



# wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 05:01 PM EST

PDB ID : 7RK8  
EMDB ID : EMD-24494  
Title : Cryo-EM Structure of Adeno-Associated Virus Serotype 9 with Engineered Peptide Domain PHP.B (AAV9-PHP.B)  
Authors : Fluck, E.C.; Pumroy, R.A.; Moiseenkova-Bell, V.Y.  
Deposited on : 2021-07-22  
Resolution : 2.27 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

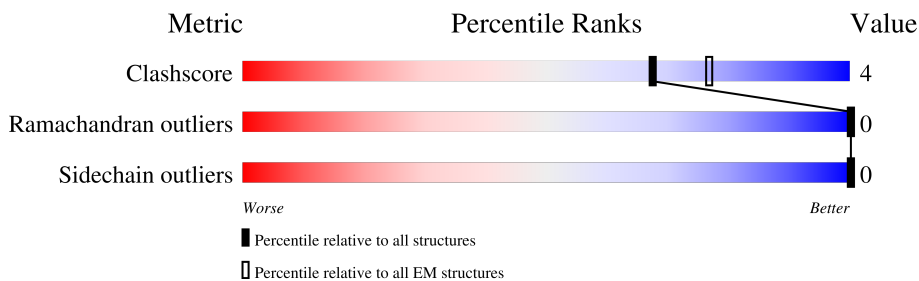
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.27 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.





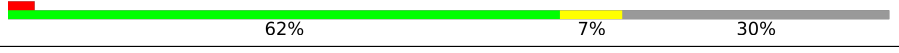
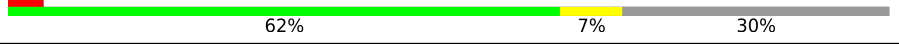



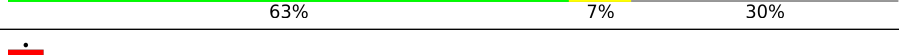
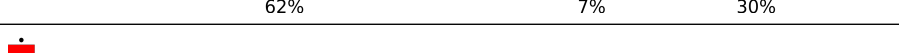
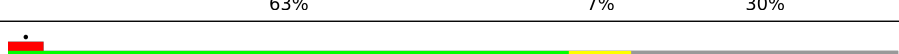
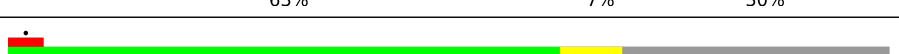

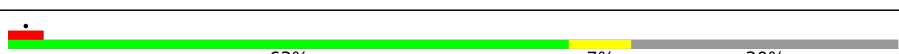
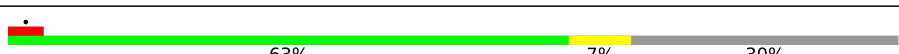
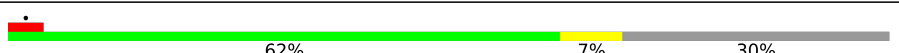




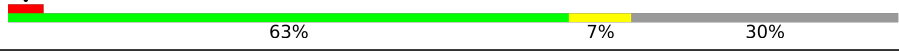





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	743	
1	AA	743	
1	AB	743	
1	B	743	
1	BA	743	
1	BB	743	
1	C	743	
1	CA	743	

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Mol	Chain	Length	Quality of chain
1	CB	743	 62% 7% 30%
1	D	743	 63% 7% 30%
1	DA	743	 62% 7% 30%
1	DB	743	 62% 7% 30%
1	E	743	 63% 7% 30%
1	EA	743	 63% 7% 30%
1	EB	743	 63% 7% 30%
1	F	743	 63% 7% 30%
1	FA	743	 62% 7% 30%
1	FB	743	 63% 7% 30%
1	G	743	 63% 7% 30%
1	GA	743	 62% 7% 30%
1	GB	743	 63% 7% 30%
1	H	743	 63% 7% 30%
1	HA	743	 63% 7% 30%
1	HB	743	 62% 7% 30%
1	I	743	 63% 6% 30%
1	IA	743	 62% 7% 30%
1	IB	743	 62% 7% 30%
1	J	743	 63% 7% 30%
1	JA	743	 63% 7% 30%
1	K	743	 62% 7% 30%
1	KA	743	 62% 7% 30%
1	L	743	 63% 7% 30%
1	LA	743	 63% 7% 30%



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Mol	Chain	Length	Quality of chain			
1	M	743		63%	7%	30%
1	MA	743		63%	6%	30%
1	N	743		62%	8%	30%
1	NA	743		63%	7%	30%
1	O	743		62%	7%	30%
1	OA	743		63%	7%	30%
1	P	743		63%	7%	30%
1	PA	743		63%	7%	30%
1	Q	743		63%	7%	30%
1	QA	743		63%	7%	30%
1	R	743		63%	7%	30%
1	RA	743		62%	7%	30%
1	S	743		63%	7%	30%
1	SA	743		63%	7%	30%
1	T	743		63%	7%	30%
1	TA	743		63%	7%	30%
1	UA	743		63%	7%	30%
1	V	743		63%	6%	30%
1	VA	743		63%	7%	30%
1	W	743		63%	7%	30%
1	WA	743		63%	6%	30%
1	X	743		63%	7%	30%
1	XA	743		62%	7%	30%
1	Y	743		63%	7%	30%
1	YA	743		63%	6%	30%

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Mol	Chain	Length	Quality of chain
1	Z	743	 63% 7% 30%
1	ZA	743	 62% 8% 30%

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 246720 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 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	517	4112	2601	714	783	14	0	0
1	B	517	4112	2601	714	783	14	0	0
1	C	517	4112	2601	714	783	14	0	0
1	D	517	4112	2601	714	783	14	0	0
1	E	517	4112	2601	714	783	14	0	0
1	F	517	4112	2601	714	783	14	0	0
1	G	517	4112	2601	714	783	14	0	0
1	H	517	4112	2601	714	783	14	0	0
1	I	517	4112	2601	714	783	14	0	0
1	J	517	4112	2601	714	783	14	0	0
1	K	517	4112	2601	714	783	14	0	0
1	L	517	4112	2601	714	783	14	0	0
1	M	517	4112	2601	714	783	14	0	0
1	N	517	4112	2601	714	783	14	0	0
1	O	517	4112	2601	714	783	14	0	0
1	P	517	4112	2601	714	783	14	0	0
1	Q	517	4112	2601	714	783	14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	S	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	T	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	V	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	W	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	X	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	Y	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	Z	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	AA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	BA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	CA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	DA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	EA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	FA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	GA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	HA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	IA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	JA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	KA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	LA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	MA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	NA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	OA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	PA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	QA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	RA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	SA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	TA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	UA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	VA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	WA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	XA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	YA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	ZA	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	AB	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	BB	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	CB	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	DB	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	EB	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	FB	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	GB	517	Total 4112	C 2601	N 714	O 783	S 14	0	0
1	HB	517	Total 4112	C 2601	N 714	O 783	S 14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	IB	517	4112	2601	714	783	14	0	0

There are 420 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	589	THR	-	insertion	UNP Q6JC40
A	590	LEU	-	insertion	UNP Q6JC40
A	591	ALA	-	insertion	UNP Q6JC40
A	592	VAL	-	insertion	UNP Q6JC40
A	593	PRO	-	insertion	UNP Q6JC40
A	594	PHE	-	insertion	UNP Q6JC40
A	595	LYS	-	insertion	UNP Q6JC40
B	589	THR	-	insertion	UNP Q6JC40
B	590	LEU	-	insertion	UNP Q6JC40
B	591	ALA	-	insertion	UNP Q6JC40
B	592	VAL	-	insertion	UNP Q6JC40
B	593	PRO	-	insertion	UNP Q6JC40
B	594	PHE	-	insertion	UNP Q6JC40
B	595	LYS	-	insertion	UNP Q6JC40
C	589	THR	-	insertion	UNP Q6JC40
C	590	LEU	-	insertion	UNP Q6JC40
C	591	ALA	-	insertion	UNP Q6JC40
C	592	VAL	-	insertion	UNP Q6JC40
C	593	PRO	-	insertion	UNP Q6JC40
C	594	PHE	-	insertion	UNP Q6JC40
C	595	LYS	-	insertion	UNP Q6JC40
D	589	THR	-	insertion	UNP Q6JC40
D	590	LEU	-	insertion	UNP Q6JC40
D	591	ALA	-	insertion	UNP Q6JC40
D	592	VAL	-	insertion	UNP Q6JC40
D	593	PRO	-	insertion	UNP Q6JC40
D	594	PHE	-	insertion	UNP Q6JC40
D	595	LYS	-	insertion	UNP Q6JC40
E	589	THR	-	insertion	UNP Q6JC40
E	590	LEU	-	insertion	UNP Q6JC40
E	591	ALA	-	insertion	UNP Q6JC40
E	592	VAL	-	insertion	UNP Q6JC40
E	593	PRO	-	insertion	UNP Q6JC40
E	594	PHE	-	insertion	UNP Q6JC40
E	595	LYS	-	insertion	UNP Q6JC40
F	589	THR	-	insertion	UNP Q6JC40

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Chain	Residue	Modelled	Actual	Comment	Reference
F	590	LEU	-	insertion	UNP Q6JC40
F	591	ALA	-	insertion	UNP Q6JC40
F	592	VAL	-	insertion	UNP Q6JC40
F	593	PRO	-	insertion	UNP Q6JC40
F	594	PHE	-	insertion	UNP Q6JC40
F	595	LYS	-	insertion	UNP Q6JC40
G	589	THR	-	insertion	UNP Q6JC40
G	590	LEU	-	insertion	UNP Q6JC40
G	591	ALA	-	insertion	UNP Q6JC40
G	592	VAL	-	insertion	UNP Q6JC40
G	593	PRO	-	insertion	UNP Q6JC40
G	594	PHE	-	insertion	UNP Q6JC40
G	595	LYS	-	insertion	UNP Q6JC40
H	589	THR	-	insertion	UNP Q6JC40
H	590	LEU	-	insertion	UNP Q6JC40
H	591	ALA	-	insertion	UNP Q6JC40
H	592	VAL	-	insertion	UNP Q6JC40
H	593	PRO	-	insertion	UNP Q6JC40
H	594	PHE	-	insertion	UNP Q6JC40
H	595	LYS	-	insertion	UNP Q6JC40
I	589	THR	-	insertion	UNP Q6JC40
I	590	LEU	-	insertion	UNP Q6JC40
I	591	ALA	-	insertion	UNP Q6JC40
I	592	VAL	-	insertion	UNP Q6JC40
I	593	PRO	-	insertion	UNP Q6JC40
I	594	PHE	-	insertion	UNP Q6JC40
I	595	LYS	-	insertion	UNP Q6JC40
J	589	THR	-	insertion	UNP Q6JC40
J	590	LEU	-	insertion	UNP Q6JC40
J	591	ALA	-	insertion	UNP Q6JC40
J	592	VAL	-	insertion	UNP Q6JC40
J	593	PRO	-	insertion	UNP Q6JC40
J	594	PHE	-	insertion	UNP Q6JC40
J	595	LYS	-	insertion	UNP Q6JC40
K	589	THR	-	insertion	UNP Q6JC40
K	590	LEU	-	insertion	UNP Q6JC40
K	591	ALA	-	insertion	UNP Q6JC40
K	592	VAL	-	insertion	UNP Q6JC40
K	593	PRO	-	insertion	UNP Q6JC40
K	594	PHE	-	insertion	UNP Q6JC40
K	595	LYS	-	insertion	UNP Q6JC40
L	589	THR	-	insertion	UNP Q6JC40

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Chain	Residue	Modelled	Actual	Comment	Reference
L	590	LEU	-	insertion	UNP Q6JC40
L	591	ALA	-	insertion	UNP Q6JC40
L	592	VAL	-	insertion	UNP Q6JC40
L	593	PRO	-	insertion	UNP Q6JC40
L	594	PHE	-	insertion	UNP Q6JC40
L	595	LYS	-	insertion	UNP Q6JC40
M	589	THR	-	insertion	UNP Q6JC40
M	590	LEU	-	insertion	UNP Q6JC40
M	591	ALA	-	insertion	UNP Q6JC40
M	592	VAL	-	insertion	UNP Q6JC40
M	593	PRO	-	insertion	UNP Q6JC40
M	594	PHE	-	insertion	UNP Q6JC40
M	595	LYS	-	insertion	UNP Q6JC40
N	589	THR	-	insertion	UNP Q6JC40
N	590	LEU	-	insertion	UNP Q6JC40
N	591	ALA	-	insertion	UNP Q6JC40
N	592	VAL	-	insertion	UNP Q6JC40
N	593	PRO	-	insertion	UNP Q6JC40
N	594	PHE	-	insertion	UNP Q6JC40
N	595	LYS	-	insertion	UNP Q6JC40
O	589	THR	-	insertion	UNP Q6JC40
O	590	LEU	-	insertion	UNP Q6JC40
O	591	ALA	-	insertion	UNP Q6JC40
O	592	VAL	-	insertion	UNP Q6JC40
O	593	PRO	-	insertion	UNP Q6JC40
O	594	PHE	-	insertion	UNP Q6JC40
O	595	LYS	-	insertion	UNP Q6JC40
P	589	THR	-	insertion	UNP Q6JC40
P	590	LEU	-	insertion	UNP Q6JC40
P	591	ALA	-	insertion	UNP Q6JC40
P	592	VAL	-	insertion	UNP Q6JC40
P	593	PRO	-	insertion	UNP Q6JC40
P	594	PHE	-	insertion	UNP Q6JC40
P	595	LYS	-	insertion	UNP Q6JC40
Q	589	THR	-	insertion	UNP Q6JC40
Q	590	LEU	-	insertion	UNP Q6JC40
Q	591	ALA	-	insertion	UNP Q6JC40
Q	592	VAL	-	insertion	UNP Q6JC40
Q	593	PRO	-	insertion	UNP Q6JC40
Q	594	PHE	-	insertion	UNP Q6JC40
Q	595	LYS	-	insertion	UNP Q6JC40
R	589	THR	-	insertion	UNP Q6JC40

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Chain	Residue	Modelled	Actual	Comment	Reference
R	590	LEU	-	insertion	UNP Q6JC40
R	591	ALA	-	insertion	UNP Q6JC40
R	592	VAL	-	insertion	UNP Q6JC40
R	593	PRO	-	insertion	UNP Q6JC40
R	594	PHE	-	insertion	UNP Q6JC40
R	595	LYS	-	insertion	UNP Q6JC40
S	589	THR	-	insertion	UNP Q6JC40
S	590	LEU	-	insertion	UNP Q6JC40
S	591	ALA	-	insertion	UNP Q6JC40
S	592	VAL	-	insertion	UNP Q6JC40
S	593	PRO	-	insertion	UNP Q6JC40
S	594	PHE	-	insertion	UNP Q6JC40
S	595	LYS	-	insertion	UNP Q6JC40
T	589	THR	-	insertion	UNP Q6JC40
T	590	LEU	-	insertion	UNP Q6JC40
T	591	ALA	-	insertion	UNP Q6JC40
T	592	VAL	-	insertion	UNP Q6JC40
T	593	PRO	-	insertion	UNP Q6JC40
T	594	PHE	-	insertion	UNP Q6JC40
T	595	LYS	-	insertion	UNP Q6JC40
V	589	THR	-	insertion	UNP Q6JC40
V	590	LEU	-	insertion	UNP Q6JC40
V	591	ALA	-	insertion	UNP Q6JC40
V	592	VAL	-	insertion	UNP Q6JC40
V	593	PRO	-	insertion	UNP Q6JC40
V	594	PHE	-	insertion	UNP Q6JC40
V	595	LYS	-	insertion	UNP Q6JC40
W	589	THR	-	insertion	UNP Q6JC40
W	590	LEU	-	insertion	UNP Q6JC40
W	591	ALA	-	insertion	UNP Q6JC40
W	592	VAL	-	insertion	UNP Q6JC40
W	593	PRO	-	insertion	UNP Q6JC40
W	594	PHE	-	insertion	UNP Q6JC40
W	595	LYS	-	insertion	UNP Q6JC40
X	589	THR	-	insertion	UNP Q6JC40
X	590	LEU	-	insertion	UNP Q6JC40
X	591	ALA	-	insertion	UNP Q6JC40
X	592	VAL	-	insertion	UNP Q6JC40
X	593	PRO	-	insertion	UNP Q6JC40
X	594	PHE	-	insertion	UNP Q6JC40
X	595	LYS	-	insertion	UNP Q6JC40
Y	589	THR	-	insertion	UNP Q6JC40

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	590	LEU	-	insertion	UNP Q6JC40
Y	591	ALA	-	insertion	UNP Q6JC40
Y	592	VAL	-	insertion	UNP Q6JC40
Y	593	PRO	-	insertion	UNP Q6JC40
Y	594	PHE	-	insertion	UNP Q6JC40
Y	595	LYS	-	insertion	UNP Q6JC40
Z	589	THR	-	insertion	UNP Q6JC40
Z	590	LEU	-	insertion	UNP Q6JC40
Z	591	ALA	-	insertion	UNP Q6JC40
Z	592	VAL	-	insertion	UNP Q6JC40
Z	593	PRO	-	insertion	UNP Q6JC40
Z	594	PHE	-	insertion	UNP Q6JC40
Z	595	LYS	-	insertion	UNP Q6JC40
AA	589	THR	-	insertion	UNP Q6JC40
AA	590	LEU	-	insertion	UNP Q6JC40
AA	591	ALA	-	insertion	UNP Q6JC40
AA	592	VAL	-	insertion	UNP Q6JC40
AA	593	PRO	-	insertion	UNP Q6JC40
AA	594	PHE	-	insertion	UNP Q6JC40
AA	595	LYS	-	insertion	UNP Q6JC40
BA	589	THR	-	insertion	UNP Q6JC40
BA	590	LEU	-	insertion	UNP Q6JC40
BA	591	ALA	-	insertion	UNP Q6JC40
BA	592	VAL	-	insertion	UNP Q6JC40
BA	593	PRO	-	insertion	UNP Q6JC40
BA	594	PHE	-	insertion	UNP Q6JC40
BA	595	LYS	-	insertion	UNP Q6JC40
CA	589	THR	-	insertion	UNP Q6JC40
CA	590	LEU	-	insertion	UNP Q6JC40
CA	591	ALA	-	insertion	UNP Q6JC40
CA	592	VAL	-	insertion	UNP Q6JC40
CA	593	PRO	-	insertion	UNP Q6JC40
CA	594	PHE	-	insertion	UNP Q6JC40
CA	595	LYS	-	insertion	UNP Q6JC40
DA	589	THR	-	insertion	UNP Q6JC40
DA	590	LEU	-	insertion	UNP Q6JC40
DA	591	ALA	-	insertion	UNP Q6JC40
DA	592	VAL	-	insertion	UNP Q6JC40
DA	593	PRO	-	insertion	UNP Q6JC40
DA	594	PHE	-	insertion	UNP Q6JC40
DA	595	LYS	-	insertion	UNP Q6JC40
EA	589	THR	-	insertion	UNP Q6JC40

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Chain	Residue	Modelled	Actual	Comment	Reference
EA	590	LEU	-	insertion	UNP Q6JC40
EA	591	ALA	-	insertion	UNP Q6JC40
EA	592	VAL	-	insertion	UNP Q6JC40
EA	593	PRO	-	insertion	UNP Q6JC40
EA	594	PHE	-	insertion	UNP Q6JC40
EA	595	LYS	-	insertion	UNP Q6JC40
FA	589	THR	-	insertion	UNP Q6JC40
FA	590	LEU	-	insertion	UNP Q6JC40
FA	591	ALA	-	insertion	UNP Q6JC40
FA	592	VAL	-	insertion	UNP Q6JC40
FA	593	PRO	-	insertion	UNP Q6JC40
FA	594	PHE	-	insertion	UNP Q6JC40
FA	595	LYS	-	insertion	UNP Q6JC40
GA	589	THR	-	insertion	UNP Q6JC40
GA	590	LEU	-	insertion	UNP Q6JC40
GA	591	ALA	-	insertion	UNP Q6JC40
GA	592	VAL	-	insertion	UNP Q6JC40
GA	593	PRO	-	insertion	UNP Q6JC40
GA	594	PHE	-	insertion	UNP Q6JC40
GA	595	LYS	-	insertion	UNP Q6JC40
HA	589	THR	-	insertion	UNP Q6JC40
HA	590	LEU	-	insertion	UNP Q6JC40
HA	591	ALA	-	insertion	UNP Q6JC40
HA	592	VAL	-	insertion	UNP Q6JC40
HA	593	PRO	-	insertion	UNP Q6JC40
HA	594	PHE	-	insertion	UNP Q6JC40
HA	595	LYS	-	insertion	UNP Q6JC40
IA	589	THR	-	insertion	UNP Q6JC40
IA	590	LEU	-	insertion	UNP Q6JC40
IA	591	ALA	-	insertion	UNP Q6JC40
IA	592	VAL	-	insertion	UNP Q6JC40
IA	593	PRO	-	insertion	UNP Q6JC40
IA	594	PHE	-	insertion	UNP Q6JC40
IA	595	LYS	-	insertion	UNP Q6JC40
JA	589	THR	-	insertion	UNP Q6JC40
JA	590	LEU	-	insertion	UNP Q6JC40
JA	591	ALA	-	insertion	UNP Q6JC40
JA	592	VAL	-	insertion	UNP Q6JC40
JA	593	PRO	-	insertion	UNP Q6JC40
JA	594	PHE	-	insertion	UNP Q6JC40
JA	595	LYS	-	insertion	UNP Q6JC40
KA	589	THR	-	insertion	UNP Q6JC40

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Chain	Residue	Modelled	Actual	Comment	Reference
KA	590	LEU	-	insertion	UNP Q6JC40
KA	591	ALA	-	insertion	UNP Q6JC40
KA	592	VAL	-	insertion	UNP Q6JC40
KA	593	PRO	-	insertion	UNP Q6JC40
KA	594	PHE	-	insertion	UNP Q6JC40
KA	595	LYS	-	insertion	UNP Q6JC40
LA	589	THR	-	insertion	UNP Q6JC40
LA	590	LEU	-	insertion	UNP Q6JC40
LA	591	ALA	-	insertion	UNP Q6JC40
LA	592	VAL	-	insertion	UNP Q6JC40
LA	593	PRO	-	insertion	UNP Q6JC40
LA	594	PHE	-	insertion	UNP Q6JC40
LA	595	LYS	-	insertion	UNP Q6JC40
MA	589	THR	-	insertion	UNP Q6JC40
MA	590	LEU	-	insertion	UNP Q6JC40
MA	591	ALA	-	insertion	UNP Q6JC40
MA	592	VAL	-	insertion	UNP Q6JC40
MA	593	PRO	-	insertion	UNP Q6JC40
MA	594	PHE	-	insertion	UNP Q6JC40
MA	595	LYS	-	insertion	UNP Q6JC40
NA	589	THR	-	insertion	UNP Q6JC40
NA	590	LEU	-	insertion	UNP Q6JC40
NA	591	ALA	-	insertion	UNP Q6JC40
NA	592	VAL	-	insertion	UNP Q6JC40
NA	593	PRO	-	insertion	UNP Q6JC40
NA	594	PHE	-	insertion	UNP Q6JC40
NA	595	LYS	-	insertion	UNP Q6JC40
OA	589	THR	-	insertion	UNP Q6JC40
OA	590	LEU	-	insertion	UNP Q6JC40
OA	591	ALA	-	insertion	UNP Q6JC40
OA	592	VAL	-	insertion	UNP Q6JC40
OA	593	PRO	-	insertion	UNP Q6JC40
OA	594	PHE	-	insertion	UNP Q6JC40
OA	595	LYS	-	insertion	UNP Q6JC40
PA	589	THR	-	insertion	UNP Q6JC40
PA	590	LEU	-	insertion	UNP Q6JC40
PA	591	ALA	-	insertion	UNP Q6JC40
PA	592	VAL	-	insertion	UNP Q6JC40
PA	593	PRO	-	insertion	UNP Q6JC40
PA	594	PHE	-	insertion	UNP Q6JC40
PA	595	LYS	-	insertion	UNP Q6JC40
QA	589	THR	-	insertion	UNP Q6JC40

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Chain	Residue	Modelled	Actual	Comment	Reference
QA	590	LEU	-	insertion	UNP Q6JC40
QA	591	ALA	-	insertion	UNP Q6JC40
QA	592	VAL	-	insertion	UNP Q6JC40
QA	593	PRO	-	insertion	UNP Q6JC40
QA	594	PHE	-	insertion	UNP Q6JC40
QA	595	LYS	-	insertion	UNP Q6JC40
RA	589	THR	-	insertion	UNP Q6JC40
RA	590	LEU	-	insertion	UNP Q6JC40
RA	591	ALA	-	insertion	UNP Q6JC40
RA	592	VAL	-	insertion	UNP Q6JC40
RA	593	PRO	-	insertion	UNP Q6JC40
RA	594	PHE	-	insertion	UNP Q6JC40
RA	595	LYS	-	insertion	UNP Q6JC40
SA	589	THR	-	insertion	UNP Q6JC40
SA	590	LEU	-	insertion	UNP Q6JC40
SA	591	ALA	-	insertion	UNP Q6JC40
SA	592	VAL	-	insertion	UNP Q6JC40
SA	593	PRO	-	insertion	UNP Q6JC40
SA	594	PHE	-	insertion	UNP Q6JC40
SA	595	LYS	-	insertion	UNP Q6JC40
TA	589	THR	-	insertion	UNP Q6JC40
TA	590	LEU	-	insertion	UNP Q6JC40
TA	591	ALA	-	insertion	UNP Q6JC40
TA	592	VAL	-	insertion	UNP Q6JC40
TA	593	PRO	-	insertion	UNP Q6JC40
TA	594	PHE	-	insertion	UNP Q6JC40
TA	595	LYS	-	insertion	UNP Q6JC40
UA	589	THR	-	insertion	UNP Q6JC40
UA	590	LEU	-	insertion	UNP Q6JC40
UA	591	ALA	-	insertion	UNP Q6JC40
UA	592	VAL	-	insertion	UNP Q6JC40
UA	593	PRO	-	insertion	UNP Q6JC40
UA	594	PHE	-	insertion	UNP Q6JC40
UA	595	LYS	-	insertion	UNP Q6JC40
VA	589	THR	-	insertion	UNP Q6JC40
VA	590	LEU	-	insertion	UNP Q6JC40
VA	591	ALA	-	insertion	UNP Q6JC40
VA	592	VAL	-	insertion	UNP Q6JC40
VA	593	PRO	-	insertion	UNP Q6JC40
VA	594	PHE	-	insertion	UNP Q6JC40
VA	595	LYS	-	insertion	UNP Q6JC40
WA	589	THR	-	insertion	UNP Q6JC40

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Chain	Residue	Modelled	Actual	Comment	Reference
WA	590	LEU	-	insertion	UNP Q6JC40
WA	591	ALA	-	insertion	UNP Q6JC40
WA	592	VAL	-	insertion	UNP Q6JC40
WA	593	PRO	-	insertion	UNP Q6JC40
WA	594	PHE	-	insertion	UNP Q6JC40
WA	595	LYS	-	insertion	UNP Q6JC40
XA	589	THR	-	insertion	UNP Q6JC40
XA	590	LEU	-	insertion	UNP Q6JC40
XA	591	ALA	-	insertion	UNP Q6JC40
XA	592	VAL	-	insertion	UNP Q6JC40
XA	593	PRO	-	insertion	UNP Q6JC40
XA	594	PHE	-	insertion	UNP Q6JC40
XA	595	LYS	-	insertion	UNP Q6JC40
YA	589	THR	-	insertion	UNP Q6JC40
YA	590	LEU	-	insertion	UNP Q6JC40
YA	591	ALA	-	insertion	UNP Q6JC40
YA	592	VAL	-	insertion	UNP Q6JC40
YA	593	PRO	-	insertion	UNP Q6JC40
YA	594	PHE	-	insertion	UNP Q6JC40
YA	595	LYS	-	insertion	UNP Q6JC40
ZA	589	THR	-	insertion	UNP Q6JC40
ZA	590	LEU	-	insertion	UNP Q6JC40
ZA	591	ALA	-	insertion	UNP Q6JC40
ZA	592	VAL	-	insertion	UNP Q6JC40
ZA	593	PRO	-	insertion	UNP Q6JC40
ZA	594	PHE	-	insertion	UNP Q6JC40
ZA	595	LYS	-	insertion	UNP Q6JC40
AB	589	THR	-	insertion	UNP Q6JC40
AB	590	LEU	-	insertion	UNP Q6JC40
AB	591	ALA	-	insertion	UNP Q6JC40
AB	592	VAL	-	insertion	UNP Q6JC40
AB	593	PRO	-	insertion	UNP Q6JC40
AB	594	PHE	-	insertion	UNP Q6JC40
AB	595	LYS	-	insertion	UNP Q6JC40
BB	589	THR	-	insertion	UNP Q6JC40
BB	590	LEU	-	insertion	UNP Q6JC40
BB	591	ALA	-	insertion	UNP Q6JC40
BB	592	VAL	-	insertion	UNP Q6JC40
BB	593	PRO	-	insertion	UNP Q6JC40
BB	594	PHE	-	insertion	UNP Q6JC40
BB	595	LYS	-	insertion	UNP Q6JC40
CB	589	THR	-	insertion	UNP Q6JC40

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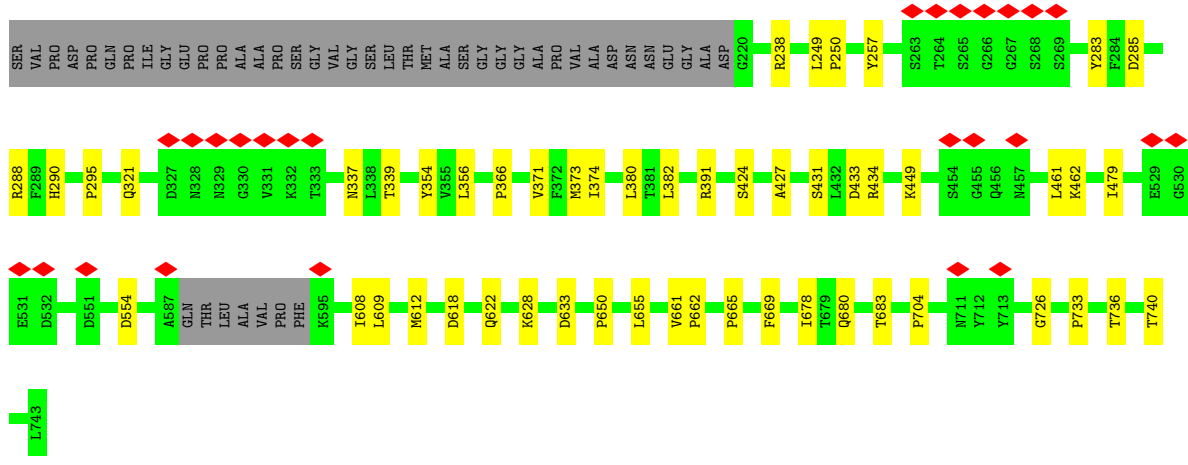
Chain	Residue	Modelled	Actual	Comment	Reference
CB	590	LEU	-	insertion	UNP Q6JC40
CB	591	ALA	-	insertion	UNP Q6JC40
CB	592	VAL	-	insertion	UNP Q6JC40
CB	593	PRO	-	insertion	UNP Q6JC40
CB	594	PHE	-	insertion	UNP Q6JC40
CB	595	LYS	-	insertion	UNP Q6JC40
DB	589	THR	-	insertion	UNP Q6JC40
DB	590	LEU	-	insertion	UNP Q6JC40
DB	591	ALA	-	insertion	UNP Q6JC40
DB	592	VAL	-	insertion	UNP Q6JC40
DB	593	PRO	-	insertion	UNP Q6JC40
DB	594	PHE	-	insertion	UNP Q6JC40
DB	595	LYS	-	insertion	UNP Q6JC40
EB	589	THR	-	insertion	UNP Q6JC40
EB	590	LEU	-	insertion	UNP Q6JC40
EB	591	ALA	-	insertion	UNP Q6JC40
EB	592	VAL	-	insertion	UNP Q6JC40
EB	593	PRO	-	insertion	UNP Q6JC40
EB	594	PHE	-	insertion	UNP Q6JC40
EB	595	LYS	-	insertion	UNP Q6JC40
FB	589	THR	-	insertion	UNP Q6JC40
FB	590	LEU	-	insertion	UNP Q6JC40
FB	591	ALA	-	insertion	UNP Q6JC40
FB	592	VAL	-	insertion	UNP Q6JC40
FB	593	PRO	-	insertion	UNP Q6JC40
FB	594	PHE	-	insertion	UNP Q6JC40
FB	595	LYS	-	insertion	UNP Q6JC40
GB	589	THR	-	insertion	UNP Q6JC40
GB	590	LEU	-	insertion	UNP Q6JC40
GB	591	ALA	-	insertion	UNP Q6JC40
GB	592	VAL	-	insertion	UNP Q6JC40
GB	593	PRO	-	insertion	UNP Q6JC40
GB	594	PHE	-	insertion	UNP Q6JC40
GB	595	LYS	-	insertion	UNP Q6JC40
HB	589	THR	-	insertion	UNP Q6JC40
HB	590	LEU	-	insertion	UNP Q6JC40
HB	591	ALA	-	insertion	UNP Q6JC40
HB	592	VAL	-	insertion	UNP Q6JC40
HB	593	PRO	-	insertion	UNP Q6JC40
HB	594	PHE	-	insertion	UNP Q6JC40
HB	595	LYS	-	insertion	UNP Q6JC40
IB	589	THR	-	insertion	UNP Q6JC40

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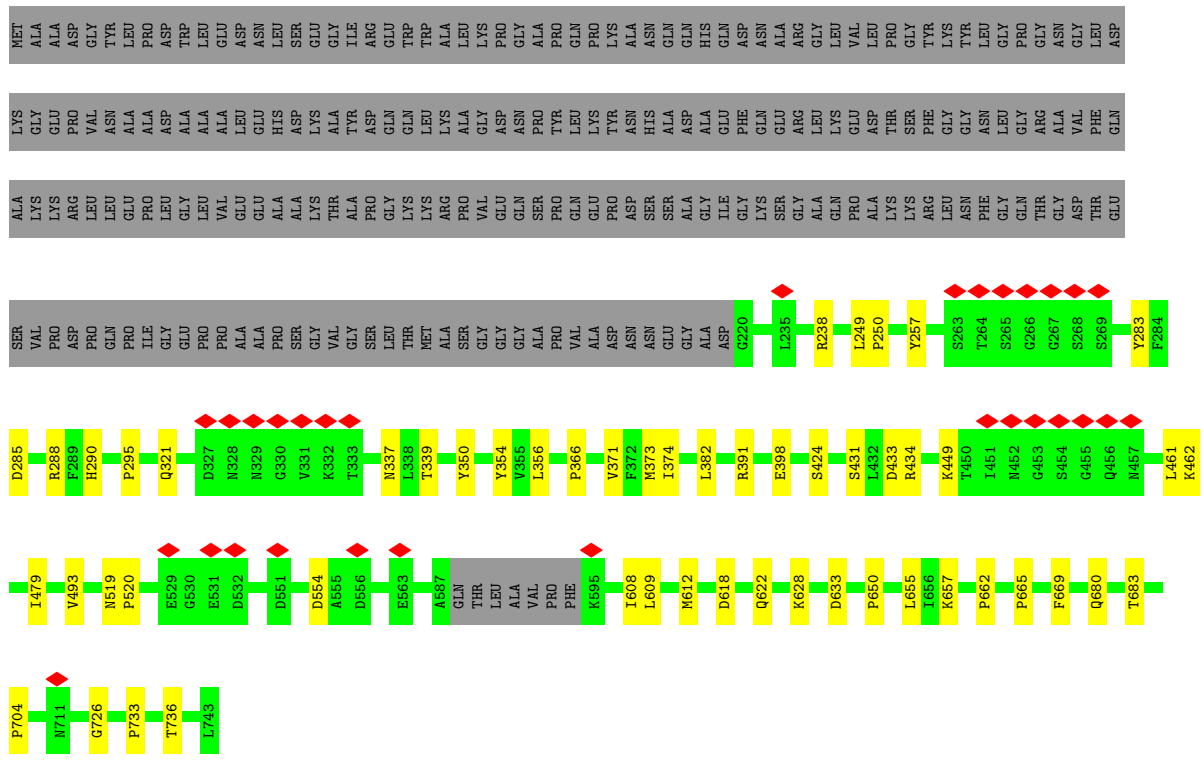
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<b>Chain</b>	<b>Residue</b>	<b>Modelled</b>	<b>Actual</b>	<b>Comment</b>	<b>Reference</b>
IB	590	LEU	-	insertion	UNP Q6JC40
IB	591	ALA	-	insertion	UNP Q6JC40
IB	592	VAL	-	insertion	UNP Q6JC40
IB	593	PRO	-	insertion	UNP Q6JC40
IB	594	PHE	-	insertion	UNP Q6JC40
IB	595	LYS	-	insertion	UNP Q6JC40

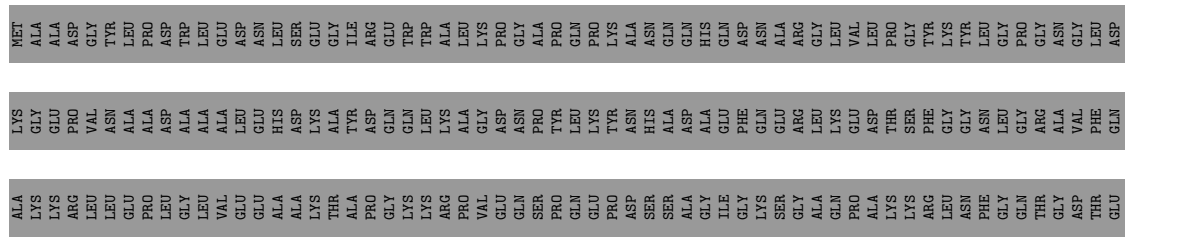




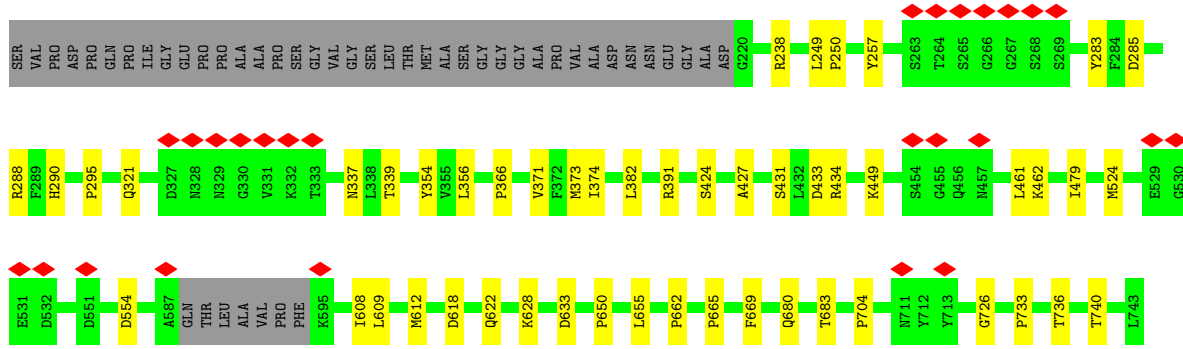
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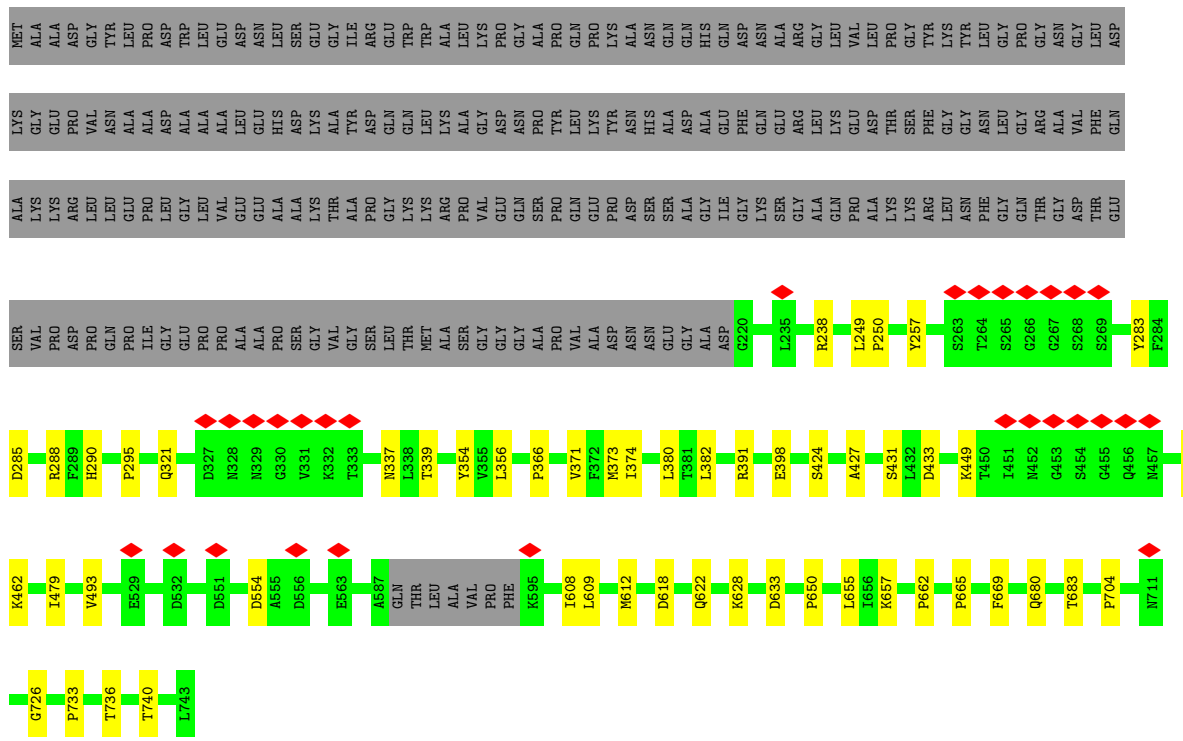
• Molecule 1: Capsid protein VP1



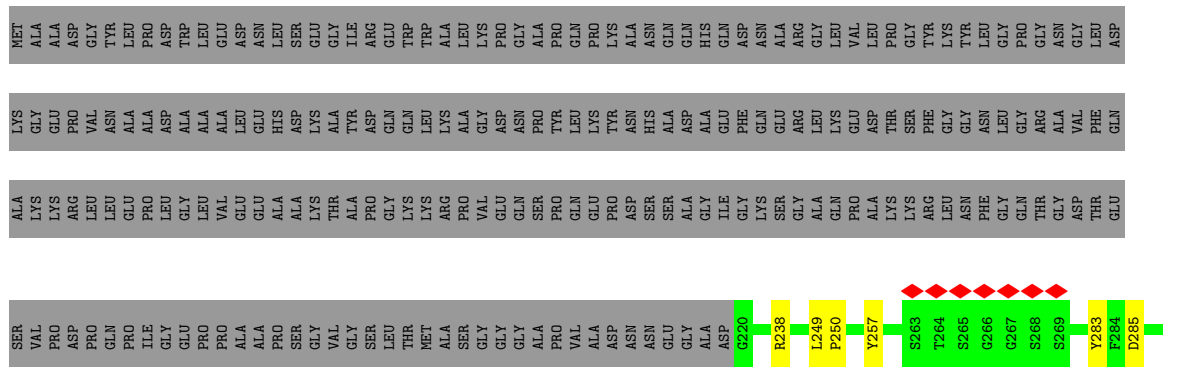




• Molecule 1: Capsid protein VP1

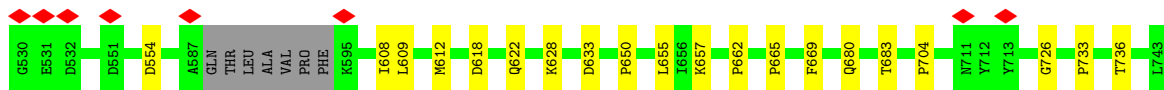


• Molecule 1: Capsid protein VP1

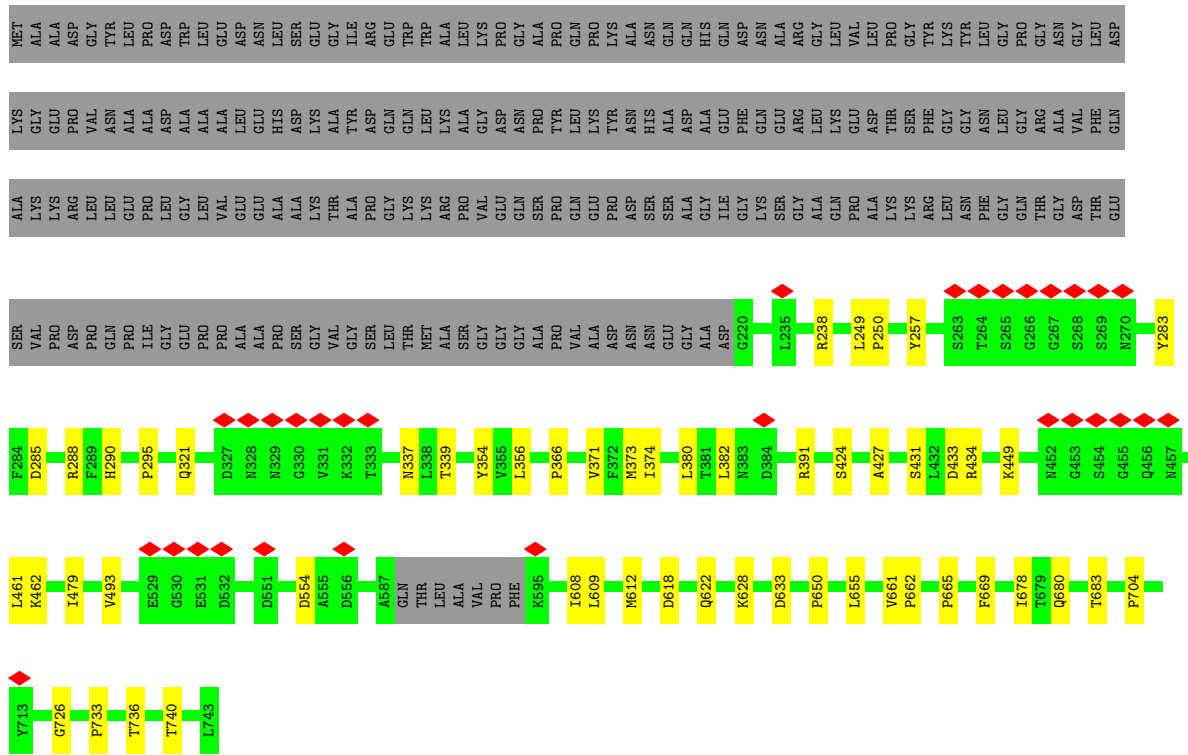




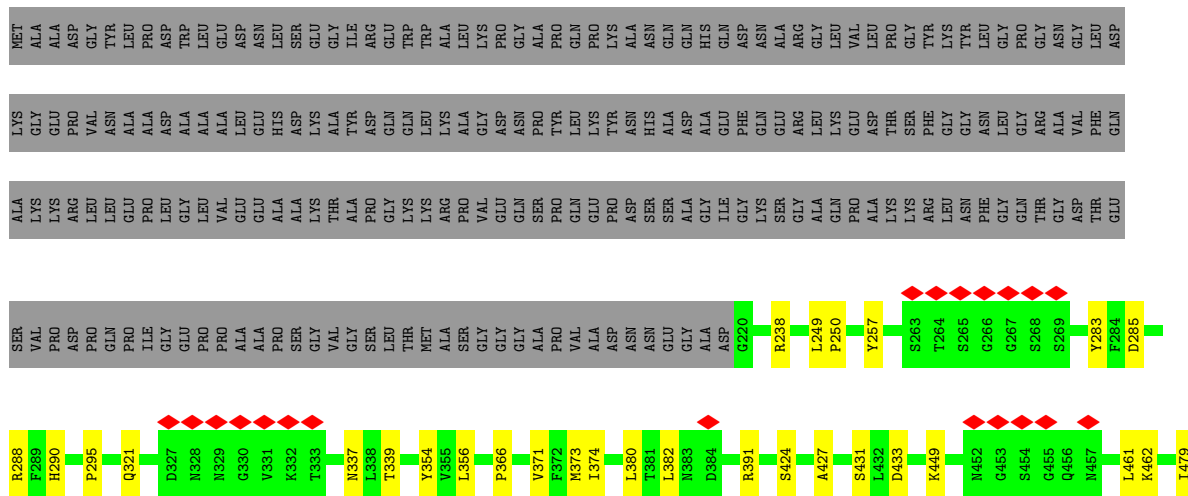




• Molecule 1: Capsid protein VP1

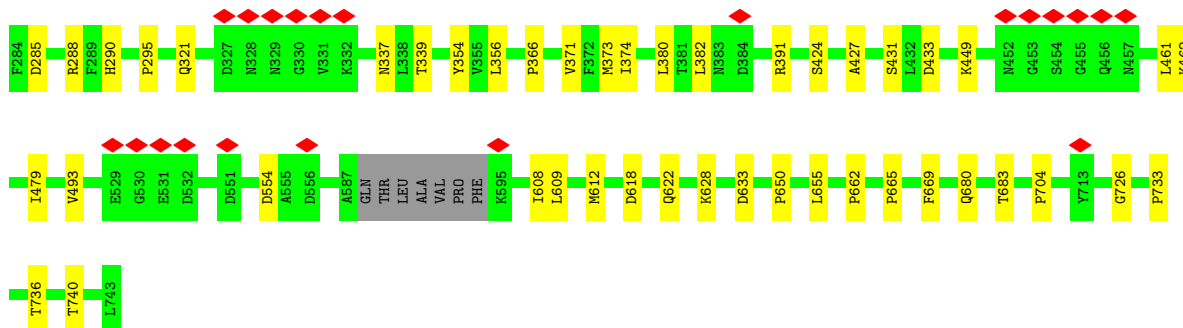


• Molecule 1: Capsid protein VP1

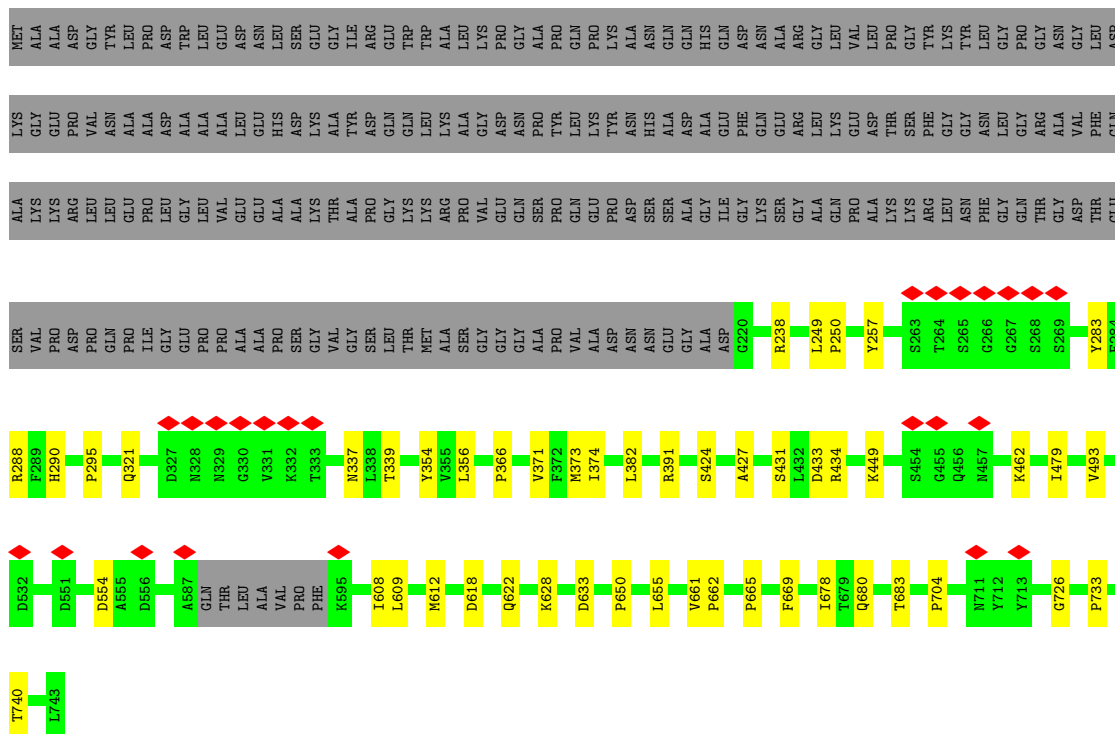




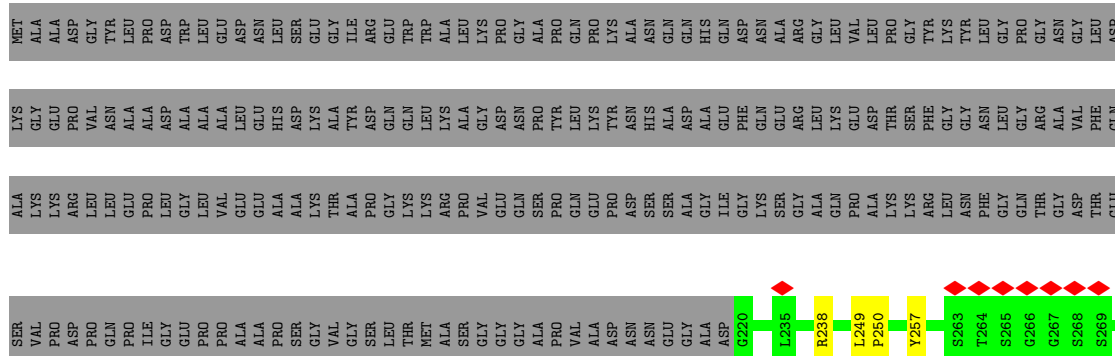




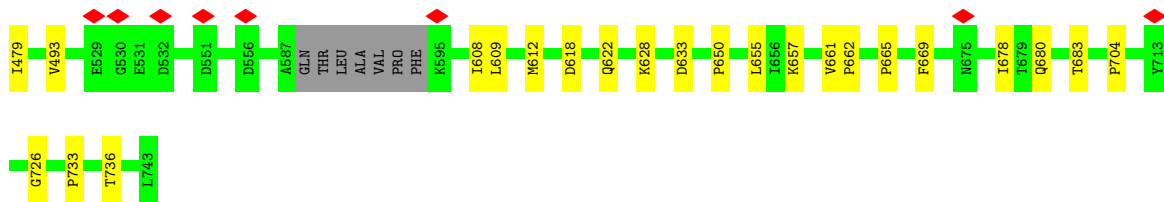
• Molecule 1: Capsid protein VP1



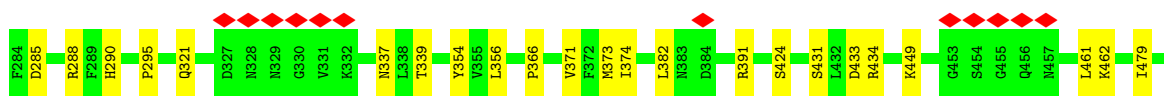
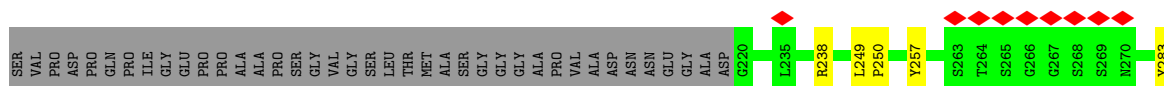
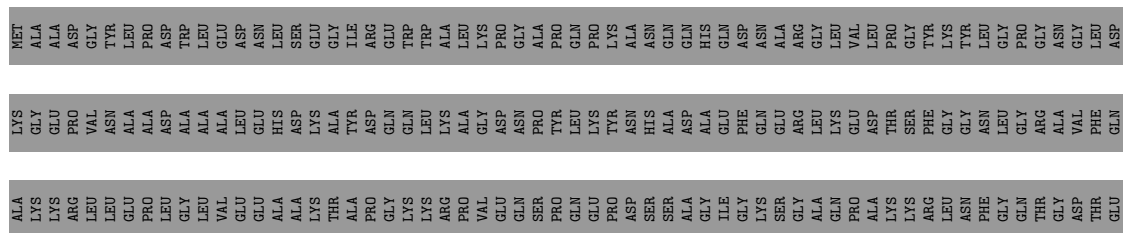
• Molecule 1: Capsid protein VP1



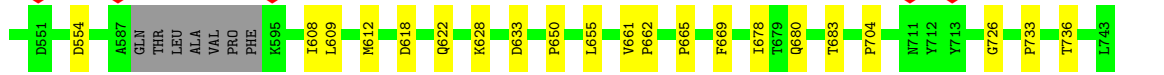
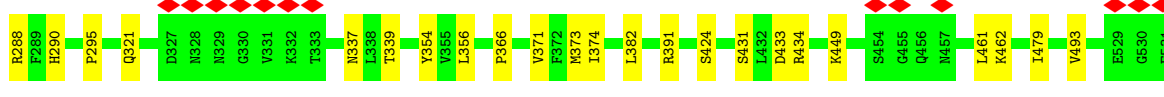
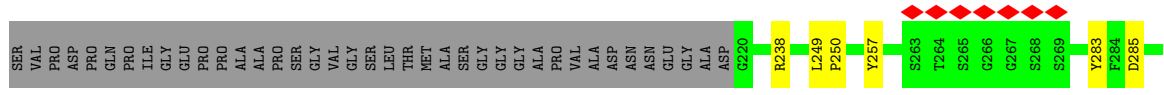
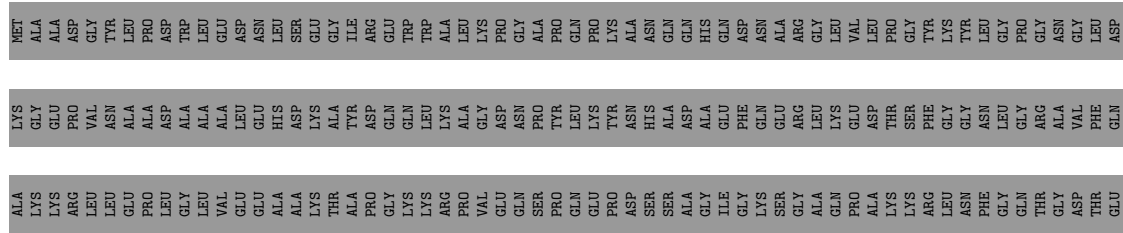




• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1







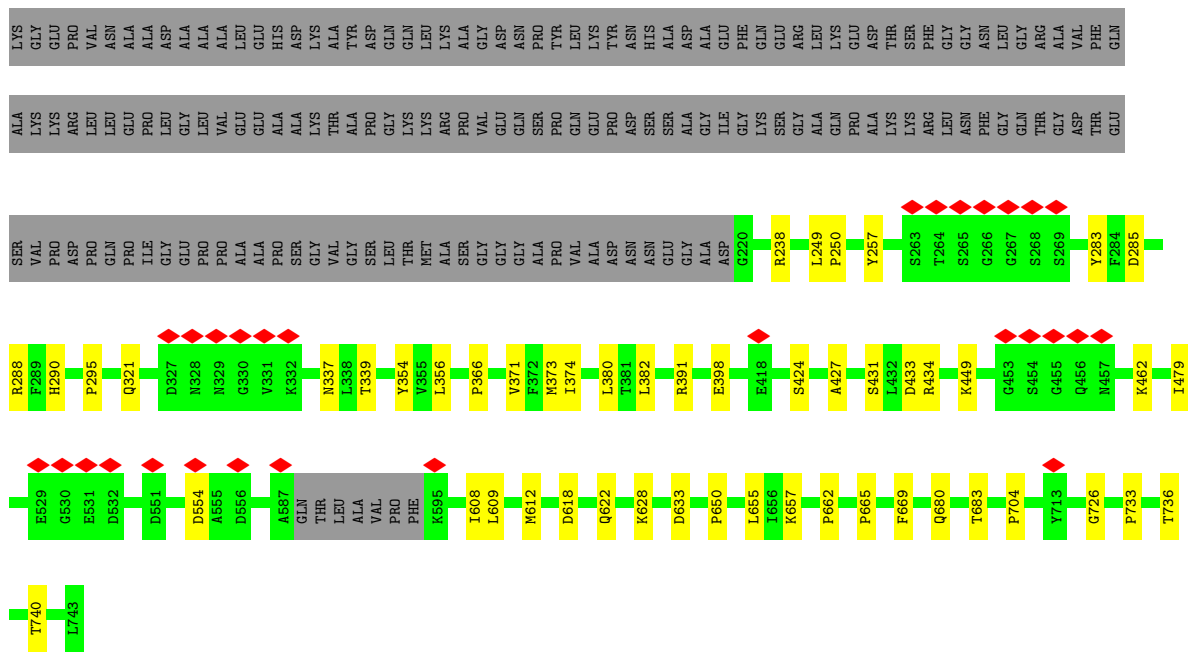




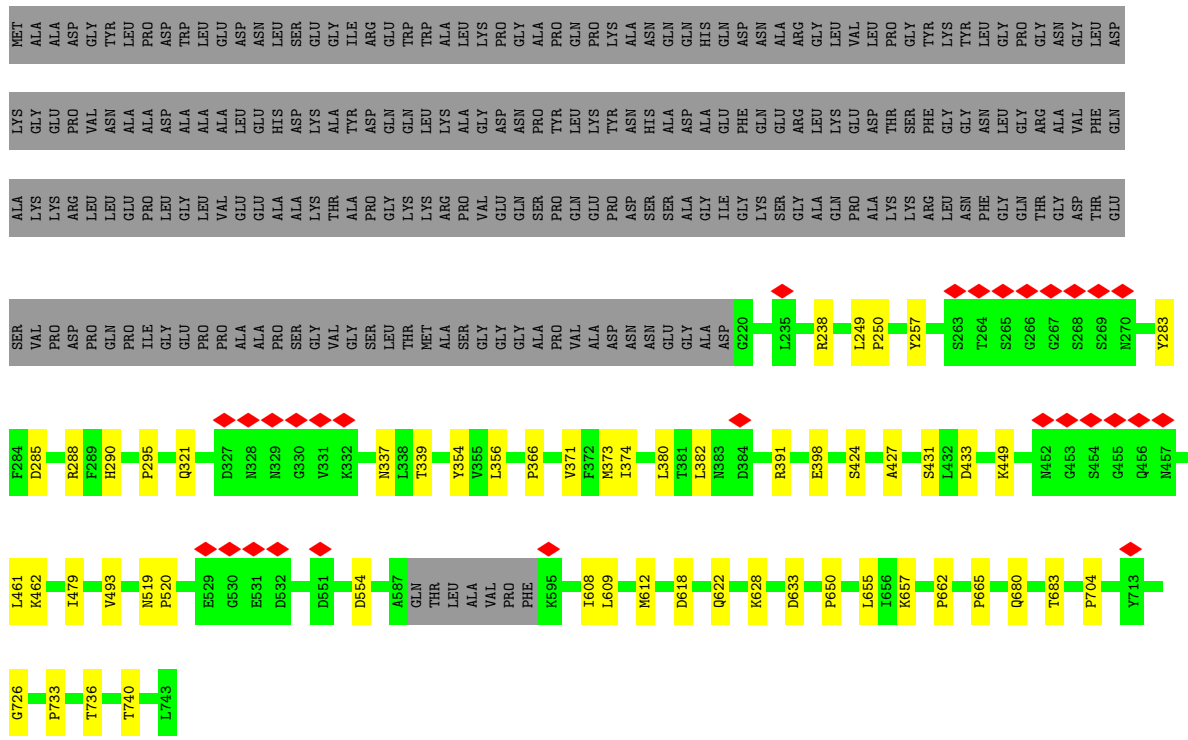






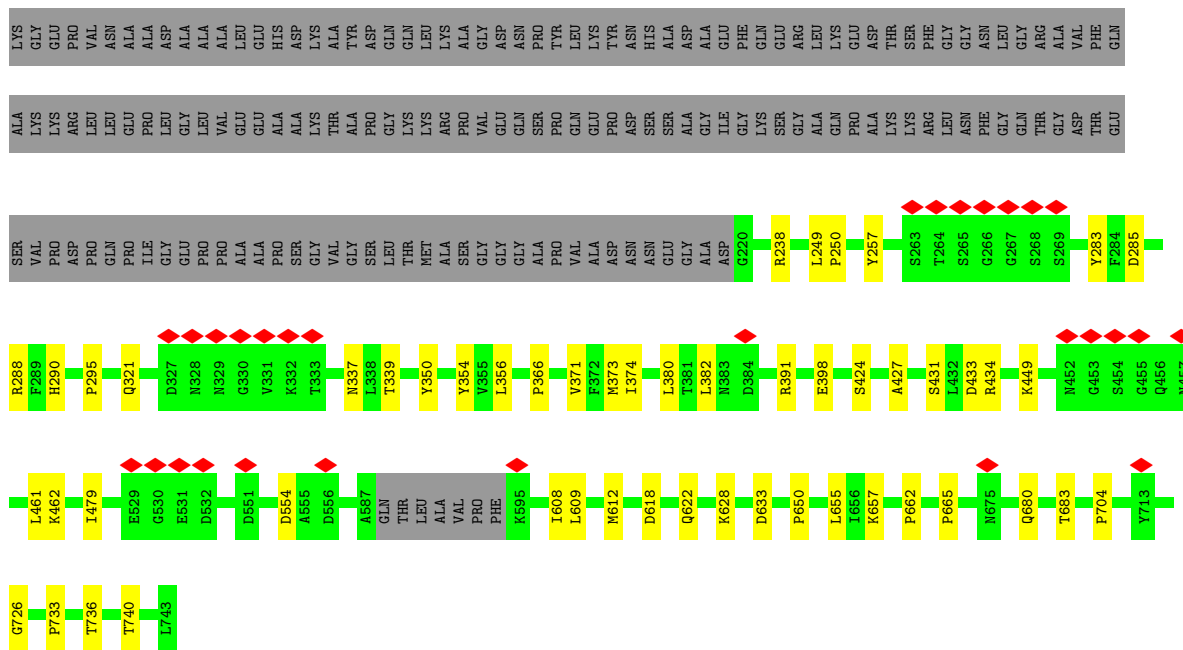


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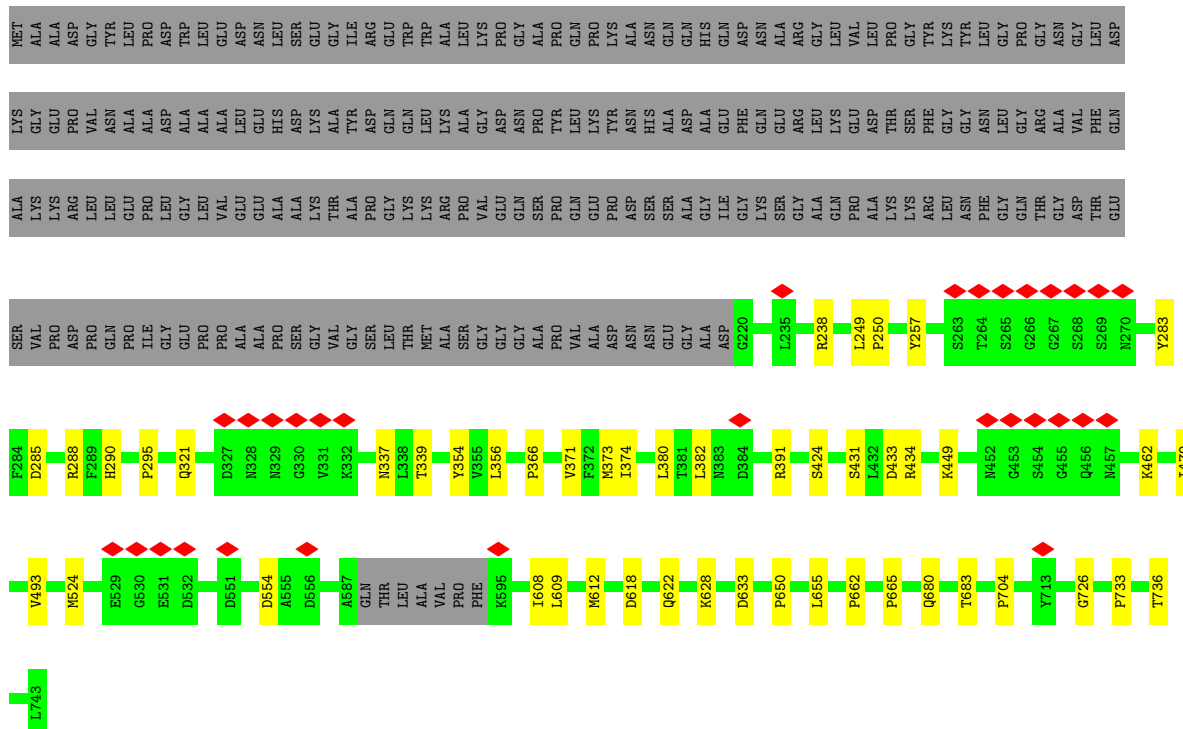


• Molecule 1: Capsid protein VP1





• Molecule 1: Capsid protein VP1



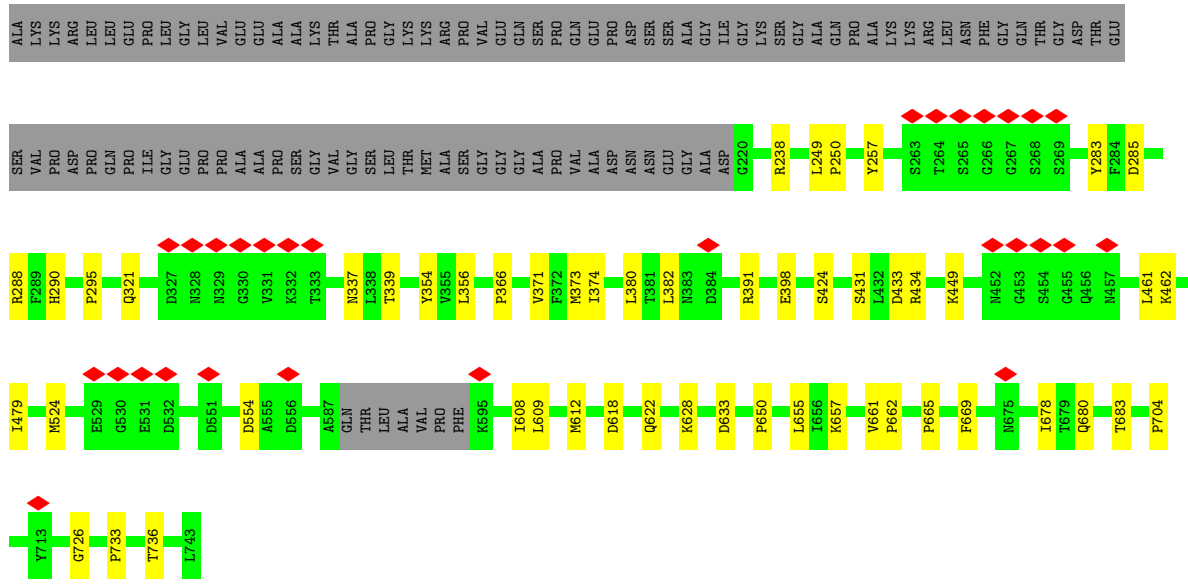
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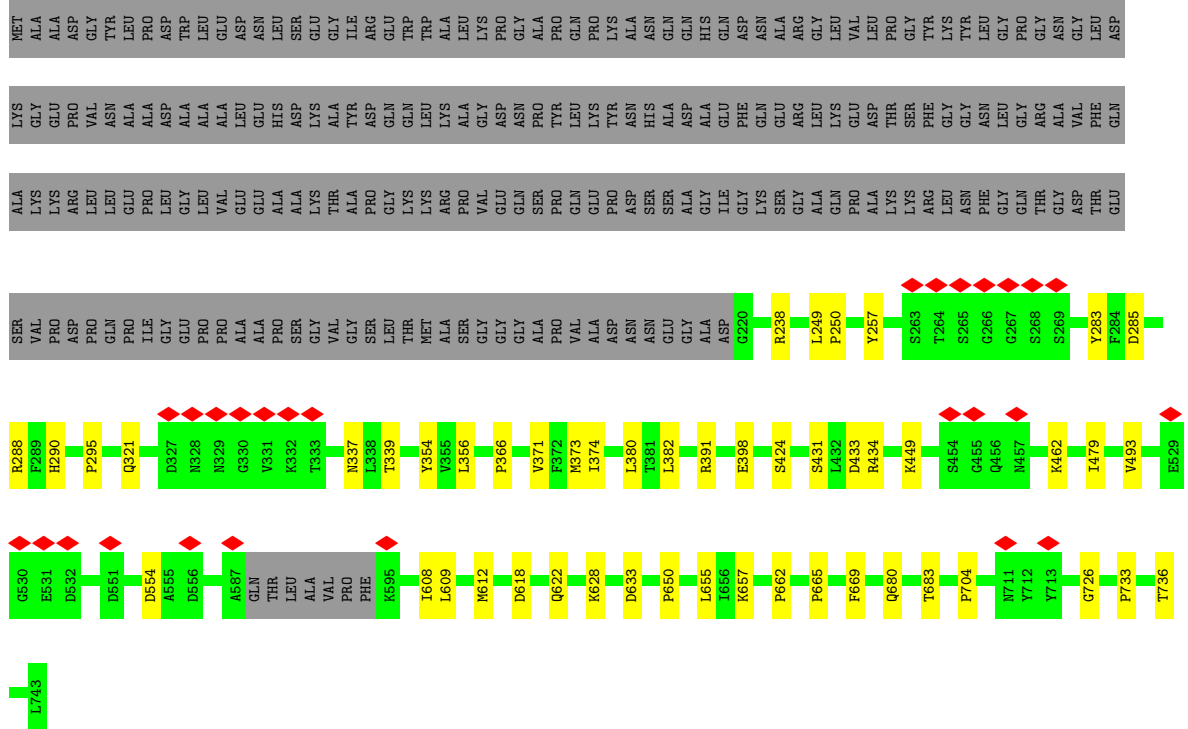




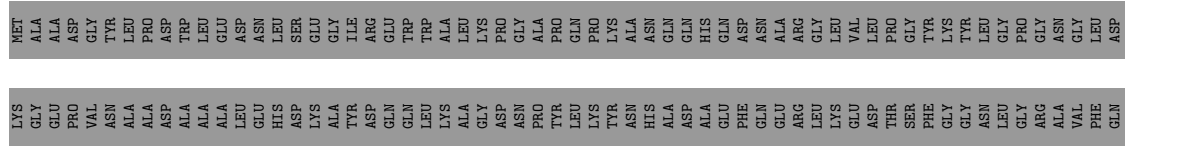




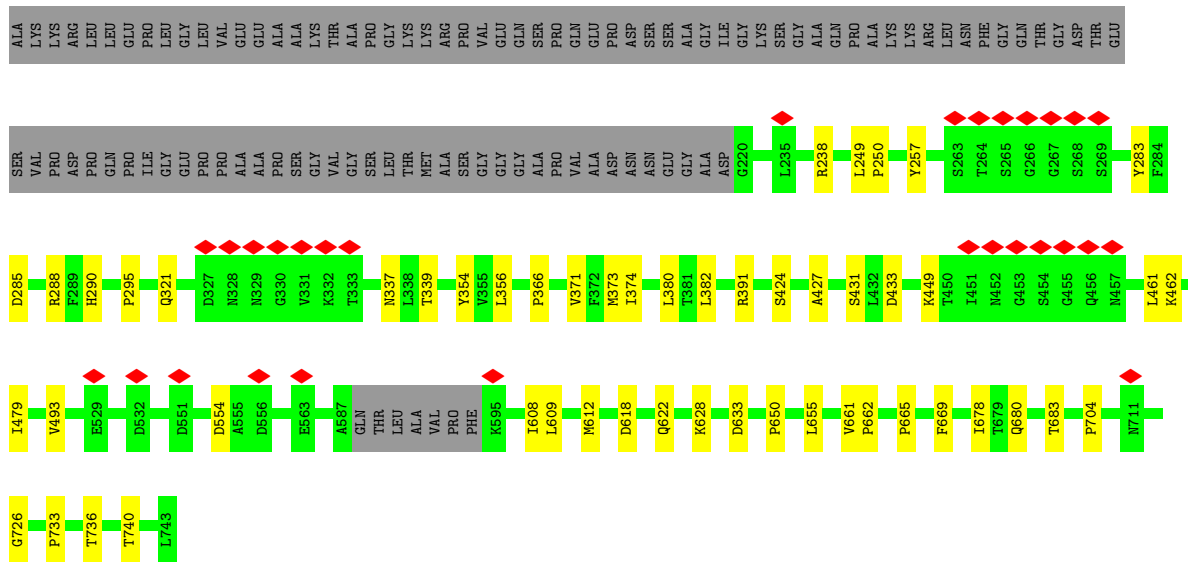
• Molecule 1: Capsid protein VP1



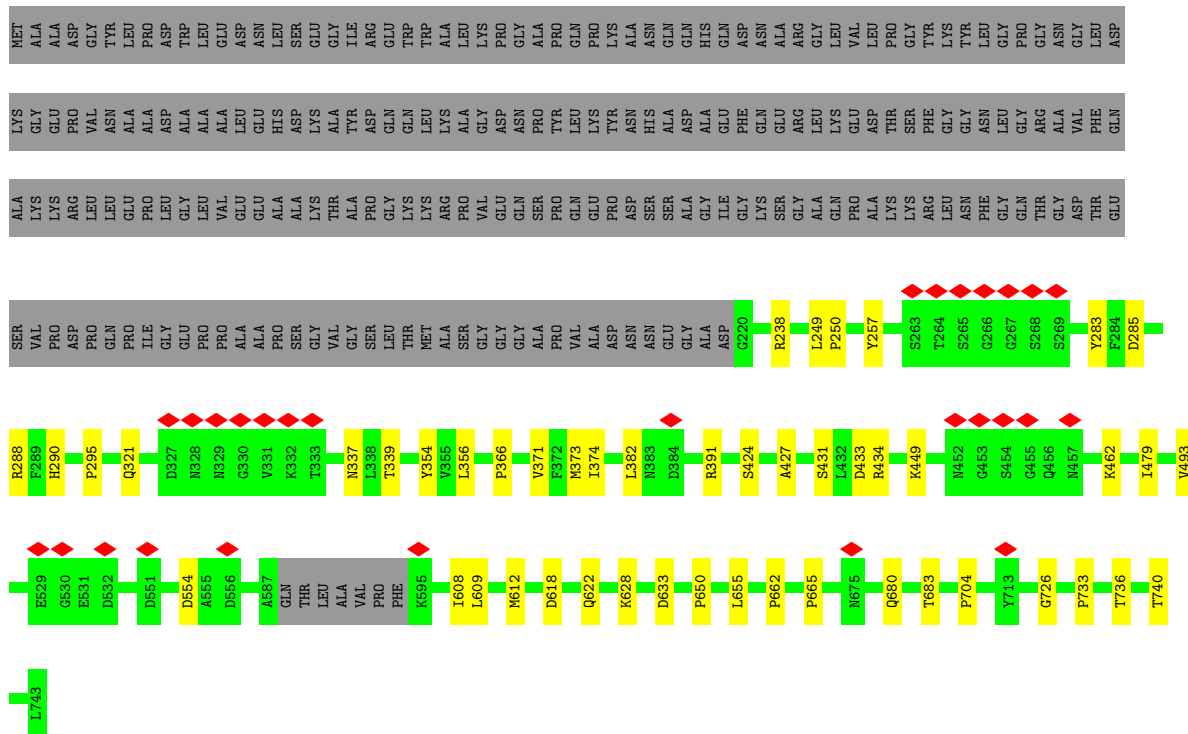
• Molecule 1: Capsid protein VP1



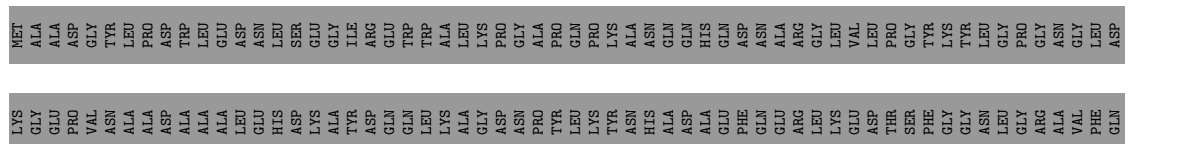




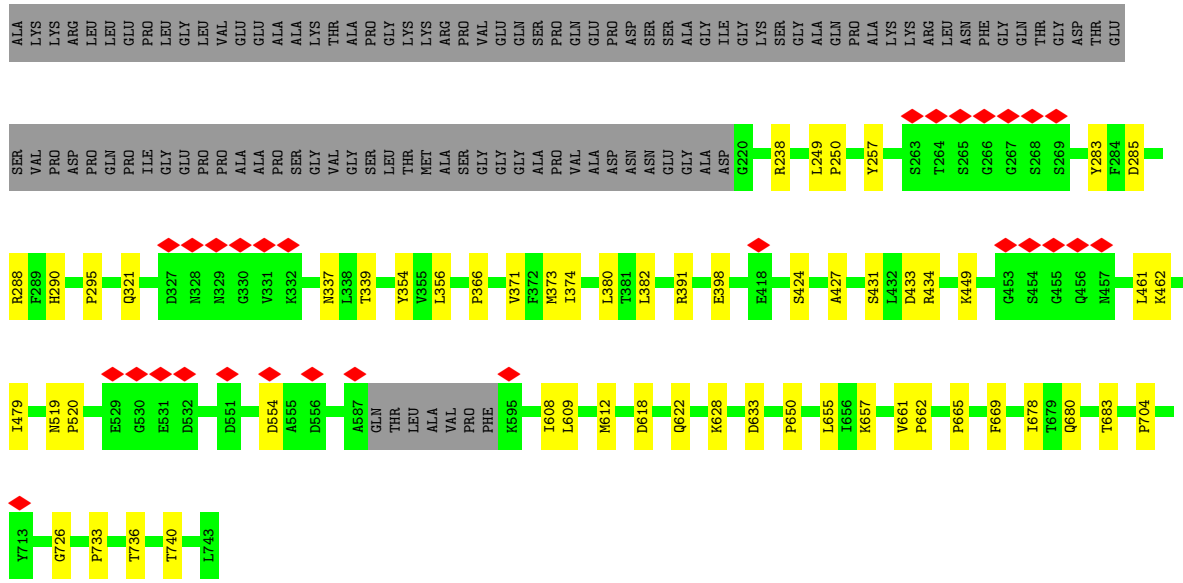
● Molecule 1: Capsid protein VP1



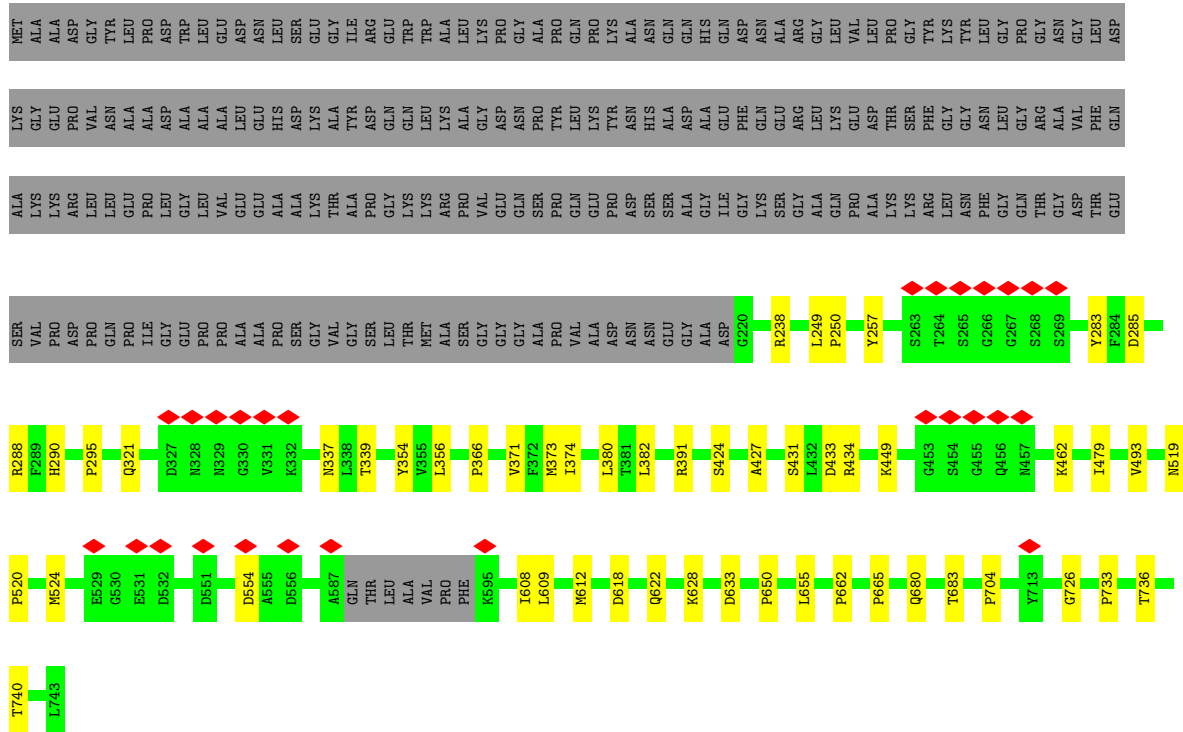
● Molecule 1: Capsid protein VP1



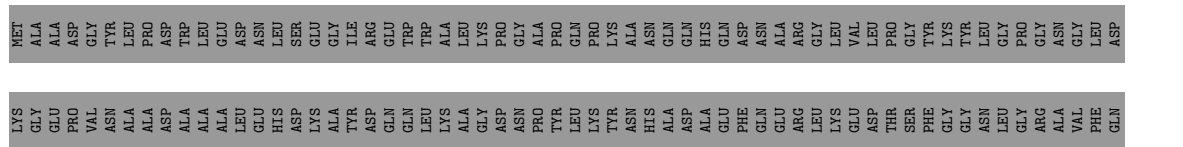




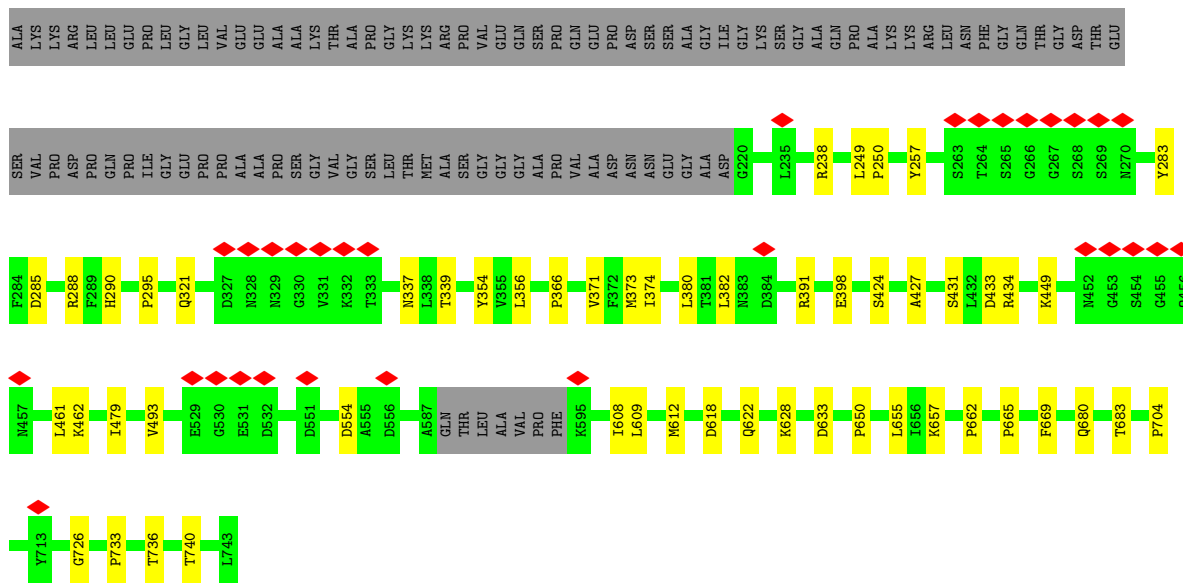
• Molecule 1: Capsid protein VP1



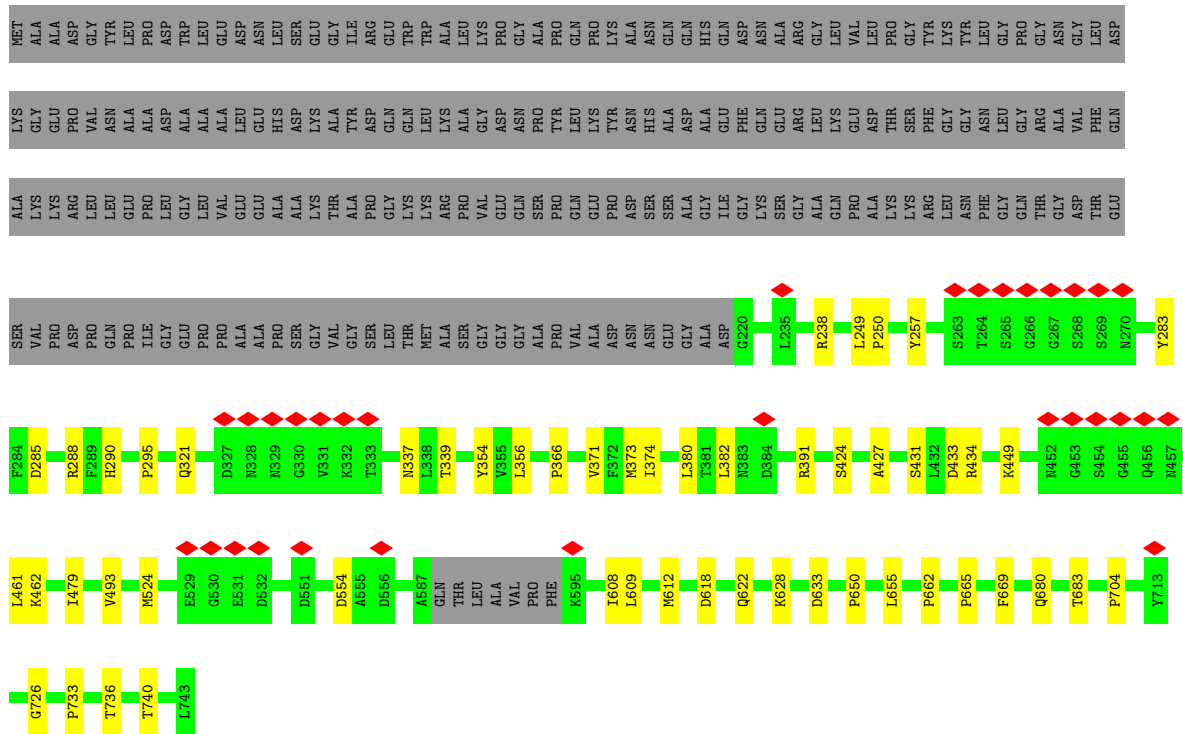
• Molecule 1: Capsid protein VP1



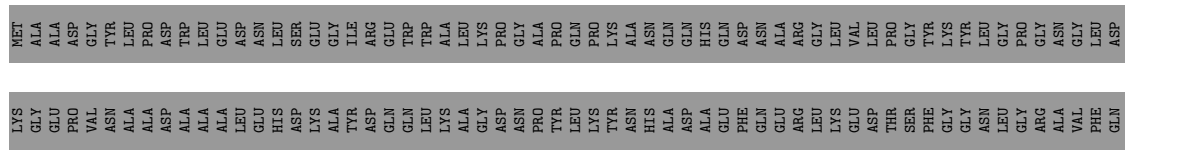


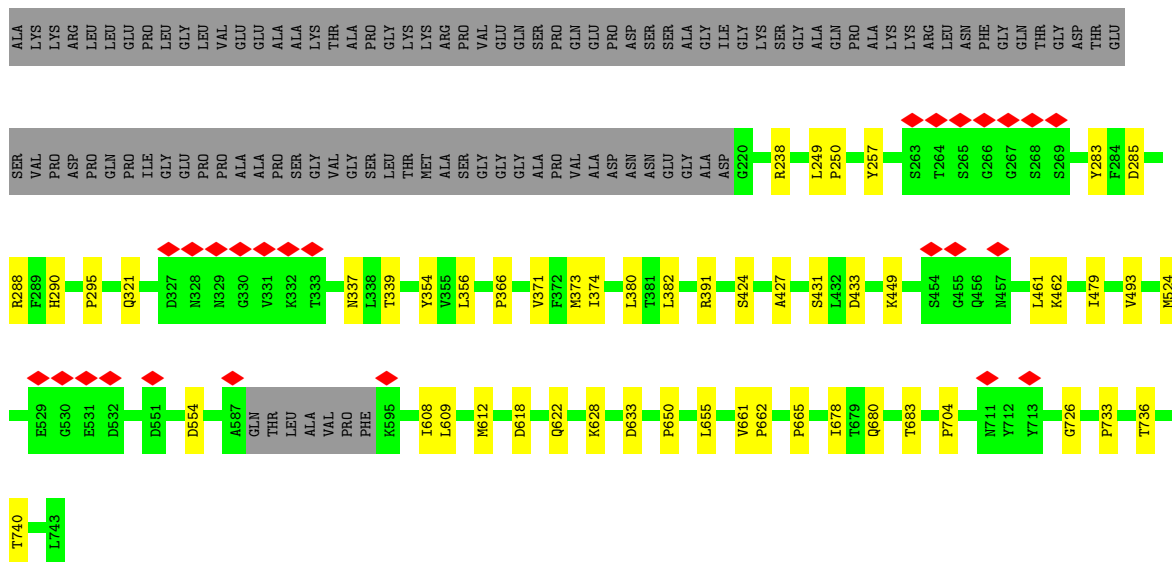


• Molecule 1: Capsid protein VP1



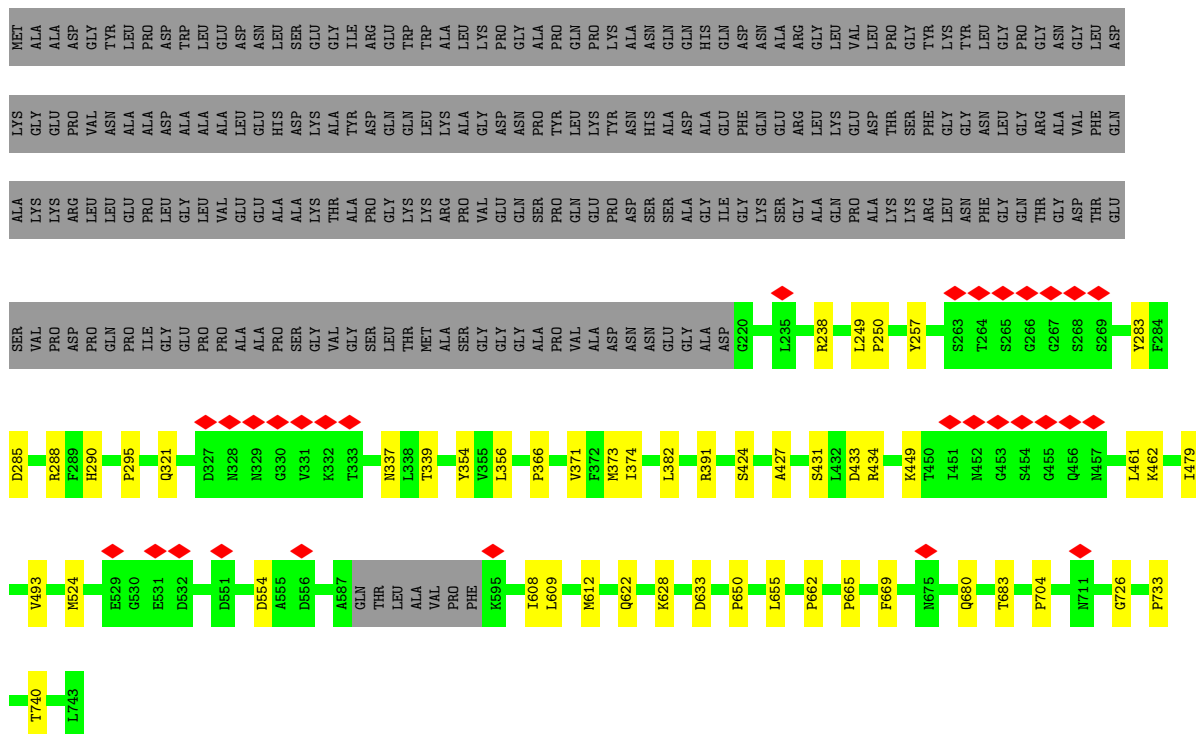
• Molecule 1: Capsid protein VP1





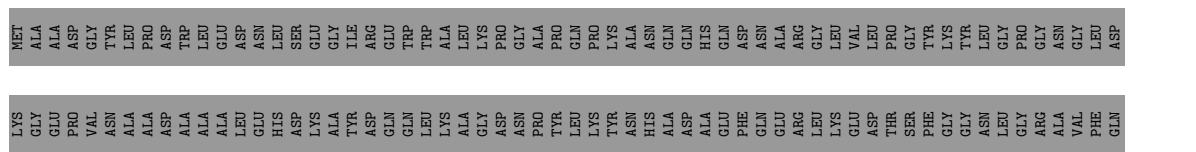
• Molecule 1: Capsid protein VP1

Chain GB: 63% 7% 30%

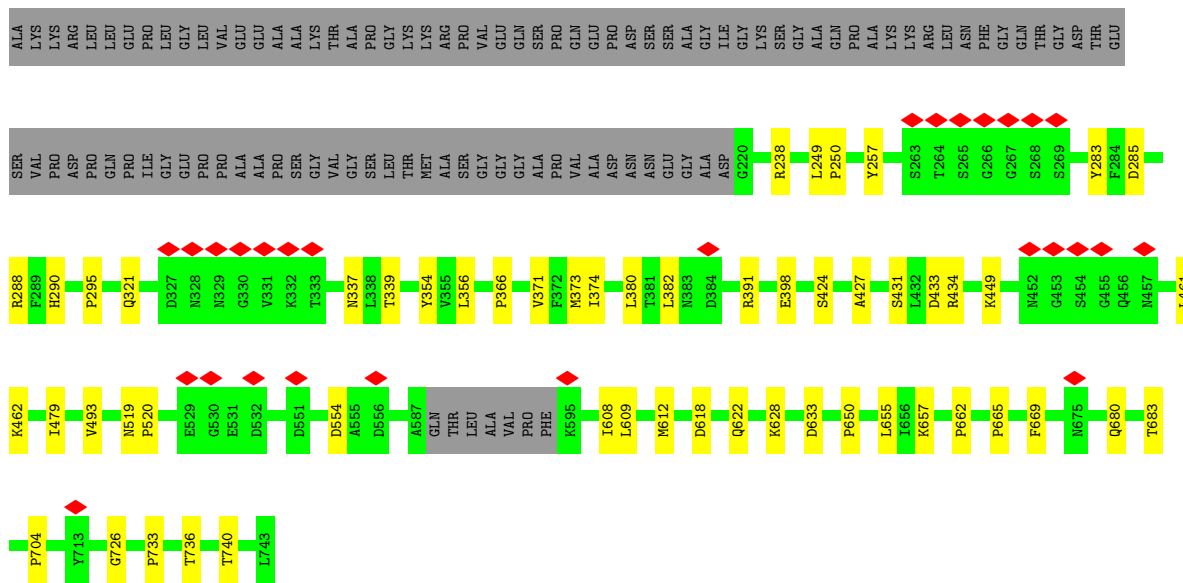


• Molecule 1: Capsid protein VP1

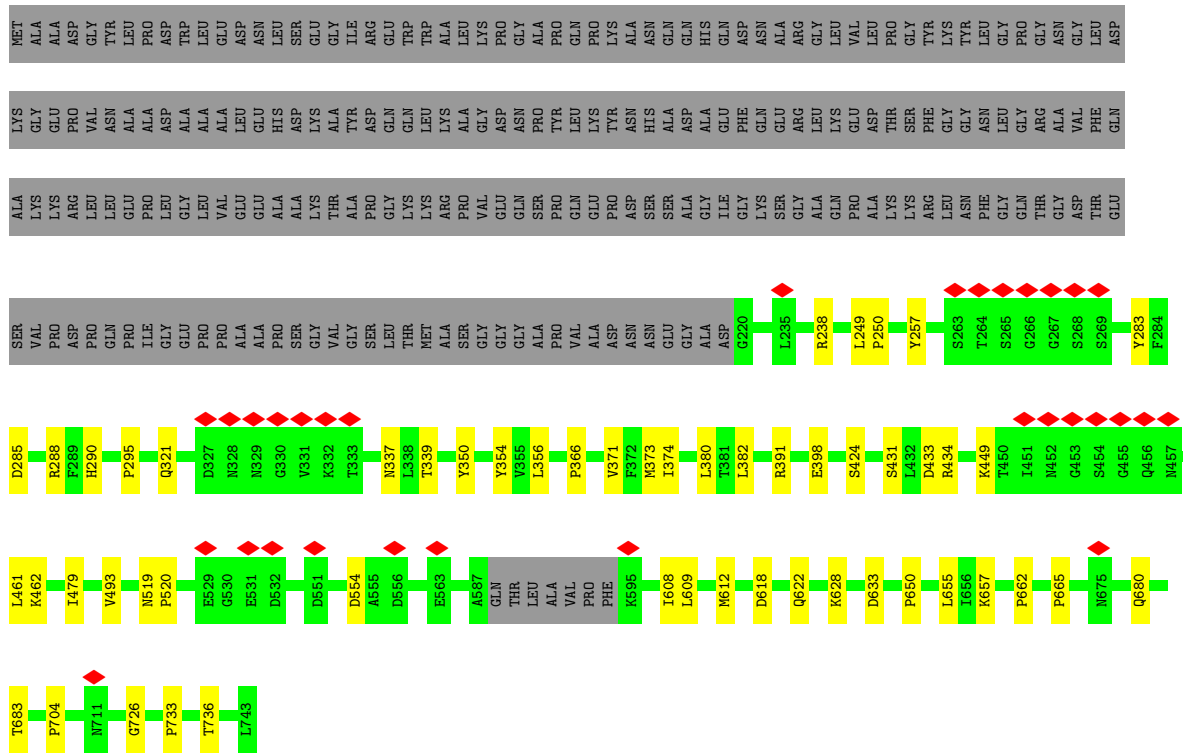
Chain HB: 62% 7% 30%







● Molecule 1: Capsid protein VP1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	42570	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	38.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.211	Depositor
Minimum map value	-0.115	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	457.91998, 457.91998, 457.91998	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.29	0/4236	0.47	0/5771
1	AA	0.29	0/4236	0.47	0/5771
1	AB	0.29	0/4236	0.47	0/5771
1	B	0.29	0/4236	0.47	0/5771
1	BA	0.29	0/4236	0.47	0/5771
1	BB	0.29	0/4236	0.47	0/5771
1	C	0.29	0/4236	0.47	0/5771
1	CA	0.29	0/4236	0.47	0/5771
1	CB	0.29	0/4236	0.47	0/5771
1	D	0.29	0/4236	0.47	0/5771
1	DA	0.29	0/4236	0.47	0/5771
1	DB	0.29	0/4236	0.47	0/5771
1	E	0.29	0/4236	0.47	0/5771
1	EA	0.29	0/4236	0.47	0/5771
1	EB	0.29	0/4236	0.47	0/5771
1	F	0.29	0/4236	0.47	0/5771
1	FA	0.29	0/4236	0.47	0/5771
1	FB	0.29	0/4236	0.47	0/5771
1	G	0.29	0/4236	0.47	0/5771
1	GA	0.29	0/4236	0.47	0/5771
1	GB	0.29	0/4236	0.47	0/5771
1	H	0.29	0/4236	0.47	0/5771
1	HA	0.29	0/4236	0.47	0/5771
1	HB	0.29	0/4236	0.47	0/5771
1	I	0.29	0/4236	0.47	0/5771
1	IA	0.29	0/4236	0.47	0/5771
1	IB	0.29	0/4236	0.47	0/5771
1	J	0.29	0/4236	0.47	0/5771
1	JA	0.29	0/4236	0.47	0/5771
1	K	0.29	0/4236	0.47	0/5771
1	KA	0.29	0/4236	0.47	0/5771
1	L	0.29	0/4236	0.47	0/5771
1	LA	0.29	0/4236	0.47	0/5771
1	M	0.29	0/4236	0.47	0/5771

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	MA	0.29	0/4236	0.47	0/5771
1	N	0.29	0/4236	0.47	0/5771
1	NA	0.29	0/4236	0.47	0/5771
1	O	0.29	0/4236	0.47	0/5771
1	OA	0.29	0/4236	0.47	0/5771
1	P	0.29	0/4236	0.47	0/5771
1	PA	0.29	0/4236	0.47	0/5771
1	Q	0.29	0/4236	0.47	0/5771
1	QA	0.29	0/4236	0.47	0/5771
1	R	0.29	0/4236	0.47	0/5771
1	RA	0.29	0/4236	0.47	0/5771
1	S	0.29	0/4236	0.47	0/5771
1	SA	0.29	0/4236	0.47	0/5771
1	T	0.29	0/4236	0.47	0/5771
1	TA	0.29	0/4236	0.47	0/5771
1	UA	0.29	0/4236	0.47	0/5771
1	V	0.29	0/4236	0.47	0/5771
1	VA	0.29	0/4236	0.47	0/5771
1	W	0.29	0/4236	0.47	0/5771
1	WA	0.29	0/4236	0.47	0/5771
1	X	0.29	0/4236	0.47	0/5771
1	XA	0.29	0/4236	0.47	0/5771
1	Y	0.29	0/4236	0.47	0/5771
1	YA	0.29	0/4236	0.47	0/5771
1	Z	0.29	0/4236	0.47	0/5771
1	ZA	0.29	0/4236	0.47	0/5771
All	All	0.29	0/254160	0.47	0/346260

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	4112	0	3868	43	0
1	AA	4112	0	3868	40	0
1	AB	4112	0	3868	41	0
1	B	4112	0	3868	42	0
1	BA	4112	0	3868	42	0
1	BB	4112	0	3868	41	0
1	C	4112	0	3868	42	0
1	CA	4112	0	3868	42	0
1	CB	4112	0	3868	43	0
1	D	4112	0	3868	41	0
1	DA	4112	0	3868	43	0
1	DB	4112	0	3868	43	0
1	E	4112	0	3868	40	0
1	EA	4112	0	3868	40	0
1	EB	4112	0	3868	42	0
1	F	4112	0	3868	40	0
1	FA	4112	0	3868	43	0
1	FB	4112	0	3868	41	0
1	G	4112	0	3868	42	0
1	GA	4112	0	3868	43	0
1	GB	4112	0	3868	40	0
1	H	4112	0	3868	41	0
1	HA	4112	0	3868	42	0
1	HB	4112	0	3868	43	0
1	I	4112	0	3868	39	0
1	IA	4112	0	3868	43	0
1	IB	4112	0	3868	42	0
1	J	4112	0	3868	41	0
1	JA	4112	0	3868	41	0
1	K	4112	0	3868	43	0
1	KA	4112	0	3868	42	0
1	L	4112	0	3868	40	0
1	LA	4112	0	3868	41	0
1	M	4112	0	3868	42	0
1	MA	4112	0	3868	39	0
1	N	4112	0	3868	45	0
1	NA	4112	0	3868	42	0
1	O	4112	0	3868	42	0
1	OA	4112	0	3868	41	0
1	P	4112	0	3868	41	0
1	PA	4112	0	3868	42	0
1	Q	4112	0	3868	40	0
1	QA	4112	0	3868	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	4112	0	3868	40	0
1	RA	4112	0	3868	42	0
1	S	4112	0	3868	41	0
1	SA	4112	0	3868	41	0
1	T	4112	0	3868	41	0
1	TA	4112	0	3868	39	0
1	UA	4112	0	3868	40	0
1	V	4112	0	3868	40	0
1	VA	4112	0	3868	42	0
1	W	4112	0	3868	41	0
1	WA	4112	0	3868	39	0
1	X	4112	0	3868	40	0
1	XA	4112	0	3868	43	0
1	Y	4112	0	3868	41	0
1	YA	4112	0	3868	39	0
1	Z	4112	0	3868	43	0
1	ZA	4112	0	3868	44	0
All	All	246720	0	232080	1873	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 4.

The worst 5 of 1873 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:N:479:ILE:HG13	1:N:612:MET:HG2	1.75	0.69
1:BA:479:ILE:HG13	1:BA:612:MET:HG2	1.75	0.69
1:LA:479:ILE:HG13	1:LA:612:MET:HG2	1.75	0.69
1:UA:479:ILE:HG13	1:UA:612:MET:HG2	1.75	0.69
1:YA:479:ILE:HG13	1:YA:612:MET:HG2	1.75	0.69

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	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	AA	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	AB	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	B	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	BA	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	BB	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	C	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	CA	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	CB	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	D	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	DA	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	DB	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	E	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	EA	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	EB	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	F	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	FA	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	FB	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	G	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	GA	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	GB	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	H	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	HA	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	HB	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	I	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	IA	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	IB	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	J	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	JA	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	K	513/743 (69%)	504 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	KA	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	L	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	LA	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	M	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	MA	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	N	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	NA	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	O	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	OA	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	P	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	PA	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	Q	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	QA	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	R	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	RA	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	S	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	SA	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	T	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	TA	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	UA	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	V	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	VA	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	W	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	WA	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	X	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	XA	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	Y	513/743 (69%)	504 (98%)	9 (2%)	0	100	100
1	YA	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	Z	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
1	ZA	513/743 (69%)	503 (98%)	10 (2%)	0	100	100
All	All	30780/44580 (69%)	30207 (98%)	573 (2%)	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	448/621 (72%)	448 (100%)	0	100	100
1	AA	448/621 (72%)	448 (100%)	0	100	100
1	AB	448/621 (72%)	448 (100%)	0	100	100
1	B	448/621 (72%)	448 (100%)	0	100	100
1	BA	448/621 (72%)	448 (100%)	0	100	100
1	BB	448/621 (72%)	448 (100%)	0	100	100
1	C	448/621 (72%)	448 (100%)	0	100	100
1	CA	448/621 (72%)	448 (100%)	0	100	100
1	CB	448/621 (72%)	448 (100%)	0	100	100
1	D	448/621 (72%)	448 (100%)	0	100	100
1	DA	448/621 (72%)	448 (100%)	0	100	100
1	DB	448/621 (72%)	448 (100%)	0	100	100
1	E	448/621 (72%)	448 (100%)	0	100	100
1	EA	448/621 (72%)	448 (100%)	0	100	100
1	EB	448/621 (72%)	448 (100%)	0	100	100
1	F	448/621 (72%)	448 (100%)	0	100	100
1	FA	448/621 (72%)	448 (100%)	0	100	100
1	FB	448/621 (72%)	448 (100%)	0	100	100
1	G	448/621 (72%)	448 (100%)	0	100	100
1	GA	448/621 (72%)	448 (100%)	0	100	100
1	GB	448/621 (72%)	448 (100%)	0	100	100
1	H	448/621 (72%)	448 (100%)	0	100	100
1	HA	448/621 (72%)	448 (100%)	0	100	100
1	HB	448/621 (72%)	448 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	448/621 (72%)	448 (100%)	0	100	100
1	IA	448/621 (72%)	448 (100%)	0	100	100
1	IB	448/621 (72%)	448 (100%)	0	100	100
1	J	448/621 (72%)	448 (100%)	0	100	100
1	JA	448/621 (72%)	448 (100%)	0	100	100
1	K	448/621 (72%)	448 (100%)	0	100	100
1	KA	448/621 (72%)	448 (100%)	0	100	100
1	L	448/621 (72%)	448 (100%)	0	100	100
1	LA	448/621 (72%)	448 (100%)	0	100	100
1	M	448/621 (72%)	448 (100%)	0	100	100
1	MA	448/621 (72%)	448 (100%)	0	100	100
1	N	448/621 (72%)	448 (100%)	0	100	100
1	NA	448/621 (72%)	448 (100%)	0	100	100
1	O	448/621 (72%)	448 (100%)	0	100	100
1	OA	448/621 (72%)	448 (100%)	0	100	100
1	P	448/621 (72%)	448 (100%)	0	100	100
1	PA	448/621 (72%)	448 (100%)	0	100	100
1	Q	448/621 (72%)	448 (100%)	0	100	100
1	QA	448/621 (72%)	448 (100%)	0	100	100
1	R	448/621 (72%)	448 (100%)	0	100	100
1	RA	448/621 (72%)	448 (100%)	0	100	100
1	S	448/621 (72%)	448 (100%)	0	100	100
1	SA	448/621 (72%)	448 (100%)	0	100	100
1	T	448/621 (72%)	448 (100%)	0	100	100
1	TA	448/621 (72%)	448 (100%)	0	100	100
1	UA	448/621 (72%)	448 (100%)	0	100	100
1	V	448/621 (72%)	448 (100%)	0	100	100
1	VA	448/621 (72%)	448 (100%)	0	100	100
1	W	448/621 (72%)	448 (100%)	0	100	100
1	WA	448/621 (72%)	448 (100%)	0	100	100
1	X	448/621 (72%)	448 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	XA	448/621 (72%)	448 (100%)	0	100	100
1	Y	448/621 (72%)	448 (100%)	0	100	100
1	YA	448/621 (72%)	448 (100%)	0	100	100
1	Z	448/621 (72%)	448 (100%)	0	100	100
1	ZA	448/621 (72%)	448 (100%)	0	100	100
All	All	26880/37260 (72%)	26880 (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 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	DA	290	HIS
1	EB	290	HIS
1	KA	290	HIS
1	DB	290	HIS
1	IB	290	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

There are no chain breaks in this entry.

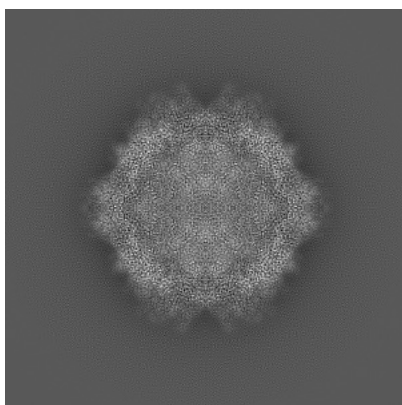
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24494. These allow visual inspection of the internal detail of the map and identification of artifacts.

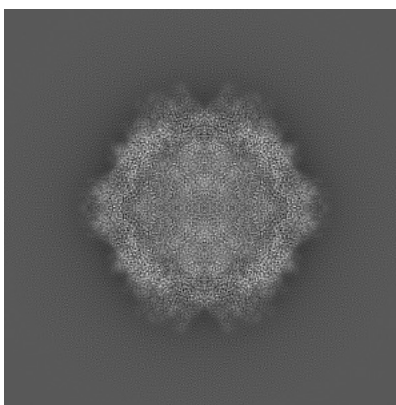
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

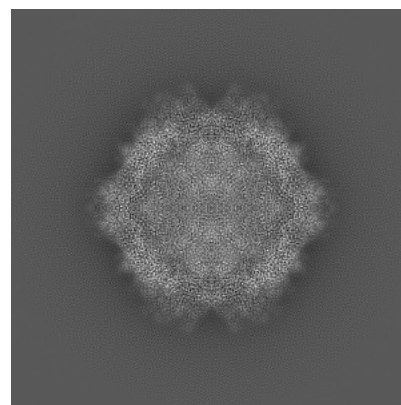
#### 6.1.1 Primary map



X



Y

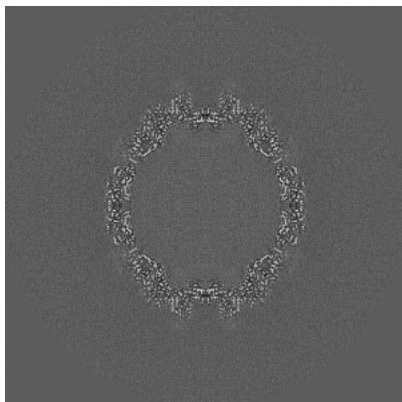


Z

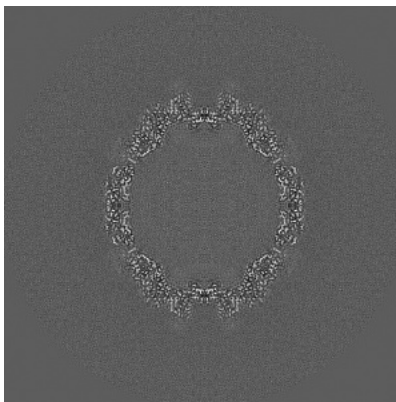
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

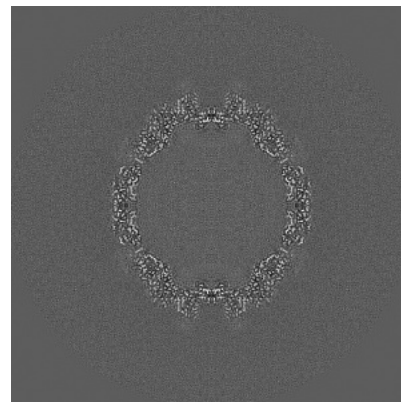
#### 6.2.1 Primary map



X Index: 216



Y Index: 216

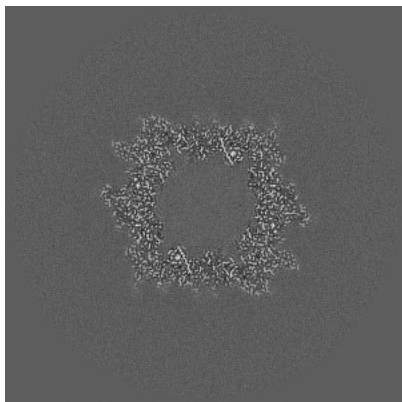


Z Index: 216

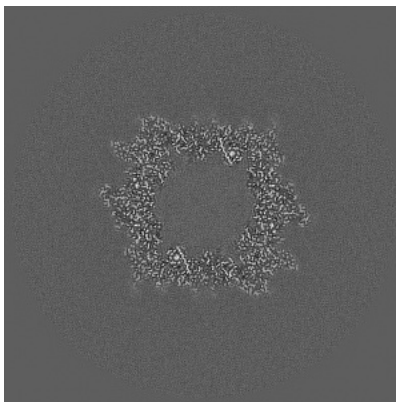
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

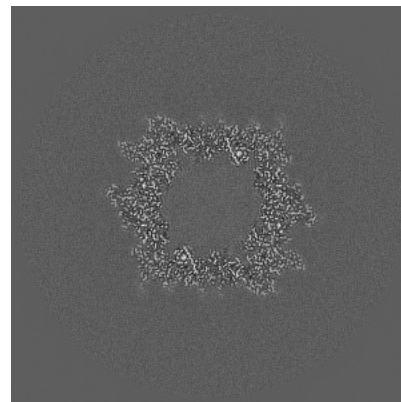
### 6.3.1 Primary map



X Index: 278



Y Index: 278

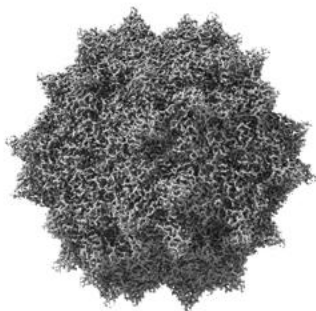


Z Index: 278

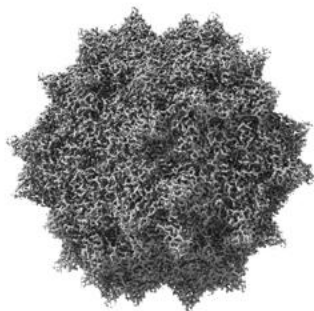
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

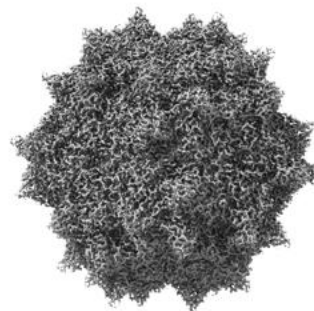
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

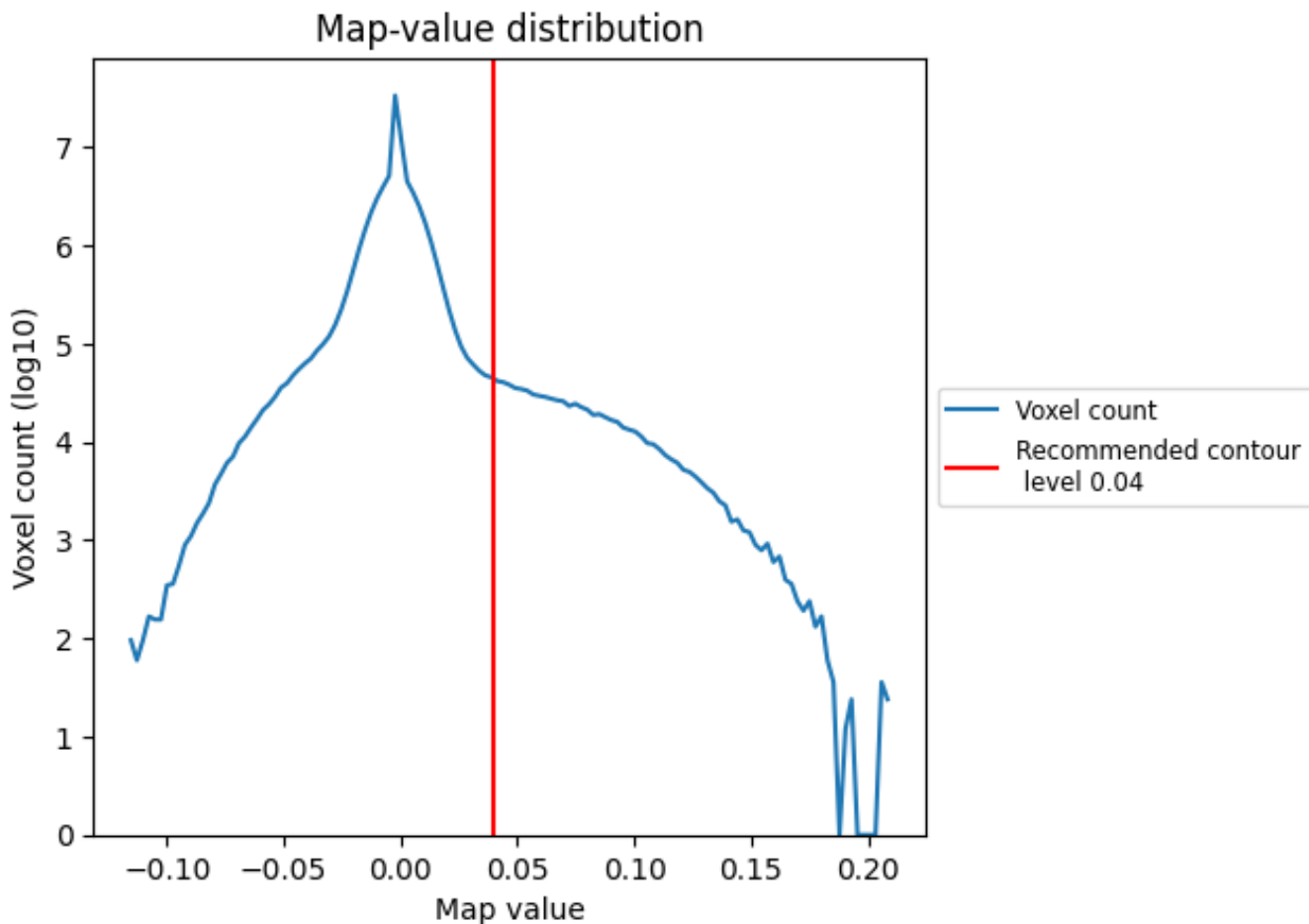
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

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

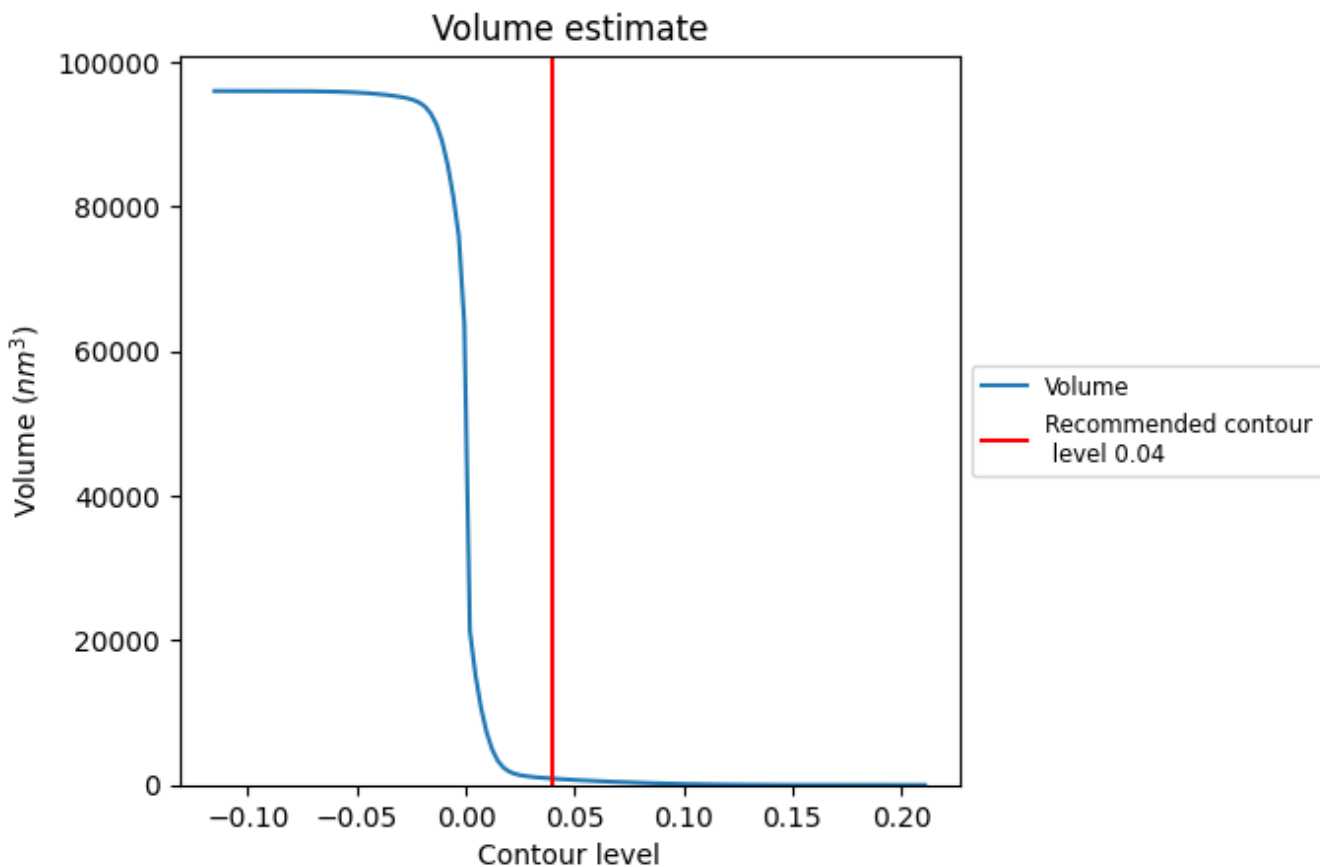
### 7.1 Map-value distribution [i](#)



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



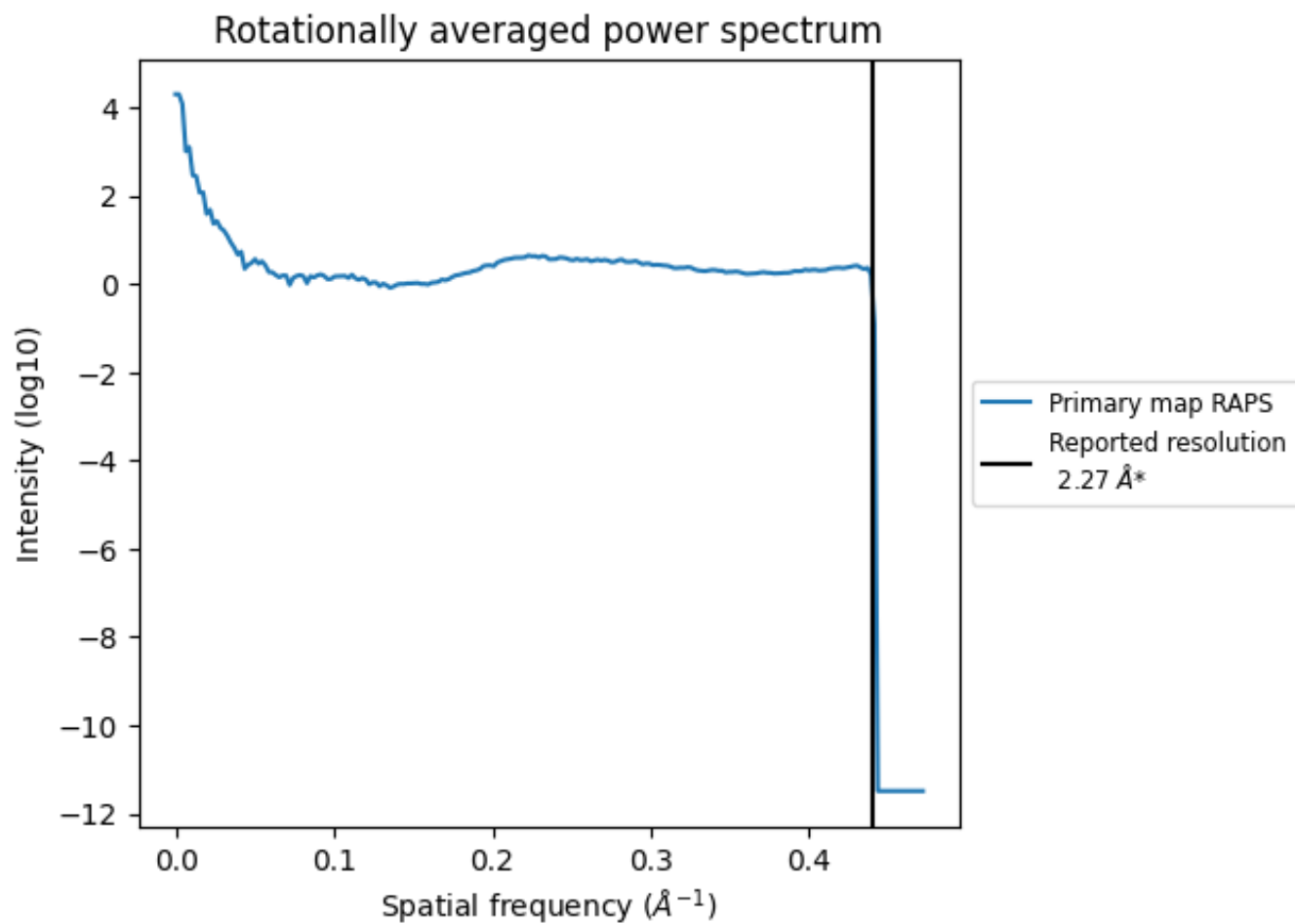
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 882  $\text{nm}^3$ ; this corresponds to an approximate mass of 796 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 [\(i\)](#)

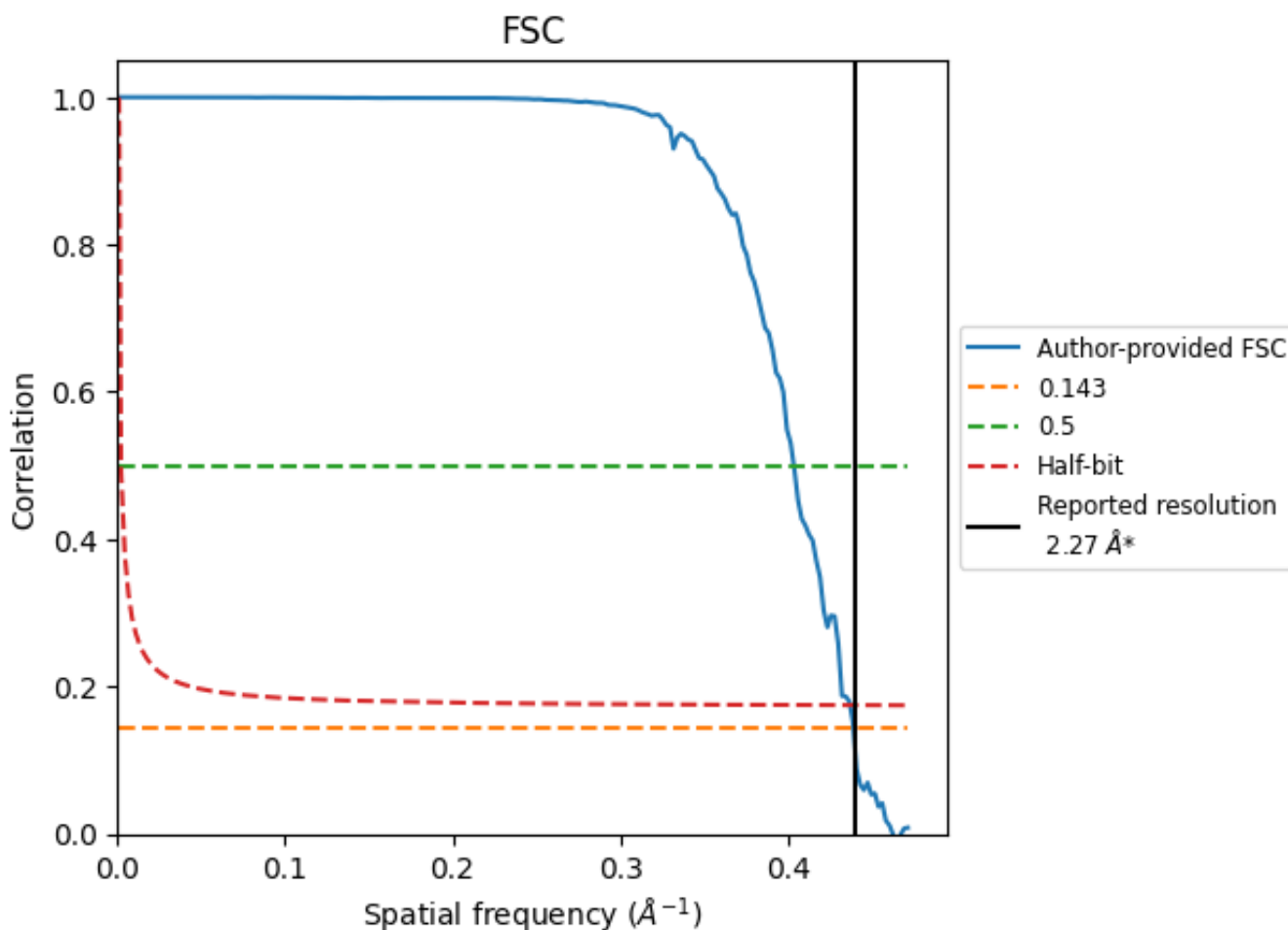


\*Reported resolution corresponds to spatial frequency of 0.441 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.441 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

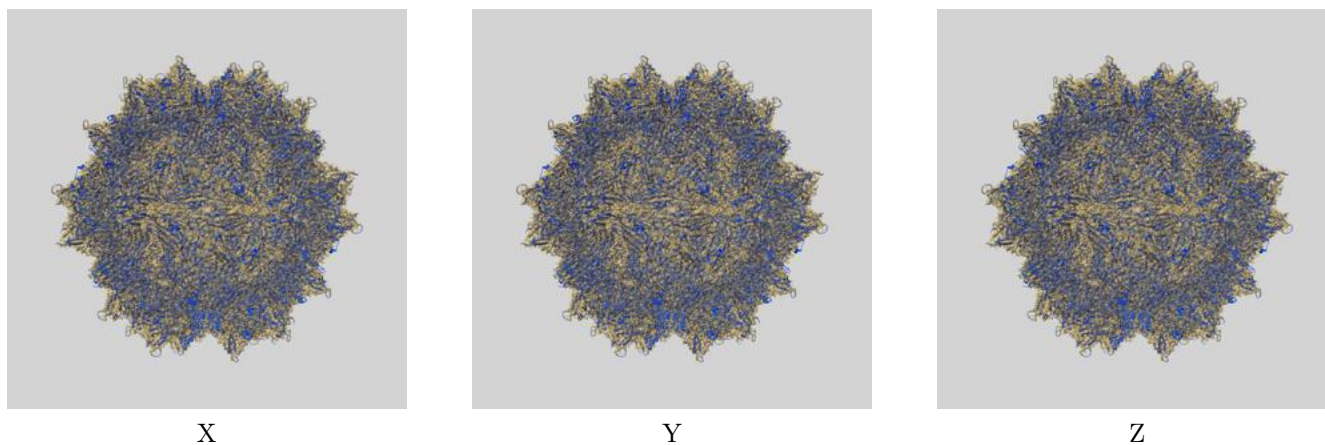
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.27	-	-
Author-provided FSC curve	2.28	2.48	2.29
Unmasked-calculated*	-	-	-

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

## 9 Map-model fit [i](#)

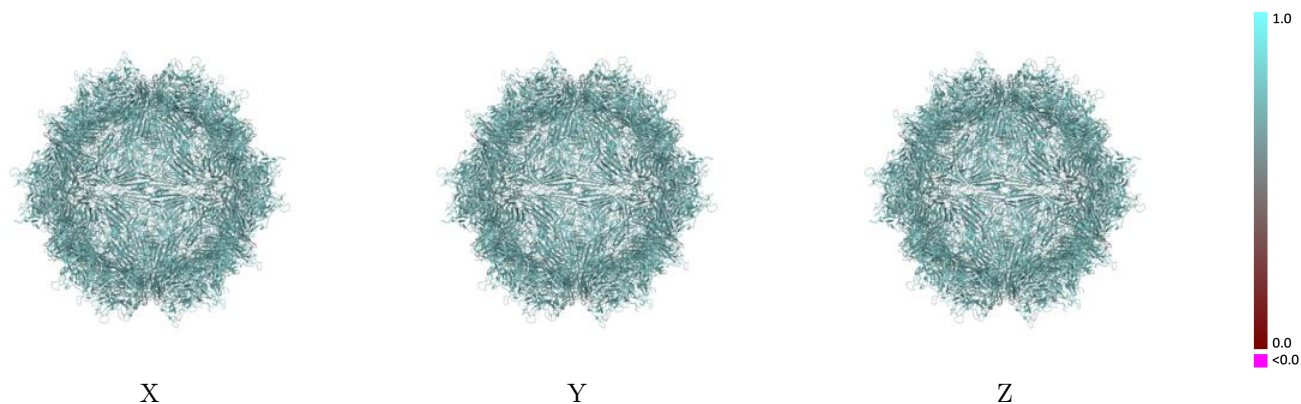
This section contains information regarding the fit between EMDB map EMD-24494 and PDB model 7RK8. Per-residue inclusion information can be found in section 3 on page 20.

### 9.1 Map-model overlay [i](#)



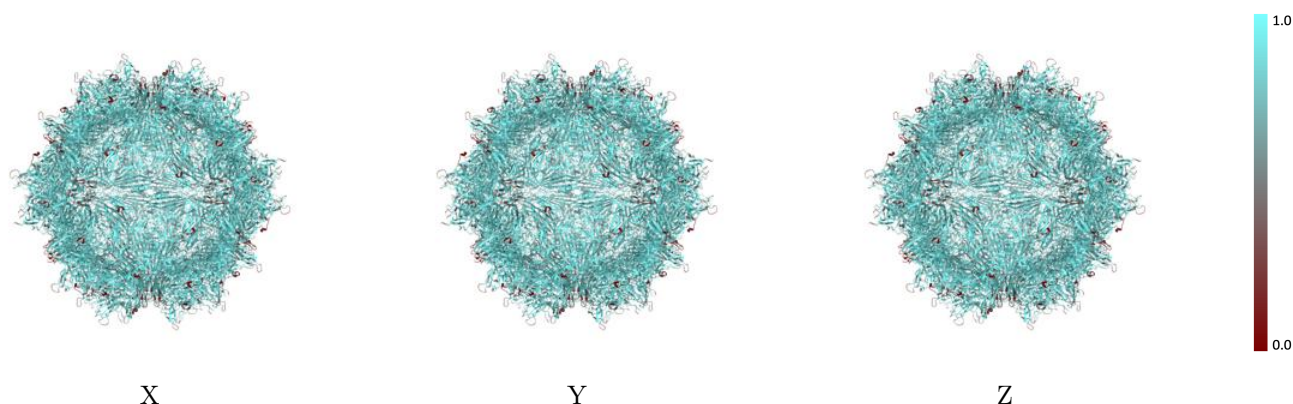
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



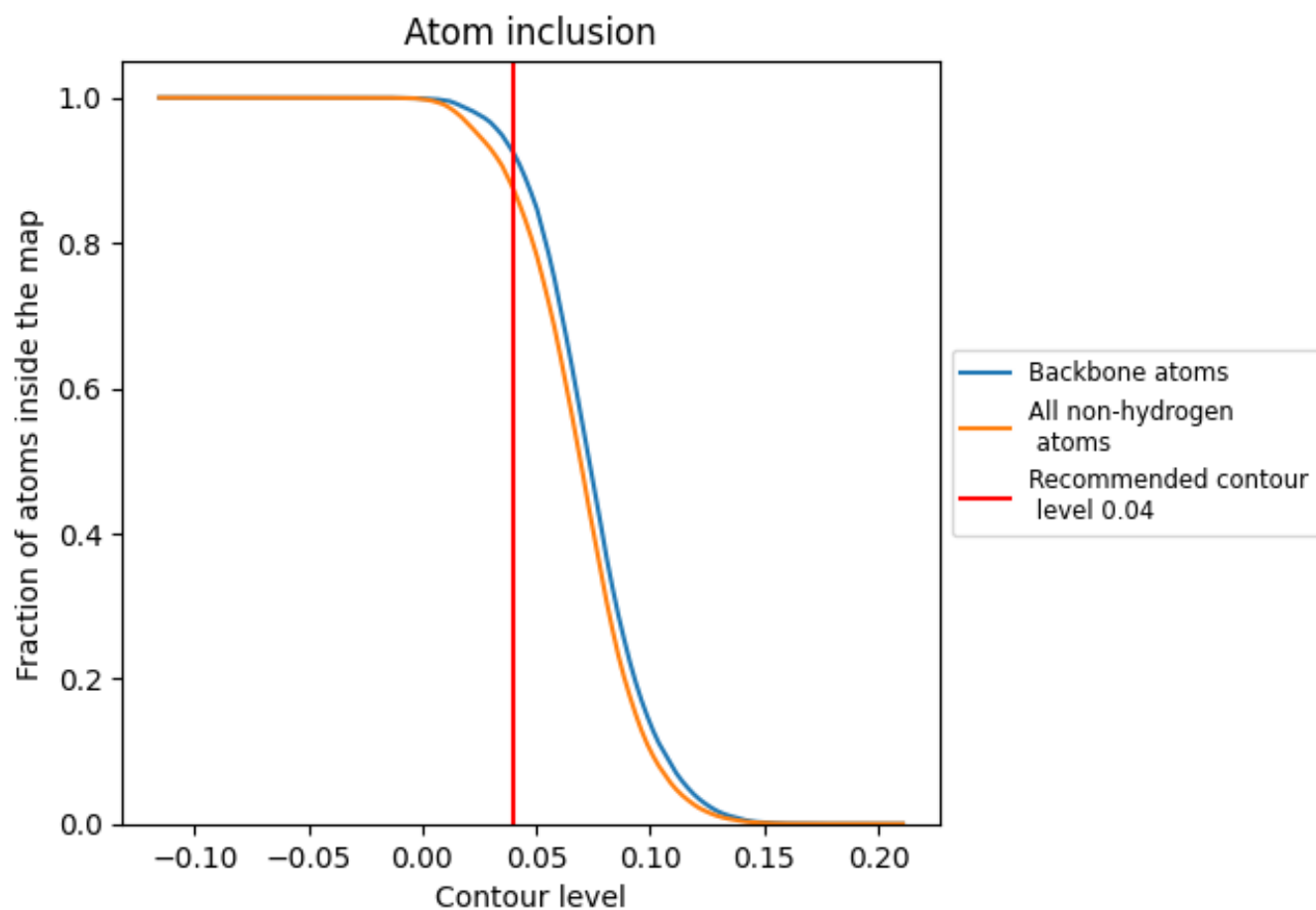
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 87% 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 (0.04) and Q-score for the entire model and for each chain.





















































Chain	Atom inclusion	Q-score
All	 0.8741	 0.7170
A	 0.8742	 0.7180
AA	 0.8710	 0.7160
AB	 0.8755	 0.7160
B	 0.8757	 0.7190
BA	 0.8750	 0.7180
BB	 0.8742	 0.7150
C	 0.8708	 0.7160
CA	 0.8757	 0.7170
CB	 0.8750	 0.7160
D	 0.8782	 0.7180
DA	 0.8760	 0.7180
DB	 0.8765	 0.7160
E	 0.8735	 0.7180
EA	 0.8760	 0.7190
EB	 0.8760	 0.7170
F	 0.8757	 0.7190
FA	 0.8735	 0.7160
FB	 0.8757	 0.7180
G	 0.8705	 0.7160
GA	 0.8730	 0.7170
GB	 0.8700	 0.7150
H	 0.8755	 0.7160
HA	 0.8762	 0.7170
HB	 0.8732	 0.7180
I	 0.8708	 0.7160
IA	 0.8735	 0.7180
IB	 0.8712	 0.7170
J	 0.8760	 0.7180
JA	 0.8745	 0.7160
K	 0.8762	 0.7170
KA	 0.8752	 0.7170
L	 0.8740	 0.7180
LA	 0.8745	 0.7180
M	 0.8755	 0.7170



*Continued on next page...*



*Continued from previous page...*

Chain	Atom inclusion	Q-score
MA	 0.8752	 0.7170
N	 0.8747	 0.7160
NA	 0.8705	 0.7160
O	 0.8735	 0.7180
OA	 0.8750	 0.7160
P	 0.8755	 0.7170
PA	 0.8747	 0.7160
Q	 0.8745	 0.7180
QA	 0.8747	 0.7160
R	 0.8710	 0.7150
RA	 0.8740	 0.7170
S	 0.8752	 0.7160
SA	 0.8750	 0.7180
T	 0.8735	 0.7170
TA	 0.8703	 0.7160
UA	 0.8752	 0.7170
V	 0.8737	 0.7170
VA	 0.8715	 0.7150
W	 0.8762	 0.7190
WA	 0.8722	 0.7170
X	 0.8757	 0.7180
XA	 0.8772	 0.7190
Y	 0.8715	 0.7160
YA	 0.8698	 0.7160
Z	 0.8745	 0.7160
ZA	 0.8750	 0.7150