Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 12:43 PM EST

PDB ID	:	6U3Q
EMDB ID	:	EMD-20630
Title	:	The atomic structure of a human adeno-associated virus capsid isolate (AAVhu69/AAVv66)
Authors	:	Hsu, H.-L.; Brown, A.; Loveland, A.; Tai, P.; Korostelev, A.; Gao, G.
Deposited on	:	2019-08-22
Resolution	:	2.46 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

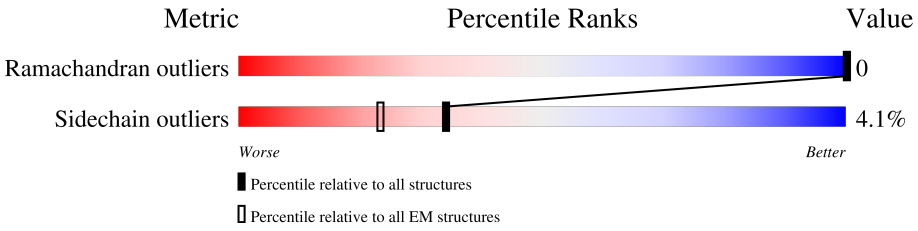
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.46 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	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	0	735	68% · 29%
1	1	735	68% · 29%
1	2	735	68% · 29%
1	3	735	68% · 29%
1	4	735	68% · 29%
1	5	735	68% · 29%
1	6	735	68% · 29%
1	7	735	68% · 29%
1	A	735	68% · 29%

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Mol	Chain	Length	Quality of chain
1	B	735	68% • 29%
1	C	735	68% • 29%
1	D	735	68% • 29%
1	E	735	68% • 29%
1	F	735	68% • 29%
1	G	735	68% • 29%
1	H	735	68% • 29%
1	I	735	68% • 29%
1	J	735	68% • 29%
1	K	735	68% • 29%
1	L	735	68% • 29%
1	M	735	68% • 29%
1	N	735	68% • 29%
1	O	735	68% • 29%
1	P	735	68% • 29%
1	Q	735	68% • 29%
1	R	735	68% • 29%
1	S	735	68% • 29%
1	T	735	68% • 29%
1	U	735	68% • 29%
1	V	735	68% • 29%
1	W	735	68% • 29%
1	X	735	68% • 29%
1	Y	735	68% • 29%
1	Z	735	68% • 29%

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Mol	Chain	Length	Quality of chain
1	a	735	68% • 29%
1	b	735	68% • 29%
1	c	735	68% • 29%
1	d	735	68% • 29%
1	e	735	68% • 29%
1	f	735	68% • 29%
1	g	735	68% • 29%
1	h	735	68% • 29%
1	i	735	68% • 29%
1	j	735	68% • 29%
1	k	735	68% • 29%
1	l	735	68% • 29%
1	m	735	68% • 29%
1	n	735	68% • 29%
1	o	735	68% • 29%
1	p	735	68% • 29%
1	q	735	68% • 29%
1	r	735	68% • 29%
1	s	735	68% • 29%
1	t	735	68% • 29%
1	u	735	68% • 29%
1	v	735	68% • 29%
1	w	735	68% • 29%
1	x	735	68% • 29%
1	y	735	68% • 29%

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Mol	Chain	Length	Quality of chain
1	z	735	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 248280 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	K	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	L	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	M	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	N	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	O	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	P	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	Q	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	R	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	S	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	T	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	B	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	U	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	V	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	W	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	X	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	Y	519	Total 4138	C 2605	N 716	O 803	S 14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Z	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	a	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	b	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	c	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	d	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	C	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	e	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	f	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	g	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	h	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	i	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	j	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	k	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	l	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	m	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	n	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	D	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	o	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	p	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	q	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		
1	r	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	s	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	t	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	u	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	v	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	w	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	x	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	E	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	y	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	z	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	0	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	1	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	2	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	3	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	4	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	5	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	6	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	7	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	F	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	G	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	H	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	I	519	Total 4138	C 2605	N 716	O 803	S 14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		

There are 360 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	GLN	LYS	conflict	UNP Q670R6
A	164	GLN	ASN	conflict	UNP Q670R6
A	312	ASN	SER	conflict	UNP Q670R6
A	447	LYS	ARG	conflict	UNP Q670R6
A	450	ALA	THR	conflict	UNP Q670R6
A	593	THR	SER	conflict	UNP Q670R6
K	39	GLN	LYS	conflict	UNP Q670R6
K	164	GLN	ASN	conflict	UNP Q670R6
K	312	ASN	SER	conflict	UNP Q670R6
K	447	LYS	ARG	conflict	UNP Q670R6
K	450	ALA	THR	conflict	UNP Q670R6
K	593	THR	SER	conflict	UNP Q670R6
L	39	GLN	LYS	conflict	UNP Q670R6
L	164	GLN	ASN	conflict	UNP Q670R6
L	312	ASN	SER	conflict	UNP Q670R6
L	447	LYS	ARG	conflict	UNP Q670R6
L	450	ALA	THR	conflict	UNP Q670R6
L	593	THR	SER	conflict	UNP Q670R6
M	39	GLN	LYS	conflict	UNP Q670R6
M	164	GLN	ASN	conflict	UNP Q670R6
M	312	ASN	SER	conflict	UNP Q670R6
M	447	LYS	ARG	conflict	UNP Q670R6
M	450	ALA	THR	conflict	UNP Q670R6
M	593	THR	SER	conflict	UNP Q670R6
N	39	GLN	LYS	conflict	UNP Q670R6
N	164	GLN	ASN	conflict	UNP Q670R6
N	312	ASN	SER	conflict	UNP Q670R6
N	447	LYS	ARG	conflict	UNP Q670R6
N	450	ALA	THR	conflict	UNP Q670R6
N	593	THR	SER	conflict	UNP Q670R6
O	39	GLN	LYS	conflict	UNP Q670R6
O	164	GLN	ASN	conflict	UNP Q670R6
O	312	ASN	SER	conflict	UNP Q670R6
O	447	LYS	ARG	conflict	UNP Q670R6
O	450	ALA	THR	conflict	UNP Q670R6
O	593	THR	SER	conflict	UNP Q670R6

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Chain	Residue	Modelled	Actual	Comment	Reference
P	39	GLN	LYS	conflict	UNP Q670R6
P	164	GLN	ASN	conflict	UNP Q670R6
P	312	ASN	SER	conflict	UNP Q670R6
P	447	LYS	ARG	conflict	UNP Q670R6
P	450	ALA	THR	conflict	UNP Q670R6
P	593	THR	SER	conflict	UNP Q670R6
Q	39	GLN	LYS	conflict	UNP Q670R6
Q	164	GLN	ASN	conflict	UNP Q670R6
Q	312	ASN	SER	conflict	UNP Q670R6
Q	447	LYS	ARG	conflict	UNP Q670R6
Q	450	ALA	THR	conflict	UNP Q670R6
Q	593	THR	SER	conflict	UNP Q670R6
R	39	GLN	LYS	conflict	UNP Q670R6
R	164	GLN	ASN	conflict	UNP Q670R6
R	312	ASN	SER	conflict	UNP Q670R6
R	447	LYS	ARG	conflict	UNP Q670R6
R	450	ALA	THR	conflict	UNP Q670R6
R	593	THR	SER	conflict	UNP Q670R6
S	39	GLN	LYS	conflict	UNP Q670R6
S	164	GLN	ASN	conflict	UNP Q670R6
S	312	ASN	SER	conflict	UNP Q670R6
S	447	LYS	ARG	conflict	UNP Q670R6
S	450	ALA	THR	conflict	UNP Q670R6
S	593	THR	SER	conflict	UNP Q670R6
T	39	GLN	LYS	conflict	UNP Q670R6
T	164	GLN	ASN	conflict	UNP Q670R6
T	312	ASN	SER	conflict	UNP Q670R6
T	447	LYS	ARG	conflict	UNP Q670R6
T	450	ALA	THR	conflict	UNP Q670R6
T	593	THR	SER	conflict	UNP Q670R6
B	39	GLN	LYS	conflict	UNP Q670R6
B	164	GLN	ASN	conflict	UNP Q670R6
B	312	ASN	SER	conflict	UNP Q670R6
B	447	LYS	ARG	conflict	UNP Q670R6
B	450	ALA	THR	conflict	UNP Q670R6
B	593	THR	SER	conflict	UNP Q670R6
U	39	GLN	LYS	conflict	UNP Q670R6
U	164	GLN	ASN	conflict	UNP Q670R6
U	312	ASN	SER	conflict	UNP Q670R6
U	447	LYS	ARG	conflict	UNP Q670R6
U	450	ALA	THR	conflict	UNP Q670R6
U	593	THR	SER	conflict	UNP Q670R6

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Chain	Residue	Modelled	Actual	Comment	Reference
V	39	GLN	LYS	conflict	UNP Q670R6
V	164	GLN	ASN	conflict	UNP Q670R6
V	312	ASN	SER	conflict	UNP Q670R6
V	447	LYS	ARG	conflict	UNP Q670R6
V	450	ALA	THR	conflict	UNP Q670R6
V	593	THR	SER	conflict	UNP Q670R6
W	39	GLN	LYS	conflict	UNP Q670R6
W	164	GLN	ASN	conflict	UNP Q670R6
W	312	ASN	SER	conflict	UNP Q670R6
W	447	LYS	ARG	conflict	UNP Q670R6
W	450	ALA	THR	conflict	UNP Q670R6
W	593	THR	SER	conflict	UNP Q670R6
X	39	GLN	LYS	conflict	UNP Q670R6
X	164	GLN	ASN	conflict	UNP Q670R6
X	312	ASN	SER	conflict	UNP Q670R6
X	447	LYS	ARG	conflict	UNP Q670R6
X	450	ALA	THR	conflict	UNP Q670R6
X	593	THR	SER	conflict	UNP Q670R6
Y	39	GLN	LYS	conflict	UNP Q670R6
Y	164	GLN	ASN	conflict	UNP Q670R6
Y	312	ASN	SER	conflict	UNP Q670R6
Y	447	LYS	ARG	conflict	UNP Q670R6
Y	450	ALA	THR	conflict	UNP Q670R6
Y	593	THR	SER	conflict	UNP Q670R6
Z	39	GLN	LYS	conflict	UNP Q670R6
Z	164	GLN	ASN	conflict	UNP Q670R6
Z	312	ASN	SER	conflict	UNP Q670R6
Z	447	LYS	ARG	conflict	UNP Q670R6
Z	450	ALA	THR	conflict	UNP Q670R6
Z	593	THR	SER	conflict	UNP Q670R6
a	39	GLN	LYS	conflict	UNP Q670R6
a	164	GLN	ASN	conflict	UNP Q670R6
a	312	ASN	SER	conflict	UNP Q670R6
a	447	LYS	ARG	conflict	UNP Q670R6
a	450	ALA	THR	conflict	UNP Q670R6
a	593	THR	SER	conflict	UNP Q670R6
b	39	GLN	LYS	conflict	UNP Q670R6
b	164	GLN	ASN	conflict	UNP Q670R6
b	312	ASN	SER	conflict	UNP Q670R6
b	447	LYS	ARG	conflict	UNP Q670R6
b	450	ALA	THR	conflict	UNP Q670R6
b	593	THR	SER	conflict	UNP Q670R6

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Chain	Residue	Modelled	Actual	Comment	Reference
c	39	GLN	LYS	conflict	UNP Q670R6
c	164	GLN	ASN	conflict	UNP Q670R6
c	312	ASN	SER	conflict	UNP Q670R6
c	447	LYS	ARG	conflict	UNP Q670R6
c	450	ALA	THR	conflict	UNP Q670R6
c	593	THR	SER	conflict	UNP Q670R6
d	39	GLN	LYS	conflict	UNP Q670R6
d	164	GLN	ASN	conflict	UNP Q670R6
d	312	ASN	SER	conflict	UNP Q670R6
d	447	LYS	ARG	conflict	UNP Q670R6
d	450	ALA	THR	conflict	UNP Q670R6
d	593	THR	SER	conflict	UNP Q670R6
C	39	GLN	LYS	conflict	UNP Q670R6
C	164	GLN	ASN	conflict	UNP Q670R6
C	312	ASN	SER	conflict	UNP Q670R6
C	447	LYS	ARG	conflict	UNP Q670R6
C	450	ALA	THR	conflict	UNP Q670R6
C	593	THR	SER	conflict	UNP Q670R6
e	39	GLN	LYS	conflict	UNP Q670R6
e	164	GLN	ASN	conflict	UNP Q670R6
e	312	ASN	SER	conflict	UNP Q670R6
e	447	LYS	ARG	conflict	UNP Q670R6
e	450	ALA	THR	conflict	UNP Q670R6
e	593	THR	SER	conflict	UNP Q670R6
f	39	GLN	LYS	conflict	UNP Q670R6
f	164	GLN	ASN	conflict	UNP Q670R6
f	312	ASN	SER	conflict	UNP Q670R6
f	447	LYS	ARG	conflict	UNP Q670R6
f	450	ALA	THR	conflict	UNP Q670R6
f	593	THR	SER	conflict	UNP Q670R6
g	39	GLN	LYS	conflict	UNP Q670R6
g	164	GLN	ASN	conflict	UNP Q670R6
g	312	ASN	SER	conflict	UNP Q670R6
g	447	LYS	ARG	conflict	UNP Q670R6
g	450	ALA	THR	conflict	UNP Q670R6
g	593	THR	SER	conflict	UNP Q670R6
h	39	GLN	LYS	conflict	UNP Q670R6
h	164	GLN	ASN	conflict	UNP Q670R6
h	312	ASN	SER	conflict	UNP Q670R6
h	447	LYS	ARG	conflict	UNP Q670R6
h	450	ALA	THR	conflict	UNP Q670R6
h	593	THR	SER	conflict	UNP Q670R6

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Chain	Residue	Modelled	Actual	Comment	Reference
i	39	GLN	LYS	conflict	UNP Q670R6
i	164	GLN	ASN	conflict	UNP Q670R6
i	312	ASN	SER	conflict	UNP Q670R6
i	447	LYS	ARG	conflict	UNP Q670R6
i	450	ALA	THR	conflict	UNP Q670R6
i	593	THR	SER	conflict	UNP Q670R6
j	39	GLN	LYS	conflict	UNP Q670R6
j	164	GLN	ASN	conflict	UNP Q670R6
j	312	ASN	SER	conflict	UNP Q670R6
j	447	LYS	ARG	conflict	UNP Q670R6
j	450	ALA	THR	conflict	UNP Q670R6
j	593	THR	SER	conflict	UNP Q670R6
k	39	GLN	LYS	conflict	UNP Q670R6
k	164	GLN	ASN	conflict	UNP Q670R6
k	312	ASN	SER	conflict	UNP Q670R6
k	447	LYS	ARG	conflict	UNP Q670R6
k	450	ALA	THR	conflict	UNP Q670R6
k	593	THR	SER	conflict	UNP Q670R6
l	39	GLN	LYS	conflict	UNP Q670R6
l	164	GLN	ASN	conflict	UNP Q670R6
l	312	ASN	SER	conflict	UNP Q670R6
l	447	LYS	ARG	conflict	UNP Q670R6
l	450	ALA	THR	conflict	UNP Q670R6
l	593	THR	SER	conflict	UNP Q670R6
m	39	GLN	LYS	conflict	UNP Q670R6
m	164	GLN	ASN	conflict	UNP Q670R6
m	312	ASN	SER	conflict	UNP Q670R6
m	447	LYS	ARG	conflict	UNP Q670R6
m	450	ALA	THR	conflict	UNP Q670R6
m	593	THR	SER	conflict	UNP Q670R6
n	39	GLN	LYS	conflict	UNP Q670R6
n	164	GLN	ASN	conflict	UNP Q670R6
n	312	ASN	SER	conflict	UNP Q670R6
n	447	LYS	ARG	conflict	UNP Q670R6
n	450	ALA	THR	conflict	UNP Q670R6
n	593	THR	SER	conflict	UNP Q670R6
D	39	GLN	LYS	conflict	UNP Q670R6
D	164	GLN	ASN	conflict	UNP Q670R6
D	312	ASN	SER	conflict	UNP Q670R6
D	447	LYS	ARG	conflict	UNP Q670R6
D	450	ALA	THR	conflict	UNP Q670R6
D	593	THR	SER	conflict	UNP Q670R6

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Chain	Residue	Modelled	Actual	Comment	Reference
o	39	GLN	LYS	conflict	UNP Q670R6
o	164	GLN	ASN	conflict	UNP Q670R6
o	312	ASN	SER	conflict	UNP Q670R6
o	447	LYS	ARG	conflict	UNP Q670R6
o	450	ALA	THR	conflict	UNP Q670R6
o	593	THR	SER	conflict	UNP Q670R6
p	39	GLN	LYS	conflict	UNP Q670R6
p	164	GLN	ASN	conflict	UNP Q670R6
p	312	ASN	SER	conflict	UNP Q670R6
p	447	LYS	ARG	conflict	UNP Q670R6
p	450	ALA	THR	conflict	UNP Q670R6
p	593	THR	SER	conflict	UNP Q670R6
q	39	GLN	LYS	conflict	UNP Q670R6
q	164	GLN	ASN	conflict	UNP Q670R6
q	312	ASN	SER	conflict	UNP Q670R6
q	447	LYS	ARG	conflict	UNP Q670R6
q	450	ALA	THR	conflict	UNP Q670R6
q	593	THR	SER	conflict	UNP Q670R6
r	39	GLN	LYS	conflict	UNP Q670R6
r	164	GLN	ASN	conflict	UNP Q670R6
r	312	ASN	SER	conflict	UNP Q670R6
r	447	LYS	ARG	conflict	UNP Q670R6
r	450	ALA	THR	conflict	UNP Q670R6
r	593	THR	SER	conflict	UNP Q670R6
s	39	GLN	LYS	conflict	UNP Q670R6
s	164	GLN	ASN	conflict	UNP Q670R6
s	312	ASN	SER	conflict	UNP Q670R6
s	447	LYS	ARG	conflict	UNP Q670R6
s	450	ALA	THR	conflict	UNP Q670R6
s	593	THR	SER	conflict	UNP Q670R6
t	39	GLN	LYS	conflict	UNP Q670R6
t	164	GLN	ASN	conflict	UNP Q670R6
t	312	ASN	SER	conflict	UNP Q670R6
t	447	LYS	ARG	conflict	UNP Q670R6
t	450	ALA	THR	conflict	UNP Q670R6
t	593	THR	SER	conflict	UNP Q670R6
u	39	GLN	LYS	conflict	UNP Q670R6
u	164	GLN	ASN	conflict	UNP Q670R6
u	312	ASN	SER	conflict	UNP Q670R6
u	447	LYS	ARG	conflict	UNP Q670R6
u	450	ALA	THR	conflict	UNP Q670R6
u	593	THR	SER	conflict	UNP Q670R6

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Chain	Residue	Modelled	Actual	Comment	Reference
v	39	GLN	LYS	conflict	UNP Q670R6
v	164	GLN	ASN	conflict	UNP Q670R6
v	312	ASN	SER	conflict	UNP Q670R6
v	447	LYS	ARG	conflict	UNP Q670R6
v	450	ALA	THR	conflict	UNP Q670R6
v	593	THR	SER	conflict	UNP Q670R6
w	39	GLN	LYS	conflict	UNP Q670R6
w	164	GLN	ASN	conflict	UNP Q670R6
w	312	ASN	SER	conflict	UNP Q670R6
w	447	LYS	ARG	conflict	UNP Q670R6
w	450	ALA	THR	conflict	UNP Q670R6
w	593	THR	SER	conflict	UNP Q670R6
x	39	GLN	LYS	conflict	UNP Q670R6
x	164	GLN	ASN	conflict	UNP Q670R6
x	312	ASN	SER	conflict	UNP Q670R6
x	447	LYS	ARG	conflict	UNP Q670R6
x	450	ALA	THR	conflict	UNP Q670R6
x	593	THR	SER	conflict	UNP Q670R6
E	39	GLN	LYS	conflict	UNP Q670R6
E	164	GLN	ASN	conflict	UNP Q670R6
E	312	ASN	SER	conflict	UNP Q670R6
E	447	LYS	ARG	conflict	UNP Q670R6
E	450	ALA	THR	conflict	UNP Q670R6
E	593	THR	SER	conflict	UNP Q670R6
y	39	GLN	LYS	conflict	UNP Q670R6
y	164	GLN	ASN	conflict	UNP Q670R6
y	312	ASN	SER	conflict	UNP Q670R6
y	447	LYS	ARG	conflict	UNP Q670R6
y	450	ALA	THR	conflict	UNP Q670R6
y	593	THR	SER	conflict	UNP Q670R6
z	39	GLN	LYS	conflict	UNP Q670R6
z	164	GLN	ASN	conflict	UNP Q670R6
z	312	ASN	SER	conflict	UNP Q670R6
z	447	LYS	ARG	conflict	UNP Q670R6
z	450	ALA	THR	conflict	UNP Q670R6
z	593	THR	SER	conflict	UNP Q670R6
0	39	GLN	LYS	conflict	UNP Q670R6
0	164	GLN	ASN	conflict	UNP Q670R6
0	312	ASN	SER	conflict	UNP Q670R6
0	447	LYS	ARG	conflict	UNP Q670R6
0	450	ALA	THR	conflict	UNP Q670R6
0	593	THR	SER	conflict	UNP Q670R6

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Chain	Residue	Modelled	Actual	Comment	Reference
1	39	GLN	LYS	conflict	UNP Q670R6
1	164	GLN	ASN	conflict	UNP Q670R6
1	312	ASN	SER	conflict	UNP Q670R6
1	447	LYS	ARG	conflict	UNP Q670R6
1	450	ALA	THR	conflict	UNP Q670R6
1	593	THR	SER	conflict	UNP Q670R6
2	39	GLN	LYS	conflict	UNP Q670R6
2	164	GLN	ASN	conflict	UNP Q670R6
2	312	ASN	SER	conflict	UNP Q670R6
2	447	LYS	ARG	conflict	UNP Q670R6
2	450	ALA	THR	conflict	UNP Q670R6
2	593	THR	SER	conflict	UNP Q670R6
3	39	GLN	LYS	conflict	UNP Q670R6
3	164	GLN	ASN	conflict	UNP Q670R6
3	312	ASN	SER	conflict	UNP Q670R6
3	447	LYS	ARG	conflict	UNP Q670R6
3	450	ALA	THR	conflict	UNP Q670R6
3	593	THR	SER	conflict	UNP Q670R6
4	39	GLN	LYS	conflict	UNP Q670R6
4	164	GLN	ASN	conflict	UNP Q670R6
4	312	ASN	SER	conflict	UNP Q670R6
4	447	LYS	ARG	conflict	UNP Q670R6
4	450	ALA	THR	conflict	UNP Q670R6
4	593	THR	SER	conflict	UNP Q670R6
5	39	GLN	LYS	conflict	UNP Q670R6
5	164	GLN	ASN	conflict	UNP Q670R6
5	312	ASN	SER	conflict	UNP Q670R6
5	447	LYS	ARG	conflict	UNP Q670R6
5	450	ALA	THR	conflict	UNP Q670R6
5	593	THR	SER	conflict	UNP Q670R6
6	39	GLN	LYS	conflict	UNP Q670R6
6	164	GLN	ASN	conflict	UNP Q670R6
6	312	ASN	SER	conflict	UNP Q670R6
6	447	LYS	ARG	conflict	UNP Q670R6
6	450	ALA	THR	conflict	UNP Q670R6
6	593	THR	SER	conflict	UNP Q670R6
7	39	GLN	LYS	conflict	UNP Q670R6
7	164	GLN	ASN	conflict	UNP Q670R6
7	312	ASN	SER	conflict	UNP Q670R6
7	447	LYS	ARG	conflict	UNP Q670R6
7	450	ALA	THR	conflict	UNP Q670R6
7	593	THR	SER	conflict	UNP Q670R6

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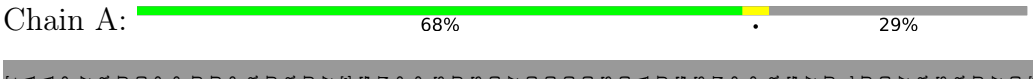
Chain	Residue	Modelled	Actual	Comment	Reference
F	39	GLN	LYS	conflict	UNP Q670R6
F	164	GLN	ASN	conflict	UNP Q670R6
F	312	ASN	SER	conflict	UNP Q670R6
F	447	LYS	ARG	conflict	UNP Q670R6
F	450	ALA	THR	conflict	UNP Q670R6
F	593	THR	SER	conflict	UNP Q670R6
G	39	GLN	LYS	conflict	UNP Q670R6
G	164	GLN	ASN	conflict	UNP Q670R6
G	312	ASN	SER	conflict	UNP Q670R6
G	447	LYS	ARG	conflict	UNP Q670R6
G	450	ALA	THR	conflict	UNP Q670R6
G	593	THR	SER	conflict	UNP Q670R6
H	39	GLN	LYS	conflict	UNP Q670R6
H	164	GLN	ASN	conflict	UNP Q670R6
H	312	ASN	SER	conflict	UNP Q670R6
H	447	LYS	ARG	conflict	UNP Q670R6
H	450	ALA	THR	conflict	UNP Q670R6
H	593	THR	SER	conflict	UNP Q670R6
I	39	GLN	LYS	conflict	UNP Q670R6
I	164	GLN	ASN	conflict	UNP Q670R6
I	312	ASN	SER	conflict	UNP Q670R6
I	447	LYS	ARG	conflict	UNP Q670R6
I	450	ALA	THR	conflict	UNP Q670R6
I	593	THR	SER	conflict	UNP Q670R6
J	39	GLN	LYS	conflict	UNP Q670R6
J	164	GLN	ASN	conflict	UNP Q670R6
J	312	ASN	SER	conflict	UNP Q670R6
J	447	LYS	ARG	conflict	UNP Q670R6
J	450	ALA	THR	conflict	UNP Q670R6
J	593	THR	SER	conflict	UNP Q670R6

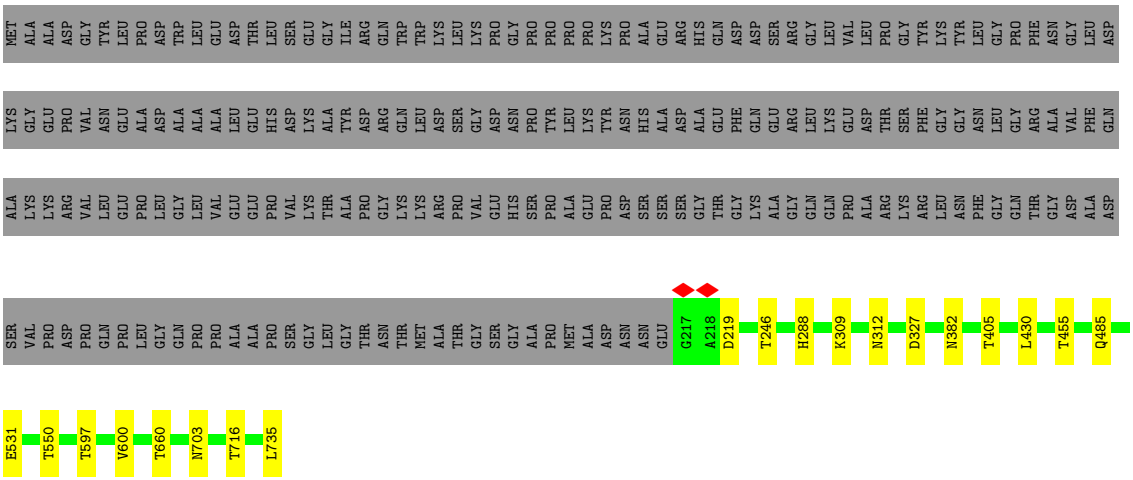
3 Residue-property plots (i)

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

- Molecule 1: Capsid protein VP1

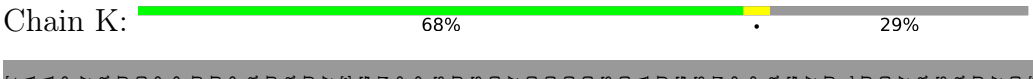
Chain A:

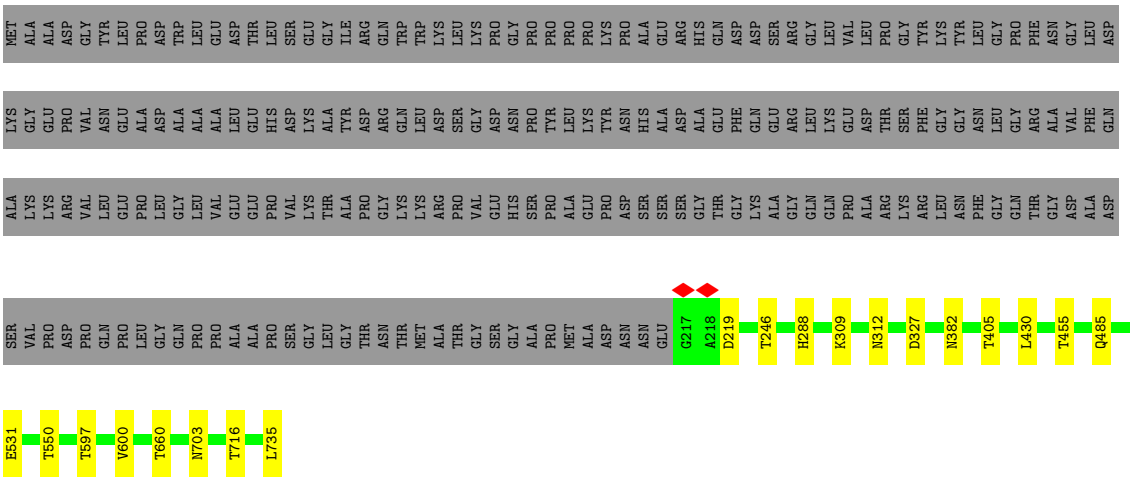




- Molecule 1: Capsid protein VP1

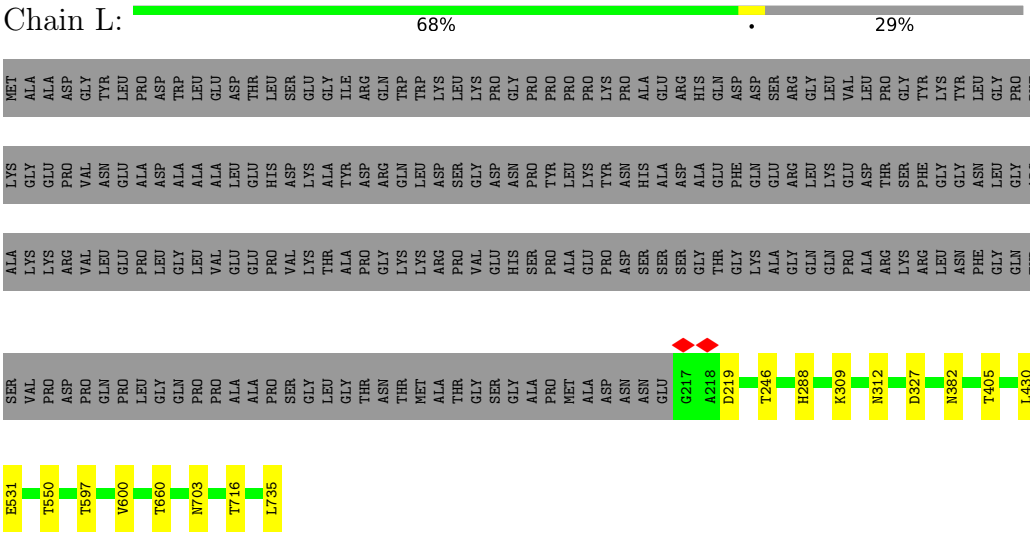
Chain K:





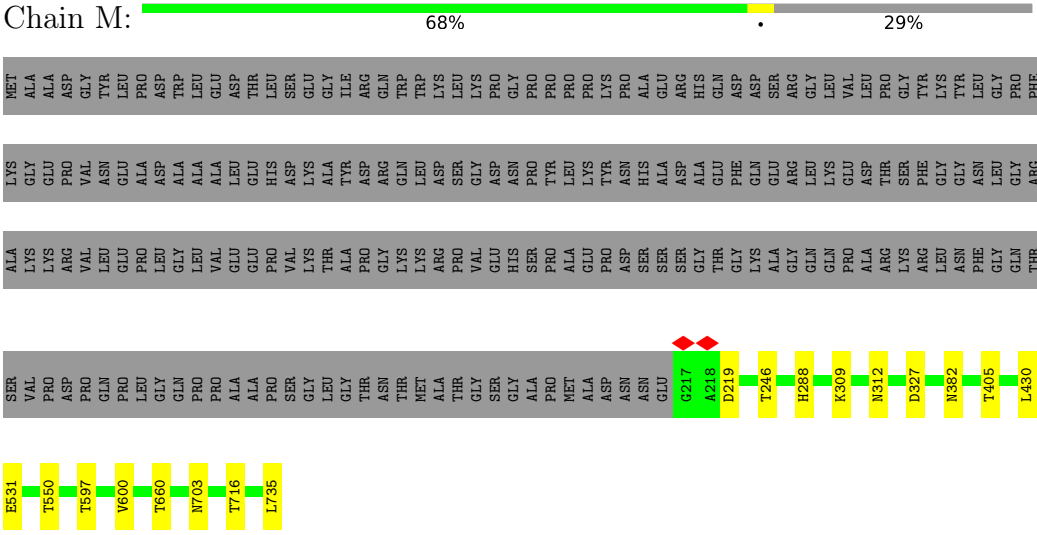
- Molecule 1: Capsid protein VP1

Chain L:



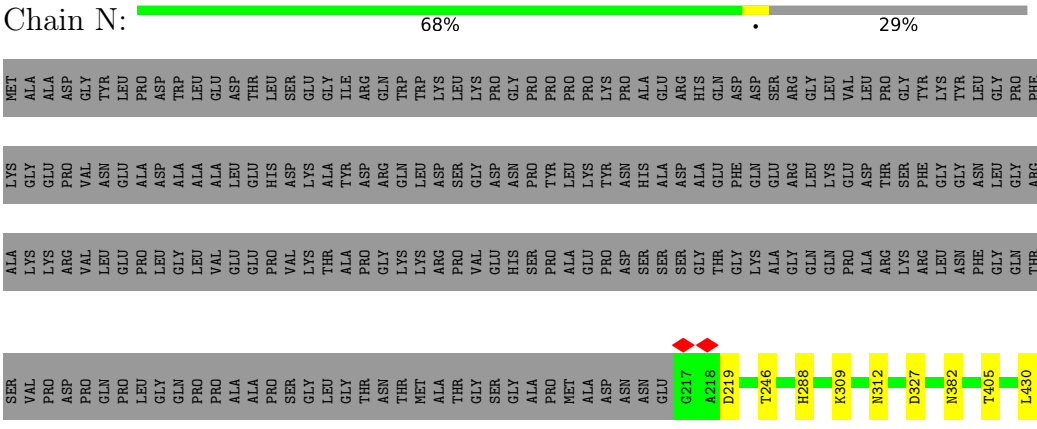
• Molecule 1: Capsid protein VP1

Chain M:



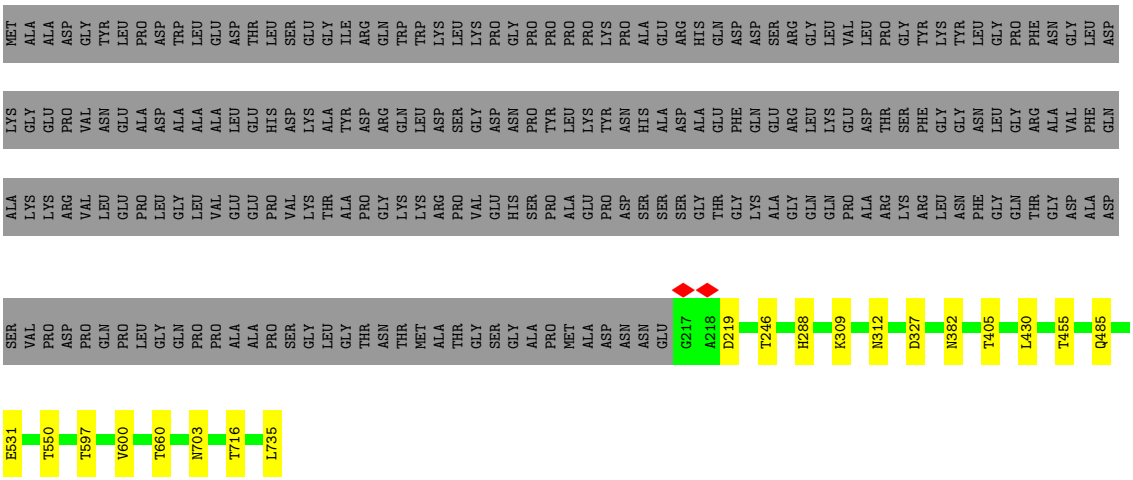
• Molecule 1: Capsid protein VP1

Chain N:



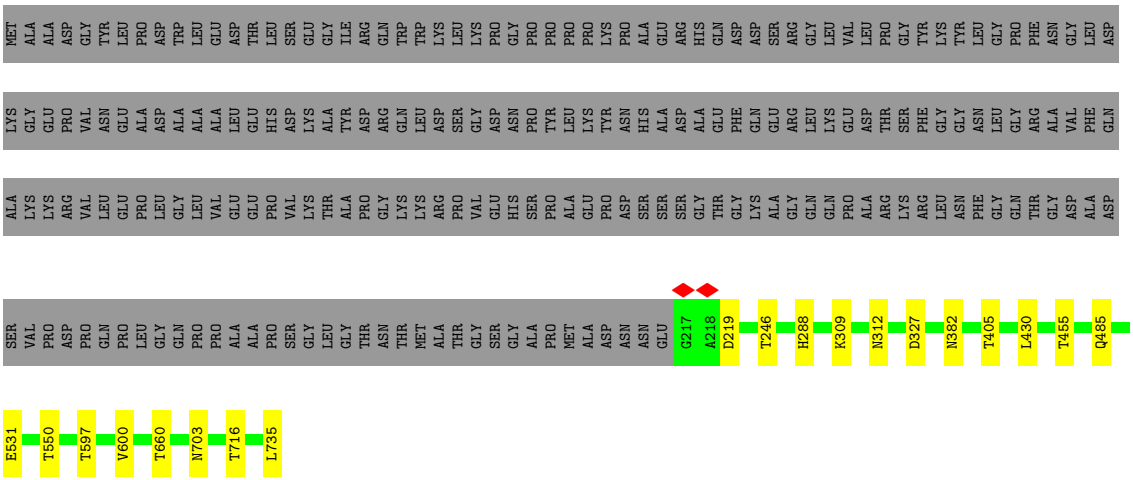
• Molecule 1: Capsid protein VP1

Chain O:



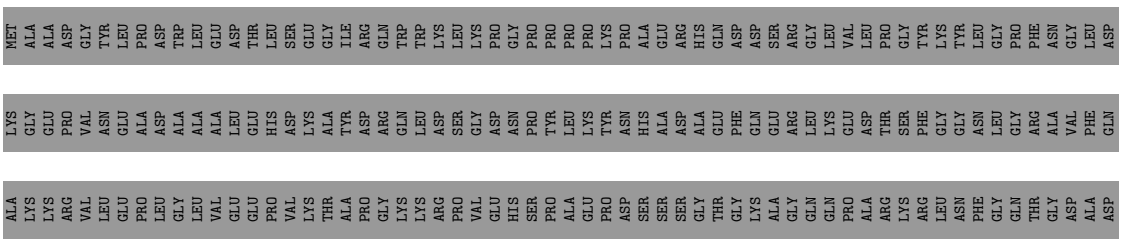
• Molecule 1: Capsid protein VP1

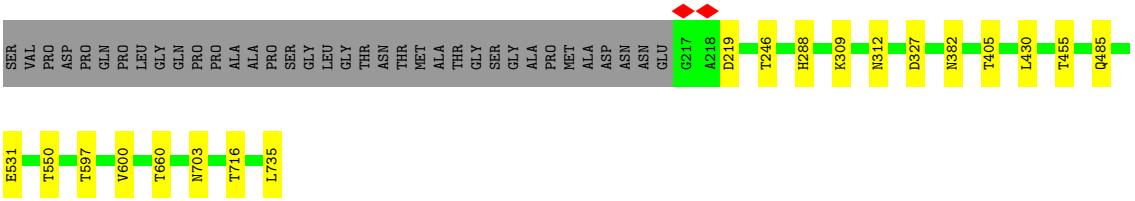
Chain P:



• Molecule 1: Capsid protein VP1

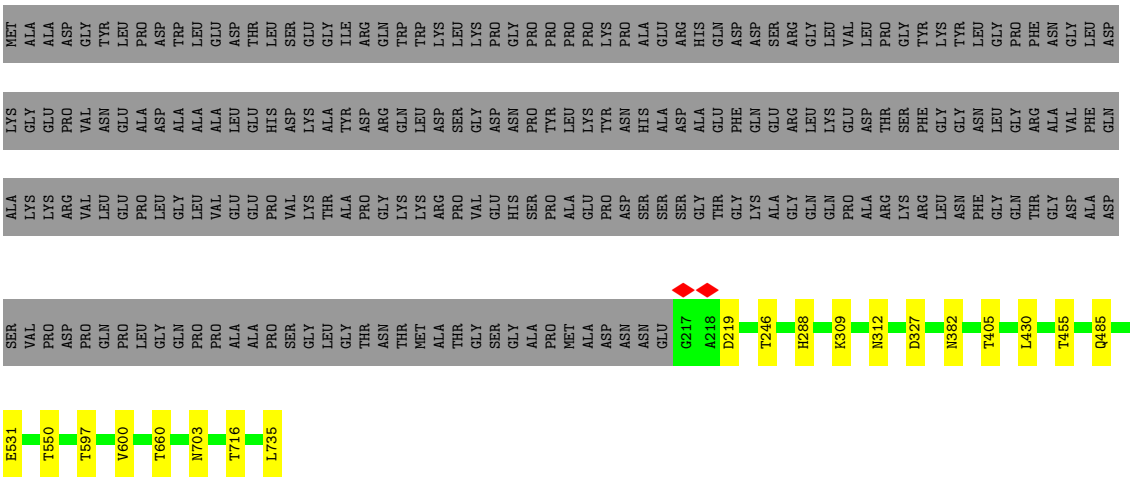
Chain Q:





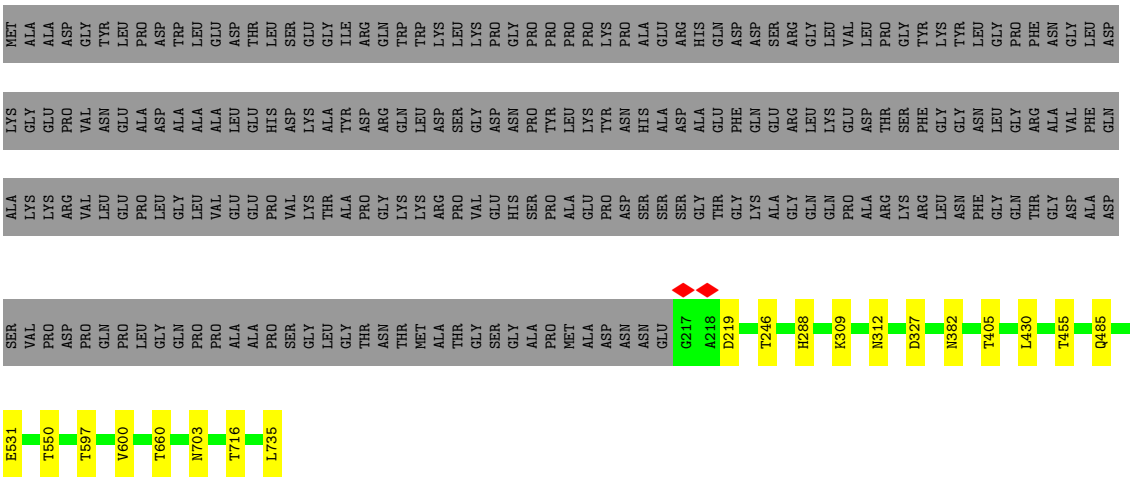
• Molecule 1: Capsid protein VP1

Chain R:



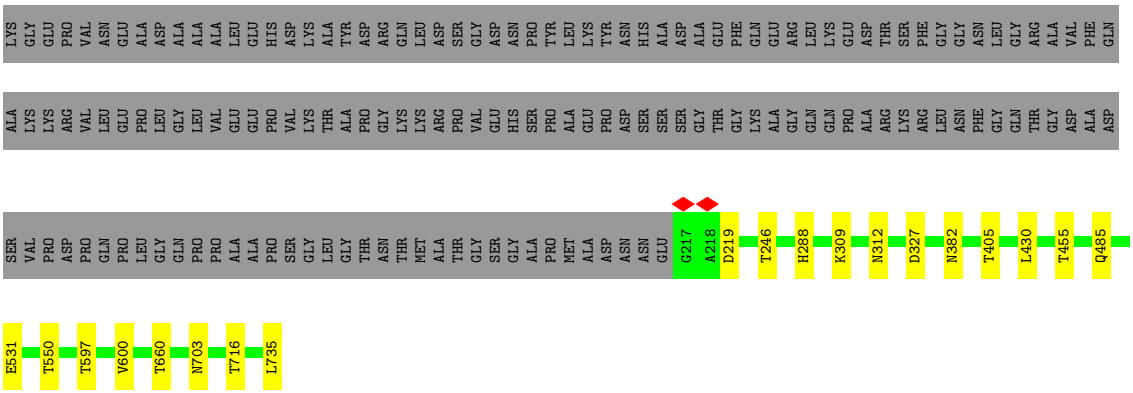
• Molecule 1: Capsid protein VP1

Chain S:



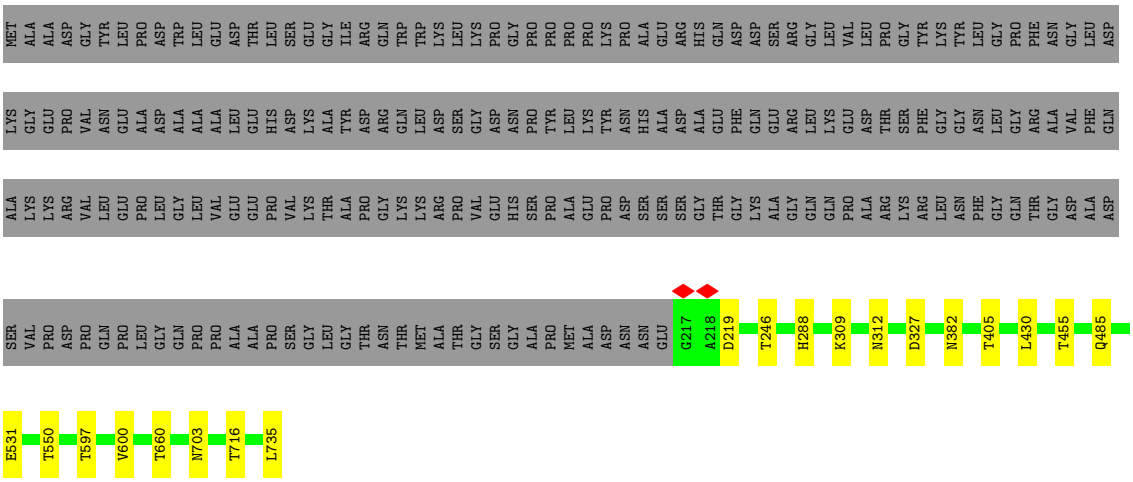
• Molecule 1: Capsid protein VP1

Chain T:



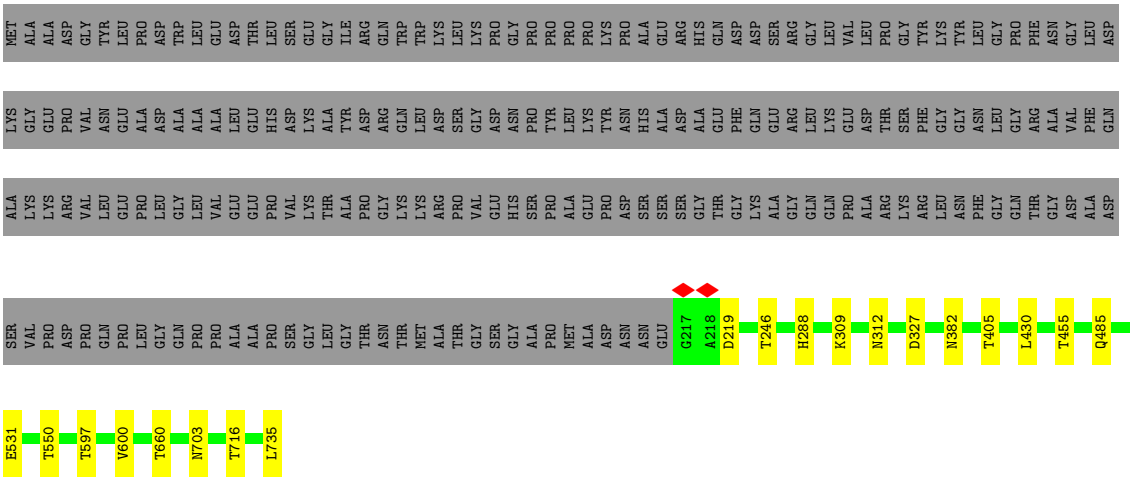
• Molecule 1: Capsid protein VP1

Chain B:



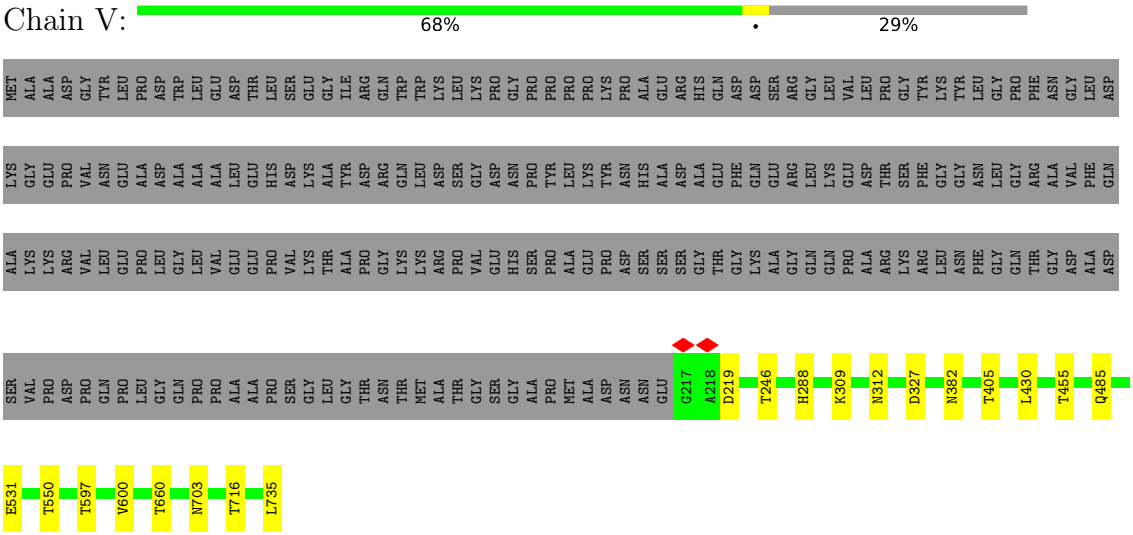
• Molecule 1: Capsid protein VP1

Chain U:



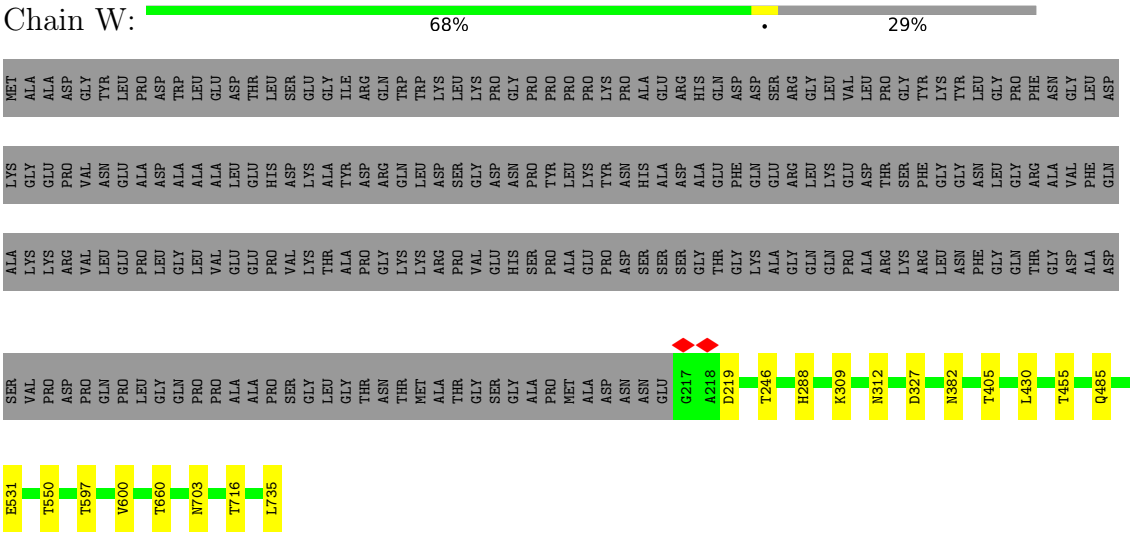
• Molecule 1: Capsid protein VP1

Chain V:



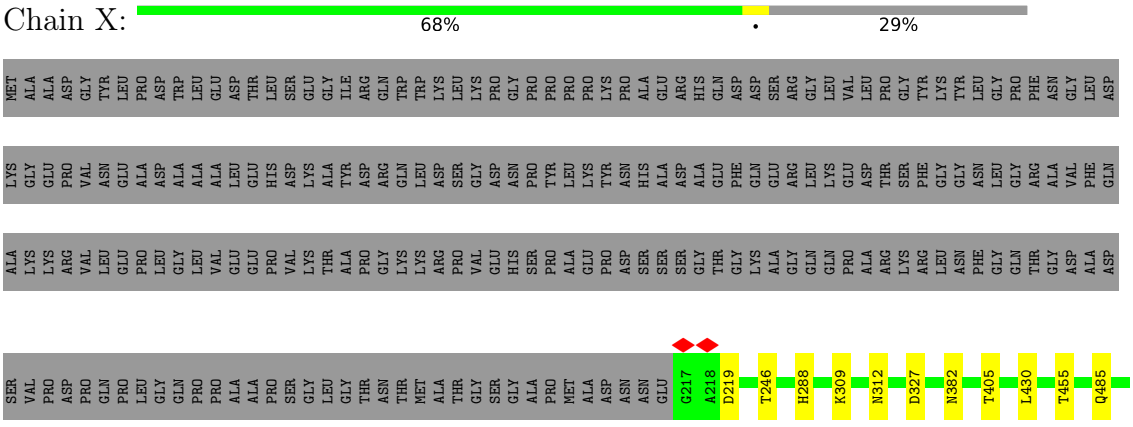
• Molecule 1: Capsid protein VP1

Chain W:



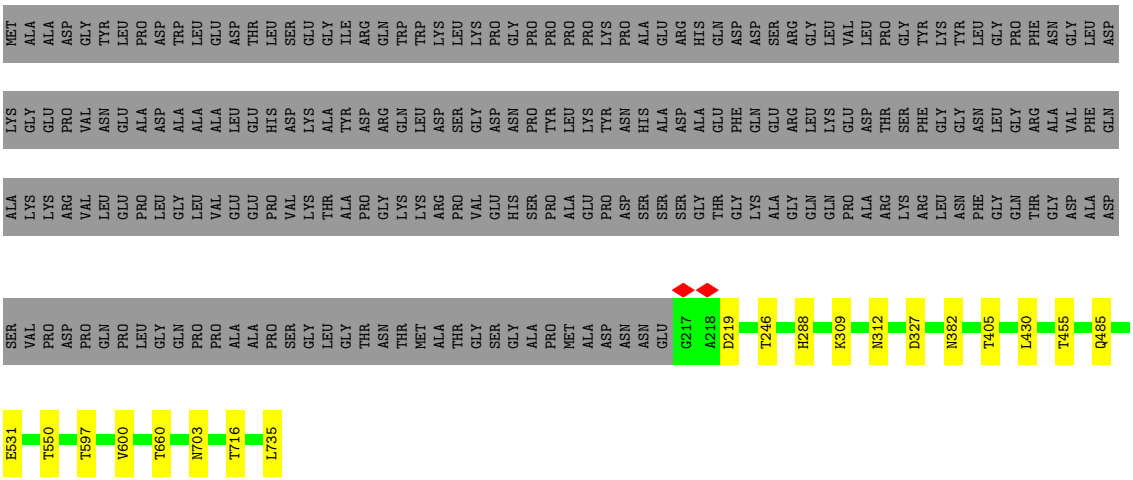
• Molecule 1: Capsid protein VP1

Chain X:



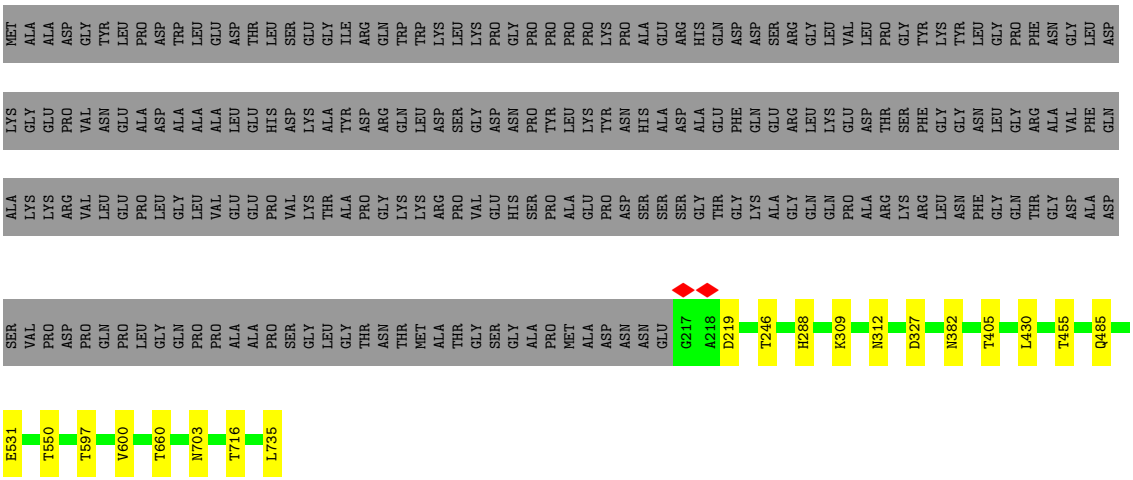
• Molecule 1: Capsid protein VP1

Chain Y:



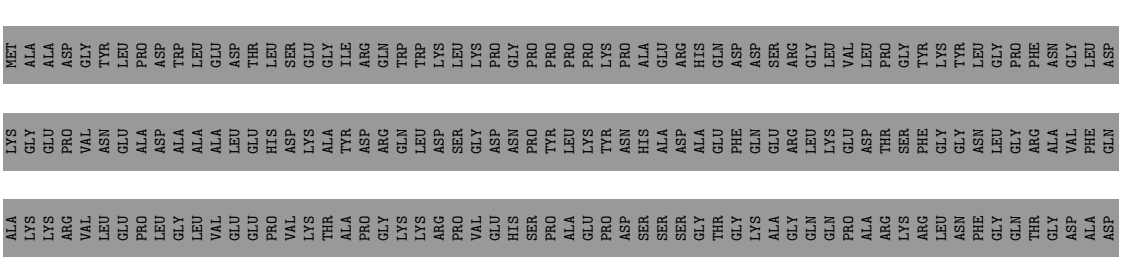
• Molecule 1: Capsid protein VP1

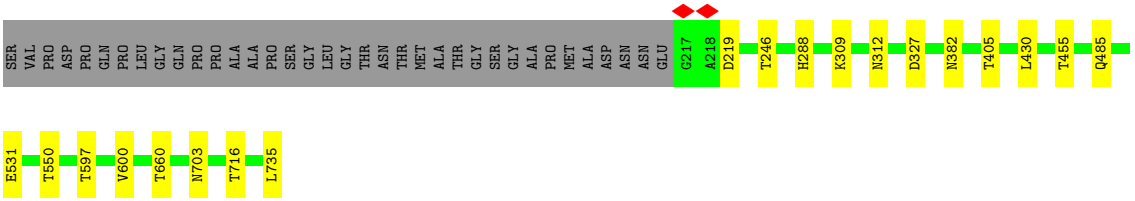
Chain Z:



• Molecule 1: Capsid protein VP1

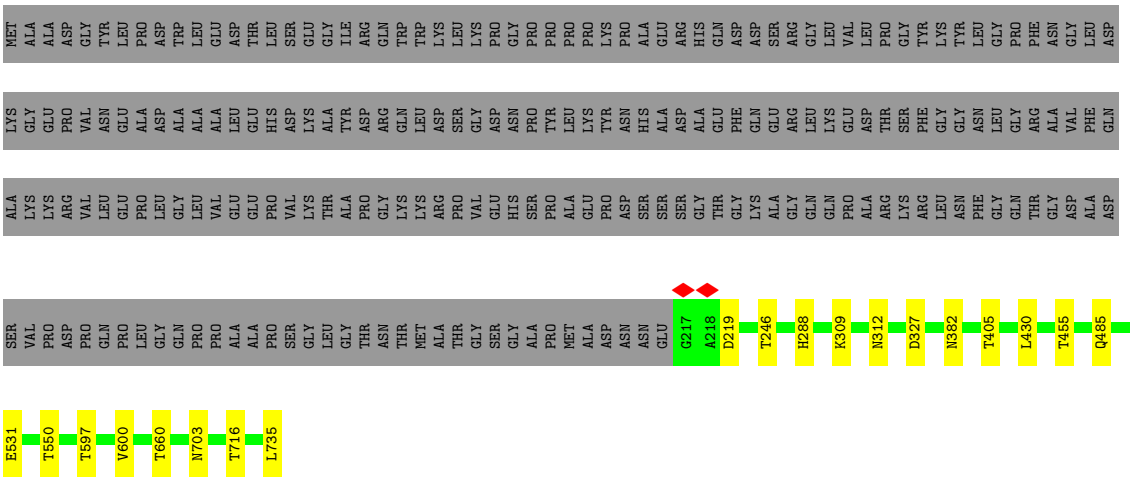
Chain a:





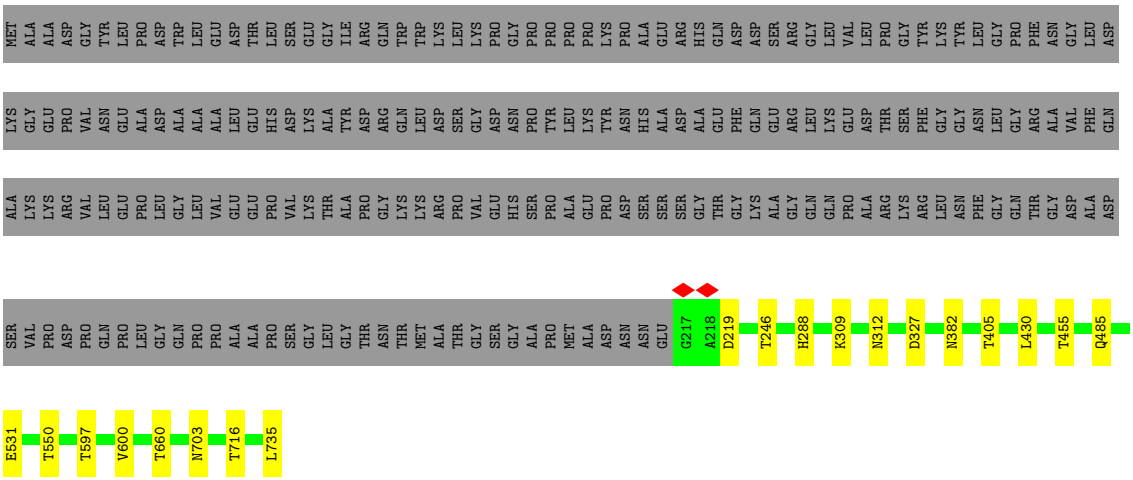
• Molecule 1: Capsid protein VP1

Chain b:



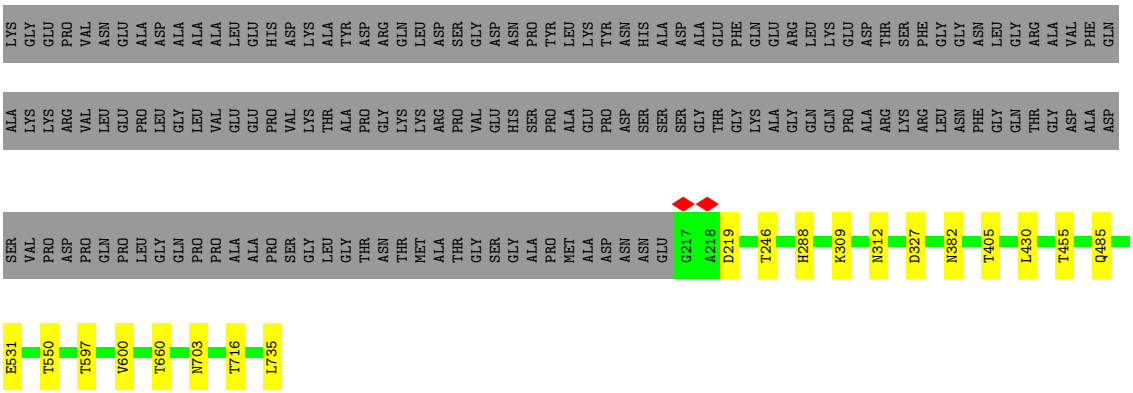
• Molecule 1: Capsid protein VP1

Chain c:



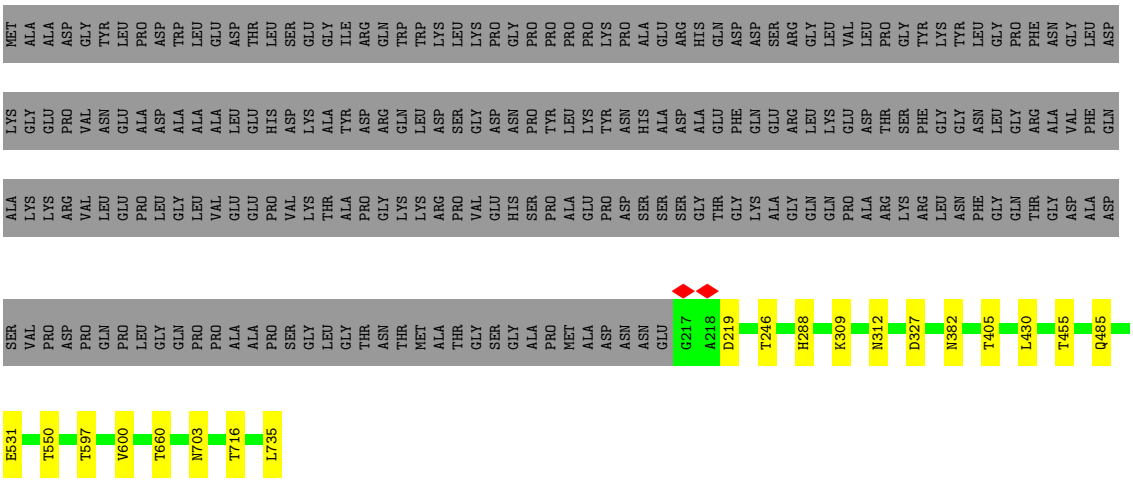
• Molecule 1: Capsid protein VP1

Chain d:



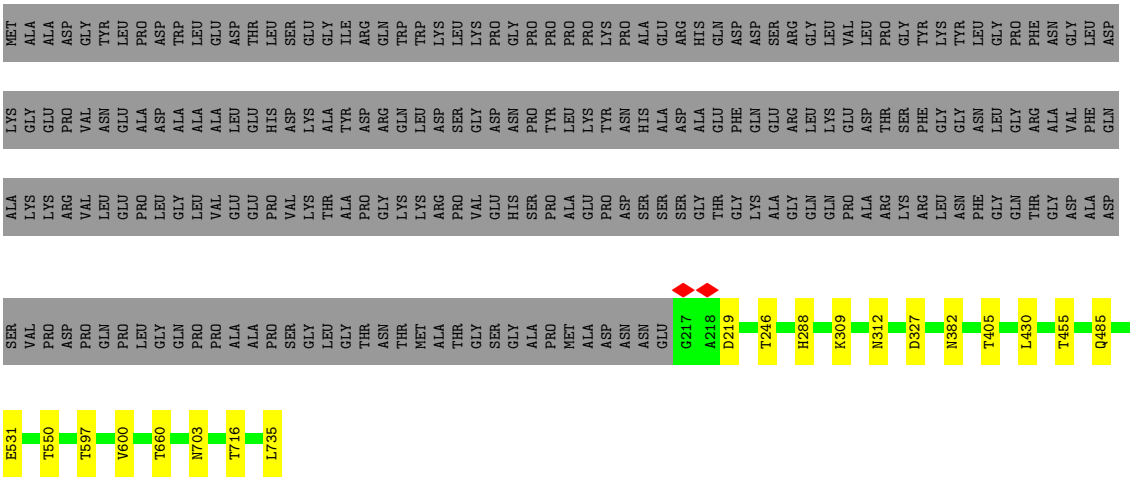
• Molecule 1: Capsid protein VP1

Chain C:



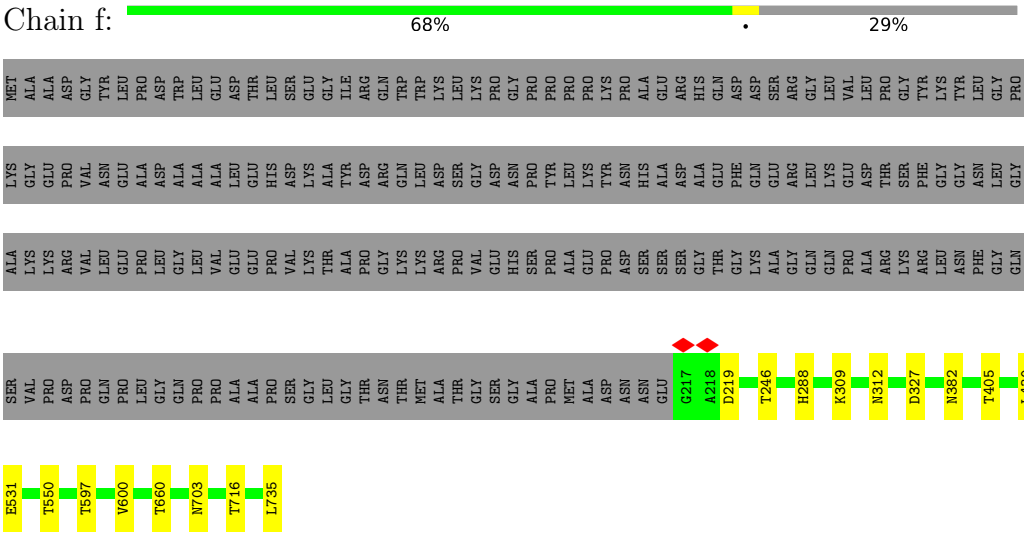
• Molecule 1: Capsid protein VP1

Chain e:



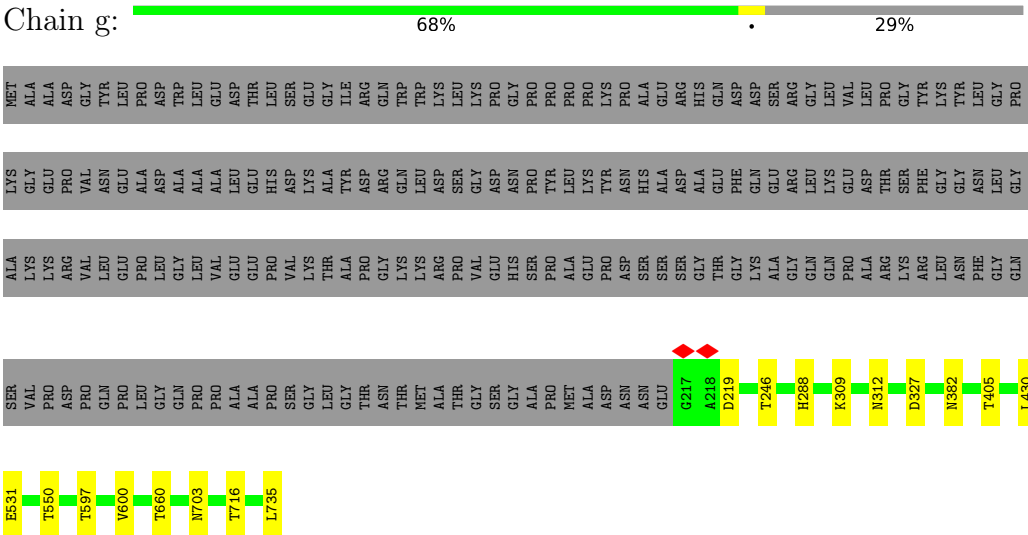
• Molecule 1: Capsid protein VP1

Chain f:



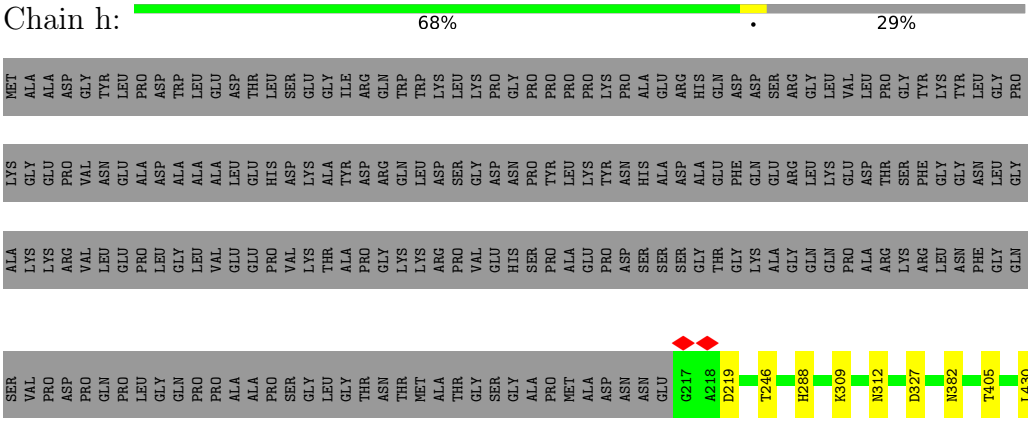
• Molecule 1: Capsid protein VP1

Chain g:



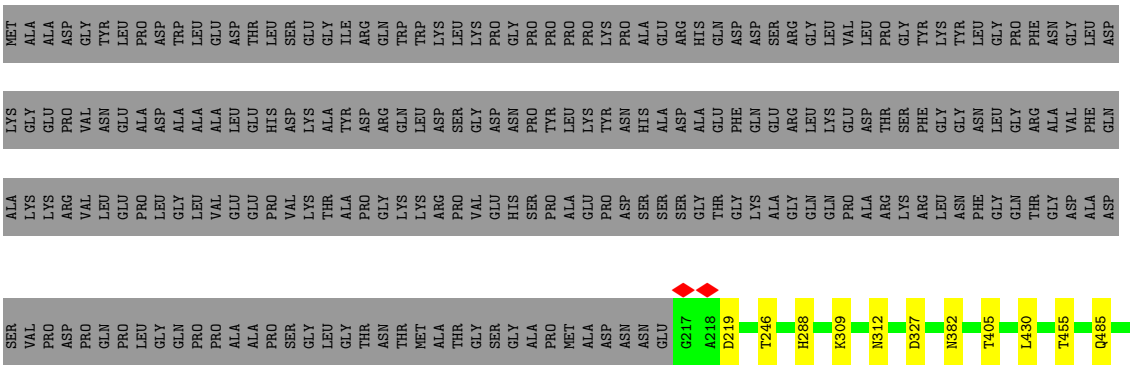
• Molecule 1: Capsid protein VP1

Chain h:



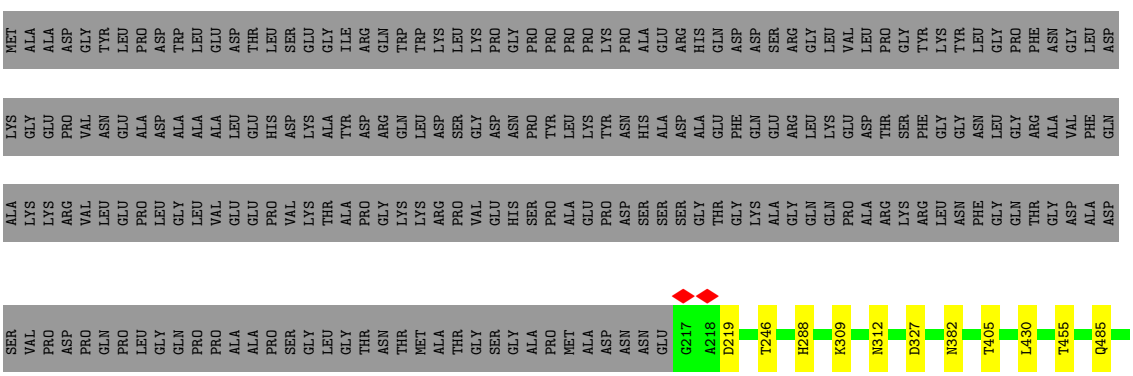
• Molecule 1: Capsid protein VP1

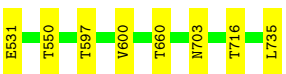
Chain i:



• Molecule 1: Capsid protein VP1

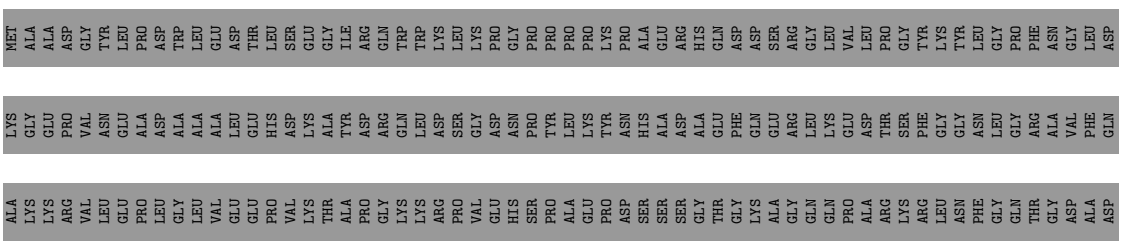
Chain j:

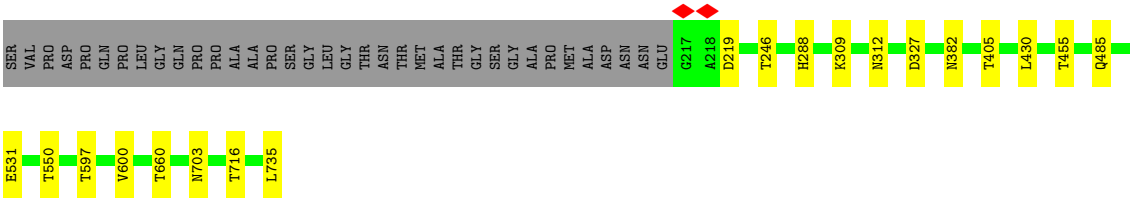




• Molecule 1: Capsid protein VP1

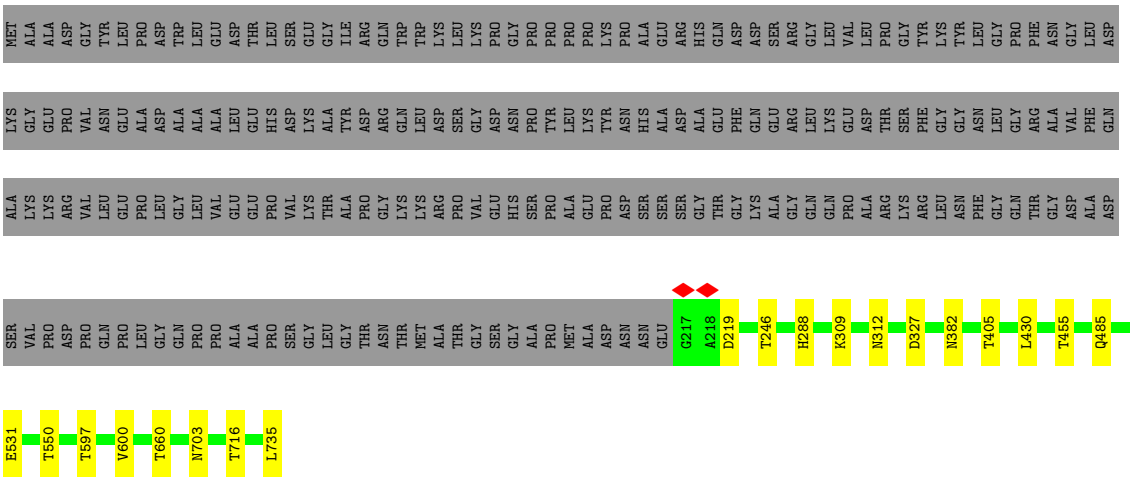
Chain k:





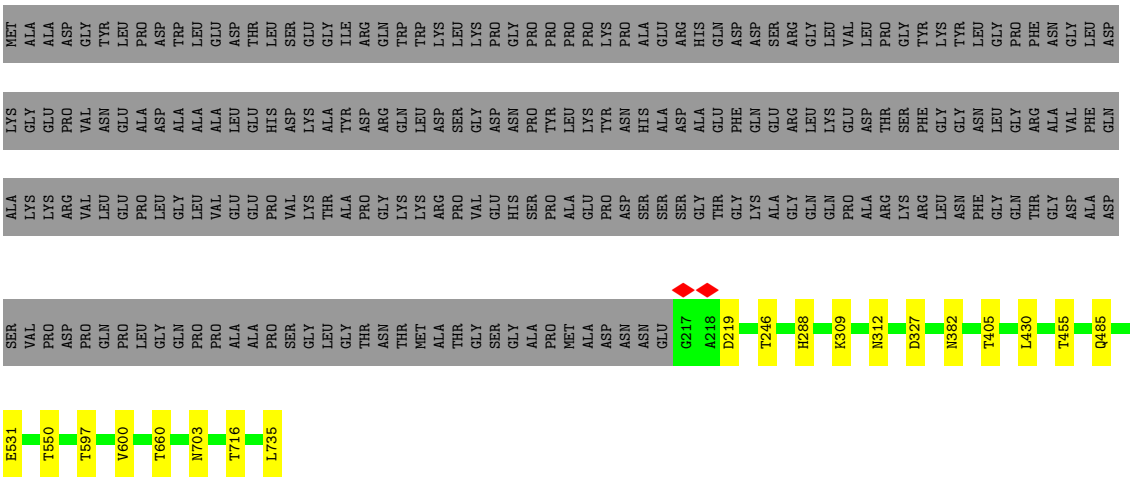
• Molecule 1: Capsid protein VP1

Chain l:



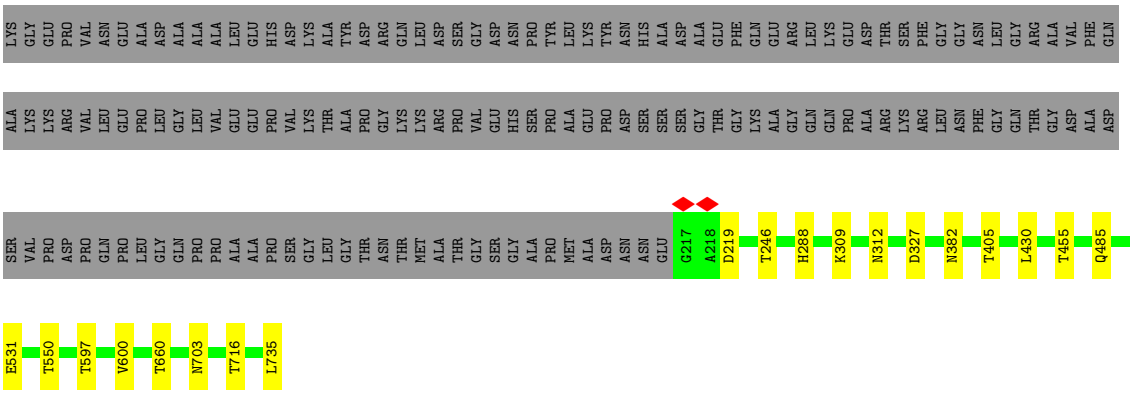
• Molecule 1: Capsid protein VP1

Chain m:



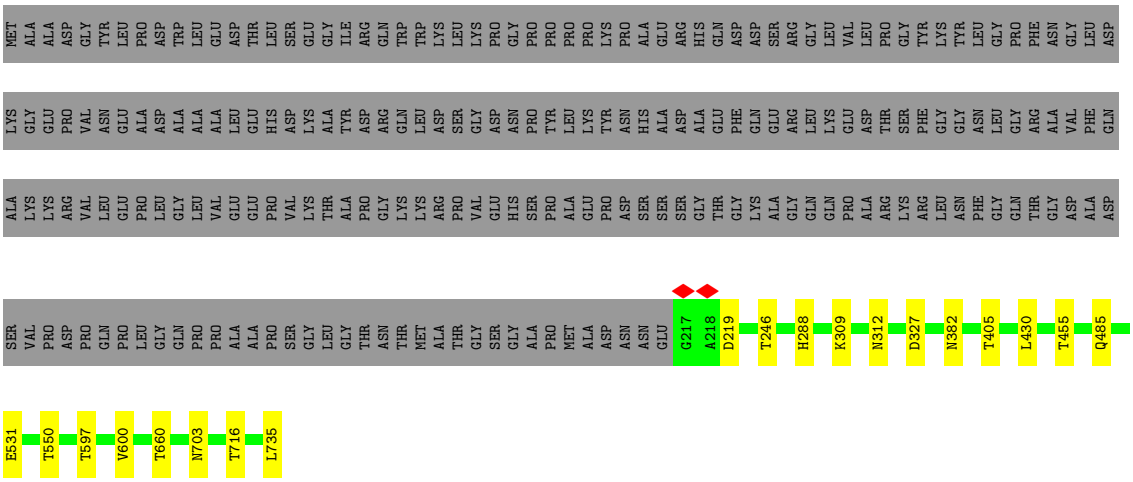
• Molecule 1: Capsid protein VP1

Chain n:



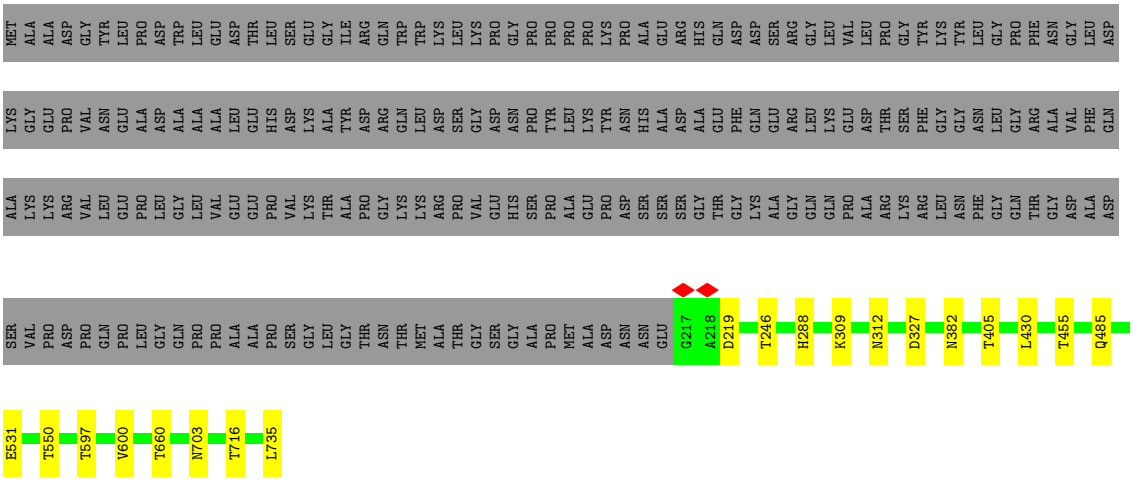
• Molecule 1: Capsid protein VP1

Chain D:



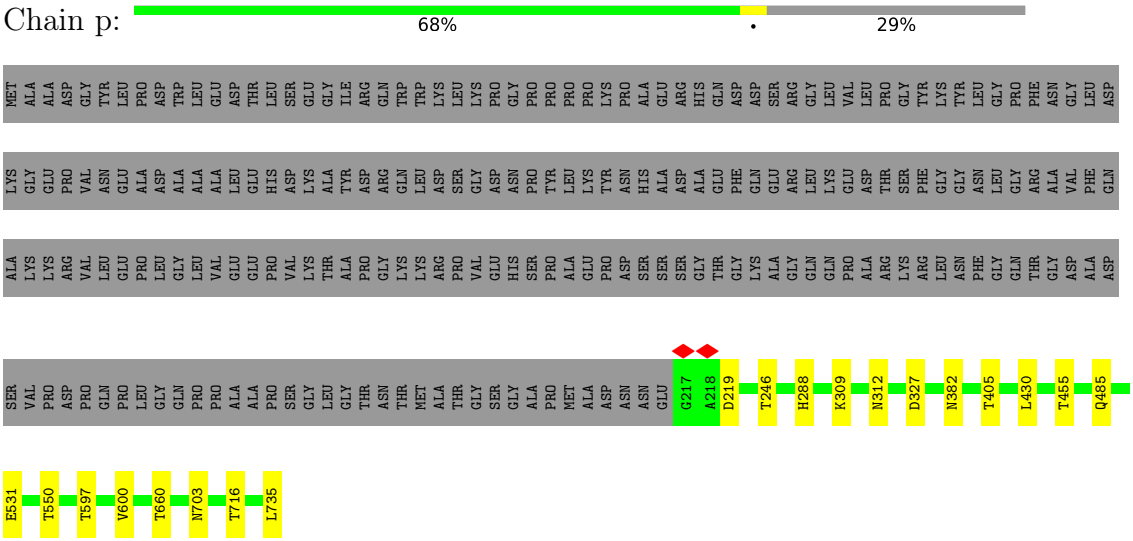
• Molecule 1: Capsid protein VP1

Chain o:



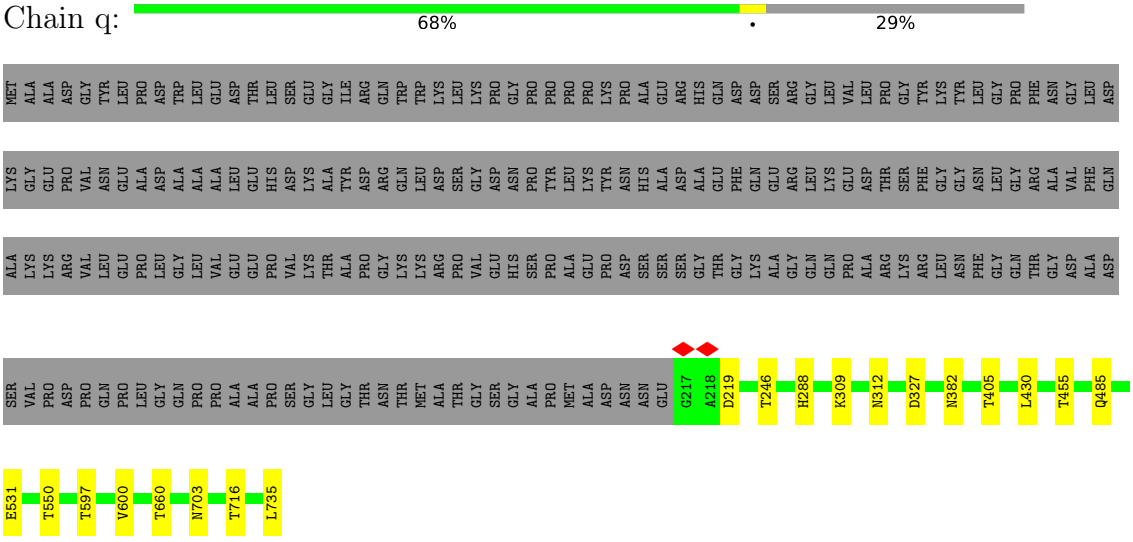
• Molecule 1: Capsid protein VP1

Chain p:



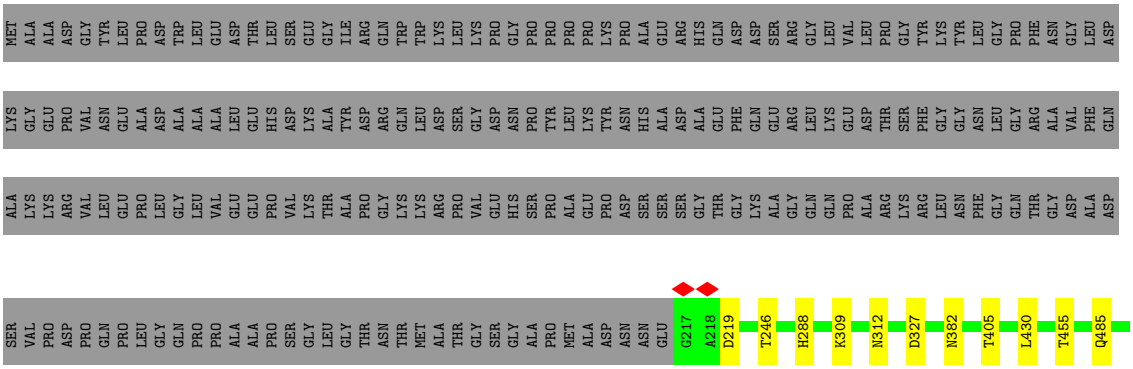
• Molecule 1: Capsid protein VP1

Chain q:



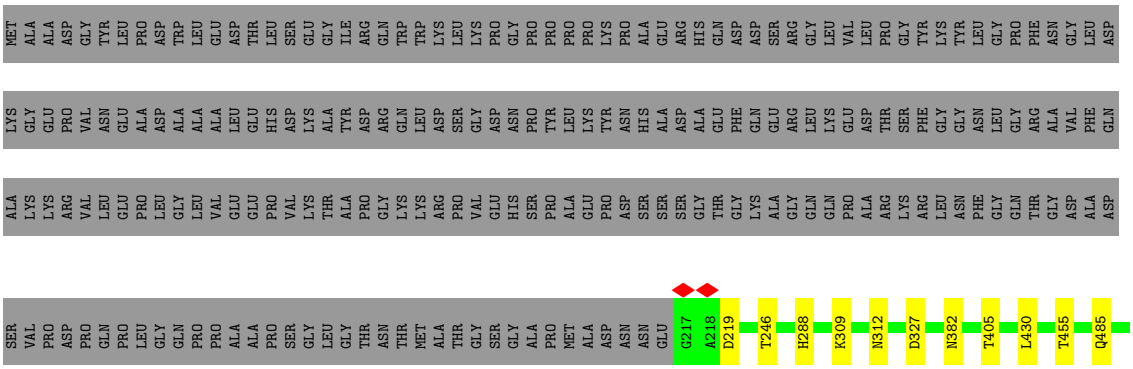
• Molecule 1: Capsid protein VP1

Chain r:



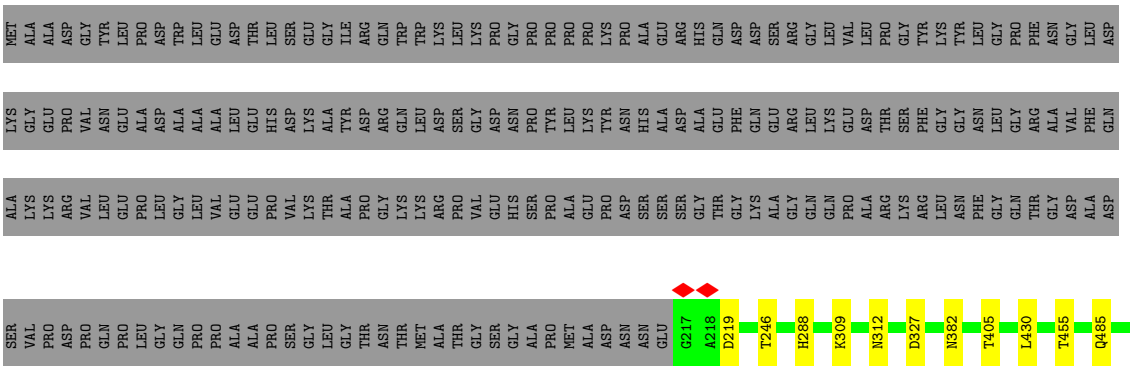
• Molecule 1: Capsid protein VP1

Chain s:



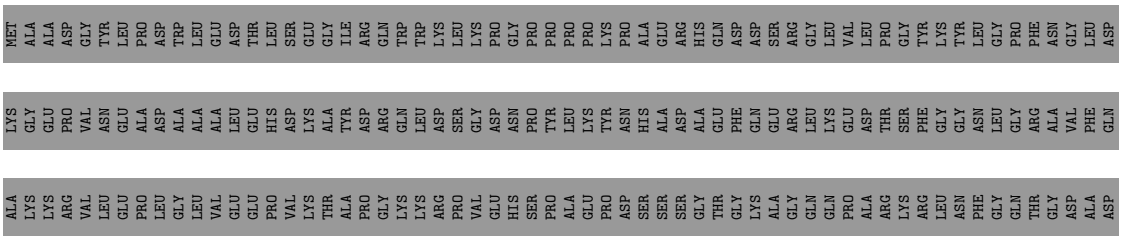
• Molecule 1: Capsid protein VP1

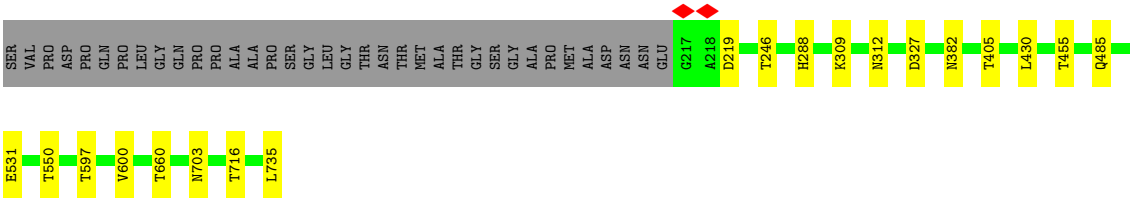
Chain t:



• Molecule 1: Capsid protein VP1

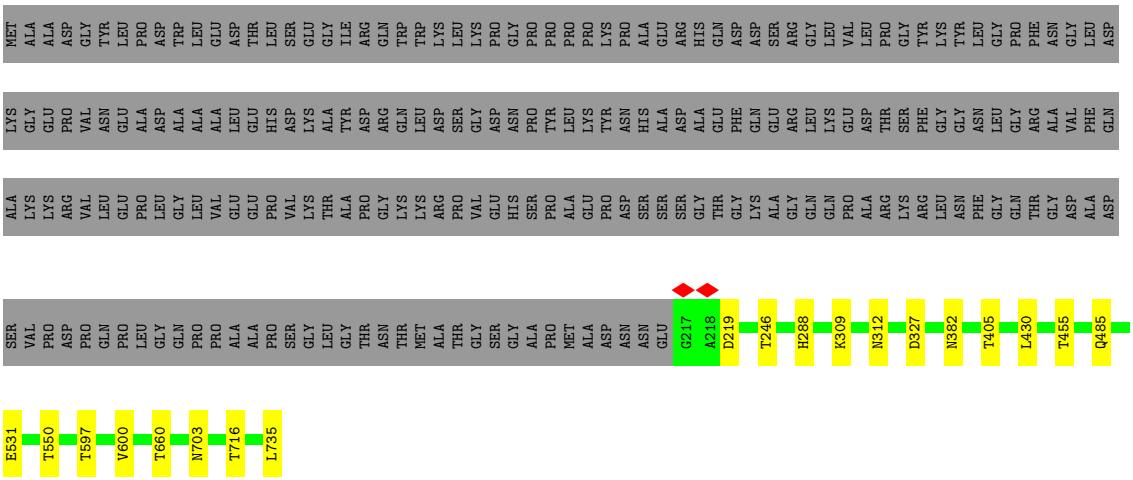
Chain u:





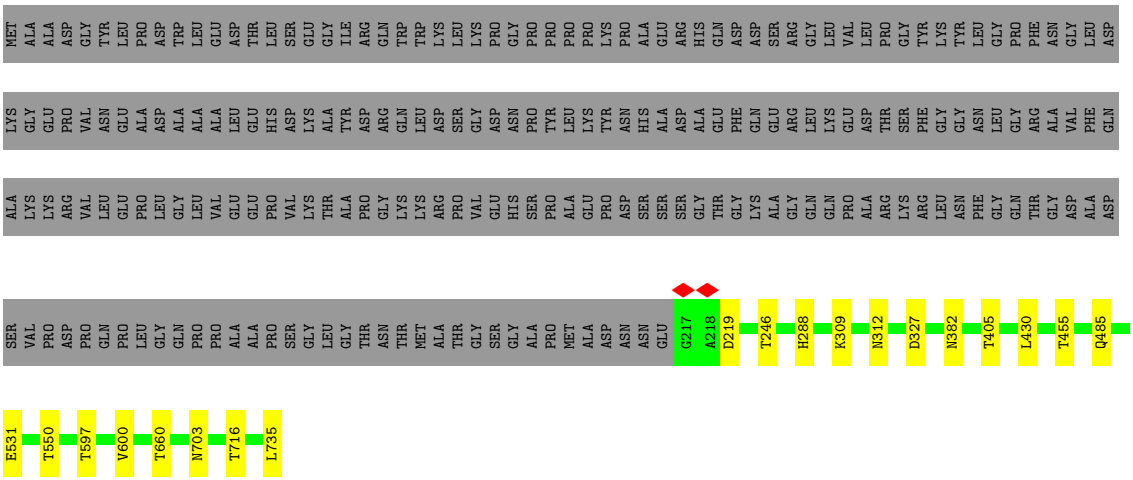
• Molecule 1: Capsid protein VP1

Chain v:



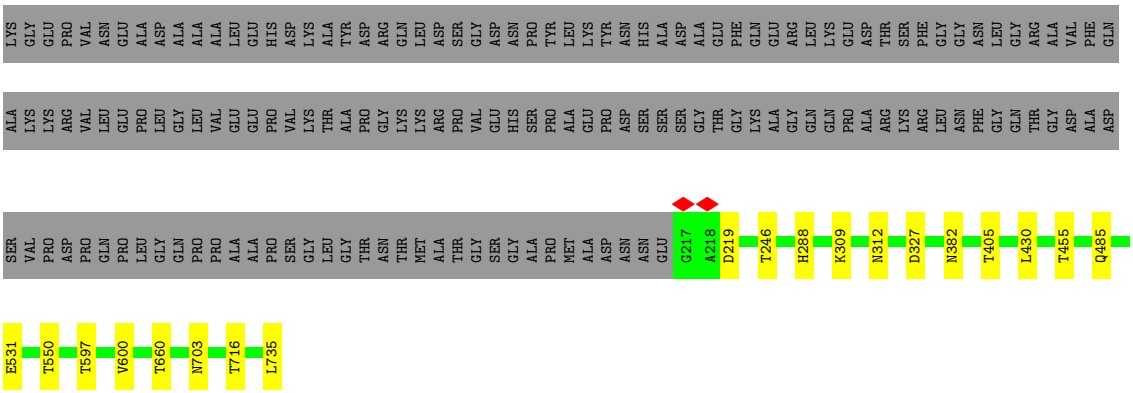
• Molecule 1: Capsid protein VP1

Chain w:



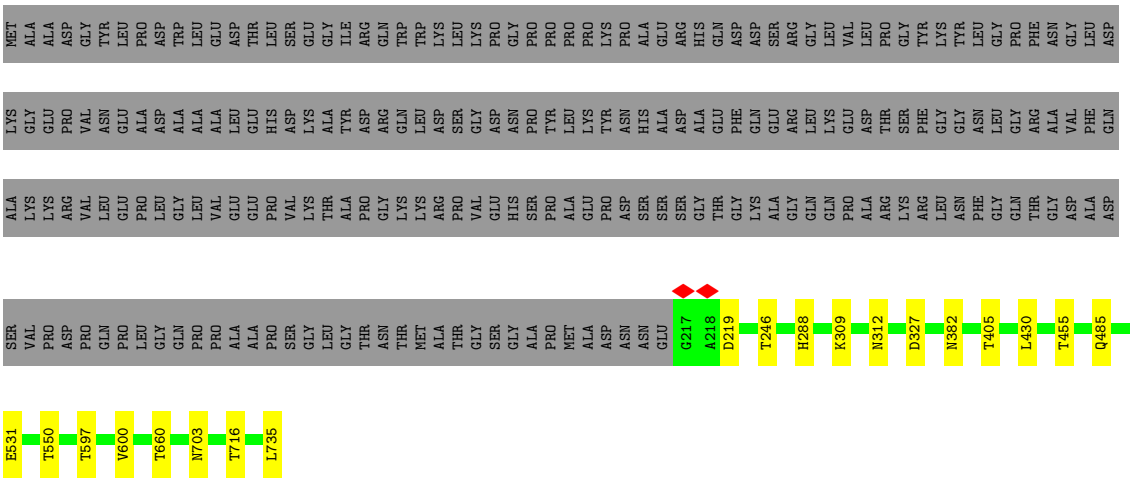
• Molecule 1: Capsid protein VP1

Chain x:



• Molecule 1: Capsid protein VP1

Chain E:

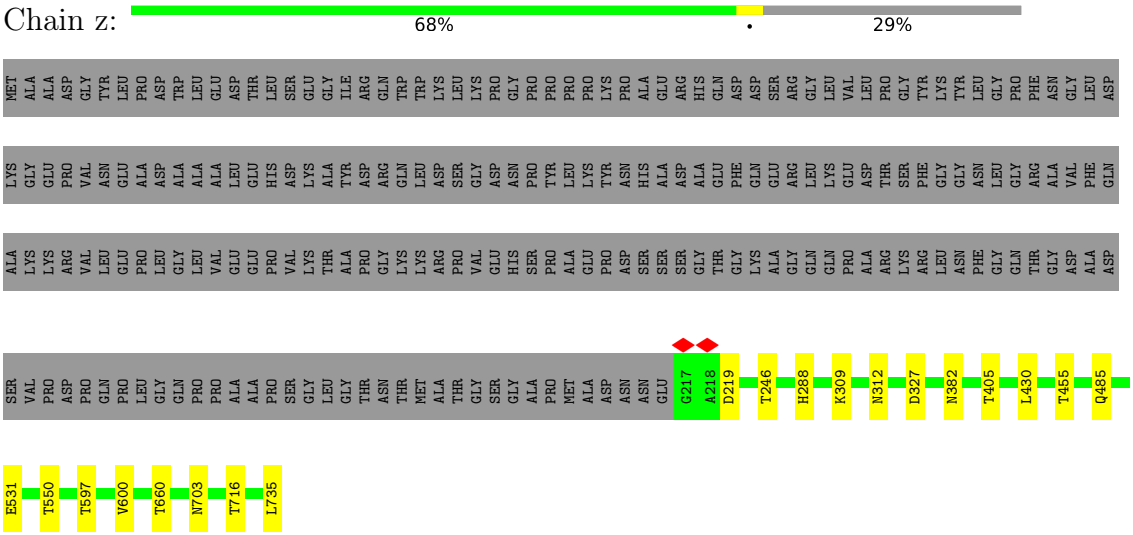


• Molecule 1: Capsid protein VP1

Chain y:

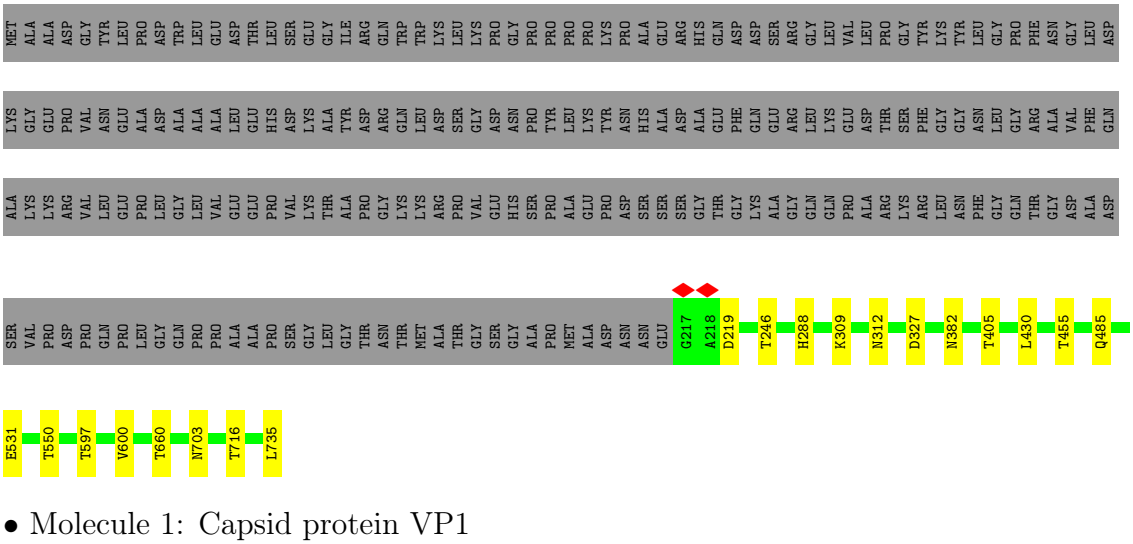
• Molecule 1: Capsid protein VP1

Chain z:



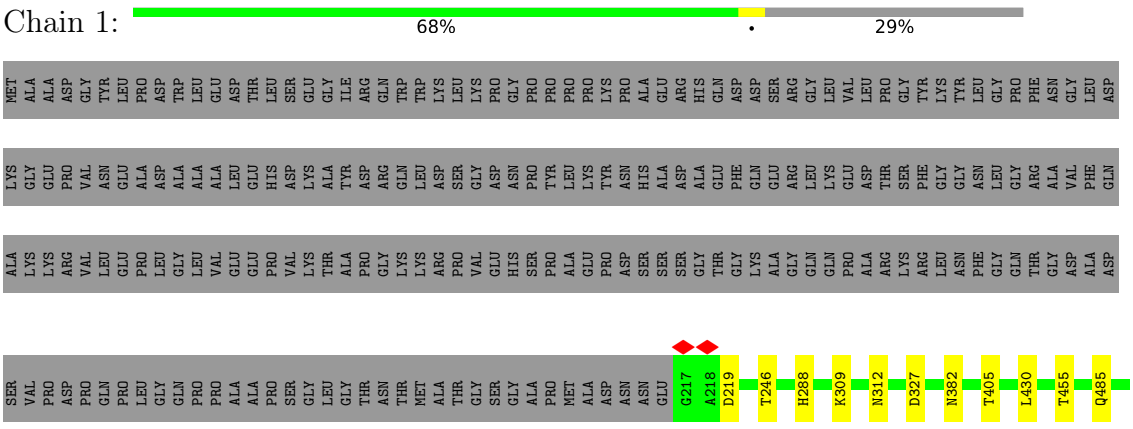
• Molecule 1: Capsid protein VP1

Chain 0:



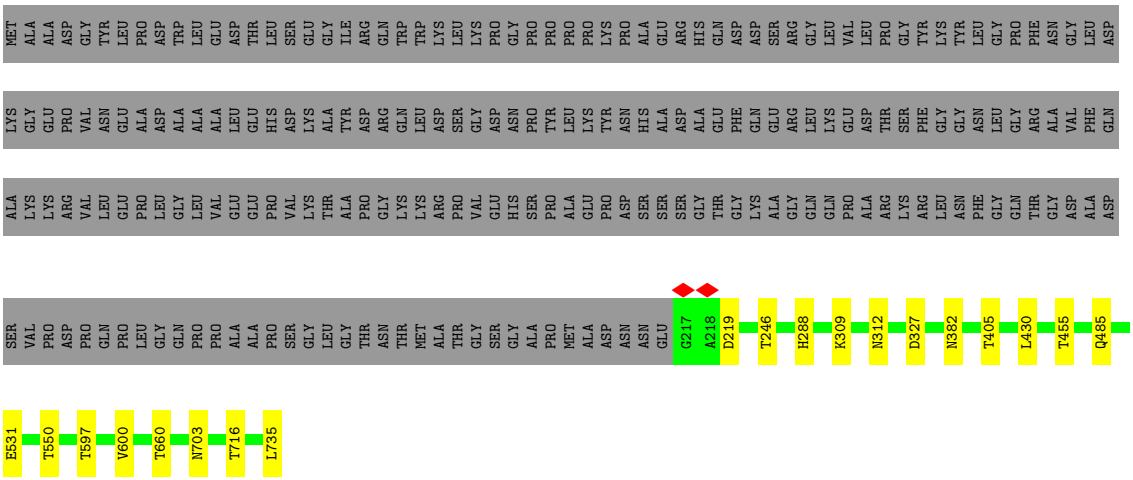
• Molecule 1: Capsid protein VP1

Chain 1:



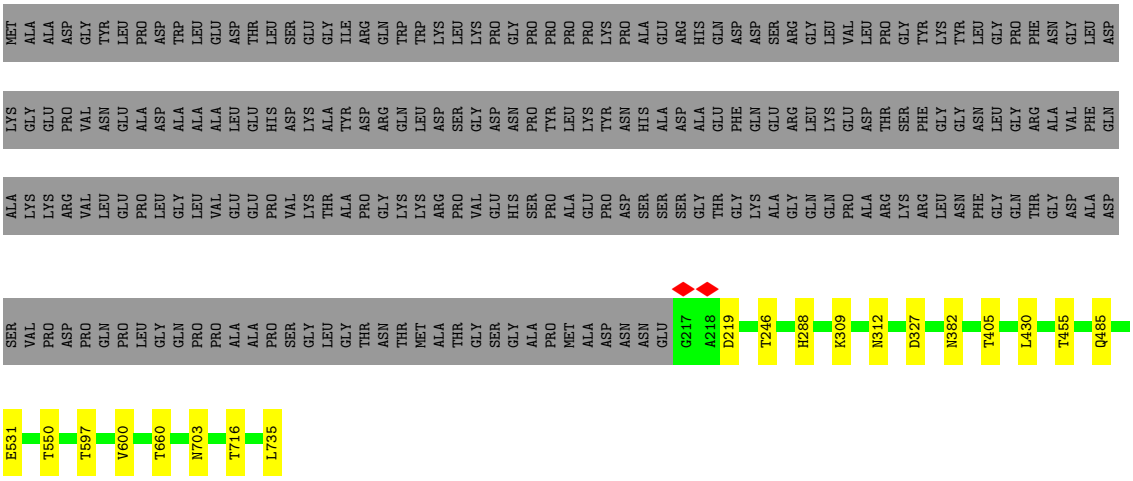
• Molecule 1: Capsid protein VP1

Chain 2:



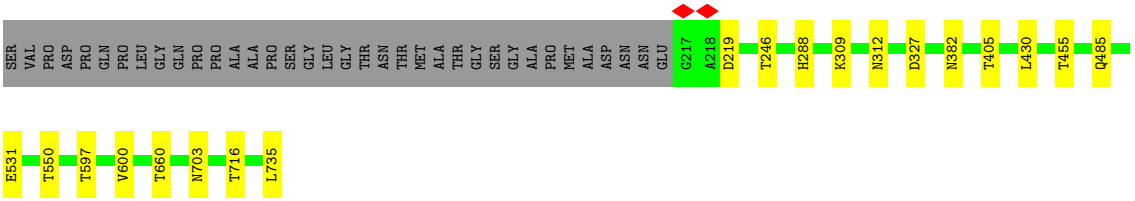
• Molecule 1: Capsid protein VP1

Chain 3:



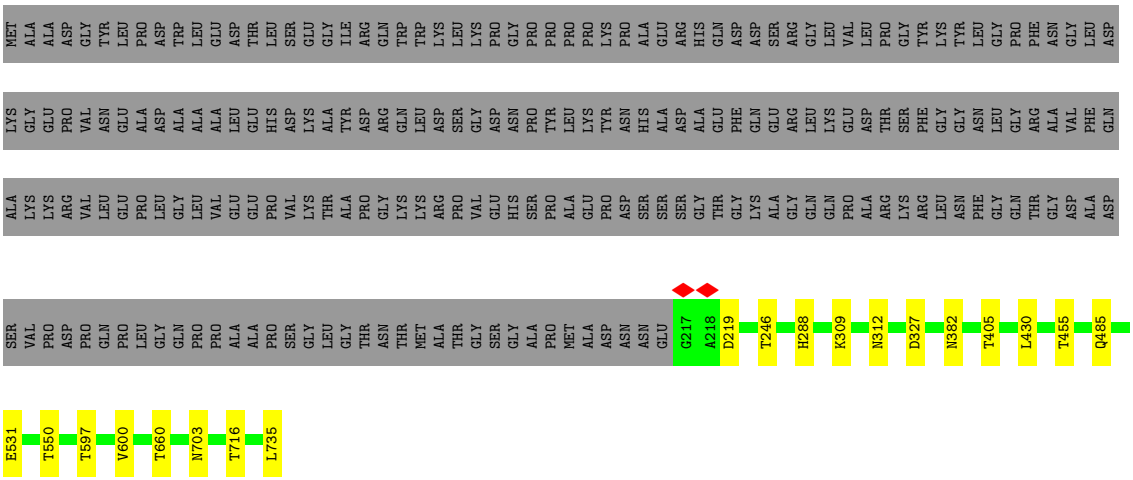
• Molecule 1: Capsid protein VP1

Chain 4:



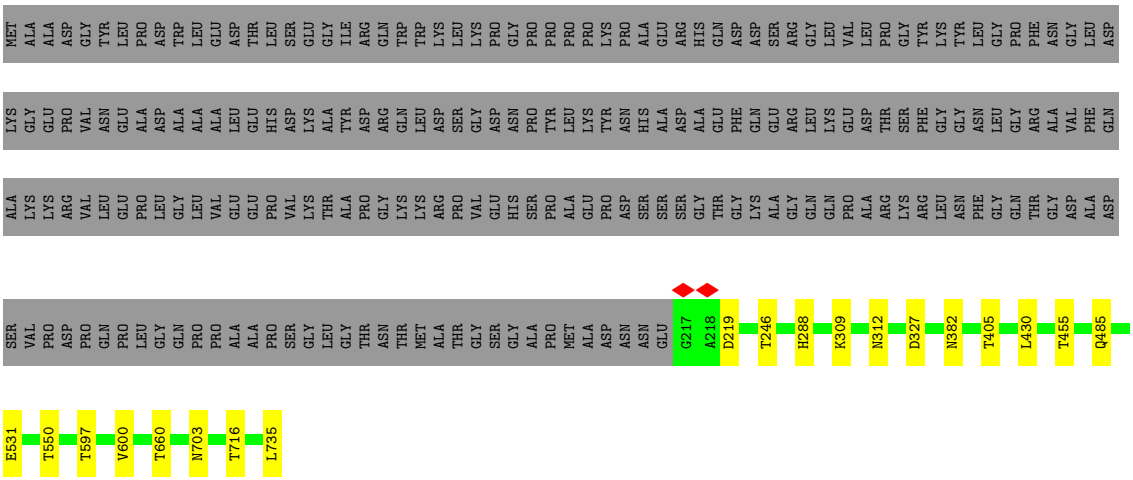
• Molecule 1: Capsid protein VP1

Chain 5:



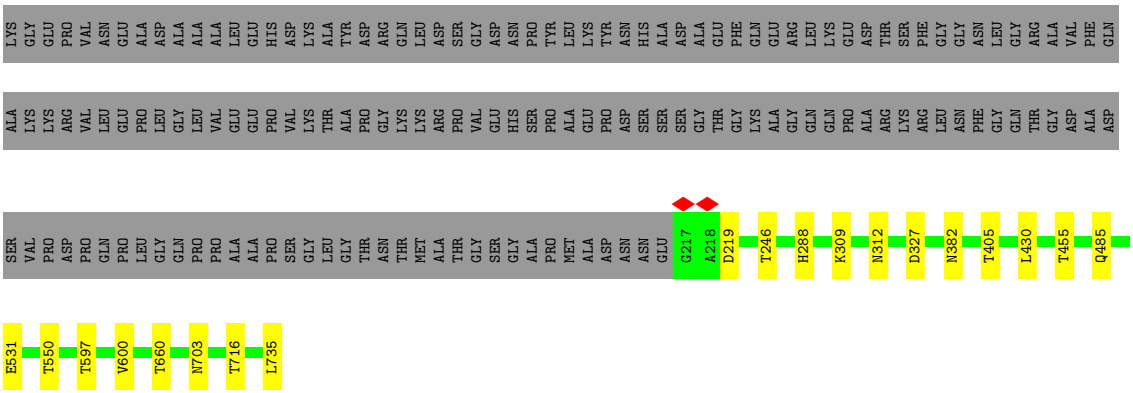
• Molecule 1: Capsid protein VP1

Chain 6:



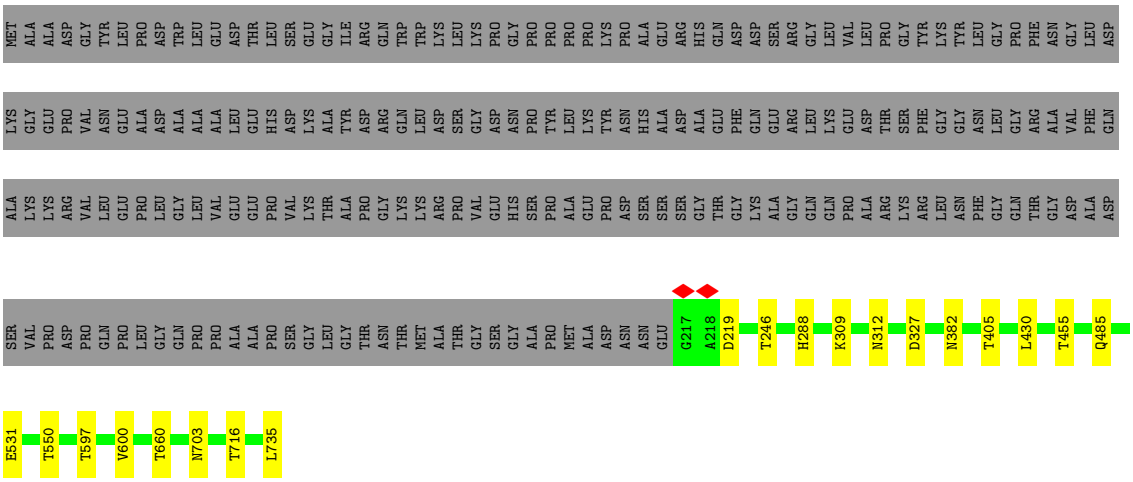
• Molecule 1: Capsid protein VP1

Chain 7:



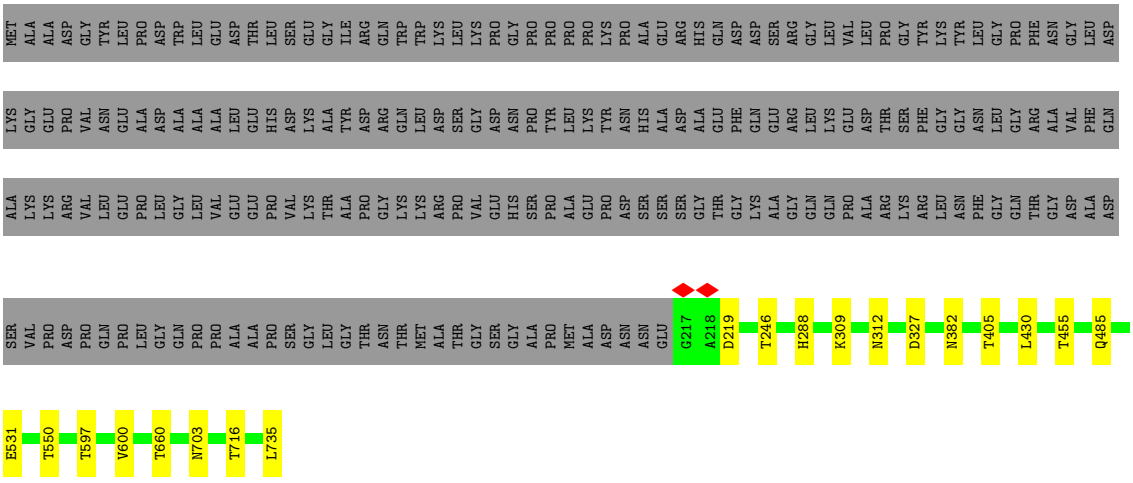
• Molecule 1: Capsid protein VP1

Chain F:



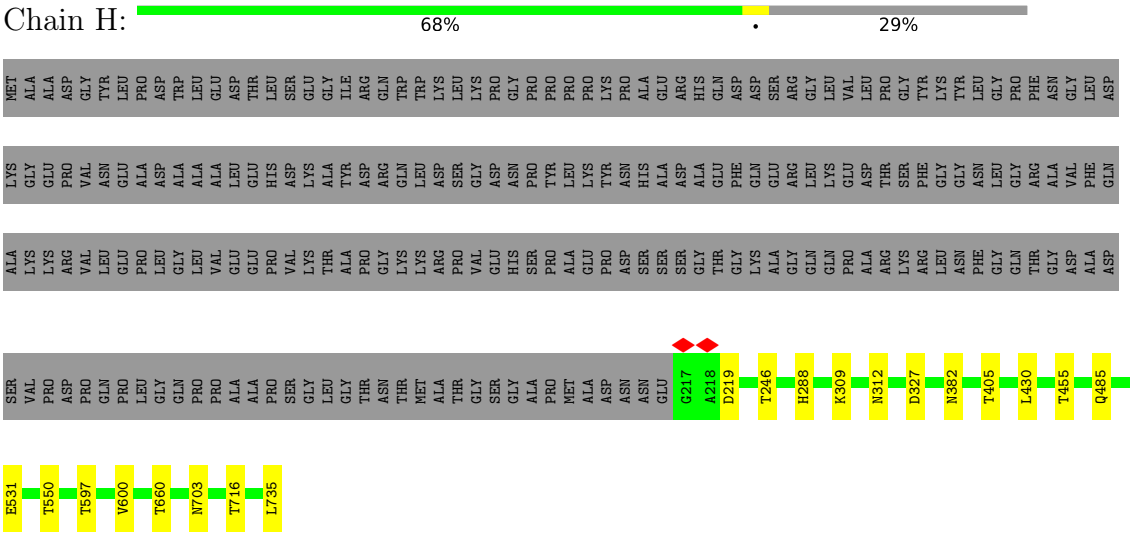
• Molecule 1: Capsid protein VP1

Chain G:



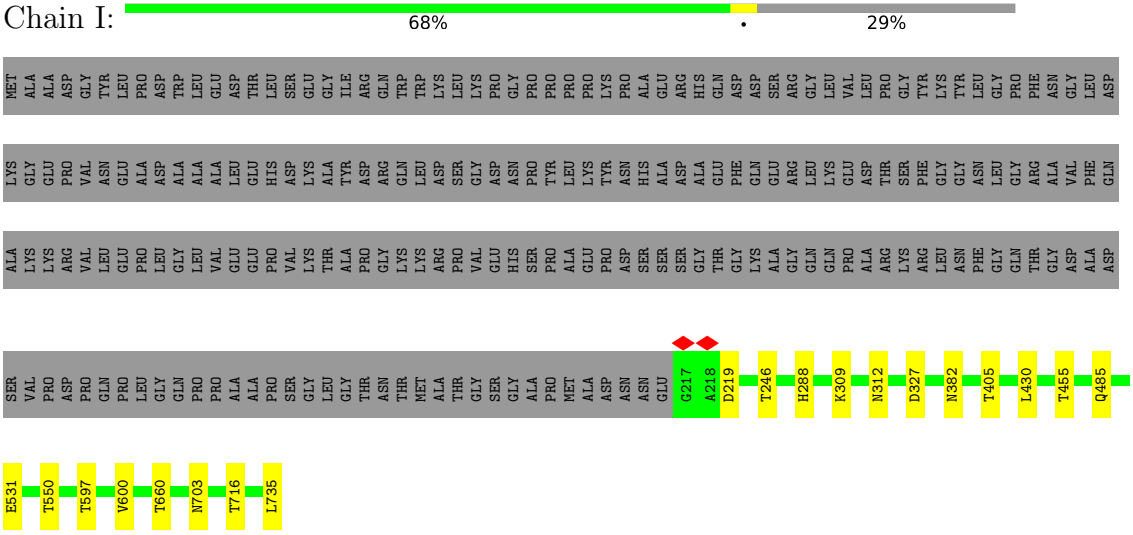
• Molecule 1: Capsid protein VP1

Chain H:



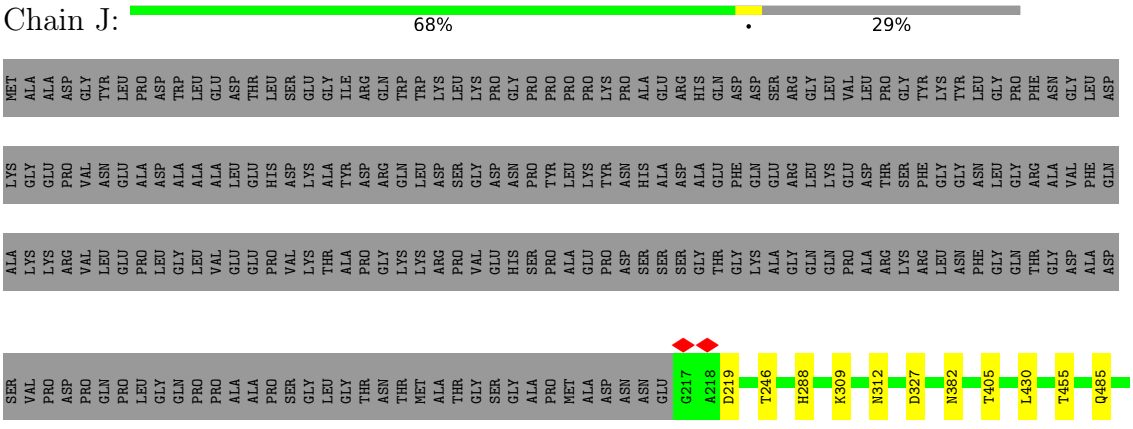
• Molecule 1: Capsid protein VP1

Chain I:



• Molecule 1: Capsid protein VP1

Chain J:



E531
T550
T597
V600
T660
N703
T716
L735

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52874	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48.62	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	22.946	Depositor
Minimum map value	-7.268	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.6	Depositor
Map size (Å)	609.984, 609.984, 609.984	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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	0.46	0/4261	0.46	0/5811
1	1	0.46	0/4261	0.46	0/5811
1	2	0.46	0/4261	0.46	0/5811
1	3	0.46	0/4261	0.46	0/5811
1	4	0.46	0/4261	0.46	0/5811
1	5	0.46	0/4261	0.46	0/5811
1	6	0.46	0/4261	0.46	0/5811
1	7	0.46	0/4261	0.46	0/5811
1	A	0.46	0/4261	0.46	0/5811
1	B	0.46	0/4261	0.46	0/5811
1	C	0.46	0/4261	0.46	0/5811
1	D	0.46	0/4261	0.46	0/5811
1	E	0.46	0/4261	0.46	0/5811
1	F	0.46	0/4261	0.46	0/5811
1	G	0.46	0/4261	0.46	0/5811
1	H	0.46	0/4261	0.46	0/5811
1	I	0.46	0/4261	0.46	0/5811
1	J	0.46	0/4261	0.46	0/5811
1	K	0.46	0/4261	0.46	0/5811
1	L	0.46	0/4261	0.46	0/5811
1	M	0.46	0/4261	0.46	0/5811
1	N	0.46	0/4261	0.46	0/5811
1	O	0.46	0/4261	0.46	0/5811
1	P	0.46	0/4261	0.46	0/5811
1	Q	0.46	0/4261	0.46	0/5811
1	R	0.46	0/4261	0.46	0/5811
1	S	0.46	0/4261	0.46	0/5811
1	T	0.46	0/4261	0.46	0/5811
1	U	0.46	0/4261	0.46	0/5811
1	V	0.46	0/4261	0.46	0/5811
1	W	0.46	0/4261	0.46	0/5811
1	X	0.46	0/4261	0.46	0/5811
1	Y	0.46	0/4261	0.46	0/5811
1	Z	0.46	0/4261	0.46	0/5811

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	a	0.46	0/4261	0.46	0/5811
1	b	0.46	0/4261	0.46	0/5811
1	c	0.46	0/4261	0.46	0/5811
1	d	0.46	0/4261	0.46	0/5811
1	e	0.46	0/4261	0.46	0/5811
1	f	0.46	0/4261	0.46	0/5811
1	g	0.46	0/4261	0.46	0/5811
1	h	0.46	0/4261	0.46	0/5811
1	i	0.46	0/4261	0.46	0/5811
1	j	0.46	0/4261	0.46	0/5811
1	k	0.46	0/4261	0.46	0/5811
1	l	0.46	0/4261	0.46	0/5811
1	m	0.46	0/4261	0.46	0/5811
1	n	0.46	0/4261	0.46	0/5811
1	o	0.46	0/4261	0.46	0/5811
1	p	0.46	0/4261	0.46	0/5811
1	q	0.46	0/4261	0.46	0/5811
1	r	0.46	0/4261	0.46	0/5811
1	s	0.46	0/4261	0.46	0/5811
1	t	0.46	0/4261	0.46	0/5811
1	u	0.46	0/4261	0.46	0/5811
1	v	0.46	0/4261	0.46	0/5811
1	w	0.46	0/4261	0.46	0/5811
1	x	0.46	0/4261	0.46	0/5811
1	y	0.46	0/4261	0.46	0/5811
1	z	0.46	0/4261	0.46	0/5811
All	All	0.46	0/255660	0.46	0/348660

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	1	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	2	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	3	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	4	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	5	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	6	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	7	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	A	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	B	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	C	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	D	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	E	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	F	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	G	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	H	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	I	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	J	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	K	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	L	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	M	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	N	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	O	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	P	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	Q	517/735 (70%)	501 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	S	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	T	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	U	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	V	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	W	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	X	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	Y	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	Z	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	a	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	b	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	c	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	d	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	e	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	f	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	g	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	h	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	i	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	j	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	k	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	l	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	m	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	n	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	o	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	p	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	q	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	r	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	s	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	t	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	u	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	v	517/735 (70%)	501 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	x	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	y	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	z	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
All	All	31020/44100 (70%)	30060 (97%)	960 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	1	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	2	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	3	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	4	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	5	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	6	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	7	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	A	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	B	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	C	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	D	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	E	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	F	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	G	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	H	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	I	458/628 (73%)	439 (96%)	19 (4%)	30	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	K	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	L	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	M	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	N	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	O	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	P	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	Q	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	R	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	S	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	T	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	U	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	V	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	W	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	X	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	Y	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	Z	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	a	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	b	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	c	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	d	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	e	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	f	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	g	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	h	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	i	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	j	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	k	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	l	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	m	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	n	458/628 (73%)	439 (96%)	19 (4%)	30	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	p	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	q	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	r	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	s	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	t	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	u	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	v	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	w	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	x	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	y	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	z	458/628 (73%)	439 (96%)	19 (4%)	30	40
All	All	27480/37680 (73%)	26340 (96%)	1140 (4%)	34	40

All (1140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	219	ASP
1	A	246	THR
1	A	288	HIS
1	A	309	LYS
1	A	312	ASN
1	A	327	ASP
1	A	382	ASN
1	A	405	THR
1	A	430	LEU
1	A	455	THR
1	A	485	GLN
1	A	531	GLU
1	A	550	THR
1	A	597	THR
1	A	600	VAL
1	A	660	THR
1	A	703	ASN
1	A	716	THR
1	A	735	LEU
1	K	219	ASP
1	K	246	THR

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Mol	Chain	Res	Type
1	K	288	HIS
1	K	309	LYS
1	K	312	ASN
1	K	327	ASP
1	K	382	ASN
1	K	405	THR
1	K	430	LEU
1	K	455	THR
1	K	485	GLN
1	K	531	GLU
1	K	550	THR
1	K	597	THR
1	K	600	VAL
1	K	660	THR
1	K	703	ASN
1	K	716	THR
1	K	735	LEU
1	L	219	ASP
1	L	246	THR
1	L	288	HIS
1	L	309	LYS
1	L	312	ASN
1	L	327	ASP
1	L	382	ASN
1	L	405	THR
1	L	430	LEU
1	L	455	THR
1	L	485	GLN
1	L	531	GLU
1	L	550	THR
1	L	597	THR
1	L	600	VAL
1	L	660	THR
1	L	703	ASN
1	L	716	THR
1	L	735	LEU
1	M	219	ASP
1	M	246	THR
1	M	288	HIS
1	M	309	LYS
1	M	312	ASN
1	M	327	ASP

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Mol	Chain	Res	Type
1	M	382	ASN
1	M	405	THR
1	M	430	LEU
1	M	455	THR
1	M	485	GLN
1	M	531	GLU
1	M	550	THR
1	M	597	THR
1	M	600	VAL
1	M	660	THR
1	M	703	ASN
1	M	716	THR
1	M	735	LEU
1	N	219	ASP
1	N	246	THR
1	N	288	HIS
1	N	309	LYS
1	N	312	ASN
1	N	327	ASP
1	N	382	ASN
1	N	405	THR
1	N	430	LEU
1	N	455	THR
1	N	485	GLN
1	N	531	GLU
1	N	550	THR
1	N	597	THR
1	N	600	VAL
1	N	660	THR
1	N	703	ASN
1	N	716	THR
1	N	735	LEU
1	O	219	ASP
1	O	246	THR
1	O	288	HIS
1	O	309	LYS
1	O	312	ASN
1	O	327	ASP
1	O	382	ASN
1	O	405	THR
1	O	430	LEU
1	O	455	THR

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Mol	Chain	Res	Type
1	O	485	GLN
1	O	531	GLU
1	O	550	THR
1	O	597	THR
1	O	600	VAL
1	O	660	THR
1	O	703	ASN
1	O	716	THR
1	O	735	LEU
1	P	219	ASP
1	P	246	THR
1	P	288	HIS
1	P	309	LYS
1	P	312	ASN
1	P	327	ASP
1	P	382	ASN
1	P	405	THR
1	P	430	LEU
1	P	455	THR
1	P	485	GLN
1	P	531	GLU
1	P	550	THR
1	P	597	THR
1	P	600	VAL
1	P	660	THR
1	P	703	ASN
1	P	716	THR
1	P	735	LEU
1	Q	219	ASP
1	Q	246	THR
1	Q	288	HIS
1	Q	309	LYS
1	Q	312	ASN
1	Q	327	ASP
1	Q	382	ASN
1	Q	405	THR
1	Q	430	LEU
1	Q	455	THR
1	Q	485	GLN
1	Q	531	GLU
1	Q	550	THR
1	Q	597	THR

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Mol	Chain	Res	Type
1	Q	600	VAL
1	Q	660	THR
1	Q	703	ASN
1	Q	716	THR
1	Q	735	LEU
1	R	219	ASP
1	R	246	THR
1	R	288	HIS
1	R	309	LYS
1	R	312	ASN
1	R	327	ASP
1	R	382	ASN
1	R	405	THR
1	R	430	LEU
1	R	455	THR
1	R	485	GLN
1	R	531	GLU
1	R	550	THR
1	R	597	THR
1	R	600	VAL
1	R	660	THR
1	R	703	ASN
1	R	716	THR
1	R	735	LEU
1	S	219	ASP
1	S	246	THR
1	S	288	HIS
1	S	309	LYS
1	S	312	ASN
1	S	327	ASP
1	S	382	ASN
1	S	405	THR
1	S	430	LEU
1	S	455	THR
1	S	485	GLN
1	S	531	GLU
1	S	550	THR
1	S	597	THR
1	S	600	VAL
1	S	660	THR
1	S	703	ASN
1	S	716	THR

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Mol	Chain	Res	Type
1	S	735	LEU
1	T	219	ASP
1	T	246	THR
1	T	288	HIS
1	T	309	LYS
1	T	312	ASN
1	T	327	ASP
1	T	382	ASN
1	T	405	THR
1	T	430	LEU
1	T	455	THR
1	T	485	GLN
1	T	531	GLU
1	T	550	THR
1	T	597	THR
1	T	600	VAL
1	T	660	THR
1	T	703	ASN
1	T	716	THR
1	T	735	LEU
1	B	219	ASP
1	B	246	THR
1	B	288	HIS
1	B	309	LYS
1	B	312	ASN
1	B	327	ASP
1	B	382	ASN
1	B	405	THR
1	B	430	LEU
1	B	455	THR
1	B	485	GLN
1	B	531	GLU
1	B	550	THR
1	B	597	THR
1	B	600	VAL
1	B	660	THR
1	B	703	ASN
1	B	716	THR
1	B	735	LEU
1	U	219	ASP
1	U	246	THR
1	U	288	HIS

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Mol	Chain	Res	Type
1	U	309	LYS
1	U	312	ASN
1	U	327	ASP
1	U	382	ASN
1	U	405	THR
1	U	430	LEU
1	U	455	THR
1	U	485	GLN
1	U	531	GLU
1	U	550	THR
1	U	597	THR
1	U	600	VAL
1	U	660	THR
1	U	703	ASN
1	U	716	THR
1	U	735	LEU
1	V	219	ASP
1	V	246	THR
1	V	288	HIS
1	V	309	LYS
1	V	312	ASN
1	V	327	ASP
1	V	382	ASN
1	V	405	THR
1	V	430	LEU
1	V	455	THR
1	V	485	GLN
1	V	531	GLU
1	V	550	THR
1	V	597	THR
1	V	600	VAL
1	V	660	THR
1	V	703	ASN
1	V	716	THR
1	V	735	LEU
1	W	219	ASP
1	W	246	THR
1	W	288	HIS
1	W	309	LYS
1	W	312	ASN
1	W	327	ASP
1	W	382	ASN

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Mol	Chain	Res	Type
1	W	405	THR
1	W	430	LEU
1	W	455	THR
1	W	485	GLN
1	W	531	GLU
1	W	550	THR
1	W	597	THR
1	W	600	VAL
1	W	660	THR
1	W	703	ASN
1	W	716	THR
1	W	735	LEU
1	X	219	ASP
1	X	246	THR
1	X	288	HIS
1	X	309	LYS
1	X	312	ASN
1	X	327	ASP
1	X	382	ASN
1	X	405	THR
1	X	430	LEU
1	X	455	THR
1	X	485	GLN
1	X	531	GLU
1	X	550	THR
1	X	597	THR
1	X	600	VAL
1	X	660	THR
1	X	703	ASN
1	X	716	THR
1	X	735	LEU
1	Y	219	ASP
1	Y	246	THR
1	Y	288	HIS
1	Y	309	LYS
1	Y	312	ASN
1	Y	327	ASP
1	Y	382	ASN
1	Y	405	THR
1	Y	430	LEU
1	Y	455	THR
1	Y	485	GLN

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Mol	Chain	Res	Type
1	Y	531	GLU
1	Y	550	THR
1	Y	597	THR
1	Y	600	VAL
1	Y	660	THR
1	Y	703	ASN
1	Y	716	THR
1	Y	735	LEU
1	Z	219	ASP
1	Z	246	THR
1	Z	288	HIS
1	Z	309	LYS
1	Z	312	ASN
1	Z	327	ASP
1	Z	382	ASN
1	Z	405	THR
1	Z	430	LEU
1	Z	455	THR
1	Z	485	GLN
1	Z	531	GLU
1	Z	550	THR
1	Z	597	THR
1	Z	600	VAL
1	Z	660	THR
1	Z	703	ASN
1	Z	716	THR
1	Z	735	LEU
1	a	219	ASP
1	a	246	THR
1	a	288	HIS
1	a	309	LYS
1	a	312	ASN
1	a	327	ASP
1	a	382	ASN
1	a	405	THR
1	a	430	LEU
1	a	455	THR
1	a	485	GLN
1	a	531	GLU
1	a	550	THR
1	a	597	THR
1	a	600	VAL

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Mol	Chain	Res	Type
1	a	660	THR
1	a	703	ASN
1	a	716	THR
1	a	735	LEU
1	b	219	ASP
1	b	246	THR
1	b	288	HIS
1	b	309	LYS
1	b	312	ASN
1	b	327	ASP
1	b	382	ASN
1	b	405	THR
1	b	430	LEU
1	b	455	THR
1	b	485	GLN
1	b	531	GLU
1	b	550	THR
1	b	597	THR
1	b	600	VAL
1	b	660	THR
1	b	703	ASN
1	b	716	THR
1	b	735	LEU
1	c	219	ASP
1	c	246	THR
1	c	288	HIS
1	c	309	LYS
1	c	312	ASN
1	c	327	ASP
1	c	382	ASN
1	c	405	THR
1	c	430	LEU
1	c	455	THR
1	c	485	GLN
1	c	531	GLU
1	c	550	THR
1	c	597	THR
1	c	600	VAL
1	c	660	THR
1	c	703	ASN
1	c	716	THR
1	c	735	LEU

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Mol	Chain	Res	Type
1	d	219	ASP
1	d	246	THR
1	d	288	HIS
1	d	309	LYS
1	d	312	ASN
1	d	327	ASP
1	d	382	ASN
1	d	405	THR
1	d	430	LEU
1	d	455	THR
1	d	485	GLN
1	d	531	GLU
1	d	550	THR
1	d	597	THR
1	d	600	VAL
1	d	660	THR
1	d	703	ASN
1	d	716	THR
1	d	735	LEU
1	C	219	ASP
1	C	246	THR
1	C	288	HIS
1	C	309	LYS
1	C	312	ASN
1	C	327	ASP
1	C	382	ASN
1	C	405	THR
1	C	430	LEU
1	C	455	THR
1	C	485	GLN
1	C	531	GLU
1	C	550	THR
1	C	597	THR
1	C	600	VAL
1	C	660	THR
1	C	703	ASN
1	C	716	THR
1	C	735	LEU
1	e	219	ASP
1	e	246	THR
1	e	288	HIS
1	e	309	LYS

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Mol	Chain	Res	Type
1	e	312	ASN
1	e	327	ASP
1	e	382	ASN
1	e	405	THR
1	e	430	LEU
1	e	455	THR
1	e	485	GLN
1	e	531	GLU
1	e	550	THR
1	e	597	THR
1	e	600	VAL
1	e	660	THR
1	e	703	ASN
1	e	716	THR
1	e	735	LEU
1	f	219	ASP
1	f	246	THR
1	f	288	HIS
1	f	309	LYS
1	f	312	ASN
1	f	327	ASP
1	f	382	ASN
1	f	405	THR
1	f	430	LEU
1	f	455	THR
1	f	485	GLN
1	f	531	GLU
1	f	550	THR
1	f	597	THR
1	f	600	VAL
1	f	660	THR
1	f	703	ASN
1	f	716	THR
1	f	735	LEU
1	g	219	ASP
1	g	246	THR
1	g	288	HIS
1	g	309	LYS
1	g	312	ASN
1	g	327	ASP
1	g	382	ASN
1	g	405	THR

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Mol	Chain	Res	Type
1	g	430	LEU
1	g	455	THR
1	g	485	GLN
1	g	531	GLU
1	g	550	THR
1	g	597	THR
1	g	600	VAL
1	g	660	THR
1	g	703	ASN
1	g	716	THR
1	g	735	LEU
1	h	219	ASP
1	h	246	THR
1	h	288	HIS
1	h	309	LYS
1	h	312	ASN
1	h	327	ASP
1	h	382	ASN
1	h	405	THR
1	h	430	LEU
1	h	455	THR
1	h	485	GLN
1	h	531	GLU
1	h	550	THR
1	h	597	THR
1	h	600	VAL
1	h	660	THR
1	h	703	ASN
1	h	716	THR
1	h	735	LEU
1	i	219	ASP
1	i	246	THR
1	i	288	HIS
1	i	309	LYS
1	i	312	ASN
1	i	327	ASP
1	i	382	ASN
1	i	405	THR
1	i	430	LEU
1	i	455	THR
1	i	485	GLN
1	i	531	GLU

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Mol	Chain	Res	Type
1	i	550	THR
1	i	597	THR
1	i	600	VAL
1	i	660	THR
1	i	703	ASN
1	i	716	THR
1	i	735	LEU
1	j	219	ASP
1	j	246	THR
1	j	288	HIS
1	j	309	LYS
1	j	312	ASN
1	j	327	ASP
1	j	382	ASN
1	j	405	THR
1	j	430	LEU
1	j	455	THR
1	j	485	GLN
1	j	531	GLU
1	j	550	THR
1	j	597	THR
1	j	600	VAL
1	j	660	THR
1	j	703	ASN
1	j	716	THR
1	j	735	LEU
1	k	219	ASP
1	k	246	THR
1	k	288	HIS
1	k	309	LYS
1	k	312	ASN
1	k	327	ASP
1	k	382	ASN
1	k	405	THR
1	k	430	LEU
1	k	455	THR
1	k	485	GLN
1	k	531	GLU
1	k	550	THR
1	k	597	THR
1	k	600	VAL
1	k	660	THR

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Mol	Chain	Res	Type
1	k	703	ASN
1	k	716	THR
1	k	735	LEU
1	l	219	ASP
1	l	246	THR
1	l	288	HIS
1	l	309	LYS
1	l	312	ASN
1	l	327	ASP
1	l	382	ASN
1	l	405	THR
1	l	430	LEU
1	l	455	THR
1	l	485	GLN
1	l	531	GLU
1	l	550	THR
1	l	597	THR
1	l	600	VAL
1	l	660	THR
1	l	703	ASN
1	l	716	THR
1	l	735	LEU
1	m	219	ASP
1	m	246	THR
1	m	288	HIS
1	m	309	LYS
1	m	312	ASN
1	m	327	ASP
1	m	382	ASN
1	m	405	THR
1	m	430	LEU
1	m	455	THR
1	m	485	GLN
1	m	531	GLU
1	m	550	THR
1	m	597	THR
1	m	600	VAL
1	m	660	THR
1	m	703	ASN
1	m	716	THR
1	m	735	LEU
1	n	219	ASP

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Mol	Chain	Res	Type
1	n	246	THR
1	n	288	HIS
1	n	309	LYS
1	n	312	ASN
1	n	327	ASP
1	n	382	ASN
1	n	405	THR
1	n	430	LEU
1	n	455	THR
1	n	485	GLN
1	n	531	GLU
1	n	550	THR
1	n	597	THR
1	n	600	VAL
1	n	660	THR
1	n	703	ASN
1	n	716	THR
1	n	735	LEU
1	D	219	ASP
1	D	246	THR
1	D	288	HIS
1	D	309	LYS
1	D	312	ASN
1	D	327	ASP
1	D	382	ASN
1	D	405	THR
1	D	430	LEU
1	D	455	THR
1	D	485	GLN
1	D	531	GLU
1	D	550	THR
1	D	597	THR
1	D	600	VAL
1	D	660	THR
1	D	703	ASN
1	D	716	THR
1	D	735	LEU
1	o	219	ASP
1	o	246	THR
1	o	288	HIS
1	o	309	LYS
1	o	312	ASN

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Mol	Chain	Res	Type
1	o	327	ASP
1	o	382	ASN
1	o	405	THR
1	o	430	LEU
1	o	455	THR
1	o	485	GLN
1	o	531	GLU
1	o	550	THR
1	o	597	THR
1	o	600	VAL
1	o	660	THR
1	o	703	ASN
1	o	716	THR
1	o	735	LEU
1	p	219	ASP
1	p	246	THR
1	p	288	HIS
1	p	309	LYS
1	p	312	ASN
1	p	327	ASP
1	p	382	ASN
1	p	405	THR
1	p	430	LEU
1	p	455	THR
1	p	485	GLN
1	p	531	GLU
1	p	550	THR
1	p	597	THR
1	p	600	VAL
1	p	660	THR
1	p	703	ASN
1	p	716	THR
1	p	735	LEU
1	q	219	ASP
1	q	246	THR
1	q	288	HIS
1	q	309	LYS
1	q	312	ASN
1	q	327	ASP
1	q	382	ASN
1	q	405	THR
1	q	430	LEU

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Mol	Chain	Res	Type
1	q	455	THR
1	q	485	GLN
1	q	531	GLU
1	q	550	THR
1	q	597	THR
1	q	600	VAL
1	q	660	THR
1	q	703	ASN
1	q	716	THR
1	q	735	LEU
1	r	219	ASP
1	r	246	THR
1	r	288	HIS
1	r	309	LYS
1	r	312	ASN
1	r	327	ASP
1	r	382	ASN
1	r	405	THR
1	r	430	LEU
1	r	455	THR
1	r	485	GLN
1	r	531	GLU
1	r	550	THR
1	r	597	THR
1	r	600	VAL
1	r	660	THR
1	r	703	ASN
1	r	716	THR
1	r	735	LEU
1	s	219	ASP
1	s	246	THR
1	s	288	HIS
1	s	309	LYS
1	s	312	ASN
1	s	327	ASP
1	s	382	ASN
1	s	405	THR
1	s	430	LEU
1	s	455	THR
1	s	485	GLN
1	s	531	GLU
1	s	550	THR

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Mol	Chain	Res	Type
1	s	597	THR
1	s	600	VAL
1	s	660	THR
1	s	703	ASN
1	s	716	THR
1	s	735	LEU
1	t	219	ASP
1	t	246	THR
1	t	288	HIS
1	t	309	LYS
1	t	312	ASN
1	t	327	ASP
1	t	382	ASN
1	t	405	THR
1	t	430	LEU
1	t	455	THR
1	t	485	GLN
1	t	531	GLU
1	t	550	THR
1	t	597	THR
1	t	600	VAL
1	t	660	THR
1	t	703	ASN
1	t	716	THR
1	t	735	LEU
1	u	219	ASP
1	u	246	THR
1	u	288	HIS
1	u	309	LYS
1	u	312	ASN
1	u	327	ASP
1	u	382	ASN
1	u	405	THR
1	u	430	LEU
1	u	455	THR
1	u	485	GLN
1	u	531	GLU
1	u	550	THR
1	u	597	THR
1	u	600	VAL
1	u	660	THR
1	u	703	ASN

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Mol	Chain	Res	Type
1	u	716	THR
1	u	735	LEU
1	v	219	ASP
1	v	246	THR
1	v	288	HIS
1	v	309	LYS
1	v	312	ASN
1	v	327	ASP
1	v	382	ASN
1	v	405	THR
1	v	430	LEU
1	v	455	THR
1	v	485	GLN
1	v	531	GLU
1	v	550	THR
1	v	597	THR
1	v	600	VAL
1	v	660	THR
1	v	703	ASN
1	v	716	THR
1	v	735	LEU
1	w	219	ASP
1	w	246	THR
1	w	288	HIS
1	w	309	LYS
1	w	312	ASN
1	w	327	ASP
1	w	382	ASN
1	w	405	THR
1	w	430	LEU
1	w	455	THR
1	w	485	GLN
1	w	531	GLU
1	w	550	THR
1	w	597	THR
1	w	600	VAL
1	w	660	THR
1	w	703	ASN
1	w	716	THR
1	w	735	LEU
1	x	219	ASP
1	x	246	THR

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Mol	Chain	Res	Type
1	x	288	HIS
1	x	309	LYS
1	x	312	ASN
1	x	327	ASP
1	x	382	ASN
1	x	405	THR
1	x	430	LEU
1	x	455	THR
1	x	485	GLN
1	x	531	GLU
1	x	550	THR
1	x	597	THR
1	x	600	VAL
1	x	660	THR
1	x	703	ASN
1	x	716	THR
1	x	735	LEU
1	E	219	ASP
1	E	246	THR
1	E	288	HIS
1	E	309	LYS
1	E	312	ASN
1	E	327	ASP
1	E	382	ASN
1	E	405	THR
1	E	430	LEU
1	E	455	THR
1	E	485	GLN
1	E	531	GLU
1	E	550	THR
1	E	597	THR
1	E	600	VAL
1	E	660	THR
1	E	703	ASN
1	E	716	THR
1	E	735	LEU
1	y	219	ASP
1	y	246	THR
1	y	288	HIS
1	y	309	LYS
1	y	312	ASN
1	y	327	ASP

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Mol	Chain	Res	Type
1	y	382	ASN
1	y	405	THR
1	y	430	LEU
1	y	455	THR
1	y	485	GLN
1	y	531	GLU
1	y	550	THR
1	y	597	THR
1	y	600	VAL
1	y	660	THR
1	y	703	ASN
1	y	716	THR
1	y	735	LEU
1	z	219	ASP
1	z	246	THR
1	z	288	HIS
1	z	309	LYS
1	z	312	ASN
1	z	327	ASP
1	z	382	ASN
1	z	405	THR
1	z	430	LEU
1	z	455	THR
1	z	485	GLN
1	z	531	GLU
1	z	550	THR
1	z	597	THR
1	z	600	VAL
1	z	660	THR
1	z	703	ASN
1	z	716	THR
1	z	735	LEU
1	0	219	ASP
1	0	246	THR
1	0	288	HIS
1	0	309	LYS
1	0	312	ASN
1	0	327	ASP
1	0	382	ASN
1	0	405	THR
1	0	430	LEU
1	0	455	THR

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Mol	Chain	Res	Type
1	0	485	GLN
1	0	531	GLU
1	0	550	THR
1	0	597	THR
1	0	600	VAL
1	0	660	THR
1	0	703	ASN
1	0	716	THR
1	0	735	LEU
1	1	219	ASP
1	1	246	THR
1	1	288	HIS
1	1	309	LYS
1	1	312	ASN
1	1	327	ASP
1	1	382	ASN
1	1	405	THR
1	1	430	LEU
1	1	455	THR
1	1	485	GLN
1	1	531	GLU
1	1	550	THR
1	1	597	THR
1	1	600	VAL
1	1	660	THR
1	1	703	ASN
1	1	716	THR
1	1	735	LEU
1	2	219	ASP
1	2	246	THR
1	2	288	HIS
1	2	309	LYS
1	2	312	ASN
1	2	327	ASP
1	2	382	ASN
1	2	405	THR
1	2	430	LEU
1	2	455	THR
1	2	485	GLN
1	2	531	GLU
1	2	550	THR
1	2	597	THR

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Mol	Chain	Res	Type
1	2	600	VAL
1	2	660	THR
1	2	703	ASN
1	2	716	THR
1	2	735	LEU
1	3	219	ASP
1	3	246	THR
1	3	288	HIS
1	3	309	LYS
1	3	312	ASN
1	3	327	ASP
1	3	382	ASN
1	3	405	THR
1	3	430	LEU
1	3	455	THR
1	3	485	GLN
1	3	531	GLU
1	3	550	THR
1	3	597	THR
1	3	600	VAL
1	3	660	THR
1	3	703	ASN
1	3	716	THR
1	3	735	LEU
1	4	219	ASP
1	4	246	THR
1	4	288	HIS
1	4	309	LYS
1	4	312	ASN
1	4	327	ASP
1	4	382	ASN
1	4	405	THR
1	4	430	LEU
1	4	455	THR
1	4	485	GLN
1	4	531	GLU
1	4	550	THR
1	4	597	THR
1	4	600	VAL
1	4	660	THR
1	4	703	ASN
1	4	716	THR

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Mol	Chain	Res	Type
1	4	735	LEU
1	5	219	ASP
1	5	246	THR
1	5	288	HIS
1	5	309	LYS
1	5	312	ASN
1	5	327	ASP
1	5	382	ASN
1	5	405	THR
1	5	430	LEU
1	5	455	THR
1	5	485	GLN
1	5	531	GLU
1	5	550	THR
1	5	597	THR
1	5	600	VAL
1	5	660	THR
1	5	703	ASN
1	5	716	THR
1	5	735	LEU
1	6	219	ASP
1	6	246	THR
1	6	288	HIS
1	6	309	LYS
1	6	312	ASN
1	6	327	ASP
1	6	382	ASN
1	6	405	THR
1	6	430	LEU
1	6	455	THR
1	6	485	GLN
1	6	531	GLU
1	6	550	THR
1	6	597	THR
1	6	600	VAL
1	6	660	THR
1	6	703	ASN
1	6	716	THR
1	6	735	LEU
1	7	219	ASP
1	7	246	THR
1	7	288	HIS

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Mol	Chain	Res	Type
1	7	309	LYS
1	7	312	ASN
1	7	327	ASP
1	7	382	ASN
1	7	405	THR
1	7	430	LEU
1	7	455	THR
1	7	485	GLN
1	7	531	GLU
1	7	550	THR
1	7	597	THR
1	7	600	VAL
1	7	660	THR
1	7	703	ASN
1	7	716	THR
1	7	735	LEU
1	F	219	ASP
1	F	246	THR
1	F	288	HIS
1	F	309	LYS
1	F	312	ASN
1	F	327	ASP
1	F	382	ASN
1	F	405	THR
1	F	430	LEU
1	F	455	THR
1	F	485	GLN
1	F	531	GLU
1	F	550	THR
1	F	597	THR
1	F	600	VAL
1	F	660	THR
1	F	703	ASN
1	F	716	THR
1	F	735	LEU
1	G	219	ASP
1	G	246	THR
1	G	288	HIS
1	G	309	LYS
1	G	312	ASN
1	G	327	ASP
1	G	382	ASN

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Mol	Chain	Res	Type
1	G	405	THR
1	G	430	LEU
1	G	455	THR
1	G	485	GLN
1	G	531	GLU
1	G	550	THR
1	G	597	THR
1	G	600	VAL
1	G	660	THR
1	G	703	ASN
1	G	716	THR
1	G	735	LEU
1	H	219	ASP
1	H	246	THR
1	H	288	HIS
1	H	309	LYS
1	H	312	ASN
1	H	327	ASP
1	H	382	ASN
1	H	405	THR
1	H	430	LEU
1	H	455	THR
1	H	485	GLN
1	H	531	GLU
1	H	550	THR
1	H	597	THR
1	H	600	VAL
1	H	660	THR
1	H	703	ASN
1	H	716	THR
1	H	735	LEU
1	I	219	ASP
1	I	246	THR
1	I	288	HIS
1	I	309	LYS
1	I	312	ASN
1	I	327	ASP
1	I	382	ASN
1	I	405	THR
1	I	430	LEU
1	I	455	THR
1	I	485	GLN

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Mol	Chain	Res	Type
1	I	531	GLU
1	I	550	THR
1	I	597	THR
1	I	600	VAL
1	I	660	THR
1	I	703	ASN
1	I	716	THR
1	I	735	LEU
1	J	219	ASP
1	J	246	THR
1	J	288	HIS
1	J	309	LYS
1	J	312	ASN
1	J	327	ASP
1	J	382	ASN
1	J	405	THR
1	J	430	LEU
1	J	455	THR
1	J	485	GLN
1	J	531	GLU
1	J	550	THR
1	J	597	THR
1	J	600	VAL
1	J	660	THR
1	J	703	ASN
1	J	716	THR
1	J	735	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (858) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	GLN
1	A	270	ASN
1	A	303	ASN
1	A	325	GLN
1	A	334	ASN
1	A	359	GLN
1	A	382	ASN
1	A	385	GLN
1	A	485	GLN
1	A	509	HIS
1	A	536	GLN

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Mol	Chain	Res	Type
1	A	589	GLN
1	A	677	GLN
1	A	709	ASN
1	K	259	GLN
1	K	263	GLN
1	K	270	ASN
1	K	303	ASN
1	K	325	GLN
1	K	334	ASN
1	K	359	GLN
1	K	385	GLN
1	K	485	GLN
1	K	509	HIS
1	K	536	GLN
1	K	589	GLN
1	K	677	GLN
1	K	709	ASN
1	L	259	GLN
1	L	263	GLN
1	L	270	ASN
1	L	303	ASN
1	L	325	GLN
1	L	334	ASN
1	L	359	GLN
1	L	385	GLN
1	L	485	GLN
1	L	509	HIS
1	L	536	GLN
1	L	589	GLN
1	L	677	GLN
1	L	709	ASN
1	M	259	GLN
1	M	263	GLN
1	M	270	ASN
1	M	303	ASN
1	M	325	GLN
1	M	334	ASN
1	M	359	GLN
1	M	385	GLN
1	M	485	GLN
1	M	509	HIS
1	M	536	GLN

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Mol	Chain	Res	Type
1	M	589	GLN
1	M	677	GLN
1	M	709	ASN
1	N	259	GLN
1	N	263	GLN
1	N	270	ASN
1	N	303	ASN
1	N	325	GLN
1	N	334	ASN
1	N	359	GLN
1	N	385	GLN
1	N	485	GLN
1	N	509	HIS
1	N	536	GLN
1	N	589	GLN
1	N	677	GLN
1	N	709	ASN
1	O	259	GLN
1	O	263	GLN
1	O	270	ASN
1	O	303	ASN
1	O	325	GLN
1	O	334	ASN
1	O	359	GLN
1	O	385	GLN
1	O	485	GLN
1	O	509	HIS
1	O	536	GLN
1	O	589	GLN
1	O	677	GLN
1	O	709	ASN
1	P	259	GLN
1	P	263	GLN
1	P	270	ASN
1	P	303	ASN
1	P	325	GLN
1	P	334	ASN
1	P	359	GLN
1	P	385	GLN
1	P	485	GLN
1	P	509	HIS
1	P	518	ASN

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Mol	Chain	Res	Type
1	P	536	GLN
1	P	589	GLN
1	P	677	GLN
1	P	709	ASN
1	Q	259	GLN
1	Q	263	GLN
1	Q	270	ASN
1	Q	303	ASN
1	Q	325	GLN
1	Q	334	ASN
1	Q	359	GLN
1	Q	382	ASN
1	Q	385	GLN
1	Q	485	GLN
1	Q	509	HIS
1	Q	536	GLN
1	Q	589	GLN
1	Q	677	GLN
1	Q	709	ASN
1	R	259	GLN
1	R	263	GLN
1	R	270	ASN
1	R	303	ASN
1	R	325	GLN
1	R	334	ASN
1	R	359	GLN
1	R	382	ASN
1	R	385	GLN
1	R	485	GLN
1	R	509	HIS
1	R	536	GLN
1	R	589	GLN
1	R	677	GLN
1	R	709	ASN
1	S	259	GLN
1	S	263	GLN
1	S	270	ASN
1	S	303	ASN
1	S	325	GLN
1	S	334	ASN
1	S	359	GLN
1	S	385	GLN

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Mol	Chain	Res	Type
1	S	485	GLN
1	S	509	HIS
1	S	536	GLN
1	S	589	GLN
1	S	677	GLN
1	S	709	ASN
1	T	259	GLN
1	T	263	GLN
1	T	270	ASN
1	T	303	ASN
1	T	325	GLN
1	T	334	ASN
1	T	359	GLN
1	T	385	GLN
1	T	485	GLN
1	T	509	HIS
1	T	536	GLN
1	T	589	GLN
1	T	677	GLN
1	T	709	ASN
1	B	259	GLN
1	B	263	GLN
1	B	270	ASN
1	B	303	ASN
1	B	325	GLN
1	B	334	ASN
1	B	359	GLN
1	B	385	GLN
1	B	485	GLN
1	B	509	HIS
1	B	536	GLN
1	B	589	GLN
1	B	677	GLN
1	B	709	ASN
1	U	263	GLN
1	U	270	ASN
1	U	303	ASN
1	U	325	GLN
1	U	334	ASN
1	U	359	GLN
1	U	382	ASN
1	U	385	GLN

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Mol	Chain	Res	Type
1	U	485	GLN
1	U	509	HIS
1	U	536	GLN
1	U	589	GLN
1	U	677	GLN
1	U	709	ASN
1	V	259	GLN
1	V	263	GLN
1	V	270	ASN
1	V	303	ASN
1	V	325	GLN
1	V	334	ASN
1	V	359	GLN
1	V	385	GLN
1	V	485	GLN
1	V	509	HIS
1	V	536	GLN
1	V	589	GLN
1	V	677	GLN
1	V	709	ASN
1	W	259	GLN
1	W	263	GLN
1	W	270	ASN
1	W	303	ASN
1	W	325	GLN
1	W	334	ASN
1	W	359	GLN
1	W	382	ASN
1	W	385	GLN
1	W	485	GLN
1	W	509	HIS
1	W	536	GLN
1	W	589	GLN
1	W	677	GLN
1	W	709	ASN
1	X	259	GLN
1	X	263	GLN
1	X	270	ASN
1	X	303	ASN
1	X	325	GLN
1	X	334	ASN
1	X	359	GLN

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Mol	Chain	Res	Type
1	X	385	GLN
1	X	485	GLN
1	X	509	HIS
1	X	536	GLN
1	X	589	GLN
1	X	677	GLN
1	X	709	ASN
1	Y	259	GLN
1	Y	263	GLN
1	Y	270	ASN
1	Y	303	ASN
1	Y	325	GLN
1	Y	334	ASN
1	Y	359	GLN
1	Y	385	GLN
1	Y	485	GLN
1	Y	509	HIS
1	Y	536	GLN
1	Y	589	GLN
1	Y	677	GLN
1	Y	709	ASN
1	Z	259	GLN
1	Z	263	GLN
1	Z	270	ASN
1	Z	303	ASN
1	Z	325	GLN
1	Z	334	ASN
1	Z	359	GLN
1	Z	385	GLN
1	Z	485	GLN
1	Z	509	HIS
1	Z	536	GLN
1	Z	589	GLN
1	Z	677	GLN
1	Z	709	ASN
1	a	259	GLN
1	a	263	GLN
1	a	270	ASN
1	a	303	ASN
1	a	325	GLN
1	a	334	ASN
1	a	359	GLN

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Mol	Chain	Res	Type
1	a	382	ASN
1	a	385	GLN
1	a	485	GLN
1	a	509	HIS
1	a	536	GLN
1	a	589	GLN
1	a	677	GLN
1	a	709	ASN
1	b	259	GLN
1	b	263	GLN
1	b	270	ASN
1	b	303	ASN
1	b	325	GLN
1	b	334	ASN
1	b	359	GLN
1	b	385	GLN
1	b	485	GLN
1	b	509	HIS
1	b	536	GLN
1	b	589	GLN
1	b	677	GLN
1	b	709	ASN
1	c	259	GLN
1	c	263	GLN
1	c	270	ASN
1	c	303	ASN
1	c	325	GLN
1	c	334	ASN
1	c	359	GLN
1	c	385	GLN
1	c	485	GLN
1	c	509	HIS
1	c	536	GLN
1	c	589	GLN
1	c	677	GLN
1	c	709	ASN
1	d	259	GLN
1	d	263	GLN
1	d	270	ASN
1	d	303	ASN
1	d	325	GLN
1	d	334	ASN

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Mol	Chain	Res	Type
1	d	359	GLN
1	d	385	GLN
1	d	485	GLN
1	d	509	HIS
1	d	536	GLN
1	d	589	GLN
1	d	677	GLN
1	d	709	ASN
1	C	259	GLN
1	C	263	GLN
1	C	270	ASN
1	C	303	ASN
1	C	325	GLN
1	C	334	ASN
1	C	359	GLN
1	C	385	GLN
1	C	485	GLN
1	C	509	HIS
1	C	536	GLN
1	C	589	GLN
1	C	677	GLN
1	C	709	ASN
1	e	259	GLN
1	e	263	GLN
1	e	270	ASN
1	e	303	ASN
1	e	325	GLN
1	e	334	ASN
1	e	359	GLN
1	e	385	GLN
1	e	485	GLN
1	e	509	HIS
1	e	536	GLN
1	e	589	GLN
1	e	677	GLN
1	e	709	ASN
1	f	259	GLN
1	f	263	GLN
1	f	270	ASN
1	f	303	ASN
1	f	325	GLN
1	f	334	ASN

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Mol	Chain	Res	Type
1	f	359	GLN
1	f	385	GLN
1	f	485	GLN
1	f	509	HIS
1	f	536	GLN
1	f	589	GLN
1	f	677	GLN
1	f	709	ASN
1	g	259	GLN
1	g	263	GLN
1	g	270	ASN
1	g	303	ASN
1	g	325	GLN
1	g	334	ASN
1	g	359	GLN
1	g	385	GLN
1	g	485	GLN
1	g	509	HIS
1	g	536	GLN
1	g	589	GLN
1	g	677	GLN
1	h	259	GLN
1	h	263	GLN
1	h	270	ASN
1	h	303	ASN
1	h	325	GLN
1	h	334	ASN
1	h	359	GLN
1	h	385	GLN
1	h	485	GLN
1	h	509	HIS
1	h	536	GLN
1	h	589	GLN
1	h	677	GLN
1	h	709	ASN
1	i	259	GLN
1	i	263	GLN
1	i	270	ASN
1	i	303	ASN
1	i	325	GLN
1	i	334	ASN
1	i	359	GLN

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Mol	Chain	Res	Type
1	i	382	ASN
1	i	385	GLN
1	i	485	GLN
1	i	509	HIS
1	i	536	GLN
1	i	589	GLN
1	i	677	GLN
1	i	709	ASN
1	j	259	GLN
1	j	263	GLN
1	j	270	ASN
1	j	303	ASN
1	j	325	GLN
1	j	334	ASN
1	j	359	GLN
1	j	385	GLN
1	j	485	GLN
1	j	509	HIS
1	j	536	GLN
1	j	589	GLN
1	j	677	GLN
1	j	709	ASN
1	k	259	GLN
1	k	263	GLN
1	k	270	ASN
1	k	303	ASN
1	k	325	GLN
1	k	334	ASN
1	k	359	GLN
1	k	385	GLN
1	k	485	GLN
1	k	509	HIS
1	k	536	GLN
1	k	589	GLN
1	k	677	GLN
1	k	709	ASN
1	l	259	GLN
1	l	263	GLN
1	l	270	ASN
1	l	303	ASN
1	l	325	GLN
1	l	334	ASN

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Mol	Chain	Res	Type
1	l	359	GLN
1	l	385	GLN
1	l	485	GLN
1	l	509	HIS
1	l	536	GLN
1	l	589	GLN
1	l	677	GLN
1	l	709	ASN
1	m	259	GLN
1	m	263	GLN
1	m	270	ASN
1	m	303	ASN
1	m	325	GLN
1	m	334	ASN
1	m	359	GLN
1	m	382	ASN
1	m	385	GLN
1	m	485	GLN
1	m	509	HIS
1	m	536	GLN
1	m	589	GLN
1	m	677	GLN
1	m	709	ASN
1	n	259	GLN
1	n	263	GLN
1	n	270	ASN
1	n	303	ASN
1	n	325	GLN
1	n	334	ASN
1	n	359	GLN
1	n	382	ASN
1	n	385	GLN
1	n	485	GLN
1	n	509	HIS
1	n	536	GLN
1	n	589	GLN
1	n	677	GLN
1	n	709	ASN
1	D	259	GLN
1	D	263	GLN
1	D	270	ASN
1	D	303	ASN

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Mol	Chain	Res	Type
1	D	325	GLN
1	D	334	ASN
1	D	359	GLN
1	D	385	GLN
1	D	485	GLN
1	D	509	HIS
1	D	536	GLN
1	D	589	GLN
1	D	677	GLN
1	D	709	ASN
1	o	259	GLN
1	o	263	GLN
1	o	270	ASN
1	o	303	ASN
1	o	325	GLN
1	o	334	ASN
1	o	359	GLN
1	o	382	ASN
1	o	385	GLN
1	o	485	GLN
1	o	509	HIS
1	o	536	GLN
1	o	589	GLN
1	o	677	GLN
1	o	709	ASN
1	p	259	GLN
1	p	263	GLN
1	p	270	ASN
1	p	303	ASN
1	p	325	GLN
1	p	334	ASN
1	p	359	GLN
1	p	385	GLN
1	p	485	GLN
1	p	509	HIS
1	p	536	GLN
1	p	589	GLN
1	p	677	GLN
1	p	709	ASN
1	q	259	GLN
1	q	263	GLN
1	q	270	ASN

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Mol	Chain	Res	Type
1	q	303	ASN
1	q	325	GLN
1	q	334	ASN
1	q	359	GLN
1	q	385	GLN
1	q	485	GLN
1	q	509	HIS
1	q	536	GLN
1	q	589	GLN
1	q	677	GLN
1	q	709	ASN
1	r	259	GLN
1	r	263	GLN
1	r	270	ASN
1	r	303	ASN
1	r	325	GLN
1	r	334	ASN
1	r	359	GLN
1	r	385	GLN
1	r	485	GLN
1	r	509	HIS
1	r	536	GLN
1	r	589	GLN
1	r	677	GLN
1	r	709	ASN
1	s	259	GLN
1	s	263	GLN
1	s	270	ASN
1	s	303	ASN
1	s	325	GLN
1	s	334	ASN
1	s	359	GLN
1	s	385	GLN
1	s	485	GLN
1	s	509	HIS
1	s	536	GLN
1	s	589	GLN
1	s	677	GLN
1	s	709	ASN
1	t	259	GLN
1	t	263	GLN
1	t	270	ASN

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Mol	Chain	Res	Type
1	t	303	ASN
1	t	325	GLN
1	t	334	ASN
1	t	359	GLN
1	t	382	ASN
1	t	385	GLN
1	t	485	GLN
1	t	509	HIS
1	t	536	GLN
1	t	589	GLN
1	t	677	GLN
1	t	709	ASN
1	u	259	GLN
1	u	263	GLN
1	u	270	ASN
1	u	303	ASN
1	u	325	GLN
1	u	334	ASN
1	u	359	GLN
1	u	385	GLN
1	u	485	GLN
1	u	509	HIS
1	u	536	GLN
1	u	589	GLN
1	u	677	GLN
1	u	709	ASN
1	v	259	GLN
1	v	263	GLN
1	v	270	ASN
1	v	303	ASN
1	v	325	GLN
1	v	334	ASN
1	v	359	GLN
1	v	385	GLN
1	v	485	GLN
1	v	509	HIS
1	v	536	GLN
1	v	589	GLN
1	v	677	GLN
1	v	709	ASN
1	w	259	GLN
1	w	263	GLN

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Mol	Chain	Res	Type
1	w	270	ASN
1	w	303	ASN
1	w	325	GLN
1	w	334	ASN
1	w	359	GLN
1	w	385	GLN
1	w	485	GLN
1	w	509	HIS
1	w	536	GLN
1	w	589	GLN
1	w	677	GLN
1	x	259	GLN
1	x	263	GLN
1	x	270	ASN
1	x	303	ASN
1	x	325	GLN
1	x	334	ASN
1	x	359	GLN
1	x	382	ASN
1	x	385	GLN
1	x	485	GLN
1	x	509	HIS
1	x	536	GLN
1	x	589	GLN
1	x	677	GLN
1	x	709	ASN
1	E	259	GLN
1	E	263	GLN
1	E	270	ASN
1	E	303	ASN
1	E	325	GLN
1	E	334	ASN
1	E	359	GLN
1	E	385	GLN
1	E	485	GLN
1	E	509	HIS
1	E	536	GLN
1	E	589	GLN
1	E	677	GLN
1	E	709	ASN
1	y	259	GLN
1	y	263	GLN

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Mol	Chain	Res	Type
1	y	270	ASN
1	y	303	ASN
1	y	325	GLN
1	y	334	ASN
1	y	359	GLN
1	y	385	GLN
1	y	485	GLN
1	y	509	HIS
1	y	536	GLN
1	y	589	GLN
1	y	677	GLN
1	y	709	ASN
1	z	259	GLN
1	z	263	GLN
1	z	270	ASN
1	z	303	ASN
1	z	325	GLN
1	z	334	ASN
1	z	359	GLN
1	z	382	ASN
1	z	385	GLN
1	z	485	GLN
1	z	509	HIS
1	z	536	GLN
1	z	589	GLN
1	z	677	GLN
1	z	709	ASN
1	0	259	GLN
1	0	263	GLN
1	0	270	ASN
1	0	303	ASN
1	0	325	GLN
1	0	334	ASN
1	0	359	GLN
1	0	382	ASN
1	0	385	GLN
1	0	485	GLN
1	0	509	HIS
1	0	518	ASN
1	0	536	GLN
1	0	589	GLN
1	0	677	GLN

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Mol	Chain	Res	Type
1	0	709	ASN
1	1	259	GLN
1	1	263	GLN
1	1	270	ASN
1	1	303	ASN
1	1	325	GLN
1	1	334	ASN
1	1	359	GLN
1	1	382	ASN
1	1	385	GLN
1	1	485	GLN
1	1	509	HIS
1	1	536	GLN
1	1	589	GLN
1	1	677	GLN
1	1	709	ASN
1	2	259	GLN
1	2	263	GLN
1	2	270	ASN
1	2	303	ASN
1	2	325	GLN
1	2	334	ASN
1	2	359	GLN
1	2	385	GLN
1	2	485	GLN
1	2	509	HIS
1	2	536	GLN
1	2	589	GLN
1	2	677	GLN
1	2	709	ASN
1	3	259	GLN
1	3	263	GLN
1	3	270	ASN
1	3	303	ASN
1	3	325	GLN
1	3	334	ASN
1	3	359	GLN
1	3	385	GLN
1	3	485	GLN
1	3	509	HIS
1	3	536	GLN
1	3	589	GLN

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Mol	Chain	Res	Type
1	3	677	GLN
1	3	709	ASN
1	4	259	GLN
1	4	263	GLN
1	4	270	ASN
1	4	303	ASN
1	4	325	GLN
1	4	334	ASN
1	4	359	GLN
1	4	382	ASN
1	4	385	GLN
1	4	485	GLN
1	4	509	HIS
1	4	536	GLN
1	4	589	GLN
1	4	677	GLN
1	4	709	ASN
1	5	259	GLN
1	5	263	GLN
1	5	270	ASN
1	5	303	ASN
1	5	325	GLN
1	5	334	ASN
1	5	359	GLN
1	5	382	ASN
1	5	385	GLN
1	5	485	GLN
1	5	509	HIS
1	5	536	GLN
1	5	589	GLN
1	5	677	GLN
1	5	709	ASN
1	6	259	GLN
1	6	263	GLN
1	6	270	ASN
1	6	303	ASN
1	6	325	GLN
1	6	334	ASN
1	6	359	GLN
1	6	385	GLN
1	6	485	GLN
1	6	509	HIS

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Mol	Chain	Res	Type
1	6	536	GLN
1	6	589	GLN
1	6	677	GLN
1	6	709	ASN
1	7	259	GLN
1	7	263	GLN
1	7	270	ASN
1	7	303	ASN
1	7	325	GLN
1	7	334	ASN
1	7	359	GLN
1	7	382	ASN
1	7	385	GLN
1	7	485	GLN
1	7	509	HIS
1	7	536	GLN
1	7	589	GLN
1	7	677	GLN
1	7	709	ASN
1	F	259	GLN
1	F	263	GLN
1	F	270	ASN
1	F	303	ASN
1	F	325	GLN
1	F	334	ASN
1	F	359	GLN
1	F	385	GLN
1	F	485	GLN
1	F	509	HIS
1	F	536	GLN
1	F	589	GLN
1	F	677	GLN
1	F	709	ASN
1	G	259	GLN
1	G	263	GLN
1	G	270	ASN
1	G	303	ASN
1	G	325	GLN
1	G	334	ASN
1	G	359	GLN
1	G	382	ASN
1	G	385	GLN

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Mol	Chain	Res	Type
1	G	485	GLN
1	G	509	HIS
1	G	536	GLN
1	G	589	GLN
1	G	677	GLN
1	G	709	ASN
1	H	259	GLN
1	H	263	GLN
1	H	270	ASN
1	H	303	ASN
1	H	325	GLN
1	H	334	ASN
1	H	359	GLN
1	H	382	ASN
1	H	385	GLN
1	H	485	GLN
1	H	509	HIS
1	H	536	GLN
1	H	589	GLN
1	H	677	GLN
1	H	709	ASN
1	I	259	GLN
1	I	263	GLN
1	I	270	ASN
1	I	303	ASN
1	I	325	GLN
1	I	334	ASN
1	I	359	GLN
1	I	385	GLN
1	I	485	GLN
1	I	509	HIS
1	I	536	GLN
1	I	589	GLN
1	I	677	GLN
1	I	709	ASN
1	J	259	GLN
1	J	263	GLN
1	J	270	ASN
1	J	303	ASN
1	J	325	GLN
1	J	334	ASN
1	J	359	GLN

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Mol	Chain	Res	Type
1	J	385	GLN
1	J	485	GLN
1	J	509	HIS
1	J	536	GLN
1	J	589	GLN
1	J	677	GLN
1	J	709	ASN

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 monosaccharides 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.

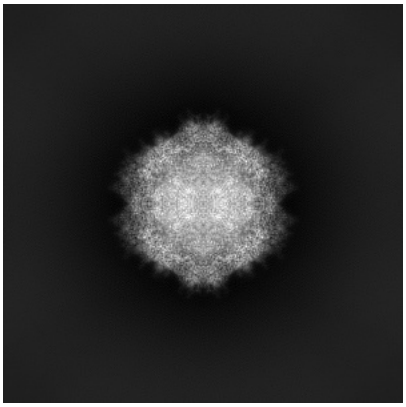
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20630. These allow visual inspection of the internal detail of the map and identification of artifacts.

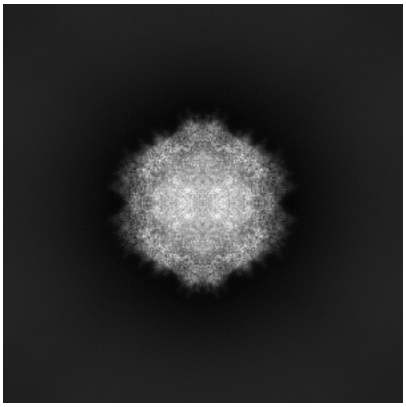
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

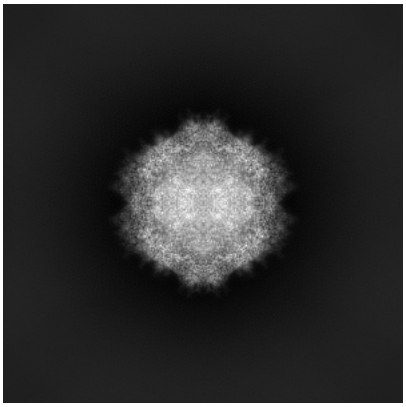
6.1.1 Primary map



X



Y

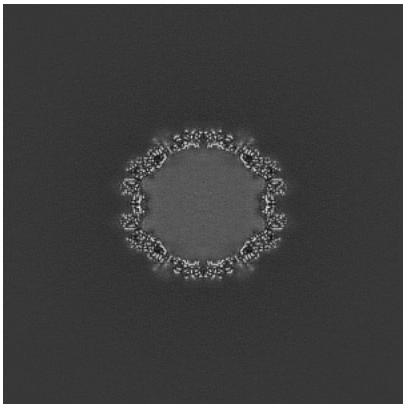


Z

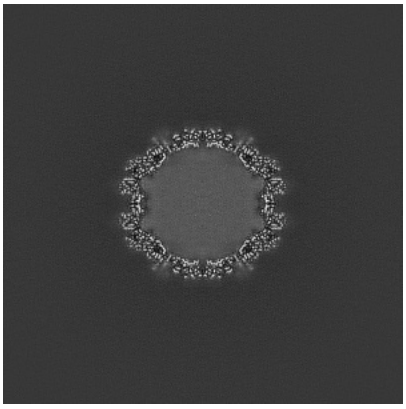
The images above show the map projected in three orthogonal directions.

6.2 Central slices

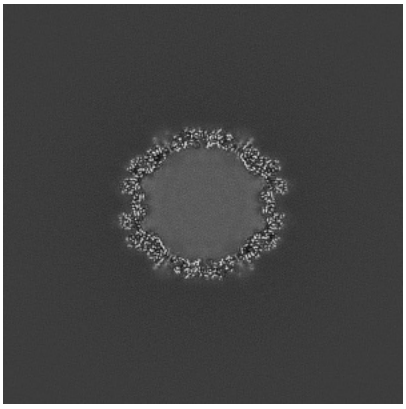
6.2.1 Primary map



X Index: 288



Y Index: 288

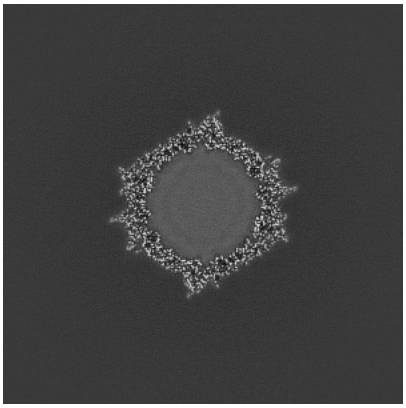


Z Index: 288

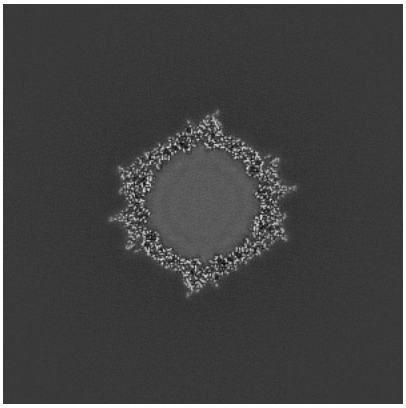
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

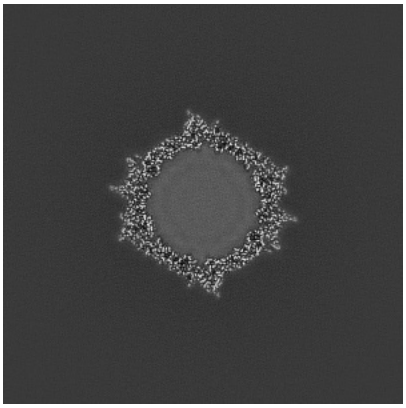
6.3.1 Primary map



X Index: 308



Y Index: 308

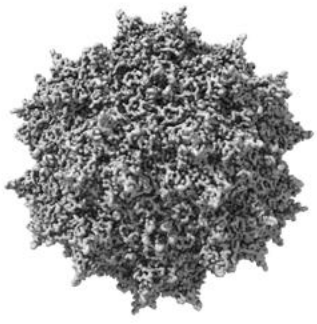


Z Index: 267

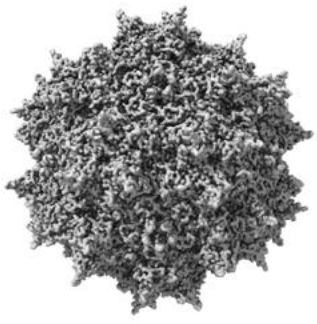
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

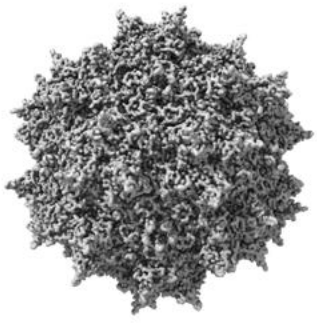
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

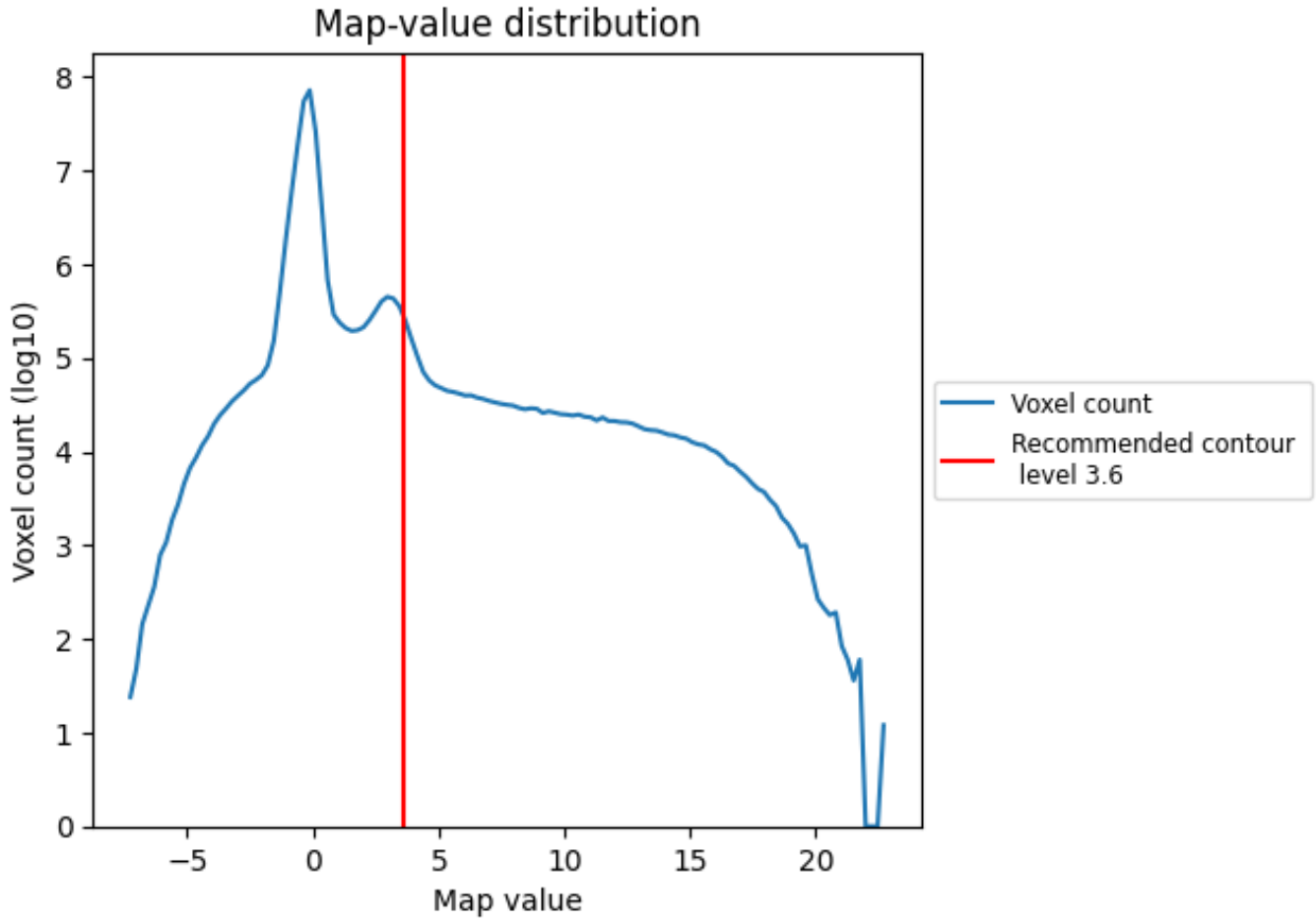
6.5 Mask visualisation (i)

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

7 Map analysis

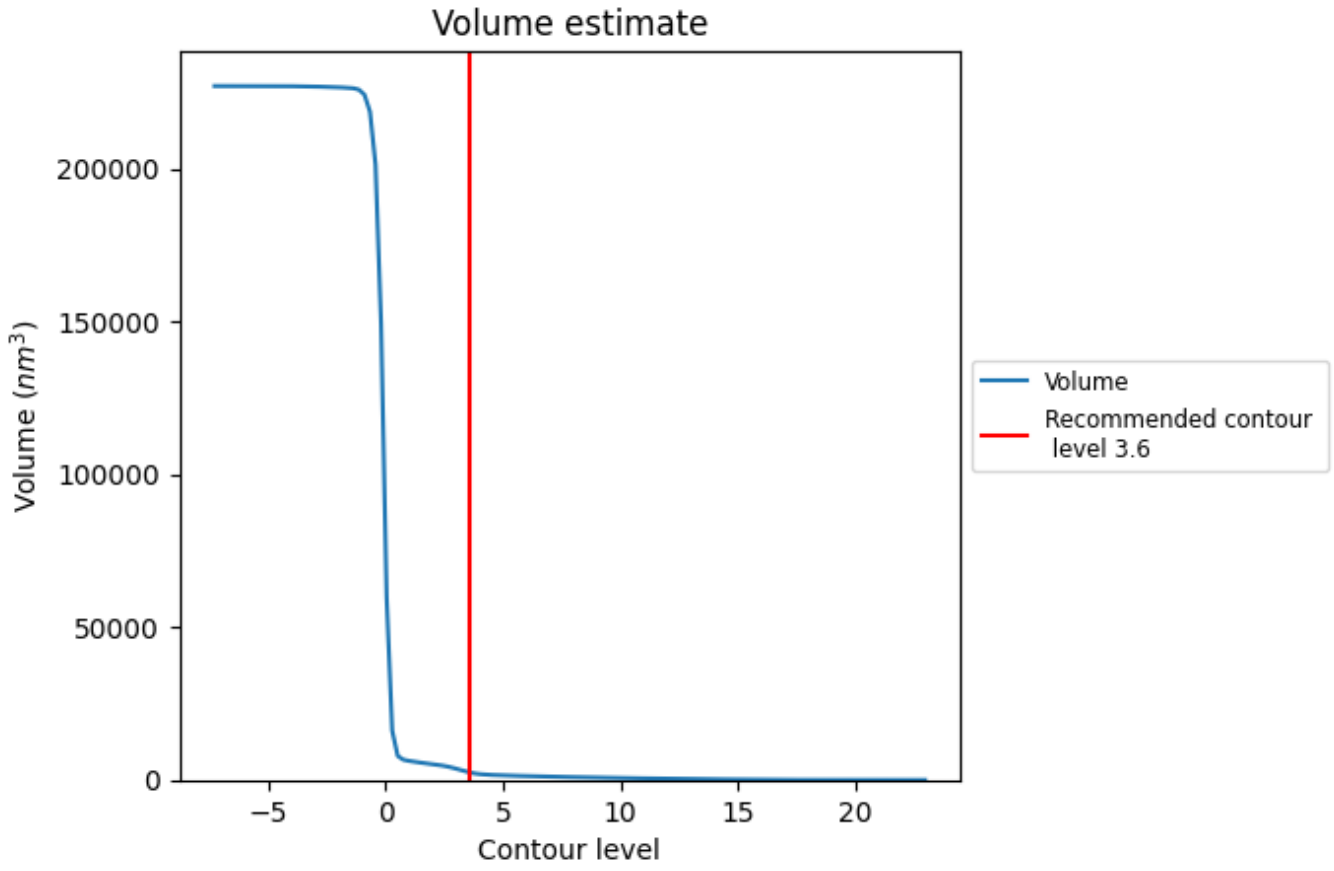
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

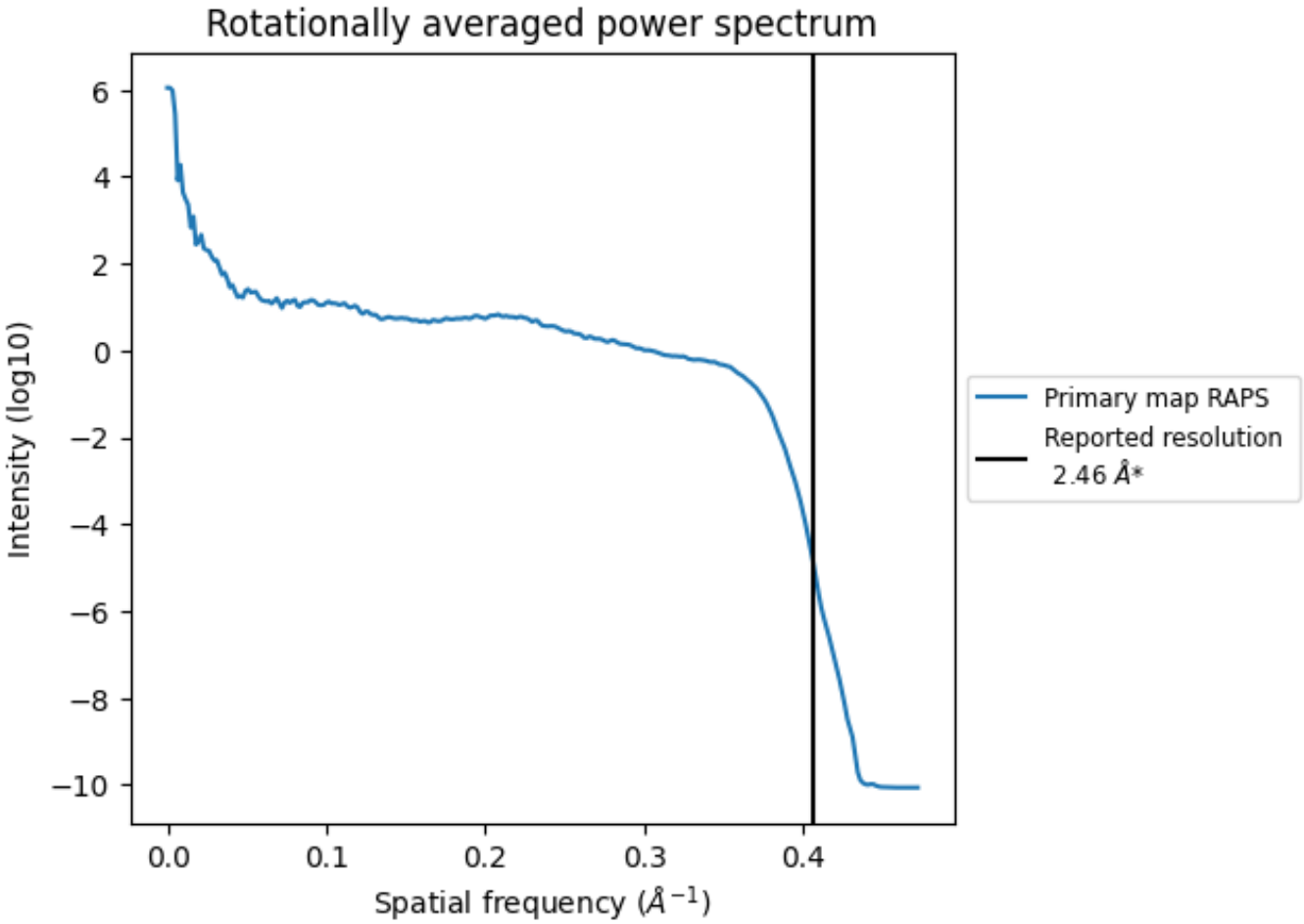
7.2 Volume estimate



The volume at the recommended contour level is 2421 nm^3; this corresponds to an approximate mass of 2187 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 0.407 Å^{-1}

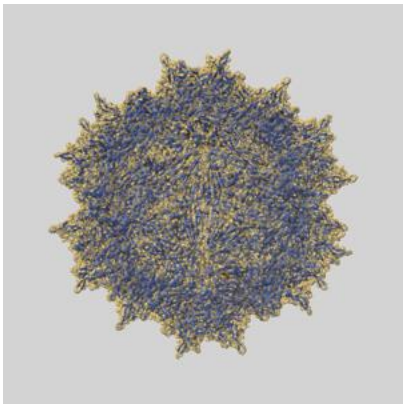
8 Fourier-Shell correlation

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

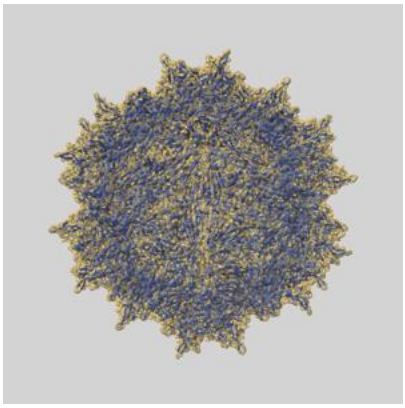
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20630 and PDB model 6U3Q. Per-residue inclusion information can be found in section 3 on page 18.

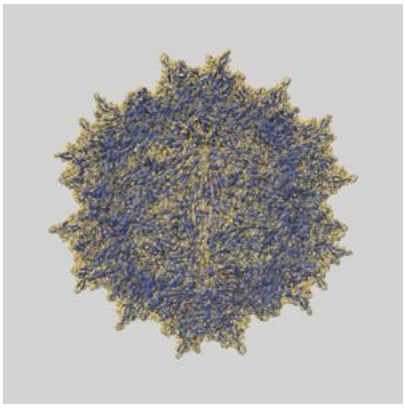
9.1 Map-model overlay



X



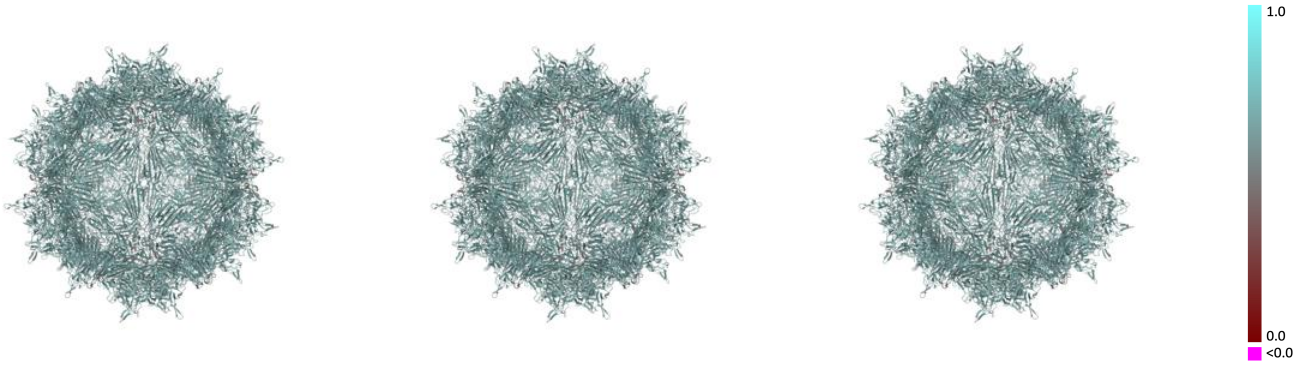
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

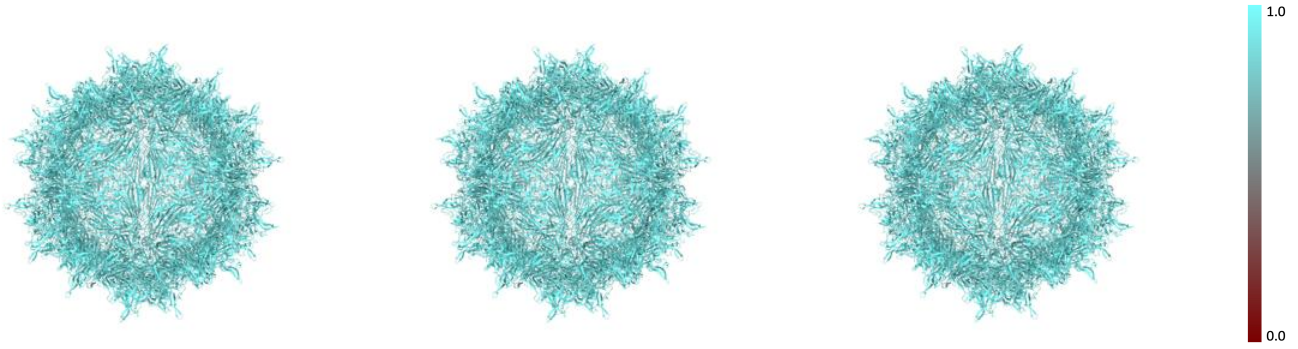
9.2 Q-score mapped to coordinate model



X Y Z

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

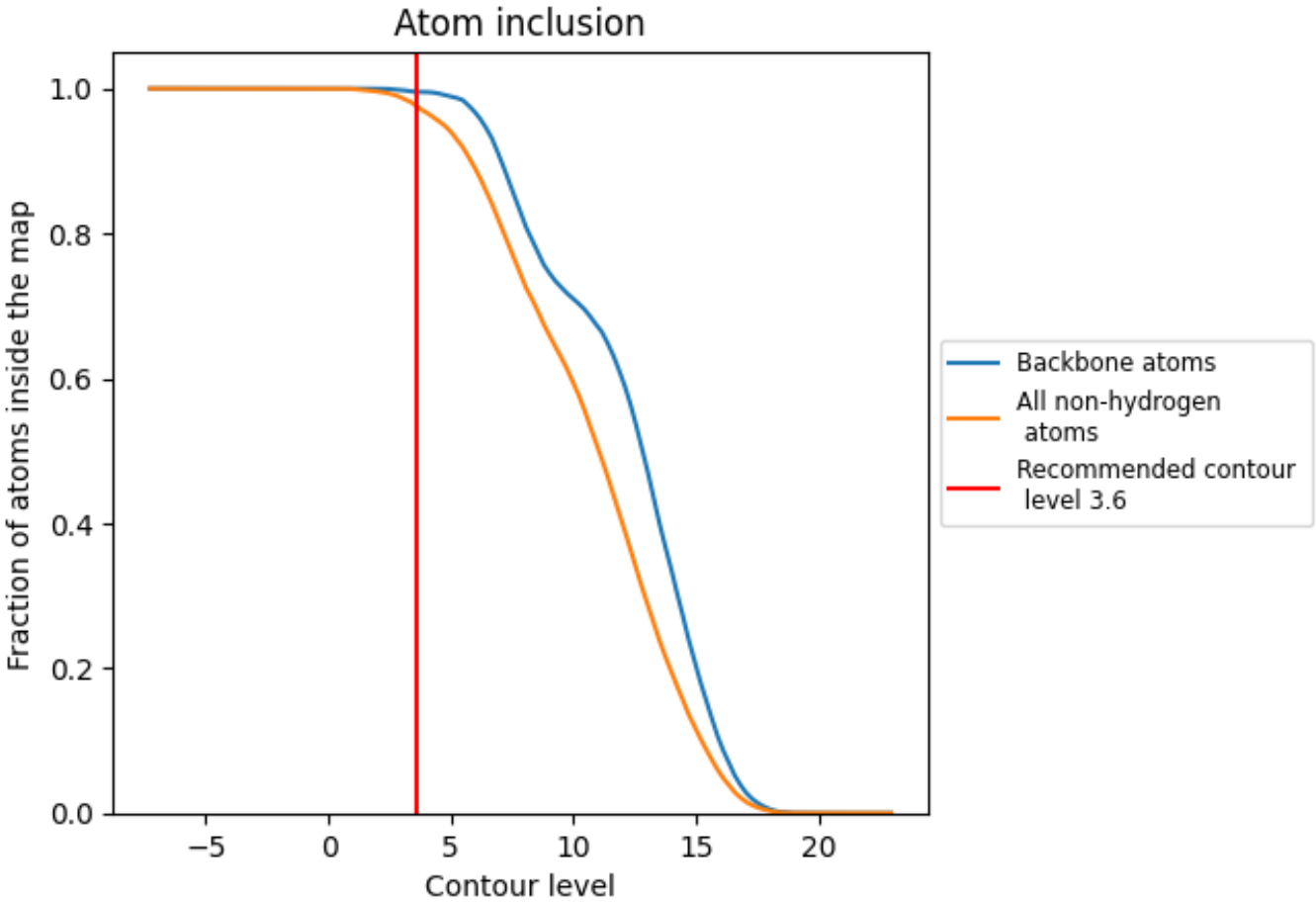
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.6).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 98% 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 (3.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9754	0.6300
0	0.9761	0.6290
1	0.9756	0.6290
2	0.9756	0.6300
3	0.9763	0.6290
4	0.9746	0.6290
5	0.9761	0.6300
6	0.9758	0.6300
7	0.9758	0.6300
A	0.9756	0.6290
B	0.9761	0.6290
C	0.9756	0.6310
D	0.9753	0.6300
E	0.9758	0.6300
F	0.9746	0.6280
G	0.9746	0.6280
H	0.9746	0.6290
I	0.9758	0.6300
J	0.9756	0.6300
K	0.9751	0.6300
L	0.9758	0.6300
M	0.9756	0.6300
N	0.9744	0.6300
O	0.9761	0.6300
P	0.9761	0.6290
Q	0.9766	0.6300
R	0.9753	0.6290
S	0.9751	0.6300
T	0.9761	0.6290
U	0.9756	0.6300
V	0.9746	0.6290
W	0.9763	0.6290
X	0.9753	0.6300
Y	0.9756	0.6300
Z	0.9761	0.6290

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Chain	Atom inclusion	Q-score
a	0.9756	0.6300
b	0.9748	0.6300
c	0.9746	0.6290
d	0.9746	0.6290
e	0.9744	0.6290
f	0.9756	0.6290
g	0.9761	0.6310
h	0.9771	0.6290
i	0.9746	0.6290
j	0.9758	0.6300
k	0.9748	0.6300
l	0.9766	0.6300
m	0.9744	0.6300
n	0.9744	0.6290
o	0.9744	0.6290
p	0.9763	0.6290
q	0.9756	0.6290
r	0.9744	0.6310
s	0.9758	0.6310
t	0.9746	0.6290
u	0.9744	0.6300
v	0.9758	0.6290
w	0.9761	0.6290
x	0.9758	0.6300
y	0.9756	0.6300
z	0.9753	0.6300