBP8
EB	594	PHE	-	insertion	UNP Q9WBP8
EB	595	LYS	-	insertion	UNP Q9WBP8
FB	589	THR	-	insertion	UNP Q9WBP8
FB	590	LEU	-	insertion	UNP Q9WBP8
FB	591	ALA	-	insertion	UNP Q9WBP8
FB	592	VAL	-	insertion	UNP Q9WBP8
FB	593	PRO	-	insertion	UNP Q9WBP8
FB	594	PHE	-	insertion	UNP Q9WBP8
FB	595	LYS	-	insertion	UNP Q9WBP8
GB	589	THR	-	insertion	UNP Q9WBP8
GB	590	LEU	-	insertion	UNP Q9WBP8
GB	591	ALA	-	insertion	UNP Q9WBP8
GB	592	VAL	-	insertion	UNP Q9WBP8
GB	593	PRO	-	insertion	UNP Q9WBP8
GB	594	PHE	-	insertion	UNP Q9WBP8
GB	595	LYS	-	insertion	UNP Q9WBP8
HB	589	THR	-	insertion	UNP Q9WBP8
HB	590	LEU	-	insertion	UNP Q9WBP8
HB	591	ALA	-	insertion	UNP Q9WBP8
HB	592	VAL	-	insertion	UNP Q9WBP8
HB	593	PRO	-	insertion	UNP Q9WBP8
HB	594	PHE	-	insertion	UNP Q9WBP8
HB	595	LYS	-	insertion	UNP Q9WBP8
IB	589	THR	-	insertion	UNP Q9WBP8

Continued on next page...

Continued from previous page...

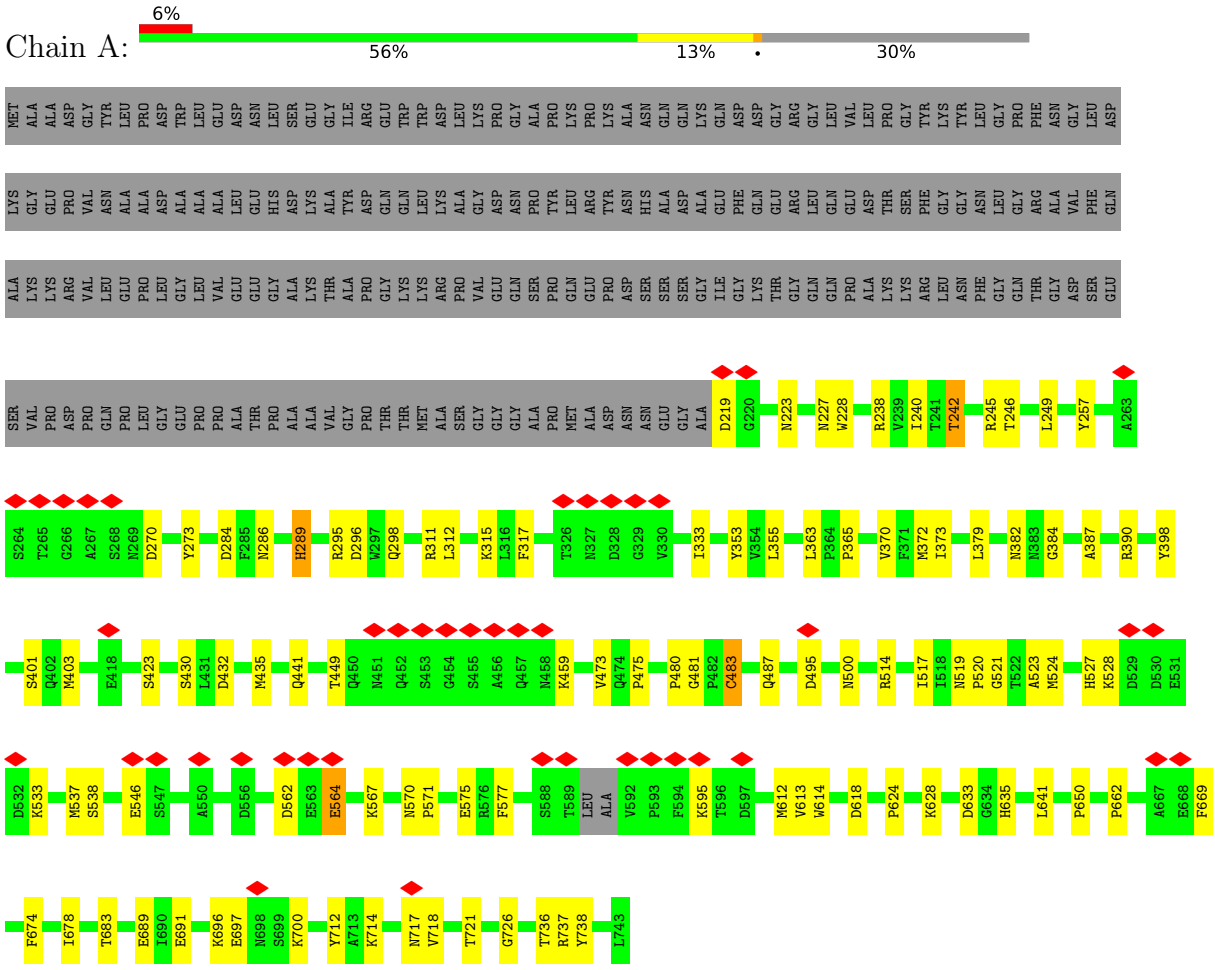
Chain	Residue	Modelled	Actual	Comment	Reference
IB	590	LEU	-	insertion	UNP Q9WBP8
IB	591	ALA	-	insertion	UNP Q9WBP8
IB	592	VAL	-	insertion	UNP Q9WBP8
IB	593	PRO	-	insertion	UNP Q9WBP8
IB	594	PHE	-	insertion	UNP Q9WBP8
IB	595	LYS	-	insertion	UNP Q9WBP8

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.

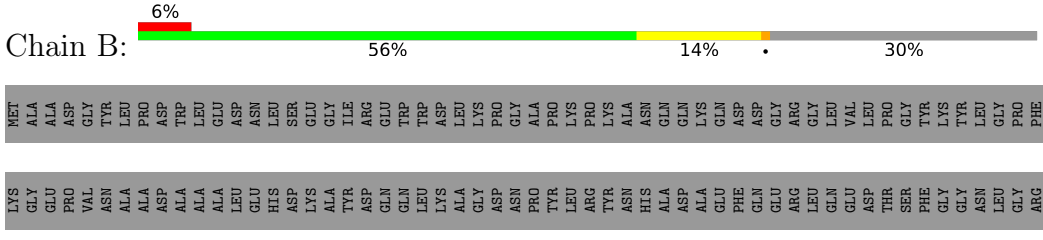
• Molecule 1: Capsid protein

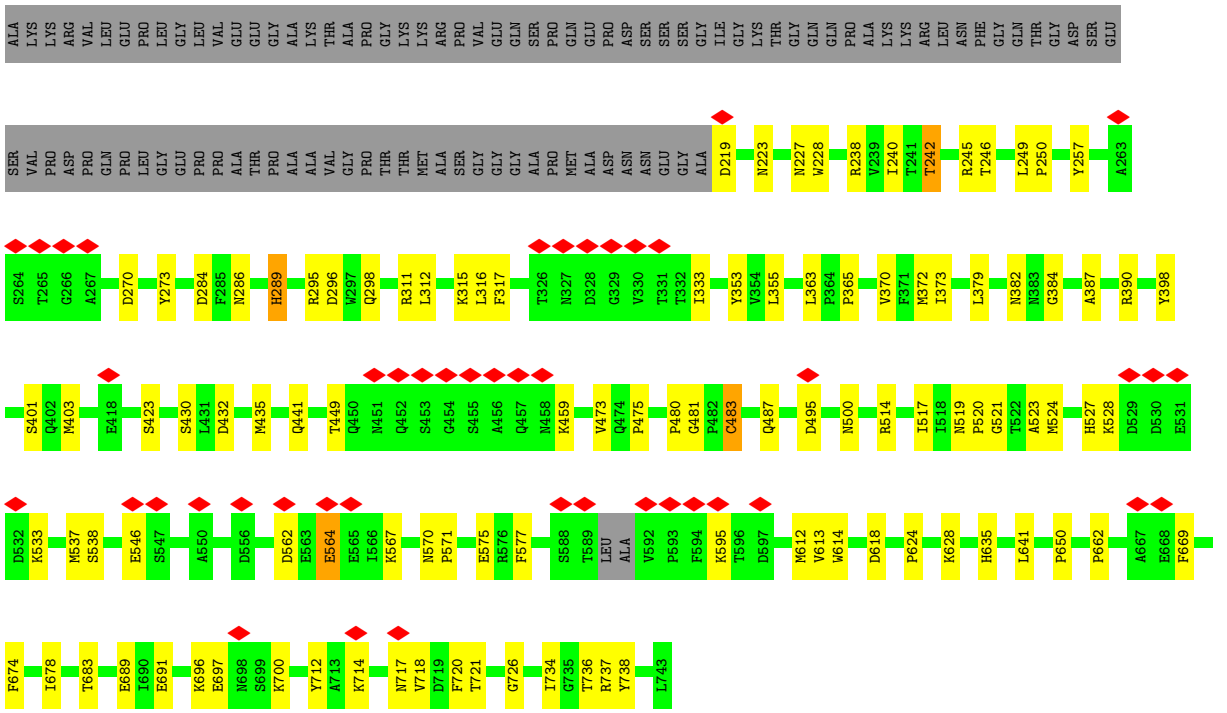
Chain A:



• Molecule 1: Capsid protein

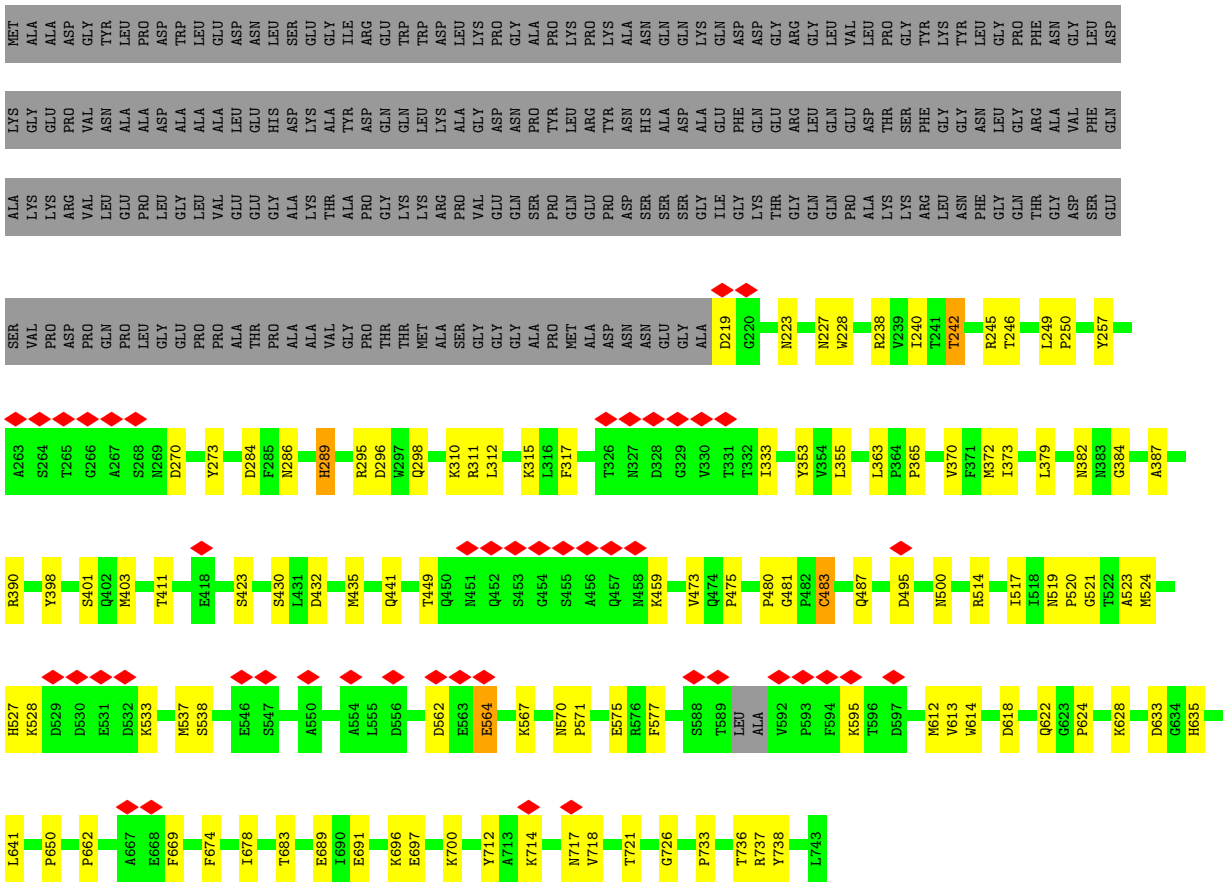
Chain B:





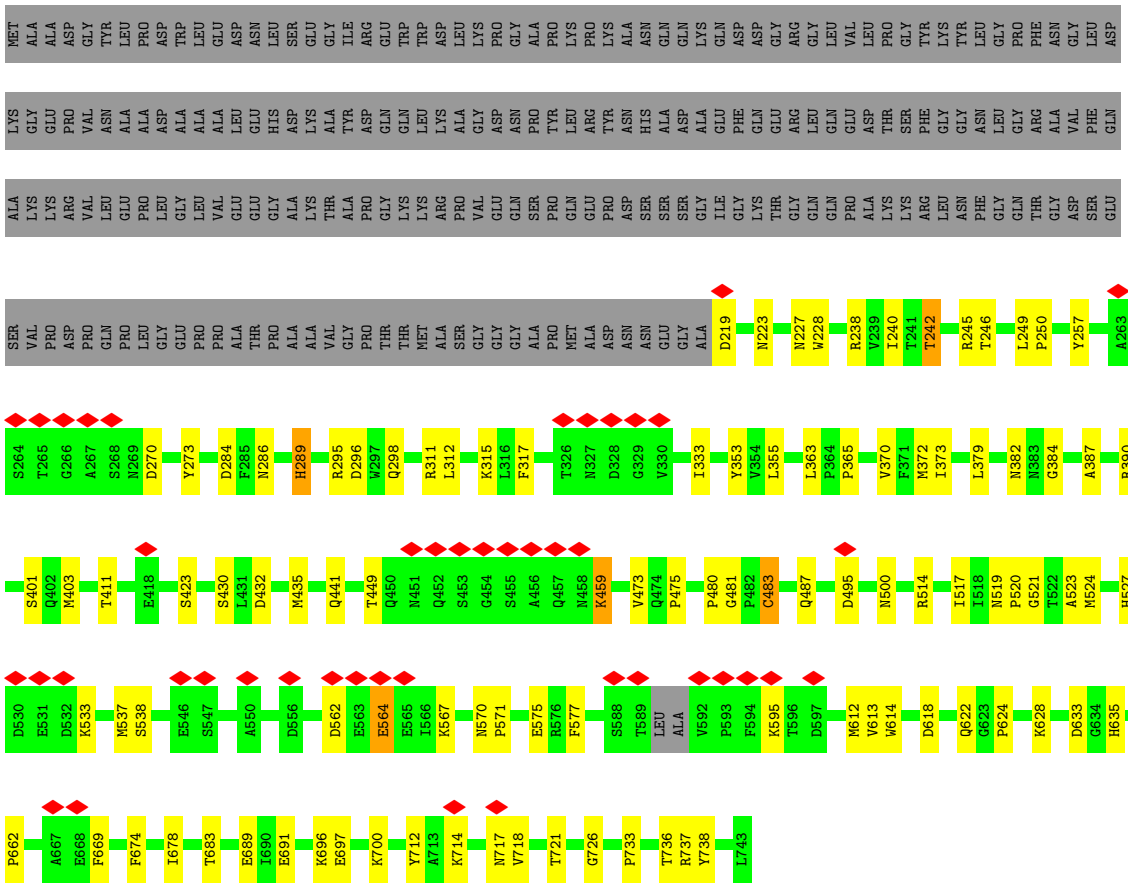
• Molecule 1: Capsid protein

Chain C:



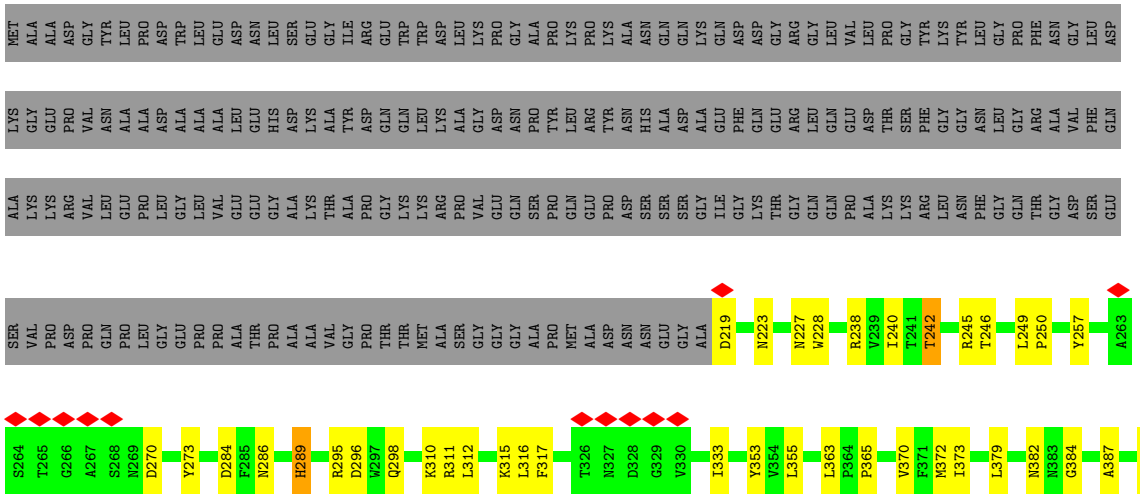
• Molecule 1: Capsid protein

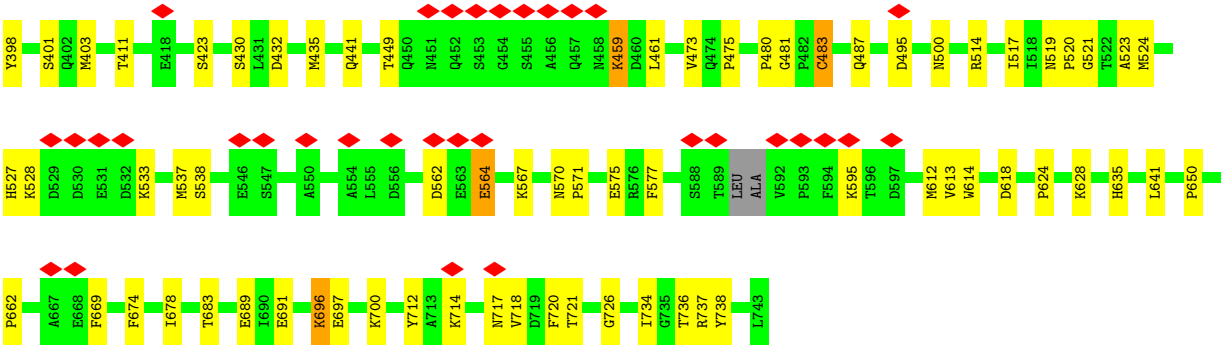
Chain D:



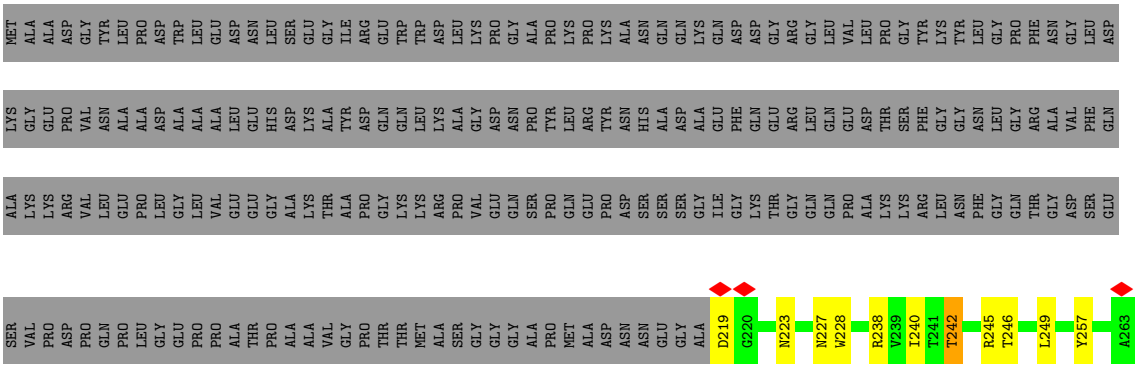
• Molecule 1: Capsid protein

Chain E:

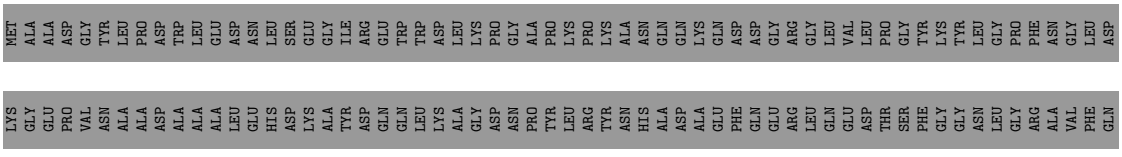


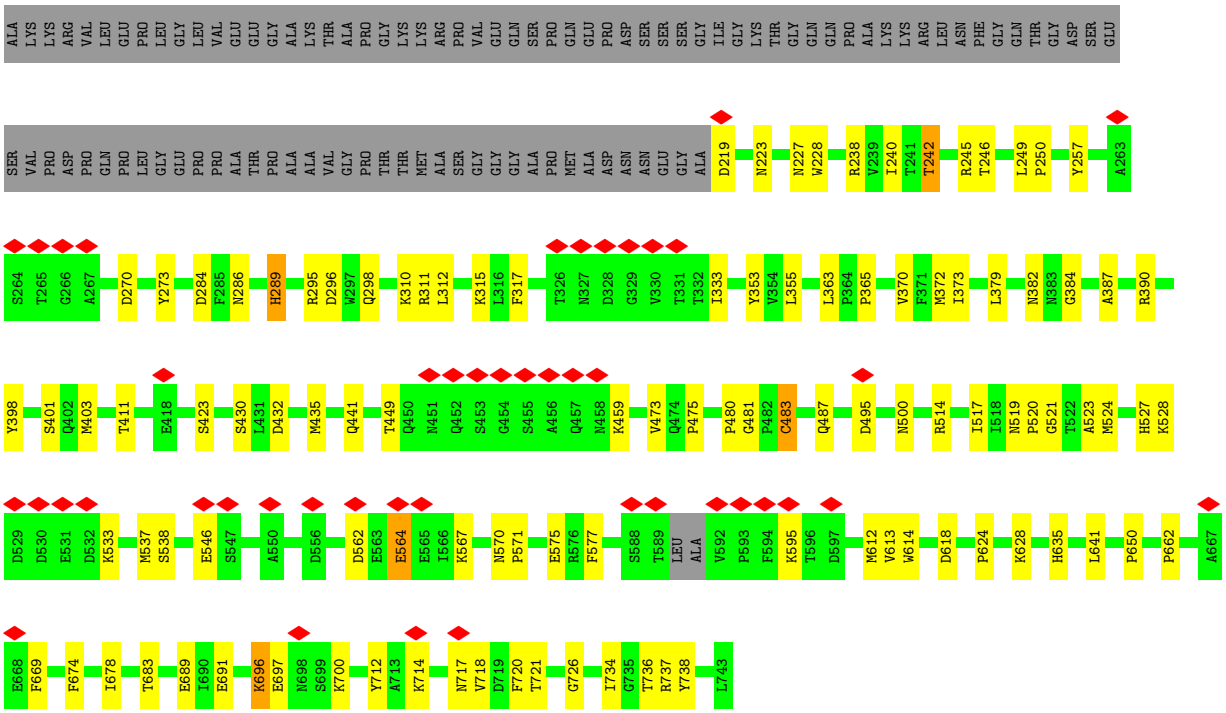


• Molecule 1: Capsid protein



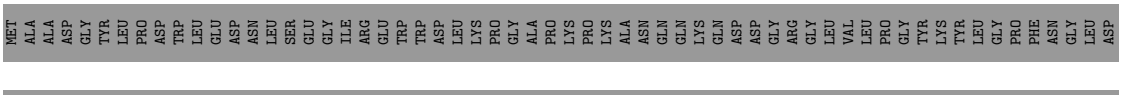
• Molecule 1: Capsid protein

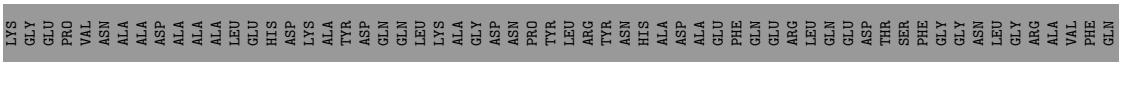


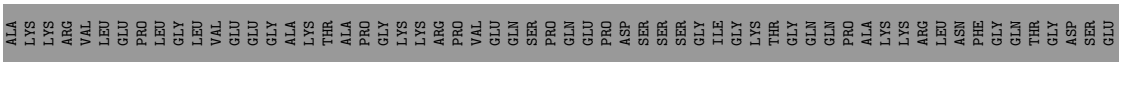


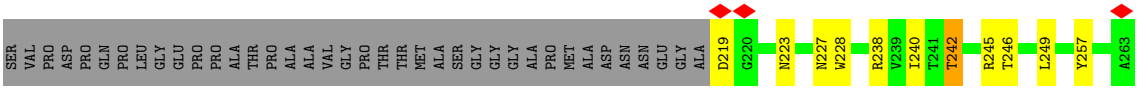
• Molecule 1: Capsid protein

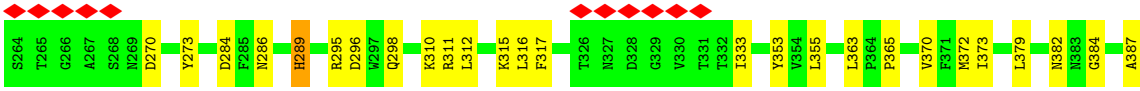
Chain H:

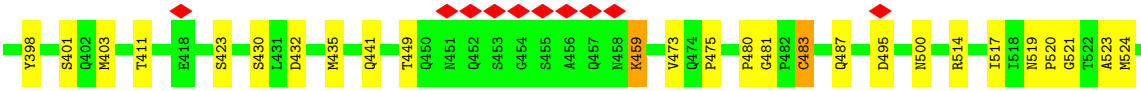


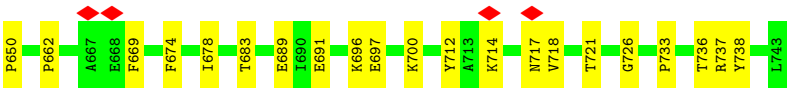






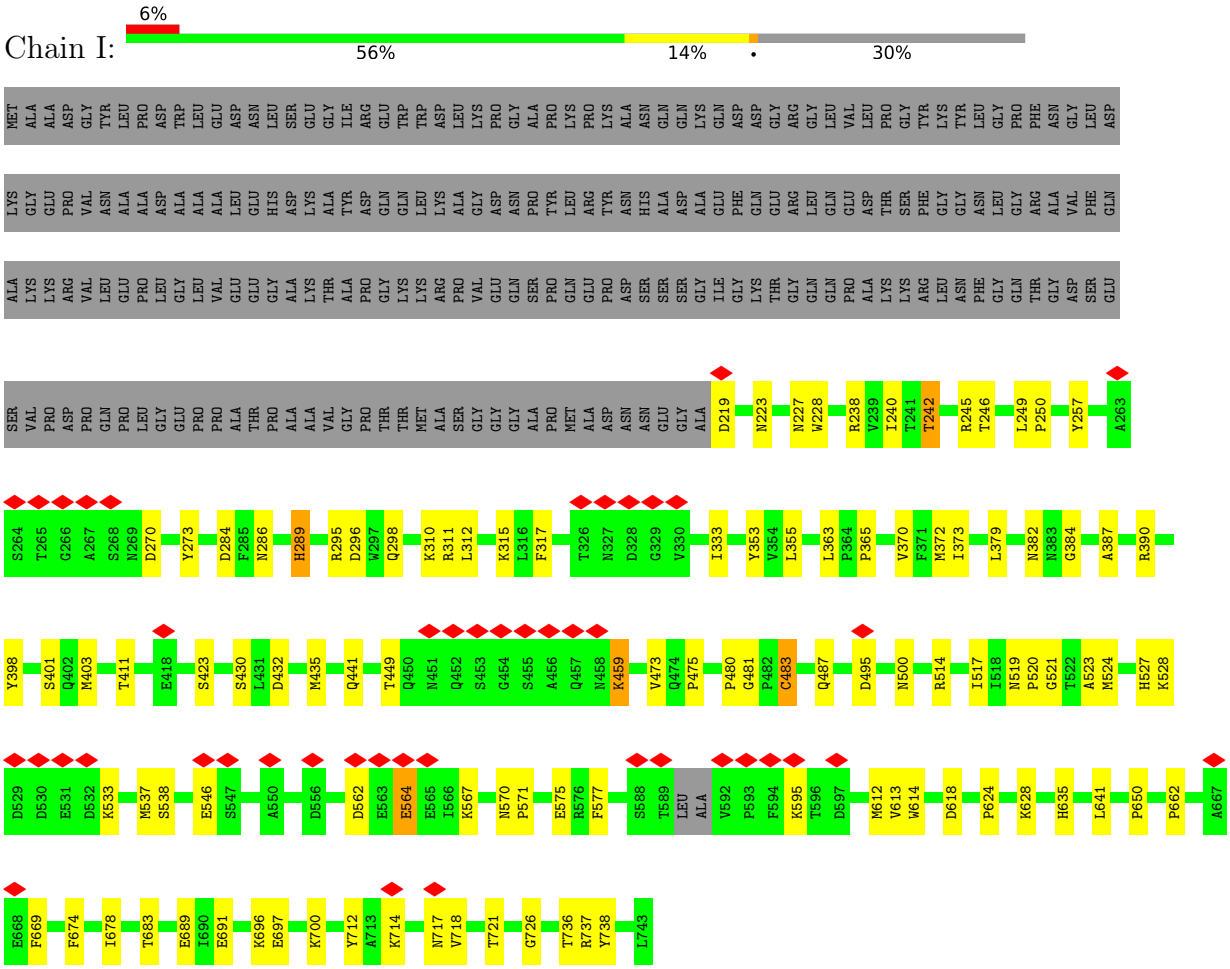






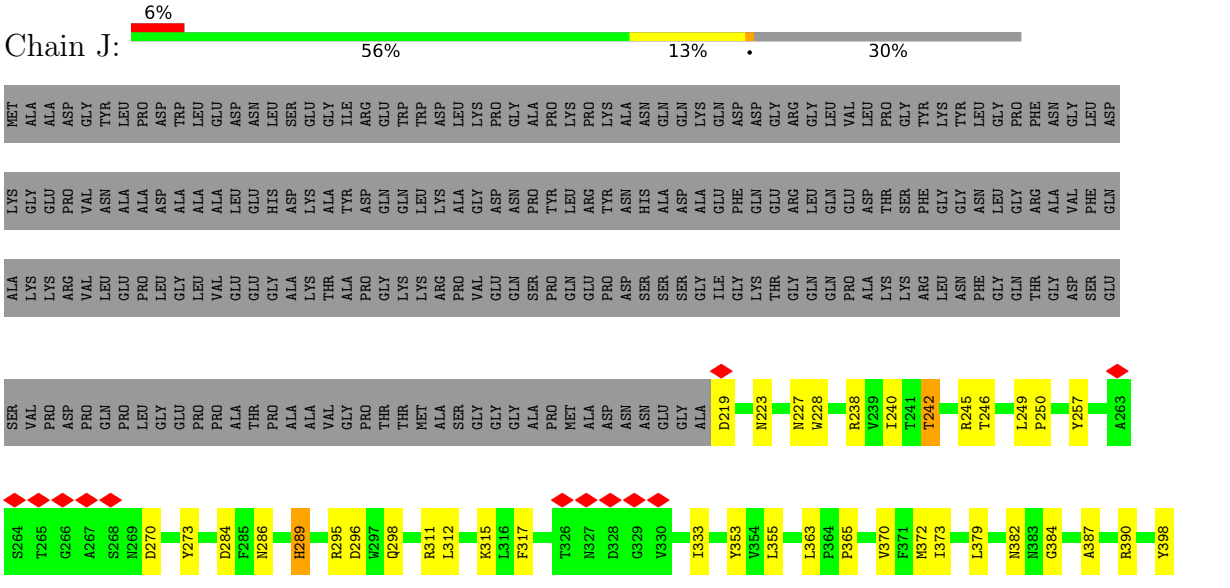
• Molecule 1: Capsid protein

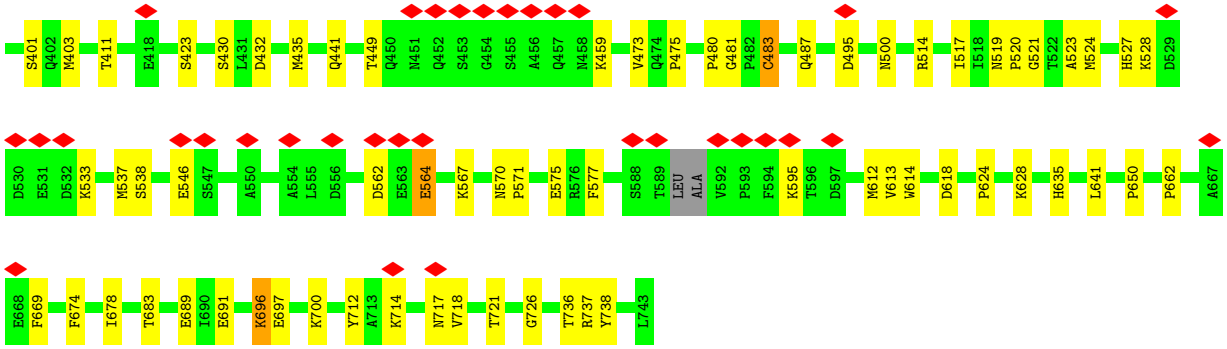
Chain I:



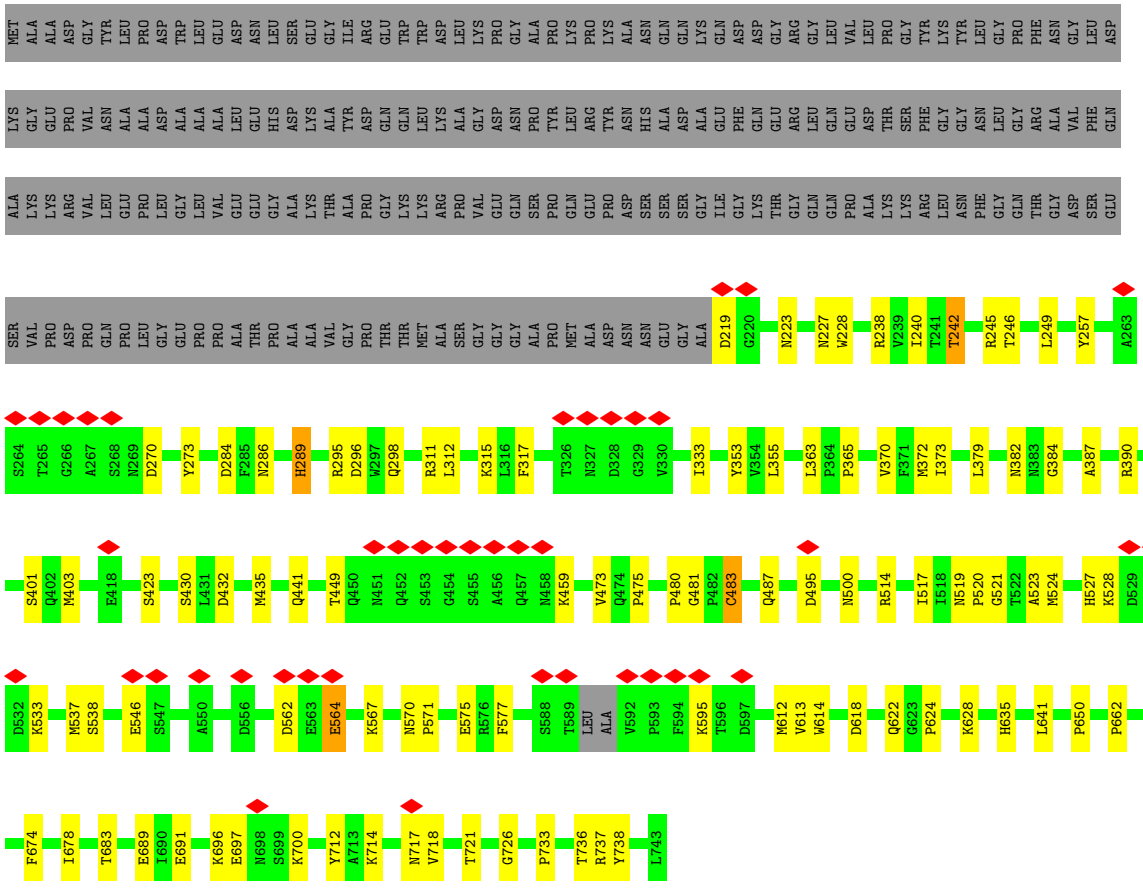
• Molecule 1: Capsid protein

Chain J:

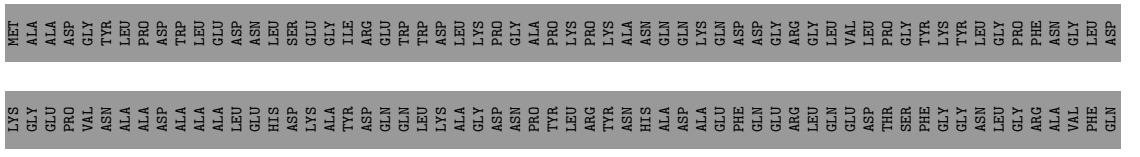


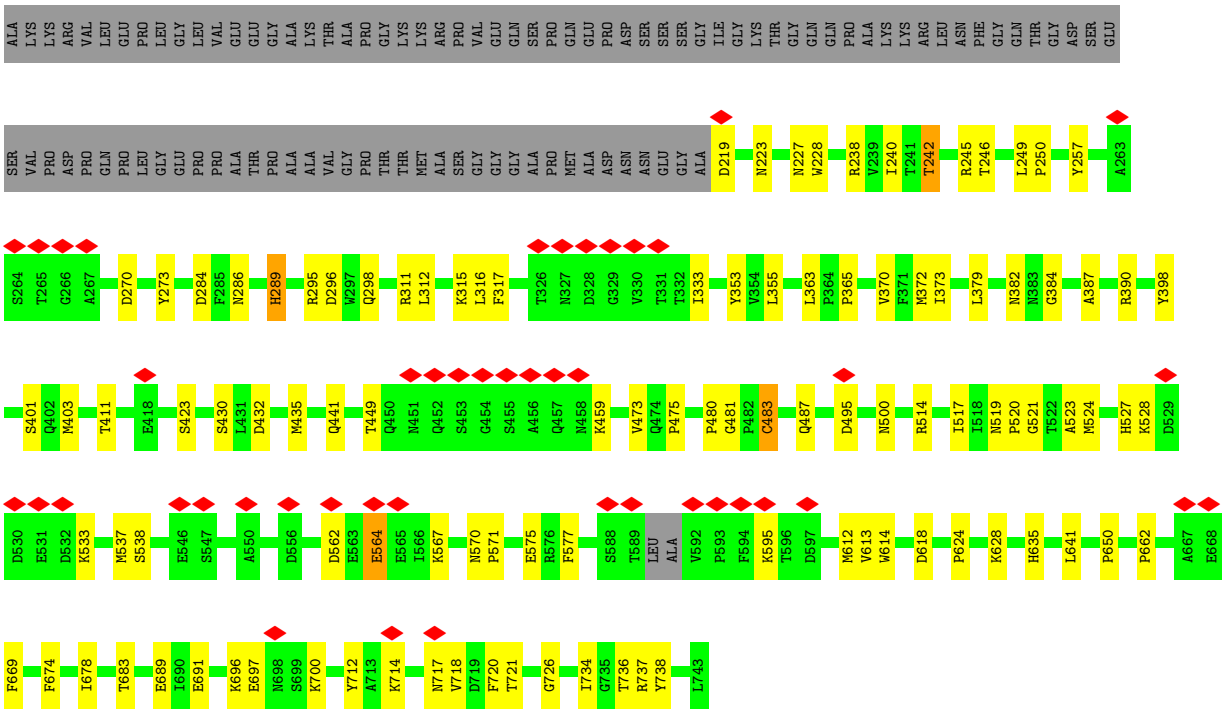


• Molecule 1: Capsid protein



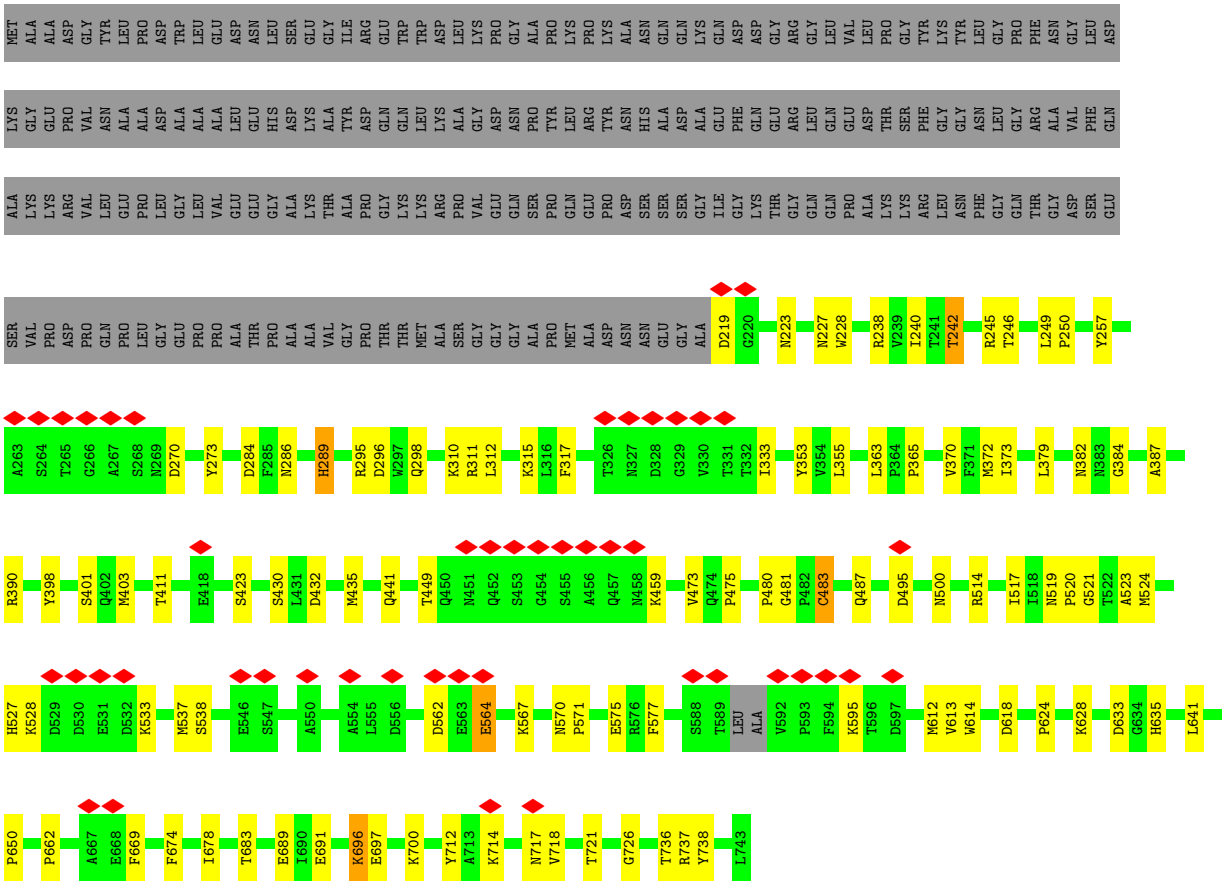
• Molecule 1: Capsid protein





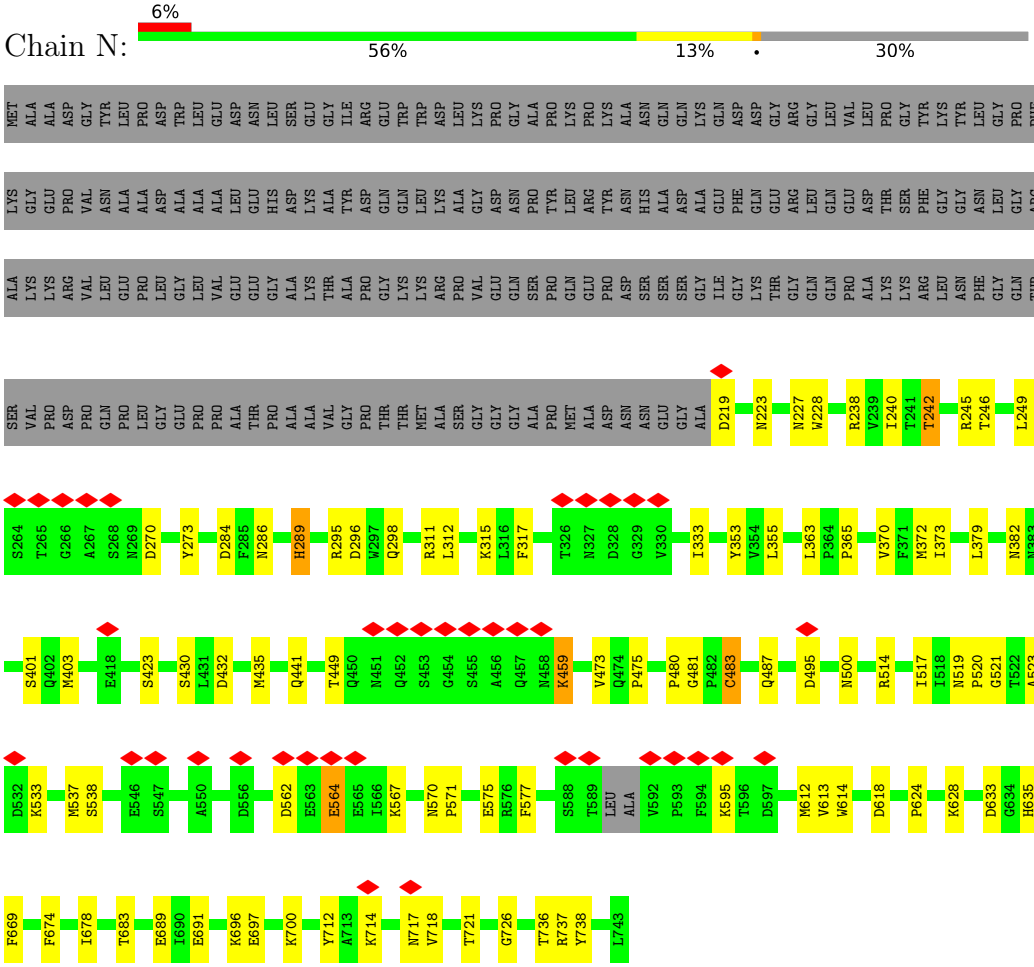
• Molecule 1: Capsid protein

Chain M:



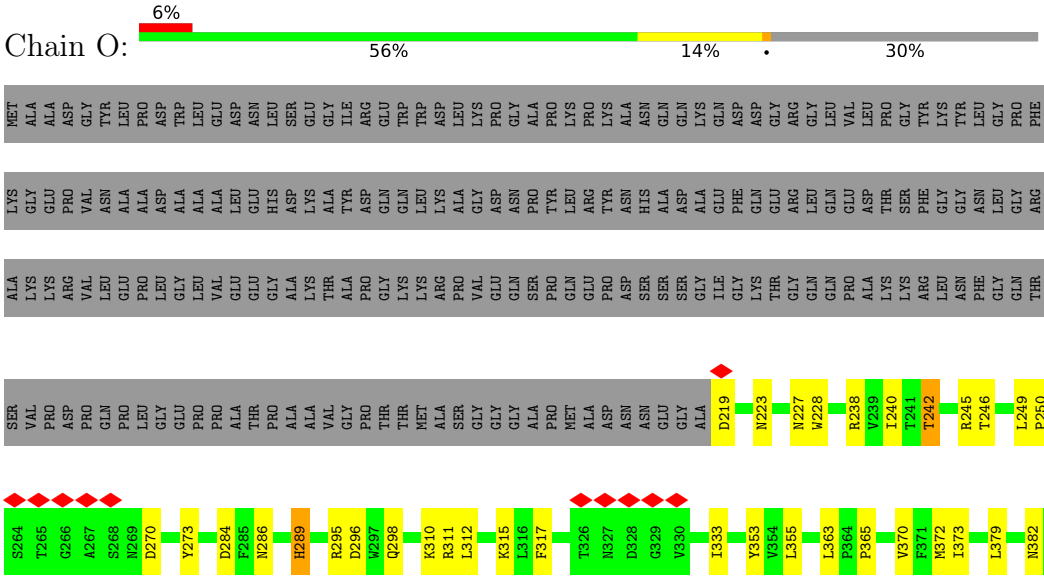
• Molecule 1: Capsid protein

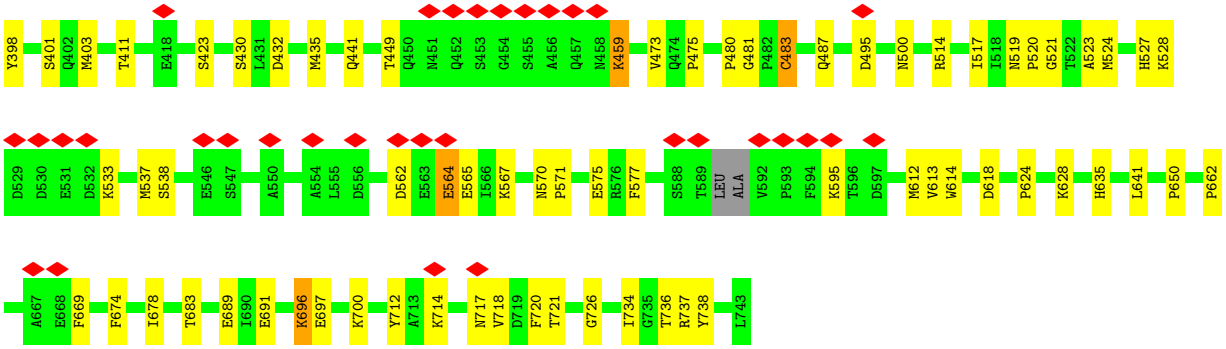
Chain N:



• Molecule 1: Capsid protein

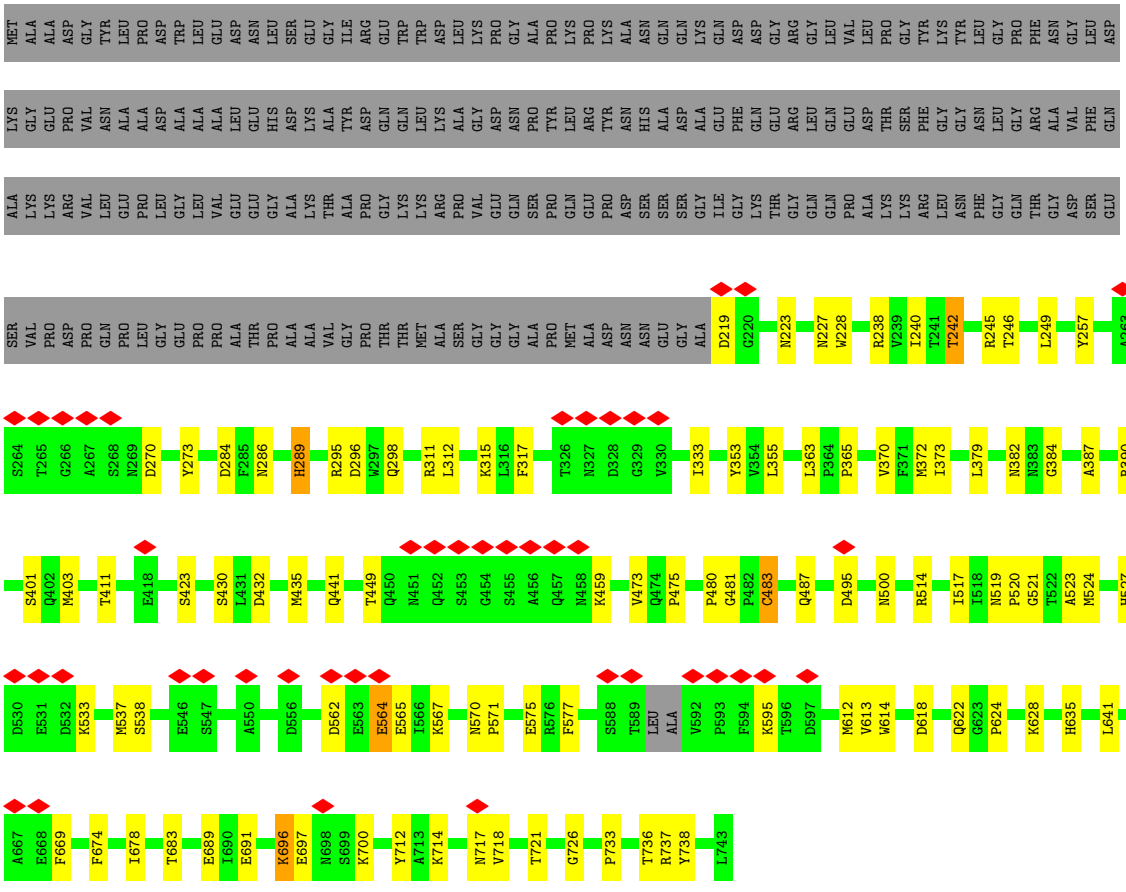
Chain O:





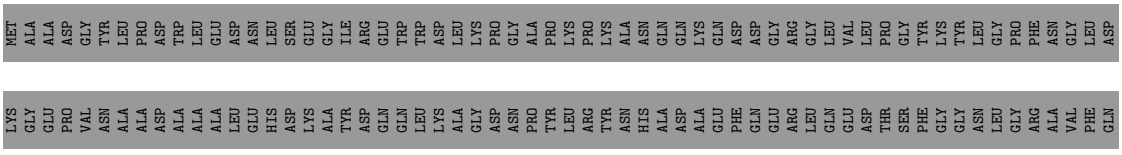
• Molecule 1: Capsid protein

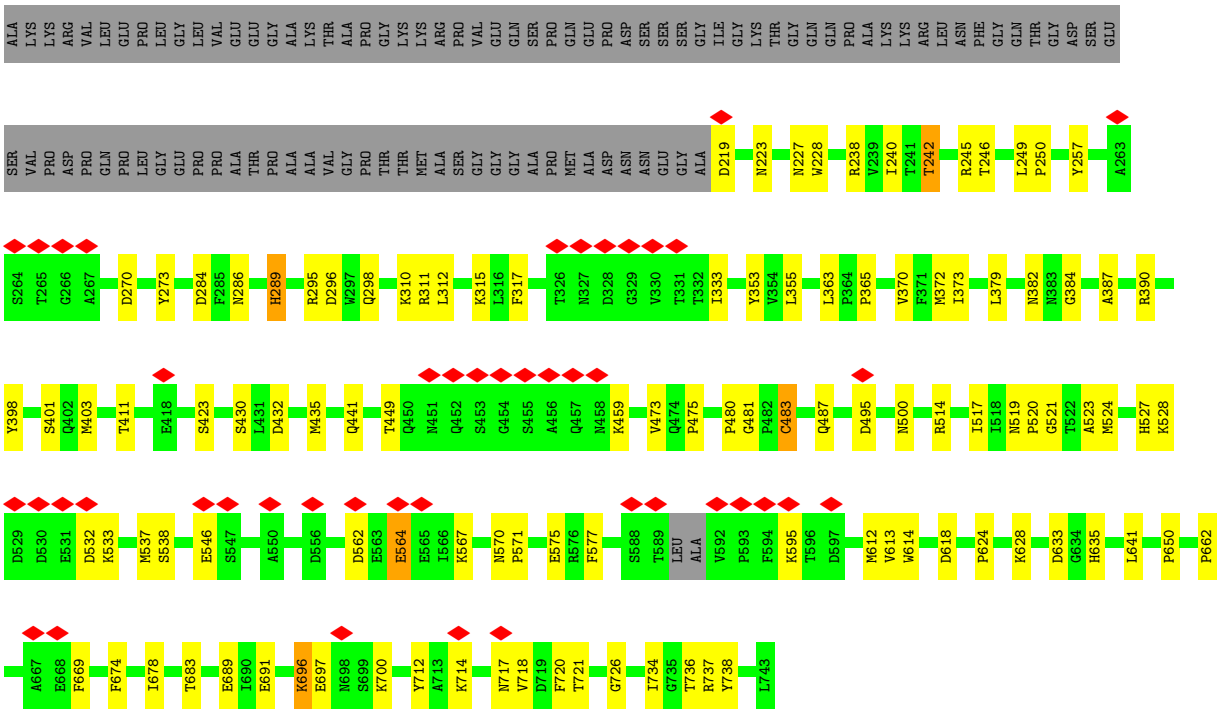
Chain P:



• Molecule 1: Capsid protein

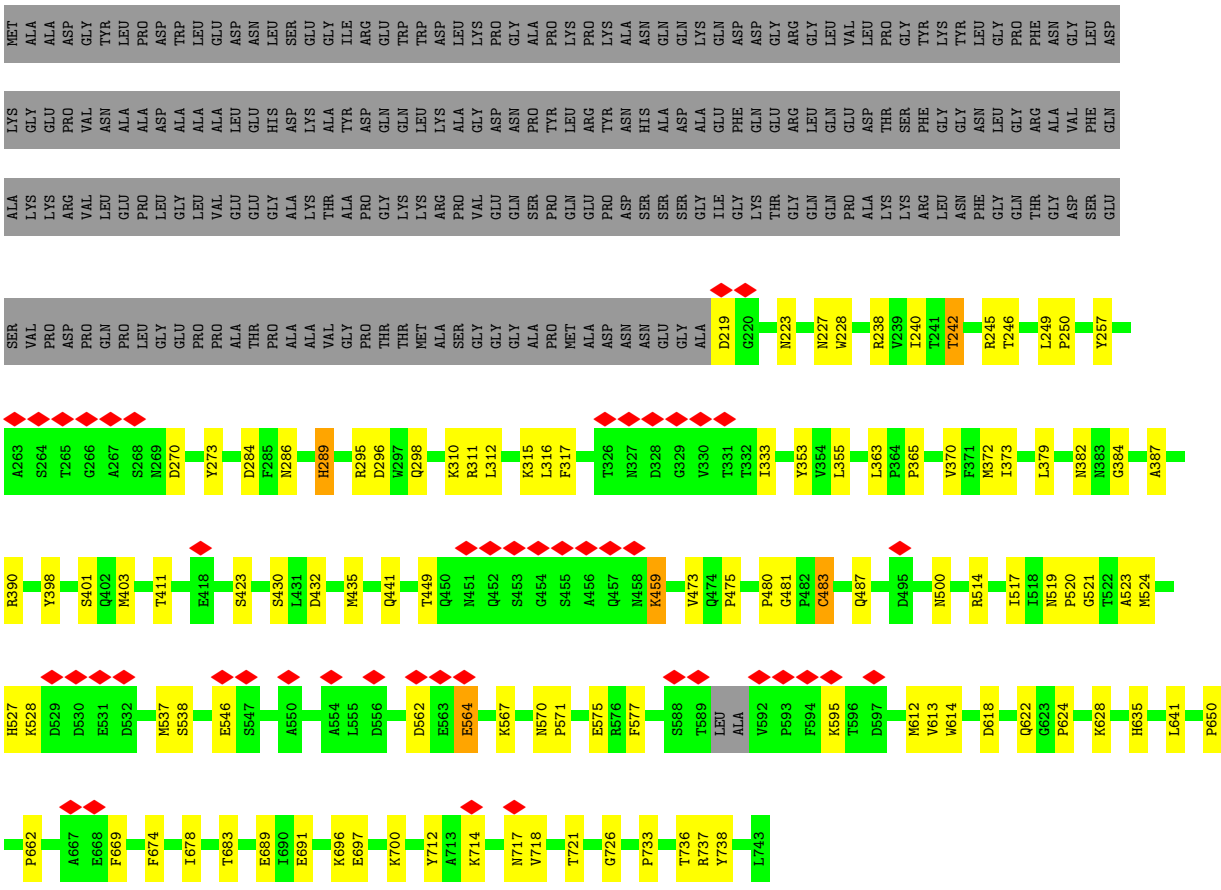
Chain Q:





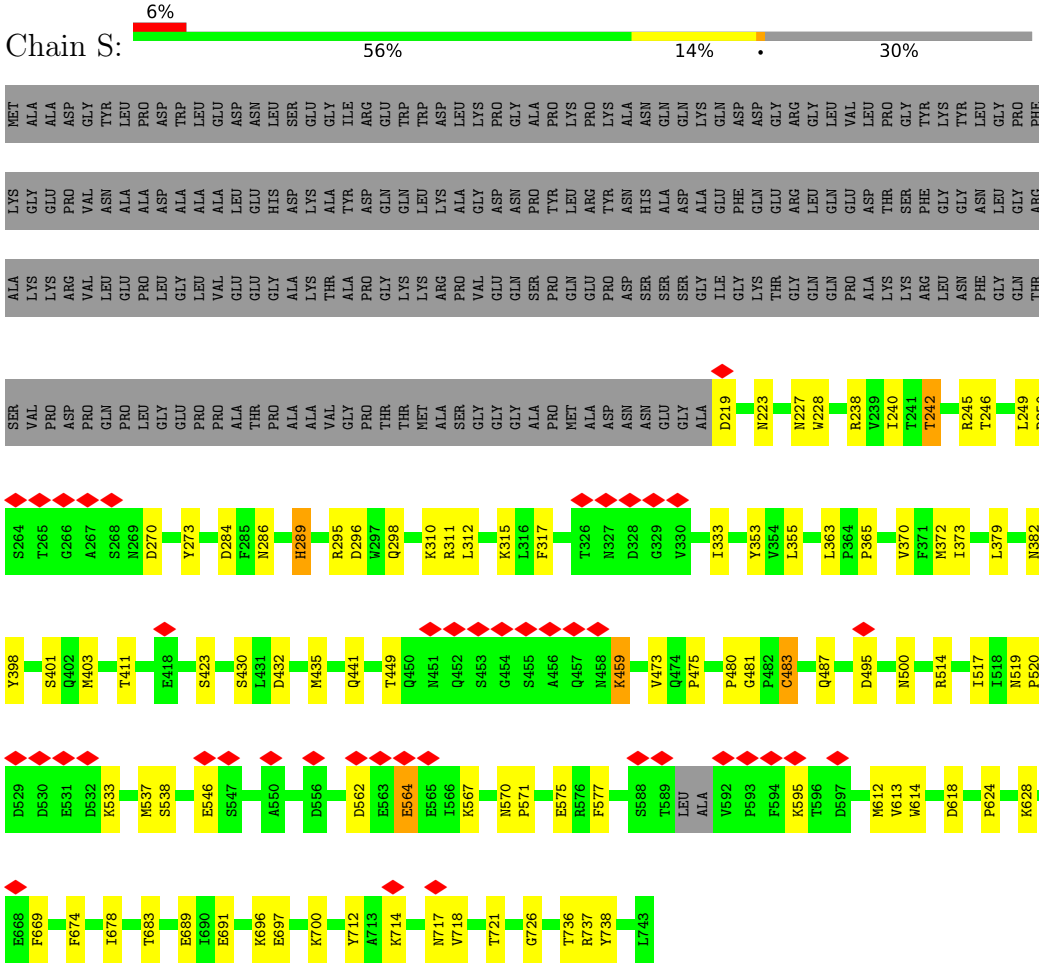
• Molecule 1: Capsid protein

Chain R:



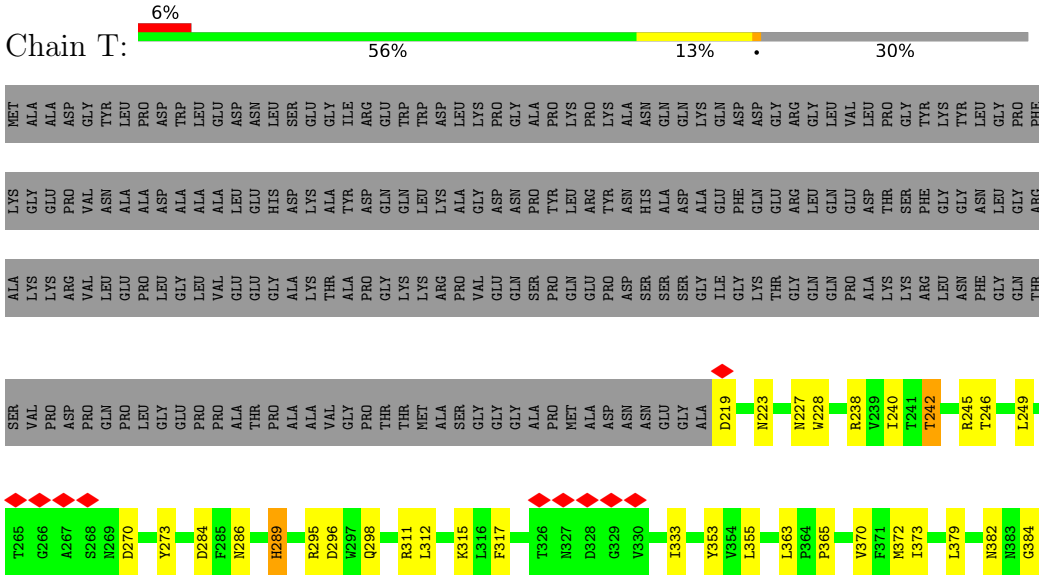
• Molecule 1: Capsid protein

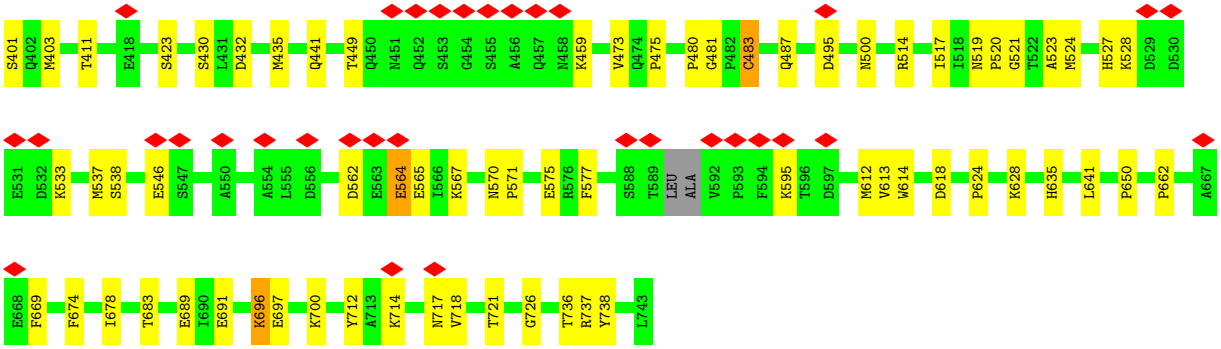
Chain S:



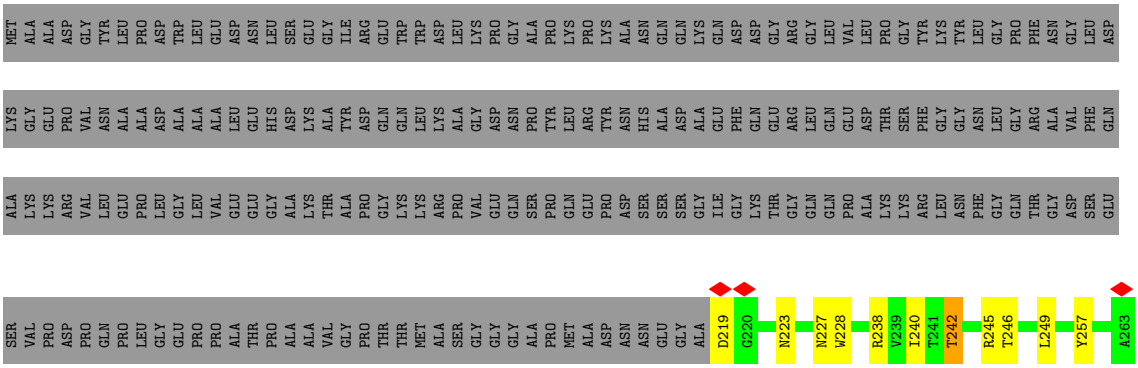
• Molecule 1: Capsid protein

Chain T:

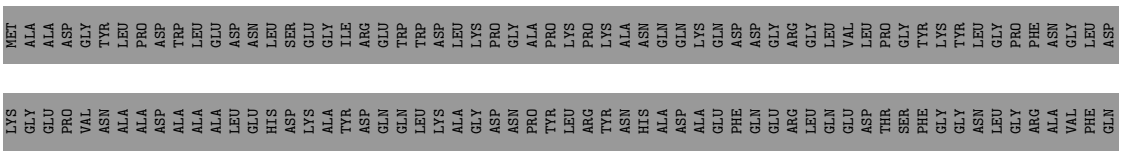


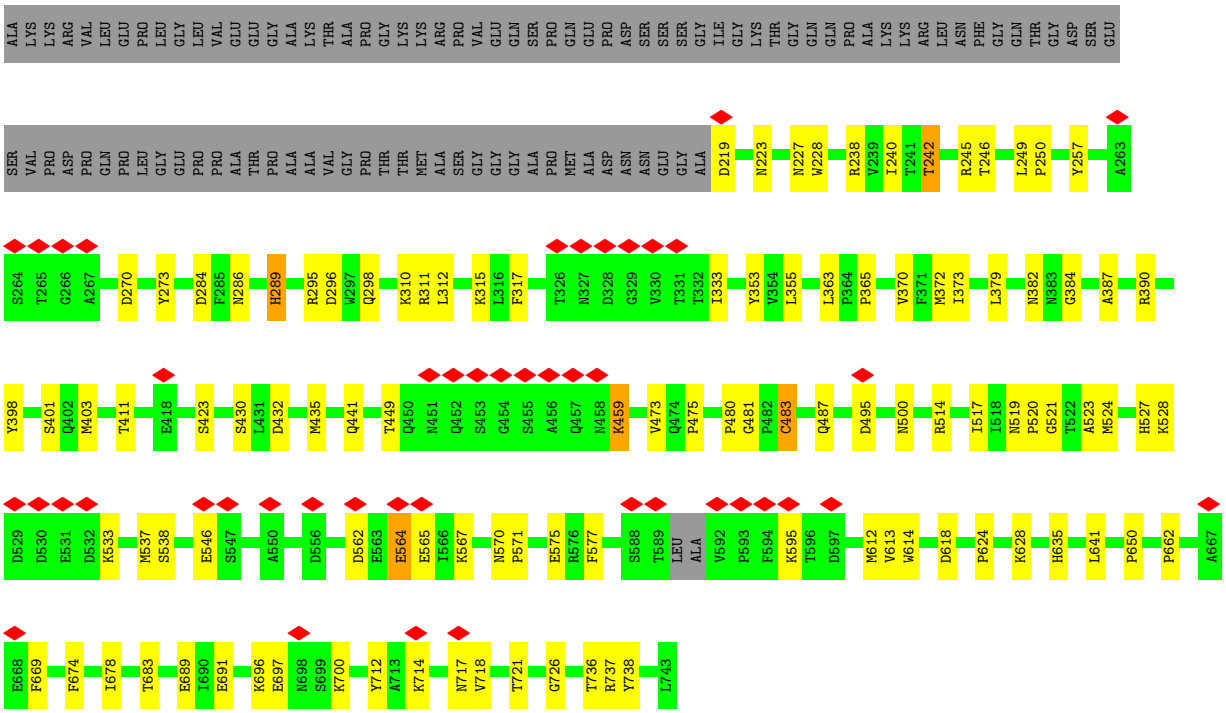


• Molecule 1: Capsid protein



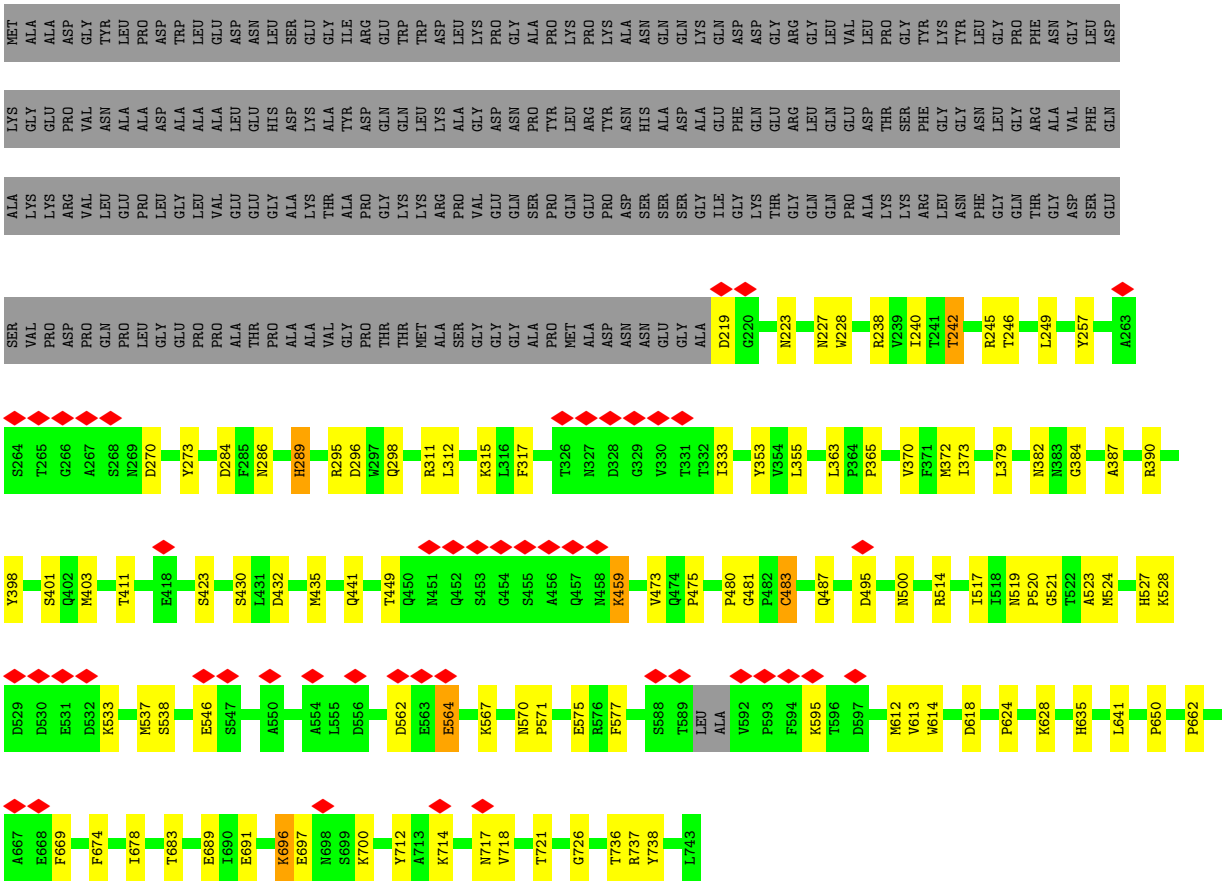
• Molecule 1: Capsid protein





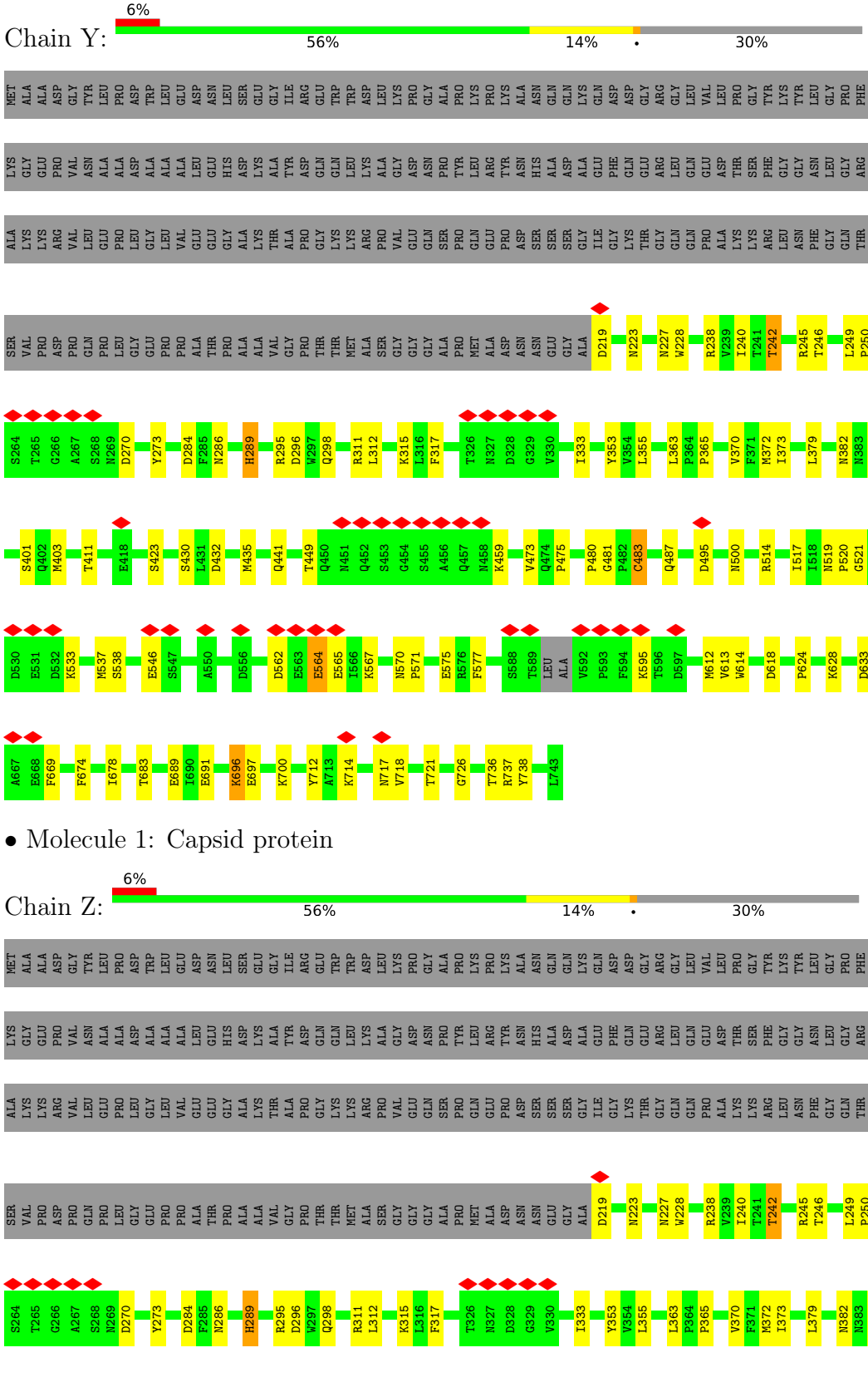
• Molecule 1: Capsid protein

Chain X:



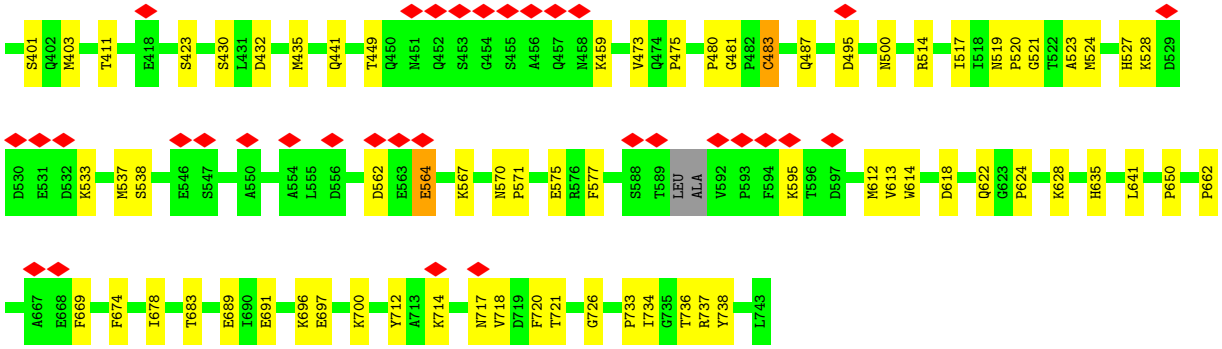
• Molecule 1: Capsid protein

Chain Y:

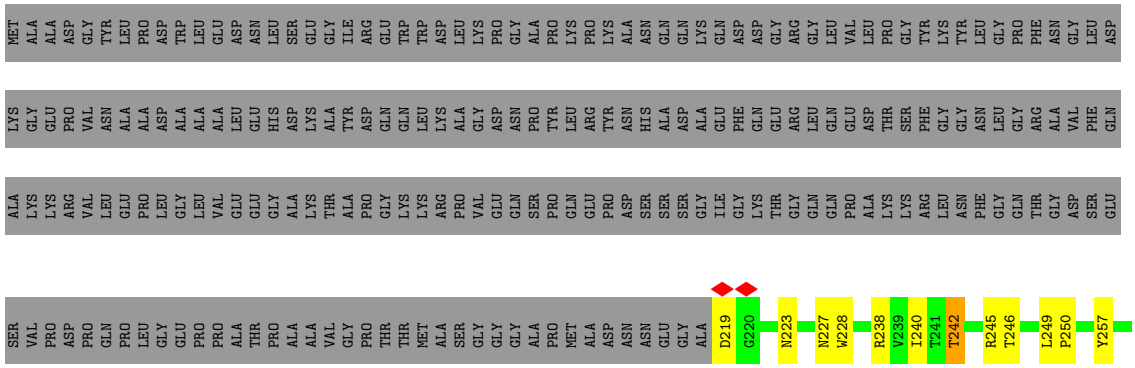


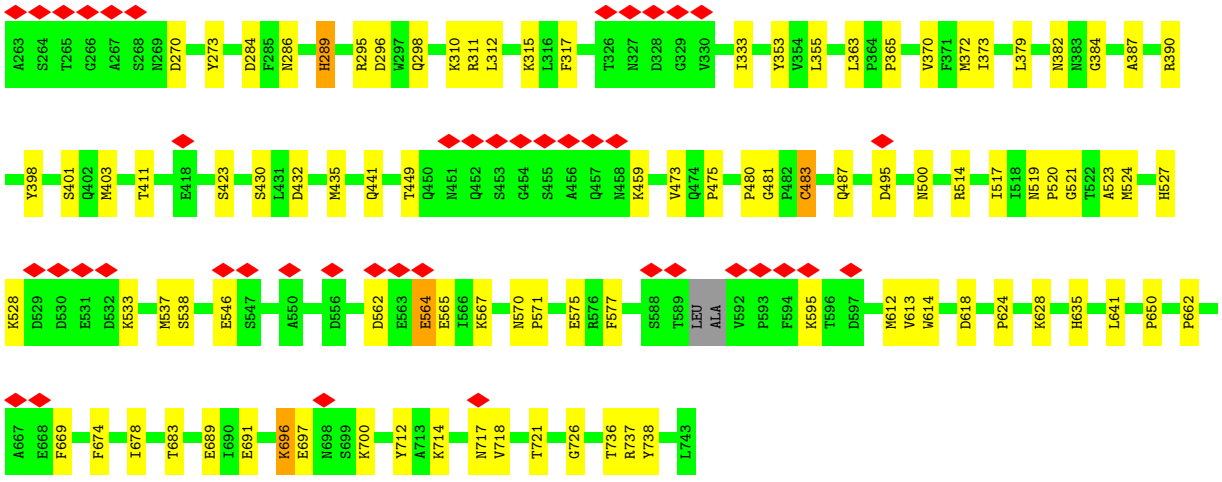
• Molecule 1: Capsid protein

Chain Z:

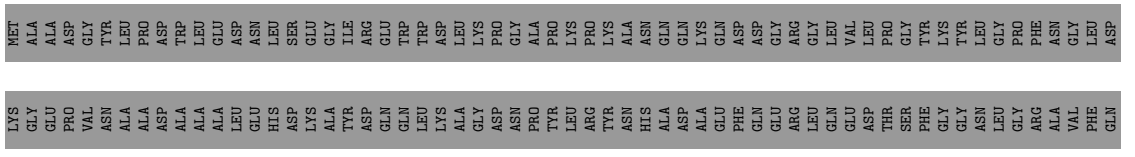


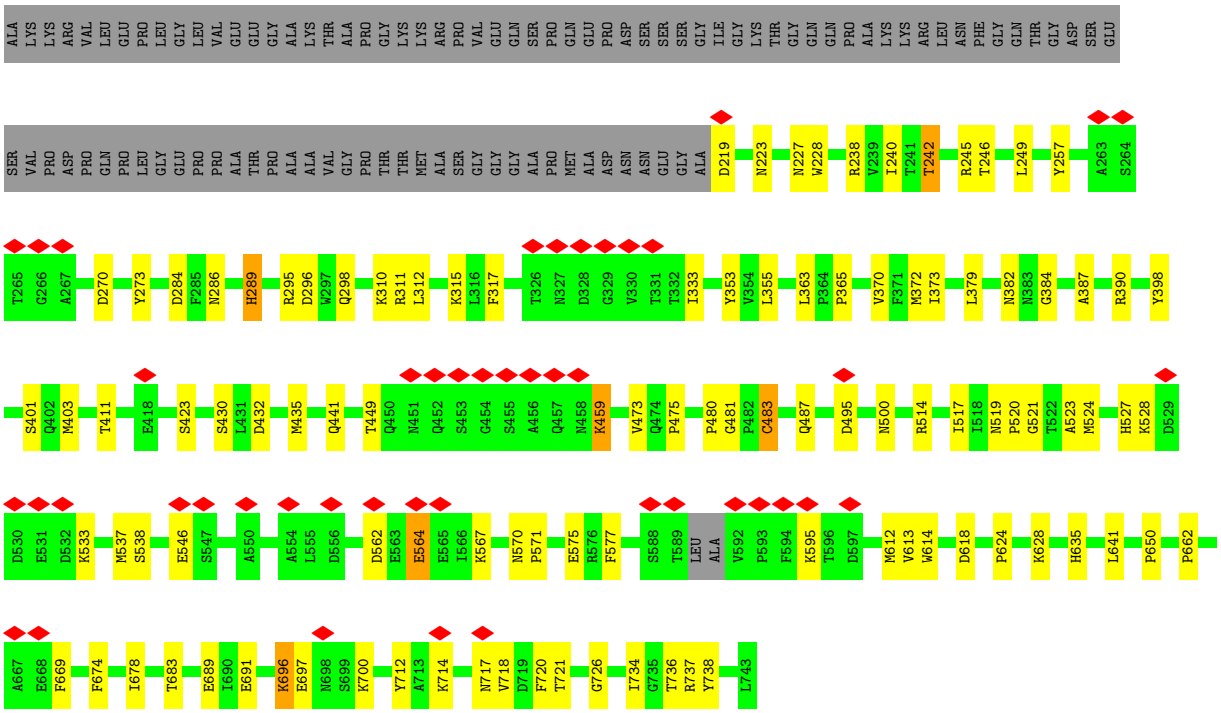
• Molecule 1: Capsid protein



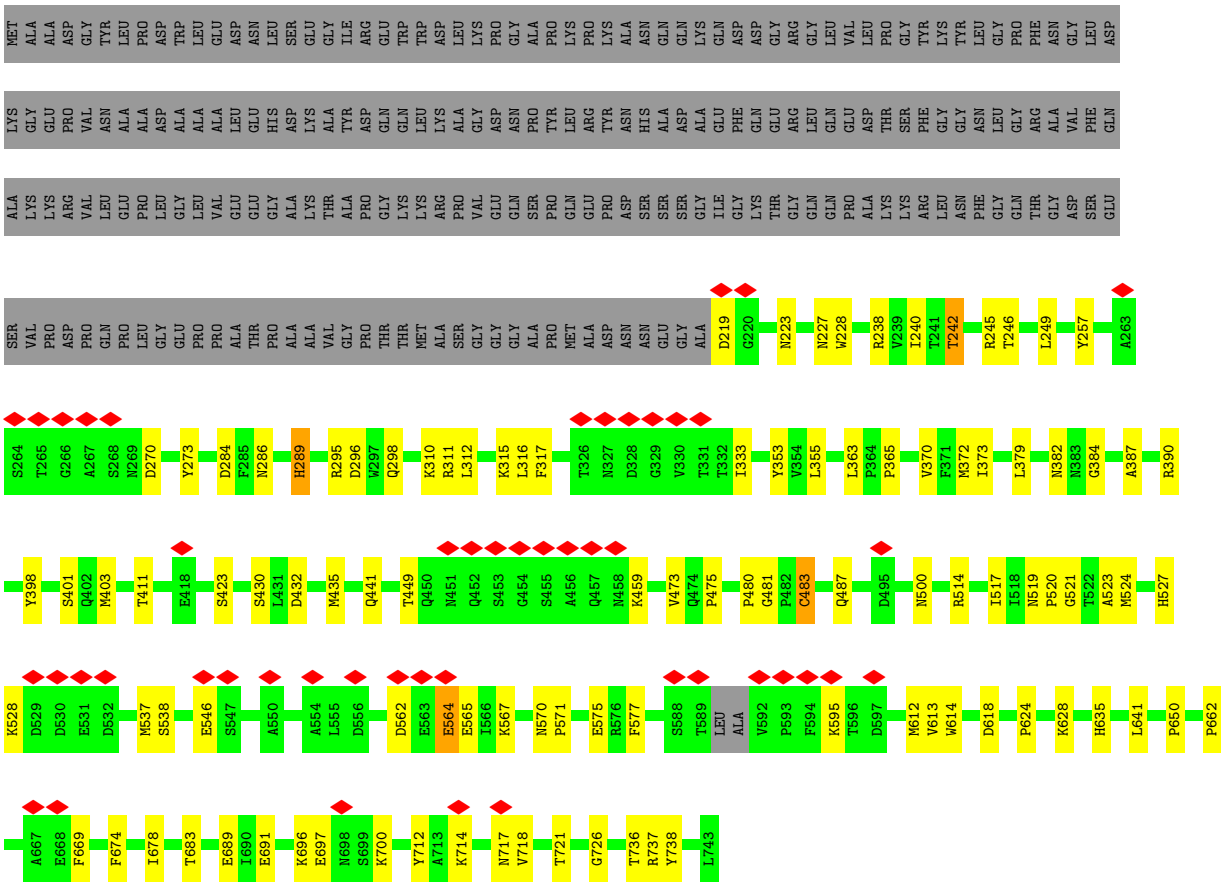


• Molecule 1: Capsid protein



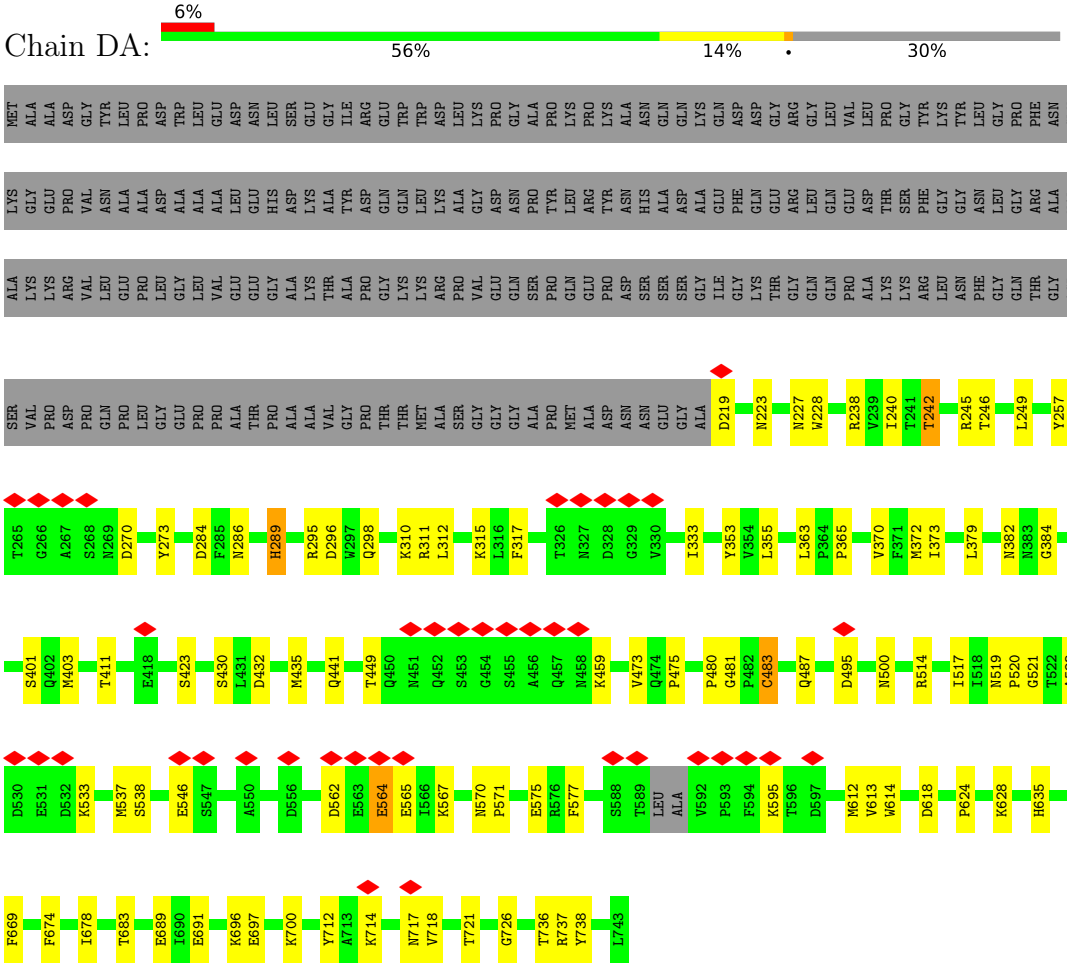


• Molecule 1: Capsid protein



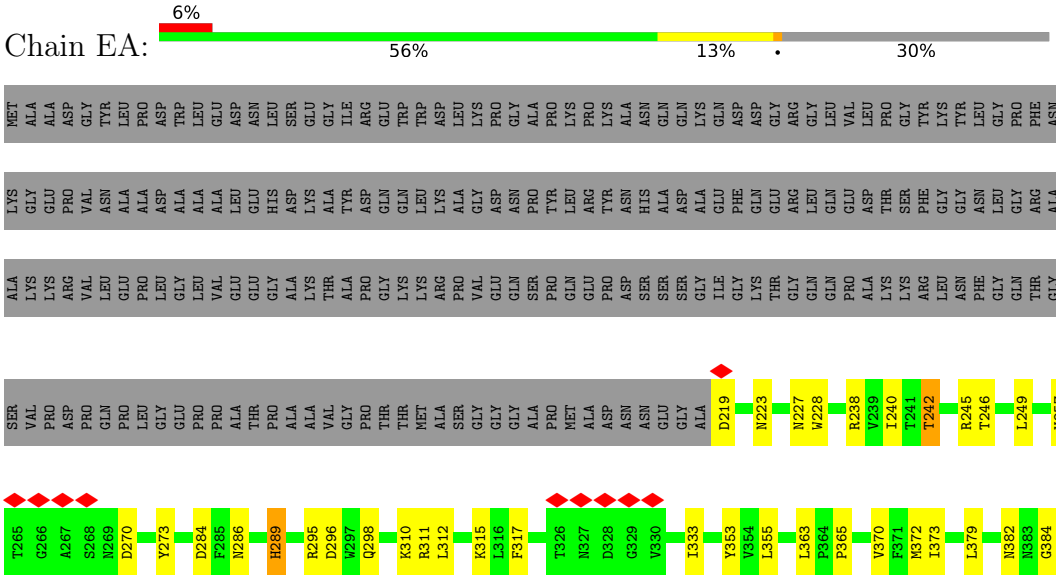
• Molecule 1: Capsid protein

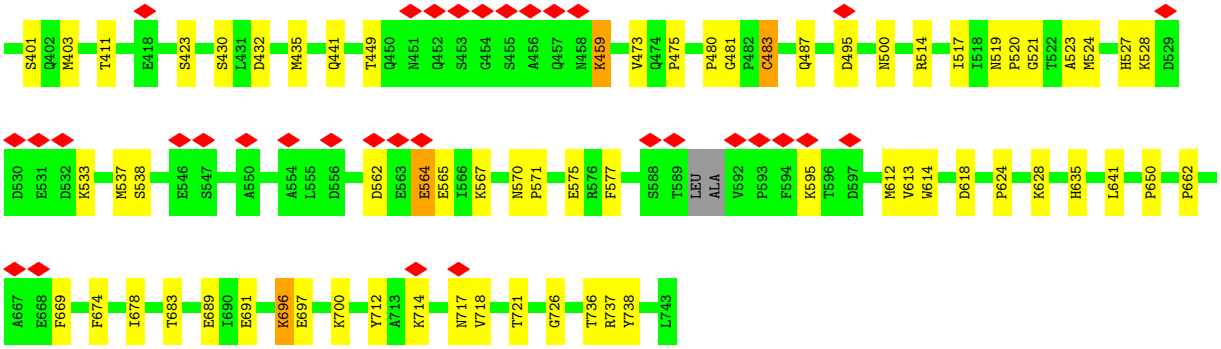
Chain DA:



• Molecule 1: Capsid protein

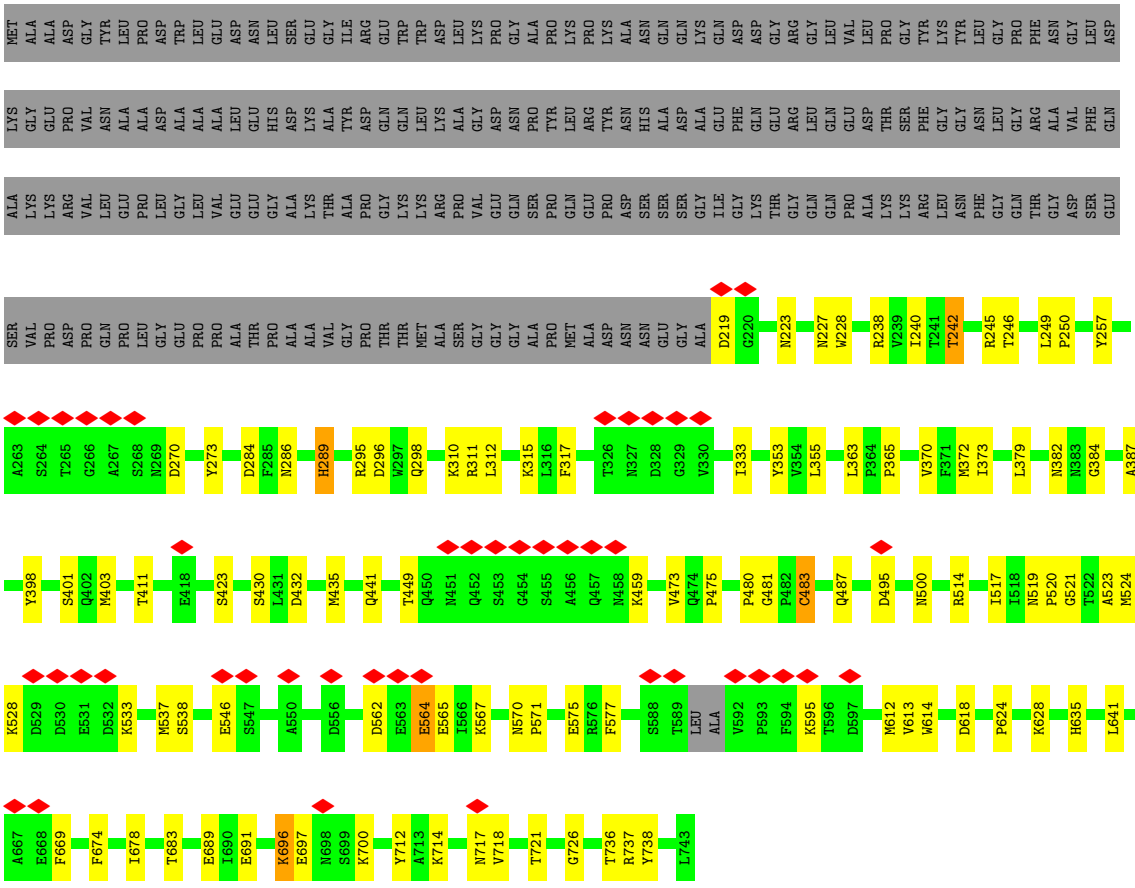
Chain EA:





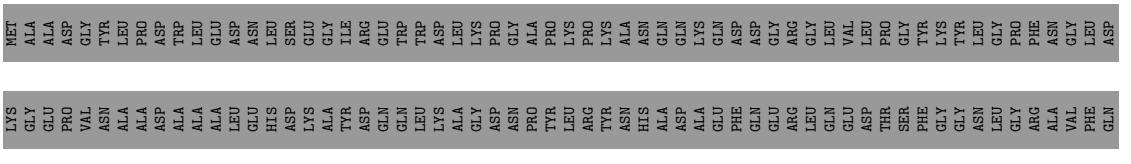
• Molecule 1: Capsid protein

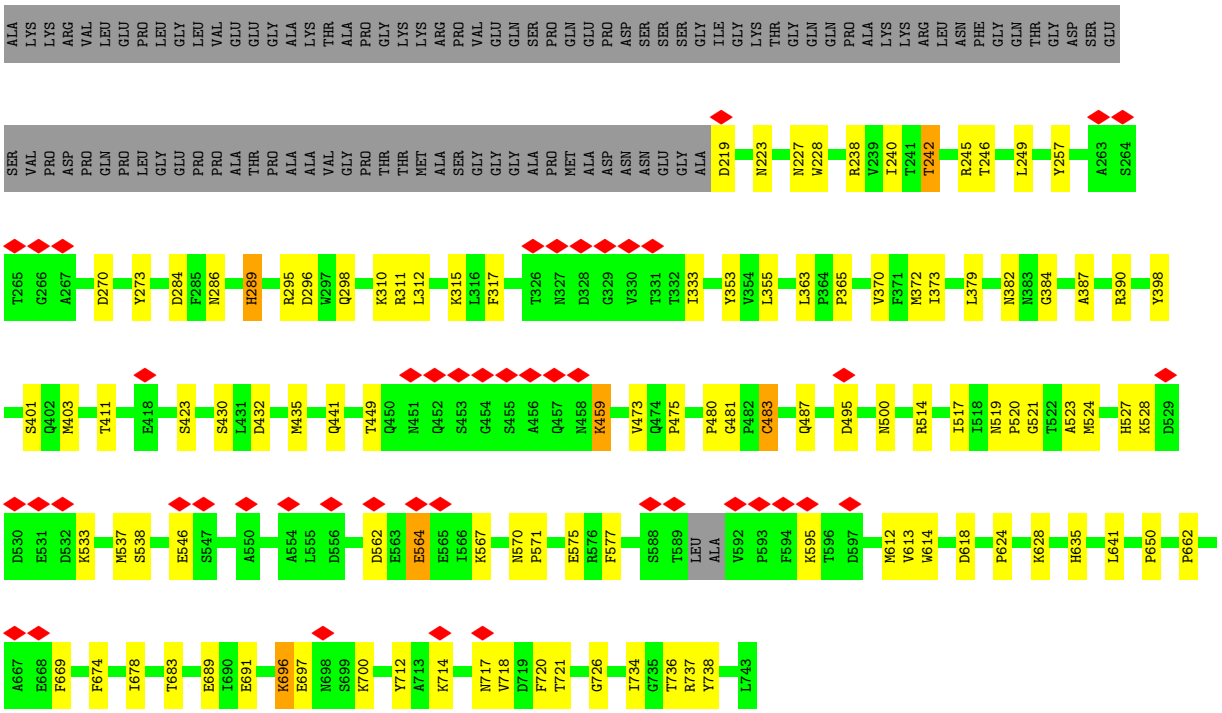
Chain FA:



• Molecule 1: Capsid protein

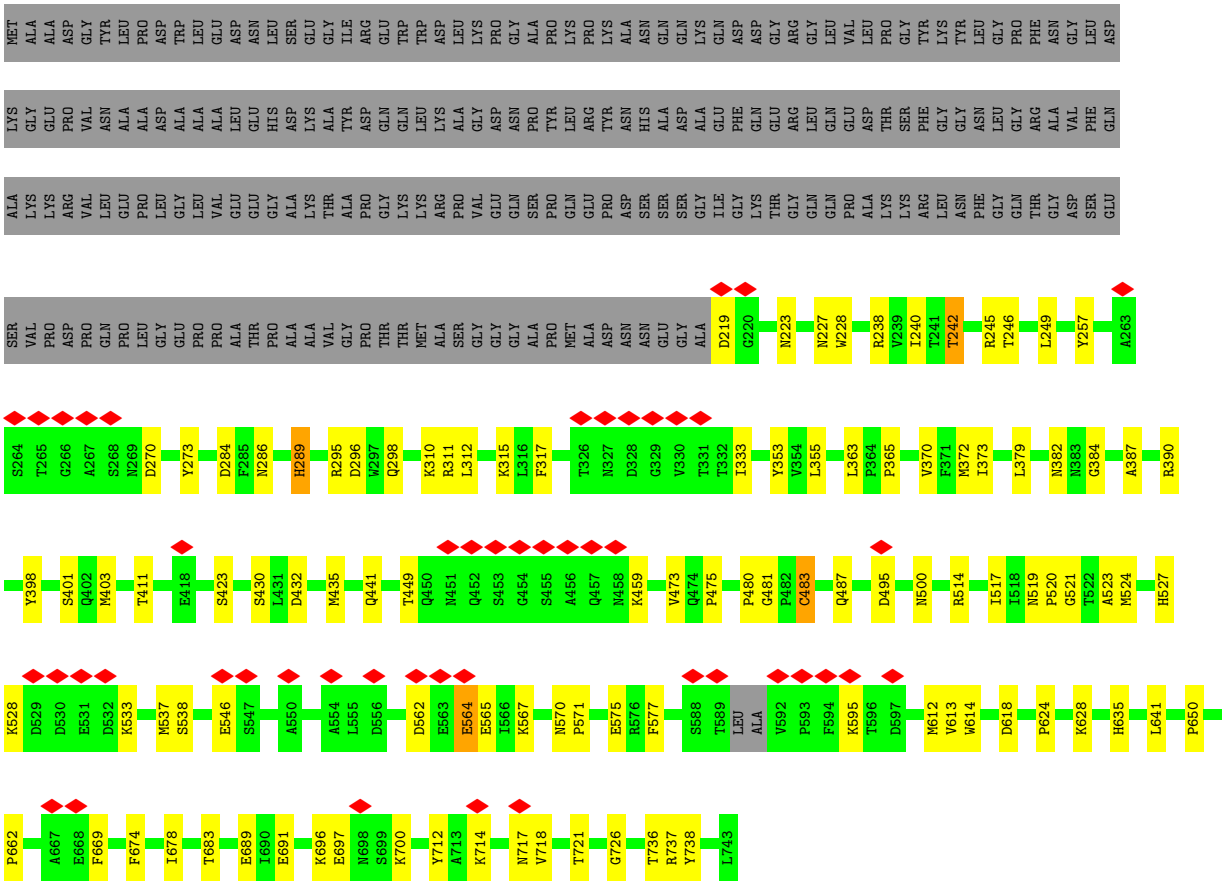
Chain GA:





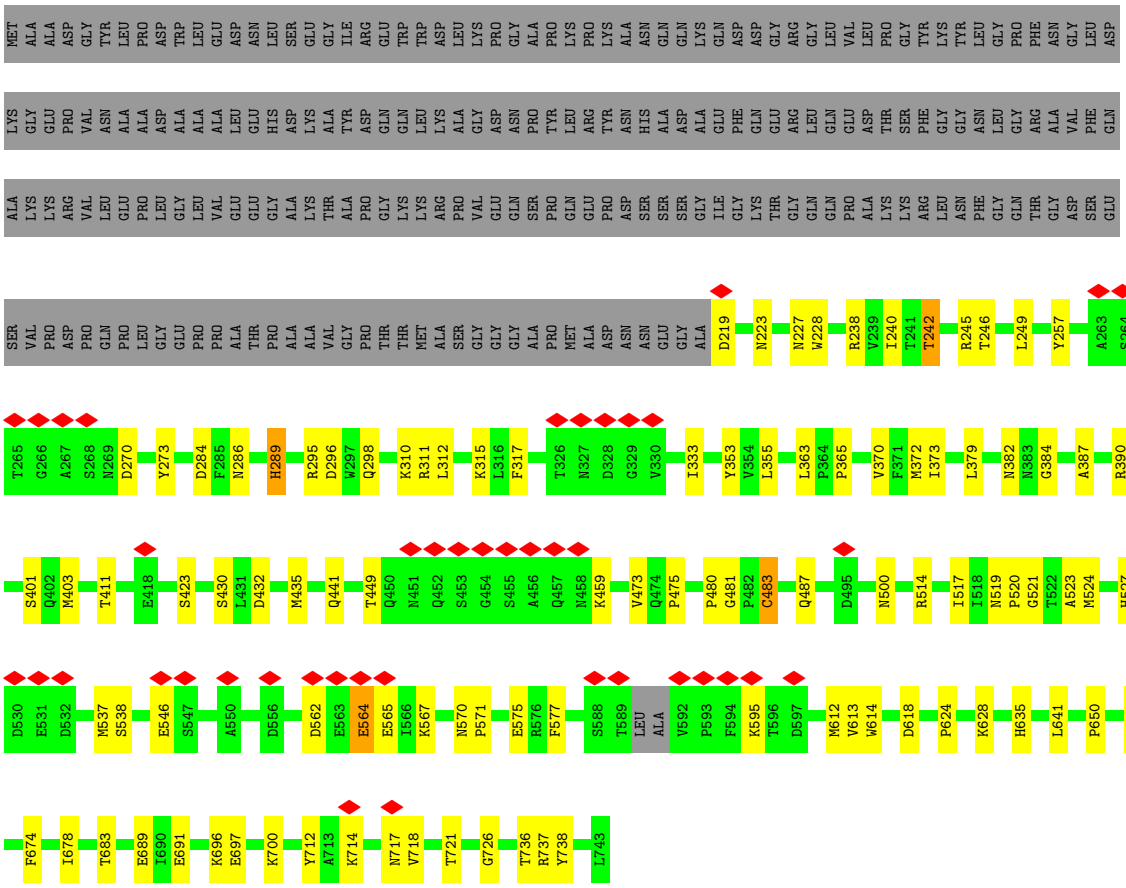
• Molecule 1: Capsid protein

Chain HA:



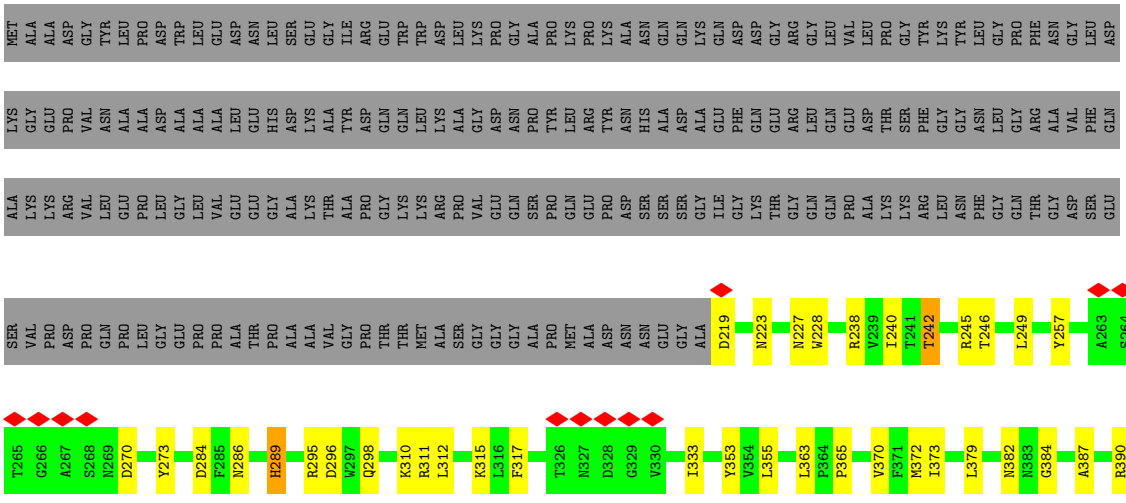
• Molecule 1: Capsid protein

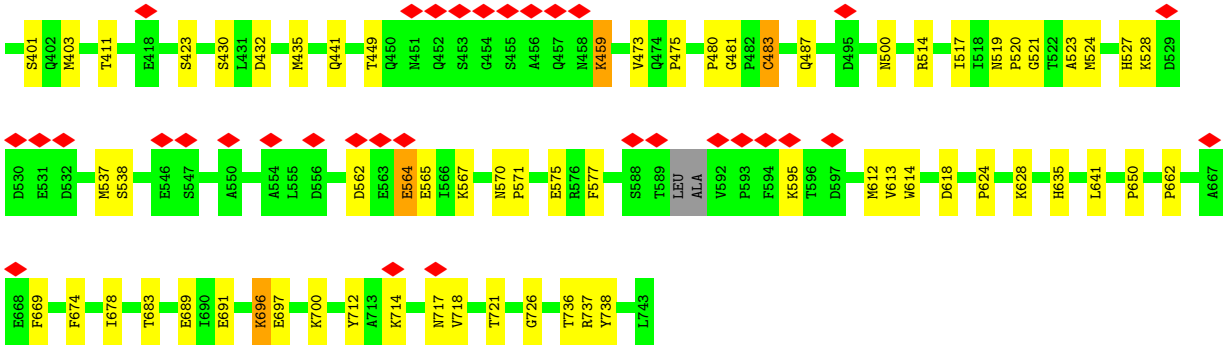
Chain IA:



• Molecule 1: Capsid protein

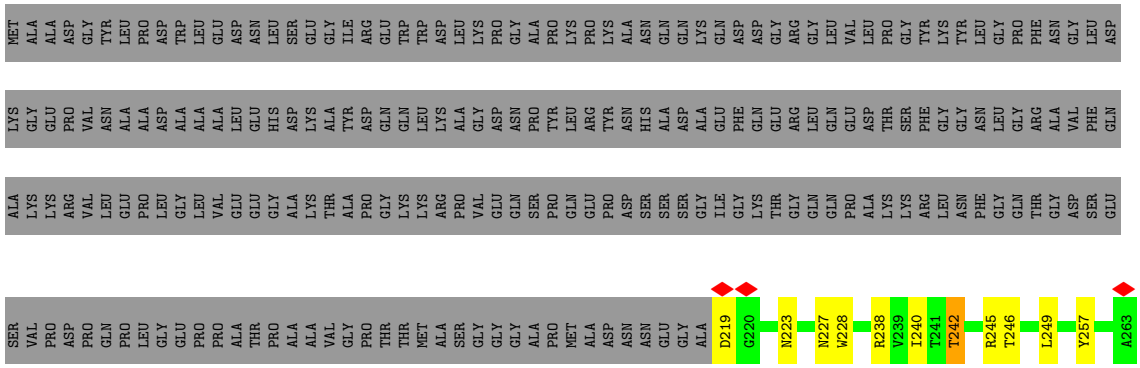
Chain JA:

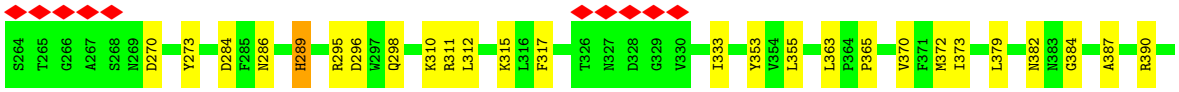


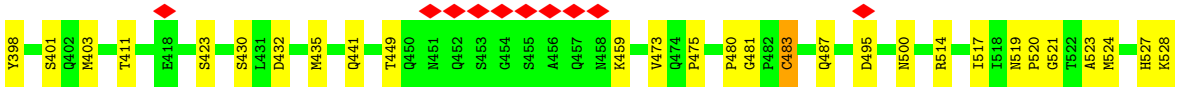


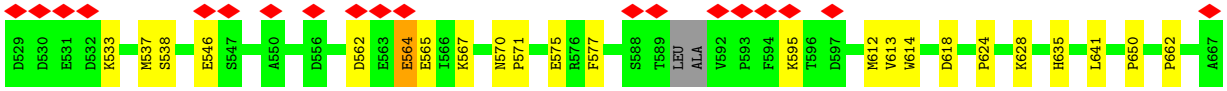
• Molecule 1: Capsid protein

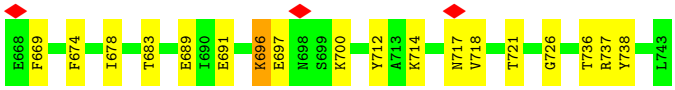
Chain KA:





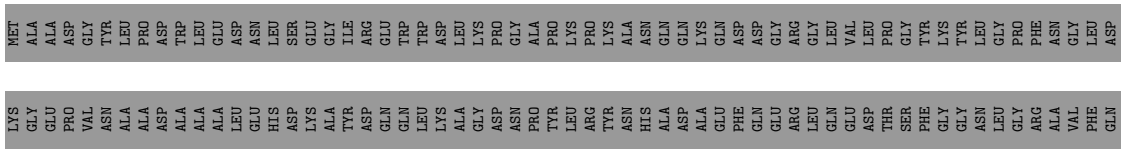


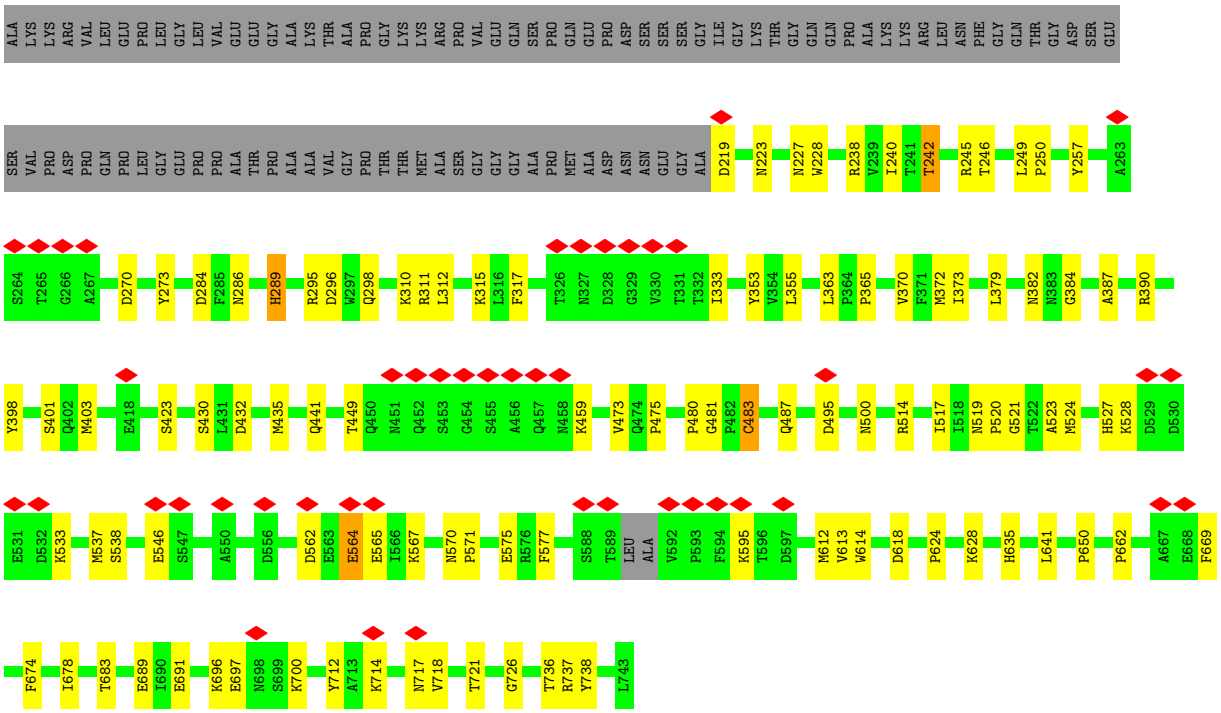


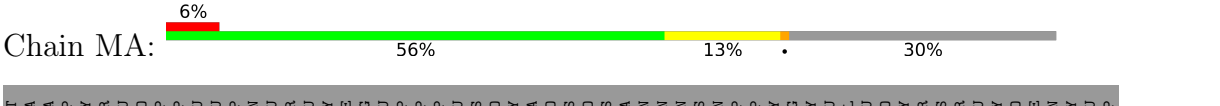


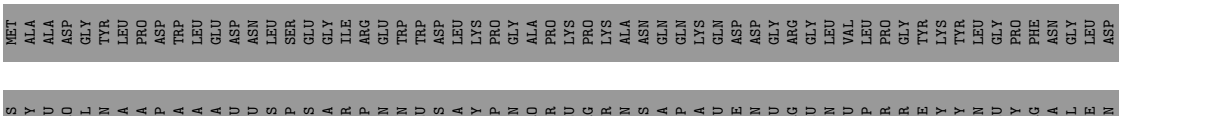
• Molecule 1: Capsid protein

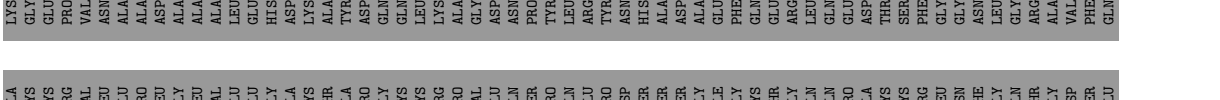
Chain LA:

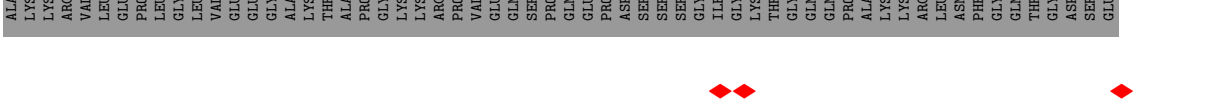


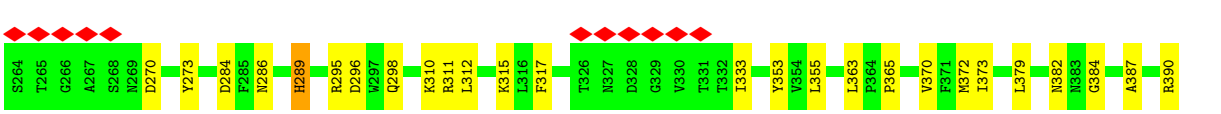


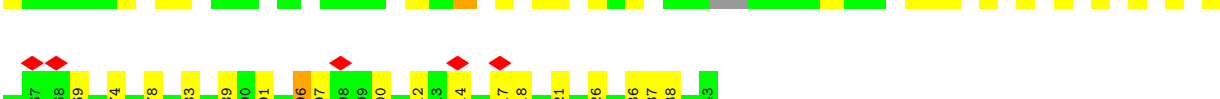










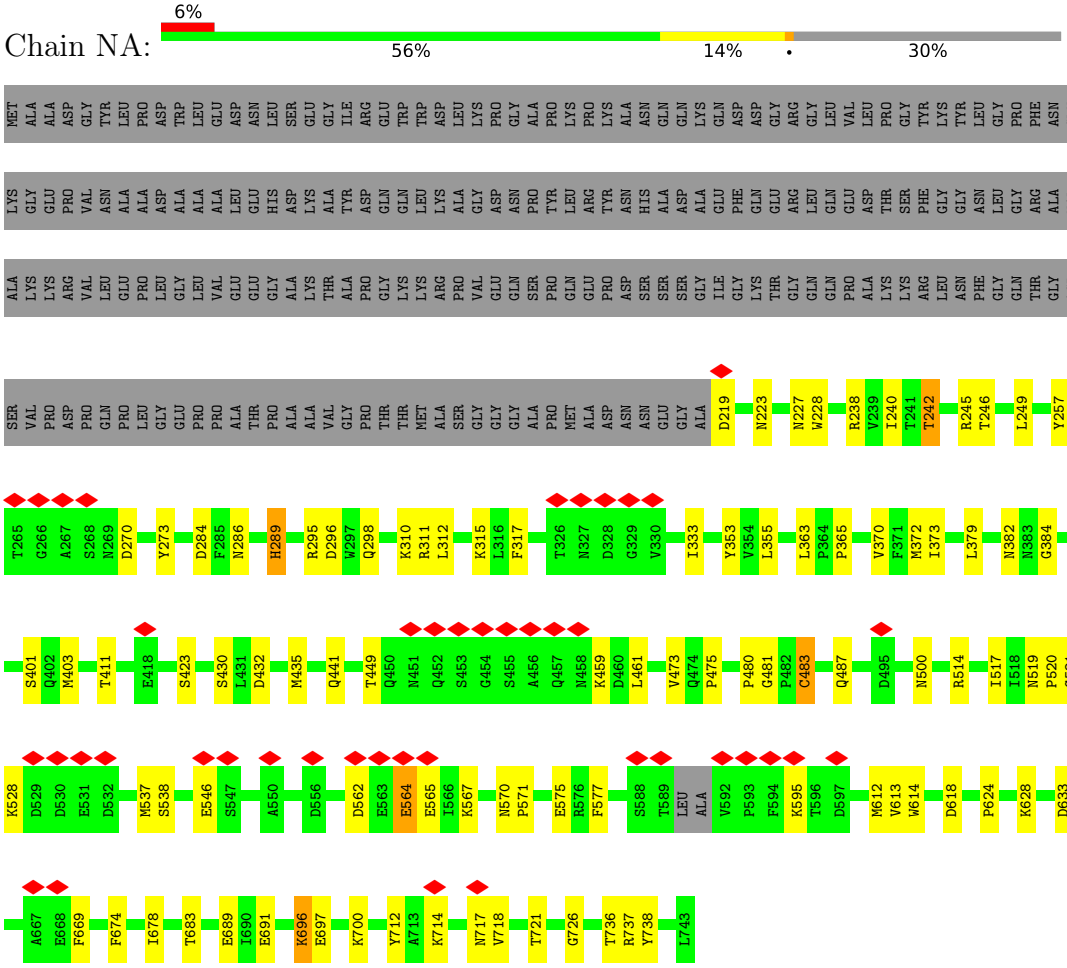


- Molecule 1: Capsid protein

Chain MA:

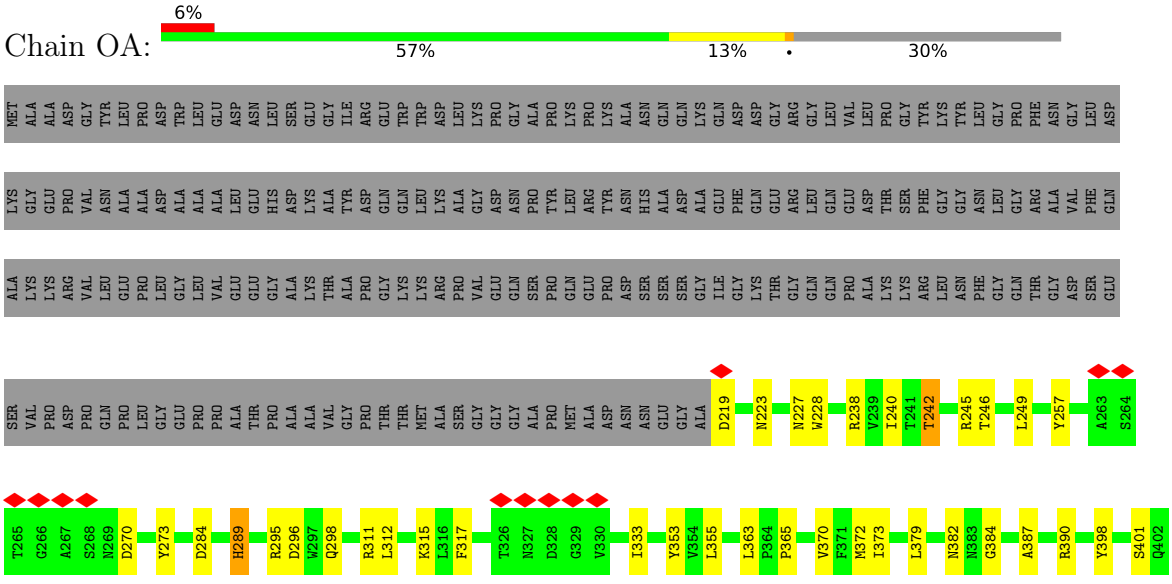
• Molecule 1: Capsid protein

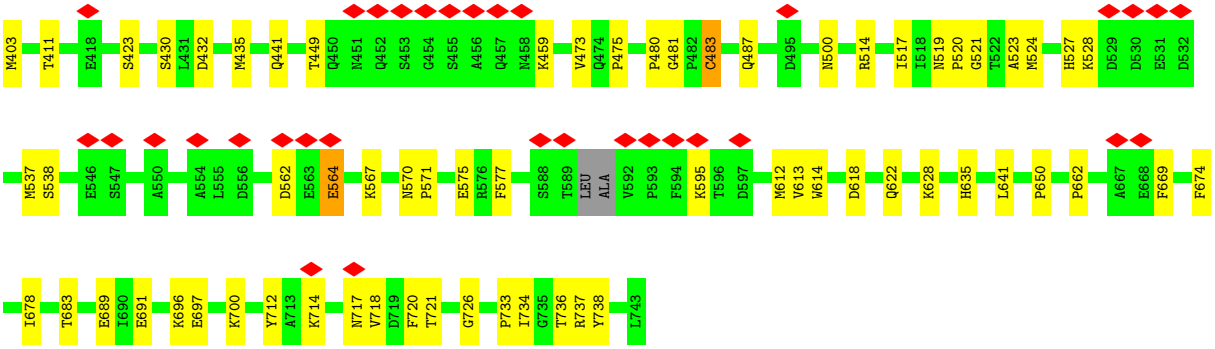
Chain NA:



• Molecule 1: Capsid protein

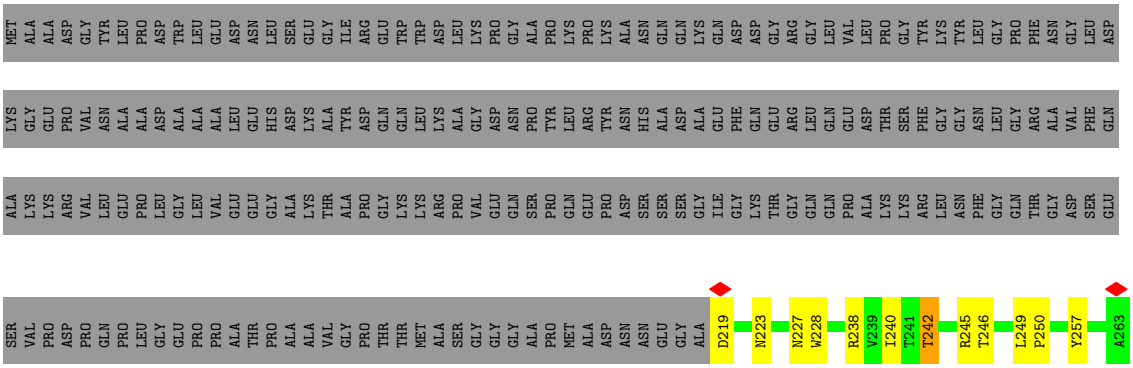
Chain OA:

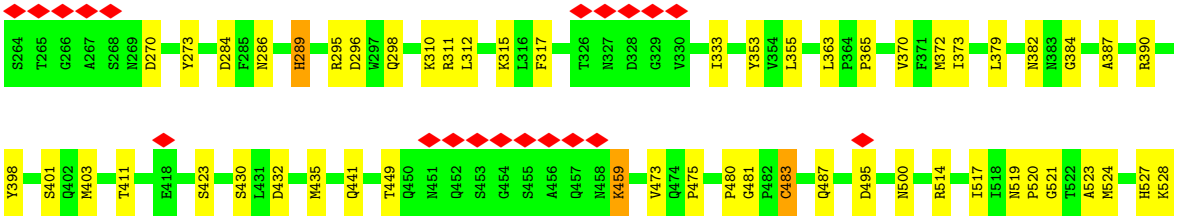




• Molecule 1: Capsid protein

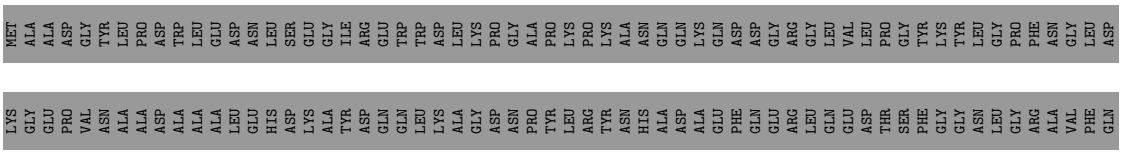
Chain PA:

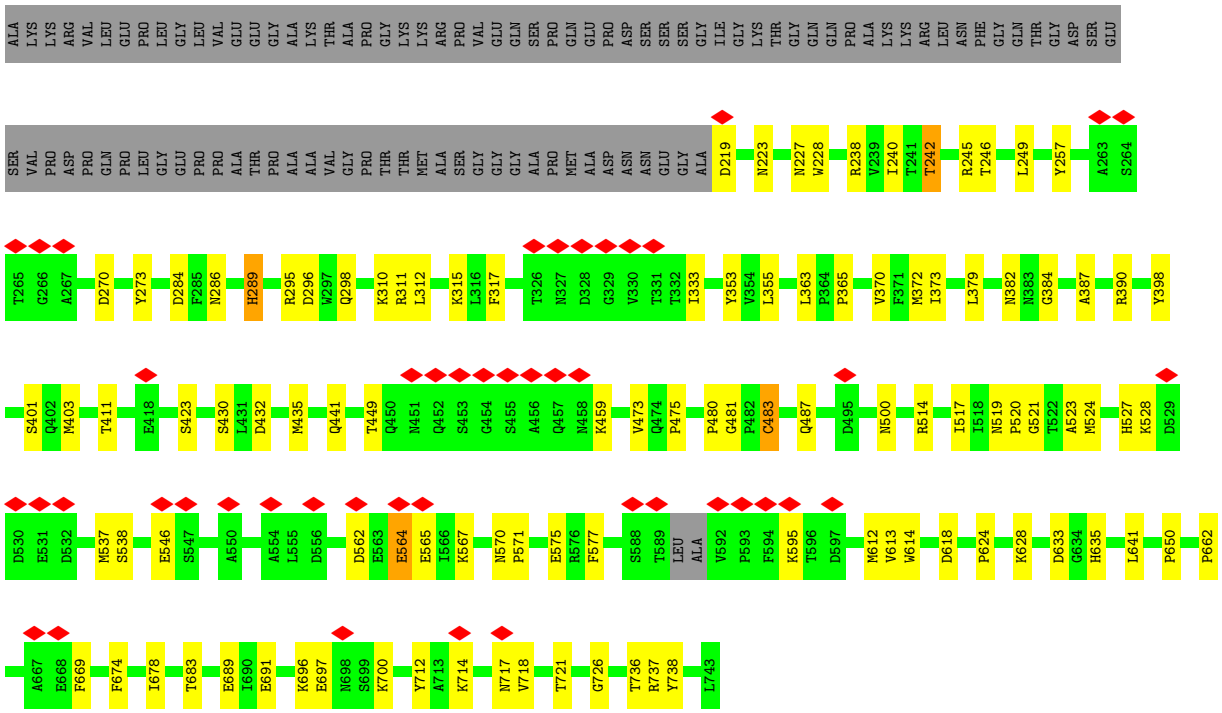




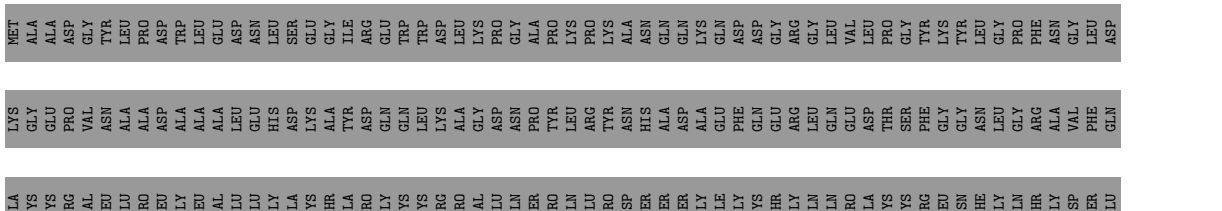
• Molecule 1: Capsid protein

Chain QA:



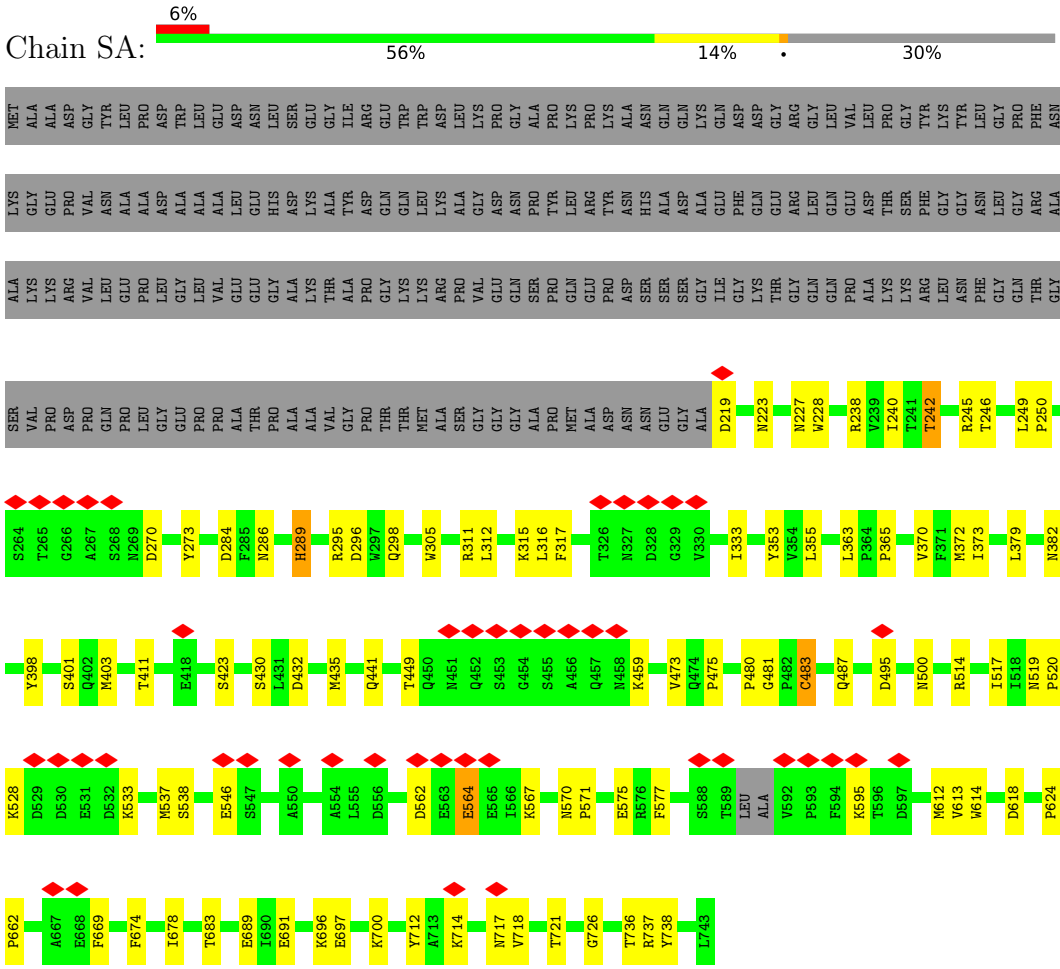


• Molecule 1: Capsid protein



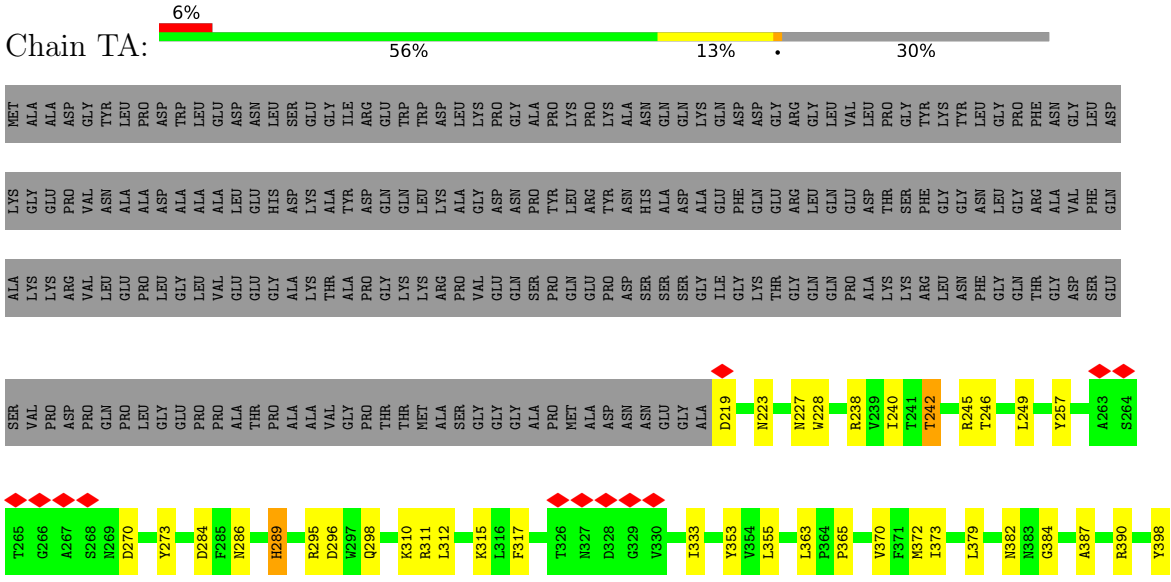
• Molecule 1: Capsid protein

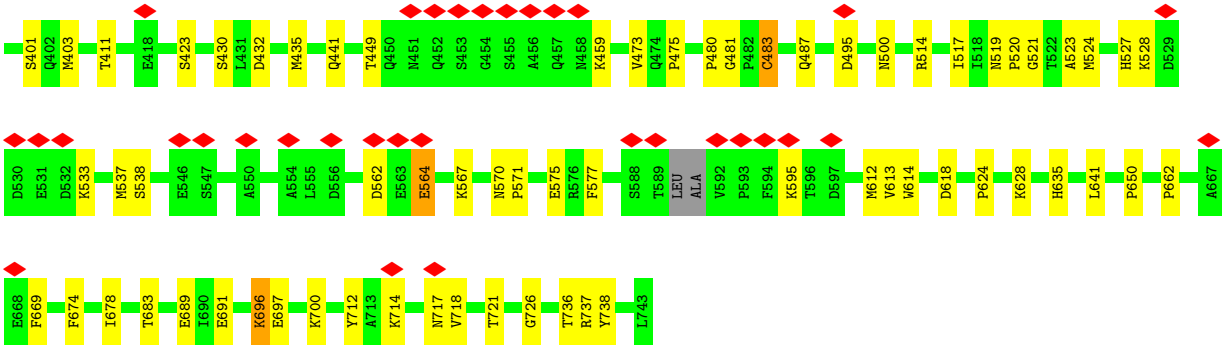
Chain SA:



• Molecule 1: Capsid protein

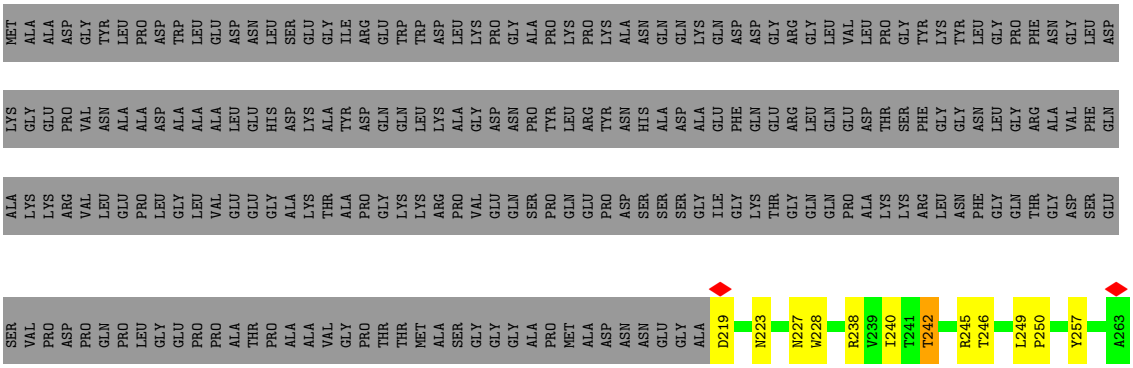
Chain TA:

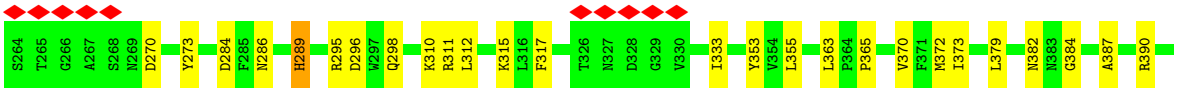


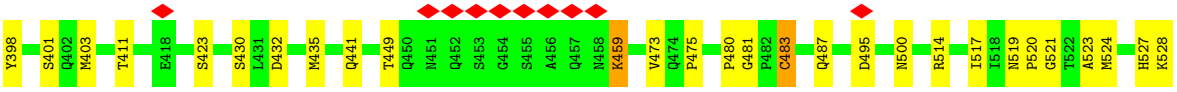


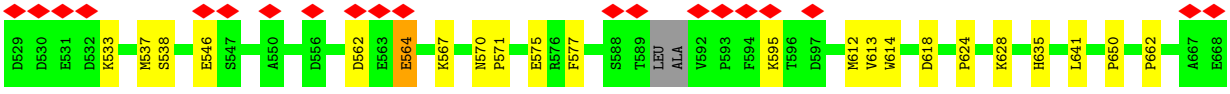
• Molecule 1: Capsid protein

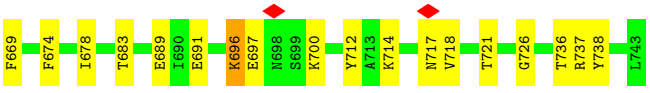
Chain UA:





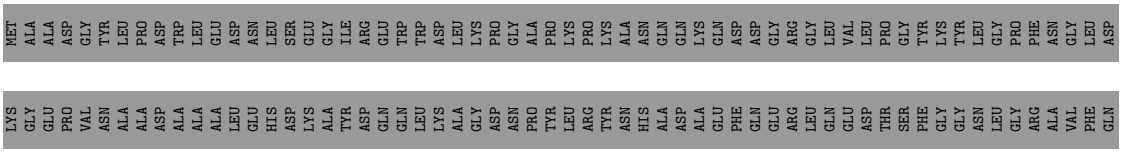


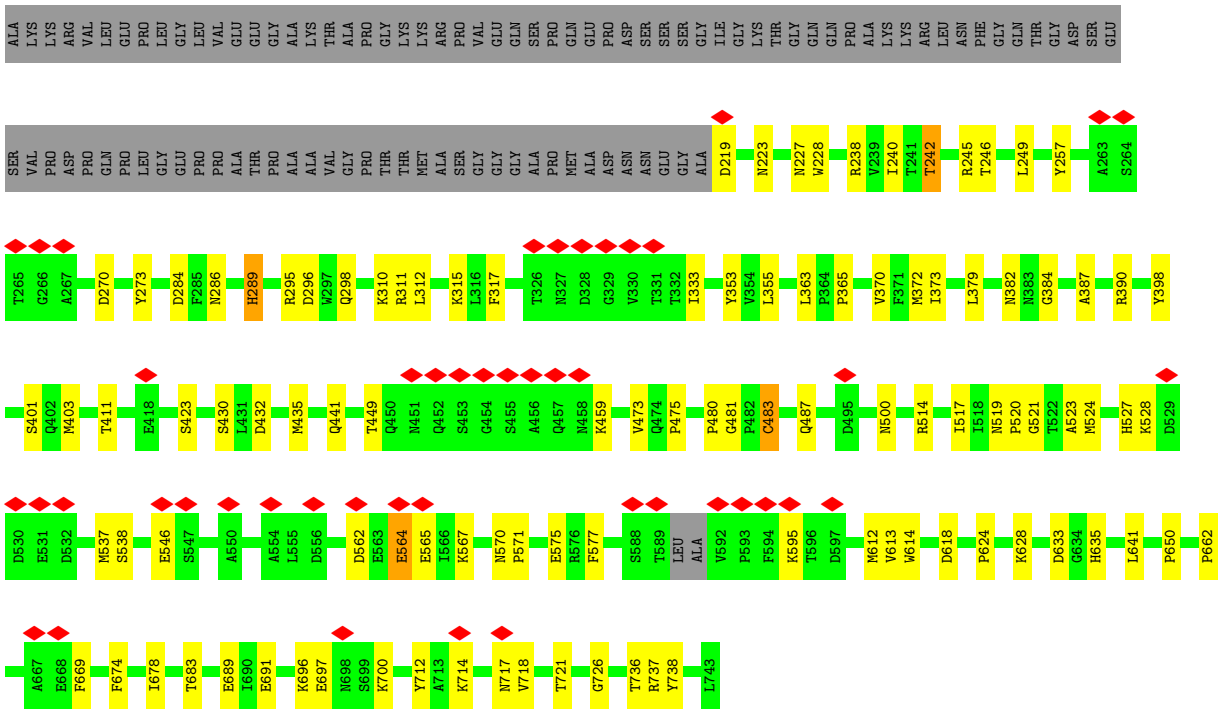




• Molecule 1: Capsid protein

Chain VA:

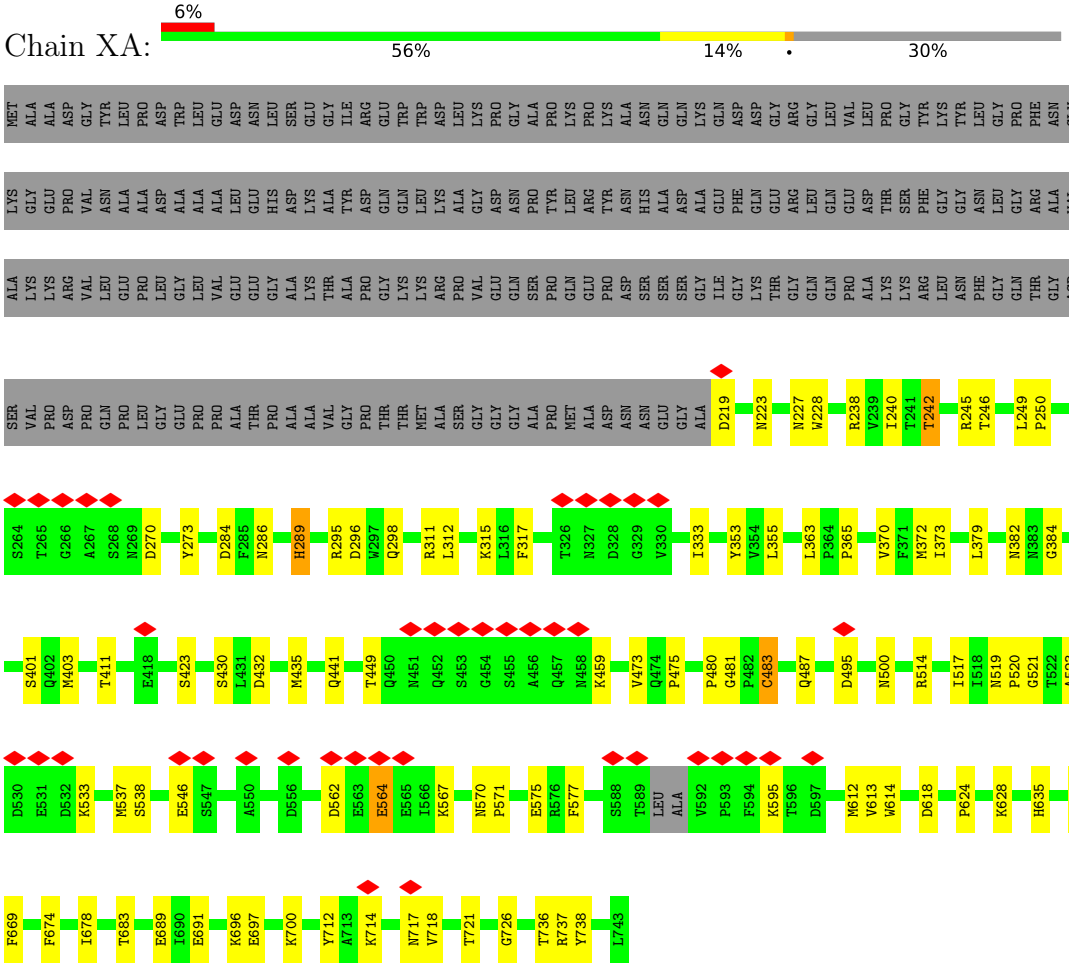




• Molecule 1: Capsid protein

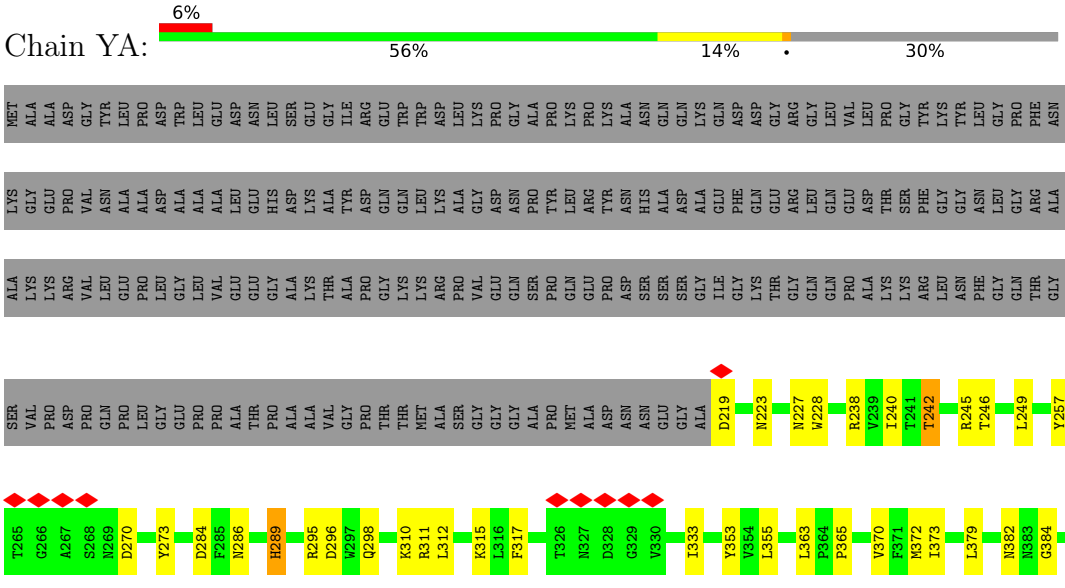
• Molecule 1: Capsid protein

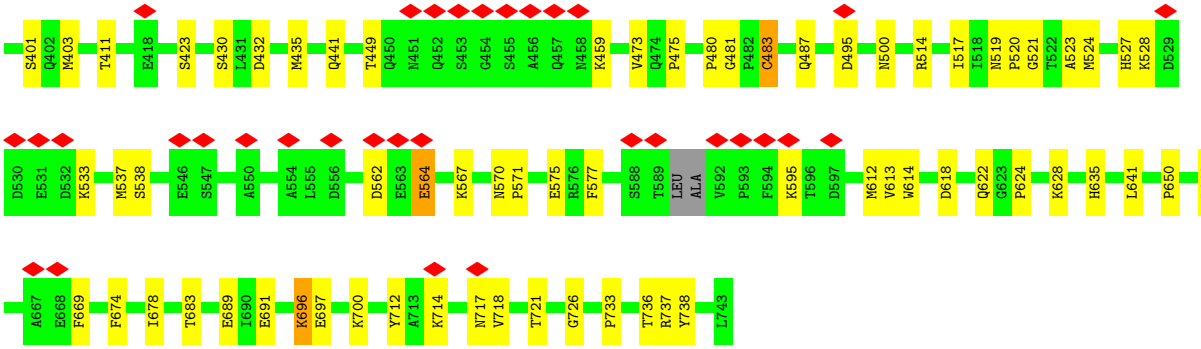
Chain XA:



• Molecule 1: Capsid protein

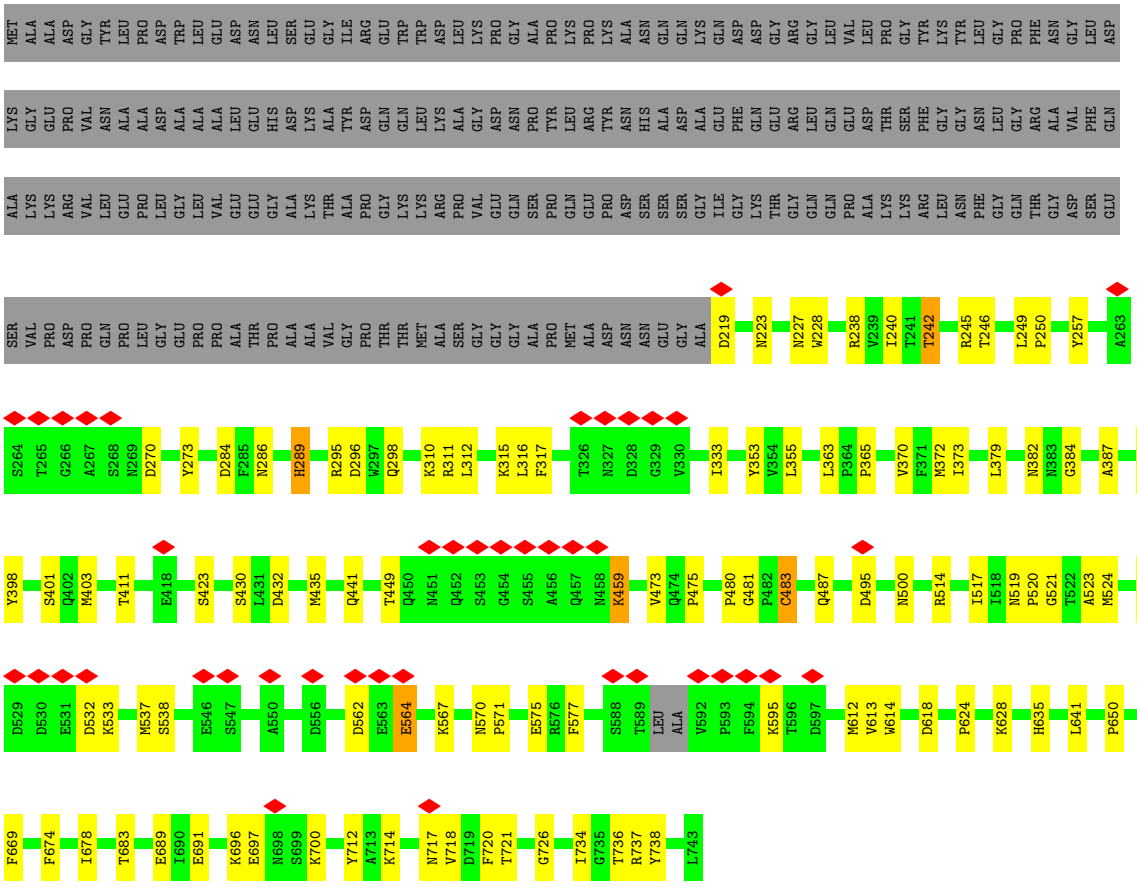
Chain YA:





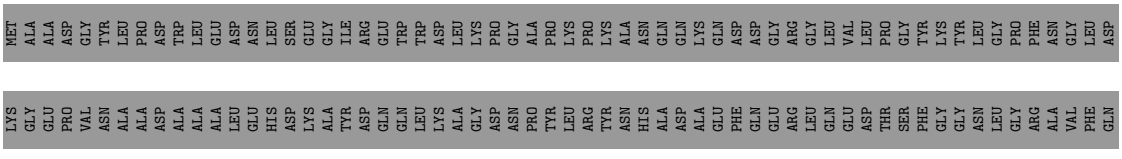
• Molecule 1: Capsid protein

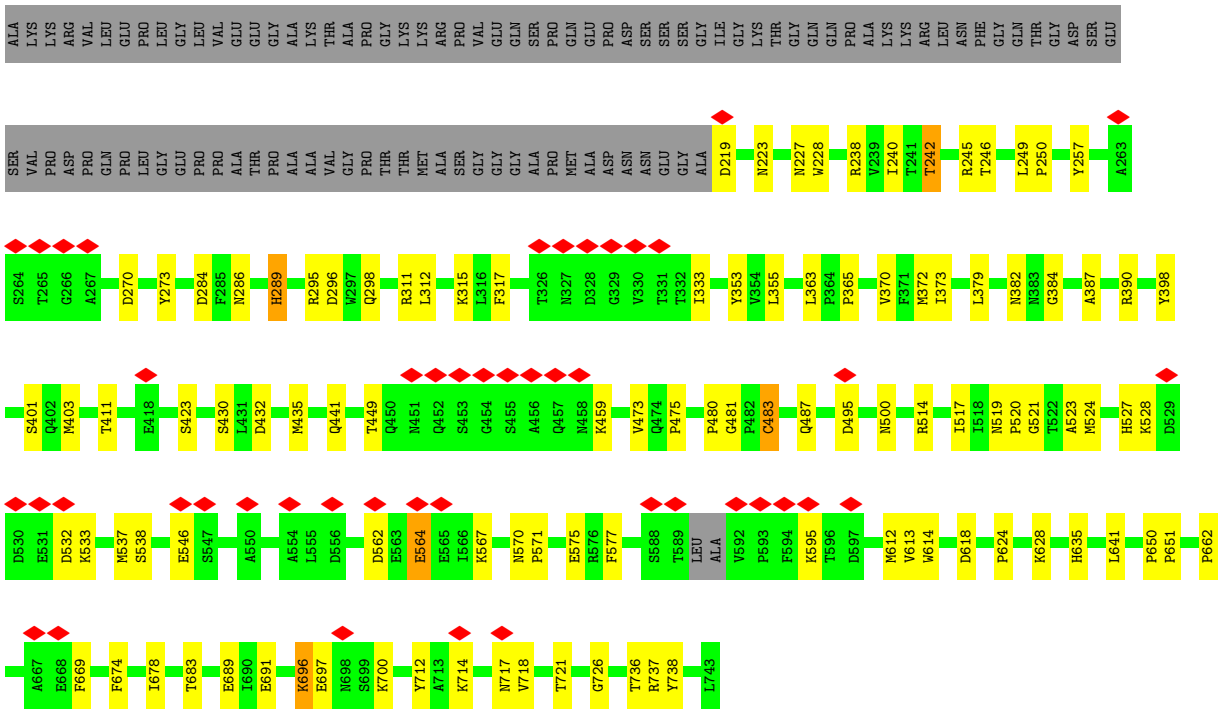
Chain ZA:

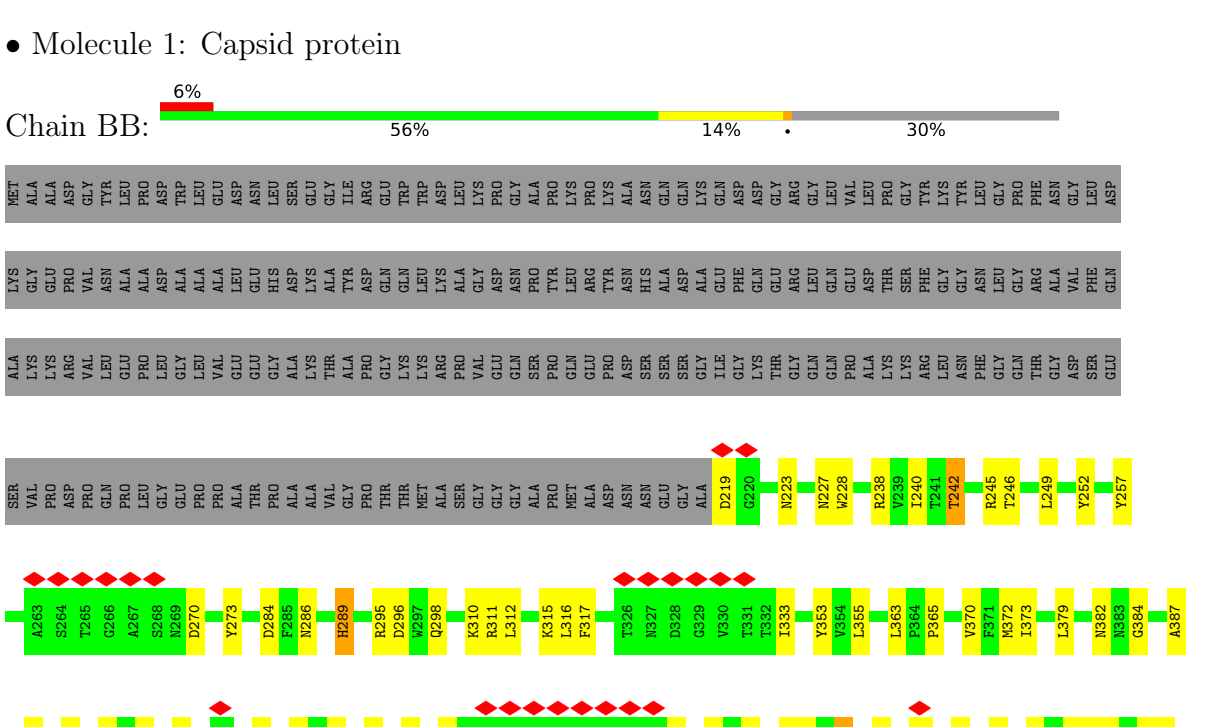


• Molecule 1: Capsid protein

Chain AB:

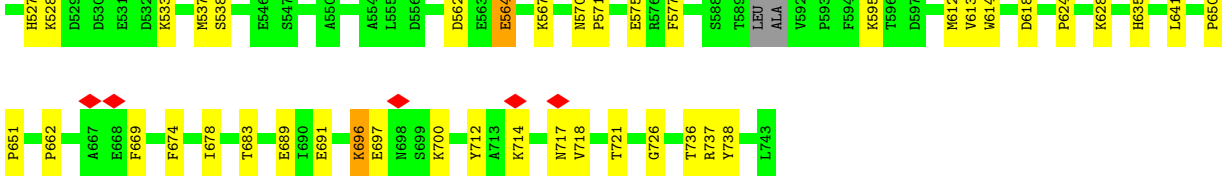






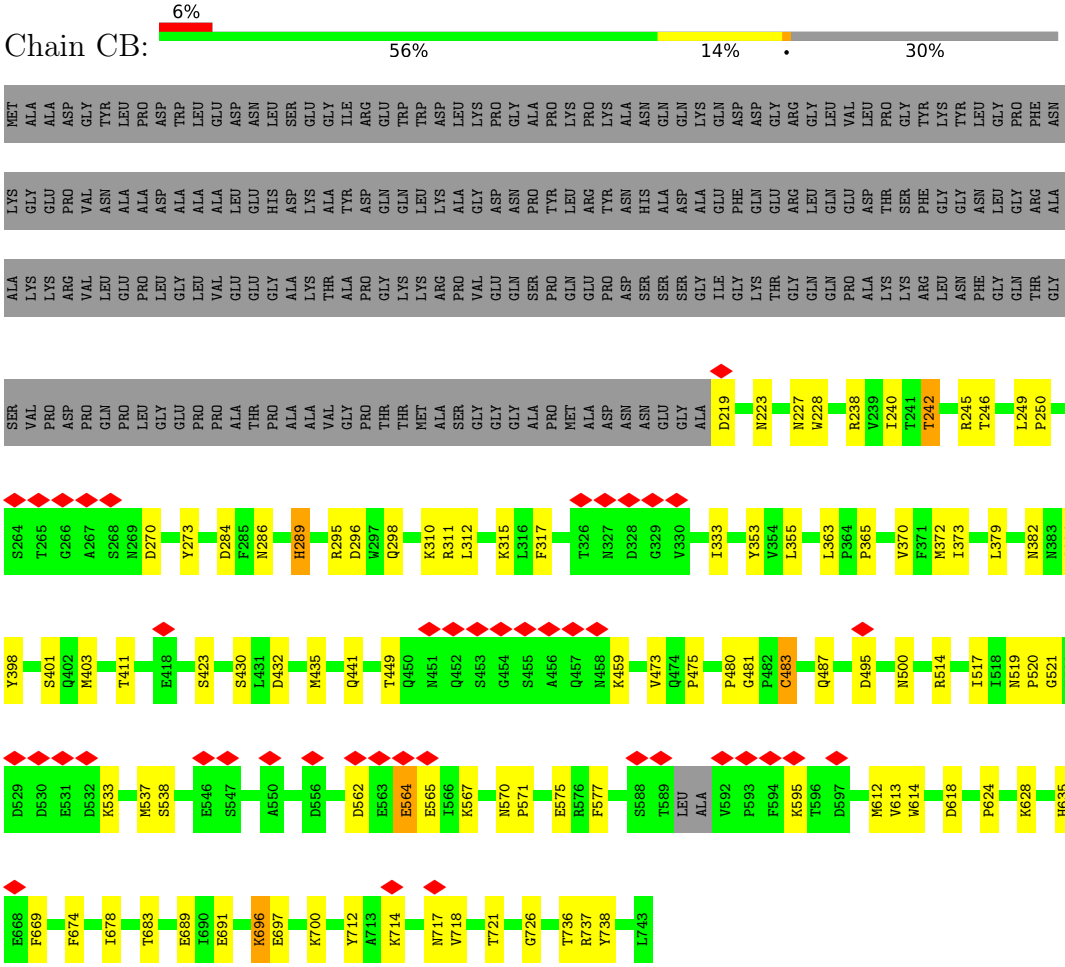
• Molecule 1: Capsid protein

Chain BB:



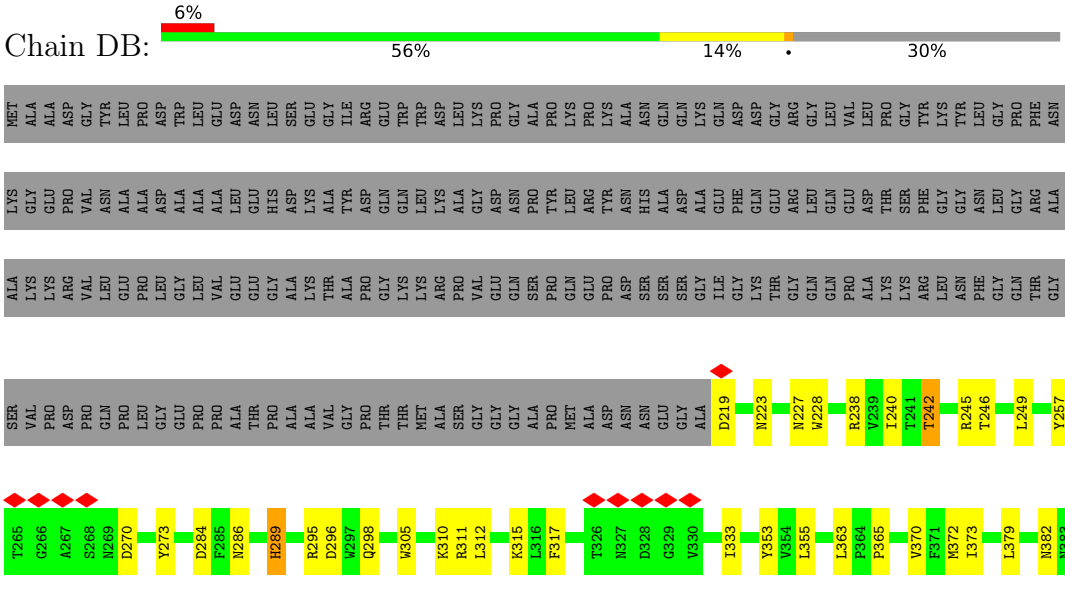
• Molecule 1: Capsid protein

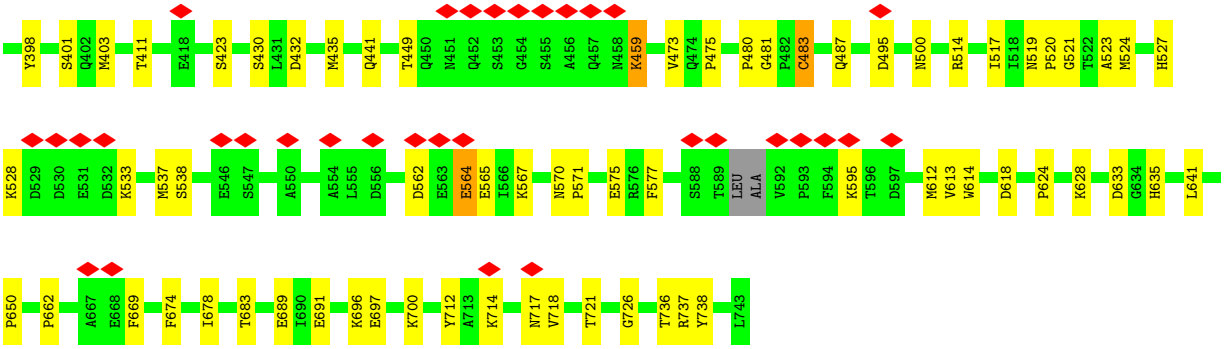
Chain CB:



• Molecule 1: Capsid protein

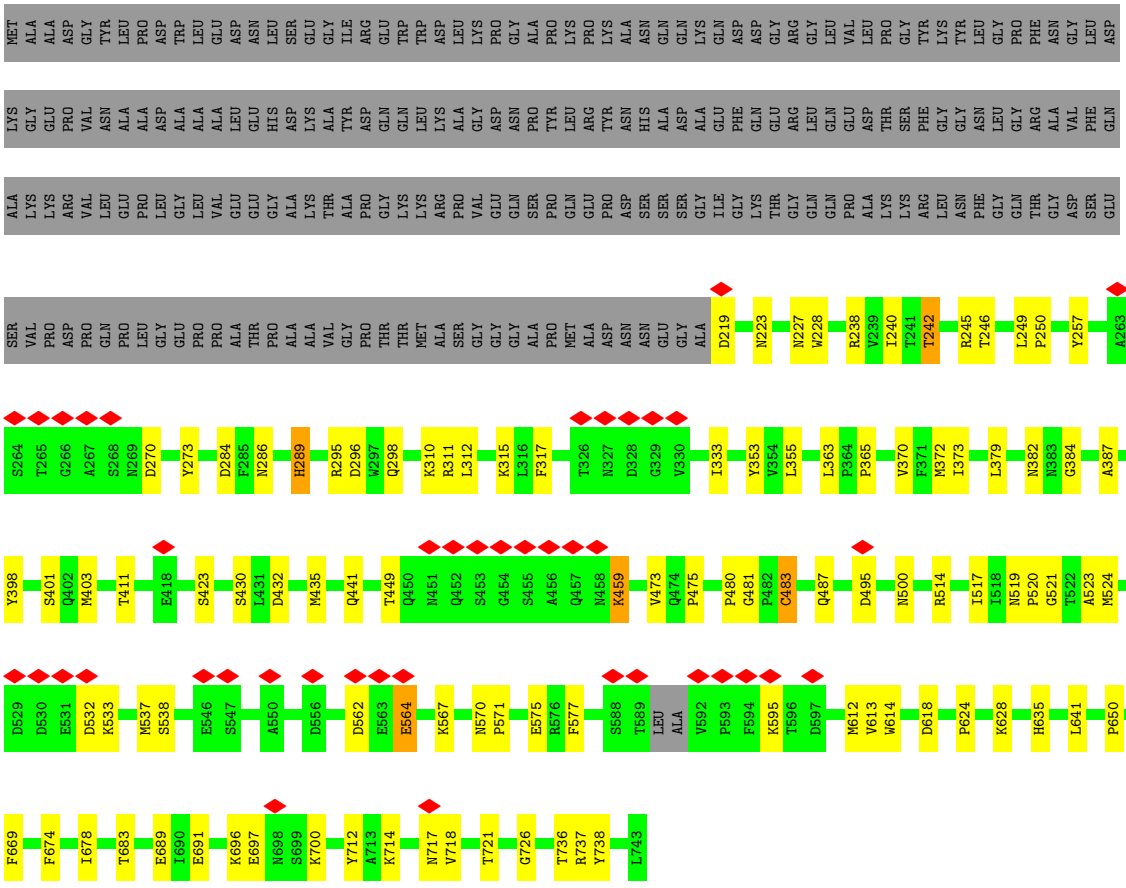
Chain DB:





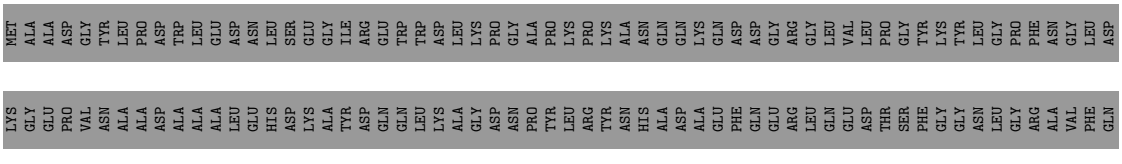
• Molecule 1: Capsid protein

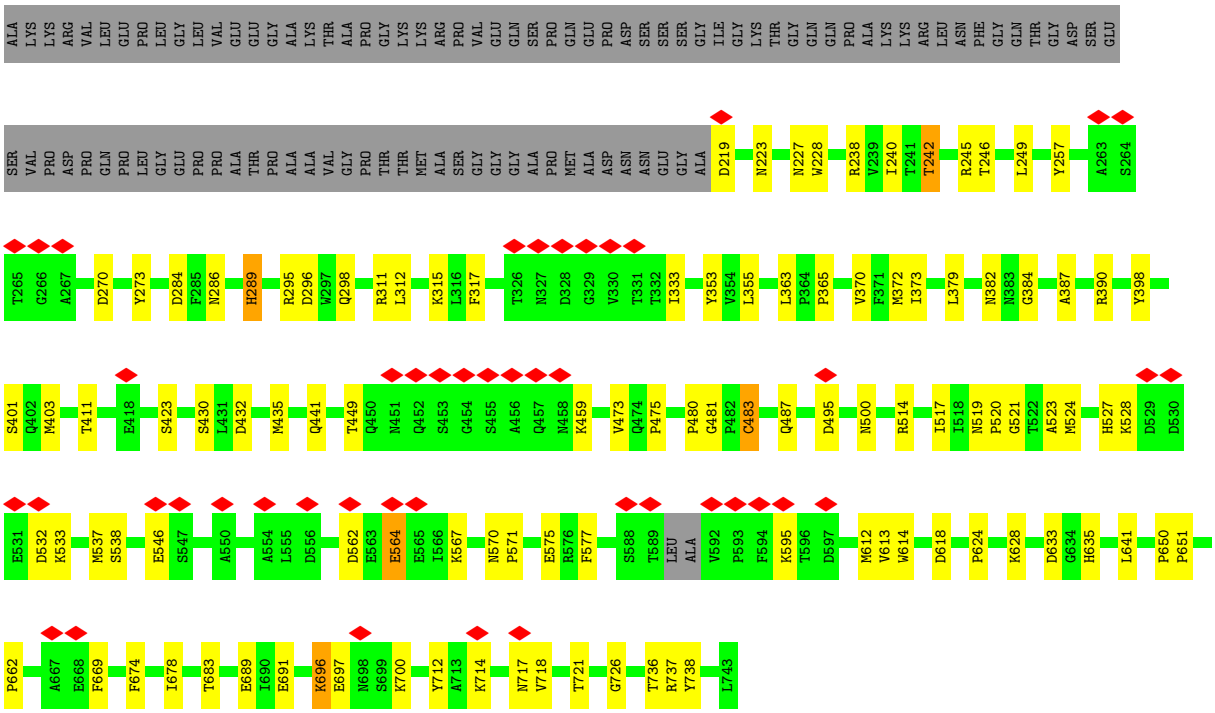
Chain EB:



• Molecule 1: Capsid protein

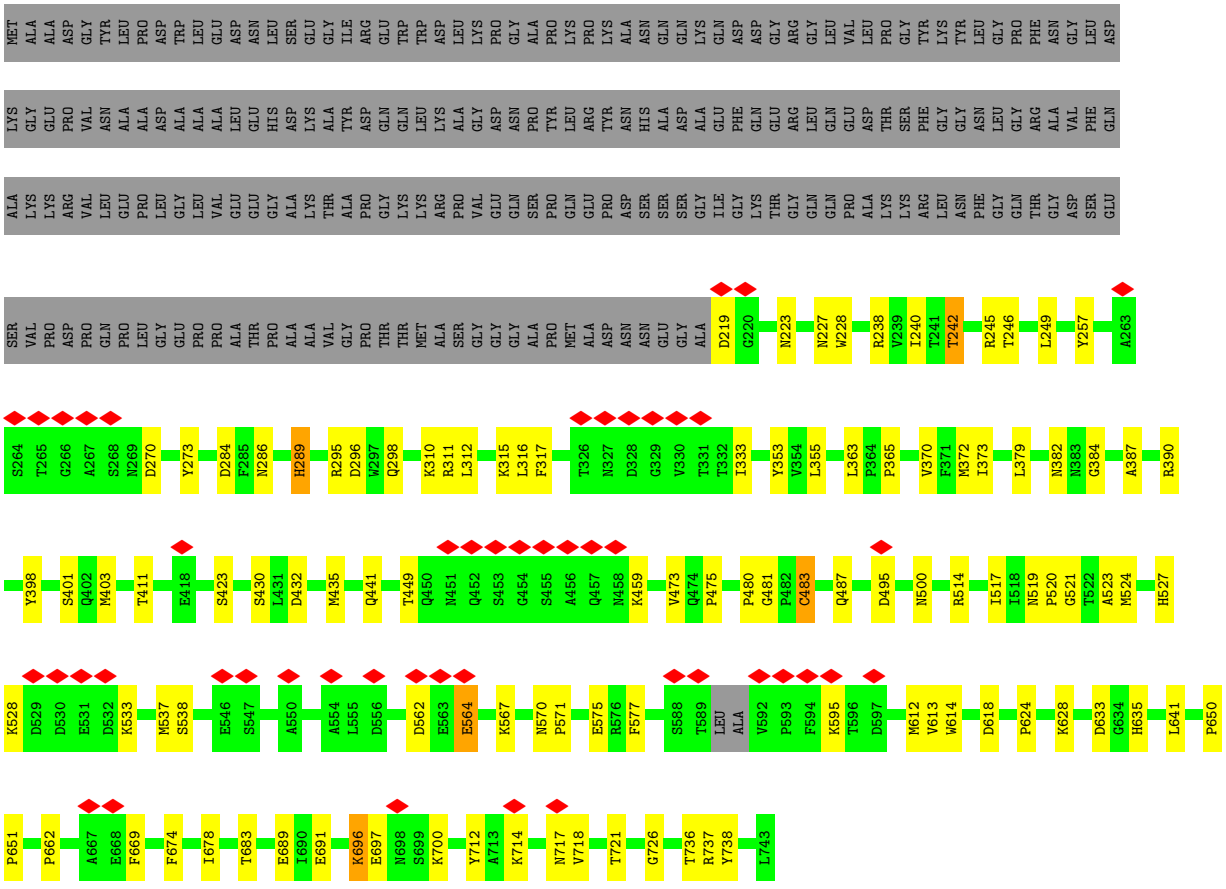
Chain FB:





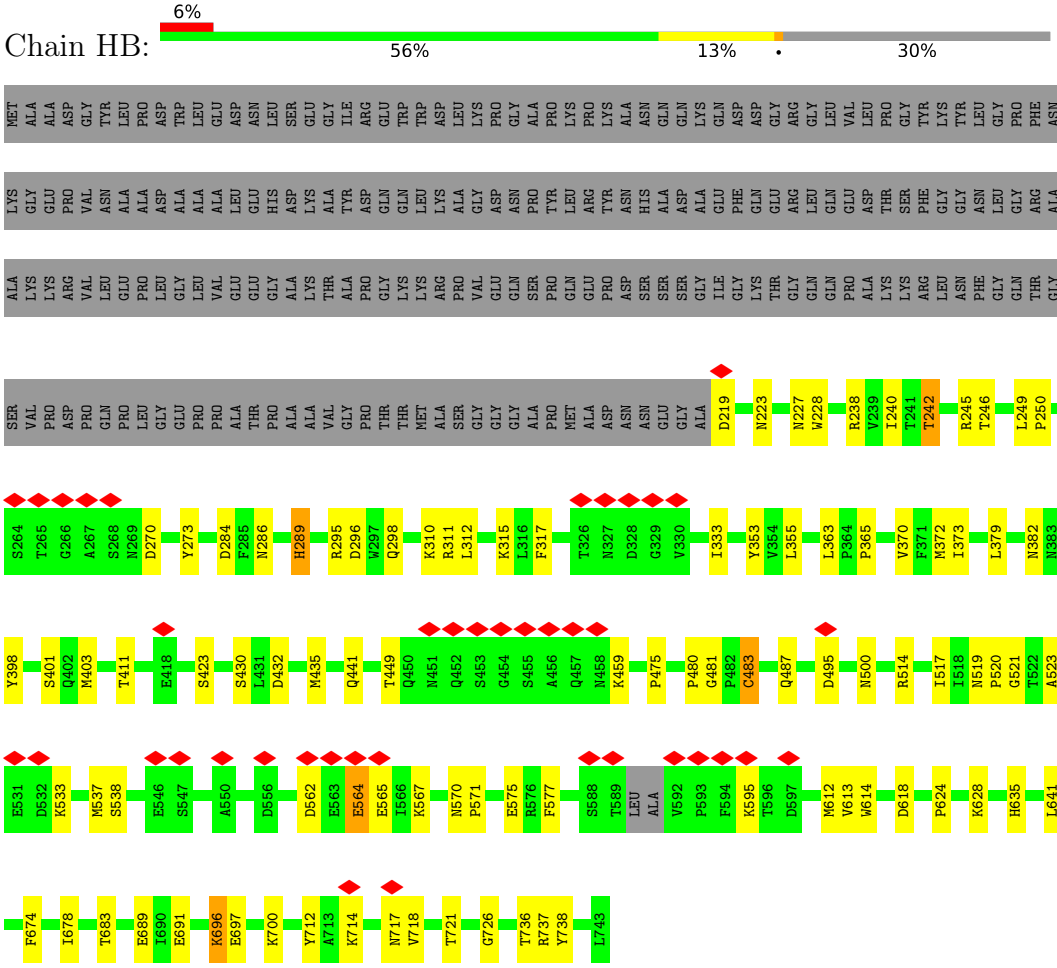
• Molecule 1: Capsid protein

Chain GB:



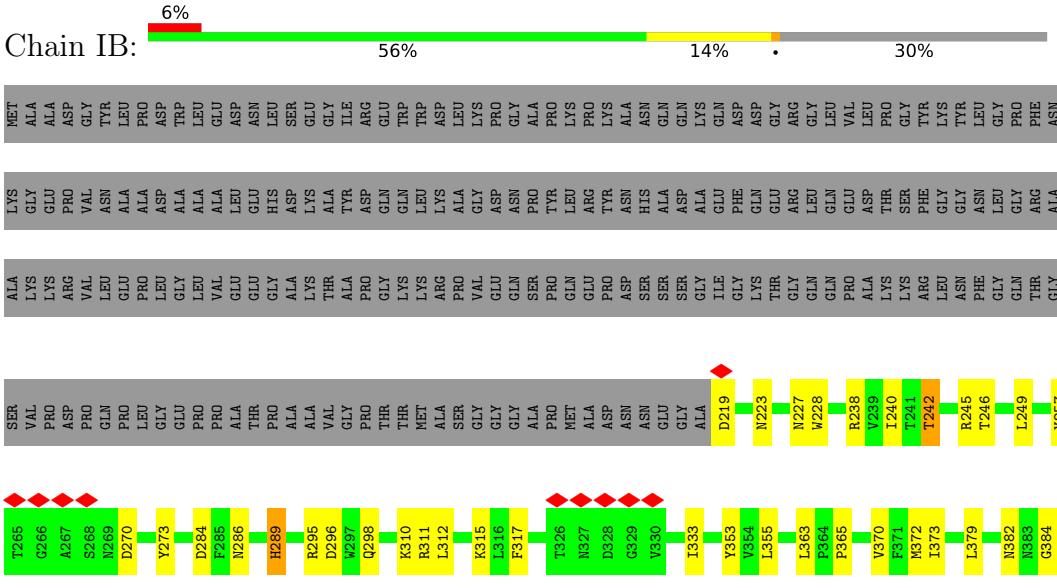
• Molecule 1: Capsid protein

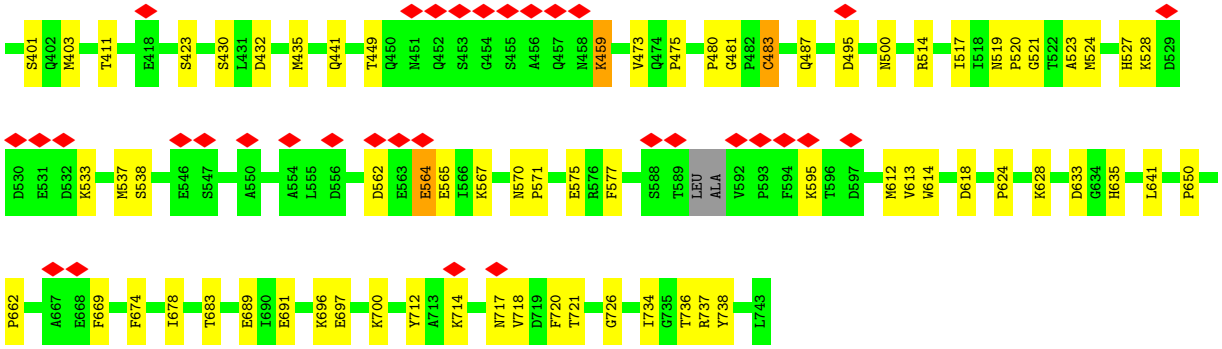
Chain HB:



• Molecule 1: Capsid protein

Chain IB:




S401 Q402 M403 T411 E418 S423 S430 L431 D432 M435 Q441 T449 Q450 N451 Q452 S453 G454 S455 A456 Q457 N458 K459 V473 Q474 P475 P480 G481 P482 C483 Q487 D495 N500 R514 I517 I518 N519 P520 G521 T522 A523 N524 H527 K528 D529
D530 E531 D532 K533 M537 S538 E546 S547 A550 A554 L555 D556 D562 E563 E564 E565 I566 K567 N570 P571 E575 R576 F577 S588 T589 LEU ALA V592 P593 F594 K595 T596 D597 M612 V613 W614 D618 P624 K628 D633 G634 H635 L641 P650
P662 A667 E668 F669 F674 I678 T683 E689 I690 E691 K696 E697 K700 Y712 A713 K714 N717 V718 D719 F720 T721 G726 I734 G735 T736 R737 Y738 L743

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	59346	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	37.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.075	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	417.6, 417.6, 417.6	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	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	A	0.42	0/4251	0.49	0/5797
1	AA	0.42	0/4251	0.49	0/5797
1	AB	0.42	0/4251	0.49	0/5797
1	B	0.42	0/4251	0.49	0/5797
1	BA	0.42	0/4251	0.49	0/5797
1	BB	0.42	0/4251	0.49	0/5797
1	C	0.42	0/4251	0.49	0/5797
1	CA	0.42	0/4251	0.49	0/5797
1	CB	0.42	0/4251	0.49	0/5797
1	D	0.42	0/4251	0.49	0/5797
1	DA	0.42	0/4251	0.49	0/5797
1	DB	0.42	0/4251	0.49	0/5797
1	E	0.42	0/4251	0.49	0/5797
1	EA	0.42	0/4251	0.49	0/5797
1	EB	0.42	0/4251	0.49	0/5797
1	F	0.42	0/4251	0.49	0/5797
1	FA	0.42	0/4251	0.49	0/5797
1	FB	0.42	0/4251	0.49	0/5797
1	G	0.42	0/4251	0.49	0/5797
1	GA	0.42	0/4251	0.49	0/5797
1	GB	0.42	0/4251	0.49	0/5797
1	H	0.42	0/4251	0.49	0/5797
1	HA	0.42	0/4251	0.49	0/5797
1	HB	0.42	0/4251	0.49	0/5797
1	I	0.42	0/4251	0.49	0/5797
1	IA	0.42	0/4251	0.49	0/5797
1	IB	0.42	0/4251	0.49	0/5797
1	J	0.42	0/4251	0.49	0/5797
1	JA	0.42	0/4251	0.49	0/5797
1	K	0.42	0/4251	0.49	0/5797
1	KA	0.42	0/4251	0.49	0/5797
1	L	0.42	0/4251	0.49	0/5797
1	LA	0.42	0/4251	0.49	0/5797
1	M	0.42	0/4251	0.49	0/5797

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	MA	0.41	0/4251	0.49	0/5797
1	N	0.42	0/4251	0.49	0/5797
1	NA	0.42	0/4251	0.49	0/5797
1	O	0.41	0/4251	0.49	0/5797
1	OA	0.42	0/4251	0.49	0/5797
1	P	0.42	0/4251	0.49	0/5797
1	PA	0.42	0/4251	0.49	0/5797
1	Q	0.42	0/4251	0.49	0/5797
1	QA	0.42	0/4251	0.49	0/5797
1	R	0.42	0/4251	0.49	0/5797
1	RA	0.42	0/4251	0.49	0/5797
1	S	0.42	0/4251	0.49	0/5797
1	SA	0.42	0/4251	0.49	0/5797
1	T	0.42	0/4251	0.49	0/5797
1	TA	0.42	0/4251	0.49	0/5797
1	UA	0.42	0/4251	0.49	0/5797
1	V	0.42	0/4251	0.49	0/5797
1	VA	0.41	0/4251	0.49	0/5797
1	W	0.42	0/4251	0.49	0/5797
1	WA	0.42	0/4251	0.49	0/5797
1	X	0.41	0/4251	0.49	0/5797
1	XA	0.42	0/4251	0.49	0/5797
1	Y	0.42	0/4251	0.49	0/5797
1	YA	0.42	0/4251	0.49	0/5797
1	Z	0.42	0/4251	0.49	0/5797
1	ZA	0.42	0/4251	0.49	0/5797
All	All	0.42	0/255060	0.49	0/347820

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	A	4125	0	3867	73	0
1	AA	4125	0	3867	76	0
1	AB	4125	0	3867	79	0
1	B	4125	0	3867	74	0
1	BA	4125	0	3867	77	0
1	BB	4125	0	3867	77	0
1	C	4125	0	3867	75	0
1	CA	4125	0	3867	75	0
1	CB	4125	0	3867	76	0
1	D	4125	0	3867	75	0
1	DA	4125	0	3867	76	0
1	DB	4125	0	3867	76	0
1	E	4125	0	3867	78	0
1	EA	4125	0	3867	75	0
1	EB	4125	0	3867	76	0
1	F	4125	0	3867	75	0
1	FA	4125	0	3867	76	0
1	FB	4125	0	3867	77	0
1	G	4125	0	3867	76	0
1	GA	4125	0	3867	78	0
1	GB	4125	0	3867	77	0
1	H	4125	0	3867	78	0
1	HA	4125	0	3867	75	0
1	HB	4125	0	3867	75	0
1	I	4125	0	3867	75	0
1	IA	4125	0	3867	75	0
1	IB	4125	0	3867	76	0
1	J	4125	0	3867	75	0
1	JA	4125	0	3867	75	0
1	K	4125	0	3867	73	0
1	KA	4125	0	3867	75	0
1	L	4125	0	3867	74	0
1	LA	4125	0	3867	75	0
1	M	4125	0	3867	75	0
1	MA	4125	0	3867	75	0
1	N	4125	0	3867	73	0
1	NA	4125	0	3867	76	0
1	O	4125	0	3867	77	0
1	OA	4125	0	3867	73	0
1	P	4125	0	3867	75	0
1	PA	4125	0	3867	76	0
1	Q	4125	0	3867	78	0
1	QA	4125	0	3867	75	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	4125	0	3867	78	0
1	RA	4125	0	3867	78	0
1	S	4125	0	3867	76	0
1	SA	4125	0	3867	75	0
1	T	4125	0	3867	74	0
1	TA	4125	0	3867	74	0
1	UA	4125	0	3867	76	0
1	V	4125	0	3867	77	0
1	VA	4125	0	3867	75	0
1	W	4125	0	3867	77	0
1	WA	4125	0	3867	77	0
1	X	4125	0	3867	76	0
1	XA	4125	0	3867	73	0
1	Y	4125	0	3867	77	0
1	YA	4125	0	3867	75	0
1	Z	4125	0	3867	75	0
1	ZA	4125	0	3867	78	0
All	All	247500	0	232020	3569	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 7.

The worst 5 of 3569 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:J:564:GLU:HG2	1:J:567:LYS:HE3	1.65	0.79
1:Q:564:GLU:HG2	1:Q:567:LYS:HE3	1.65	0.79
1:T:564:GLU:HG2	1:T:567:LYS:HE3	1.65	0.79
1:X:564:GLU:HG2	1:X:567:LYS:HE3	1.65	0.79
1:TA:564:GLU:HG2	1:TA:567:LYS:HE3	1.65	0.79

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	A	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	AA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	AB	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	B	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	BA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	BB	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	C	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	CA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	CB	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	D	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	DA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	DB	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	E	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	EA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	EB	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	F	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	FA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	FB	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	G	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	GA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	GB	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	H	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	HA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	HB	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	I	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	IA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	IB	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	J	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	JA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	K	519/743 (70%)	504 (97%)	15 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	KA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	L	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	LA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	M	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	MA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	N	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	NA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	O	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	OA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	P	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	PA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	Q	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	QA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	R	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	RA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	S	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	SA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	T	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	TA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	UA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	V	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	VA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	W	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	WA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	X	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	XA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	Y	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	YA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	Z	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
1	ZA	519/743 (70%)	504 (97%)	15 (3%)	0	100	100
All	All	31140/44580 (70%)	30240 (97%)	900 (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	A	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	AA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	AB	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	B	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	BA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	BB	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	C	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	CA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	CB	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	D	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	DA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	DB	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	E	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	EA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	EB	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	F	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	FA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	FB	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	G	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	GA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	GB	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	H	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	HA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	HB	444/623 (71%)	432 (97%)	12 (3%)	44	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	IA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	IB	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	J	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	JA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	K	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	KA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	L	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	LA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	M	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	MA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	N	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	NA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	O	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	OA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	P	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	PA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	Q	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	QA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	R	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	RA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	S	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	SA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	T	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	TA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	UA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	V	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	VA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	W	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	WA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	X	444/623 (71%)	432 (97%)	12 (3%)	44	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	XA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	Y	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	YA	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	Z	444/623 (71%)	432 (97%)	12 (3%)	44	60
1	ZA	444/623 (71%)	432 (97%)	12 (3%)	44	60
All	All	26640/37380 (71%)	25920 (97%)	720 (3%)	48	60

5 of 720 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	NA	564	GLU
1	WA	674	PHE
1	OA	595	LYS
1	NA	562	ASP
1	SA	459	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
1	GA	289	HIS
1	NA	289	HIS
1	EB	289	HIS
1	HA	289	HIS
1	KA	289	HIS

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 monosaccharides 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.

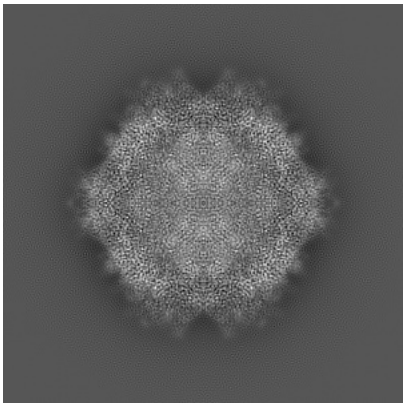
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24495. These allow visual inspection of the internal detail of the map and identification of artifacts.

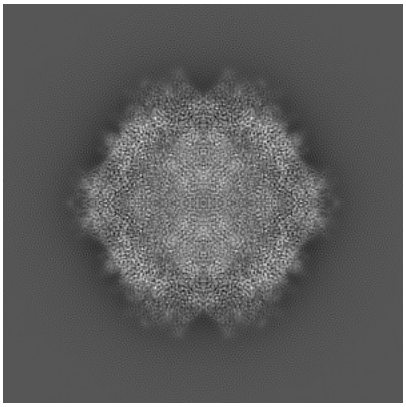
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

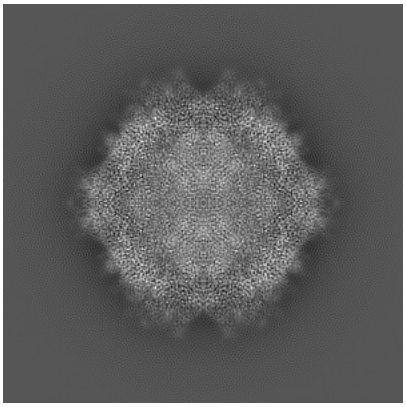
6.1.1 Primary map



X



Y

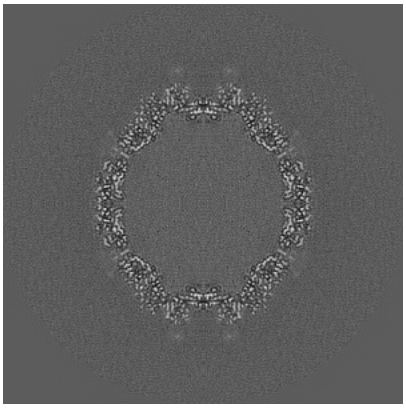


Z

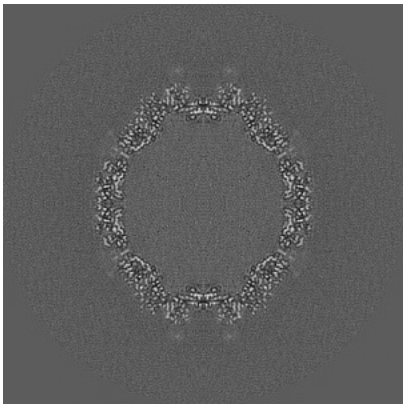
The images above show the map projected in three orthogonal directions.

6.2 Central slices

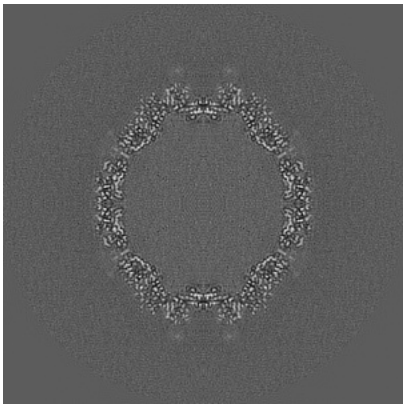
6.2.1 Primary map



X Index: 240



Y Index: 240

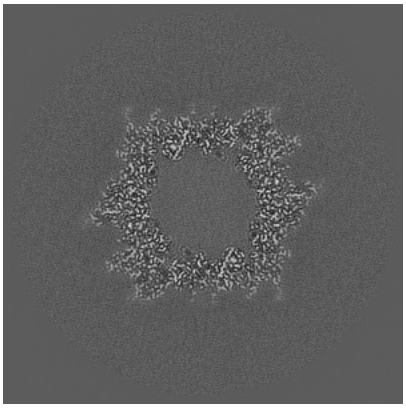


Z Index: 240

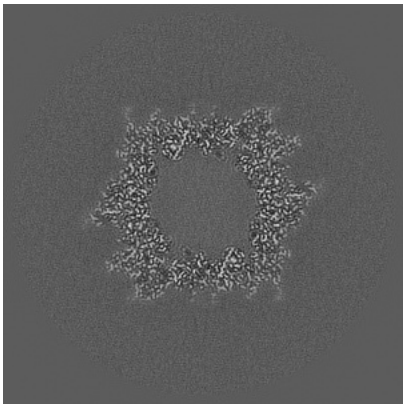
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

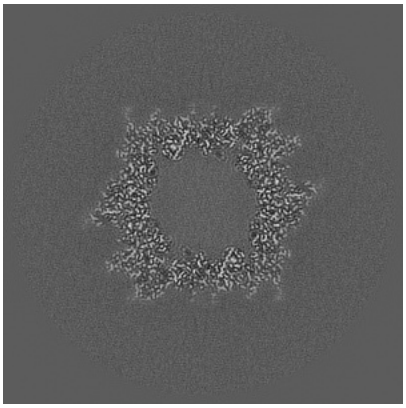
6.3.1 Primary map



X Index: 165



Y Index: 165

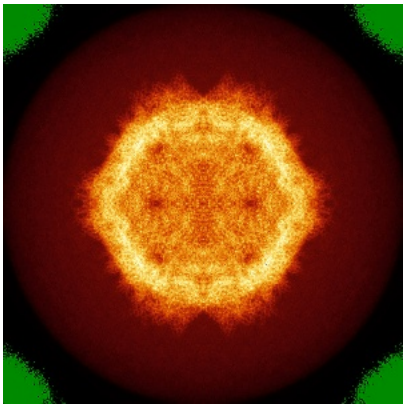


Z Index: 165

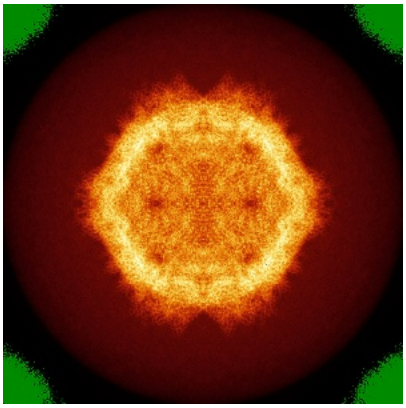
The images above show the largest variance slices of the map in three orthogonal directions.

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

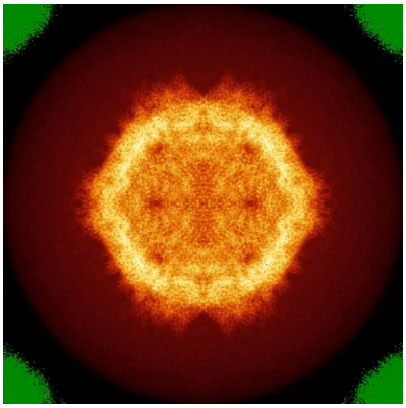
6.4.1 Primary map



X



Y

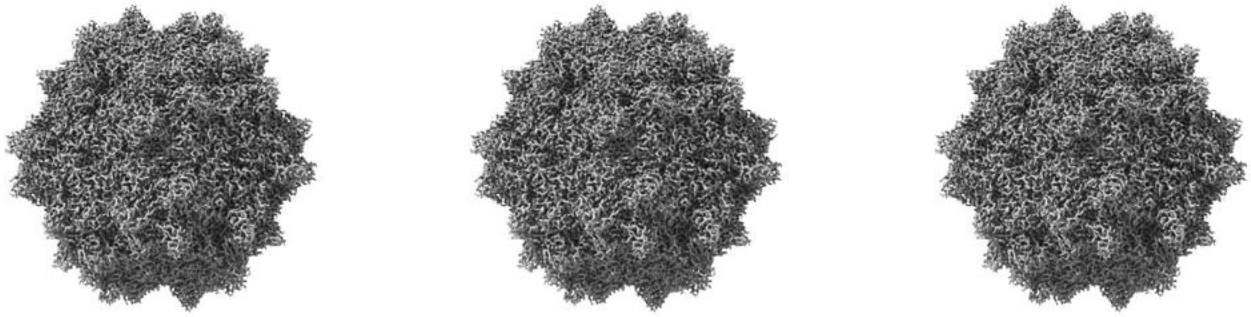


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

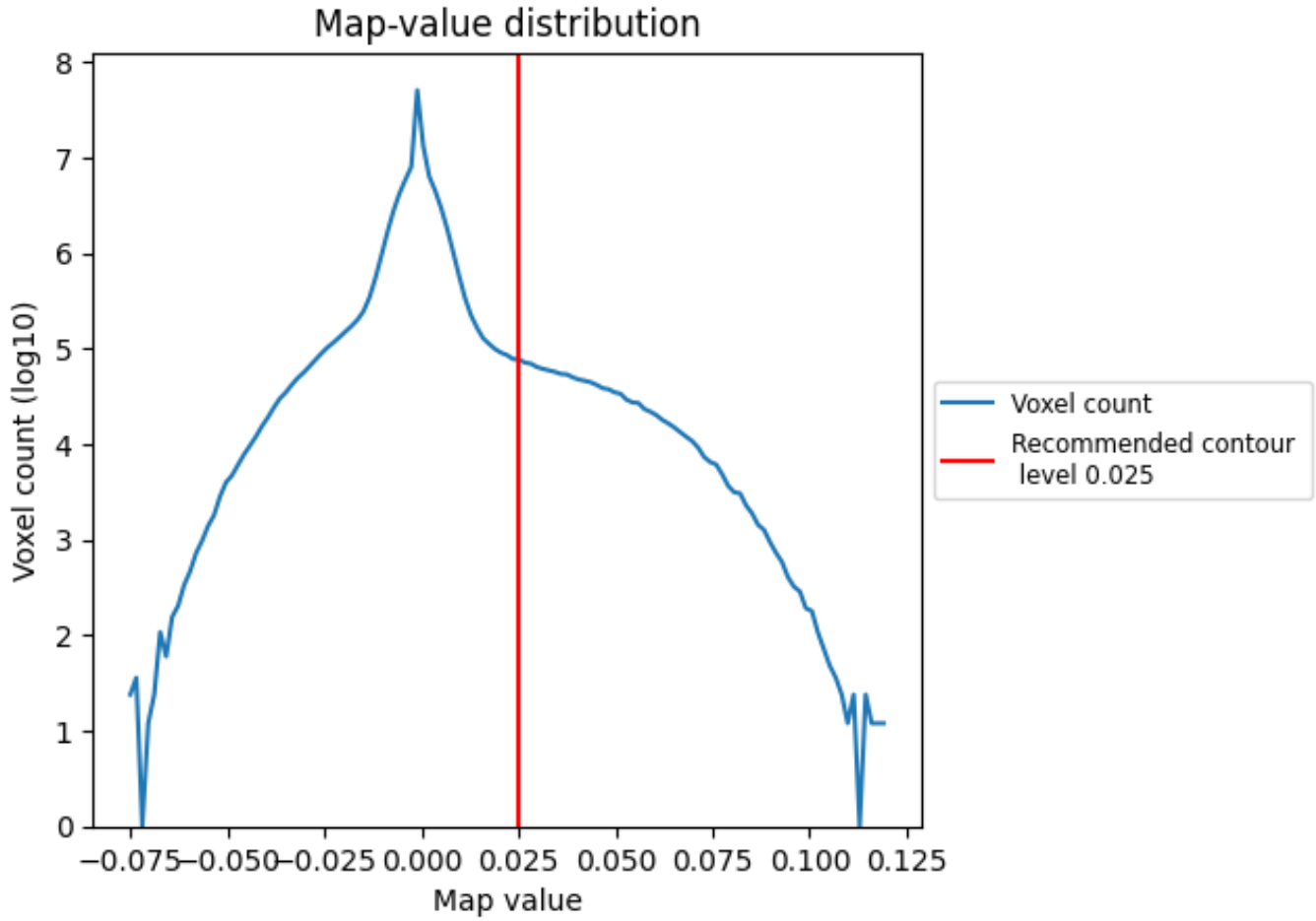
6.6 Mask visualisation (i)

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

7 Map analysis

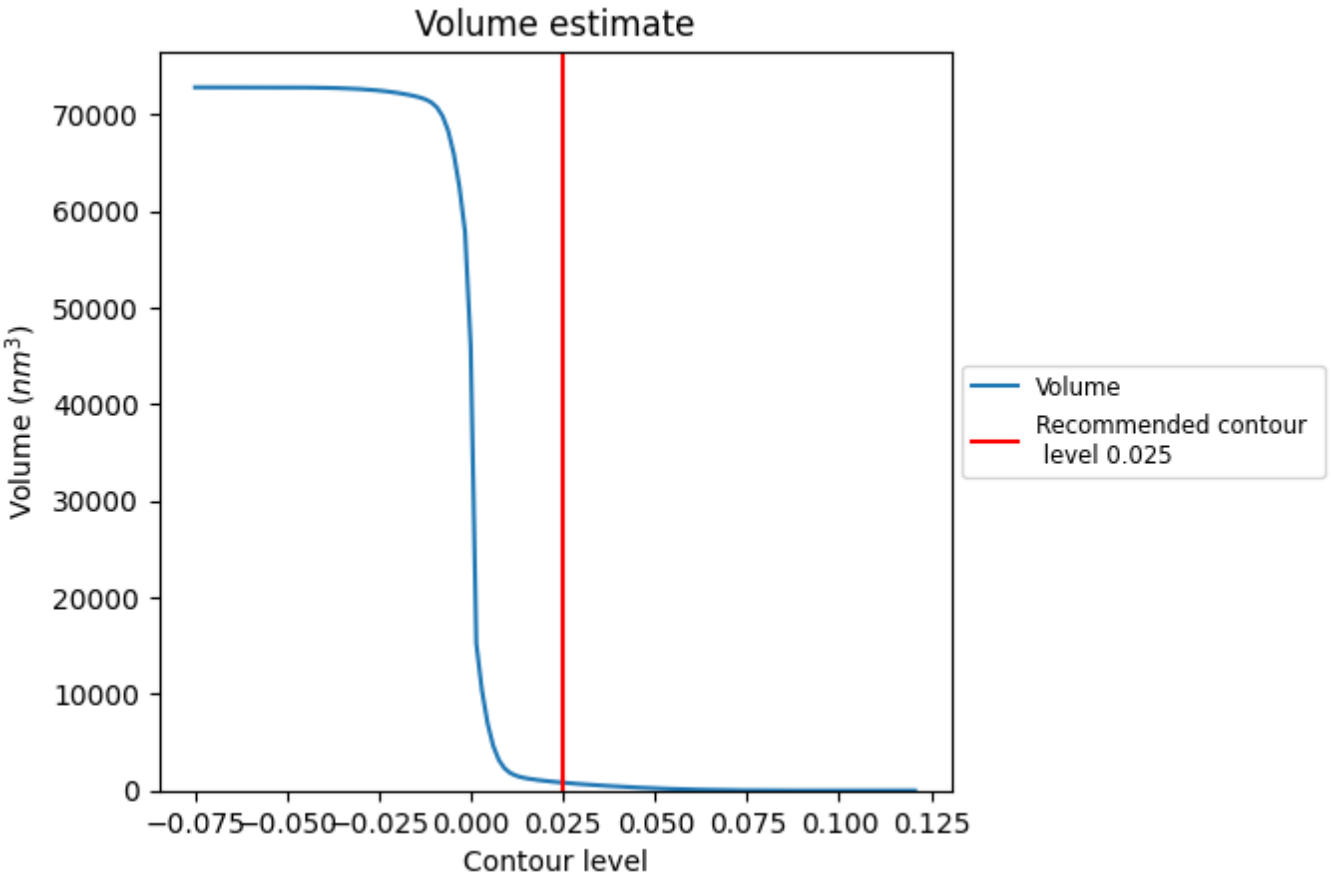
This section contains the results of statistical analysis of the map.

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.

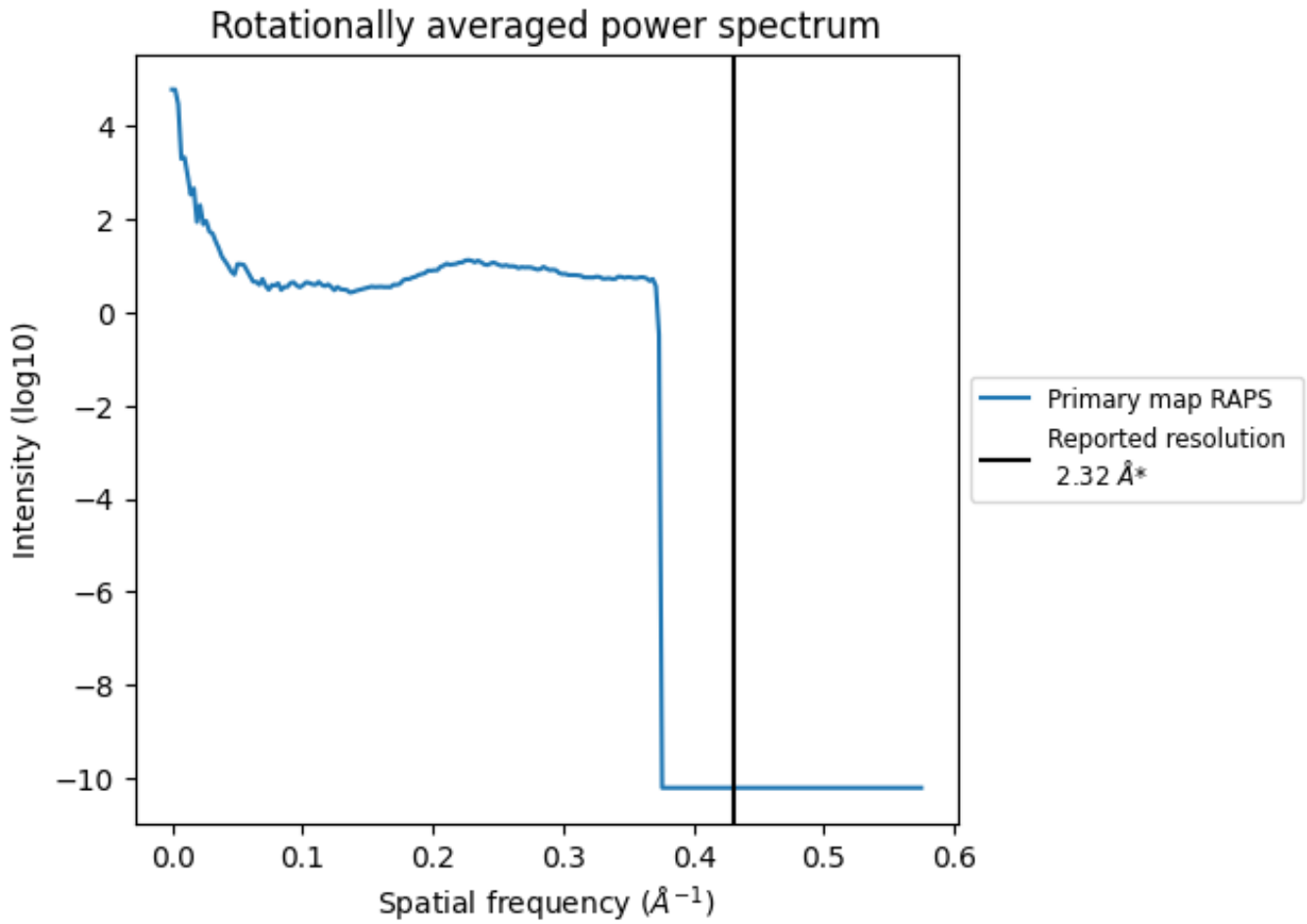
7.2 Volume estimate (i)



The volume at the recommended contour level is 818 nm^3; this corresponds to an approximate mass of 739 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)

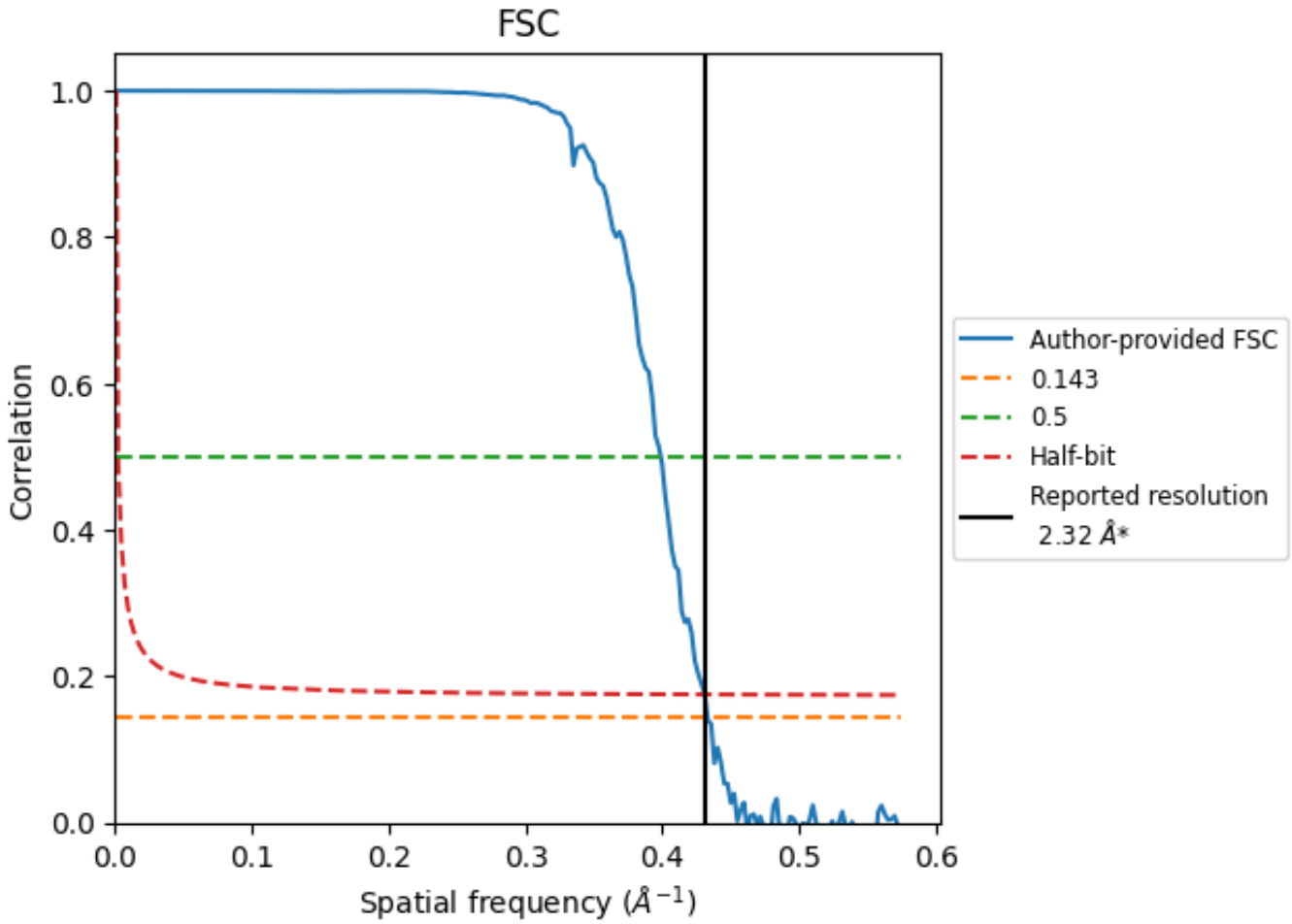


*Reported resolution corresponds to spatial frequency of 0.431 Å^{-1}

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 0.431 Å^{-1}

8.2 Resolution estimates (i)

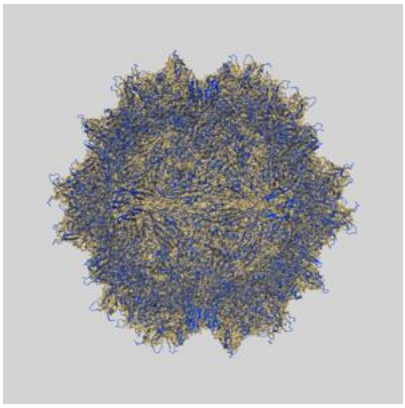
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.32	-	-
Author-provided FSC curve	2.31	2.51	2.32
Unmasked-calculated*	-	-	-

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

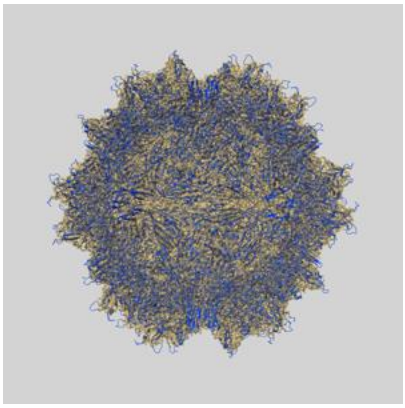
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24495 and PDB model 7RK9. Per-residue inclusion information can be found in section 3 on page 20.

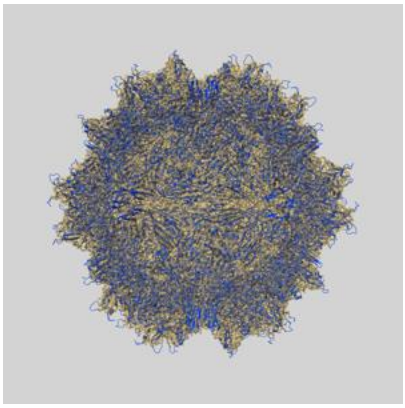
9.1 Map-model overlay



X



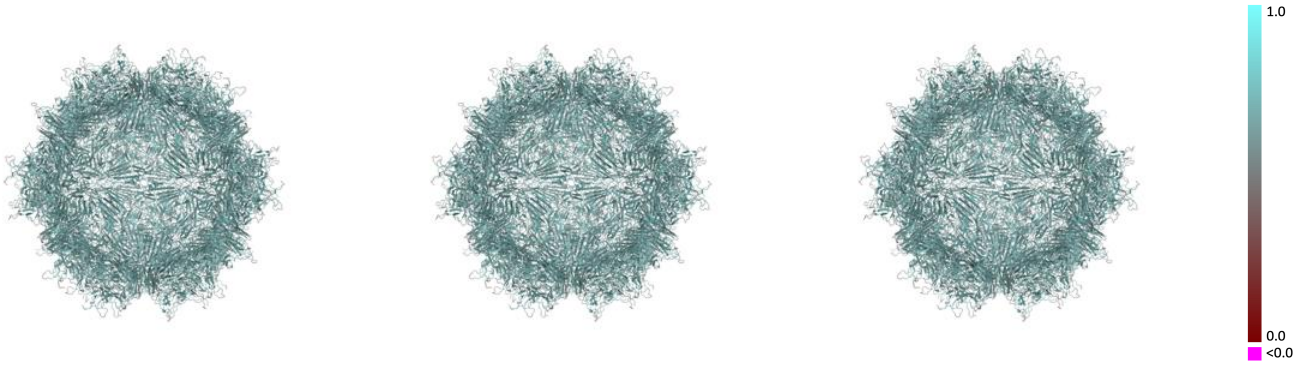
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

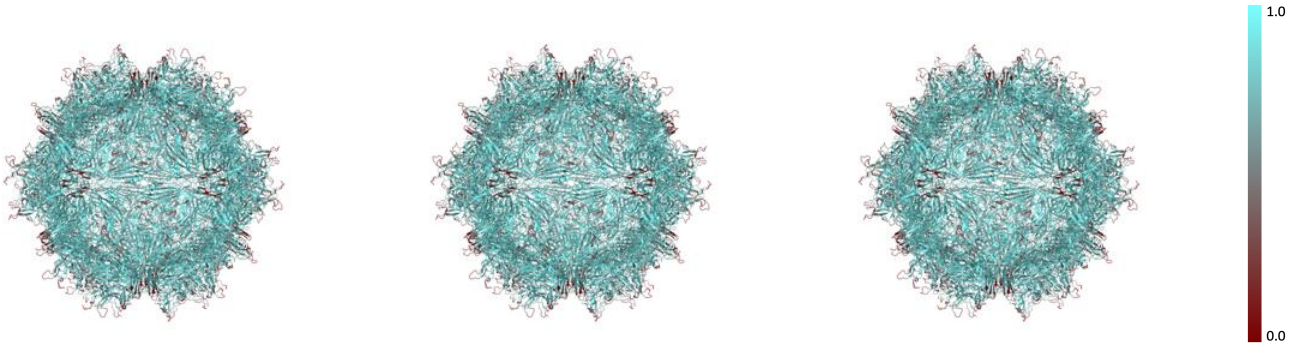
9.2 Q-score mapped to coordinate model



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.

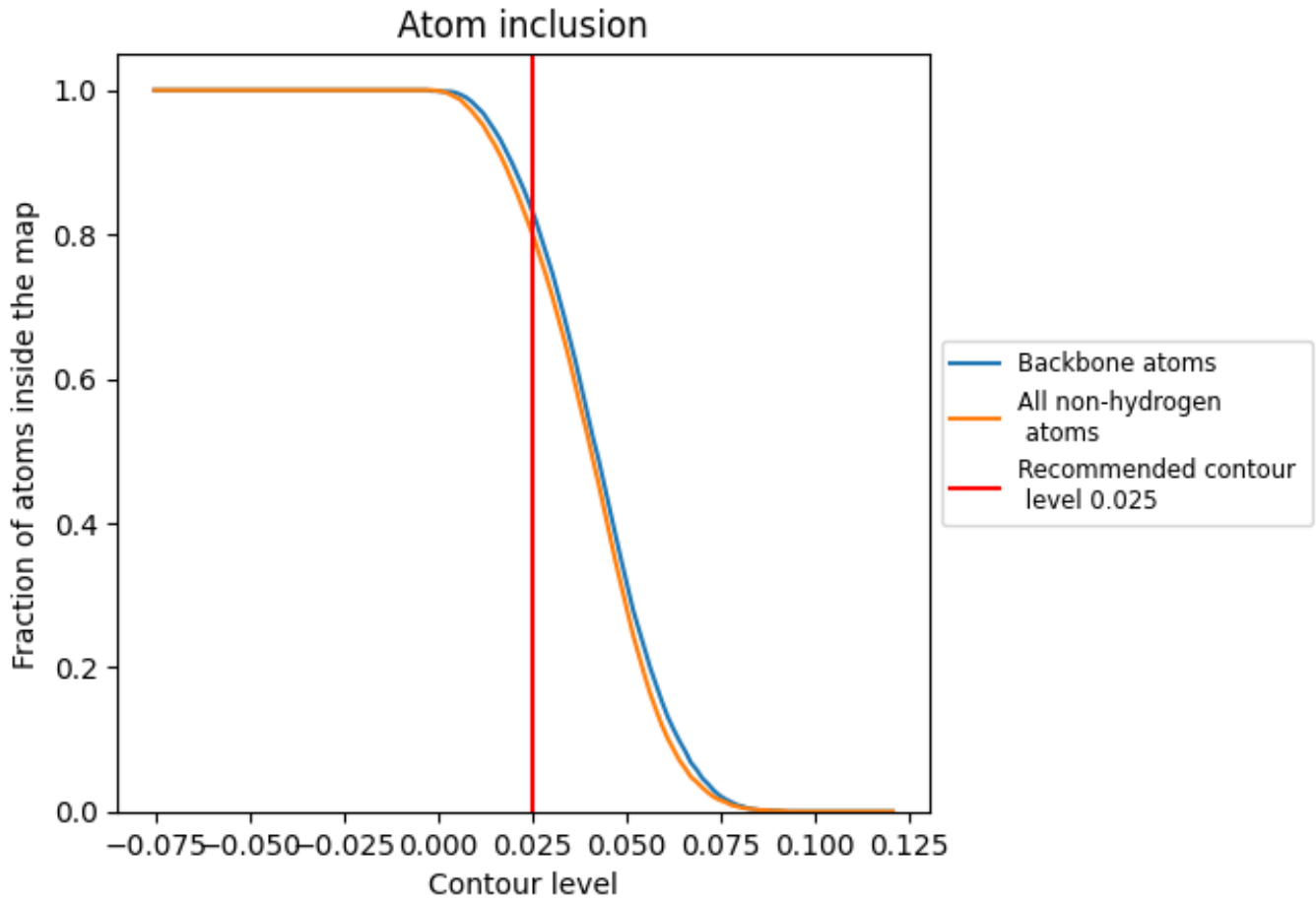
9.3 Atom inclusion mapped to coordinate model



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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8020	0.6640
A	0.8010	0.6630
AA	0.8020	0.6640
AB	0.8010	0.6640
B	0.8020	0.6640
BA	0.8010	0.6640
BB	0.8010	0.6640
C	0.8010	0.6650
CA	0.8010	0.6640
CB	0.8000	0.6630
D	0.8000	0.6640
DA	0.8000	0.6640
DB	0.8040	0.6640
E	0.8040	0.6630
EA	0.8040	0.6640
EB	0.8020	0.6640
F	0.8020	0.6630
FA	0.8020	0.6640
FB	0.8010	0.6630
G	0.8010	0.6630
GA	0.8010	0.6640
GB	0.8010	0.6640
H	0.8010	0.6640
HA	0.8010	0.6640
HB	0.8000	0.6640
I	0.8000	0.6630
IA	0.8000	0.6640
IB	0.8040	0.6640
J	0.8040	0.6630
JA	0.8040	0.6640
K	0.8020	0.6630
KA	0.8020	0.6640
L	0.8010	0.6640
LA	0.8020	0.6640
M	0.8010	0.6640

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
MA	0.8010	0.6630
N	0.8000	0.6640
NA	0.8010	0.6640
O	0.8040	0.6630
OA	0.8040	0.6640
P	0.8020	0.6640
PA	0.8020	0.6650
Q	0.8020	0.6640
QA	0.8010	0.6650
R	0.8010	0.6640
RA	0.8010	0.6640
S	0.8000	0.6640
SA	0.8000	0.6630
T	0.8040	0.6630
TA	0.8040	0.6630
UA	0.8020	0.6640
V	0.8020	0.6640
VA	0.8010	0.6640
W	0.8010	0.6640
WA	0.8010	0.6640
X	0.8010	0.6630
XA	0.8000	0.6630
Y	0.8000	0.6640
YA	0.8040	0.6640
Z	0.8040	0.6650
ZA	0.8020	0.6640