wwPDB EM Validation Summary Report

Dec 31, 2024 – 06:44 AM EST

PDB ID	:	8GMO
EMDB ID	:	EMD-40228
Title	:	Bacteriophage T4 capsid shell containing 9DE insertions into the gp23* major capsid protein subunits
Authors	:	Fokine, A.; Rao, V.B.
Deposited on	:	2023-03-26
Resolution	:	3.90 Å(reported)
Based on initial model	:	7VS5

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 (i) 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 (i)) were used in the production of this report:

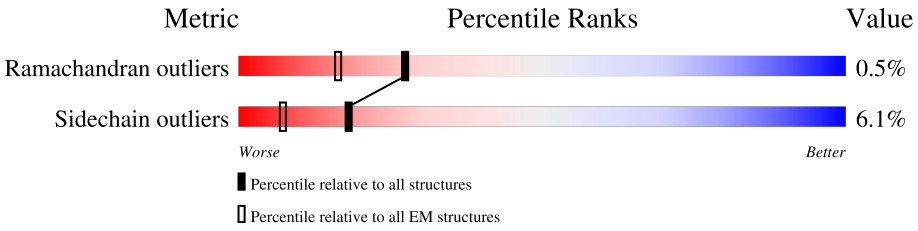
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.90 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	465	94% 6%
1	1	465	96%
1	2	465	94% 6%
1	3	465	96%
1	4	465	94% 6%
1	5	465	95% 5%
1	6	465	97%
1	7	465	97%
1	8	465	92% 8%

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Mol	Chain	Length	Quality of chain
1	9	465	96%
1	AA	465	96%
1	AB	465	94% 6%
1	AC	465	94% 6%
1	AD	465	90% 5% 6%
1	AE	465	95% 5%
1	AF	465	92% 8%
1	AG	465	96%
1	AH	465	92% 8%
1	AI	465	93% 7%
1	AJ	465	94% 6%
1	AK	465	95% 5%
1	AL	465	94% 6%
1	AM	465	95% 5%
1	AN	465	97%
1	AO	465	97%
1	AP	465	96%
1	AQ	465	94% 6%
1	AR	465	95% 5%
1	AS	465	96%
1	AT	465	92% 8%
1	AU	465	95% 5%
1	AV	465	93% 7%
1	AW	465	96%
1	AX	465	94% 6%

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Mol	Chain	Length	Quality of chain
1	AY	465	95% 5%
1	AZ	465	97%
1	Aa	465	97%
1	Ab	465	95% 5%
1	Ac	465	96%
1	Ad	465	96%
1	Ae	465	96%
1	Af	465	91% 9%
1	Ag	465	95% 5%
1	Ah	465	94% 6%
1	Ai	465	95% 5%
1	Aj	465	95% 5%
1	Ak	465	96%
1	Al	465	97%
1	Am	465	98%
1	G	465	94% 6%
1	H	465	95% 5%
1	J	465	95%
1	K	465	95% 5%
1	L	465	97%
1	M	465	96%
1	N	465	97%
1	O	465	91% 9%
1	P	465	94% 6%
1	Q	465	94% 6%

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Mol	Chain	Length	Quality of chain
1	R	465	95% 5%
1	S	465	94% 6%
1	T	465	95% 5%
1	U	465	95% 5%
1	V	465	96%
1	W	465	96%
1	X	465	97%
1	Y	465	93% 7%
1	Z	465	94% 6%
1	b	465	94% 6%
1	c	465	97%
1	d	465	96%
1	e	465	96%
1	f	465	92% 8%
1	g	465	97%
1	h	465	97%
1	i	465	97%
1	j	465	98%
1	k	465	95% 5%
1	l	465	95% 5%
1	m	465	95% 5%
1	n	465	96%
1	o	465	95% 5%
1	p	465	94% 6%
1	q	465	95% 5%

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Mol	Chain	Length	Quality of chain
1	r	465	94% 6%
1	s	465	96%
1	t	465	94% 6%
1	u	465	96%
1	v	465	97%
1	w	465	97%
1	x	465	96%
1	y	465	95% 5%
1	z	465	91% 9%
2	A	415	91% 8%
2	B	415	90% 10%
2	C	415	89% 11%
2	D	415	90% 10%
2	a	415	90% 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 341379 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 Mature major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	1	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	2	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	3	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	4	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	5	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	6	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	7	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	8	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	9	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AA	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AB	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AC	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AD	439	Total 3312	C 2092	N 559	O 646	S 15	0	0
1	AE	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AF	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AG	465	Total 3501	C 2207	N 593	O 686	S 15	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AH	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AI	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AJ	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AK	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AL	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AM	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AN	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AO	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AP	465	Total 3488	C 2197	N 591	O 685	S 15	0	0
1	AQ	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AR	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AS	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AT	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AU	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AV	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AW	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AX	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AY	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	AZ	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	Aa	465	Total 3501	C 2207	N 593	O 686	S 15	0	0
1	Ab	465	Total 3488	C 2197	N 591	O 685	S 15	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ac	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	Ad	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	Ae	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	Af	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	Ag	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	Ah	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	Ai	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	Aj	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	Ak	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	Al	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	Am	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	G	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	H	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	J	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	K	465	Total	C	N	O	S	0	0
			3488	2197	591	685	15		
1	L	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	M	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	N	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	O	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	P	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	Q	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	S	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	T	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	U	465	Total	C	N	O	S	0	0
			3488	2197	591	685	15		
1	V	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	W	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	X	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	Y	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	Z	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	b	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	c	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	d	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	e	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	f	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	g	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	h	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	i	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	j	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	k	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	l	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	m	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	n	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	o	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	p	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	q	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	r	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	s	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	t	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	u	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	v	465	Total	C	N	O	S	0	0
			3488	2197	591	685	15		
1	w	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	x	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	y	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		
1	z	465	Total	C	N	O	S	0	0
			3501	2207	593	686	15		

There are 837 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	201A	ASP	-	insertion	UNP P04535
0	201B	GLU	-	insertion	UNP P04535
0	201C	ASP	-	insertion	UNP P04535
0	201D	GLU	-	insertion	UNP P04535
0	201E	ASP	-	insertion	UNP P04535
0	201F	GLU	-	insertion	UNP P04535
0	201G	ASP	-	insertion	UNP P04535
0	201H	GLU	-	insertion	UNP P04535
0	201I	ASP	-	insertion	UNP P04535
1	201A	ASP	-	insertion	UNP P04535
1	201B	GLU	-	insertion	UNP P04535
1	201C	ASP	-	insertion	UNP P04535
1	201D	GLU	-	insertion	UNP P04535

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Chain	Residue	Modelled	Actual	Comment	Reference
1	201E	ASP	-	insertion	UNP P04535
1	201F	GLU	-	insertion	UNP P04535
1	201G	ASP	-	insertion	UNP P04535
1	201H	GLU	-	insertion	UNP P04535
1	201I	ASP	-	insertion	UNP P04535
2	201A	ASP	-	insertion	UNP P04535
2	201B	GLU	-	insertion	UNP P04535
2	201C	ASP	-	insertion	UNP P04535
2	201D	GLU	-	insertion	UNP P04535
2	201E	ASP	-	insertion	UNP P04535
2	201F	GLU	-	insertion	UNP P04535
2	201G	ASP	-	insertion	UNP P04535
2	201H	GLU	-	insertion	UNP P04535
2	201I	ASP	-	insertion	UNP P04535
3	201A	ASP	-	insertion	UNP P04535
3	201B	GLU	-	insertion	UNP P04535
3	201C	ASP	-	insertion	UNP P04535
3	201D	GLU	-	insertion	UNP P04535
3	201E	ASP	-	insertion	UNP P04535
3	201F	GLU	-	insertion	UNP P04535
3	201G	ASP	-	insertion	UNP P04535
3	201H	GLU	-	insertion	UNP P04535
3	201I	ASP	-	insertion	UNP P04535
4	201A	ASP	-	insertion	UNP P04535
4	201B	GLU	-	insertion	UNP P04535
4	201C	ASP	-	insertion	UNP P04535
4	201D	GLU	-	insertion	UNP P04535
4	201E	ASP	-	insertion	UNP P04535
4	201F	GLU	-	insertion	UNP P04535
4	201G	ASP	-	insertion	UNP P04535
4	201H	GLU	-	insertion	UNP P04535
4	201I	ASP	-	insertion	UNP P04535
5	201A	ASP	-	insertion	UNP P04535
5	201B	GLU	-	insertion	UNP P04535
5	201C	ASP	-	insertion	UNP P04535
5	201D	GLU	-	insertion	UNP P04535
5	201E	ASP	-	insertion	UNP P04535
5	201F	GLU	-	insertion	UNP P04535
5	201G	ASP	-	insertion	UNP P04535
5	201H	GLU	-	insertion	UNP P04535
5	201I	ASP	-	insertion	UNP P04535
6	201A	ASP	-	insertion	UNP P04535

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Chain	Residue	Modelled	Actual	Comment	Reference
6	201B	GLU	-	insertion	UNP P04535
6	201C	ASP	-	insertion	UNP P04535
6	201D	GLU	-	insertion	UNP P04535
6	201E	ASP	-	insertion	UNP P04535
6	201F	GLU	-	insertion	UNP P04535
6	201G	ASP	-	insertion	UNP P04535
6	201H	GLU	-	insertion	UNP P04535
6	201I	ASP	-	insertion	UNP P04535
7	201A	ASP	-	insertion	UNP P04535
7	201B	GLU	-	insertion	UNP P04535
7	201C	ASP	-	insertion	UNP P04535
7	201D	GLU	-	insertion	UNP P04535
7	201E	ASP	-	insertion	UNP P04535
7	201F	GLU	-	insertion	UNP P04535
7	201G	ASP	-	insertion	UNP P04535
7	201H	GLU	-	insertion	UNP P04535
7	201I	ASP	-	insertion	UNP P04535
8	201A	ASP	-	insertion	UNP P04535
8	201B	GLU	-	insertion	UNP P04535
8	201C	ASP	-	insertion	UNP P04535
8	201D	GLU	-	insertion	UNP P04535
8	201E	ASP	-	insertion	UNP P04535
8	201F	GLU	-	insertion	UNP P04535
8	201G	ASP	-	insertion	UNP P04535
8	201H	GLU	-	insertion	UNP P04535
8	201I	ASP	-	insertion	UNP P04535
9	201A	ASP	-	insertion	UNP P04535
9	201B	GLU	-	insertion	UNP P04535
9	201C	ASP	-	insertion	UNP P04535
9	201D	GLU	-	insertion	UNP P04535
9	201E	ASP	-	insertion	UNP P04535
9	201F	GLU	-	insertion	UNP P04535
9	201G	ASP	-	insertion	UNP P04535
9	201H	GLU	-	insertion	UNP P04535
9	201I	ASP	-	insertion	UNP P04535
AA	201A	ASP	-	insertion	UNP P04535
AA	201B	GLU	-	insertion	UNP P04535
AA	201C	ASP	-	insertion	UNP P04535
AA	201D	GLU	-	insertion	UNP P04535
AA	201E	ASP	-	insertion	UNP P04535
AA	201F	GLU	-	insertion	UNP P04535
AA	201G	ASP	-	insertion	UNP P04535

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Chain	Residue	Modelled	Actual	Comment	Reference
AA	201H	GLU	-	insertion	UNP P04535
AA	201I	ASP	-	insertion	UNP P04535
AB	201A	ASP	-	insertion	UNP P04535
AB	201B	GLU	-	insertion	UNP P04535
AB	201C	ASP	-	insertion	UNP P04535
AB	201D	GLU	-	insertion	UNP P04535
AB	201E	ASP	-	insertion	UNP P04535
AB	201F	GLU	-	insertion	UNP P04535
AB	201G	ASP	-	insertion	UNP P04535
AB	201H	GLU	-	insertion	UNP P04535
AB	201I	ASP	-	insertion	UNP P04535
AC	201A	ASP	-	insertion	UNP P04535
AC	201B	GLU	-	insertion	UNP P04535
AC	201C	ASP	-	insertion	UNP P04535
AC	201D	GLU	-	insertion	UNP P04535
AC	201E	ASP	-	insertion	UNP P04535
AC	201F	GLU	-	insertion	UNP P04535
AC	201G	ASP	-	insertion	UNP P04535
AC	201H	GLU	-	insertion	UNP P04535
AC	201I	ASP	-	insertion	UNP P04535
AD	201A	ASP	-	insertion	UNP P04535
AD	201B	GLU	-	insertion	UNP P04535
AD	201C	ASP	-	insertion	UNP P04535
AD	201D	GLU	-	insertion	UNP P04535
AD	201E	ASP	-	insertion	UNP P04535
AD	201F	GLU	-	insertion	UNP P04535
AD	201G	ASP	-	insertion	UNP P04535
AD	201H	GLU	-	insertion	UNP P04535
AD	201I	ASP	-	insertion	UNP P04535
AE	201A	ASP	-	insertion	UNP P04535
AE	201B	GLU	-	insertion	UNP P04535
AE	201C	ASP	-	insertion	UNP P04535
AE	201D	GLU	-	insertion	UNP P04535
AE	201E	ASP	-	insertion	UNP P04535
AE	201F	GLU	-	insertion	UNP P04535
AE	201G	ASP	-	insertion	UNP P04535
AE	201H	GLU	-	insertion	UNP P04535
AE	201I	ASP	-	insertion	UNP P04535
AF	201A	ASP	-	insertion	UNP P04535
AF	201B	GLU	-	insertion	UNP P04535
AF	201C	ASP	-	insertion	UNP P04535
AF	201D	GLU	-	insertion	UNP P04535

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Chain	Residue	Modelled	Actual	Comment	Reference
AF	201E	ASP	-	insertion	UNP P04535
AF	201F	GLU	-	insertion	UNP P04535
AF	201G	ASP	-	insertion	UNP P04535
AF	201H	GLU	-	insertion	UNP P04535
AF	201I	ASP	-	insertion	UNP P04535
AG	201A	ASP	-	insertion	UNP P04535
AG	201B	GLU	-	insertion	UNP P04535
AG	201C	ASP	-	insertion	UNP P04535
AG	201D	GLU	-	insertion	UNP P04535
AG	201E	ASP	-	insertion	UNP P04535
AG	201F	GLU	-	insertion	UNP P04535
AG	201G	ASP	-	insertion	UNP P04535
AG	201H	GLU	-	insertion	UNP P04535
AG	201I	ASP	-	insertion	UNP P04535
AH	201A	ASP	-	insertion	UNP P04535
AH	201B	GLU	-	insertion	UNP P04535
AH	201C	ASP	-	insertion	UNP P04535
AH	201D	GLU	-	insertion	UNP P04535
AH	201E	ASP	-	insertion	UNP P04535
AH	201F	GLU	-	insertion	UNP P04535
AH	201G	ASP	-	insertion	UNP P04535
AH	201H	GLU	-	insertion	UNP P04535
AH	201I	ASP	-	insertion	UNP P04535
AI	201A	ASP	-	insertion	UNP P04535
AI	201B	GLU	-	insertion	UNP P04535
AI	201C	ASP	-	insertion	UNP P04535
AI	201D	GLU	-	insertion	UNP P04535
AI	201E	ASP	-	insertion	UNP P04535
AI	201F	GLU	-	insertion	UNP P04535
AI	201G	ASP	-	insertion	UNP P04535
AI	201H	GLU	-	insertion	UNP P04535
AI	201I	ASP	-	insertion	UNP P04535
AJ	201A	ASP	-	insertion	UNP P04535
AJ	201B	GLU	-	insertion	UNP P04535
AJ	201C	ASP	-	insertion	UNP P04535
AJ	201D	GLU	-	insertion	UNP P04535
AJ	201E	ASP	-	insertion	UNP P04535
AJ	201F	GLU	-	insertion	UNP P04535
AJ	201G	ASP	-	insertion	UNP P04535
AJ	201H	GLU	-	insertion	UNP P04535
AJ	201I	ASP	-	insertion	UNP P04535
AK	201A	ASP	-	insertion	UNP P04535

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Chain	Residue	Modelled	Actual	Comment	Reference
AK	201B	GLU	-	insertion	UNP P04535
AK	201C	ASP	-	insertion	UNP P04535
AK	201D	GLU	-	insertion	UNP P04535
AK	201E	ASP	-	insertion	UNP P04535
AK	201F	GLU	-	insertion	UNP P04535
AK	201G	ASP	-	insertion	UNP P04535
AK	201H	GLU	-	insertion	UNP P04535
AK	201I	ASP	-	insertion	UNP P04535
AL	201A	ASP	-	insertion	UNP P04535
AL	201B	GLU	-	insertion	UNP P04535
AL	201C	ASP	-	insertion	UNP P04535
AL	201D	GLU	-	insertion	UNP P04535
AL	201E	ASP	-	insertion	UNP P04535
AL	201F	GLU	-	insertion	UNP P04535
AL	201G	ASP	-	insertion	UNP P04535
AL	201H	GLU	-	insertion	UNP P04535
AL	201I	ASP	-	insertion	UNP P04535
AM	201A	ASP	-	insertion	UNP P04535
AM	201B	GLU	-	insertion	UNP P04535
AM	201C	ASP	-	insertion	UNP P04535
AM	201D	GLU	-	insertion	UNP P04535
AM	201E	ASP	-	insertion	UNP P04535
AM	201F	GLU	-	insertion	UNP P04535
AM	201G	ASP	-	insertion	UNP P04535
AM	201H	GLU	-	insertion	UNP P04535
AM	201I	ASP	-	insertion	UNP P04535
AN	201A	ASP	-	insertion	UNP P04535
AN	201B	GLU	-	insertion	UNP P04535
AN	201C	ASP	-	insertion	UNP P04535
AN	201D	GLU	-	insertion	UNP P04535
AN	201E	ASP	-	insertion	UNP P04535
AN	201F	GLU	-	insertion	UNP P04535
AN	201G	ASP	-	insertion	UNP P04535
AN	201H	GLU	-	insertion	UNP P04535
AN	201I	ASP	-	insertion	UNP P04535
AO	201A	ASP	-	insertion	UNP P04535
AO	201B	GLU	-	insertion	UNP P04535
AO	201C	ASP	-	insertion	UNP P04535
AO	201D	GLU	-	insertion	UNP P04535
AO	201E	ASP	-	insertion	UNP P04535
AO	201F	GLU	-	insertion	UNP P04535
AO	201G	ASP	-	insertion	UNP P04535

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Chain	Residue	Modelled	Actual	Comment	Reference
AO	201H	GLU	-	insertion	UNP P04535
AO	201I	ASP	-	insertion	UNP P04535
AP	201A	ASP	-	insertion	UNP P04535
AP	201B	GLU	-	insertion	UNP P04535
AP	201C	ASP	-	insertion	UNP P04535
AP	201D	GLU	-	insertion	UNP P04535
AP	201E	ASP	-	insertion	UNP P04535
AP	201F	GLU	-	insertion	UNP P04535
AP	201G	ASP	-	insertion	UNP P04535
AP	201H	GLU	-	insertion	UNP P04535
AP	201I	ASP	-	insertion	UNP P04535
AQ	201A	ASP	-	insertion	UNP P04535
AQ	201B	GLU	-	insertion	UNP P04535
AQ	201C	ASP	-	insertion	UNP P04535
AQ	201D	GLU	-	insertion	UNP P04535
AQ	201E	ASP	-	insertion	UNP P04535
AQ	201F	GLU	-	insertion	UNP P04535
AQ	201G	ASP	-	insertion	UNP P04535
AQ	201H	GLU	-	insertion	UNP P04535
AQ	201I	ASP	-	insertion	UNP P04535
AR	201A	ASP	-	insertion	UNP P04535
AR	201B	GLU	-	insertion	UNP P04535
AR	201C	ASP	-	insertion	UNP P04535
AR	201D	GLU	-	insertion	UNP P04535
AR	201E	ASP	-	insertion	UNP P04535
AR	201F	GLU	-	insertion	UNP P04535
AR	201G	ASP	-	insertion	UNP P04535
AR	201H	GLU	-	insertion	UNP P04535
AR	201I	ASP	-	insertion	UNP P04535
AS	201A	ASP	-	insertion	UNP P04535
AS	201B	GLU	-	insertion	UNP P04535
AS	201C	ASP	-	insertion	UNP P04535
AS	201D	GLU	-	insertion	UNP P04535
AS	201E	ASP	-	insertion	UNP P04535
AS	201F	GLU	-	insertion	UNP P04535
AS	201G	ASP	-	insertion	UNP P04535
AS	201H	GLU	-	insertion	UNP P04535
AS	201I	ASP	-	insertion	UNP P04535
AT	201A	ASP	-	insertion	UNP P04535
AT	201B	GLU	-	insertion	UNP P04535
AT	201C	ASP	-	insertion	UNP P04535
AT	201D	GLU	-	insertion	UNP P04535

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Chain	Residue	Modelled	Actual	Comment	Reference
AT	201E	ASP	-	insertion	UNP P04535
AT	201F	GLU	-	insertion	UNP P04535
AT	201G	ASP	-	insertion	UNP P04535
AT	201H	GLU	-	insertion	UNP P04535
AT	201I	ASP	-	insertion	UNP P04535
AU	201A	ASP	-	insertion	UNP P04535
AU	201B	GLU	-	insertion	UNP P04535
AU	201C	ASP	-	insertion	UNP P04535
AU	201D	GLU	-	insertion	UNP P04535
AU	201E	ASP	-	insertion	UNP P04535
AU	201F	GLU	-	insertion	UNP P04535
AU	201G	ASP	-	insertion	UNP P04535
AU	201H	GLU	-	insertion	UNP P04535
AU	201I	ASP	-	insertion	UNP P04535
AV	201A	ASP	-	insertion	UNP P04535
AV	201B	GLU	-	insertion	UNP P04535
AV	201C	ASP	-	insertion	UNP P04535
AV	201D	GLU	-	insertion	UNP P04535
AV	201E	ASP	-	insertion	UNP P04535
AV	201F	GLU	-	insertion	UNP P04535
AV	201G	ASP	-	insertion	UNP P04535
AV	201H	GLU	-	insertion	UNP P04535
AV	201I	ASP	-	insertion	UNP P04535
AW	201A	ASP	-	insertion	UNP P04535
AW	201B	GLU	-	insertion	UNP P04535
AW	201C	ASP	-	insertion	UNP P04535
AW	201D	GLU	-	insertion	UNP P04535
AW	201E	ASP	-	insertion	UNP P04535
AW	201F	GLU	-	insertion	UNP P04535
AW	201G	ASP	-	insertion	UNP P04535
AW	201H	GLU	-	insertion	UNP P04535
AW	201I	ASP	-	insertion	UNP P04535
AX	201A	ASP	-	insertion	UNP P04535
AX	201B	GLU	-	insertion	UNP P04535
AX	201C	ASP	-	insertion	UNP P04535
AX	201D	GLU	-	insertion	UNP P04535
AX	201E	ASP	-	insertion	UNP P04535
AX	201F	GLU	-	insertion	UNP P04535
AX	201G	ASP	-	insertion	UNP P04535
AX	201H	GLU	-	insertion	UNP P04535
AX	201I	ASP	-	insertion	UNP P04535
AY	201A	ASP	-	insertion	UNP P04535

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Chain	Residue	Modelled	Actual	Comment	Reference
AY	201B	GLU	-	insertion	UNP P04535
AY	201C	ASP	-	insertion	UNP P04535
AY	201D	GLU	-	insertion	UNP P04535
AY	201E	ASP	-	insertion	UNP P04535
AY	201F	GLU	-	insertion	UNP P04535
AY	201G	ASP	-	insertion	UNP P04535
AY	201H	GLU	-	insertion	UNP P04535
AY	201I	ASP	-	insertion	UNP P04535
AZ	201A	ASP	-	insertion	UNP P04535
AZ	201B	GLU	-	insertion	UNP P04535
AZ	201C	ASP	-	insertion	UNP P04535
AZ	201D	GLU	-	insertion	UNP P04535
AZ	201E	ASP	-	insertion	UNP P04535
AZ	201F	GLU	-	insertion	UNP P04535
AZ	201G	ASP	-	insertion	UNP P04535
AZ	201H	GLU	-	insertion	UNP P04535
AZ	201I	ASP	-	insertion	UNP P04535
Aa	201A	ASP	-	insertion	UNP P04535
Aa	201B	GLU	-	insertion	UNP P04535
Aa	201C	ASP	-	insertion	UNP P04535
Aa	201D	GLU	-	insertion	UNP P04535
Aa	201E	ASP	-	insertion	UNP P04535
Aa	201F	GLU	-	insertion	UNP P04535
Aa	201G	ASP	-	insertion	UNP P04535
Aa	201H	GLU	-	insertion	UNP P04535
Aa	201I	ASP	-	insertion	UNP P04535
Ab	201A	ASP	-	insertion	UNP P04535
Ab	201B	GLU	-	insertion	UNP P04535
Ab	201C	ASP	-	insertion	UNP P04535
Ab	201D	GLU	-	insertion	UNP P04535
Ab	201E	ASP	-	insertion	UNP P04535
Ab	201F	GLU	-	insertion	UNP P04535
Ab	201G	ASP	-	insertion	UNP P04535
Ab	201H	GLU	-	insertion	UNP P04535
Ab	201I	ASP	-	insertion	UNP P04535
Ac	201A	ASP	-	insertion	UNP P04535
Ac	201B	GLU	-	insertion	UNP P04535
Ac	201C	ASP	-	insertion	UNP P04535
Ac	201D	GLU	-	insertion	UNP P04535
Ac	201E	ASP	-	insertion	UNP P04535
Ac	201F	GLU	-	insertion	UNP P04535
Ac	201G	ASP	-	insertion	UNP P04535

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Chain	Residue	Modelled	Actual	Comment	Reference
Ac	201H	GLU	-	insertion	UNP P04535
Ac	201I	ASP	-	insertion	UNP P04535
Ad	201A	ASP	-	insertion	UNP P04535
Ad	201B	GLU	-	insertion	UNP P04535
Ad	201C	ASP	-	insertion	UNP P04535
Ad	201D	GLU	-	insertion	UNP P04535
Ad	201E	ASP	-	insertion	UNP P04535
Ad	201F	GLU	-	insertion	UNP P04535
Ad	201G	ASP	-	insertion	UNP P04535
Ad	201H	GLU	-	insertion	UNP P04535
Ad	201I	ASP	-	insertion	UNP P04535
Ae	201A	ASP	-	insertion	UNP P04535
Ae	201B	GLU	-	insertion	UNP P04535
Ae	201C	ASP	-	insertion	UNP P04535
Ae	201D	GLU	-	insertion	UNP P04535
Ae	201E	ASP	-	insertion	UNP P04535
Ae	201F	GLU	-	insertion	UNP P04535
Ae	201G	ASP	-	insertion	UNP P04535
Ae	201H	GLU	-	insertion	UNP P04535
Ae	201I	ASP	-	insertion	UNP P04535
Af	201A	ASP	-	insertion	UNP P04535
Af	201B	GLU	-	insertion	UNP P04535
Af	201C	ASP	-	insertion	UNP P04535
Af	201D	GLU	-	insertion	UNP P04535
Af	201E	ASP	-	insertion	UNP P04535
Af	201F	GLU	-	insertion	UNP P04535
Af	201G	ASP	-	insertion	UNP P04535
Af	201H	GLU	-	insertion	UNP P04535
Af	201I	ASP	-	insertion	UNP P04535
Ag	201A	ASP	-	insertion	UNP P04535
Ag	201B	GLU	-	insertion	UNP P04535
Ag	201C	ASP	-	insertion	UNP P04535
Ag	201D	GLU	-	insertion	UNP P04535
Ag	201E	ASP	-	insertion	UNP P04535
Ag	201F	GLU	-	insertion	UNP P04535
Ag	201G	ASP	-	insertion	UNP P04535
Ag	201H	GLU	-	insertion	UNP P04535
Ag	201I	ASP	-	insertion	UNP P04535
Ah	201A	ASP	-	insertion	UNP P04535
Ah	201B	GLU	-	insertion	UNP P04535
Ah	201C	ASP	-	insertion	UNP P04535
Ah	201D	GLU	-	insertion	UNP P04535

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Chain	Residue	Modelled	Actual	Comment	Reference
Ah	201E	ASP	-	insertion	UNP P04535
Ah	201F	GLU	-	insertion	UNP P04535
Ah	201G	ASP	-	insertion	UNP P04535
Ah	201H	GLU	-	insertion	UNP P04535
Ah	201I	ASP	-	insertion	UNP P04535
Ai	201A	ASP	-	insertion	UNP P04535
Ai	201B	GLU	-	insertion	UNP P04535
Ai	201C	ASP	-	insertion	UNP P04535
Ai	201D	GLU	-	insertion	UNP P04535
Ai	201E	ASP	-	insertion	UNP P04535
Ai	201F	GLU	-	insertion	UNP P04535
Ai	201G	ASP	-	insertion	UNP P04535
Ai	201H	GLU	-	insertion	UNP P04535
Ai	201I	ASP	-	insertion	UNP P04535
Aj	201A	ASP	-	insertion	UNP P04535
Aj	201B	GLU	-	insertion	UNP P04535
Aj	201C	ASP	-	insertion	UNP P04535
Aj	201D	GLU	-	insertion	UNP P04535
Aj	201E	ASP	-	insertion	UNP P04535
Aj	201F	GLU	-	insertion	UNP P04535
Aj	201G	ASP	-	insertion	UNP P04535
Aj	201H	GLU	-	insertion	UNP P04535
Aj	201I	ASP	-	insertion	UNP P04535
Ak	201A	ASP	-	insertion	UNP P04535
Ak	201B	GLU	-	insertion	UNP P04535
Ak	201C	ASP	-	insertion	UNP P04535
Ak	201D	GLU	-	insertion	UNP P04535
Ak	201E	ASP	-	insertion	UNP P04535
Ak	201F	GLU	-	insertion	UNP P04535
Ak	201G	ASP	-	insertion	UNP P04535
Ak	201H	GLU	-	insertion	UNP P04535
Ak	201I	ASP	-	insertion	UNP P04535
Al	201A	ASP	-	insertion	UNP P04535
Al	201B	GLU	-	insertion	UNP P04535
Al	201C	ASP	-	insertion	UNP P04535
Al	201D	GLU	-	insertion	UNP P04535
Al	201E	ASP	-	insertion	UNP P04535
Al	201F	GLU	-	insertion	UNP P04535
Al	201G	ASP	-	insertion	UNP P04535
Al	201H	GLU	-	insertion	UNP P04535
Al	201I	ASP	-	insertion	UNP P04535
Am	201A	ASP	-	insertion	UNP P04535

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Chain	Residue	Modelled	Actual	Comment	Reference
Am	201B	GLU	-	insertion	UNP P04535
Am	201C	ASP	-	insertion	UNP P04535
Am	201D	GLU	-	insertion	UNP P04535
Am	201E	ASP	-	insertion	UNP P04535
Am	201F	GLU	-	insertion	UNP P04535
Am	201G	ASP	-	insertion	UNP P04535
Am	201H	GLU	-	insertion	UNP P04535
Am	201I	ASP	-	insertion	UNP P04535
G	201A	ASP	-	insertion	UNP P04535
G	201B	GLU	-	insertion	UNP P04535
G	201C	ASP	-	insertion	UNP P04535
G	201D	GLU	-	insertion	UNP P04535
G	201E	ASP	-	insertion	UNP P04535
G	201F	GLU	-	insertion	UNP P04535
G	201G	ASP	-	insertion	UNP P04535
G	201H	GLU	-	insertion	UNP P04535
G	201I	ASP	-	insertion	UNP P04535
H	201A	ASP	-	insertion	UNP P04535
H	201B	GLU	-	insertion	UNP P04535
H	201C	ASP	-	insertion	UNP P04535
H	201D	GLU	-	insertion	UNP P04535
H	201E	ASP	-	insertion	UNP P04535
H	201F	GLU	-	insertion	UNP P04535
H	201G	ASP	-	insertion	UNP P04535
H	201H	GLU	-	insertion	UNP P04535
H	201I	ASP	-	insertion	UNP P04535
J	201A	ASP	-	insertion	UNP P04535
J	201B	GLU	-	insertion	UNP P04535
J	201C	ASP	-	insertion	UNP P04535
J	201D	GLU	-	insertion	UNP P04535
J	201E	ASP	-	insertion	UNP P04535
J	201F	GLU	-	insertion	UNP P04535
J	201G	ASP	-	insertion	UNP P04535
J	201H	GLU	-	insertion	UNP P04535
J	201I	ASP	-	insertion	UNP P04535
K	201A	ASP	-	insertion	UNP P04535
K	201B	GLU	-	insertion	UNP P04535
K	201C	ASP	-	insertion	UNP P04535
K	201D	GLU	-	insertion	UNP P04535
K	201E	ASP	-	insertion	UNP P04535
K	201F	GLU	-	insertion	UNP P04535
K	201G	ASP	-	insertion	UNP P04535

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Chain	Residue	Modelled	Actual	Comment	Reference
K	201H	GLU	-	insertion	UNP P04535
K	201I	ASP	-	insertion	UNP P04535
L	201A	ASP	-	insertion	UNP P04535
L	201B	GLU	-	insertion	UNP P04535
L	201C	ASP	-	insertion	UNP P04535
L	201D	GLU	-	insertion	UNP P04535
L	201E	ASP	-	insertion	UNP P04535
L	201F	GLU	-	insertion	UNP P04535
L	201G	ASP	-	insertion	UNP P04535
L	201H	GLU	-	insertion	UNP P04535
L	201I	ASP	-	insertion	UNP P04535
M	201A	ASP	-	insertion	UNP P04535
M	201B	GLU	-	insertion	UNP P04535
M	201C	ASP	-	insertion	UNP P04535
M	201D	GLU	-	insertion	UNP P04535
M	201E	ASP	-	insertion	UNP P04535
M	201F	GLU	-	insertion	UNP P04535
M	201G	ASP	-	insertion	UNP P04535
M	201H	GLU	-	insertion	UNP P04535
M	201I	ASP	-	insertion	UNP P04535
N	201A	ASP	-	insertion	UNP P04535
N	201B	GLU	-	insertion	UNP P04535
N	201C	ASP	-	insertion	UNP P04535
N	201D	GLU	-	insertion	UNP P04535
N	201E	ASP	-	insertion	UNP P04535
N	201F	GLU	-	insertion	UNP P04535
N	201G	ASP	-	insertion	UNP P04535
N	201H	GLU	-	insertion	UNP P04535
N	201I	ASP	-	insertion	UNP P04535
O	201A	ASP	-	insertion	UNP P04535
O	201B	GLU	-	insertion	UNP P04535
O	201C	ASP	-	insertion	UNP P04535
O	201D	GLU	-	insertion	UNP P04535
O	201E	ASP	-	insertion	UNP P04535
O	201F	GLU	-	insertion	UNP P04535
O	201G	ASP	-	insertion	UNP P04535
O	201H	GLU	-	insertion	UNP P04535
O	201I	ASP	-	insertion	UNP P04535
P	201A	ASP	-	insertion	UNP P04535
P	201B	GLU	-	insertion	UNP P04535
P	201C	ASP	-	insertion	UNP P04535
P	201D	GLU	-	insertion	UNP P04535

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Chain	Residue	Modelled	Actual	Comment	Reference
P	201E	ASP	-	insertion	UNP P04535
P	201F	GLU	-	insertion	UNP P04535
P	201G	ASP	-	insertion	UNP P04535
P	201H	GLU	-	insertion	UNP P04535
P	201I	ASP	-	insertion	UNP P04535
Q	201A	ASP	-	insertion	UNP P04535
Q	201B	GLU	-	insertion	UNP P04535
Q	201C	ASP	-	insertion	UNP P04535
Q	201D	GLU	-	insertion	UNP P04535
Q	201E	ASP	-	insertion	UNP P04535
Q	201F	GLU	-	insertion	UNP P04535
Q	201G	ASP	-	insertion	UNP P04535
Q	201H	GLU	-	insertion	UNP P04535
Q	201I	ASP	-	insertion	UNP P04535
R	201A	ASP	-	insertion	UNP P04535
R	201B	GLU	-	insertion	UNP P04535
R	201C	ASP	-	insertion	UNP P04535
R	201D	GLU	-	insertion	UNP P04535
R	201E	ASP	-	insertion	UNP P04535
R	201F	GLU	-	insertion	UNP P04535
R	201G	ASP	-	insertion	UNP P04535
R	201H	GLU	-	insertion	UNP P04535
R	201I	ASP	-	insertion	UNP P04535
S	201A	ASP	-	insertion	UNP P04535
S	201B	GLU	-	insertion	UNP P04535
S	201C	ASP	-	insertion	UNP P04535
S	201D	GLU	-	insertion	UNP P04535
S	201E	ASP	-	insertion	UNP P04535
S	201F	GLU	-	insertion	UNP P04535
S	201G	ASP	-	insertion	UNP P04535
S	201H	GLU	-	insertion	UNP P04535
S	201I	ASP	-	insertion	UNP P04535
T	201A	ASP	-	insertion	UNP P04535
T	201B	GLU	-	insertion	UNP P04535
T	201C	ASP	-	insertion	UNP P04535
T	201D	GLU	-	insertion	UNP P04535
T	201E	ASP	-	insertion	UNP P04535
T	201F	GLU	-	insertion	UNP P04535
T	201G	ASP	-	insertion	UNP P04535
T	201H	GLU	-	insertion	UNP P04535
T	201I	ASP	-	insertion	UNP P04535
U	201A	ASP	-	insertion	UNP P04535

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Chain	Residue	Modelled	Actual	Comment	Reference
U	201B	GLU	-	insertion	UNP P04535
U	201C	ASP	-	insertion	UNP P04535
U	201D	GLU	-	insertion	UNP P04535
U	201E	ASP	-	insertion	UNP P04535
U	201F	GLU	-	insertion	UNP P04535
U	201G	ASP	-	insertion	UNP P04535
U	201H	GLU	-	insertion	UNP P04535
U	201I	ASP	-	insertion	UNP P04535
V	201A	ASP	-	insertion	UNP P04535
V	201B	GLU	-	insertion	UNP P04535
V	201C	ASP	-	insertion	UNP P04535
V	201D	GLU	-	insertion	UNP P04535
V	201E	ASP	-	insertion	UNP P04535
V	201F	GLU	-	insertion	UNP P04535
V	201G	ASP	-	insertion	UNP P04535
V	201H	GLU	-	insertion	UNP P04535
V	201I	ASP	-	insertion	UNP P04535
W	201A	ASP	-	insertion	UNP P04535
W	201B	GLU	-	insertion	UNP P04535
W	201C	ASP	-	insertion	UNP P04535
W	201D	GLU	-	insertion	UNP P04535
W	201E	ASP	-	insertion	UNP P04535
W	201F	GLU	-	insertion	UNP P04535
W	201G	ASP	-	insertion	UNP P04535
W	201H	GLU	-	insertion	UNP P04535
W	201I	ASP	-	insertion	UNP P04535
X	201A	ASP	-	insertion	UNP P04535
X	201B	GLU	-	insertion	UNP P04535
X	201C	ASP	-	insertion	UNP P04535
X	201D	GLU	-	insertion	UNP P04535
X	201E	ASP	-	insertion	UNP P04535
X	201F	GLU	-	insertion	UNP P04535
X	201G	ASP	-	insertion	UNP P04535
X	201H	GLU	-	insertion	UNP P04535
X	201I	ASP	-	insertion	UNP P04535
Y	201A	ASP	-	insertion	UNP P04535
Y	201B	GLU	-	insertion	UNP P04535
Y	201C	ASP	-	insertion	UNP P04535
Y	201D	GLU	-	insertion	UNP P04535
Y	201E	ASP	-	insertion	UNP P04535
Y	201F	GLU	-	insertion	UNP P04535
Y	201G	ASP	-	insertion	UNP P04535

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	201H	GLU	-	insertion	UNP P04535
Y	201I	ASP	-	insertion	UNP P04535
Z	201A	ASP	-	insertion	UNP P04535
Z	201B	GLU	-	insertion	UNP P04535
Z	201C	ASP	-	insertion	UNP P04535
Z	201D	GLU	-	insertion	UNP P04535
Z	201E	ASP	-	insertion	UNP P04535
Z	201F	GLU	-	insertion	UNP P04535
Z	201G	ASP	-	insertion	UNP P04535
Z	201H	GLU	-	insertion	UNP P04535
Z	201I	ASP	-	insertion	UNP P04535
b	201A	ASP	-	insertion	UNP P04535
b	201B	GLU	-	insertion	UNP P04535
b	201C	ASP	-	insertion	UNP P04535
b	201D	GLU	-	insertion	UNP P04535
b	201E	ASP	-	insertion	UNP P04535
b	201F	GLU	-	insertion	UNP P04535
b	201G	ASP	-	insertion	UNP P04535
b	201H	GLU	-	insertion	UNP P04535
b	201I	ASP	-	insertion	UNP P04535
c	201A	ASP	-	insertion	UNP P04535
c	201B	GLU	-	insertion	UNP P04535
c	201C	ASP	-	insertion	UNP P04535
c	201D	GLU	-	insertion	UNP P04535
c	201E	ASP	-	insertion	UNP P04535
c	201F	GLU	-	insertion	UNP P04535
c	201G	ASP	-	insertion	UNP P04535
c	201H	GLU	-	insertion	UNP P04535
c	201I	ASP	-	insertion	UNP P04535
d	201A	ASP	-	insertion	UNP P04535
d	201B	GLU	-	insertion	UNP P04535
d	201C	ASP	-	insertion	UNP P04535
d	201D	GLU	-	insertion	UNP P04535
d	201E	ASP	-	insertion	UNP P04535
d	201F	GLU	-	insertion	UNP P04535
d	201G	ASP	-	insertion	UNP P04535
d	201H	GLU	-	insertion	UNP P04535
d	201I	ASP	-	insertion	UNP P04535
e	201A	ASP	-	insertion	UNP P04535
e	201B	GLU	-	insertion	UNP P04535
e	201C	ASP	-	insertion	UNP P04535
e	201D	GLU	-	insertion	UNP P04535

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Chain	Residue	Modelled	Actual	Comment	Reference
e	201E	ASP	-	insertion	UNP P04535
e	201F	GLU	-	insertion	UNP P04535
e	201G	ASP	-	insertion	UNP P04535
e	201H	GLU	-	insertion	UNP P04535
e	201I	ASP	-	insertion	UNP P04535
f	201A	ASP	-	insertion	UNP P04535
f	201B	GLU	-	insertion	UNP P04535
f	201C	ASP	-	insertion	UNP P04535
f	201D	GLU	-	insertion	UNP P04535
f	201E	ASP	-	insertion	UNP P04535
f	201F	GLU	-	insertion	UNP P04535
f	201G	ASP	-	insertion	UNP P04535
f	201H	GLU	-	insertion	UNP P04535
f	201I	ASP	-	insertion	UNP P04535
g	201A	ASP	-	insertion	UNP P04535
g	201B	GLU	-	insertion	UNP P04535
g	201C	ASP	-	insertion	UNP P04535
g	201D	GLU	-	insertion	UNP P04535
g	201E	ASP	-	insertion	UNP P04535
g	201F	GLU	-	insertion	UNP P04535
g	201G	ASP	-	insertion	UNP P04535
g	201H	GLU	-	insertion	UNP P04535
g	201I	ASP	-	insertion	UNP P04535
h	201A	ASP	-	insertion	UNP P04535
h	201B	GLU	-	insertion	UNP P04535
h	201C	ASP	-	insertion	UNP P04535
h	201D	GLU	-	insertion	UNP P04535
h	201E	ASP	-	insertion	UNP P04535
h	201F	GLU	-	insertion	UNP P04535
h	201G	ASP	-	insertion	UNP P04535
h	201H	GLU	-	insertion	UNP P04535
h	201I	ASP	-	insertion	UNP P04535
i	201A	ASP	-	insertion	UNP P04535
i	201B	GLU	-	insertion	UNP P04535
i	201C	ASP	-	insertion	UNP P04535
i	201D	GLU	-	insertion	UNP P04535
i	201E	ASP	-	insertion	UNP P04535
i	201F	GLU	-	insertion	UNP P04535
i	201G	ASP	-	insertion	UNP P04535
i	201H	GLU	-	insertion	UNP P04535
i	201I	ASP	-	insertion	UNP P04535
j	201A	ASP	-	insertion	UNP P04535

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Chain	Residue	Modelled	Actual	Comment	Reference
j	201B	GLU	-	insertion	UNP P04535
j	201C	ASP	-	insertion	UNP P04535
j	201D	GLU	-	insertion	UNP P04535
j	201E	ASP	-	insertion	UNP P04535
j	201F	GLU	-	insertion	UNP P04535
j	201G	ASP	-	insertion	UNP P04535
j	201H	GLU	-	insertion	UNP P04535
j	201I	ASP	-	insertion	UNP P04535
k	201A	ASP	-	insertion	UNP P04535
k	201B	GLU	-	insertion	UNP P04535
k	201C	ASP	-	insertion	UNP P04535
k	201D	GLU	-	insertion	UNP P04535
k	201E	ASP	-	insertion	UNP P04535
k	201F	GLU	-	insertion	UNP P04535
k	201G	ASP	-	insertion	UNP P04535
k	201H	GLU	-	insertion	UNP P04535
k	201I	ASP	-	insertion	UNP P04535
l	201A	ASP	-	insertion	UNP P04535
l	201B	GLU	-	insertion	UNP P04535
l	201C	ASP	-	insertion	UNP P04535
l	201D	GLU	-	insertion	UNP P04535
l	201E	ASP	-	insertion	UNP P04535
l	201F	GLU	-	insertion	UNP P04535
l	201G	ASP	-	insertion	UNP P04535
l	201H	GLU	-	insertion	UNP P04535
l	201I	ASP	-	insertion	UNP P04535
m	201A	ASP	-	insertion	UNP P04535
m	201B	GLU	-	insertion	UNP P04535
m	201C	ASP	-	insertion	UNP P04535
m	201D	GLU	-	insertion	UNP P04535
m	201E	ASP	-	insertion	UNP P04535
m	201F	GLU	-	insertion	UNP P04535
m	201G	ASP	-	insertion	UNP P04535
m	201H	GLU	-	insertion	UNP P04535
m	201I	ASP	-	insertion	UNP P04535
n	201A	ASP	-	insertion	UNP P04535
n	201B	GLU	-	insertion	UNP P04535
n	201C	ASP	-	insertion	UNP P04535
n	201D	GLU	-	insertion	UNP P04535
n	201E	ASP	-	insertion	UNP P04535
n	201F	GLU	-	insertion	UNP P04535
n	201G	ASP	-	insertion	UNP P04535

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Chain	Residue	Modelled	Actual	Comment	Reference
n	201H	GLU	-	insertion	UNP P04535
n	201I	ASP	-	insertion	UNP P04535
o	201A	ASP	-	insertion	UNP P04535
o	201B	GLU	-	insertion	UNP P04535
o	201C	ASP	-	insertion	UNP P04535
o	201D	GLU	-	insertion	UNP P04535
o	201E	ASP	-	insertion	UNP P04535
o	201F	GLU	-	insertion	UNP P04535
o	201G	ASP	-	insertion	UNP P04535
o	201H	GLU	-	insertion	UNP P04535
o	201I	ASP	-	insertion	UNP P04535
p	201A	ASP	-	insertion	UNP P04535
p	201B	GLU	-	insertion	UNP P04535
p	201C	ASP	-	insertion	UNP P04535
p	201D	GLU	-	insertion	UNP P04535
p	201E	ASP	-	insertion	UNP P04535
p	201F	GLU	-	insertion	UNP P04535
p	201G	ASP	-	insertion	UNP P04535
p	201H	GLU	-	insertion	UNP P04535
p	201I	ASP	-	insertion	UNP P04535
q	201A	ASP	-	insertion	UNP P04535
q	201B	GLU	-	insertion	UNP P04535
q	201C	ASP	-	insertion	UNP P04535
q	201D	GLU	-	insertion	UNP P04535
q	201E	ASP	-	insertion	UNP P04535
q	201F	GLU	-	insertion	UNP P04535
q	201G	ASP	-	insertion	UNP P04535
q	201H	GLU	-	insertion	UNP P04535
q	201I	ASP	-	insertion	UNP P04535
r	201A	ASP	-	insertion	UNP P04535
r	201B	GLU	-	insertion	UNP P04535
r	201C	ASP	-	insertion	UNP P04535
r	201D	GLU	-	insertion	UNP P04535
r	201E	ASP	-	insertion	UNP P04535
r	201F	GLU	-	insertion	UNP P04535
r	201G	ASP	-	insertion	UNP P04535
r	201H	GLU	-	insertion	UNP P04535
r	201I	ASP	-	insertion	UNP P04535
s	201A	ASP	-	insertion	UNP P04535
s	201B	GLU	-	insertion	UNP P04535
s	201C	ASP	-	insertion	UNP P04535
s	201D	GLU	-	insertion	UNP P04535

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Chain	Residue	Modelled	Actual	Comment	Reference
s	201E	ASP	-	insertion	UNP P04535
s	201F	GLU	-	insertion	UNP P04535
s	201G	ASP	-	insertion	UNP P04535
s	201H	GLU	-	insertion	UNP P04535
s	201I	ASP	-	insertion	UNP P04535
t	201A	ASP	-	insertion	UNP P04535
t	201B	GLU	-	insertion	UNP P04535
t	201C	ASP	-	insertion	UNP P04535
t	201D	GLU	-	insertion	UNP P04535
t	201E	ASP	-	insertion	UNP P04535
t	201F	GLU	-	insertion	UNP P04535
t	201G	ASP	-	insertion	UNP P04535
t	201H	GLU	-	insertion	UNP P04535
t	201I	ASP	-	insertion	UNP P04535
u	201A	ASP	-	insertion	UNP P04535
u	201B	GLU	-	insertion	UNP P04535
u	201C	ASP	-	insertion	UNP P04535
u	201D	GLU	-	insertion	UNP P04535
u	201E	ASP	-	insertion	UNP P04535
u	201F	GLU	-	insertion	UNP P04535
u	201G	ASP	-	insertion	UNP P04535
u	201H	GLU	-	insertion	UNP P04535
u	201I	ASP	-	insertion	UNP P04535
v	201A	ASP	-	insertion	UNP P04535
v	201B	GLU	-	insertion	UNP P04535
v	201C	ASP	-	insertion	UNP P04535
v	201D	GLU	-	insertion	UNP P04535
v	201E	ASP	-	insertion	UNP P04535
v	201F	GLU	-	insertion	UNP P04535
v	201G	ASP	-	insertion	UNP P04535
v	201H	GLU	-	insertion	UNP P04535
v	201I	ASP	-	insertion	UNP P04535
w	201A	ASP	-	insertion	UNP P04535
w	201B	GLU	-	insertion	UNP P04535
w	201C	ASP	-	insertion	UNP P04535
w	201D	GLU	-	insertion	UNP P04535
w	201E	ASP	-	insertion	UNP P04535
w	201F	GLU	-	insertion	UNP P04535
w	201G	ASP	-	insertion	UNP P04535
w	201H	GLU	-	insertion	UNP P04535
w	201I	ASP	-	insertion	UNP P04535
x	201A	ASP	-	insertion	UNP P04535

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Chain	Residue	Modelled	Actual	Comment	Reference
x	201B	GLU	-	insertion	UNP P04535
x	201C	ASP	-	insertion	UNP P04535
x	201D	GLU	-	insertion	UNP P04535
x	201E	ASP	-	insertion	UNP P04535
x	201F	GLU	-	insertion	UNP P04535
x	201G	ASP	-	insertion	UNP P04535
x	201H	GLU	-	insertion	UNP P04535
x	201I	ASP	-	insertion	UNP P04535
y	201A	ASP	-	insertion	UNP P04535
y	201B	GLU	-	insertion	UNP P04535
y	201C	ASP	-	insertion	UNP P04535
y	201D	GLU	-	insertion	UNP P04535
y	201E	ASP	-	insertion	UNP P04535
y	201F	GLU	-	insertion	UNP P04535
y	201G	ASP	-	insertion	UNP P04535
y	201H	GLU	-	insertion	UNP P04535
y	201I	ASP	-	insertion	UNP P04535
z	201A	ASP	-	insertion	UNP P04535
z	201B	GLU	-	insertion	UNP P04535
z	201C	ASP	-	insertion	UNP P04535
z	201D	GLU	-	insertion	UNP P04535
z	201E	ASP	-	insertion	UNP P04535
z	201F	GLU	-	insertion	UNP P04535
z	201G	ASP	-	insertion	UNP P04535
z	201H	GLU	-	insertion	UNP P04535
z	201I	ASP	-	insertion	UNP P04535

- Molecule 2 is a protein called Mature capsid vertex protein.

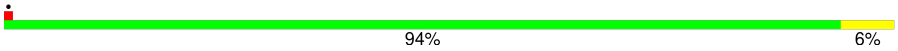
Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	415	Total	C	N	O	S	0	0
			3208	2039	521	640	8		
2	B	415	Total	C	N	O	S	0	0
			3208	2039	521	640	8		
2	C	415	Total	C	N	O	S	0	0
			3208	2039	521	640	8		
2	D	415	Total	C	N	O	S	0	0
			3208	2039	521	640	8		
2	a	415	Total	C	N	O	S	0	0
			3208	2039	521	640	8		

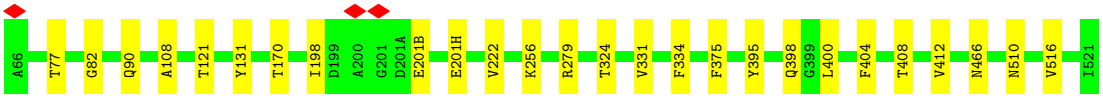
3 Residue-property plots (i)

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

• Molecule 1: Mature major capsid protein

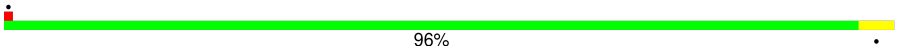
Chain 0:

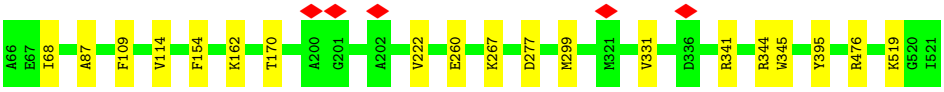




• Molecule 1: Mature major capsid protein

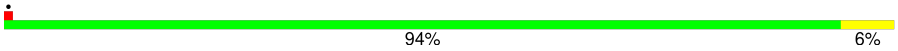
Chain 1:

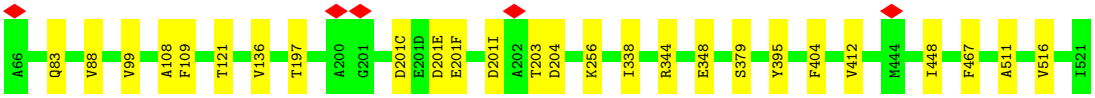




• Molecule 1: Mature major capsid protein

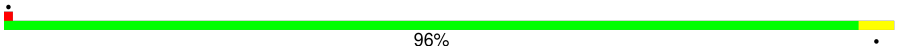
Chain 2:

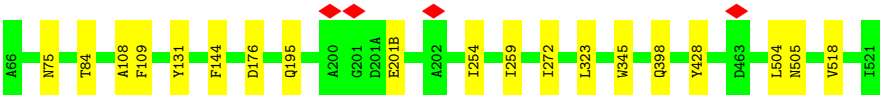




• Molecule 1: Mature major capsid protein

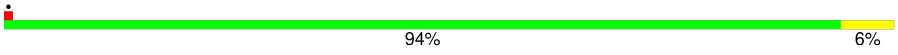
Chain 3:

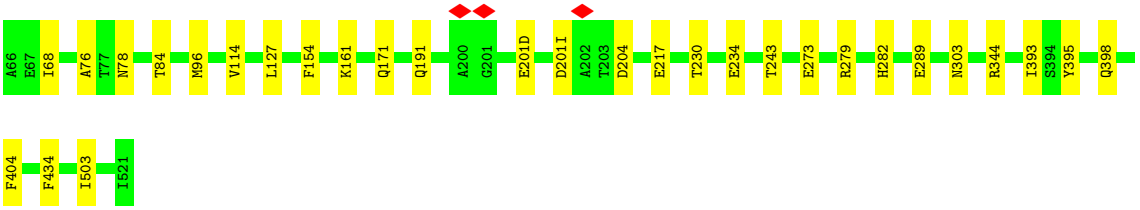




• Molecule 1: Mature major capsid protein

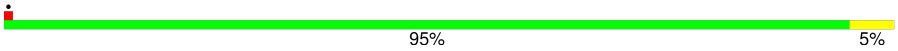
Chain 4:

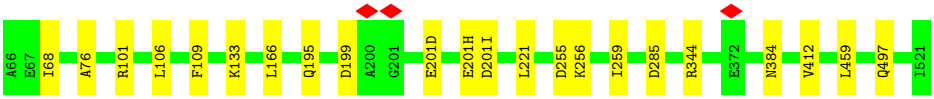




• Molecule 1: Mature major capsid protein

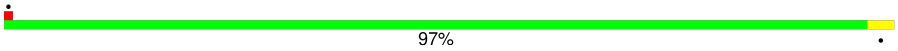
Chain 5:

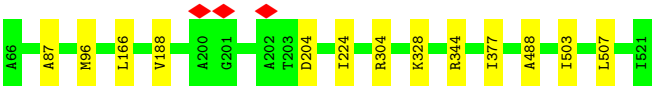




• Molecule 1: Mature major capsid protein

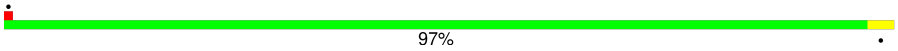
Chain 6:





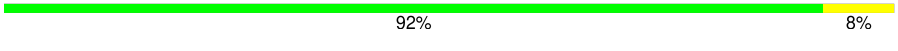
• Molecule 1: Mature major capsid protein

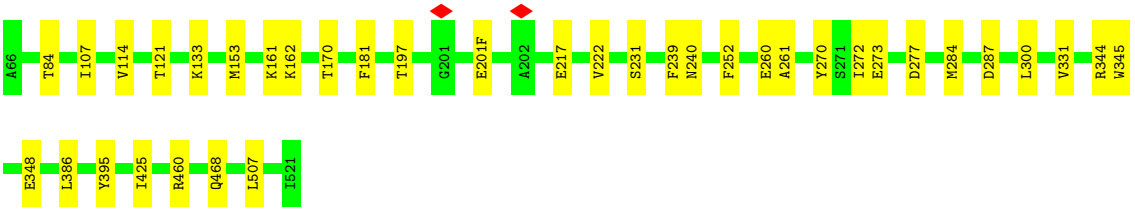
Chain 7:



• Molecule 1: Mature major capsid protein

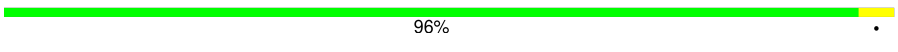
Chain 8:

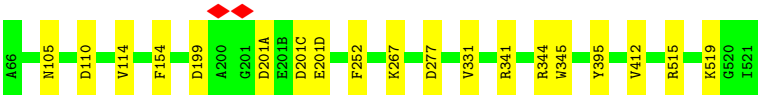




• Molecule 1: Mature major capsid protein

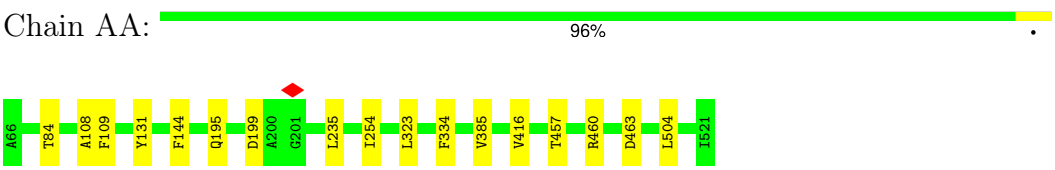
Chain 9:





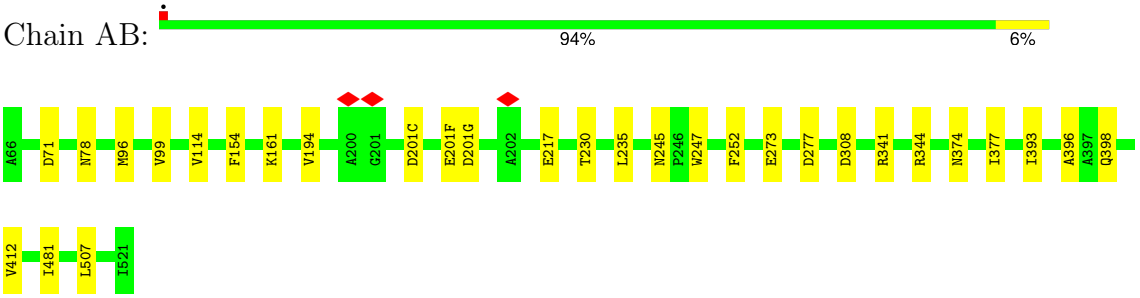
• Molecule 1: Mature major capsid protein

Chain AA:



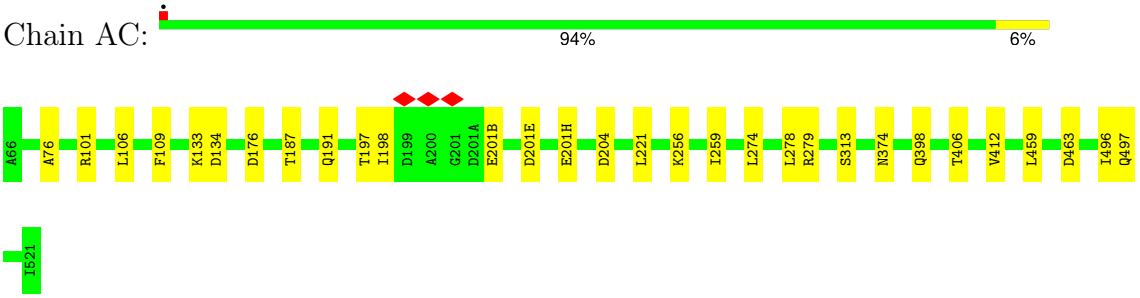
• Molecule 1: Mature major capsid protein

Chain AB:



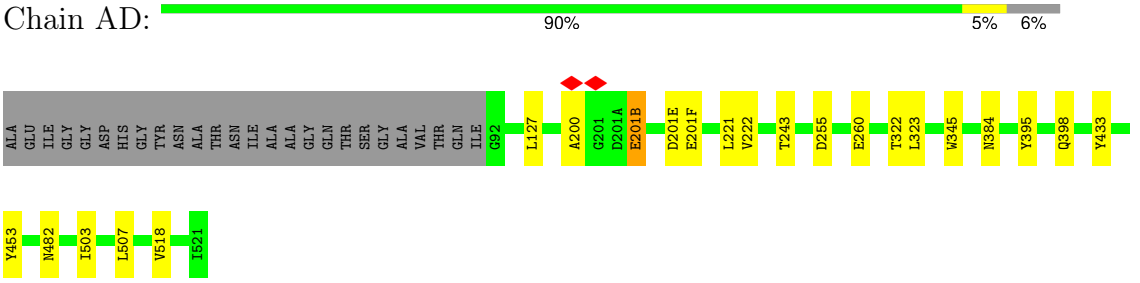
• Molecule 1: Mature major capsid protein

Chain AC:



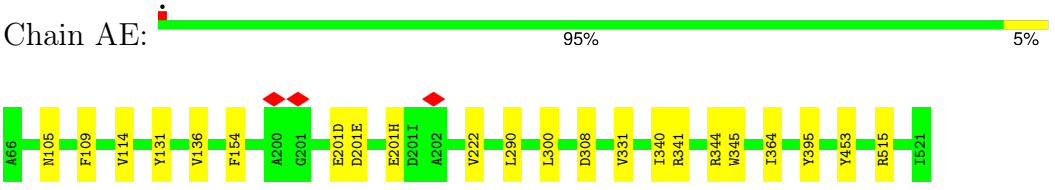
• Molecule 1: Mature major capsid protein

Chain AD:



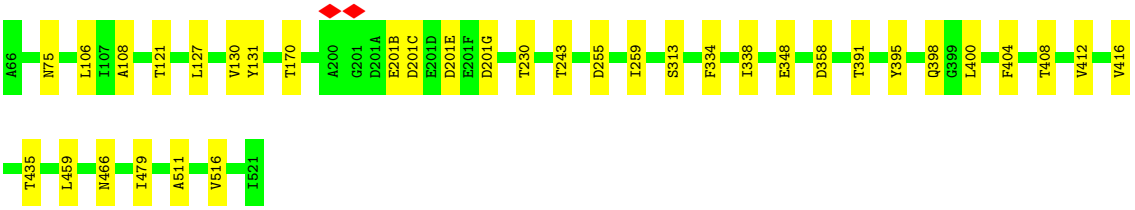
• Molecule 1: Mature major capsid protein

Chain AE:



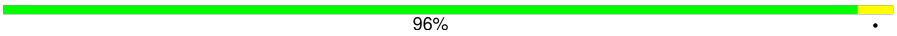
• Molecule 1: Mature major capsid protein

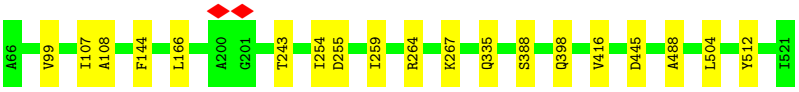
Chain AF:



• Molecule 1: Mature major capsid protein

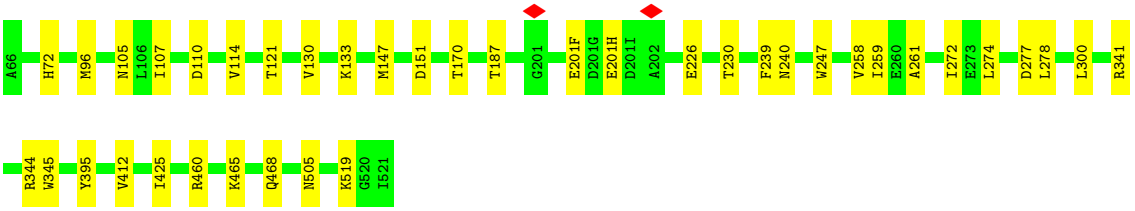
Chain AG:





• Molecule 1: Mature major capsid protein

Chain AH:

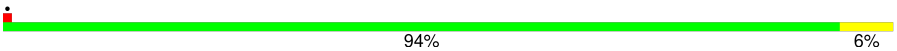


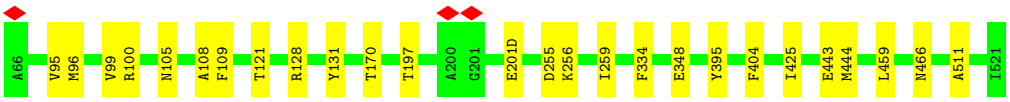
• Molecule 1: Mature major capsid protein

Chain AI:

• Molecule 1: Mature major capsid protein

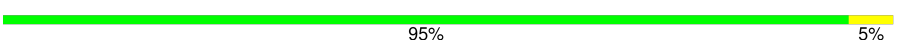
Chain AJ:

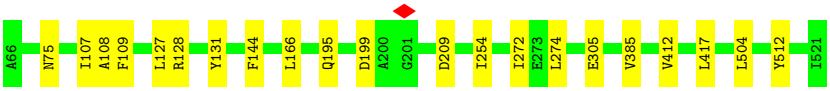




• Molecule 1: Mature major capsid protein

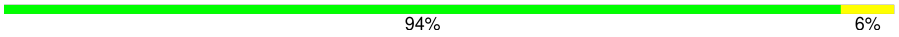
Chain AK:





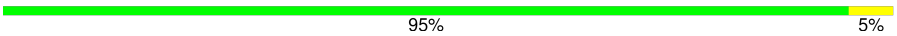
• Molecule 1: Mature major capsid protein

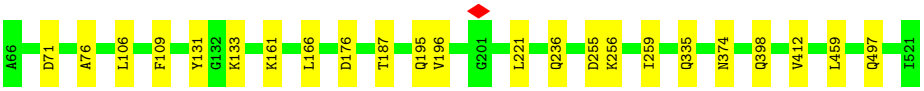
Chain AL:



• Molecule 1: Mature major capsid protein

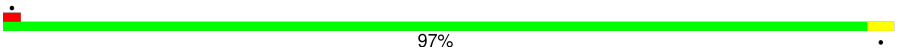
Chain AM:





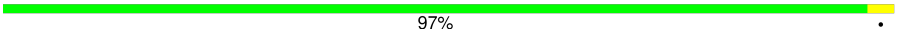
• Molecule 1: Mature major capsid protein

Chain AN:



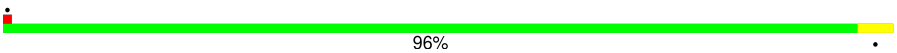
• Molecule 1: Mature major capsid protein

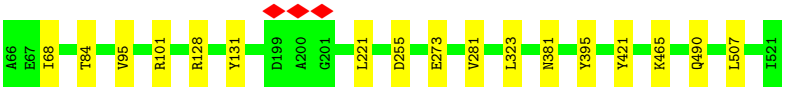
Chain AO:



• Molecule 1: Mature major capsid protein

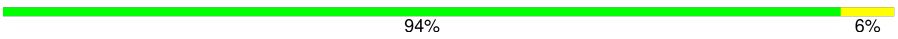
Chain AP:

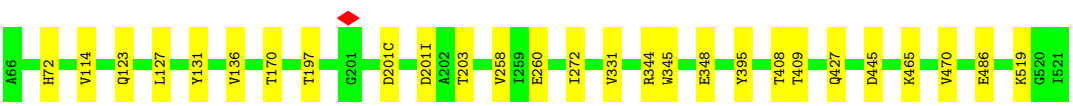




• Molecule 1: Mature major capsid protein

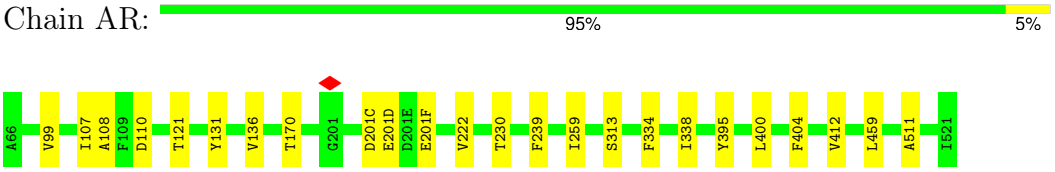
Chain AQ:





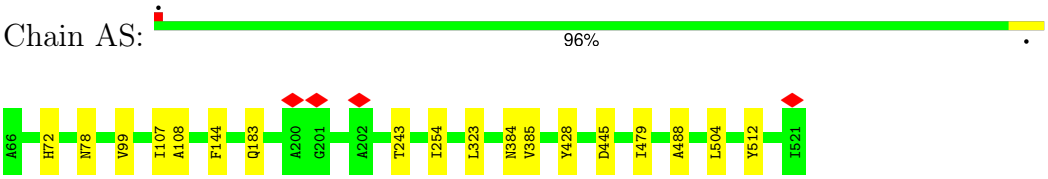
• Molecule 1: Mature major capsid protein

Chain AR:



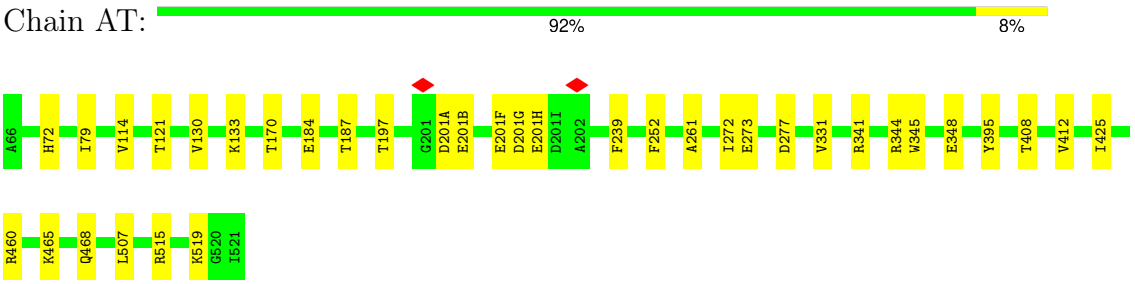
• Molecule 1: Mature major capsid protein

Chain AS:



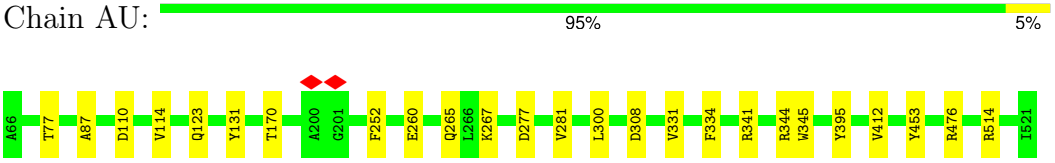
• Molecule 1: Mature major capsid protein

Chain AT:



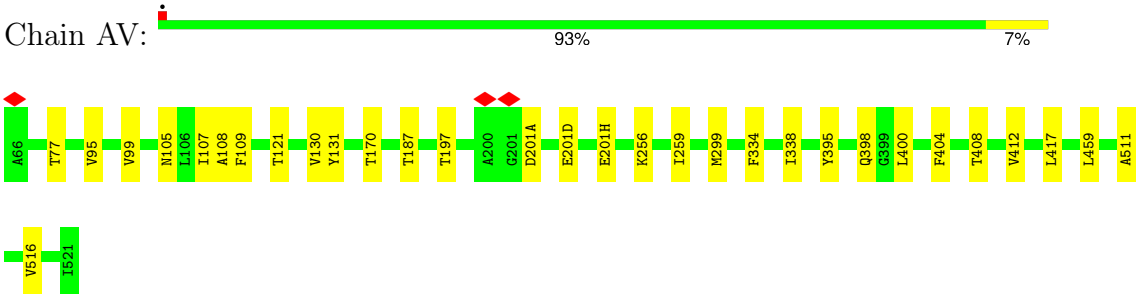
• Molecule 1: Mature major capsid protein

Chain AU:



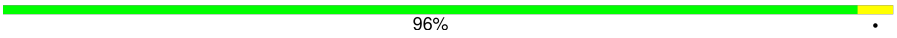
• Molecule 1: Mature major capsid protein

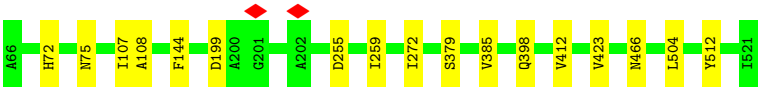
Chain AV:



• Molecule 1: Mature major capsid protein

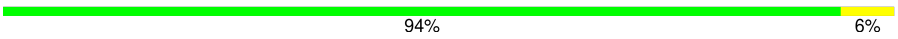
Chain AW:

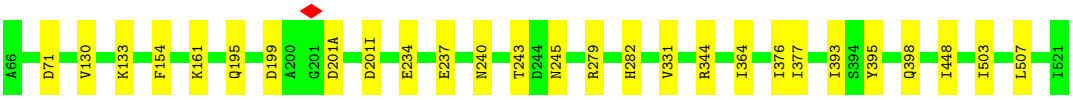




• Molecule 1: Mature major capsid protein

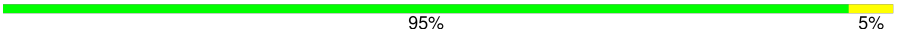
Chain AX:

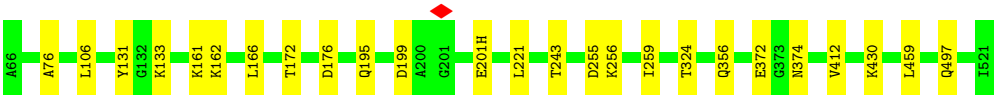




• Molecule 1: Mature major capsid protein

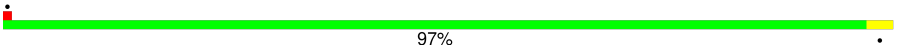
Chain AY:





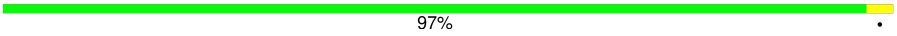
• Molecule 1: Mature major capsid protein

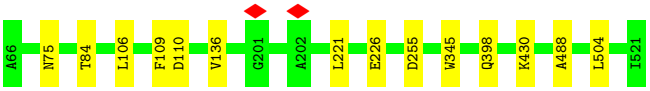
Chain AZ:



• Molecule 1: Mature major capsid protein

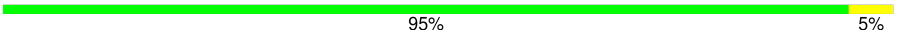
Chain Aa:

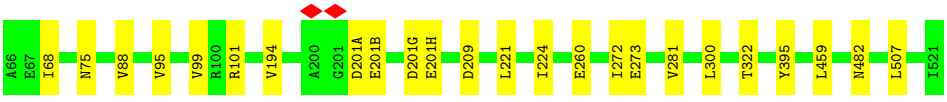




• Molecule 1: Mature major capsid protein

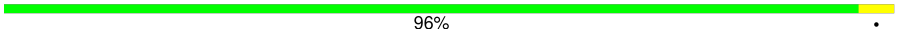
Chain Ab:

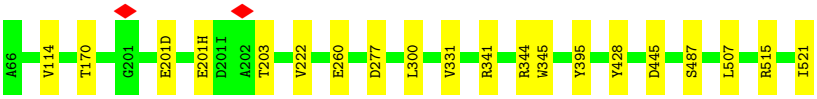




• Molecule 1: Mature major capsid protein

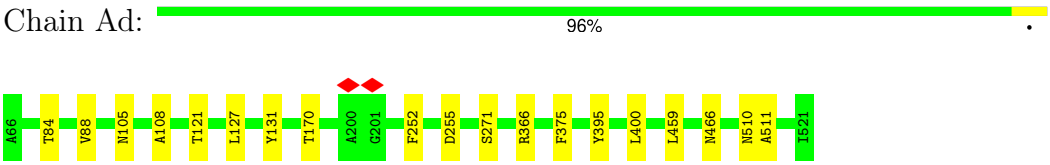
Chain Ac:





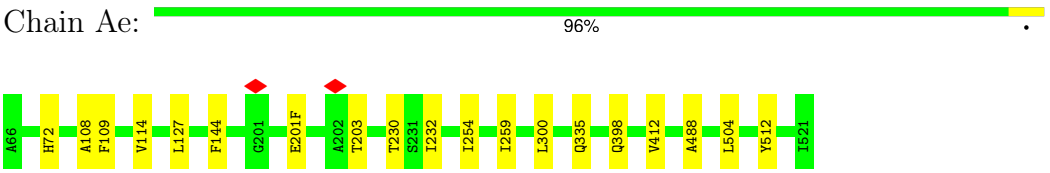
• Molecule 1: Mature major capsid protein

Chain Ad:



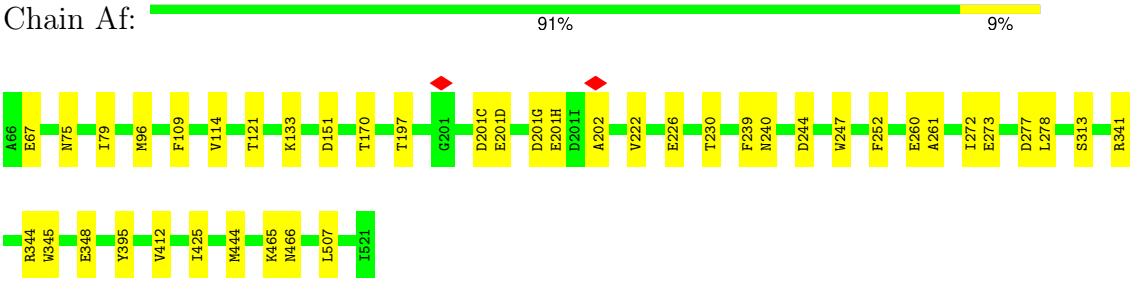
• Molecule 1: Mature major capsid protein

Chain Ae:



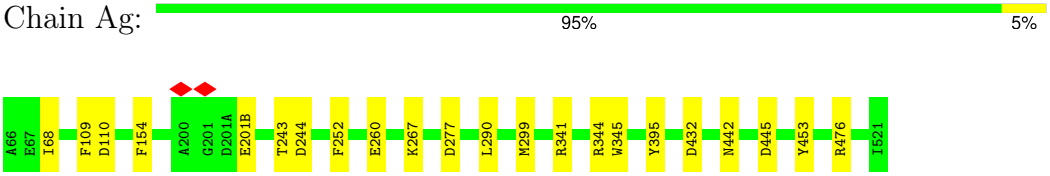
• Molecule 1: Mature major capsid protein

Chain Af:



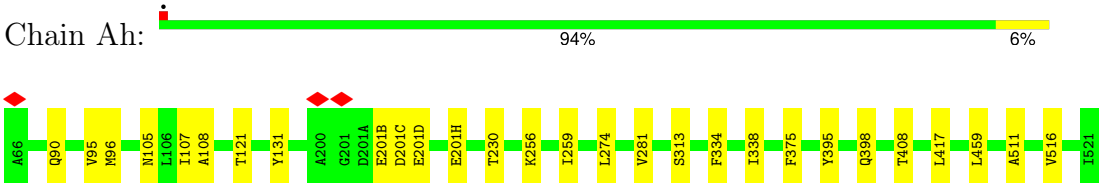
• Molecule 1: Mature major capsid protein

Chain Ag:



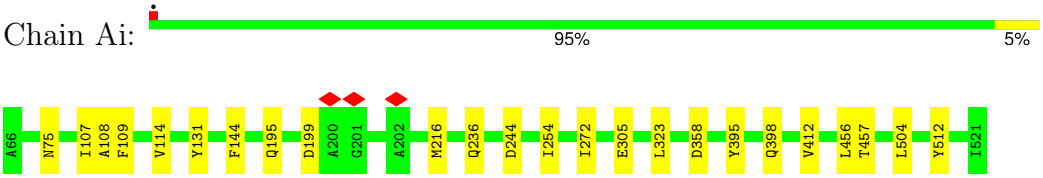
• Molecule 1: Mature major capsid protein

Chain Ah:



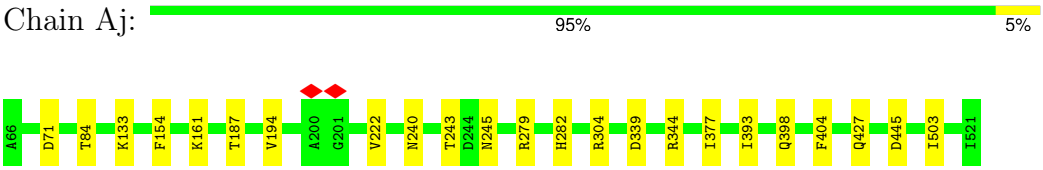
• Molecule 1: Mature major capsid protein

Chain Ai:



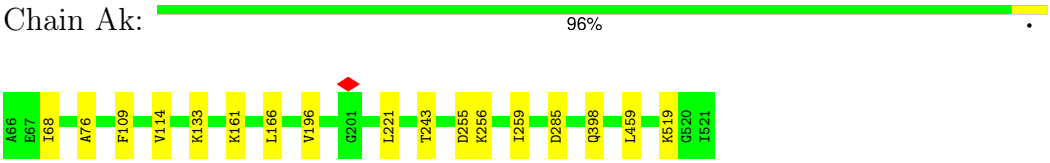
• Molecule 1: Mature major capsid protein

Chain Aj:



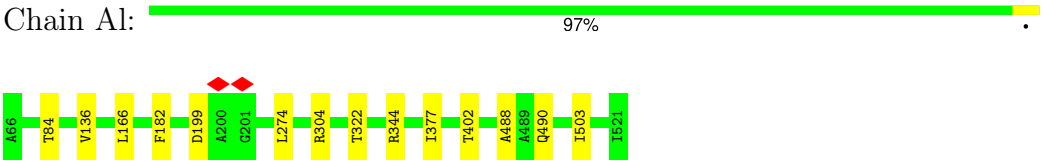
• Molecule 1: Mature major capsid protein

Chain Ak:



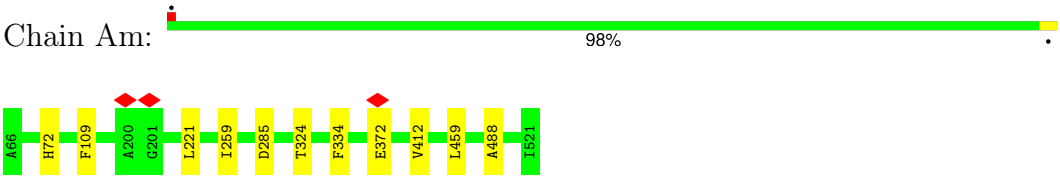
• Molecule 1: Mature major capsid protein

Chain Al:



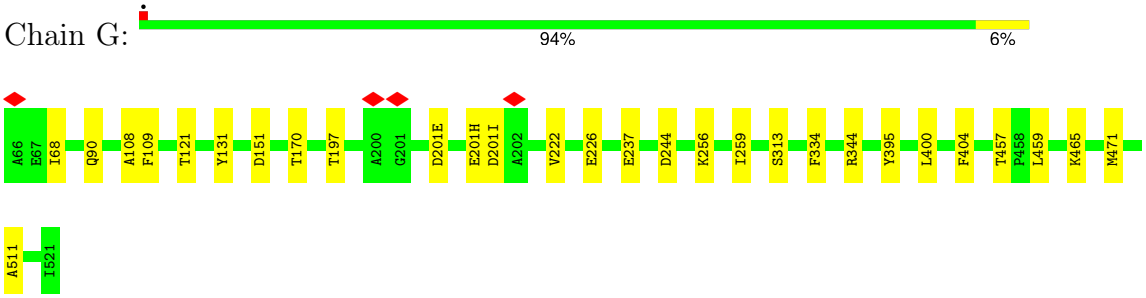
• Molecule 1: Mature major capsid protein

Chain Am:



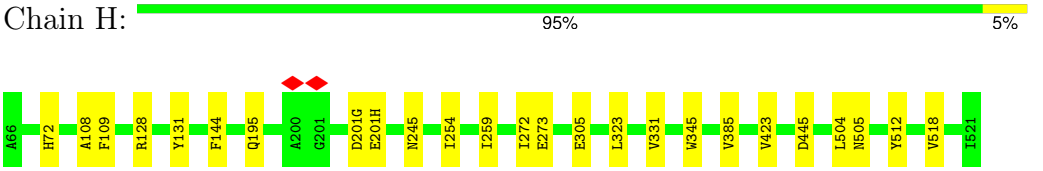
• Molecule 1: Mature major capsid protein

Chain G:



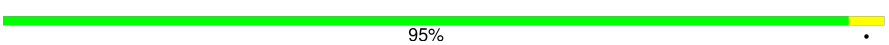
• Molecule 1: Mature major capsid protein

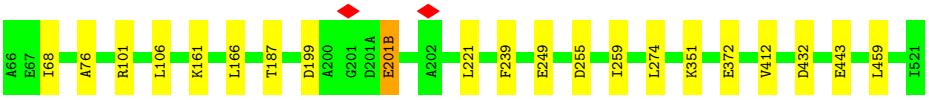
Chain H:



• Molecule 1: Mature major capsid protein

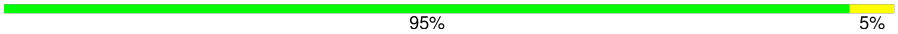
Chain J:

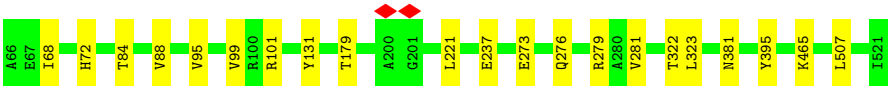




• Molecule 1: Mature major capsid protein

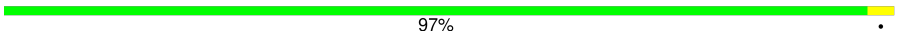
Chain K:

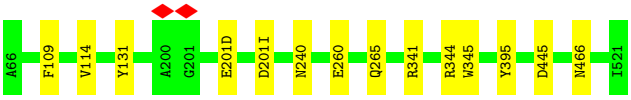




• Molecule 1: Mature major capsid protein

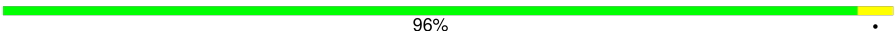
Chain L:

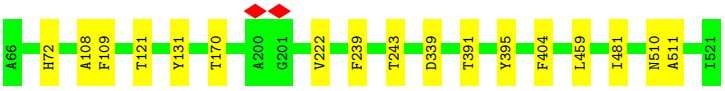




• Molecule 1: Mature major capsid protein

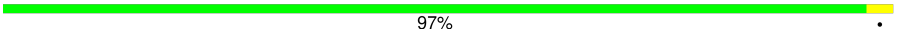
Chain M:

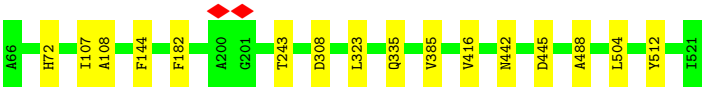




• Molecule 1: Mature major capsid protein

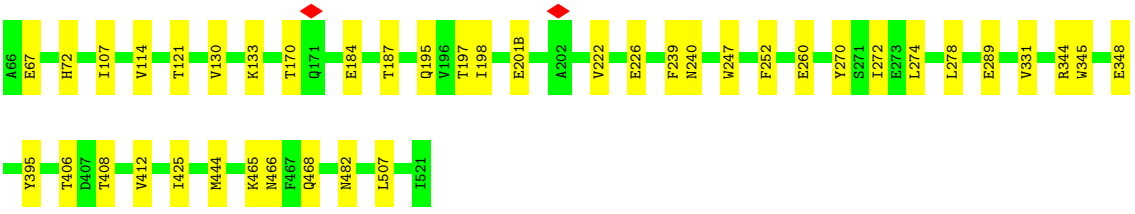
Chain N:





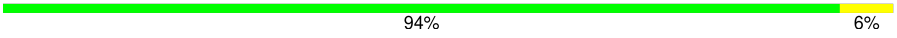
• Molecule 1: Mature major capsid protein

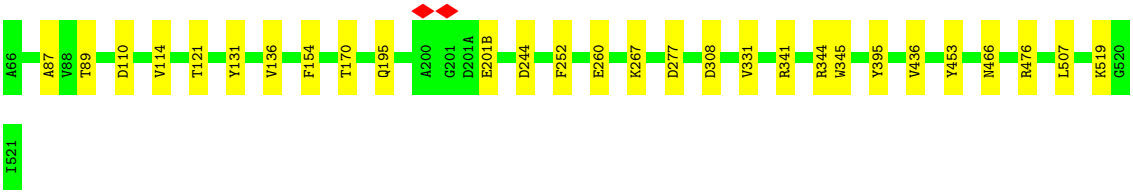
Chain O:



• Molecule 1: Mature major capsid protein

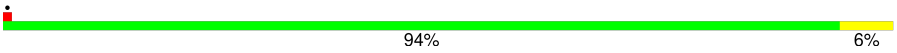
Chain P:

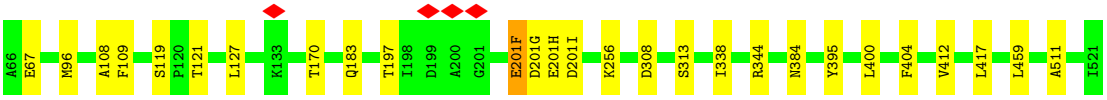




• Molecule 1: Mature major capsid protein

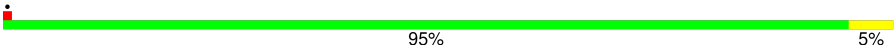
Chain Q:





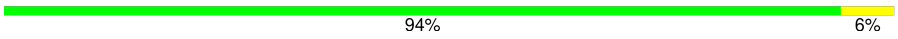
• Molecule 1: Mature major capsid protein

Chain R:



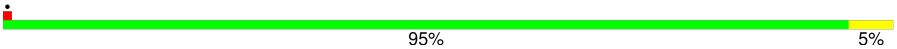
• Molecule 1: Mature major capsid protein

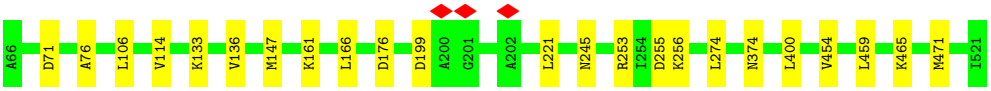
Chain S:



• Molecule 1: Mature major capsid protein

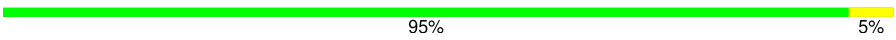
Chain T:





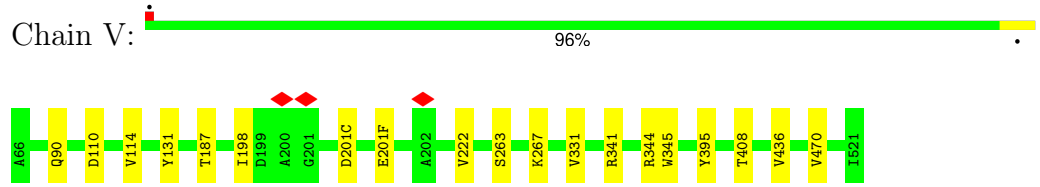
• Molecule 1: Mature major capsid protein

Chain U:



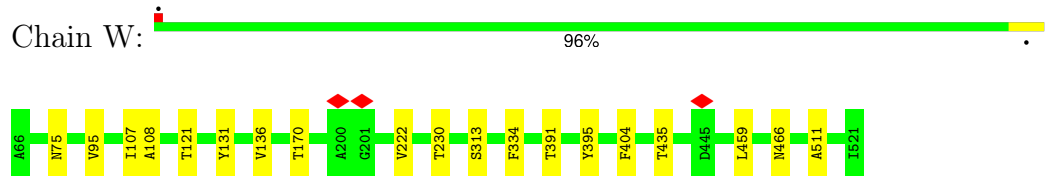
• Molecule 1: Mature major capsid protein

Chain V:



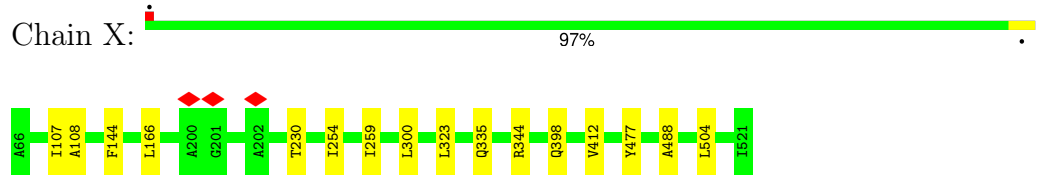
• Molecule 1: Mature major capsid protein

Chain W:



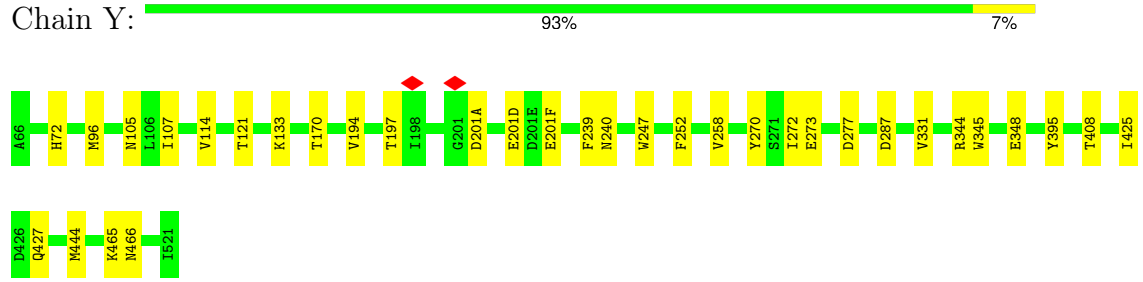
• Molecule 1: Mature major capsid protein

Chain X:



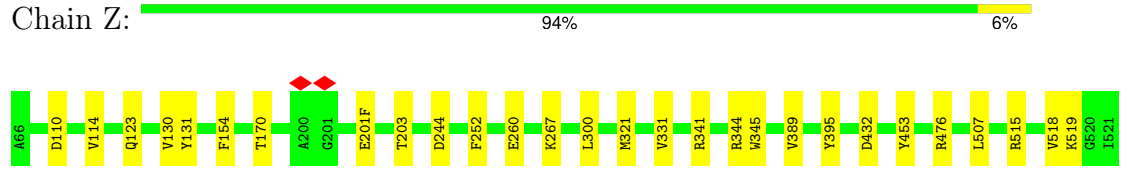
• Molecule 1: Mature major capsid protein

Chain Y:



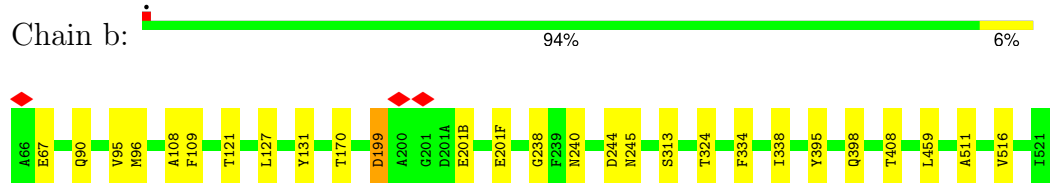
• Molecule 1: Mature major capsid protein

Chain Z:



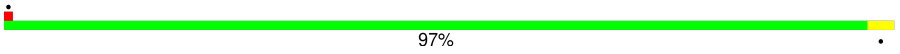
• Molecule 1: Mature major capsid protein

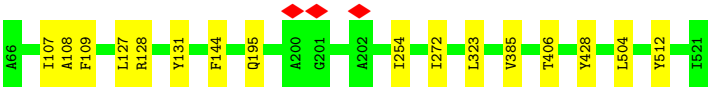
Chain b:



• Molecule 1: Mature major capsid protein

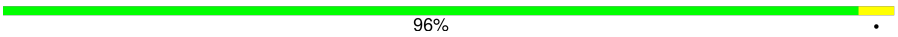
Chain c:

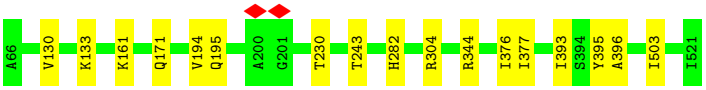




• Molecule 1: Mature major capsid protein

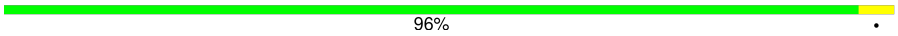
Chain d:

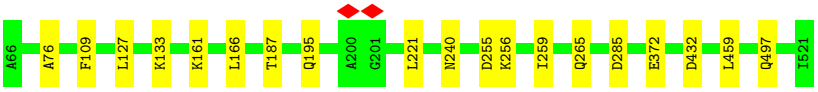




• Molecule 1: Mature major capsid protein

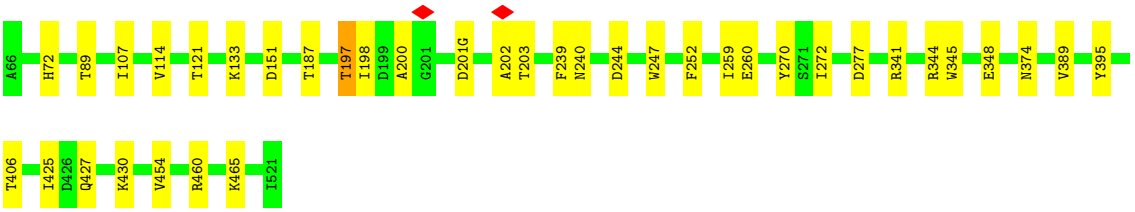
Chain e:





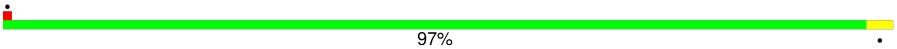
• Molecule 1: Mature major capsid protein

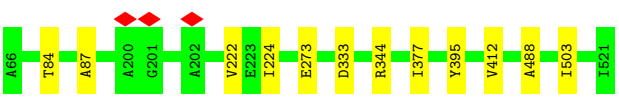
Chain f:



• Molecule 1: Mature major capsid protein

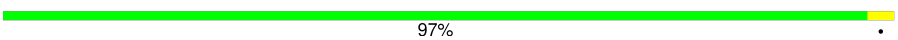
Chain g:





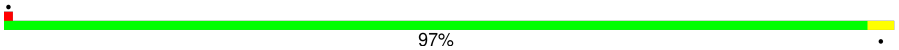
• Molecule 1: Mature major capsid protein

Chain h:



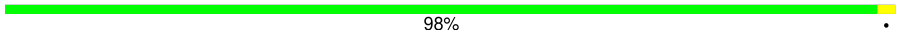
• Molecule 1: Mature major capsid protein

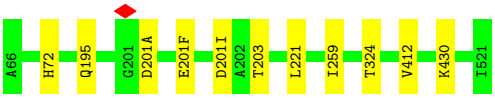
Chain i:



• Molecule 1: Mature major capsid protein

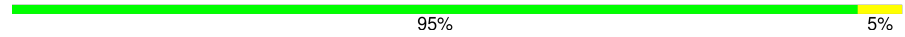
Chain j:

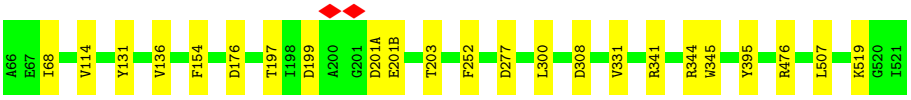




• Molecule 1: Mature major capsid protein

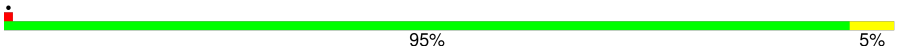
Chain k:

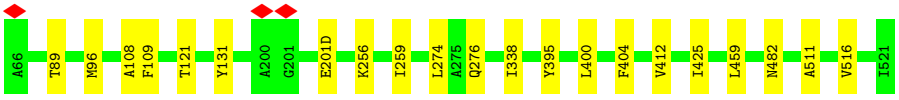




• Molecule 1: Mature major capsid protein

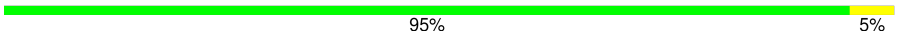
Chain l:

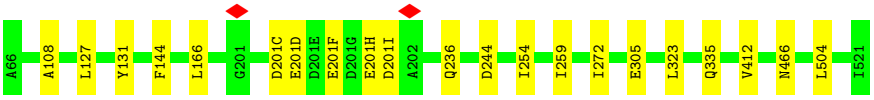




• Molecule 1: Mature major capsid protein

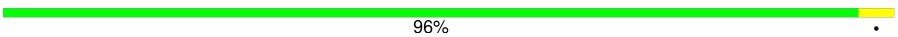
Chain m:

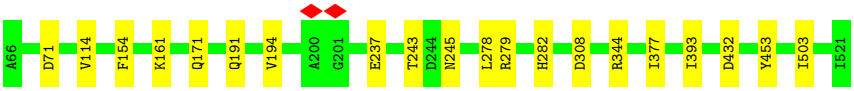




• Molecule 1: Mature major capsid protein

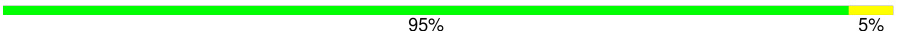
Chain n:

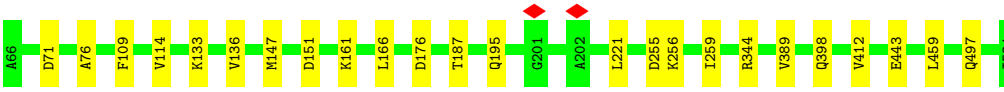




• Molecule 1: Mature major capsid protein

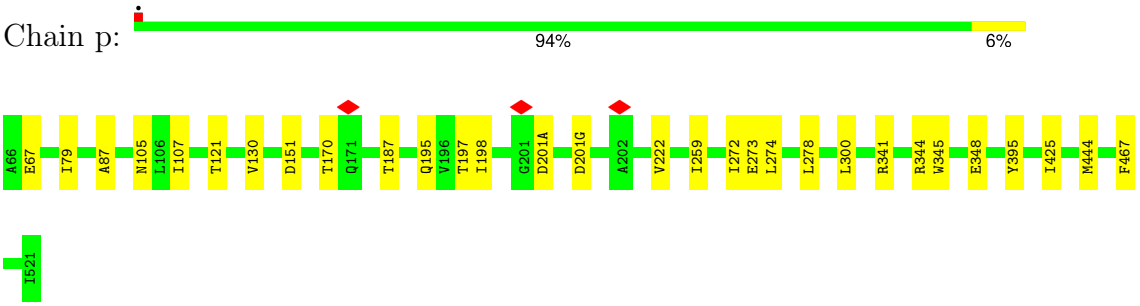
Chain o:





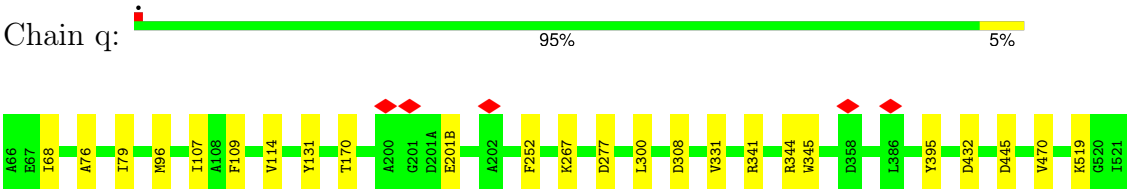
• Molecule 1: Mature major capsid protein

Chain p:



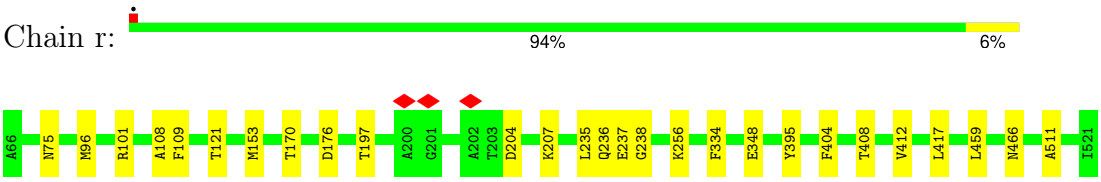
• Molecule 1: Mature major capsid protein

Chain q:



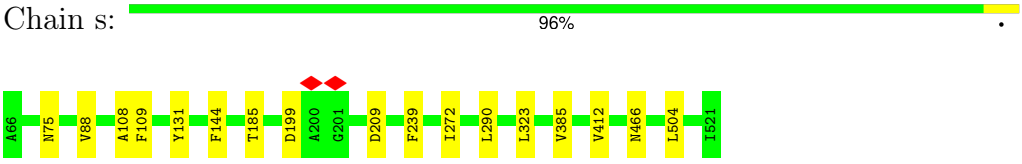
• Molecule 1: Mature major capsid protein

Chain r:



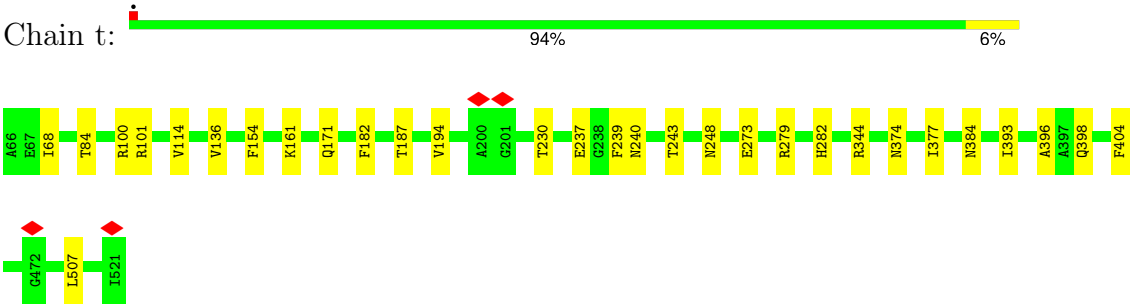
• Molecule 1: Mature major capsid protein

Chain s:



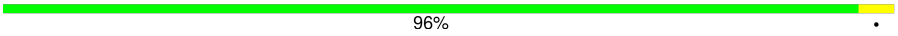
• Molecule 1: Mature major capsid protein

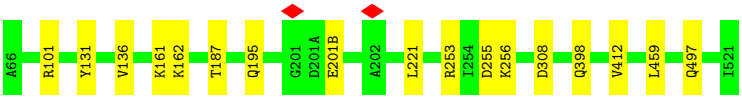
Chain t:



• Molecule 1: Mature major capsid protein

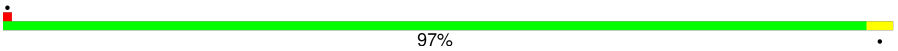
Chain u:

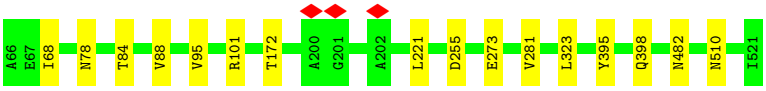




• Molecule 1: Mature major capsid protein

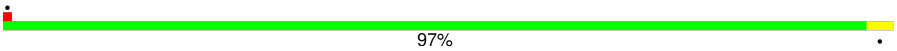
Chain v:

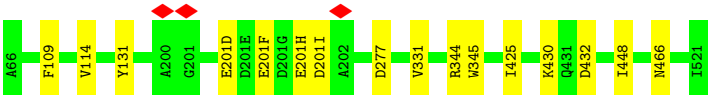




• Molecule 1: Mature major capsid protein

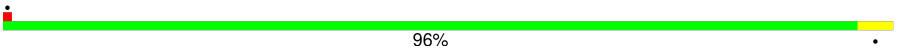
Chain w:

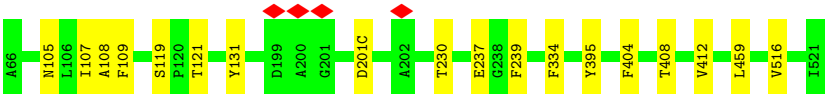




• Molecule 1: Mature major capsid protein

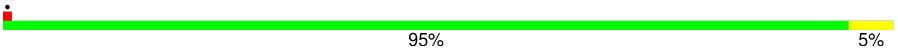
Chain x:





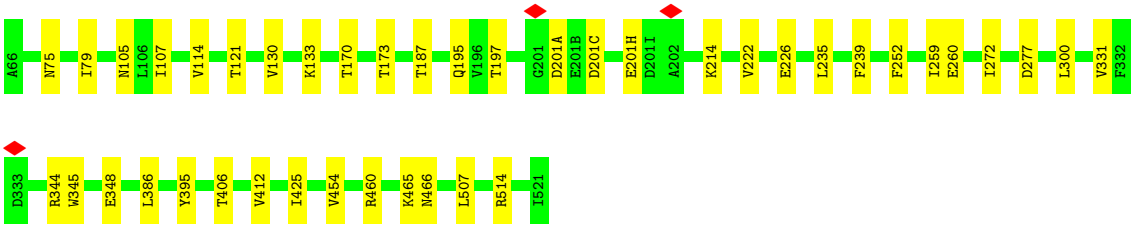
• Molecule 1: Mature major capsid protein

Chain y:



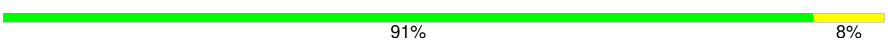
• Molecule 1: Mature major capsid protein

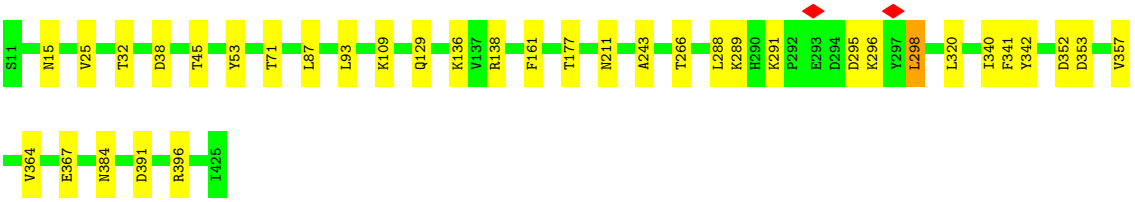
Chain z:



• Molecule 2: Mature capsid vertex protein

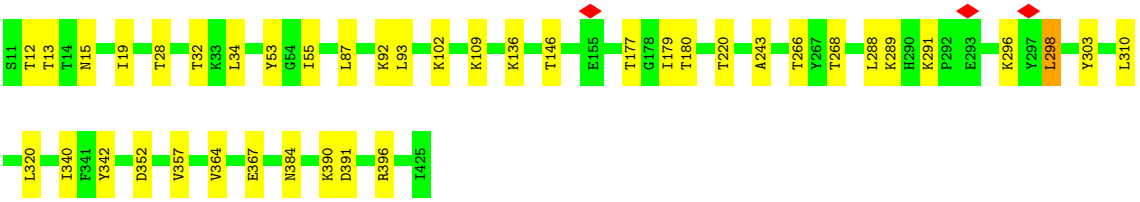
Chain A:





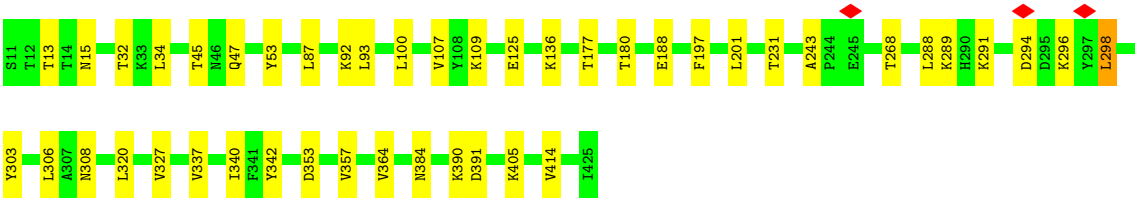
• Molecule 2: Mature capsid vertex protein

Chain B:



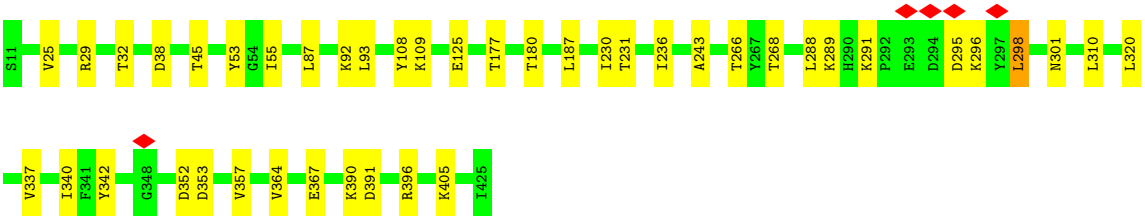
• Molecule 2: Mature capsid vertex protein

Chain C:



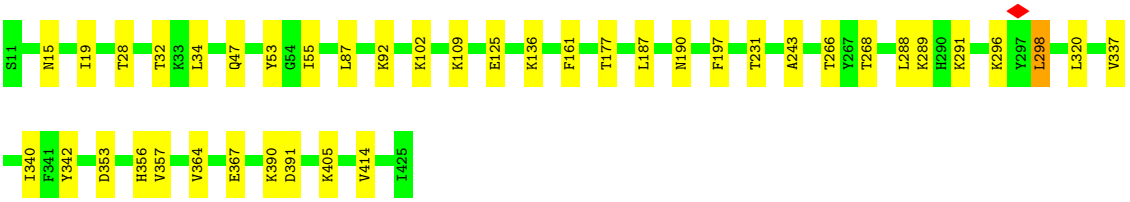
• Molecule 2: Mature capsid vertex protein

Chain D:



• Molecule 2: Mature capsid vertex protein

Chain a:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D5	Depositor
Number of particles used	70340	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	36	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.084	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	1332.0, 1332.0, 1332.0	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.85, 1.85, 1.85	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0	0.28	0/3569	0.49	0/4834
1	1	0.28	0/3569	0.48	0/4834
1	2	0.27	0/3569	0.49	0/4834
1	3	0.27	0/3569	0.48	0/4834
1	4	0.27	0/3569	0.48	0/4834
1	5	0.27	0/3569	0.48	0/4834
1	6	0.28	0/3569	0.48	0/4834
1	7	0.28	0/3569	0.48	0/4834
1	8	0.28	0/3569	0.49	0/4834
1	9	0.29	0/3569	0.50	0/4834
1	AA	0.28	0/3569	0.49	0/4834
1	AB	0.27	0/3569	0.48	0/4834
1	AC	0.27	0/3569	0.49	0/4834
1	AD	0.30	0/3376	0.49	0/4570
1	AE	0.29	0/3569	0.48	0/4834
1	AF	0.29	0/3569	0.49	0/4834
1	AG	0.29	0/3569	0.49	0/4834
1	AH	0.30	0/3569	0.51	0/4834
1	AI	0.29	0/3569	0.49	0/4834
1	AJ	0.29	0/3569	0.50	0/4834
1	AK	0.29	0/3569	0.49	0/4834
1	AL	0.29	0/3569	0.48	0/4834
1	AM	0.29	0/3569	0.48	0/4834
1	AN	0.29	0/3569	0.48	0/4834
1	AO	0.29	0/3569	0.49	0/4834
1	AP	0.29	0/3554	0.48	0/4813
1	AQ	0.29	0/3569	0.49	0/4834
1	AR	0.28	0/3569	0.48	0/4834
1	AS	0.29	0/3569	0.48	0/4834
1	AT	0.28	0/3569	0.50	0/4834
1	AU	0.29	0/3569	0.48	0/4834
1	AV	0.29	0/3569	0.49	0/4834
1	AW	0.28	0/3569	0.49	0/4834
1	AX	0.28	0/3569	0.48	0/4834

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	AY	0.29	0/3569	0.48	0/4834
1	AZ	0.29	0/3569	0.47	0/4834
1	Aa	0.29	0/3569	0.49	0/4834
1	Ab	0.29	0/3554	0.48	0/4813
1	Ac	0.29	0/3569	0.49	0/4834
1	Ad	0.29	0/3569	0.49	0/4834
1	Ae	0.29	0/3569	0.48	0/4834
1	Af	0.29	0/3569	0.50	0/4834
1	Ag	0.29	0/3569	0.49	0/4834
1	Ah	0.30	0/3569	0.49	0/4834
1	Ai	0.29	0/3569	0.49	0/4834
1	Aj	0.28	0/3569	0.48	0/4834
1	Ak	0.29	0/3569	0.48	0/4834
1	Al	0.29	0/3569	0.48	0/4834
1	Am	0.28	0/3569	0.48	0/4834
1	G	0.27	0/3569	0.49	0/4834
1	H	0.27	0/3569	0.48	0/4834
1	J	0.27	0/3569	0.48	0/4834
1	K	0.29	0/3554	0.48	0/4813
1	L	0.29	0/3569	0.49	0/4834
1	M	0.28	0/3569	0.48	0/4834
1	N	0.28	0/3569	0.48	0/4834
1	O	0.28	0/3569	0.48	0/4834
1	P	0.28	0/3569	0.48	0/4834
1	Q	0.28	0/3569	0.49	0/4834
1	R	0.28	0/3569	0.48	0/4834
1	S	0.27	0/3569	0.48	0/4834
1	T	0.27	0/3569	0.48	0/4834
1	U	0.29	0/3554	0.48	0/4813
1	V	0.29	0/3569	0.49	0/4834
1	W	0.28	0/3569	0.48	0/4834
1	X	0.28	0/3569	0.48	0/4834
1	Y	0.28	0/3569	0.49	0/4834
1	Z	0.28	0/3569	0.49	0/4834
1	b	0.31	0/3569	0.50	0/4834
1	c	0.28	0/3569	0.49	0/4834
1	d	0.28	0/3569	0.48	0/4834
1	e	0.28	0/3569	0.48	0/4834
1	f	0.30	0/3569	0.51	0/4834
1	g	0.28	0/3569	0.48	0/4834
1	h	0.28	0/3569	0.48	0/4834
1	i	0.29	0/3569	0.48	0/4834
1	j	0.29	0/3569	0.48	0/4834

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	k	0.27	0/3569	0.49	0/4834
1	l	0.28	0/3569	0.49	0/4834
1	m	0.27	0/3569	0.49	0/4834
1	n	0.27	0/3569	0.48	0/4834
1	o	0.28	0/3569	0.48	0/4834
1	p	0.27	0/3569	0.49	0/4834
1	q	0.27	0/3569	0.49	0/4834
1	r	0.30	0/3569	0.50	0/4834
1	s	0.27	0/3569	0.49	0/4834
1	t	0.27	0/3569	0.48	0/4834
1	u	0.27	0/3569	0.49	0/4834
1	v	0.28	0/3554	0.48	0/4813
1	w	0.29	0/3569	0.49	0/4834
1	x	0.28	0/3569	0.49	0/4834
1	y	0.28	0/3569	0.48	0/4834
1	z	0.27	0/3569	0.48	0/4834
2	A	0.28	0/3263	0.49	0/4430
2	B	0.28	0/3263	0.48	0/4430
2	C	0.28	0/3263	0.48	0/4430
2	D	0.28	0/3263	0.48	0/4430
2	a	0.28	0/3263	0.49	0/4430
All	All	0.28	0/347964	0.49	0/471343

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	0	463/465 (100%)	408 (88%)	53 (11%)	2 (0%)	30	65
1	1	463/465 (100%)	408 (88%)	54 (12%)	1 (0%)	44	75
1	2	463/465 (100%)	409 (88%)	50 (11%)	4 (1%)	14	48
1	3	463/465 (100%)	410 (89%)	51 (11%)	2 (0%)	30	65
1	4	463/465 (100%)	405 (88%)	56 (12%)	2 (0%)	30	65
1	5	463/465 (100%)	403 (87%)	59 (13%)	1 (0%)	44	75
1	6	463/465 (100%)	415 (90%)	46 (10%)	2 (0%)	30	65
1	7	463/465 (100%)	416 (90%)	46 (10%)	1 (0%)	44	75
1	8	463/465 (100%)	397 (86%)	63 (14%)	3 (1%)	22	57
1	9	463/465 (100%)	409 (88%)	53 (11%)	1 (0%)	44	75
1	AA	463/465 (100%)	404 (87%)	56 (12%)	3 (1%)	22	57
1	AB	463/465 (100%)	405 (88%)	56 (12%)	2 (0%)	30	65
1	AC	463/465 (100%)	408 (88%)	53 (11%)	2 (0%)	30	65
1	AD	437/465 (94%)	395 (90%)	40 (9%)	2 (0%)	25	60
1	AE	463/465 (100%)	412 (89%)	51 (11%)	0	100	100
1	AF	463/465 (100%)	404 (87%)	57 (12%)	2 (0%)	30	65
1	AG	463/465 (100%)	411 (89%)	49 (11%)	3 (1%)	22	57
1	AH	463/465 (100%)	400 (86%)	59 (13%)	4 (1%)	14	48
1	AI	463/465 (100%)	403 (87%)	59 (13%)	1 (0%)	44	75
1	AJ	463/465 (100%)	404 (87%)	57 (12%)	2 (0%)	30	65
1	AK	463/465 (100%)	401 (87%)	59 (13%)	3 (1%)	22	57
1	AL	463/465 (100%)	399 (86%)	63 (14%)	1 (0%)	44	75
1	AM	463/465 (100%)	404 (87%)	58 (12%)	1 (0%)	44	75
1	AN	463/465 (100%)	405 (88%)	54 (12%)	4 (1%)	14	48
1	AO	463/465 (100%)	409 (88%)	53 (11%)	1 (0%)	44	75
1	AP	463/465 (100%)	425 (92%)	37 (8%)	1 (0%)	44	75
1	AQ	463/465 (100%)	412 (89%)	49 (11%)	2 (0%)	30	65
1	AR	463/465 (100%)	410 (89%)	50 (11%)	3 (1%)	22	57
1	AS	463/465 (100%)	415 (90%)	45 (10%)	3 (1%)	22	57
1	AT	463/465 (100%)	396 (86%)	63 (14%)	4 (1%)	14	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AU	463/465 (100%)	414 (89%)	48 (10%)	1 (0%)	44	75
1	AV	463/465 (100%)	405 (88%)	55 (12%)	3 (1%)	22	57
1	AW	463/465 (100%)	406 (88%)	54 (12%)	3 (1%)	22	57
1	AX	463/465 (100%)	406 (88%)	56 (12%)	1 (0%)	44	75
1	AY	463/465 (100%)	405 (88%)	57 (12%)	1 (0%)	44	75
1	AZ	463/465 (100%)	413 (89%)	48 (10%)	2 (0%)	30	65
1	Aa	463/465 (100%)	414 (89%)	48 (10%)	1 (0%)	44	75
1	Ab	463/465 (100%)	420 (91%)	40 (9%)	3 (1%)	22	57
1	Ac	463/465 (100%)	413 (89%)	50 (11%)	0	100	100
1	Ad	463/465 (100%)	413 (89%)	48 (10%)	2 (0%)	30	65
1	Ae	463/465 (100%)	410 (89%)	50 (11%)	3 (1%)	22	57
1	Af	463/465 (100%)	402 (87%)	56 (12%)	5 (1%)	12	45
1	Ag	463/465 (100%)	403 (87%)	60 (13%)	0	100	100
1	Ah	463/465 (100%)	407 (88%)	54 (12%)	2 (0%)	30	65
1	Ai	463/465 (100%)	400 (86%)	60 (13%)	3 (1%)	22	57
1	Aj	463/465 (100%)	406 (88%)	56 (12%)	1 (0%)	44	75
1	Ak	463/465 (100%)	404 (87%)	58 (12%)	1 (0%)	44	75
1	Al	463/465 (100%)	409 (88%)	53 (11%)	1 (0%)	44	75
1	Am	463/465 (100%)	411 (89%)	51 (11%)	1 (0%)	44	75
1	G	463/465 (100%)	407 (88%)	52 (11%)	4 (1%)	14	48
1	H	463/465 (100%)	406 (88%)	54 (12%)	3 (1%)	22	57
1	J	463/465 (100%)	403 (87%)	57 (12%)	3 (1%)	22	57
1	K	463/465 (100%)	422 (91%)	39 (8%)	2 (0%)	30	65
1	L	463/465 (100%)	408 (88%)	55 (12%)	0	100	100
1	M	463/465 (100%)	409 (88%)	52 (11%)	2 (0%)	30	65
1	N	463/465 (100%)	414 (89%)	46 (10%)	3 (1%)	22	57
1	O	463/465 (100%)	398 (86%)	63 (14%)	2 (0%)	30	65
1	P	463/465 (100%)	405 (88%)	56 (12%)	2 (0%)	30	65
1	Q	463/465 (100%)	404 (87%)	53 (11%)	6 (1%)	10	41
1	R	463/465 (100%)	408 (88%)	52 (11%)	3 (1%)	22	57
1	S	463/465 (100%)	398 (86%)	64 (14%)	1 (0%)	44	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	T	463/465 (100%)	412 (89%)	50 (11%)	1 (0%)	44 75
1	U	463/465 (100%)	426 (92%)	34 (7%)	3 (1%)	22 57
1	V	463/465 (100%)	413 (89%)	50 (11%)	0	100 100
1	W	463/465 (100%)	413 (89%)	48 (10%)	2 (0%)	30 65
1	X	463/465 (100%)	409 (88%)	51 (11%)	3 (1%)	22 57
1	Y	463/465 (100%)	405 (88%)	56 (12%)	2 (0%)	30 65
1	Z	463/465 (100%)	414 (89%)	49 (11%)	0	100 100
1	b	463/465 (100%)	408 (88%)	48 (10%)	7 (2%)	8 39
1	c	463/465 (100%)	410 (89%)	51 (11%)	2 (0%)	30 65
1	d	463/465 (100%)	405 (88%)	56 (12%)	2 (0%)	30 65
1	e	463/465 (100%)	403 (87%)	59 (13%)	1 (0%)	44 75
1	f	463/465 (100%)	399 (86%)	57 (12%)	7 (2%)	8 39
1	g	463/465 (100%)	414 (89%)	47 (10%)	2 (0%)	30 65
1	h	463/465 (100%)	411 (89%)	51 (11%)	1 (0%)	44 75
1	i	463/465 (100%)	405 (88%)	57 (12%)	1 (0%)	44 75
1	j	463/465 (100%)	404 (87%)	58 (12%)	1 (0%)	44 75
1	k	463/465 (100%)	411 (89%)	52 (11%)	0	100 100
1	l	463/465 (100%)	401 (87%)	60 (13%)	2 (0%)	30 65
1	m	463/465 (100%)	398 (86%)	63 (14%)	2 (0%)	30 65
1	n	463/465 (100%)	401 (87%)	61 (13%)	1 (0%)	44 75
1	o	463/465 (100%)	408 (88%)	54 (12%)	1 (0%)	44 75
1	p	463/465 (100%)	404 (87%)	56 (12%)	3 (1%)	22 57
1	q	463/465 (100%)	411 (89%)	51 (11%)	1 (0%)	44 75
1	r	463/465 (100%)	397 (86%)	61 (13%)	5 (1%)	12 45
1	s	463/465 (100%)	405 (88%)	54 (12%)	4 (1%)	14 48
1	t	463/465 (100%)	405 (88%)	55 (12%)	3 (1%)	22 57
1	u	463/465 (100%)	391 (84%)	72 (16%)	0	100 100
1	v	463/465 (100%)	421 (91%)	40 (9%)	2 (0%)	30 65
1	w	463/465 (100%)	420 (91%)	43 (9%)	0	100 100
1	x	463/465 (100%)	415 (90%)	47 (10%)	1 (0%)	44 75
1	y	463/465 (100%)	412 (89%)	48 (10%)	3 (1%)	22 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	z	463/465 (100%)	410 (89%)	51 (11%)	2 (0%)	30 65
2	A	413/415 (100%)	364 (88%)	42 (10%)	7 (2%)	7 36
2	B	413/415 (100%)	361 (87%)	46 (11%)	6 (2%)	8 39
2	C	413/415 (100%)	362 (88%)	45 (11%)	6 (2%)	8 39
2	D	413/415 (100%)	362 (88%)	44 (11%)	7 (2%)	7 36
2	a	413/415 (100%)	365 (88%)	41 (10%)	7 (2%)	7 36
All	All	45098/45320 (100%)	39720 (88%)	5152 (11%)	226 (0%)	27 60

5 of 226 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	88	VAL
1	2	108	ALA
1	2	201(I)	ASP
1	3	108	ALA
1	6	488	ALA

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	0	354/354 (100%)	330 (93%)	24 (7%)	13 38
1	1	354/354 (100%)	336 (95%)	18 (5%)	20 45
1	2	354/354 (100%)	332 (94%)	22 (6%)	15 40
1	3	354/354 (100%)	337 (95%)	17 (5%)	21 46
1	4	354/354 (100%)	326 (92%)	28 (8%)	10 33
1	5	354/354 (100%)	333 (94%)	21 (6%)	16 41
1	6	354/354 (100%)	343 (97%)	11 (3%)	35 56
1	7	354/354 (100%)	341 (96%)	13 (4%)	29 53
1	8	354/354 (100%)	320 (90%)	34 (10%)	7 25
1	9	354/354 (100%)	336 (95%)	18 (5%)	20 45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	354/354 (100%)	340 (96%)	14 (4%)	27	51
1	AB	354/354 (100%)	326 (92%)	28 (8%)	10	33
1	AC	354/354 (100%)	326 (92%)	28 (8%)	10	33
1	AD	336/354 (95%)	315 (94%)	21 (6%)	15	40
1	AE	354/354 (100%)	332 (94%)	22 (6%)	15	40
1	AF	354/354 (100%)	321 (91%)	33 (9%)	7	27
1	AG	354/354 (100%)	338 (96%)	16 (4%)	23	48
1	AH	354/354 (100%)	319 (90%)	35 (10%)	6	24
1	AI	354/354 (100%)	322 (91%)	32 (9%)	8	28
1	AJ	354/354 (100%)	330 (93%)	24 (7%)	13	38
1	AK	354/354 (100%)	336 (95%)	18 (5%)	20	45
1	AL	354/354 (100%)	328 (93%)	26 (7%)	11	35
1	AM	354/354 (100%)	332 (94%)	22 (6%)	15	40
1	AN	354/354 (100%)	342 (97%)	12 (3%)	32	55
1	AO	354/354 (100%)	339 (96%)	15 (4%)	25	49
1	AP	352/354 (99%)	336 (96%)	16 (4%)	23	48
1	AQ	354/354 (100%)	329 (93%)	25 (7%)	12	36
1	AR	354/354 (100%)	333 (94%)	21 (6%)	16	41
1	AS	354/354 (100%)	339 (96%)	15 (4%)	25	49
1	AT	354/354 (100%)	322 (91%)	32 (9%)	8	28
1	AU	354/354 (100%)	330 (93%)	24 (7%)	13	38
1	AV	354/354 (100%)	326 (92%)	28 (8%)	10	33
1	AW	354/354 (100%)	340 (96%)	14 (4%)	27	51
1	AX	354/354 (100%)	328 (93%)	26 (7%)	11	35
1	AY	354/354 (100%)	330 (93%)	24 (7%)	13	38
1	AZ	354/354 (100%)	344 (97%)	10 (3%)	38	59
1	Aa	354/354 (100%)	341 (96%)	13 (4%)	29	53
1	Ab	352/354 (99%)	331 (94%)	21 (6%)	16	41
1	Ac	354/354 (100%)	334 (94%)	20 (6%)	17	43
1	Ad	354/354 (100%)	337 (95%)	17 (5%)	21	46
1	Ae	354/354 (100%)	338 (96%)	16 (4%)	23	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Af	354/354 (100%)	317 (90%)	37 (10%)	5 22
1	Ag	354/354 (100%)	332 (94%)	22 (6%)	15 40
1	Ah	354/354 (100%)	328 (93%)	26 (7%)	11 35
1	Ai	354/354 (100%)	333 (94%)	21 (6%)	16 41
1	Aj	354/354 (100%)	332 (94%)	22 (6%)	15 40
1	Ak	354/354 (100%)	338 (96%)	16 (4%)	23 48
1	Al	354/354 (100%)	341 (96%)	13 (4%)	29 53
1	Am	354/354 (100%)	344 (97%)	10 (3%)	38 59
1	G	354/354 (100%)	329 (93%)	25 (7%)	12 36
1	H	354/354 (100%)	332 (94%)	22 (6%)	15 40
1	J	354/354 (100%)	335 (95%)	19 (5%)	18 44
1	K	352/354 (99%)	333 (95%)	19 (5%)	18 44
1	L	354/354 (100%)	340 (96%)	14 (4%)	27 51
1	M	354/354 (100%)	339 (96%)	15 (4%)	25 49
1	N	354/354 (100%)	341 (96%)	13 (4%)	29 53
1	O	354/354 (100%)	315 (89%)	39 (11%)	5 21
1	P	354/354 (100%)	328 (93%)	26 (7%)	11 35
1	Q	354/354 (100%)	332 (94%)	22 (6%)	15 40
1	R	354/354 (100%)	334 (94%)	20 (6%)	17 43
1	S	354/354 (100%)	326 (92%)	28 (8%)	10 33
1	T	354/354 (100%)	332 (94%)	22 (6%)	15 40
1	U	352/354 (99%)	334 (95%)	18 (5%)	20 45
1	V	354/354 (100%)	335 (95%)	19 (5%)	18 44
1	W	354/354 (100%)	337 (95%)	17 (5%)	21 46
1	X	354/354 (100%)	341 (96%)	13 (4%)	29 53
1	Y	354/354 (100%)	322 (91%)	32 (9%)	8 28
1	Z	354/354 (100%)	326 (92%)	28 (8%)	10 33
1	b	354/354 (100%)	333 (94%)	21 (6%)	16 41
1	c	354/354 (100%)	340 (96%)	14 (4%)	27 51
1	d	354/354 (100%)	339 (96%)	15 (4%)	25 49
1	e	354/354 (100%)	336 (95%)	18 (5%)	20 45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	f	354/354 (100%)	322 (91%)	32 (9%)	8 28
1	g	354/354 (100%)	344 (97%)	10 (3%)	38 59
1	h	354/354 (100%)	341 (96%)	13 (4%)	29 53
1	i	354/354 (100%)	343 (97%)	11 (3%)	35 56
1	j	354/354 (100%)	344 (97%)	10 (3%)	38 59
1	k	354/354 (100%)	331 (94%)	23 (6%)	14 39
1	l	354/354 (100%)	335 (95%)	19 (5%)	18 44
1	m	354/354 (100%)	335 (95%)	19 (5%)	18 44
1	n	354/354 (100%)	335 (95%)	19 (5%)	18 44
1	o	354/354 (100%)	331 (94%)	23 (6%)	14 39
1	p	354/354 (100%)	327 (92%)	27 (8%)	11 34
1	q	354/354 (100%)	331 (94%)	23 (6%)	14 39
1	r	354/354 (100%)	332 (94%)	22 (6%)	15 40
1	s	354/354 (100%)	341 (96%)	13 (4%)	29 53
1	t	354/354 (100%)	327 (92%)	27 (8%)	11 34
1	u	354/354 (100%)	337 (95%)	17 (5%)	21 46
1	v	352/354 (99%)	338 (96%)	14 (4%)	27 51
1	w	354/354 (100%)	338 (96%)	16 (4%)	23 48
1	x	354/354 (100%)	337 (95%)	17 (5%)	21 46
1	y	354/354 (100%)	334 (94%)	20 (6%)	17 43
1	z	354/354 (100%)	314 (89%)	40 (11%)	4 21
2	A	350/350 (100%)	320 (91%)	30 (9%)	8 31
2	B	350/350 (100%)	314 (90%)	36 (10%)	6 23
2	C	350/350 (100%)	310 (89%)	40 (11%)	4 20
2	D	350/350 (100%)	313 (89%)	37 (11%)	5 22
2	a	350/350 (100%)	315 (90%)	35 (10%)	6 24
All	All	34644/34672 (100%)	32531 (94%)	2113 (6%)	18 41

5 of 2113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	n	453	TYR
1	q	107	ILE

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Mol	Chain	Res	Type
1	n	377	ILE
1	z	170	THR
1	AX	377	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 141 such sidechains are listed below:

Mol	Chain	Res	Type
1	e	171	GLN
1	f	195	GLN
1	o	236	GLN
1	AN	276	GLN
1	AN	265	GLN

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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

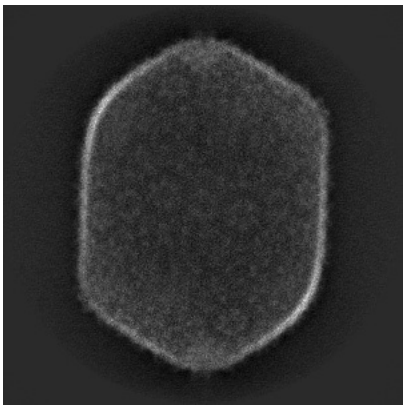
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40228. These allow visual inspection of the internal detail of the map and identification of artifacts.

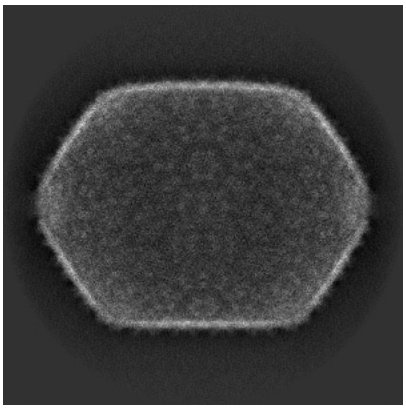
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

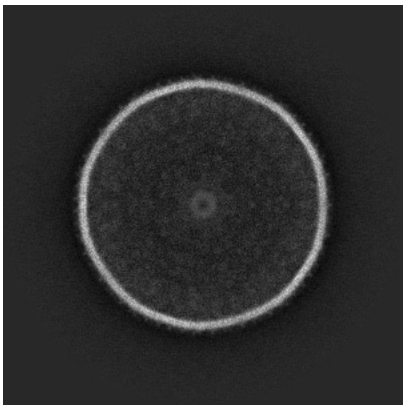
6.1.1 Primary map



X

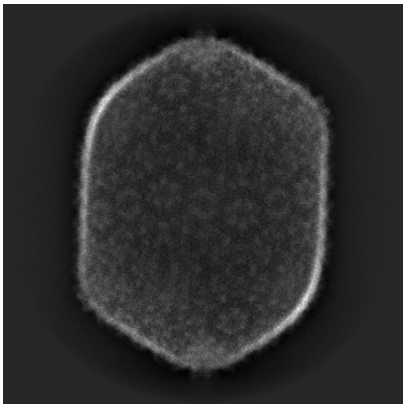


Y

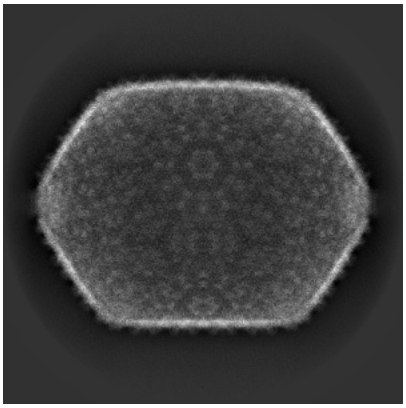


Z

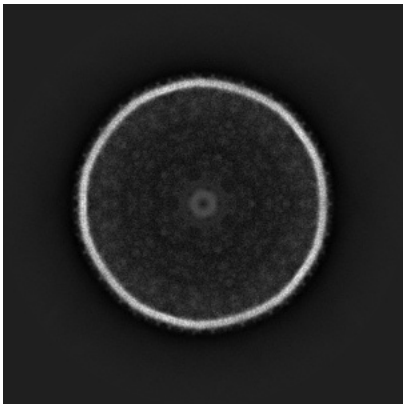
6.1.2 Raw map



X



Y

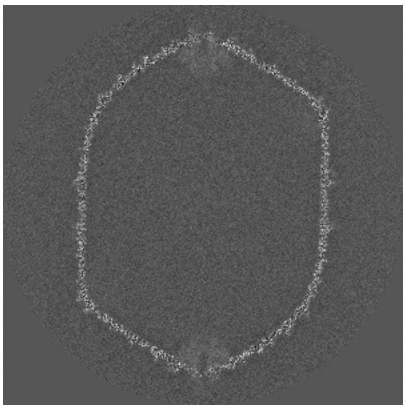


Z

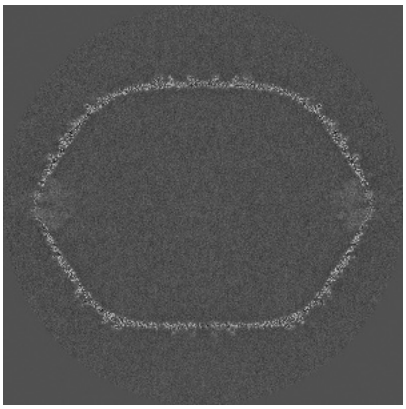
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

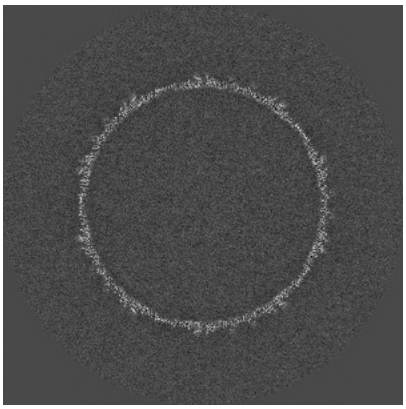
6.2.1 Primary map



X Index: 360

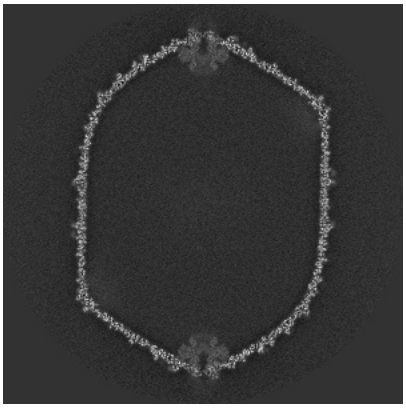


Y Index: 360

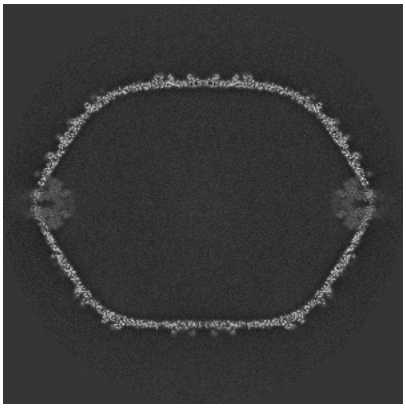


Z Index: 360

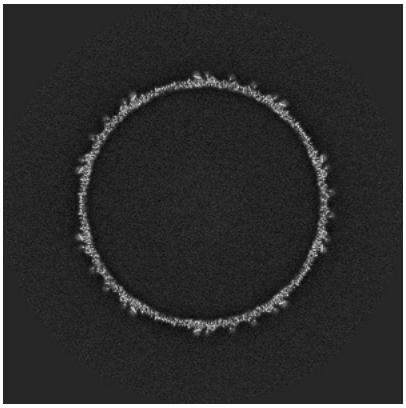
6.2.2 Raw map



X Index: 360



Y Index: 360

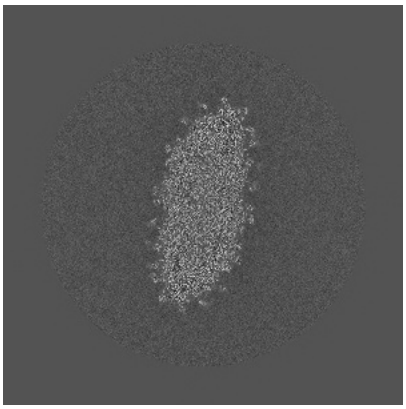


Z Index: 360

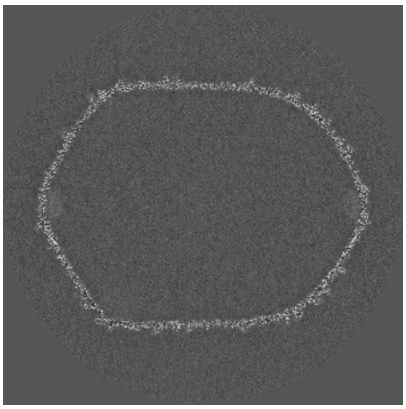
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

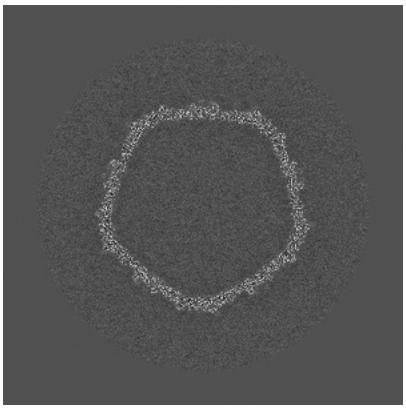
6.3.1 Primary map



X Index: 147

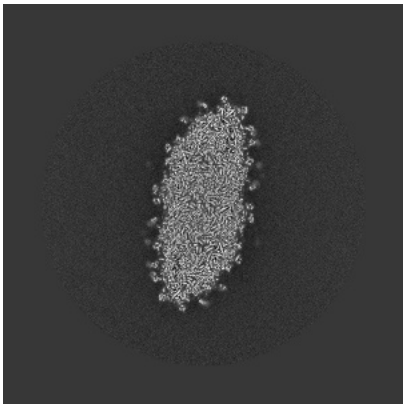


Y Index: 323

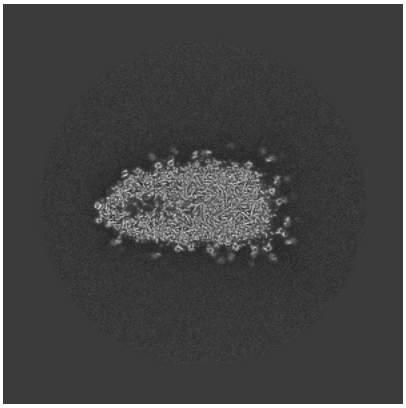


Z Index: 157

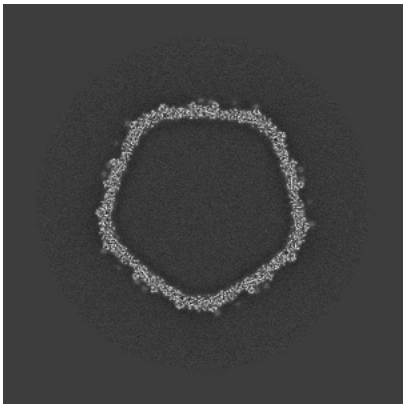
6.3.2 Raw map



X Index: 147



Y Index: 147

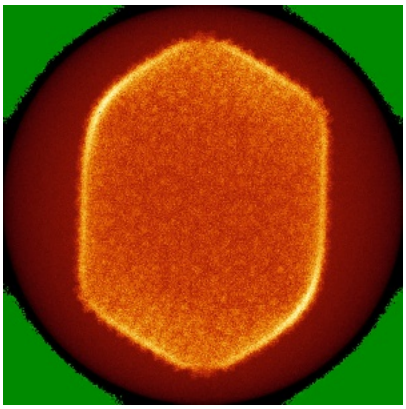


Z Index: 157

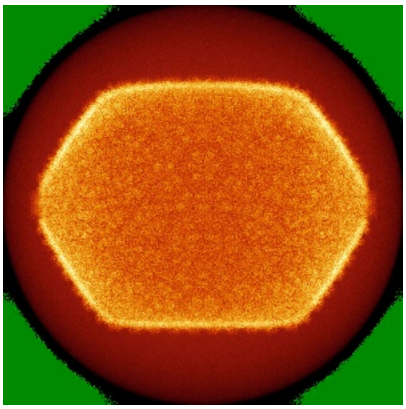
The images above show the largest variance slices of the map in three orthogonal directions.

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

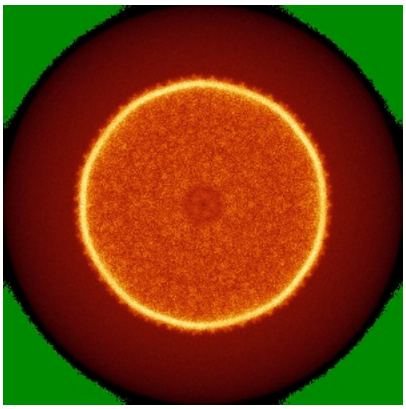
6.4.1 Primary map



X

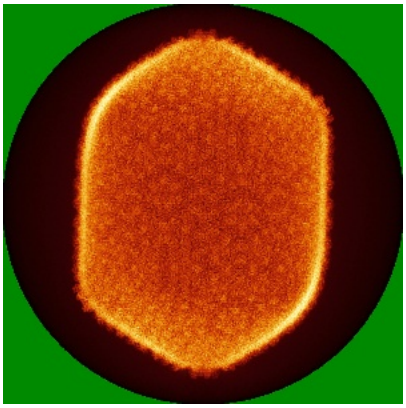


Y

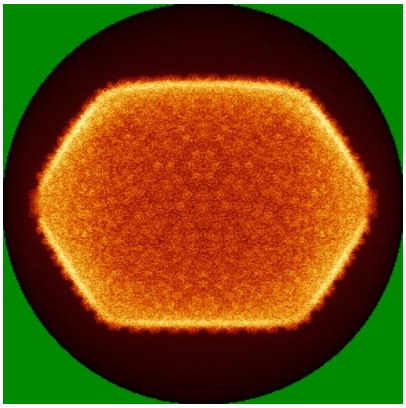


Z

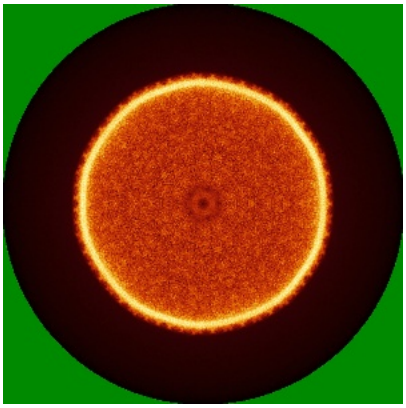
6.4.2 Raw map



X



Y

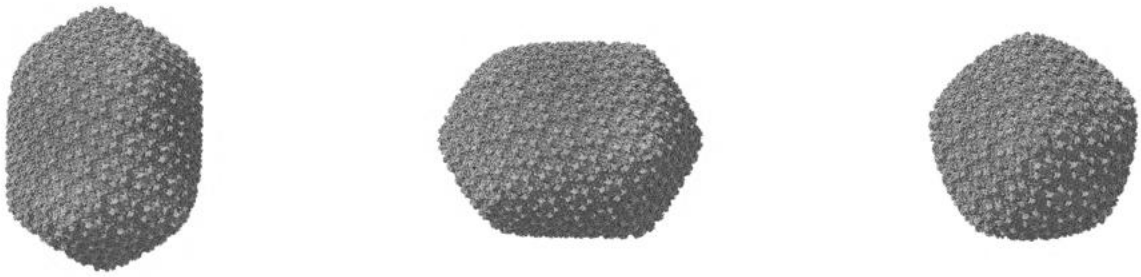


Z

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

6.5 Orthogonal surface views (i)

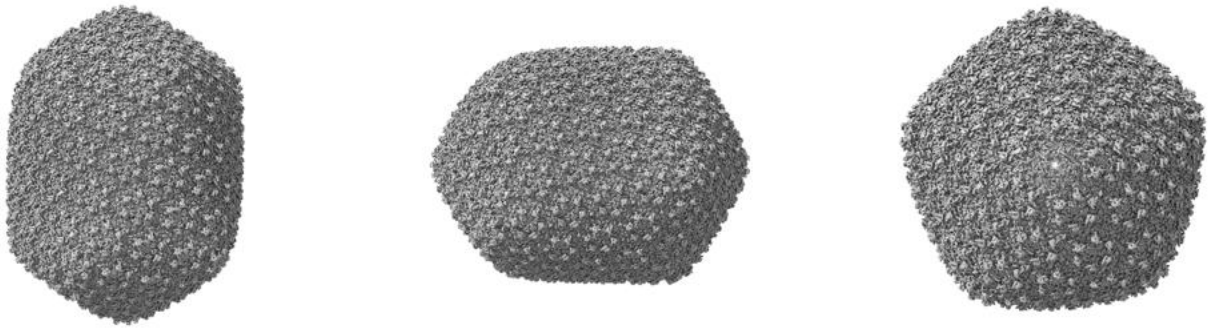
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

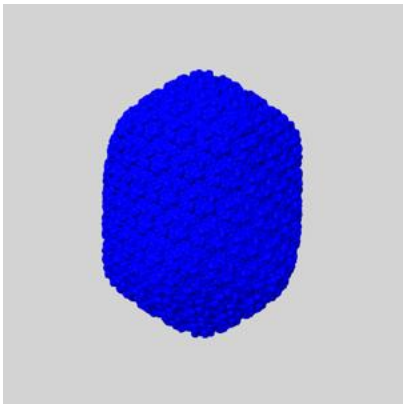
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

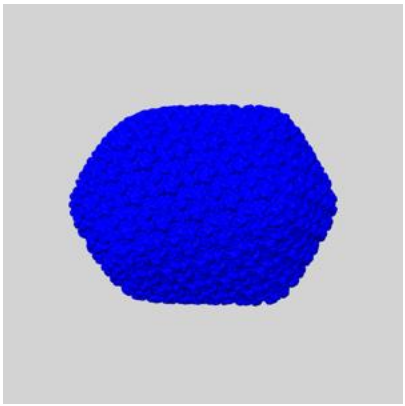
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

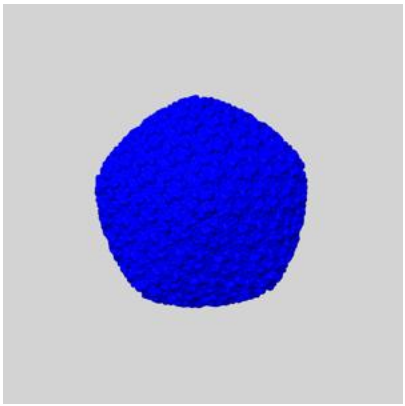
6.6.1 emd_40228_msk_1.map (i)



X



Y

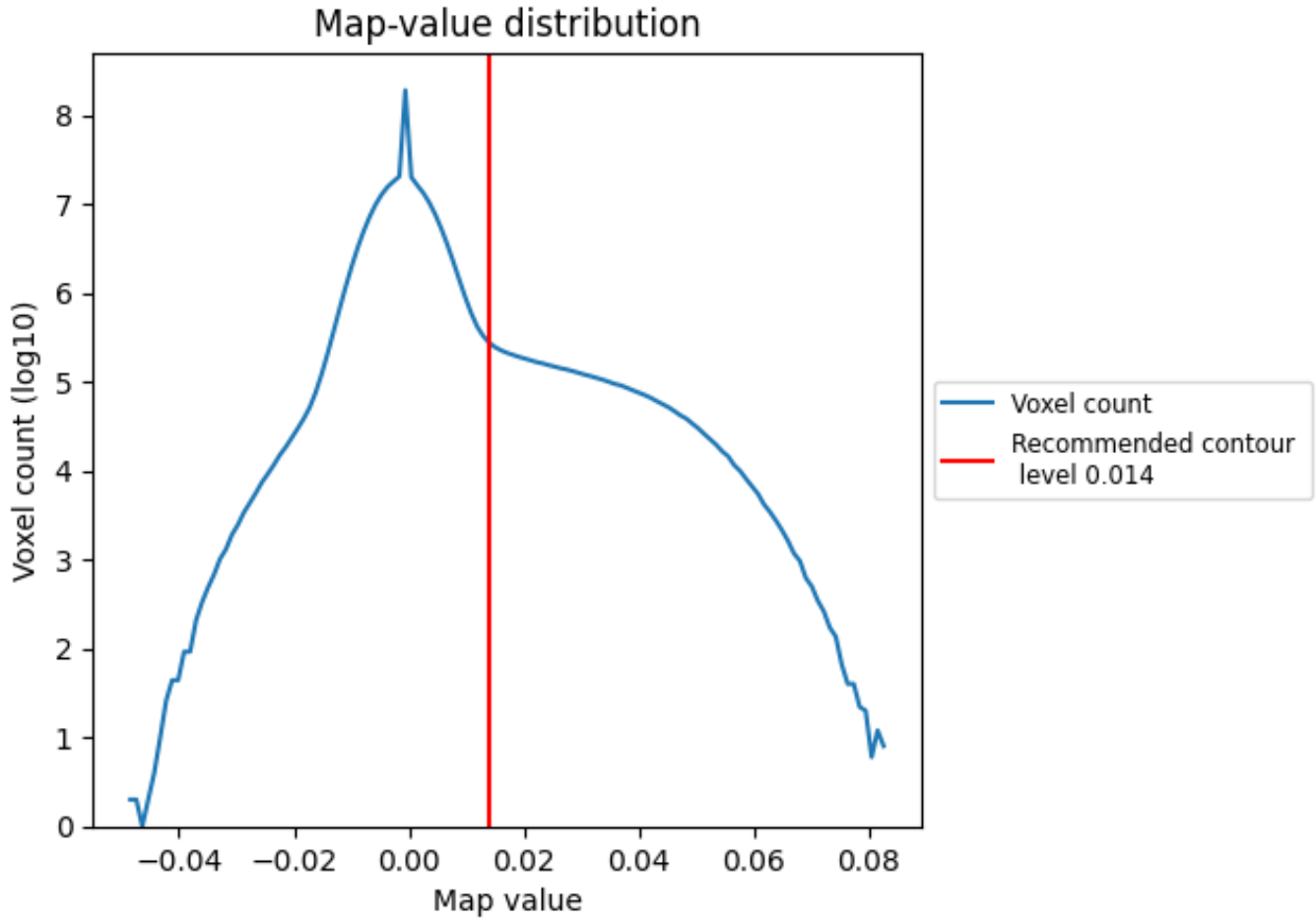


Z

7 Map analysis

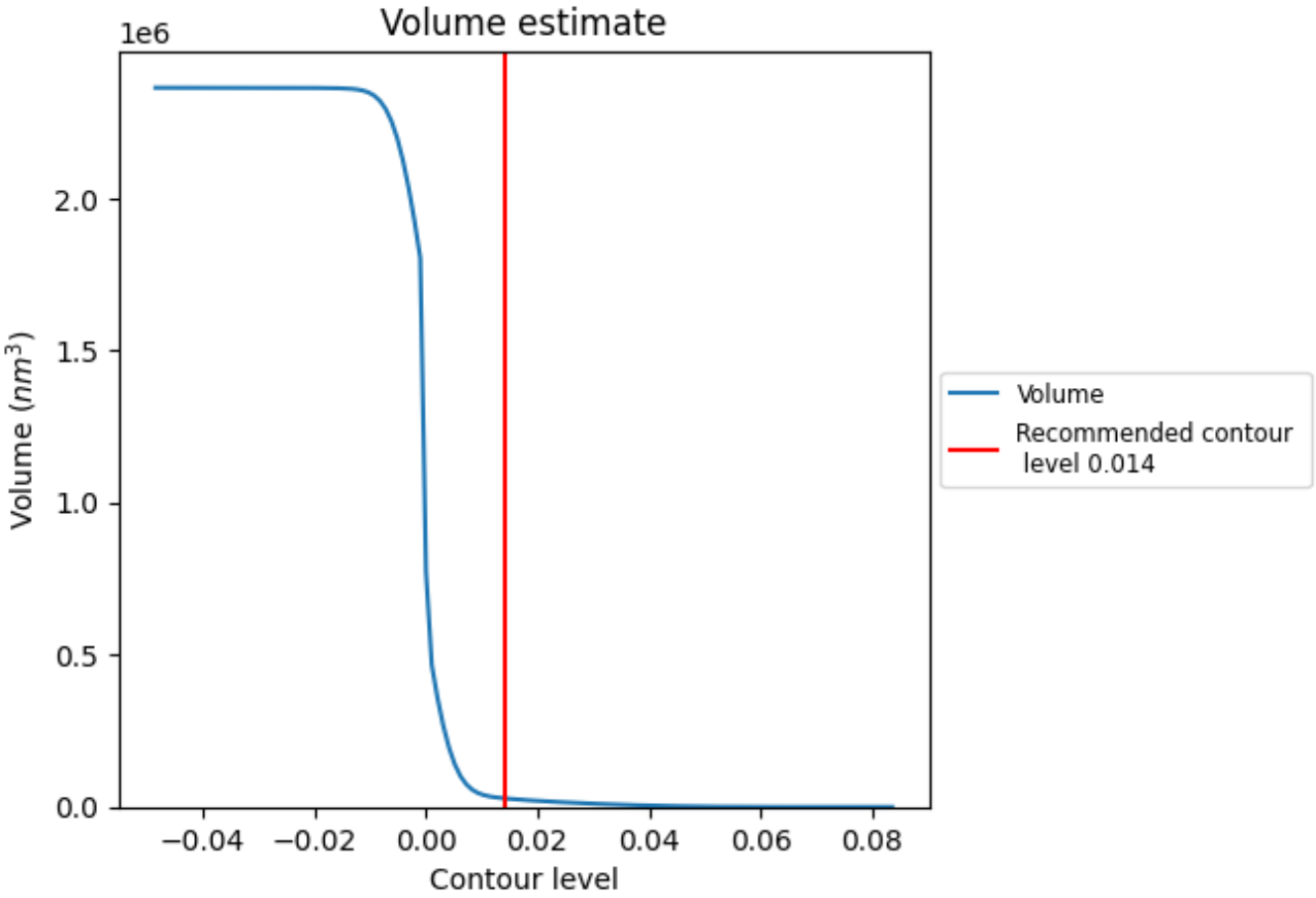
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

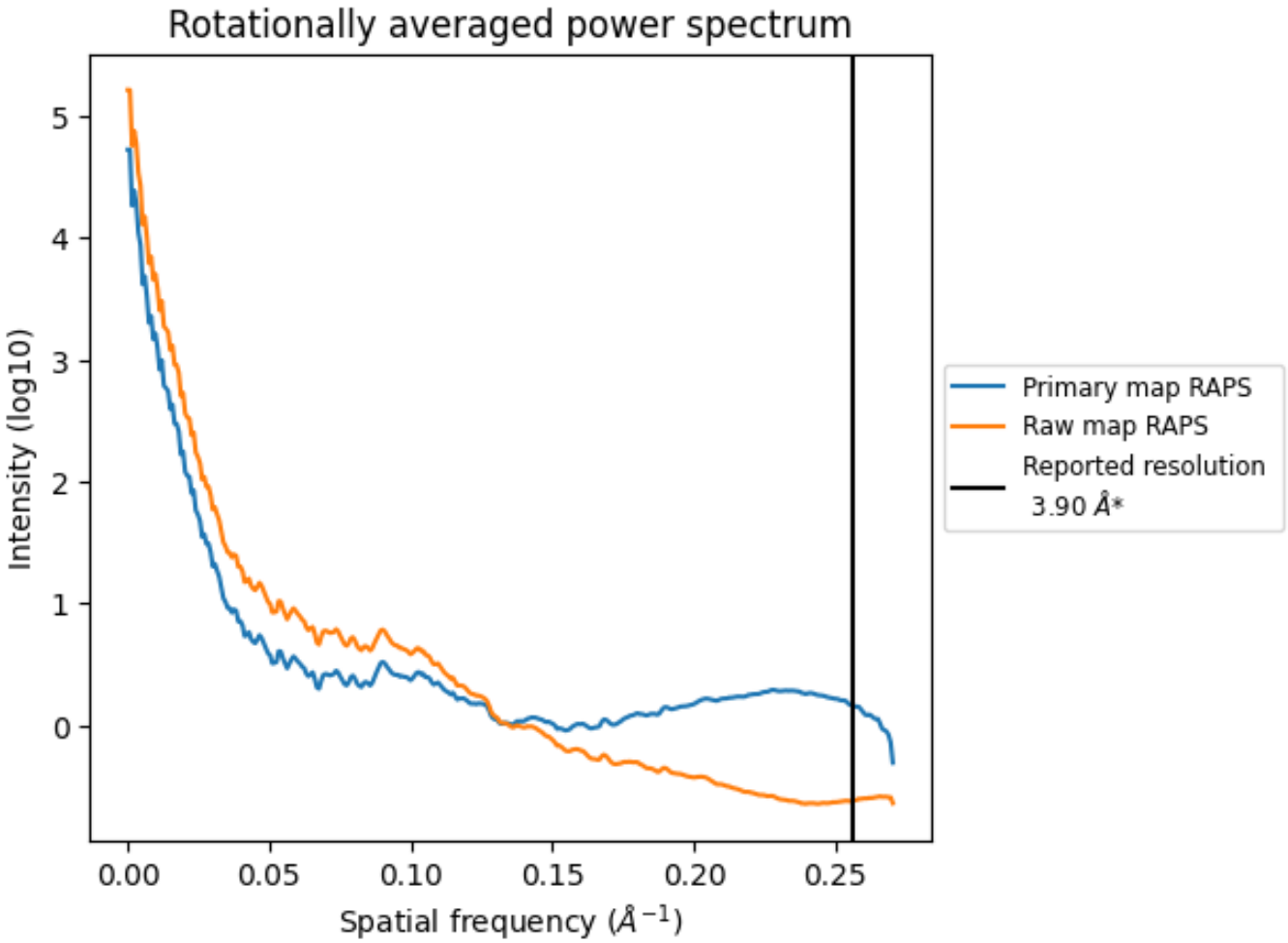
7.2 Volume estimate (i)



The volume at the recommended contour level is 28460 nm^3; this corresponds to an approximate mass of 25708 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)

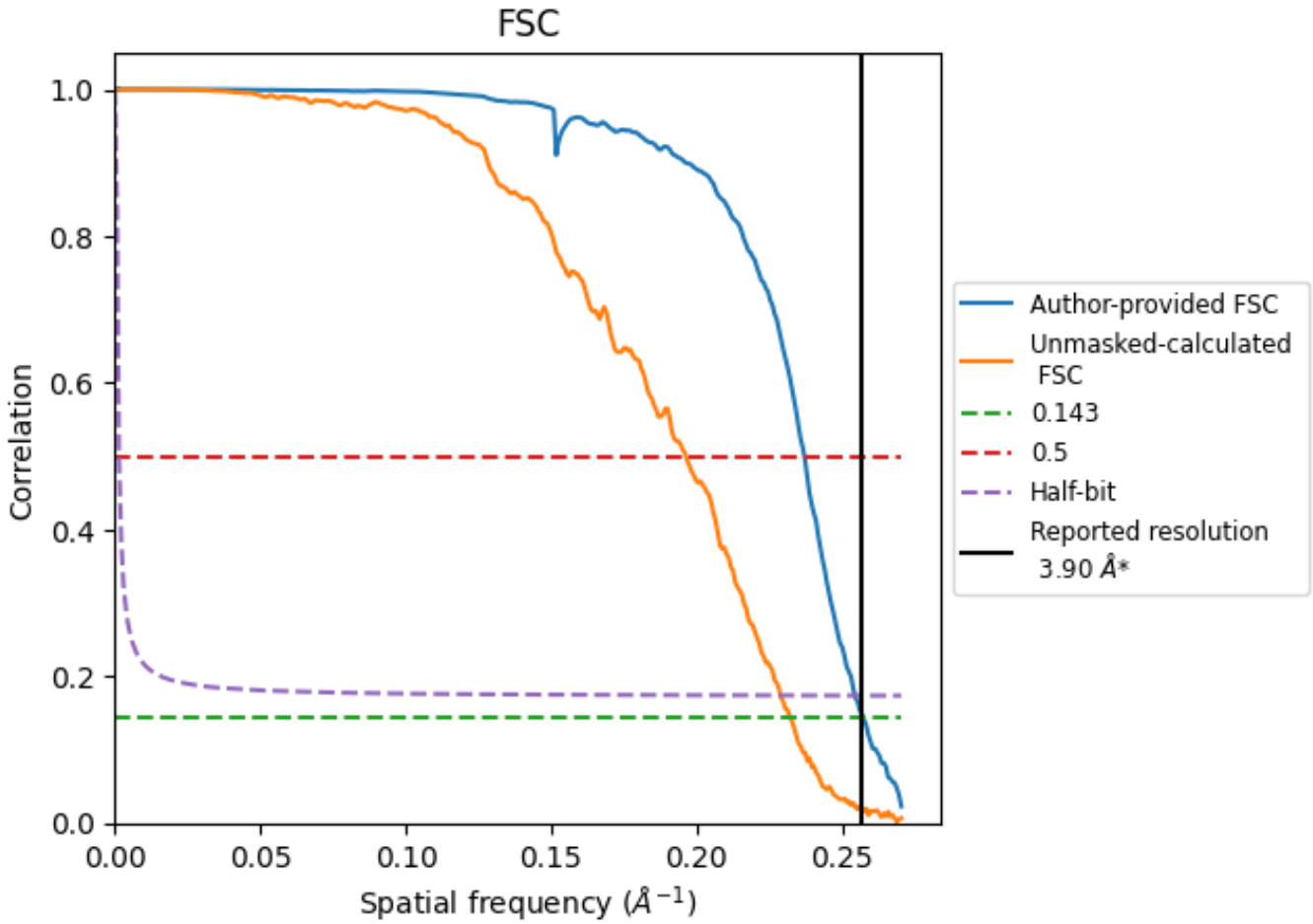


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.89	4.22	3.93
Unmasked-calculated*	4.31	5.09	4.37

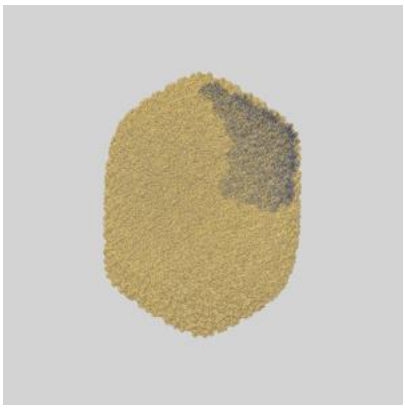
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.31 differs from the reported value 3.9 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40228 and PDB model 8GMO. Per-residue inclusion information can be found in section 3 on page 32.

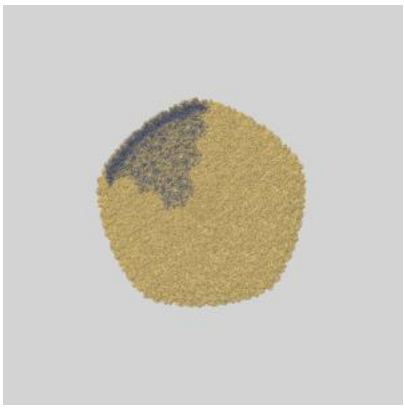
9.1 Map-model overlays

9.1.1 Map-model overlay



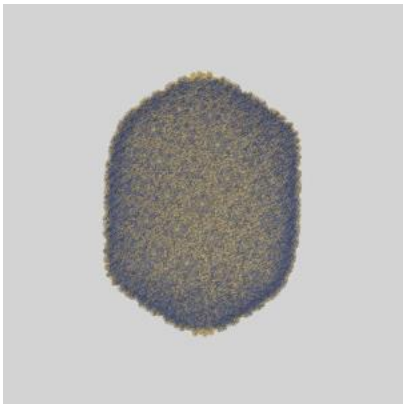
X

Y

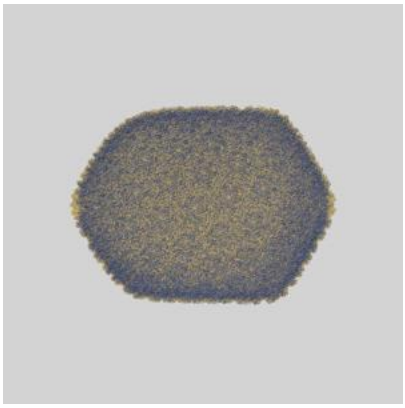


Z

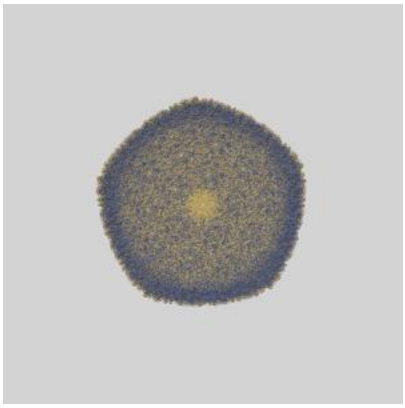
9.1.2 Map-model assembly overlay



X



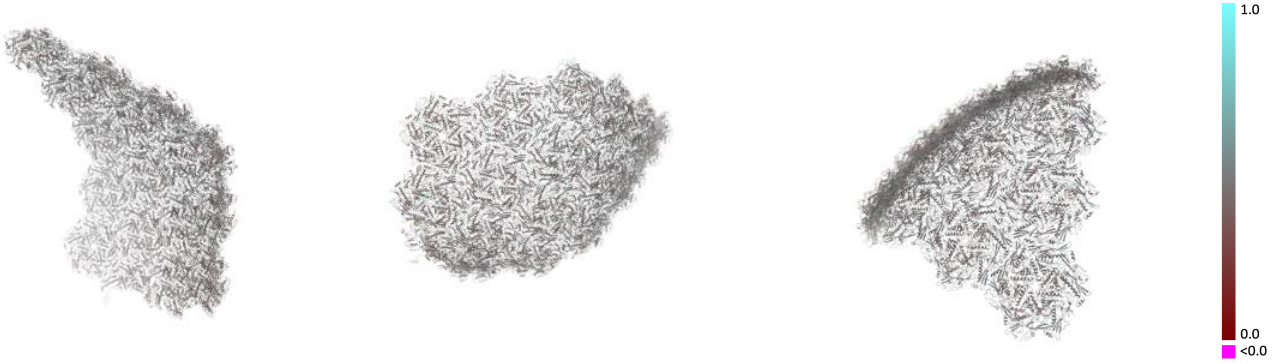
Y



Z

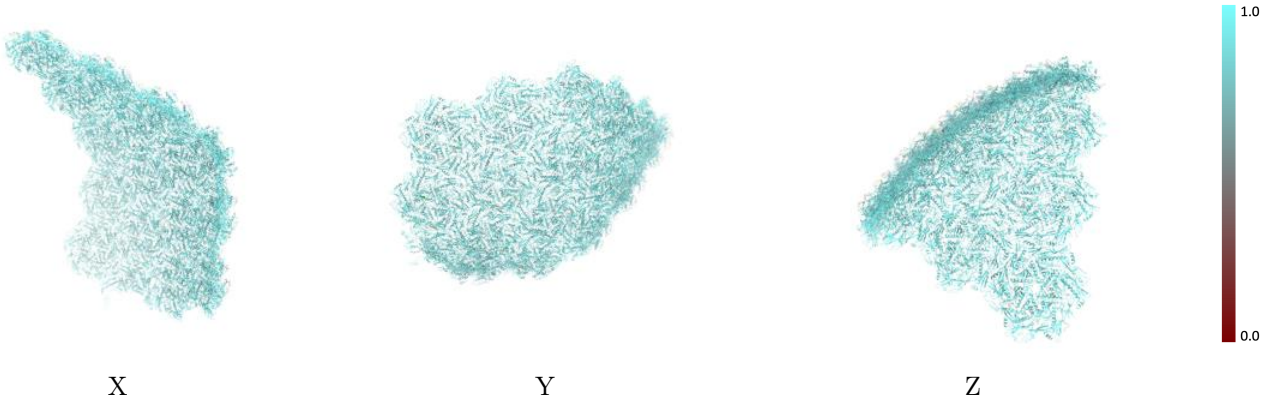
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



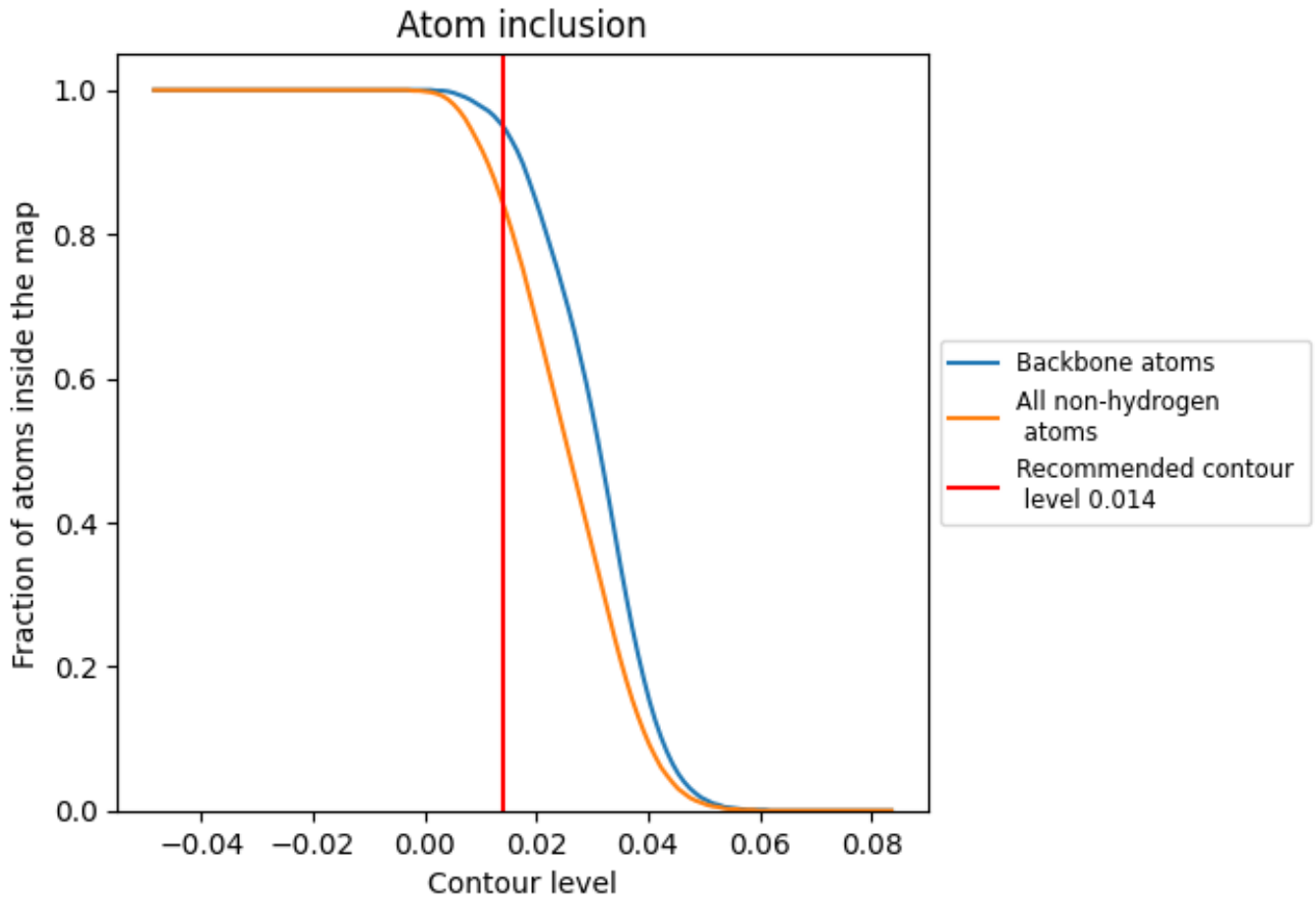
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 84% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8430	0.4520
0	0.8340	0.4450
1	0.8150	0.4420
2	0.8060	0.4330
3	0.8040	0.4330
4	0.8170	0.4380
5	0.8180	0.4310
6	0.8380	0.4530
7	0.8260	0.4400
8	0.8270	0.4430
9	0.8260	0.4420
A	0.8280	0.4520
AA	0.8370	0.4430
AB	0.8290	0.4390
AC	0.8290	0.4440
AD	0.8600	0.4630
AE	0.8600	0.4600
AF	0.8730	0.4640
AG	0.8650	0.4570
AH	0.8670	0.4680
AI	0.8710	0.4690
AJ	0.8540	0.4570
AK	0.8660	0.4670
AL	0.8680	0.4690
AM	0.8610	0.4560
AN	0.8510	0.4520
AO	0.8650	0.4650
AP	0.8610	0.4620
AQ	0.8550	0.4620
AR	0.8610	0.4660
AS	0.8630	0.4610
AT	0.8640	0.4560
AU	0.8600	0.4600
AV	0.8670	0.4600
AW	0.8670	0.4620

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Chain	Atom inclusion	Q-score
AX	0.8670	0.4600
AY	0.8590	0.4570
AZ	0.8630	0.4620
Aa	0.8690	0.4600
Ab	0.8600	0.4650
Ac	0.8550	0.4650
Ad	0.8610	0.4620
Ae	0.8620	0.4640
Af	0.8620	0.4590
Ag	0.8580	0.4590
Ah	0.8590	0.4620
Ai	0.8640	0.4610
Aj	0.8620	0.4620
Ak	0.8550	0.4580
Al	0.8580	0.4610
Am	0.8560	0.4620
B	0.8320	0.4540
C	0.8350	0.4480
D	0.8390	0.4530
G	0.8190	0.4370
H	0.8230	0.4380
J	0.8200	0.4350
K	0.8520	0.4630
L	0.8500	0.4580
M	0.8440	0.4560
N	0.8480	0.4580
O	0.8370	0.4530
P	0.8390	0.4430
Q	0.8240	0.4430
R	0.8280	0.4430
S	0.8310	0.4410
T	0.8280	0.4350
U	0.8520	0.4610
V	0.8460	0.4560
W	0.8520	0.4610
X	0.8480	0.4570
Y	0.8410	0.4500
Z	0.8460	0.4570
a	0.8380	0.4530
b	0.8460	0.4600
c	0.8410	0.4490
d	0.8550	0.4600

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Chain	Atom inclusion	Q-score
e	0.8380	0.4550
f	0.8310	0.4450
g	0.8410	0.4530
h	0.8450	0.4530
i	0.8570	0.4600
j	0.8490	0.4610
k	0.8180	0.4470
l	0.8390	0.4520
m	0.8370	0.4500
n	0.8230	0.4420
o	0.8390	0.4500
p	0.8180	0.4290
q	0.8110	0.4340
r	0.8050	0.4350
s	0.8170	0.4340
t	0.8050	0.4300
u	0.8150	0.4310
v	0.8340	0.4470
w	0.8390	0.4560
x	0.8350	0.4450
y	0.8380	0.4490
z	0.8160	0.4340