



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2022 – 02:48 PM EDT

PDB ID : 5VF3
EMDB ID : EMD-8661
Title : Bacteriophage T4 isometric capsid
Authors : Chen, Z.; Sun, L.; Zhang, Z.; Fokine, A.; Padilla-Sanchez, V.; Hanein, D.;
Jiang, W.; Rossmann, M.G.; Rao, V.B.
Deposited on : 2017-04-06
Resolution : 3.30 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:

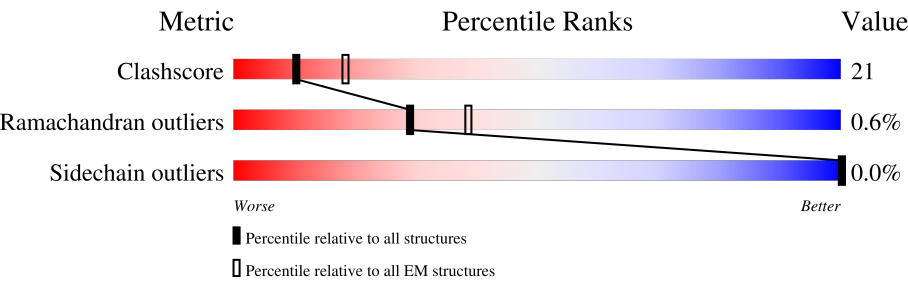
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 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.









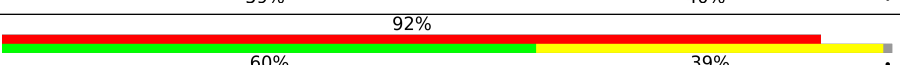

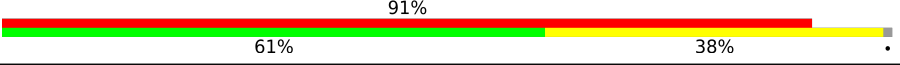
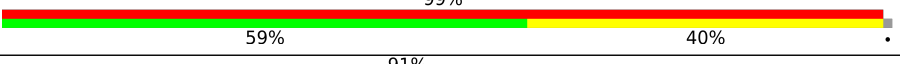
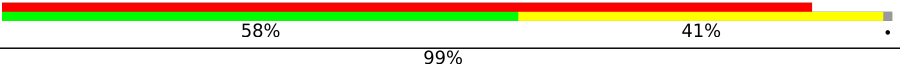

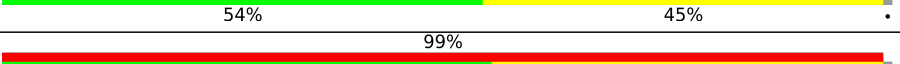
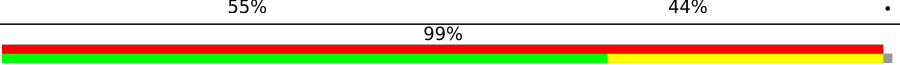
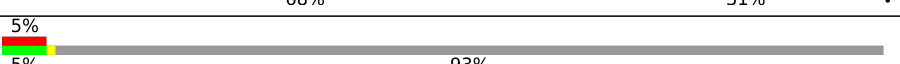
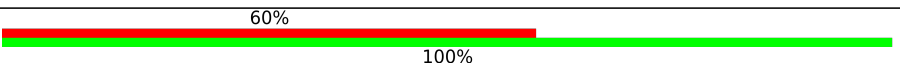


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. 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	417	<div><div>14%</div><div>98%</div><div></div></div>
2	A	456	<div><div></div><div>59%</div><div>40%</div><div></div></div>
2	B	456	<div><div></div><div>53%</div><div>47%</div><div></div></div>
2	C	456	<div><div></div><div>57%</div><div>43%</div><div></div></div>
2	D	456	<div><div></div><div>55%</div><div>44%</div><div></div></div>
2	E	456	<div><div></div><div>53%</div><div>47%</div><div></div></div>
2	F	456	<div><div></div><div>57%</div><div>43%</div><div></div></div>
2	G	456	<div><div></div><div>60%</div><div>39%</div><div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	456	 60%40%
2	I	456	 58%42%
2	J	456	 60%39%
2	K	456	 59%40%
2	L	456	 57%42%
3	O	80	 64%30%
3	P	80	 56%40%
3	Q	80	 92%39%
3	R	80	 85%36%
3	S	80	 91%38%
3	T	80	 99%40%
3	U	80	 91%41%
3	V	80	 99%36%
3	W	80	 81%45%
3	X	80	 99%44%
3	Y	80	 99%31%
4	Z	376	 5%93%
5	z	15	 60%100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 51584 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 vertex protein gp24.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	415	Total	C	N	O	S	0	0
			3208	2039	521	640	8		

- Molecule 2 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	B	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	C	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	D	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	E	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	F	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	G	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	H	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	I	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	J	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	K	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		
2	L	456	Total	C	N	O	S	0	0
			3427	2168	584	660	15		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	275	THR	ALA	conflict	UNP P04535
B	275	THR	ALA	conflict	UNP P04535
C	275	THR	ALA	conflict	UNP P04535
D	275	THR	ALA	conflict	UNP P04535
E	275	THR	ALA	conflict	UNP P04535
F	275	THR	ALA	conflict	UNP P04535
G	275	THR	ALA	conflict	UNP P04535
H	275	THR	ALA	conflict	UNP P04535
I	275	THR	ALA	conflict	UNP P04535
J	275	THR	ALA	conflict	UNP P04535
K	275	THR	ALA	conflict	UNP P04535
L	275	THR	ALA	conflict	UNP P04535

- Molecule 3 is a protein called Small outer capsid protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	O	79	Total 633	C 403	N 106	O 124	0	0
3	P	79	Total 633	C 403	N 106	O 124	0	0
3	Q	79	Total 633	C 403	N 106	O 124	0	0
3	R	79	Total 633	C 403	N 106	O 124	0	0
3	S	79	Total 633	C 403	N 106	O 124	0	0
3	T	79	Total 633	C 403	N 106	O 124	0	0
3	U	79	Total 633	C 403	N 106	O 124	0	0
3	V	79	Total 633	C 403	N 106	O 124	0	0
3	W	79	Total 633	C 403	N 106	O 124	0	0
3	X	79	Total 633	C 403	N 106	O 124	0	0
3	Y	79	Total 633	C 403	N 106	O 124	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	4	ALA	THR	conflict	UNP P03715

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
O	28	VAL	ILE	conflict	UNP P03715
P	4	ALA	THR	conflict	UNP P03715
P	28	VAL	ILE	conflict	UNP P03715
Q	4	ALA	THR	conflict	UNP P03715
Q	28	VAL	ILE	conflict	UNP P03715
R	4	ALA	THR	conflict	UNP P03715
R	28	VAL	ILE	conflict	UNP P03715
S	4	ALA	THR	conflict	UNP P03715
S	28	VAL	ILE	conflict	UNP P03715
T	4	ALA	THR	conflict	UNP P03715
T	28	VAL	ILE	conflict	UNP P03715
U	4	ALA	THR	conflict	UNP P03715
U	28	VAL	ILE	conflict	UNP P03715
V	4	ALA	THR	conflict	UNP P03715
V	28	VAL	ILE	conflict	UNP P03715
W	4	ALA	THR	conflict	UNP P03715
W	28	VAL	ILE	conflict	UNP P03715
X	4	ALA	THR	conflict	UNP P03715
X	28	VAL	ILE	conflict	UNP P03715
Y	4	ALA	THR	conflict	UNP P03715
Y	28	VAL	ILE	conflict	UNP P03715

- Molecule 4 is a protein called Highly immunogenic outer capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Z	25	Total	C	N	O	S	0	0
			214	140	32	39	3		

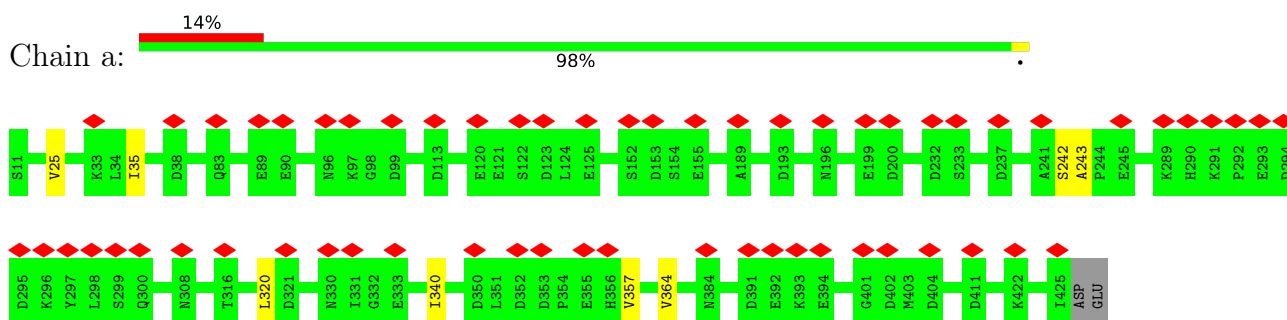
- Molecule 5 is a protein called Highly immunogenic outer capsid protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	z	15	Total	C	N	O	0	0
			75	45	15	15		

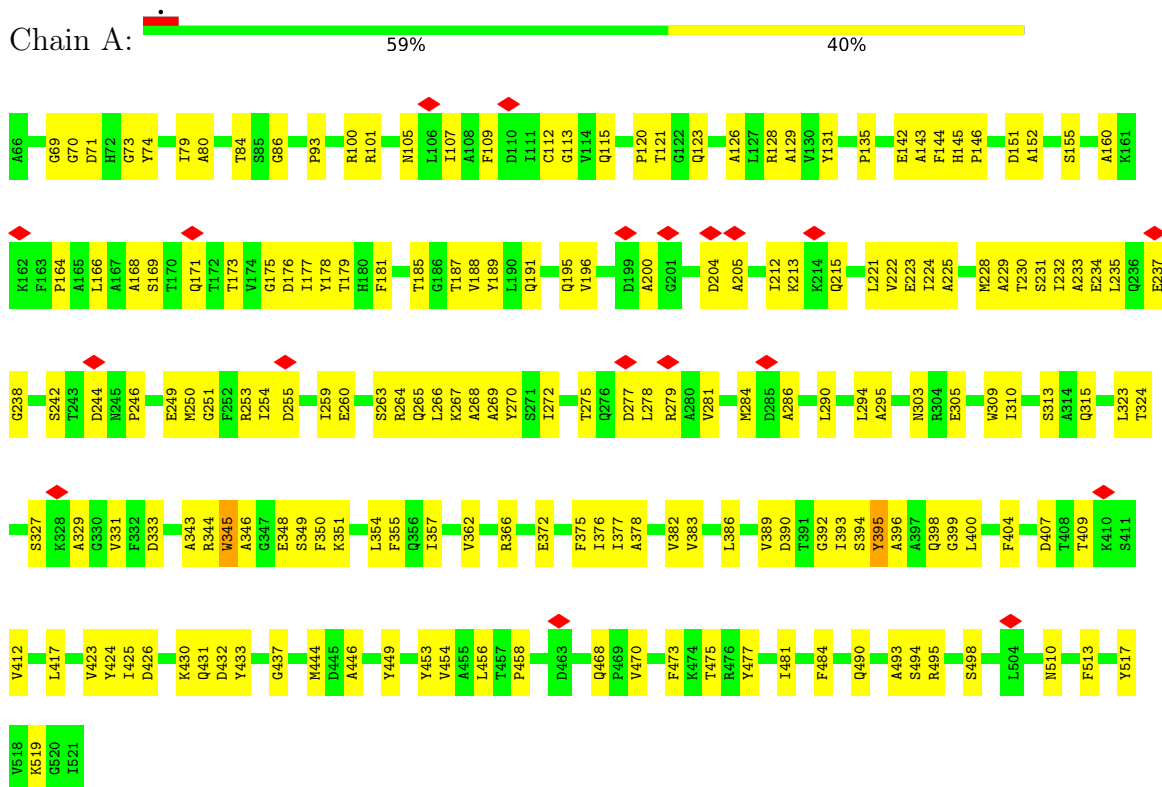
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

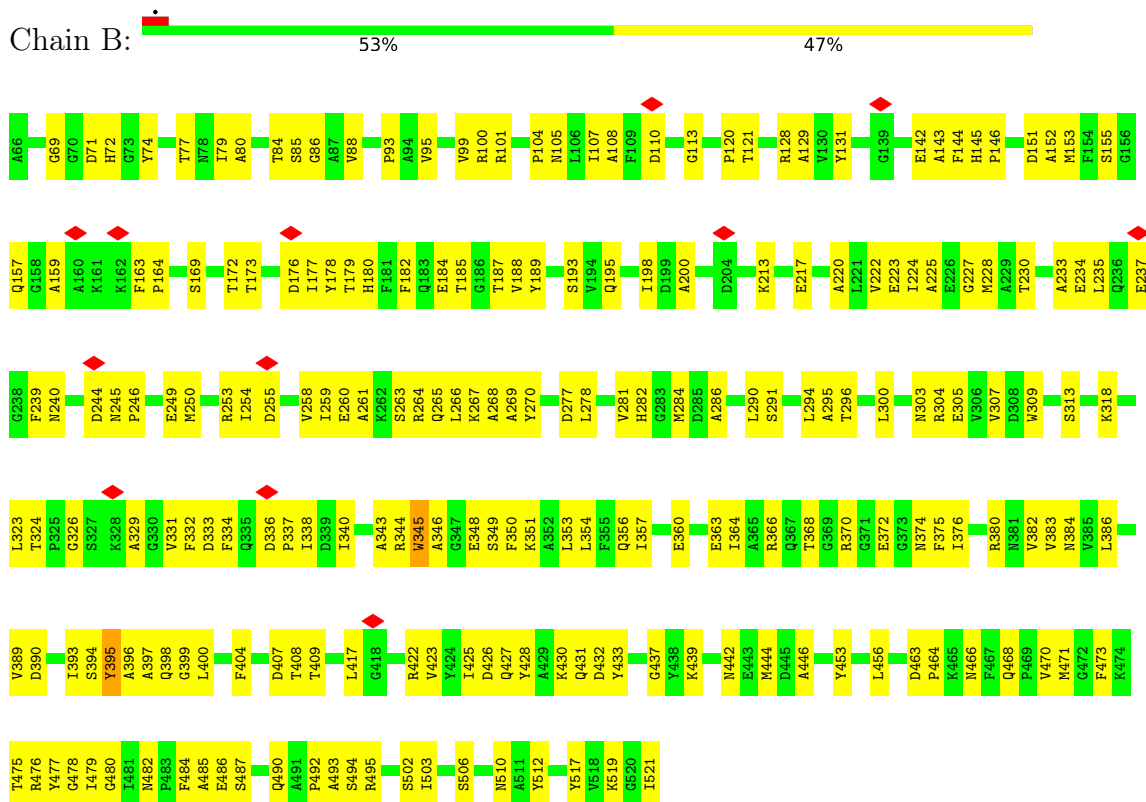
- Molecule 1: Capsid vertex protein gp24



- Molecule 2: Major capsid protein



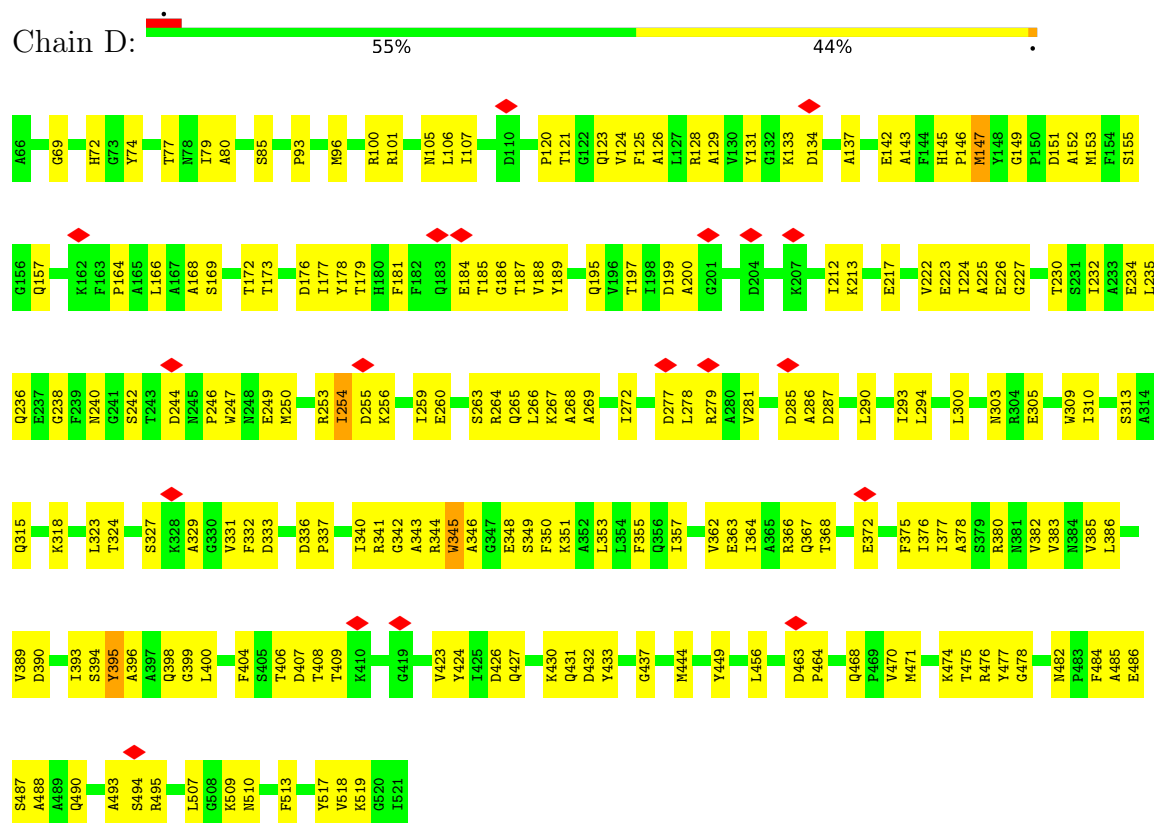
- Molecule 2: Major capsid protein



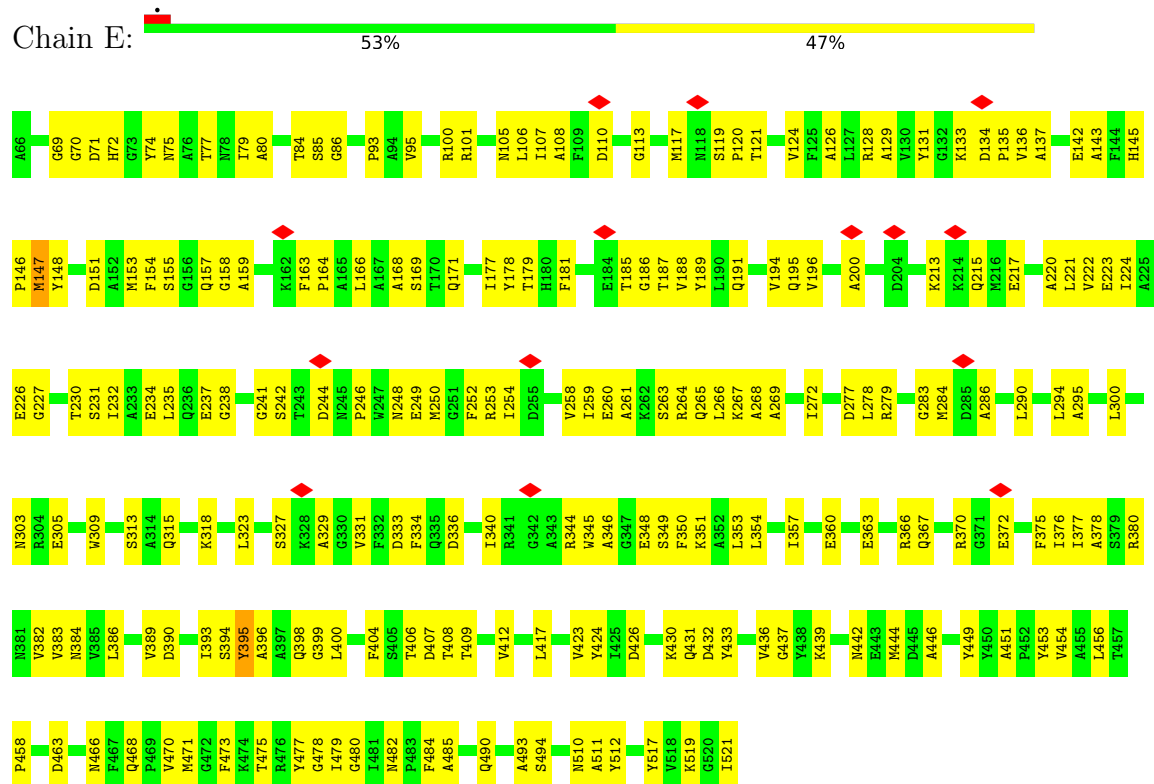
- Molecule 2: Major capsid protein



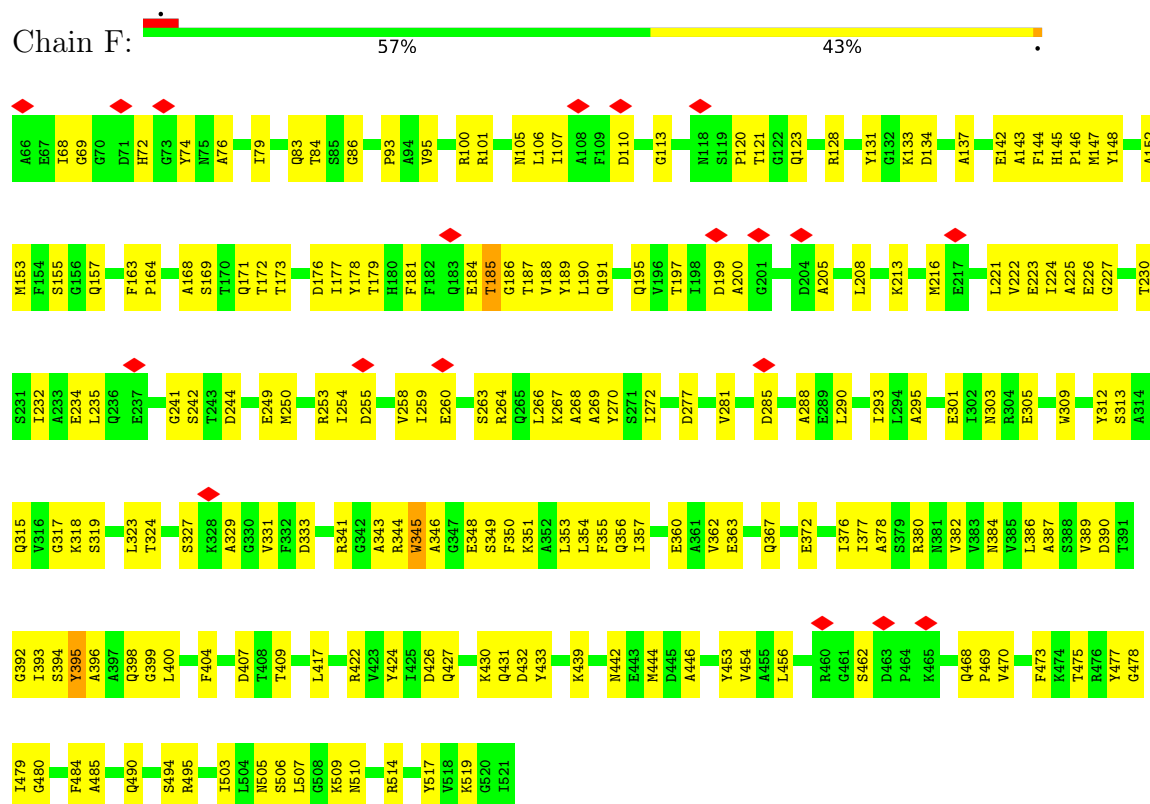
- Molecule 2: Major capsid protein

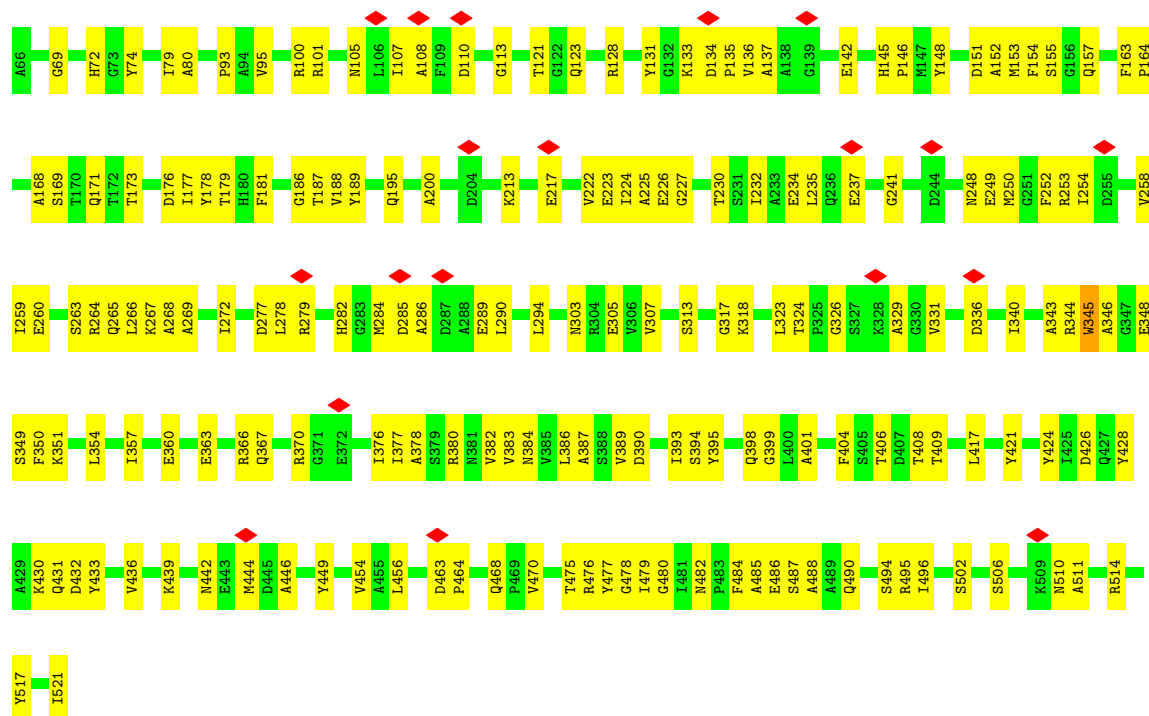


• Molecule 2: Major capsid protein



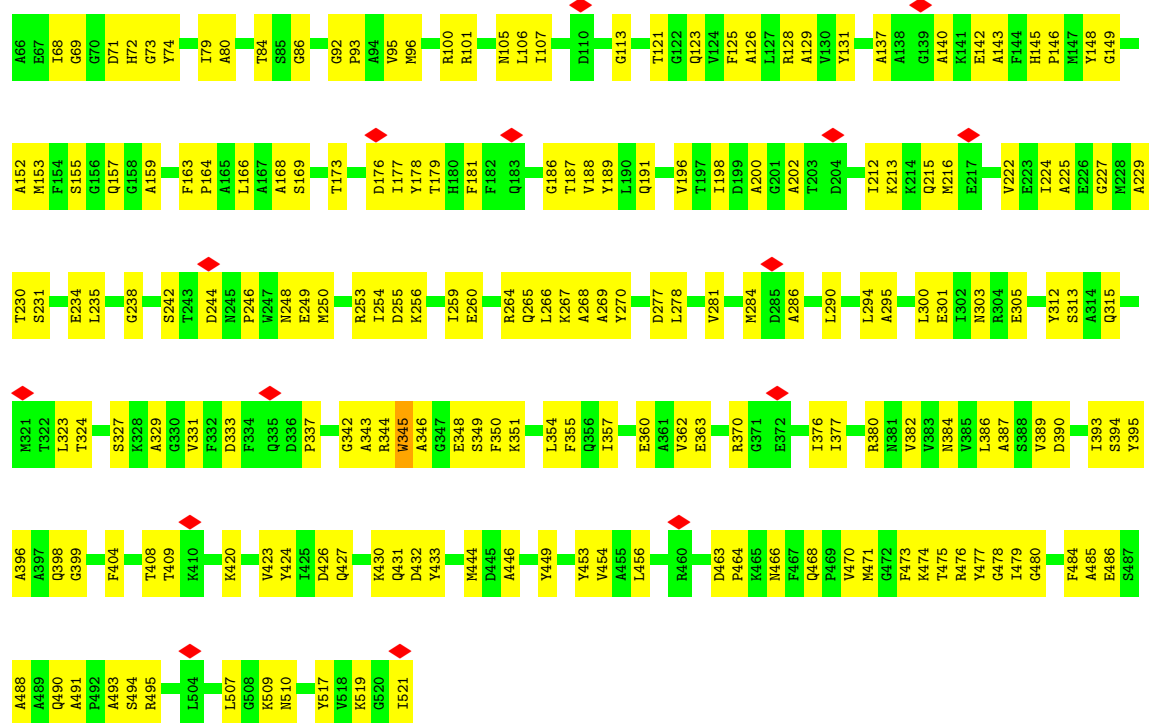
• Molecule 2: Major capsid protein





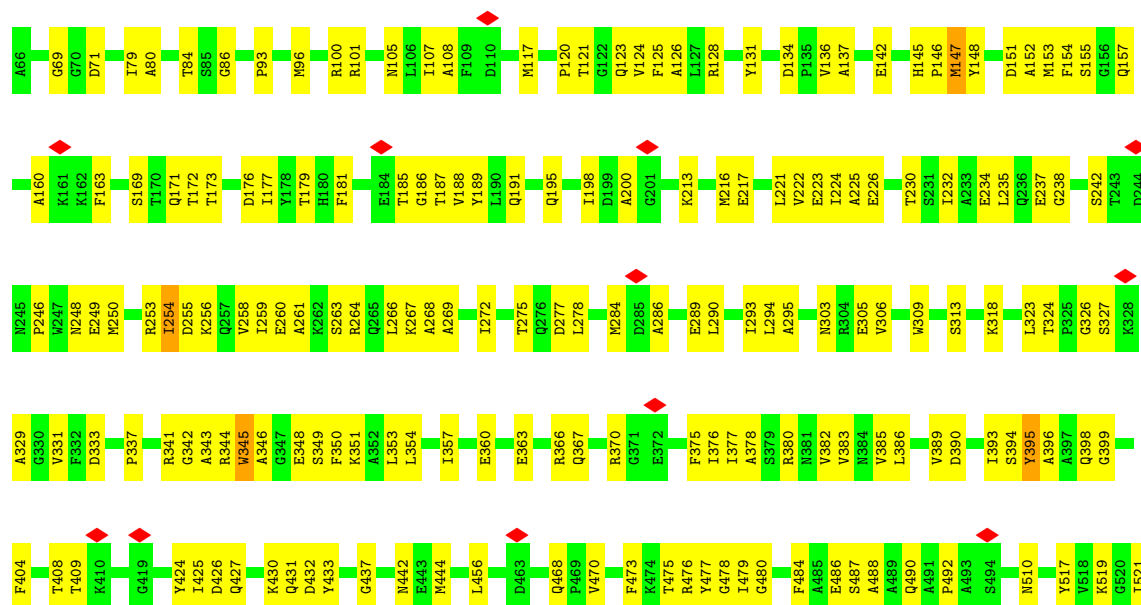
• Molecule 2: Major capsid protein

Chain I: 58% 42%



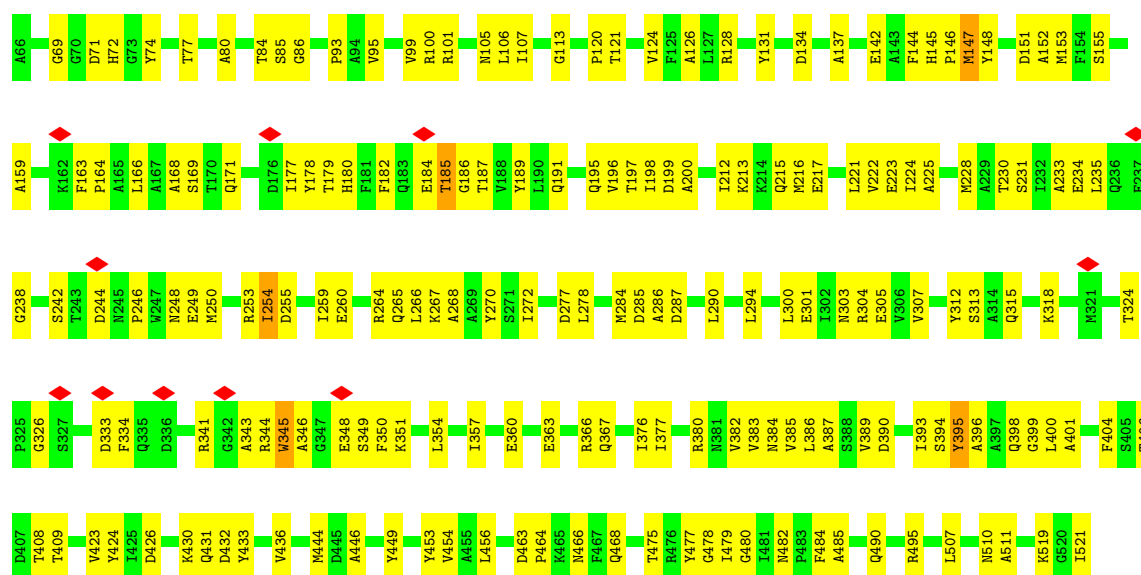
• Molecule 2: Major capsid protein

Chain J: 60% 39%



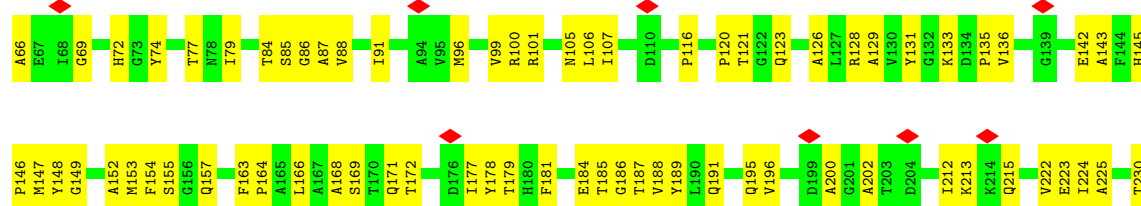
• Molecule 2: Major capsid protein

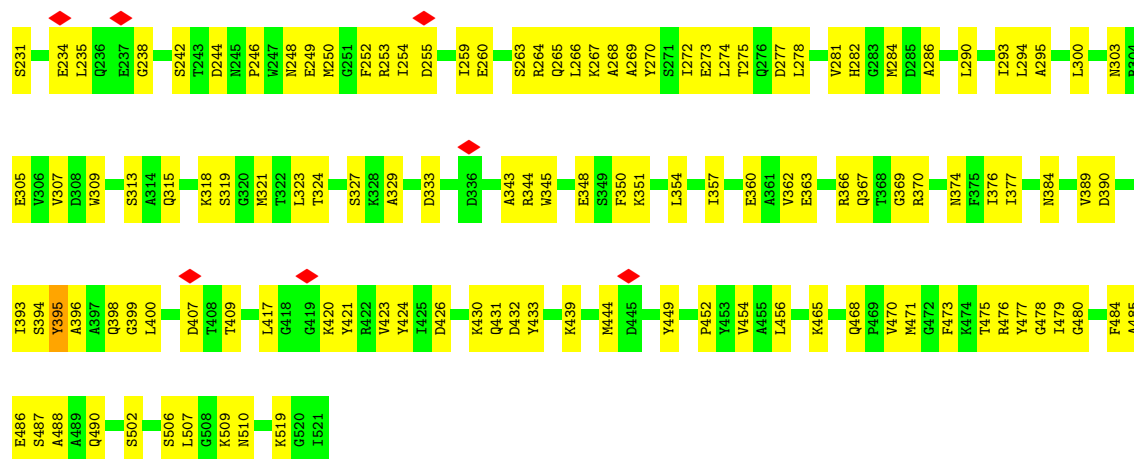
Chain K: 59% 40% .



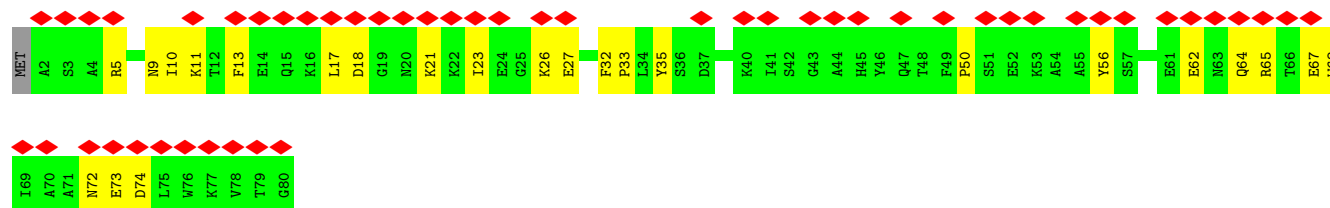
• Molecule 2: Major capsid protein

Chain L: 57% 42%

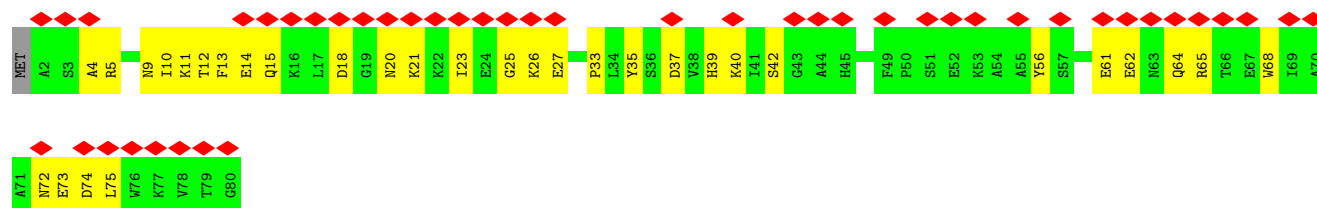




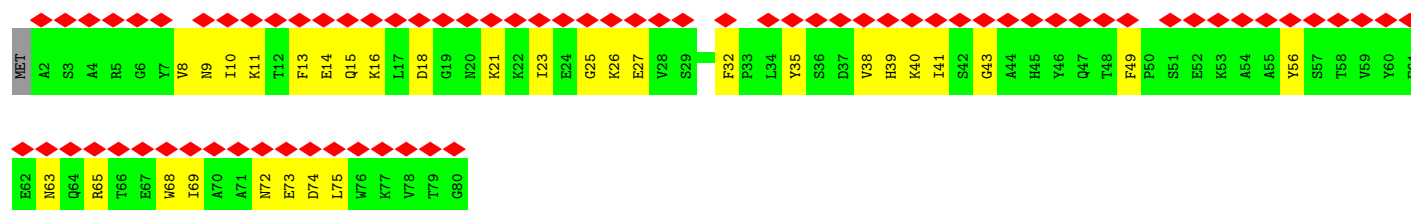
• Molecule 3: Small outer capsid protein



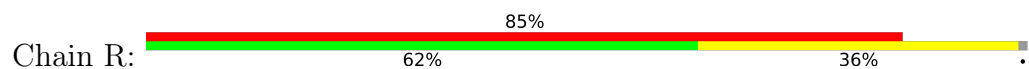
• Molecule 3: Small outer capsid protein

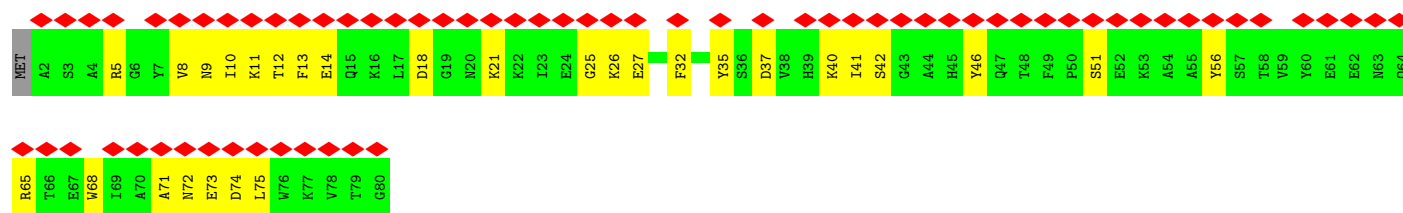


• Molecule 3: Small outer capsid protein



• Molecule 3: Small outer capsid protein

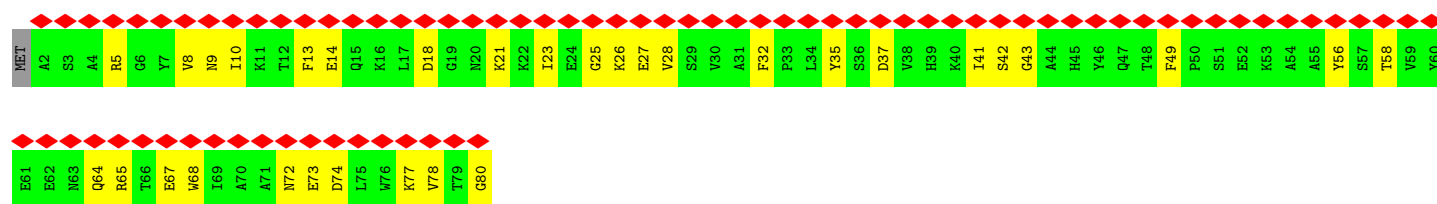




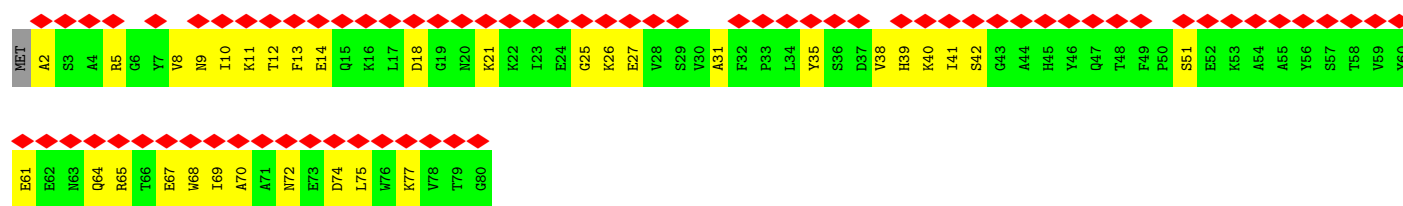
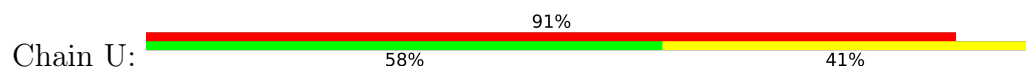
• Molecule 3: Small outer capsid protein



• Molecule 3: Small outer capsid protein



• Molecule 3: Small outer capsid protein



• Molecule 3: Small outer capsid protein

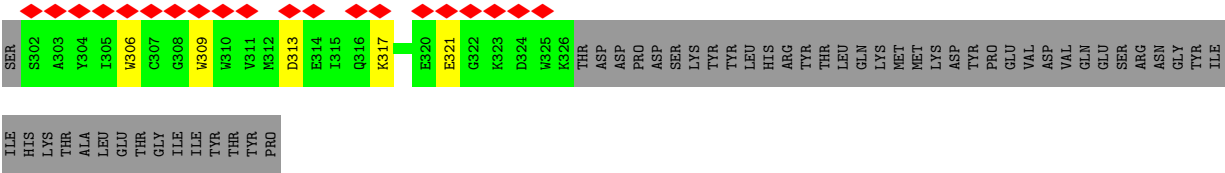


Q64	R65	T66	E67	W68	I69	A70	A71	N72	E73	D74	L75	W76	K77	V78	T79	G80																																									
A2	S3	A4	R5	G6	Y7	V8	N9	I10	K11	T12	F13	E14	Q15	K16	L17	D18	G19	N20	K21	K22	I23	E24	Q25	K26	E27	F32	P33	L34	Y35	S36	D37	V38	H39	K40	I41	S42	G43	A44	H45	Y46	Q47	T48	F49	P50	S51	E52	K53	A54	A55	Y56	S57	T58	V59	Y60	E61	E62	W63

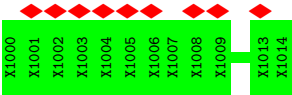
E61	E62	N63	Q64	R65	T66	E67	W68	I69	A70	A71	N72	E73	D74	L75	W76	K77	V78	T79	G80																																						
A2	S3	A4	R5	G6	T7	V8	N9	I10	K11	T12	F13	E14	Q15	K16	L17	D18	G19	I20	K21	K22	E24	G25	K26	E27	V28	S29	V30	A31	F32	P33	L34	Y35	S36	D37	V38	H39	K40	I41	S42	G43	A44	H45	Y46	Q47	T48	F49	P50	S51	E52	K53	A54	A55	Y56	S57	T58	V59	V60

E61	E62	E63	E64	E65	E66	E67	E68	E69	E70	E71	E72	E73	E74	E75	E76	E77	E78	E79	E80
A2	A3	A4	A5	A6	A7	A8	A9	A10	A11	A12	A13	A14	A15	A16	A17	A18	A19	A20	A21
B2	B3	B4	B5	B6	B7	B8	B9	B10	B11	B12	B13	B14	B15	B16	B17	B18	B19	B20	B21
C2	C3	C4	C5	C6	C7	C8	C9	C10	C11	C12	C13	C14	C15	C16	C17	C18	C19	C20	C21
D2	D3	D4	D5	D6	D7	D8	D9	D10	D11	D12	D13	D14	D15	D16	D17	D18	D19	D20	D21
E2	E3	E4	E5	E6	E7	E8	E9	E10	E11	E12	E13	E14	E15	E16	E17	E18	E19	E20	E21
F2	F3	F4	F5	F6	F7	F8	F9	F10	F11	F12	F13	F14	F15	F16	F17	F18	F19	F20	F21
G2	G3	G4	G5	G6	G7	G8	G9	G10	G11	G12	G13	G14	G15	G16	G17	G18	G19	G20	G21
H2	H3	H4	H5	H6	H7	H8	H9	H10	H11	H12	H13	H14	H15	H16	H17	H18	H19	H20	H21
I2	I3	I4	I5	I6	I7	I8	I9	I10	I11	I12	I13	I14	I15	I16	I17	I18	I19	I20	I21
J2	J3	J4	J5	J6	J7	J8	J9	J10	J11	J12	J13	J14	J15	J16	J17	J18	J19	J20	J21
K2	K3	K4	K5	K6	K7	K8	K9	K10	K11	K12	K13	K14	K15	K16	K17	K18	K19	K20	K21
L2	L3	L4	L5	L6	L7	L8	L9	L10	L11	L12	L13	L14	L15	L16	L17	L18	L19	L20	L21
M2	M3	M4	M5	M6	M7	M8	M9	M10	M11	M12	M13	M14	M15	M16	M17	M18	M19	M20	M21
N2	N3	N4	N5	N6	N7	N8	N9	N10	N11	N12	N13	N14	N15	N16	N17	N18	N19	N20	N21
O2	O3	O4	O5	O6	O7	O8	O9	O10	O11	O12	O13	O14	O15	O16	O17	O18	O19	O20	O21
P2	P3	P4	P5	P6	P7	P8	P9	P10	P11	P12	P13	P14	P15	P16	P17	P18	P19	P20	P21
Q2	Q3	Q4	Q5	Q6	Q7	Q8	Q9	Q10	Q11	Q12	Q13	Q14	Q15	Q16	Q17	Q18	Q19	Q20	Q21
R2	R3	R4	R5	R6	R7	R8	R9	R10	R11	R12	R13	R14	R15	R16	R17	R18	R19	R20	R21
S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15	S16	S17	S18	S19	S20	S21
T2	T3	T4	T5	T6	T7	T8	T9	T10	T11	T12	T13	T14	T15	T16	T17	T18	T19	T20	T21
U2	U3	U4	U5	U6	U7	U8	U9	U10	U11	U12	U13	U14	U15	U16	U17	U18	U19	U20	U21
V2	V3	V4	V5	V6	V7	V8	V9	V10	V11	V12	V13	V14	V15	V16	V17	V18	V19	V20	V21
W2	W3	W4	W5	W6	W7	W8	W9	W10	W11	W12	W13	W14	W15	W16	W17	W18	W19	W20	W21
X2	X3	X4	X5	X6	X7	X8	X9	X10	X11	X12	X13	X14	X15	X16	X17	X18	X19	X20	X21
Y2	Y3	Y4	Y5	Y6	Y7	Y8	Y9	Y10	Y11	Y12	Y13	Y14	Y15	Y16	Y17	Y18	Y19	Y20	Y21
Z2	Z3	Z4	Z5	Z6	Z7	Z8	Z9	Z10	Z11	Z12	Z13	Z14	Z15	Z16	Z17	Z18	Z19	Z20	Z21

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



● Molecule 5: Highly immunogenic outer capsid protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	18000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; CTF amplitude correction was performed during 3D reconstruction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	26	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-3500	Depositor
Magnification	18000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	42.346	Depositor
Minimum map value	-31.033	Depositor
Average map value	0.006	Depositor
Map value standard deviation	1.708	Depositor
Recommended contour level	8.0	Depositor
Map size (Å)	1244.16, 1244.16, 1244.16	wwPDB
Map dimensions	1536, 1536, 1536	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	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	0.56	0/3263	0.62	0/4430
2	A	0.61	0/3495	0.64	1/4734 (0.0%)
2	B	0.62	0/3495	0.64	1/4734 (0.0%)
2	C	0.63	0/3495	0.64	1/4734 (0.0%)
2	D	0.61	0/3495	0.64	1/4734 (0.0%)
2	E	0.63	0/3495	0.64	0/4734
2	F	0.62	0/3495	0.64	1/4734 (0.0%)
2	G	0.61	0/3495	0.64	1/4734 (0.0%)
2	H	0.61	0/3495	0.64	1/4734 (0.0%)
2	I	0.61	0/3495	0.64	1/4734 (0.0%)
2	J	0.61	0/3495	0.64	1/4734 (0.0%)
2	K	0.61	0/3495	0.64	1/4734 (0.0%)
2	L	0.61	0/3495	0.64	0/4734
3	O	0.41	0/648	0.49	0/876
3	P	0.41	0/648	0.51	0/876
3	Q	0.37	0/648	0.49	0/876
3	R	0.37	0/648	0.52	0/876
3	S	0.36	0/648	0.49	0/876
3	T	0.32	0/648	0.48	0/876
3	U	0.34	0/648	0.48	0/876
3	V	0.29	0/648	0.47	0/876
3	W	0.36	0/648	0.51	0/876
3	X	0.32	0/648	0.48	0/876
3	Y	0.33	0/648	0.47	0/876
4	Z	0.27	0/222	0.43	0/301
All	All	0.58	0/52553	0.62	10/71175 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
-----	-------	---------------------	---------------------

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	3
2	E	0	1
2	F	0	1
2	G	0	1
2	K	0	1
3	Q	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	345	TRP	CA-CB-CG	5.85	124.81	113.70
2	H	345	TRP	CA-CB-CG	5.79	124.71	113.70
2	C	345	TRP	CA-CB-CG	5.67	124.48	113.70
2	D	345	TRP	CA-CB-CG	5.59	124.32	113.70
2	F	345	TRP	CA-CB-CG	5.58	124.30	113.70

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	185	THR	Peptide
2	F	185	THR	Peptide
1	a	242	SER	Peptide
1	a	320	LEU	Peptide
1	a	35	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3208	0	3205	0	0
2	A	3427	0	3373	174	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3427	0	3373	195	0
2	C	3427	0	3373	194	0
2	D	3427	0	3373	191	0
2	E	3427	0	3373	201	0
2	F	3427	0	3373	183	0
2	G	3427	0	3373	174	0
2	H	3427	0	3373	158	0
2	I	3427	0	3373	177	0
2	J	3427	0	3373	166	0
2	K	3427	0	3373	174	0
2	L	3427	0	3373	186	0
3	O	633	0	608	22	0
3	P	633	0	608	26	0
3	Q	633	0	608	28	0
3	R	633	0	608	25	0
3	S	633	0	608	29	0
3	T	633	0	608	33	0
3	U	633	0	608	24	0
3	V	633	0	608	23	0
3	W	633	0	608	28	0
3	X	633	0	608	30	0
3	Y	633	0	608	22	0
4	Z	214	0	187	3	0
5	z	75	0	19	0	0
All	All	51584	0	50575	2035	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 21.

The worst 5 of 2035 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)
2:A:152:ALA:HB1	2:A:225:ALA:HB2	1.51	0.92
2:J:431:GLN:HE22	2:K:217:GLU:HB2	1.35	0.92
2:J:152:ALA:HB1	2:J:225:ALA:HB2	1.51	0.91
2:H:152:ALA:HB1	2:H:225:ALA:HB2	1.54	0.89
2:F:152:ALA:HB1	2:F:225:ALA:HB2	1.55	0.89

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	413/417 (99%)	374 (91%)	34 (8%)	5 (1%)	13	42
2	A	454/456 (100%)	411 (90%)	41 (9%)	2 (0%)	34	66
2	B	454/456 (100%)	407 (90%)	44 (10%)	3 (1%)	22	54
2	C	454/456 (100%)	408 (90%)	43 (10%)	3 (1%)	22	54
2	D	454/456 (100%)	410 (90%)	41 (9%)	3 (1%)	22	54
2	E	454/456 (100%)	406 (89%)	44 (10%)	4 (1%)	17	48
2	F	454/456 (100%)	413 (91%)	39 (9%)	2 (0%)	34	66
2	G	454/456 (100%)	413 (91%)	38 (8%)	3 (1%)	22	54
2	H	454/456 (100%)	407 (90%)	44 (10%)	3 (1%)	22	54
2	I	454/456 (100%)	408 (90%)	44 (10%)	2 (0%)	34	66
2	J	454/456 (100%)	413 (91%)	37 (8%)	4 (1%)	17	48
2	K	454/456 (100%)	410 (90%)	41 (9%)	3 (1%)	22	54
2	L	454/456 (100%)	409 (90%)	43 (10%)	2 (0%)	34	66
3	O	77/80 (96%)	69 (90%)	8 (10%)	0	100	100
3	P	77/80 (96%)	70 (91%)	7 (9%)	0	100	100
3	Q	77/80 (96%)	70 (91%)	7 (9%)	0	100	100
3	R	77/80 (96%)	70 (91%)	7 (9%)	0	100	100
3	S	77/80 (96%)	70 (91%)	7 (9%)	0	100	100
3	T	77/80 (96%)	71 (92%)	6 (8%)	0	100	100
3	U	77/80 (96%)	72 (94%)	5 (6%)	0	100	100
3	V	77/80 (96%)	69 (90%)	8 (10%)	0	100	100
3	W	77/80 (96%)	70 (91%)	7 (9%)	0	100	100
3	X	77/80 (96%)	69 (90%)	8 (10%)	0	100	100
3	Y	77/80 (96%)	71 (92%)	6 (8%)	0	100	100
4	Z	23/376 (6%)	23 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	6731/7145 (94%)	6083 (90%)	609 (9%)	39 (1%)	29	57

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	395	TYR
2	H	395	TYR
2	I	395	TYR
2	J	395	TYR
2	L	395	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	350/352 (99%)	350 (100%)	0	100	100
2	A	346/346 (100%)	346 (100%)	0	100	100
2	B	346/346 (100%)	346 (100%)	0	100	100
2	C	346/346 (100%)	346 (100%)	0	100	100
2	D	346/346 (100%)	346 (100%)	0	100	100
2	E	346/346 (100%)	346 (100%)	0	100	100
2	F	346/346 (100%)	346 (100%)	0	100	100
2	G	346/346 (100%)	346 (100%)	0	100	100
2	H	346/346 (100%)	346 (100%)	0	100	100
2	I	346/346 (100%)	346 (100%)	0	100	100
2	J	346/346 (100%)	346 (100%)	0	100	100
2	K	346/346 (100%)	346 (100%)	0	100	100
2	L	346/346 (100%)	346 (100%)	0	100	100
3	O	66/67 (98%)	66 (100%)	0	100	100
3	P	66/67 (98%)	66 (100%)	0	100	100
3	Q	66/67 (98%)	66 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	R	66/67 (98%)	66 (100%)	0	100	100
3	S	66/67 (98%)	66 (100%)	0	100	100
3	T	66/67 (98%)	66 (100%)	0	100	100
3	U	66/67 (98%)	66 (100%)	0	100	100
3	V	66/67 (98%)	66 (100%)	0	100	100
3	W	66/67 (98%)	66 (100%)	0	100	100
3	X	66/67 (98%)	66 (100%)	0	100	100
3	Y	66/67 (98%)	66 (100%)	0	100	100
4	Z	21/319 (7%)	19 (90%)	2 (10%)	8	29
All	All	5249/5560 (94%)	5247 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Z	317	LYS
4	Z	321	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 111 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	282	HIS
3	X	15	GLN
2	I	236	GLN
3	T	45	HIS
2	L	282	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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.

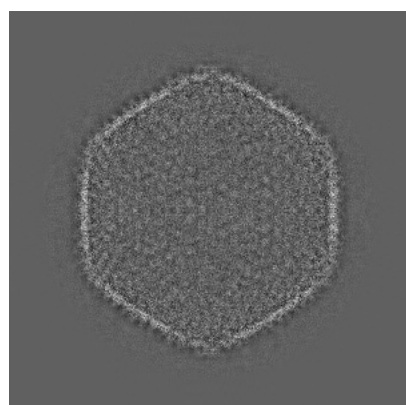
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8661. These allow visual inspection of the internal detail of the map and identification of artifacts.

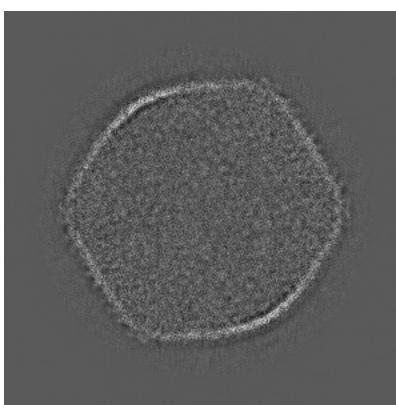
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

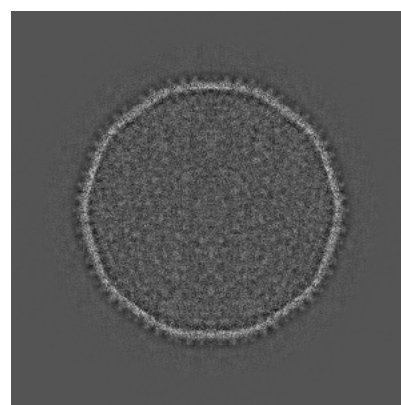
6.1.1 Primary map



X



Y

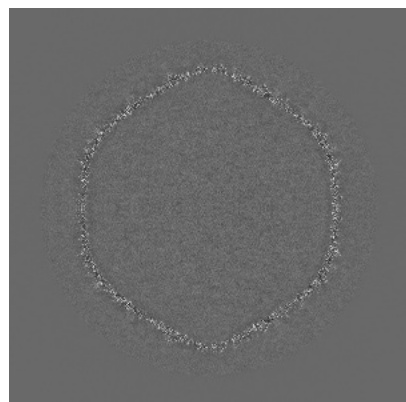


Z

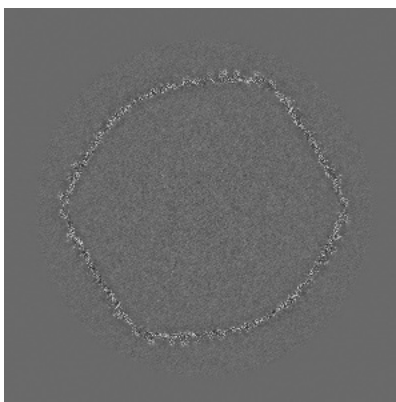
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

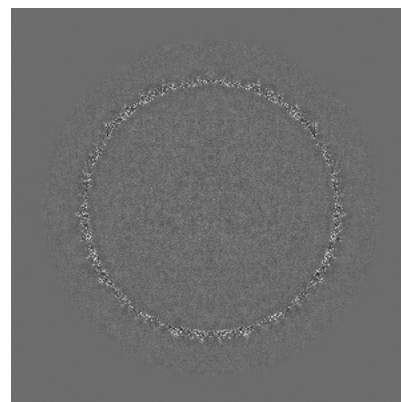
6.2.1 Primary map



X Index: 768



Y Index: 768

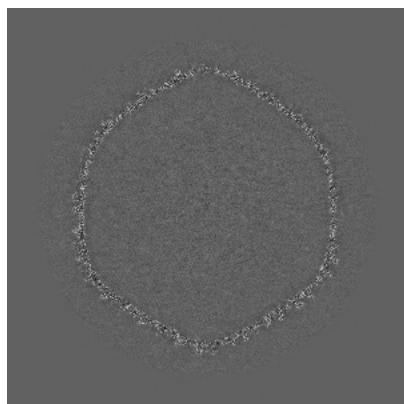


Z Index: 768

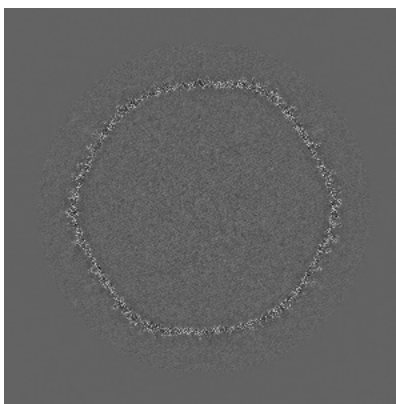
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

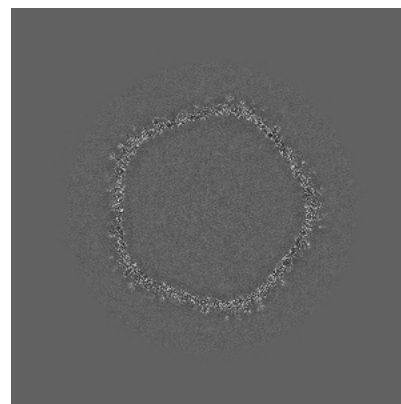
6.3.1 Primary map



X Index: 734



Y Index: 666



Z Index: 1095

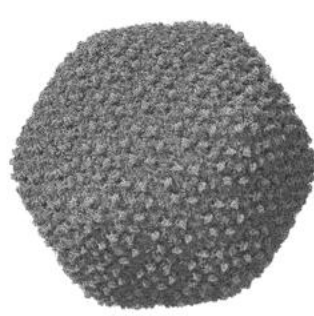
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

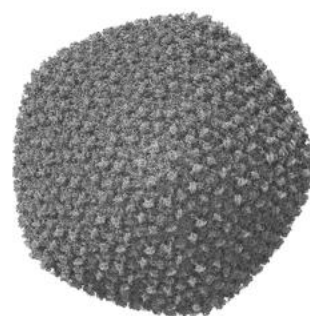
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

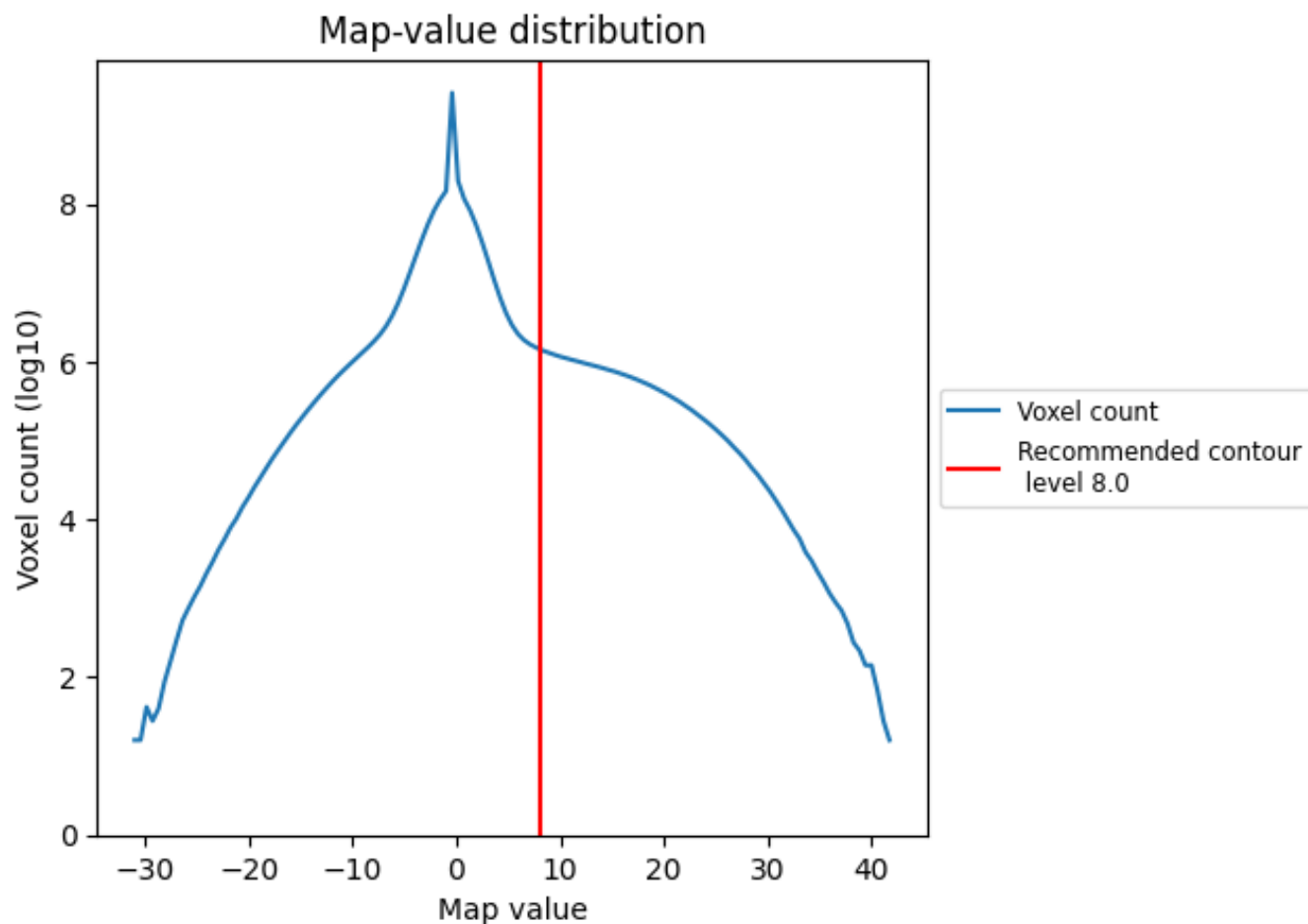
6.5 Mask visualisation

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

7 Map analysis [i](#)

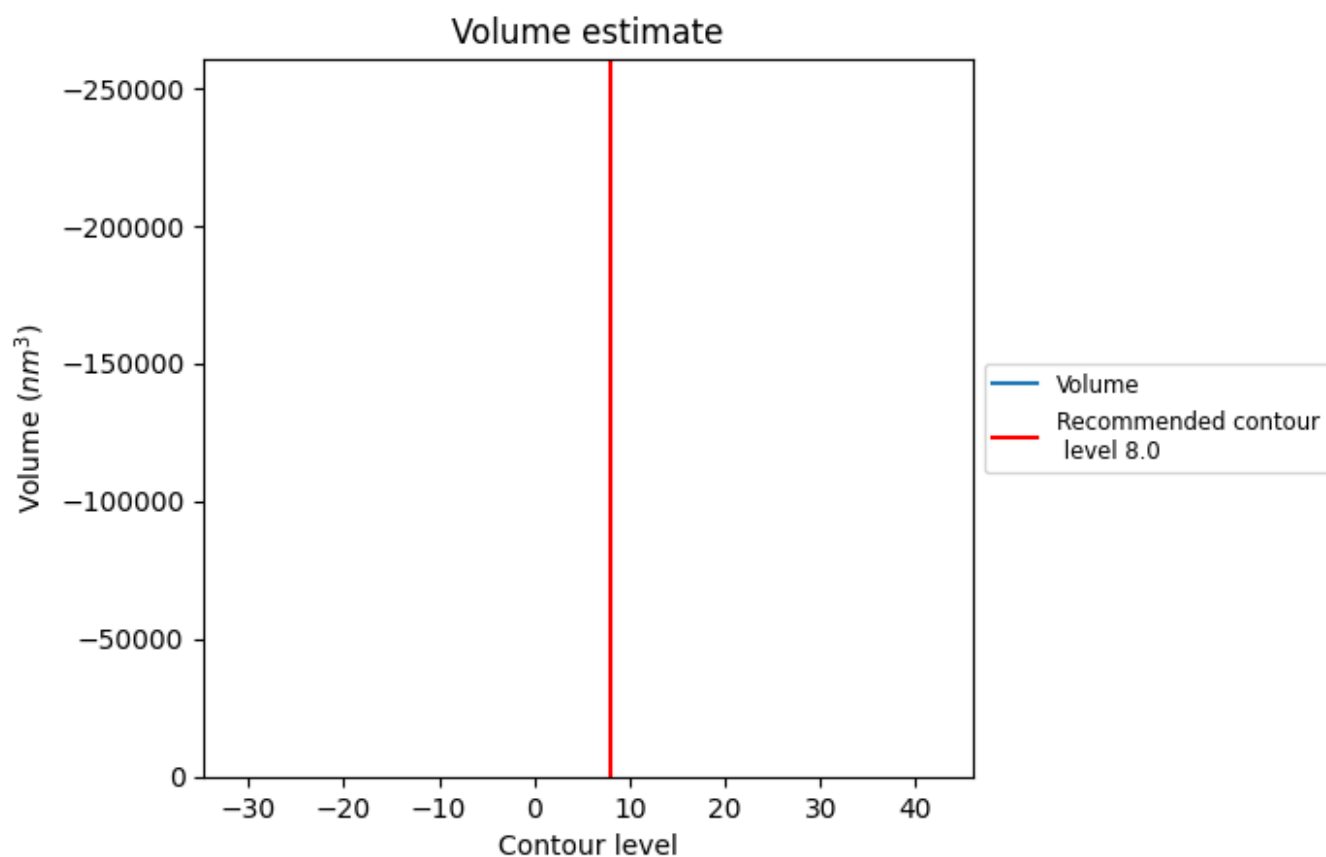
This section contains the results of statistical analysis of the map.

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.

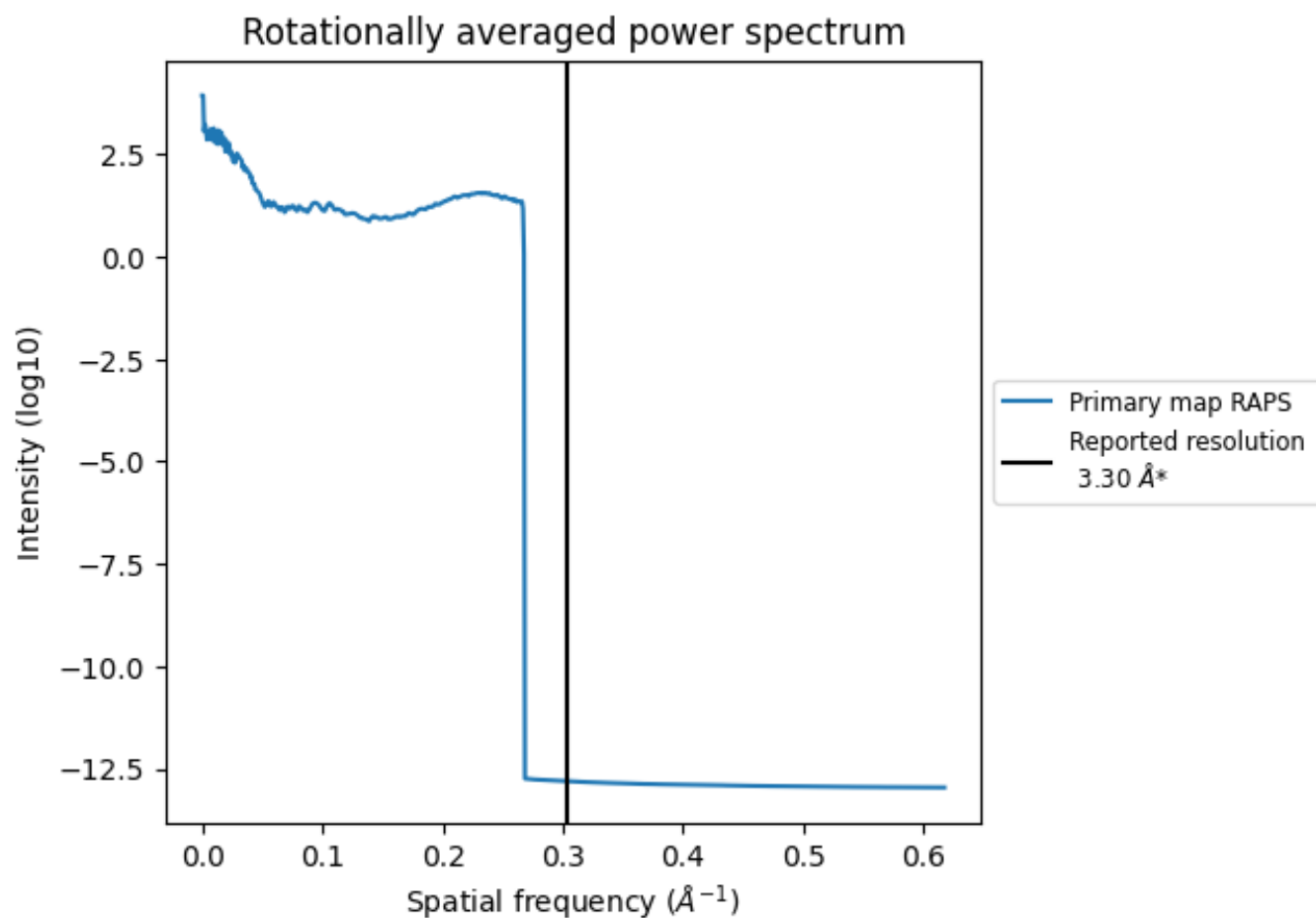
7.2 Volume estimate [i](#)



The volume at the recommended contour level is -2271095 nm³; this corresponds to an approximate mass of -2051540 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation ⓘ

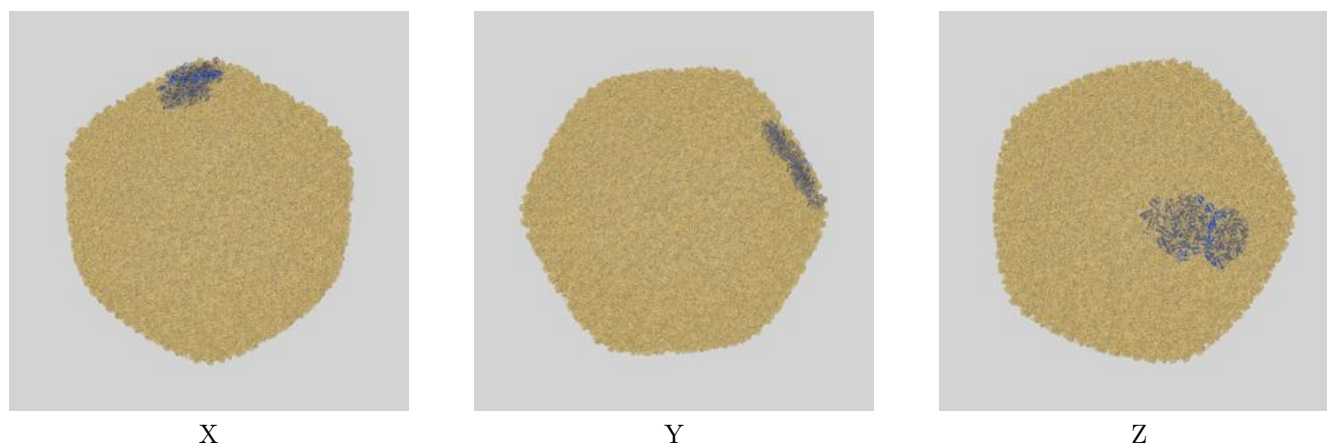
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

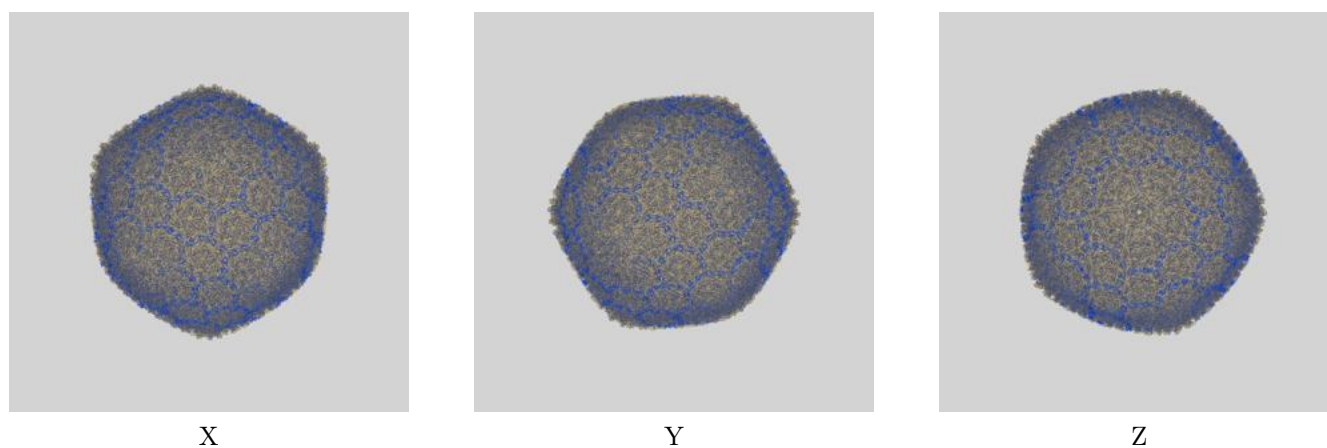
This section contains information regarding the fit between EMDB map EMD-8661 and PDB model 5VF3. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

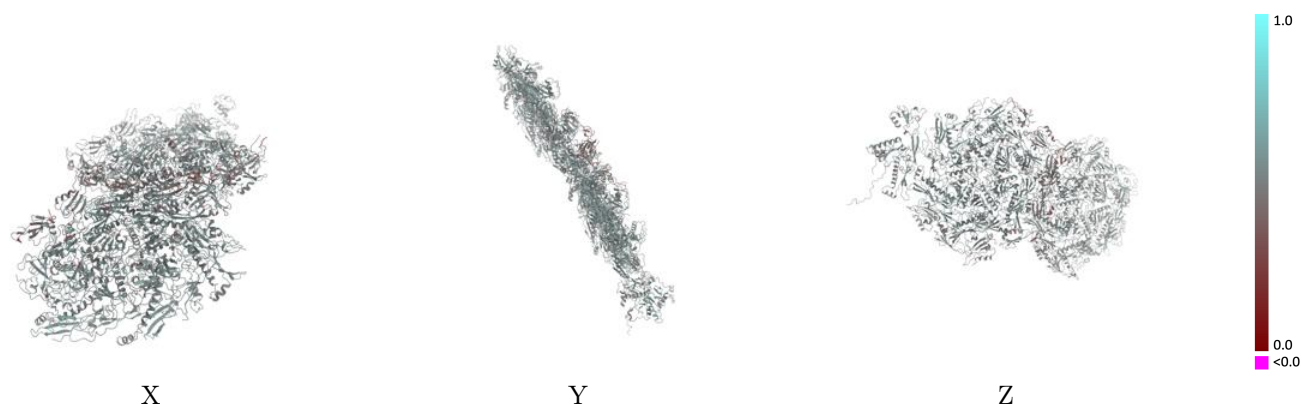


9.1.2 Map-model assembly overlay [i](#)



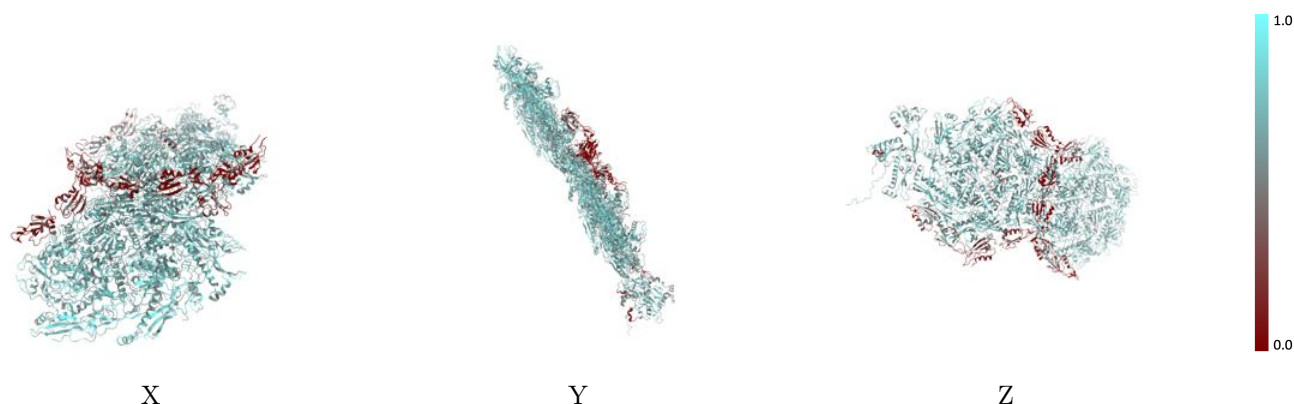
The images above show the 3D surface view of the map at the recommended contour level 8.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



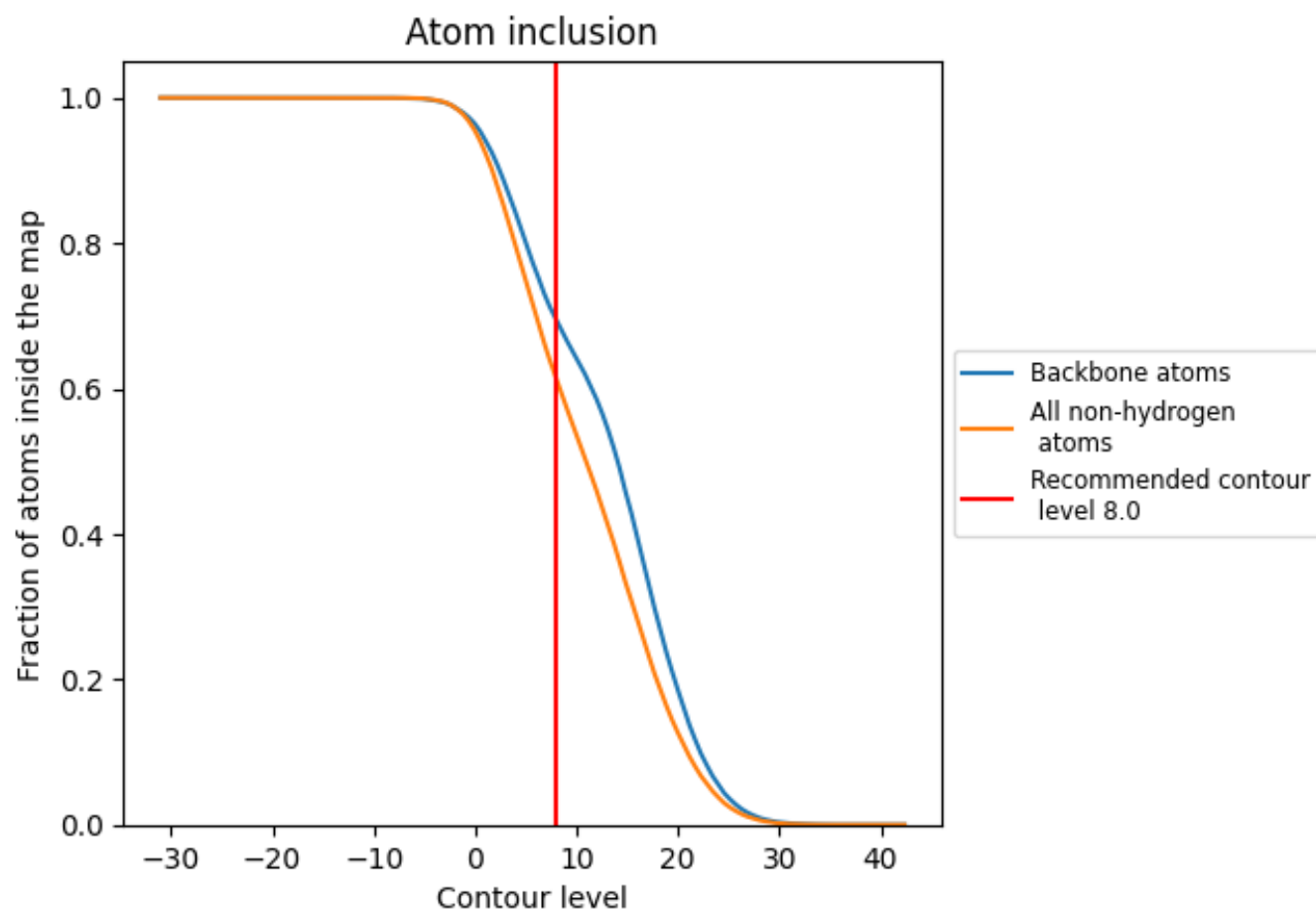
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (8.0).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 61% 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 (8.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6135	 0.5050
A	 0.6863	 0.5210
B	 0.7002	 0.5190
C	 0.6972	 0.5160
D	 0.6990	 0.5160
E	 0.7053	 0.5180
F	 0.6978	 0.5180
G	 0.6999	 0.5170
H	 0.6961	 0.5160
I	 0.6990	 0.5120
J	 0.7064	 0.5150
K	 0.7026	 0.5150
L	 0.7020	 0.5170
O	 0.2814	 0.4740
P	 0.3505	 0.4830
Q	 0.1174	 0.4570
R	 0.1527	 0.4490
S	 0.1367	 0.4520
T	 0.0145	 0.4090
U	 0.1254	 0.4380
V	 0.0032	 0.3920
W	 0.1768	 0.4470
X	 0.0177	 0.4140
Y	 0.0386	 0.4050
Z	 0.2392	 0.4650
a	 0.5942	 0.5010
z	 0.4267	 0.4650

