



Full wwPDB EM Validation Report ⓘ

Mar 4, 2024 – 08:47 PM EST

PDB ID : 6E9D
EMDB ID : EMD-9012
Title : Sub-2 Angstrom Ewald Curvature-Corrected Single-Particle Cryo-EM Reconstruction of AAV-2 L336C
Authors : Tan, Y.Z.; Aiyer, S.; Mietzsch, M.; Hull, J.A.; McKenna, R.; Baker, T.S.; Agbandje-McKenna, M.; Lyumkis, D.
Deposited on : 2018-07-31
Resolution : 1.86 Å (reported)
Based on initial model : 1LP3

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:

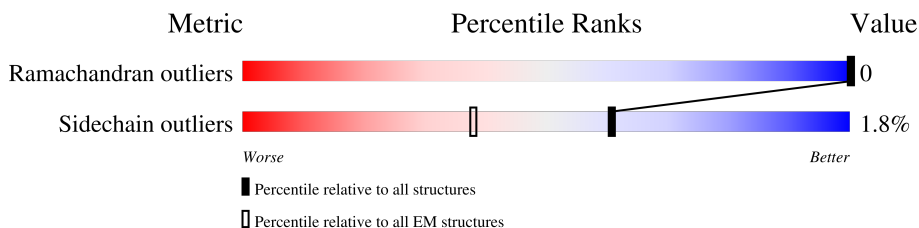
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 1.86 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.






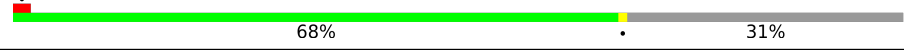
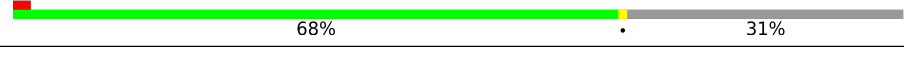



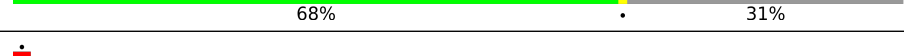
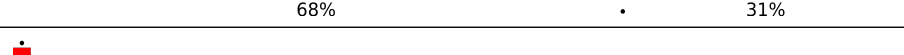
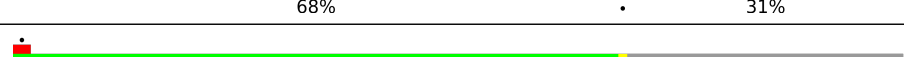
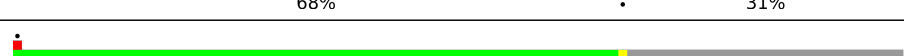

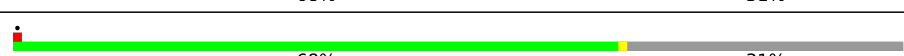
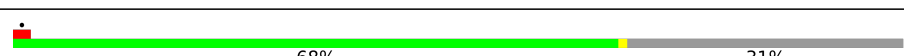
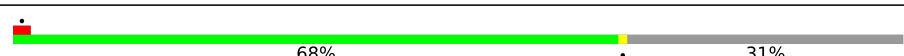





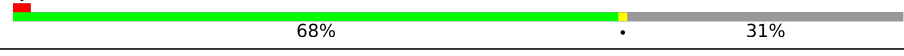



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	735	68% 31%
1	2	735	68% 31%
1	3	735	68% 31%
1	4	735	68% 31%
1	5	735	68% 31%
1	6	735	68% 31%
1	7	735	68% 31%
1	8	735	68% 31%
1	A	735	68% 31%




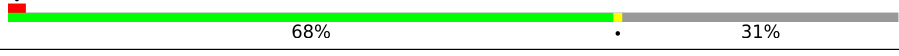
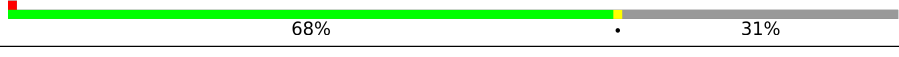



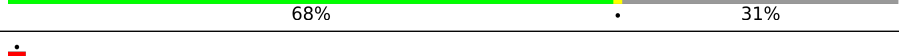
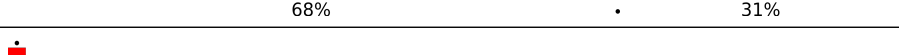
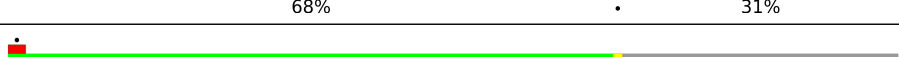
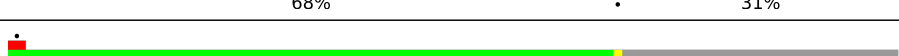

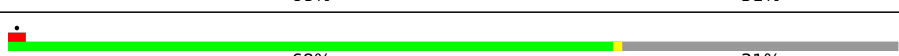
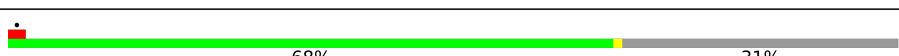
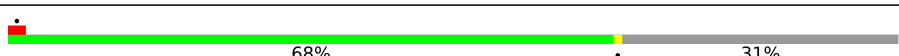





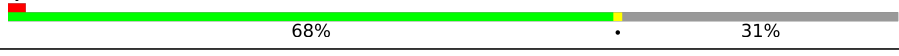



Continued on next page...

Continued from previous page...

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


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	a	735	 68% 31%
1	b	735	 68% 31%
1	c	735	 68% 31%
1	d	735	 68% 31%
1	e	735	 68% 31%
1	f	735	 68% 31%
1	g	735	 68% 31%
1	h	735	 68% 31%
1	i	735	 68% 31%
1	j	735	 68% 31%
1	k	735	 68% 31%
1	l	735	 68% 31%
1	m	735	 68% 31%
1	n	735	 68% 31%
1	o	735	 68% 31%
1	p	735	 68% 31%
1	q	735	 68% 31%
1	r	735	 68% 31%
1	s	735	 68% 31%
1	t	735	 68% 31%
1	u	735	 68% 31%
1	v	735	 68% 31%
1	w	735	 68% 31%
1	x	735	 68% 31%
1	y	735	 68% 31%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	z	735	 A horizontal bar chart representing the quality of the chain. The bar is divided into two segments: a green segment on the left representing 68% and a grey segment on the right representing 31%. A small red square is at the beginning of the green segment, and a small black dot is at the end of the grey segment.

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 489900 atoms, of which 232200 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	510	7968	2581	3870	715	788	14	0	0
1	B	510	7968	2581	3870	715	788	14	0	0
1	C	510	7968	2581	3870	715	788	14	0	0
1	D	510	7968	2581	3870	715	788	14	0	0
1	E	510	7968	2581	3870	715	788	14	0	0
1	F	510	7968	2581	3870	715	788	14	0	0
1	G	510	7968	2581	3870	715	788	14	0	0
1	H	510	7968	2581	3870	715	788	14	0	0
1	I	510	7968	2581	3870	715	788	14	0	0
1	J	510	7968	2581	3870	715	788	14	0	0
1	K	510	7968	2581	3870	715	788	14	0	0
1	L	510	7968	2581	3870	715	788	14	0	0
1	M	510	7968	2581	3870	715	788	14	0	0
1	N	510	7968	2581	3870	715	788	14	0	0
1	O	510	7968	2581	3870	715	788	14	0	0
1	P	510	7968	2581	3870	715	788	14	0	0
1	Q	510	7968	2581	3870	715	788	14	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace	
1	R	510	Total 7968	C 2581	H 3870	N 715	O 788	S 14	0	0
1	S	510	Total 7968	C 2581	H 3870	N 715	O 788	S 14	0	0
1	T	510	Total 7968	C 2581	H 3870	N 715	O 788	S 14	0	0
1	U	510	Total 7968	C 2581	H 3870	N 715	O 788	S 14	0	0
1	V	510	Total 7968	C 2581	H 3870	N 715	O 788	S 14	0	0
1	W	510	Total 7968	C 2581	H 3870	N 715	O 788	S 14	0	0
1	X	510	Total 7968	C 2581	H 3870	N 715	O 788	S 14	0	0
1	Y	510	Total 7968	C 2581	H 3870	N 715	O 788	S 14	0	0
1	Z	510	Total 7968	C 2581	H 3870	N 715	O 788	S 14	0	0
1	1	510	Total 7968	C 2581	H 3870	N 715	O 788	S 14	0	0
1	2	510	Total 7968	C 2581	H 3870	N 715	O 788	S 14	0	0
1	3	510	Total 7968	C 2581	H 3870	N 715	O 788	S 14	0	0
1	4	510	Total 7968	C 2581	H 3870	N 715	O 788	S 14	0	0
1	5	510	Total 7968	C 2581	H 3870	N 715	O 788	S 14	0	0
1	6	510	Total 7968	C 2581	H 3870	N 715	O 788	S 14	0	0
1	a	510	Total 7968	C 2581	H 3870	N 715	O 788	S 14	0	0
1	b	510	Total 7968	C 2581	H 3870	N 715	O 788	S 14	0	0
1	c	510	Total 7968	C 2581	H 3870	N 715	O 788	S 14	0	0
1	d	510	Total 7968	C 2581	H 3870	N 715	O 788	S 14	0	0
1	e	510	Total 7968	C 2581	H 3870	N 715	O 788	S 14	0	0
1	f	510	Total 7968	C 2581	H 3870	N 715	O 788	S 14	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
1	g	510	Total	C	H	N	O	S	0	0
			7968	2581	3870	715	788	14		
1	h	510	Total	C	H	N	O	S	0	0
			7968	2581	3870	715	788	14		
1	i	510	Total	C	H	N	O	S	0	0
			7968	2581	3870	715	788	14		
1	j	510	Total	C	H	N	O	S	0	0
			7968	2581	3870	715	788	14		
1	k	510	Total	C	H	N	O	S	0	0
			7968	2581	3870	715	788	14		
1	l	510	Total	C	H	N	O	S	0	0
			7968	2581	3870	715	788	14		
1	m	510	Total	C	H	N	O	S	0	0
			7968	2581	3870	715	788	14		
1	n	510	Total	C	H	N	O	S	0	0
			7968	2581	3870	715	788	14		
1	o	510	Total	C	H	N	O	S	0	0
			7968	2581	3870	715	788	14		
1	p	510	Total	C	H	N	O	S	0	0
			7968	2581	3870	715	788	14		
1	q	510	Total	C	H	N	O	S	0	0
			7968	2581	3870	715	788	14		
1	r	510	Total	C	H	N	O	S	0	0
			7968	2581	3870	715	788	14		
1	s	510	Total	C	H	N	O	S	0	0
			7968	2581	3870	715	788	14		
1	t	510	Total	C	H	N	O	S	0	0
			7968	2581	3870	715	788	14		
1	u	510	Total	C	H	N	O	S	0	0
			7968	2581	3870	715	788	14		
1	v	510	Total	C	H	N	O	S	0	0
			7968	2581	3870	715	788	14		
1	w	510	Total	C	H	N	O	S	0	0
			7968	2581	3870	715	788	14		
1	x	510	Total	C	H	N	O	S	0	0
			7968	2581	3870	715	788	14		
1	y	510	Total	C	H	N	O	S	0	0
			7968	2581	3870	715	788	14		
1	z	510	Total	C	H	N	O	S	0	0
			7968	2581	3870	715	788	14		
1	7	510	Total	C	H	N	O	S	0	0
			7968	2581	3870	715	788	14		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	8	510	7968	2581	3870	715	788	14	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	336	CYS	LEU	engineered mutation	UNP P03135
B	336	CYS	LEU	engineered mutation	UNP P03135
C	336	CYS	LEU	engineered mutation	UNP P03135
D	336	CYS	LEU	engineered mutation	UNP P03135
E	336	CYS	LEU	engineered mutation	UNP P03135
F	336	CYS	LEU	engineered mutation	UNP P03135
G	336	CYS	LEU	engineered mutation	UNP P03135
H	336	CYS	LEU	engineered mutation	UNP P03135
I	336	CYS	LEU	engineered mutation	UNP P03135
J	336	CYS	LEU	engineered mutation	UNP P03135
K	336	CYS	LEU	engineered mutation	UNP P03135
L	336	CYS	LEU	engineered mutation	UNP P03135
M	336	CYS	LEU	engineered mutation	UNP P03135
N	336	CYS	LEU	engineered mutation	UNP P03135
O	336	CYS	LEU	engineered mutation	UNP P03135
P	336	CYS	LEU	engineered mutation	UNP P03135
Q	336	CYS	LEU	engineered mutation	UNP P03135
R	336	CYS	LEU	engineered mutation	UNP P03135
S	336	CYS	LEU	engineered mutation	UNP P03135
T	336	CYS	LEU	engineered mutation	UNP P03135
U	336	CYS	LEU	engineered mutation	UNP P03135
V	336	CYS	LEU	engineered mutation	UNP P03135
W	336	CYS	LEU	engineered mutation	UNP P03135
X	336	CYS	LEU	engineered mutation	UNP P03135
Y	336	CYS	LEU	engineered mutation	UNP P03135
Z	336	CYS	LEU	engineered mutation	UNP P03135
1	336	CYS	LEU	engineered mutation	UNP P03135
2	336	CYS	LEU	engineered mutation	UNP P03135
3	336	CYS	LEU	engineered mutation	UNP P03135
4	336	CYS	LEU	engineered mutation	UNP P03135
5	336	CYS	LEU	engineered mutation	UNP P03135
6	336	CYS	LEU	engineered mutation	UNP P03135
a	336	CYS	LEU	engineered mutation	UNP P03135
b	336	CYS	LEU	engineered mutation	UNP P03135
c	336	CYS	LEU	engineered mutation	UNP P03135
d	336	CYS	LEU	engineered mutation	UNP P03135

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
e	336	CYS	LEU	engineered mutation	UNP P03135
f	336	CYS	LEU	engineered mutation	UNP P03135
g	336	CYS	LEU	engineered mutation	UNP P03135
h	336	CYS	LEU	engineered mutation	UNP P03135
i	336	CYS	LEU	engineered mutation	UNP P03135
j	336	CYS	LEU	engineered mutation	UNP P03135
k	336	CYS	LEU	engineered mutation	UNP P03135
l	336	CYS	LEU	engineered mutation	UNP P03135
m	336	CYS	LEU	engineered mutation	UNP P03135
n	336	CYS	LEU	engineered mutation	UNP P03135
o	336	CYS	LEU	engineered mutation	UNP P03135
p	336	CYS	LEU	engineered mutation	UNP P03135
q	336	CYS	LEU	engineered mutation	UNP P03135
r	336	CYS	LEU	engineered mutation	UNP P03135
s	336	CYS	LEU	engineered mutation	UNP P03135
t	336	CYS	LEU	engineered mutation	UNP P03135
u	336	CYS	LEU	engineered mutation	UNP P03135
v	336	CYS	LEU	engineered mutation	UNP P03135
w	336	CYS	LEU	engineered mutation	UNP P03135
x	336	CYS	LEU	engineered mutation	UNP P03135
y	336	CYS	LEU	engineered mutation	UNP P03135
z	336	CYS	LEU	engineered mutation	UNP P03135
7	336	CYS	LEU	engineered mutation	UNP P03135
8	336	CYS	LEU	engineered mutation	UNP P03135

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	AltConf
2	A	197	Total O 197 197	0
2	B	199	Total O 199 199	0
2	C	198	Total O 198 198	0
2	D	197	Total O 197 197	0
2	E	197	Total O 197 197	0
2	F	196	Total O 196 196	0
2	G	197	Total O 197 197	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
2	H	197	Total 197	O 197	0
2	I	197	Total 197	O 197	0
2	J	196	Total 196	O 196	0
2	K	197	Total 197	O 197	0
2	L	196	Total 196	O 196	0
2	M	196	Total 196	O 196	0
2	N	197	Total 197	O 197	0
2	O	197	Total 197	O 197	0
2	P	197	Total 197	O 197	0
2	Q	198	Total 198	O 198	0
2	R	197	Total 197	O 197	0
2	S	197	Total 197	O 197	0
2	T	197	Total 197	O 197	0
2	U	197	Total 197	O 197	0
2	V	197	Total 197	O 197	0
2	W	197	Total 197	O 197	0
2	X	197	Total 197	O 197	0
2	Y	197	Total 197	O 197	0
2	Z	197	Total 197	O 197	0
2	1	197	Total 197	O 197	0
2	2	197	Total 197	O 197	0

Continued on next page...

Continued from previous page...

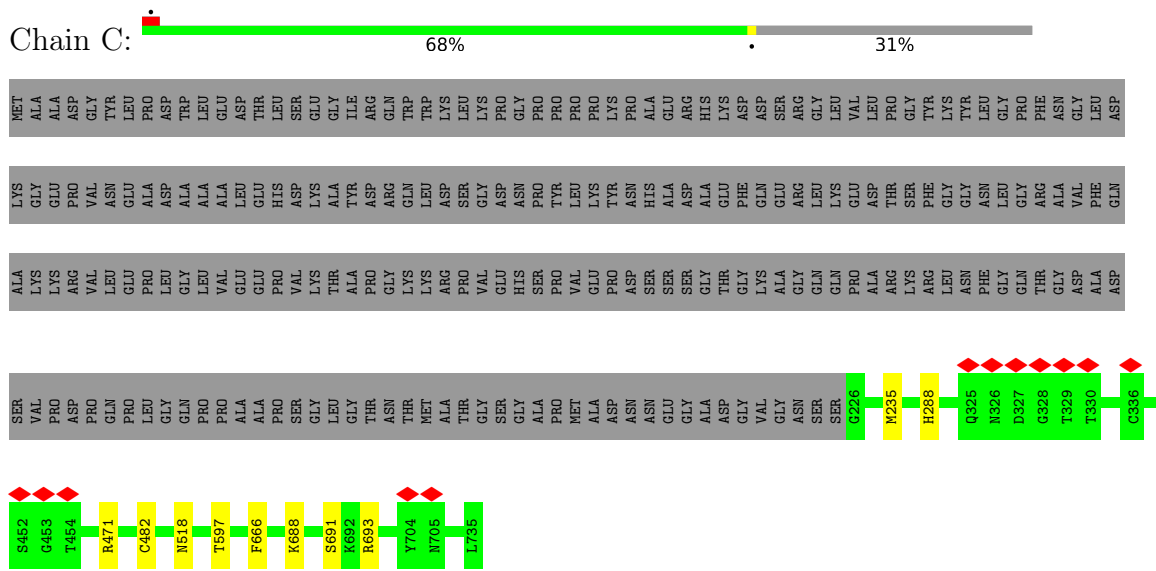
Mol	Chain	Residues	Atoms		AltConf
2	3	197	Total 197	O 197	0
2	4	197	Total 197	O 197	0
2	5	197	Total 197	O 197	0
2	6	197	Total 197	O 197	0
2	a	197	Total 197	O 197	0
2	b	197	Total 197	O 197	0
2	c	197	Total 197	O 197	0
2	d	197	Total 197	O 197	0
2	e	197	Total 197	O 197	0
2	f	197	Total 197	O 197	0
2	g	197	Total 197	O 197	0
2	h	197	Total 197	O 197	0
2	i	197	Total 197	O 197	0
2	j	197	Total 197	O 197	0
2	k	197	Total 197	O 197	0
2	l	197	Total 197	O 197	0
2	m	197	Total 197	O 197	0
2	n	197	Total 197	O 197	0
2	o	197	Total 197	O 197	0
2	p	197	Total 197	O 197	0
2	q	197	Total 197	O 197	0

Continued on next page...

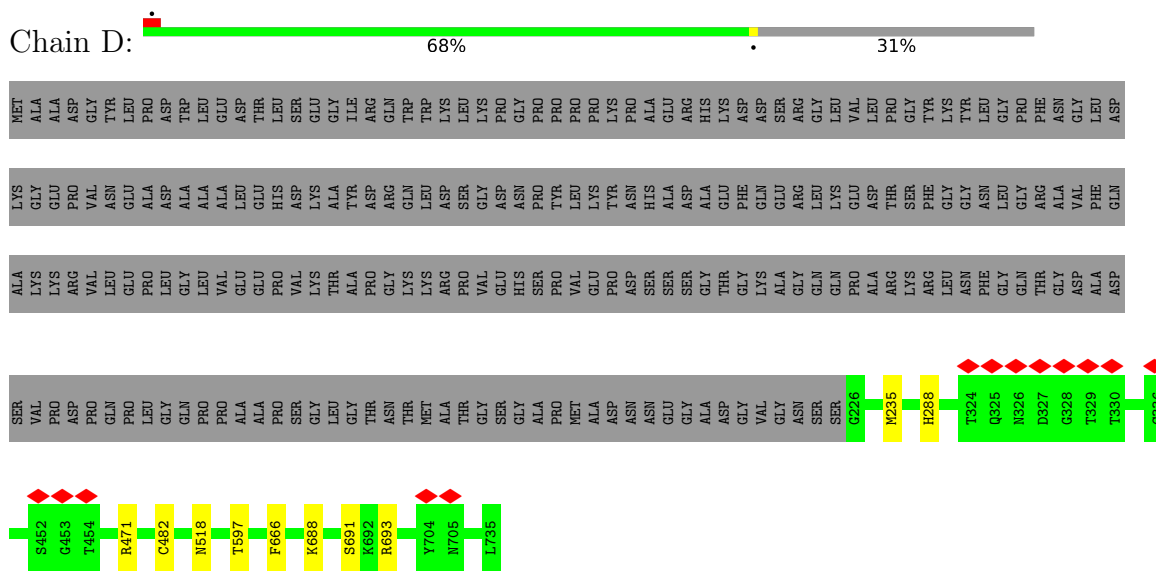
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
2	r	197	Total 197	O 197	0
2	s	197	Total 197	O 197	0
2	t	197	Total 197	O 197	0
2	u	197	Total 197	O 197	0
2	v	197	Total 197	O 197	0
2	w	197	Total 197	O 197	0
2	x	197	Total 197	O 197	0
2	y	197	Total 197	O 197	0
2	z	197	Total 197	O 197	0
2	7	197	Total 197	O 197	0
2	8	197	Total 197	O 197	0

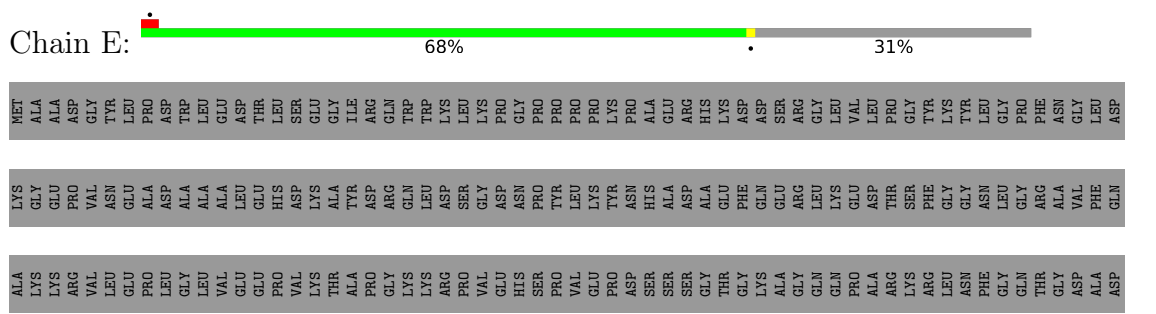
Molecule 1: Capsid protein VP1

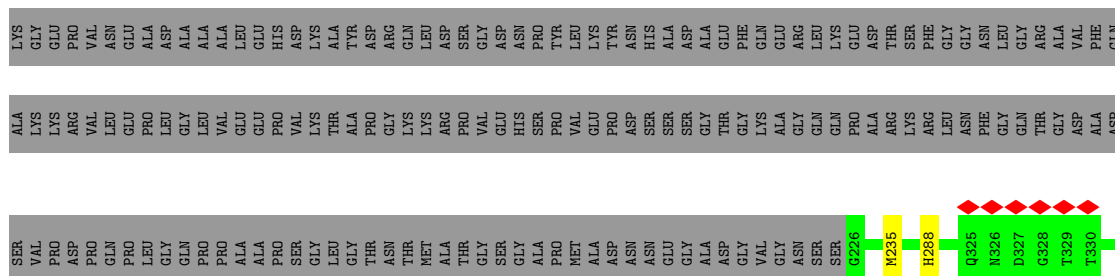


Molecule 1: Capsid protein VP1

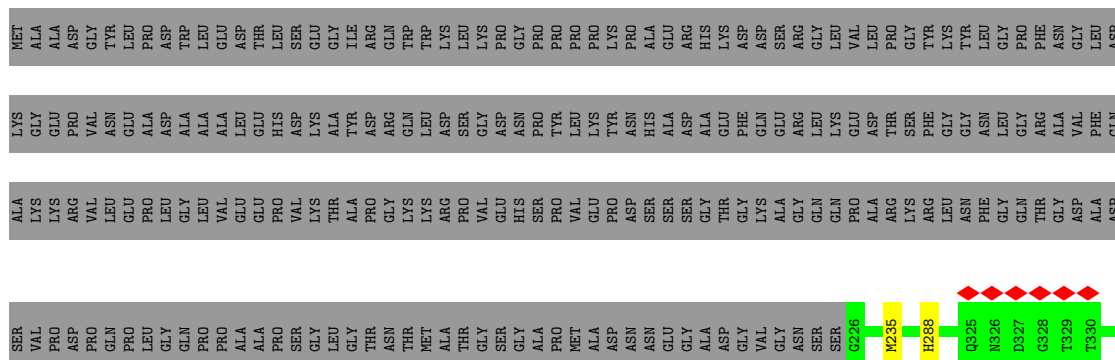


Molecule 1: Capsid protein VP1

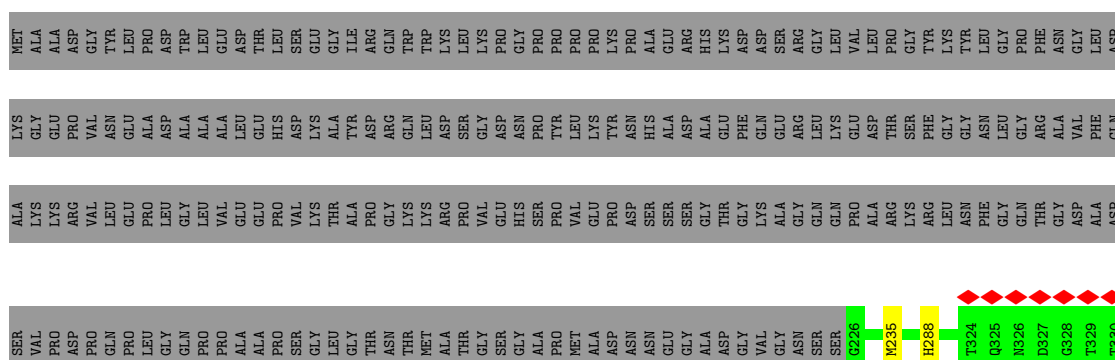




● Molecule 1: Capsid protein VP1



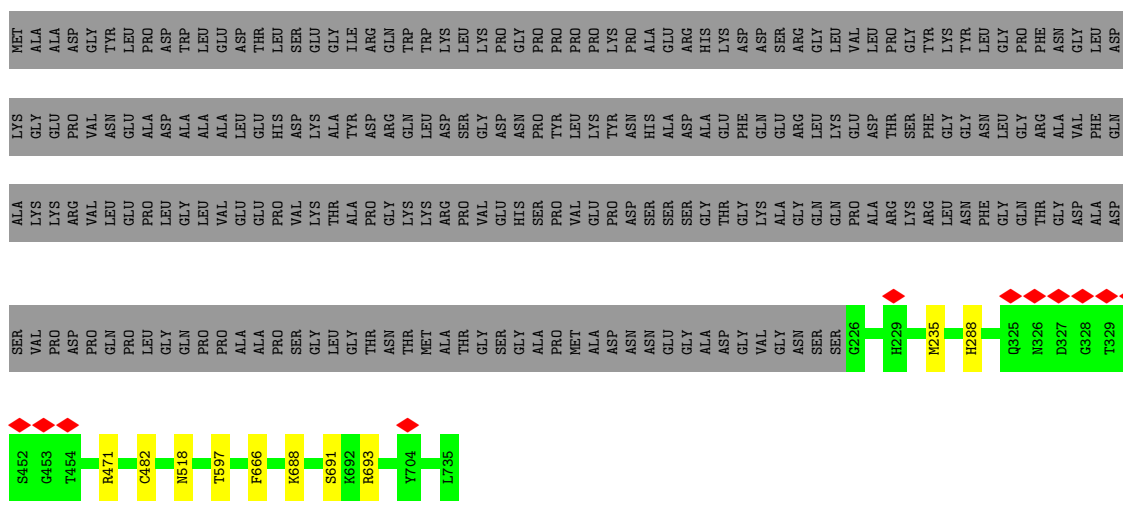
● Molecule 1: Capsid protein VP1



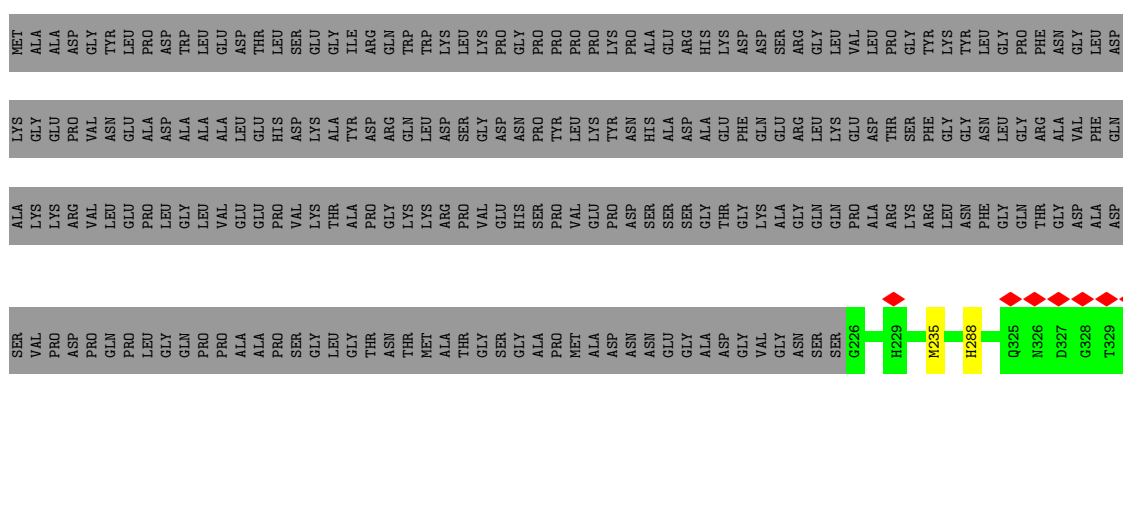
● Molecule 1: Capsid protein VP1

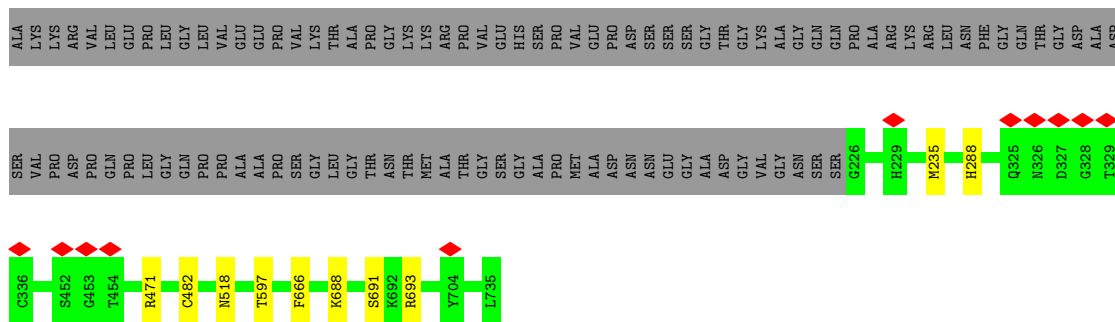


• Molecule 1: Capsid protein VP1

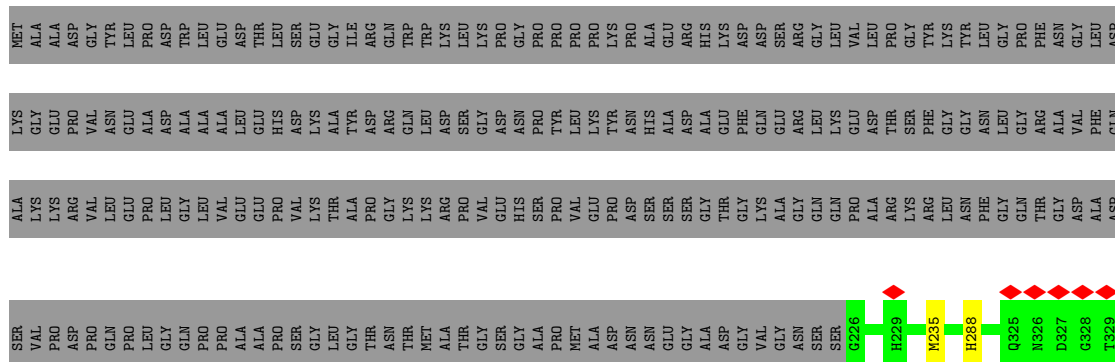


• Molecule 1: Capsid protein VP1

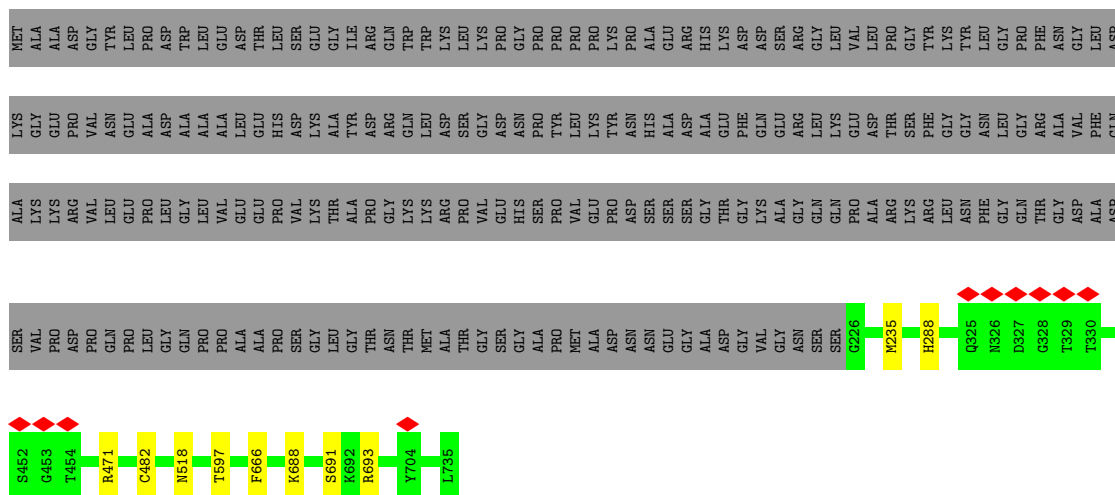




● Molecule 1: Capsid protein VP1

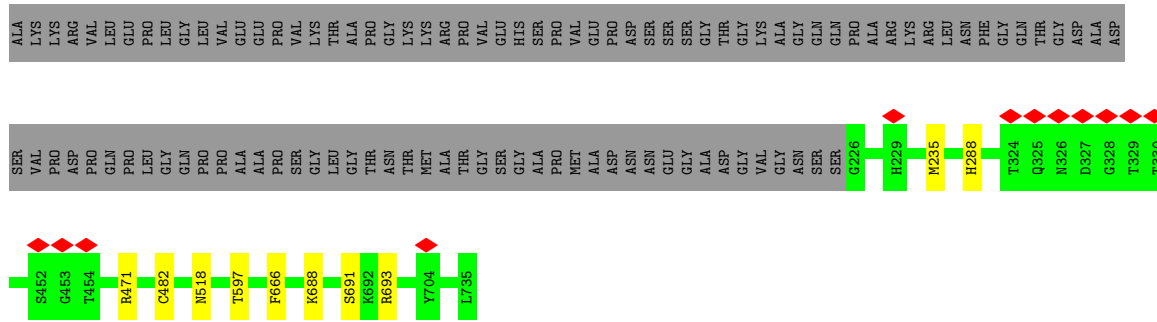


● Molecule 1: Capsid protein VP1

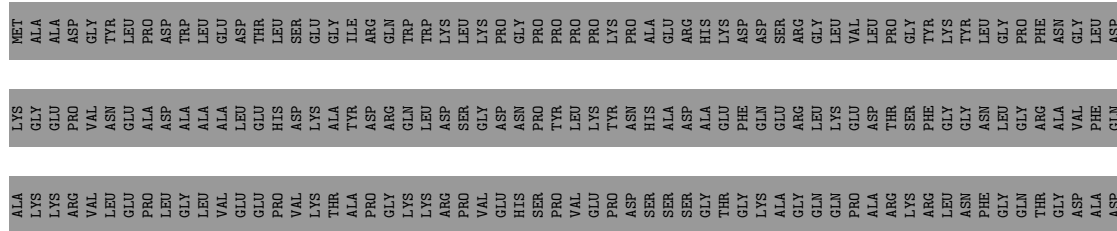


● Molecule 1: Capsid protein VP1

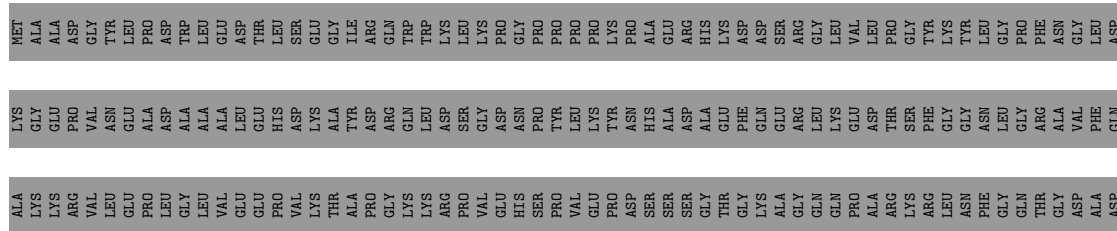




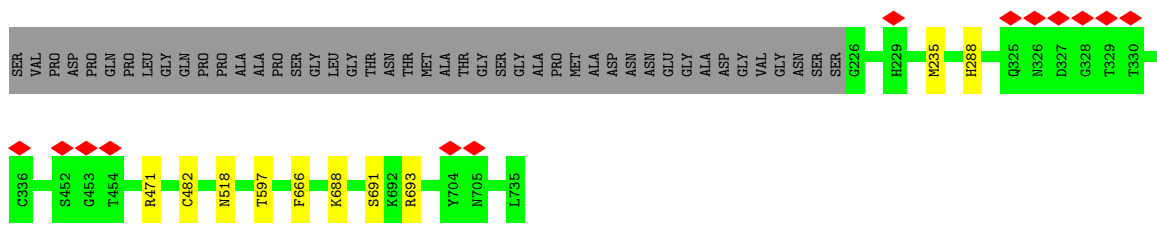
● Molecule 1: Capsid protein VP1

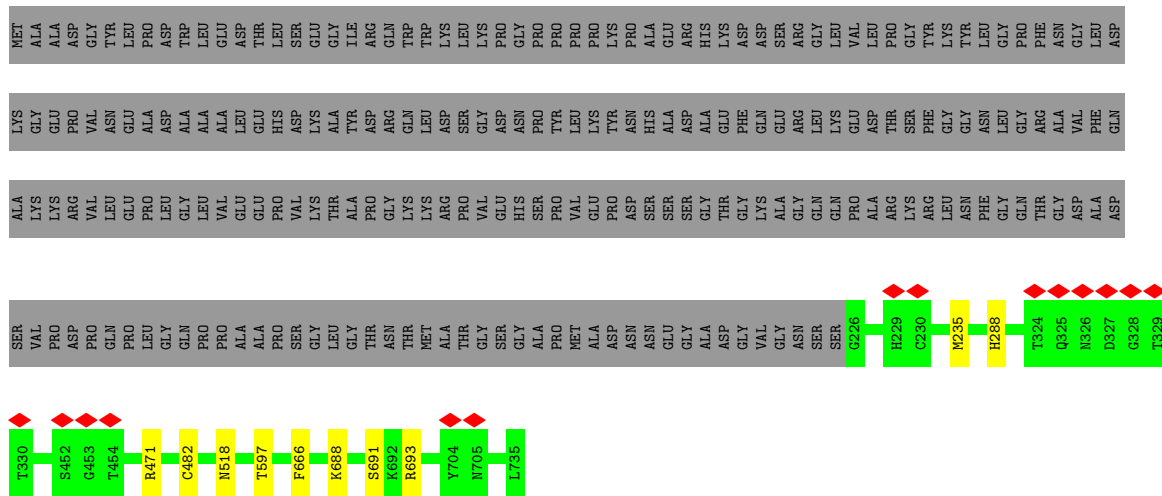


● Molecule 1: Capsid protein VP1

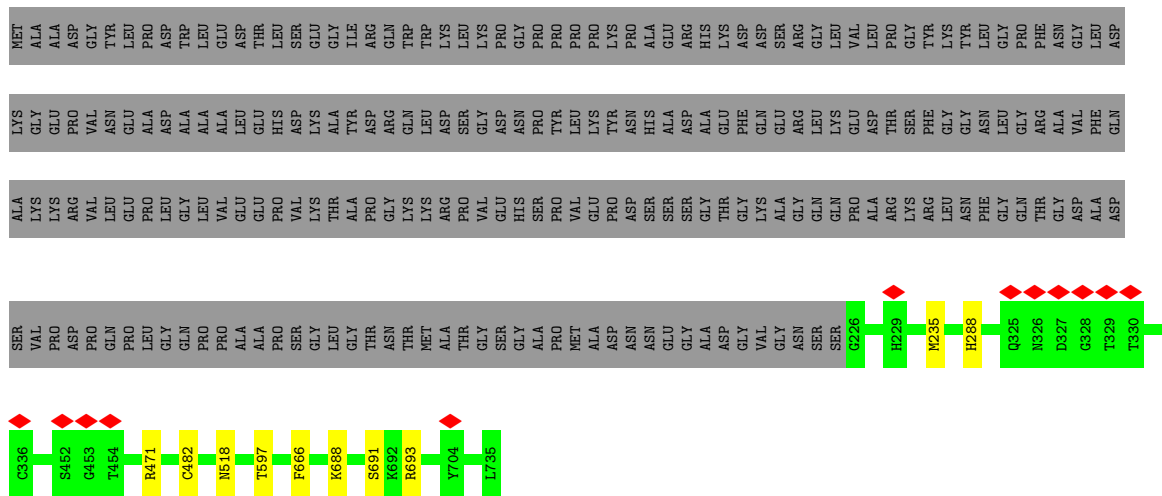


● Molecule 1: Capsid protein VP1

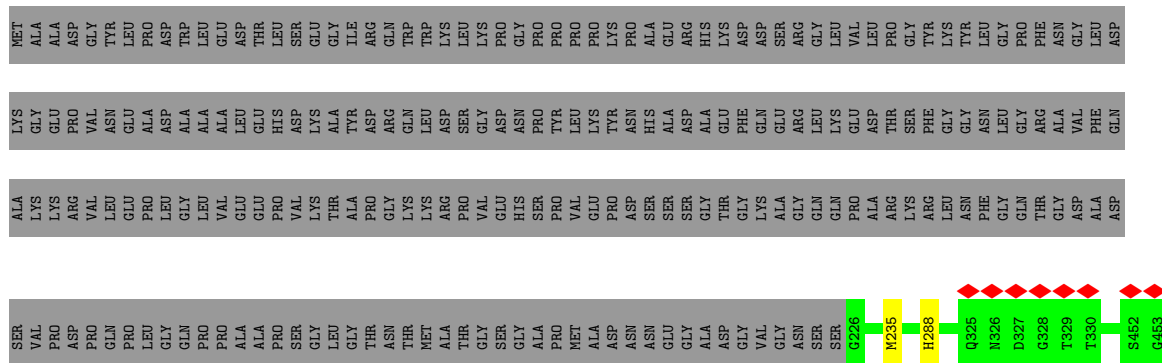




● Molecule 1: Capsid protein VP1



● Molecule 1: Capsid protein VP1



ALA
LYS
LYS
ARG
PRO
VAL
LEU
LEU
GLU
PRO
LEU
GLY
GLY
PRO
VAL
VAL
GLU
GLU
PRO
VAL
VAL
VAL
VAL
GLY
LEU
LEU
LEU
THR
THR
ALA
PRO
GLY
LYS
LYS
LYS
ARG
PRO
PRO
VAL
GLU
GLY
HIS
SER
SER
MET
MET
VAL
VAL
GLY
PRO
SER
SER
SER
SER
GLY
GLY
THR

SER
VAL
PRO
ASP
PRO
GLN
PRO
LEU
GLY
GLN
PRO
PRO
PRO
ALA
ALA
PRO
SER
SER
GLY
GLY
THR
THR
MET
ALA
ALA
GLY
ASP
ASN
THR
MET
LYS
ARG
ALA
SER
SER
SER
GLY
GLY
ALA
ASP
GLY
VAL
GLY
GLY
ASN
SER
SER
SER
G226
H229
M235
H288
T324
Q325
N326
D327
G328
T329
T330



- Molecule 1: Capsid protein VP1

Chain i: 68% 31%

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

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

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

SER
VAL
PRO
ASP
PRO
GLN
PRO
LEU
GLY
GLN
PRO
PRO
PRO
ALA
ALA
PRO
SER
SER
GLY
GLY
THR
THR
MET
ALA
ALA
GLY
ASP
ASN
THR
MET
LYS
ARG
ALA
SER
SER
SER
GLY
ALA
ASP
GLY
VAL
GLY
VAL
GLN
SER
SER
SER
SER
SER
SER
SER
SER
SER
SER
SER
G226
H229
M235
H288
T324
Q325
N326
D327
G328
T329
T330



- Molecule 1: Capsid protein VP1

Chain j: 68% 31%

MET
ALA
ALA
ASP
GLY
TYR
LEU
PRO
LEU
ASP
TRP
LEU
LEU
ALA
VAL
GLU
ASP
THR
LEU
SER
SER
GLY
GLY
THR
TLE
ARG
GLN
LEU
TRP
LEU
LEU
SER
ALA
TYR
ASP
ASP
GLY
SER
GLY
ASN
GLY
HIS
PRO
PRO
TYR
PRO
MET
LEU
VAL
PRO
PRO
LYS
LEU
VAL
VAL
GLY
SER

LYS
GLY
GLU
PRO
VAL
ASN
GLU
ALA
ASP
TRP
LEU
LEU
ALA
VAL
GLU
LEU
GLU
HIS
ASP
SER
VAL
SER
GLY
TYR
ASP
GLN
LEU
TRP
LEU
LEU
SER
ALA
TYR
ASP
ASP
GLY
SER
GLY
ASN
GLY
HIS
PRO
PRO
TYR
PRO
MET
LEU
VAL
PRO
PRO
LYS
LEU
VAL
VAL
GLY
SER

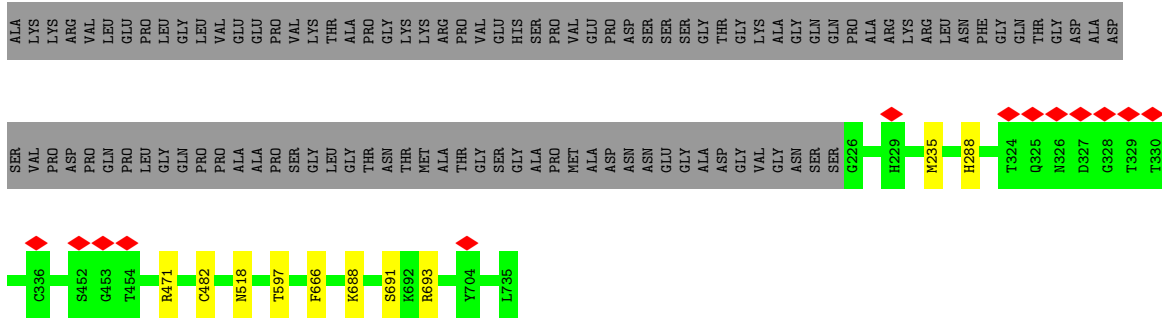
ALA
LYS
LYS
ARG
PRO
VAL
LEU
LEU
GLU
PRO
LEU
ASP
THR
LEU
SER
SER
GLY
GLY
THR
TLE
ARG
GLN
LEU
TRP
LEU
LEU
SER
ALA
TYR
ASP
ASP
GLY
SER
GLY
ASN
GLY
HIS
PRO
PRO
TYR
PRO
MET
LEU
VAL
PRO
PRO
LYS
LEU
VAL
VAL
GLY
SER

SER
VAL
PRO
ASP
GLM
PRO
LEU
GLY
GLN
PRO
PRO
PRO
ALA
ALA
PRO
SER
SER
GLY
GLY
THR
THR
MET
ALA
ALA
GLY
ASP
ASN
THR
MET
LYS
ARG
ALA
SER
SER
SER
GLY
ALA
ASP
VAL
GLY
VAL
GLN
SER
SER
SER
SER
SER
SER
SER
SER
SER
SER
G226
H229
M235
H288
T324
Q325
N326
D327
G328
T329
T330

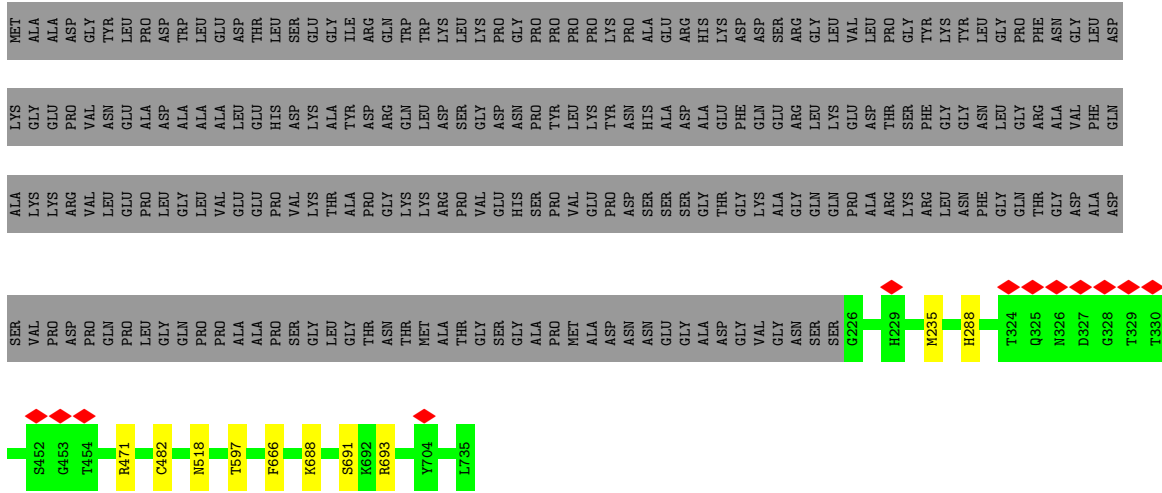


- Molecule 1: Capsid protein VP1

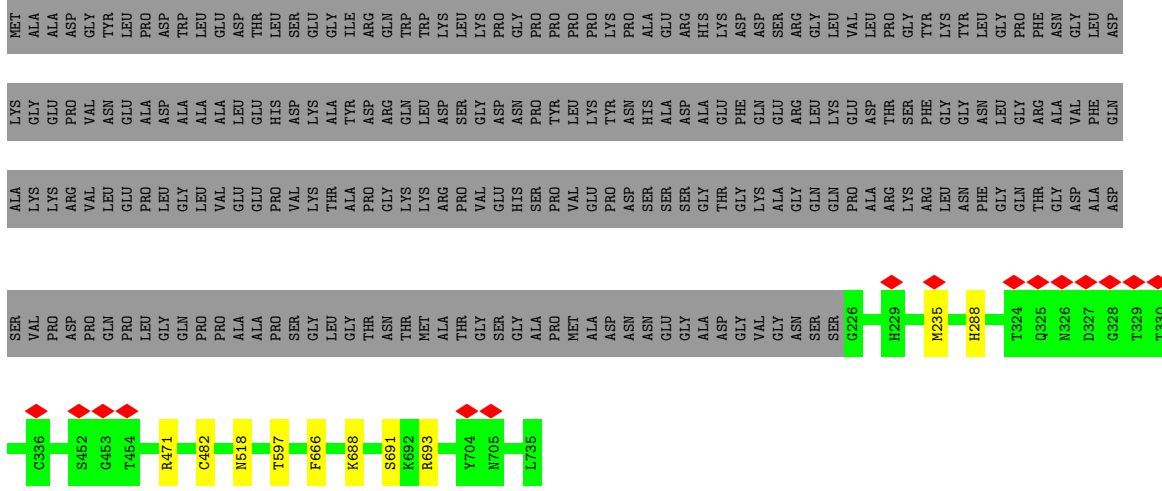
Chain k: 68% 31%



● Molecule 1: Capsid protein VP1



● Molecule 1: Capsid protein VP1



● Molecule 1: Capsid protein VP1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	30515	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF estimation per particle - Gctf, CTF estimation per micrograph - CTFFIND4	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22.5	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	37000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.416	Depositor
Minimum map value	-0.223	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.06	Depositor
Map size (\AA)	283.68, 283.68, 283.68	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.394, 0.394, 0.394	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	1	0.51	0/4221	0.66	2/5754 (0.0%)
1	2	0.51	0/4221	0.66	2/5754 (0.0%)
1	3	0.51	0/4221	0.66	2/5754 (0.0%)
1	4	0.51	0/4221	0.66	2/5754 (0.0%)
1	5	0.51	0/4221	0.66	2/5754 (0.0%)
1	6	0.51	0/4221	0.66	2/5754 (0.0%)
1	7	0.51	0/4221	0.66	2/5754 (0.0%)
1	8	0.51	0/4221	0.66	2/5754 (0.0%)
1	A	0.51	0/4221	0.66	2/5754 (0.0%)
1	B	0.51	0/4221	0.66	2/5754 (0.0%)
1	C	0.51	0/4221	0.66	2/5754 (0.0%)
1	D	0.51	0/4221	0.66	2/5754 (0.0%)
1	E	0.51	0/4221	0.66	2/5754 (0.0%)
1	F	0.51	0/4221	0.66	2/5754 (0.0%)
1	G	0.51	0/4221	0.66	2/5754 (0.0%)
1	H	0.51	0/4221	0.66	2/5754 (0.0%)
1	I	0.51	0/4221	0.66	2/5754 (0.0%)
1	J	0.51	0/4221	0.66	2/5754 (0.0%)
1	K	0.51	0/4221	0.66	2/5754 (0.0%)
1	L	0.51	0/4221	0.66	2/5754 (0.0%)
1	M	0.51	0/4221	0.66	2/5754 (0.0%)
1	N	0.51	0/4221	0.66	2/5754 (0.0%)
1	O	0.51	0/4221	0.66	2/5754 (0.0%)
1	P	0.51	0/4221	0.66	2/5754 (0.0%)
1	Q	0.51	0/4221	0.66	2/5754 (0.0%)
1	R	0.51	0/4221	0.66	2/5754 (0.0%)
1	S	0.51	0/4221	0.66	2/5754 (0.0%)
1	T	0.51	0/4221	0.66	2/5754 (0.0%)
1	U	0.51	0/4221	0.66	2/5754 (0.0%)
1	V	0.51	0/4221	0.66	2/5754 (0.0%)
1	W	0.51	0/4221	0.66	2/5754 (0.0%)
1	X	0.51	0/4221	0.66	2/5754 (0.0%)
1	Y	0.51	0/4221	0.66	2/5754 (0.0%)
1	Z	0.51	0/4221	0.66	2/5754 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.51	0/4221	0.66	2/5754 (0.0%)
1	b	0.51	0/4221	0.66	2/5754 (0.0%)
1	c	0.51	0/4221	0.66	2/5754 (0.0%)
1	d	0.51	0/4221	0.66	2/5754 (0.0%)
1	e	0.51	0/4221	0.66	2/5754 (0.0%)
1	f	0.51	0/4221	0.66	2/5754 (0.0%)
1	g	0.51	0/4221	0.66	2/5754 (0.0%)
1	h	0.51	0/4221	0.66	2/5754 (0.0%)
1	i	0.51	0/4221	0.66	2/5754 (0.0%)
1	j	0.51	0/4221	0.66	2/5754 (0.0%)
1	k	0.51	0/4221	0.66	2/5754 (0.0%)
1	l	0.51	0/4221	0.66	2/5754 (0.0%)
1	m	0.51	0/4221	0.66	2/5754 (0.0%)
1	n	0.51	0/4221	0.66	2/5754 (0.0%)
1	o	0.51	0/4221	0.66	2/5754 (0.0%)
1	p	0.51	0/4221	0.66	2/5754 (0.0%)
1	q	0.51	0/4221	0.66	2/5754 (0.0%)
1	r	0.51	0/4221	0.66	2/5754 (0.0%)
1	s	0.51	0/4221	0.66	2/5754 (0.0%)
1	t	0.51	0/4221	0.66	2/5754 (0.0%)
1	u	0.51	0/4221	0.66	2/5754 (0.0%)
1	v	0.51	0/4221	0.66	2/5754 (0.0%)
1	w	0.51	0/4221	0.66	2/5754 (0.0%)
1	x	0.51	0/4221	0.66	2/5754 (0.0%)
1	y	0.51	0/4221	0.66	2/5754 (0.0%)
1	z	0.51	0/4221	0.66	2/5754 (0.0%)
All	All	0.51	0/253260	0.66	120/345240 (0.0%)

There are no bond length outliers.

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	471	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	w	471	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	7	471	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	N	471	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	Q	471	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	G	471	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	W	471	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	p	471	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	Z	471	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	o	471	ARG	NE-CZ-NH2	-6.36	117.12	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	471	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	D	471	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	r	471	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	F	471	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	K	471	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	C	471	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	e	471	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	M	471	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	n	471	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	4	471	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	6	471	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	I	471	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	v	471	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	l	471	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	H	471	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	S	471	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	J	471	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	q	471	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	z	471	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	t	471	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	O	471	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	d	471	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	471	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	h	471	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	P	471	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	i	471	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	u	471	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	2	471	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	Y	471	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	y	471	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	b	471	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	L	471	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	k	471	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	T	471	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	V	471	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	U	471	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	X	471	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	l	471	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	s	471	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	c	471	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	3	471	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	f	471	ARG	NE-CZ-NH2	-6.24	117.18	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	j	471	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	m	471	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	g	471	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	x	471	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	5	471	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	R	471	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	8	471	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	a	471	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	Y	518	ASN	N-CA-CB	-5.30	101.05	110.60
1	o	518	ASN	N-CA-CB	-5.30	101.06	110.60
1	Q	518	ASN	N-CA-CB	-5.30	101.06	110.60
1	g	518	ASN	N-CA-CB	-5.30	101.06	110.60
1	B	518	ASN	N-CA-CB	-5.29	101.07	110.60
1	2	518	ASN	N-CA-CB	-5.29	101.07	110.60
1	p	518	ASN	N-CA-CB	-5.29	101.07	110.60
1	5	518	ASN	N-CA-CB	-5.29	101.08	110.60
1	J	518	ASN	N-CA-CB	-5.29	101.08	110.60
1	c	518	ASN	N-CA-CB	-5.29	101.08	110.60
1	f	518	ASN	N-CA-CB	-5.29	101.08	110.60
1	w	518	ASN	N-CA-CB	-5.29	101.08	110.60
1	H	518	ASN	N-CA-CB	-5.29	101.09	110.60
1	K	518	ASN	N-CA-CB	-5.29	101.08	110.60
1	V	518	ASN	N-CA-CB	-5.29	101.09	110.60
1	3	518	ASN	N-CA-CB	-5.29	101.09	110.60
1	a	518	ASN	N-CA-CB	-5.29	101.09	110.60
1	q	518	ASN	N-CA-CB	-5.29	101.09	110.60
1	C	518	ASN	N-CA-CB	-5.28	101.09	110.60
1	n	518	ASN	N-CA-CB	-5.28	101.09	110.60
1	j	518	ASN	N-CA-CB	-5.28	101.09	110.60
1	m	518	ASN	N-CA-CB	-5.28	101.09	110.60
1	6	518	ASN	N-CA-CB	-5.28	101.09	110.60
1	u	518	ASN	N-CA-CB	-5.28	101.09	110.60
1	z	518	ASN	N-CA-CB	-5.28	101.09	110.60
1	P	518	ASN	N-CA-CB	-5.28	101.10	110.60
1	e	518	ASN	N-CA-CB	-5.28	101.10	110.60
1	A	518	ASN	N-CA-CB	-5.28	101.10	110.60
1	I	518	ASN	N-CA-CB	-5.28	101.10	110.60
1	L	518	ASN	N-CA-CB	-5.28	101.10	110.60
1	R	518	ASN	N-CA-CB	-5.28	101.10	110.60
1	b	518	ASN	N-CA-CB	-5.28	101.10	110.60
1	d	518	ASN	N-CA-CB	-5.27	101.11	110.60
1	1	518	ASN	N-CA-CB	-5.27	101.11	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	v	518	ASN	N-CA-CB	-5.27	101.11	110.60
1	S	518	ASN	N-CA-CB	-5.27	101.11	110.60
1	4	518	ASN	N-CA-CB	-5.27	101.11	110.60
1	M	518	ASN	N-CA-CB	-5.27	101.12	110.60
1	O	518	ASN	N-CA-CB	-5.27	101.12	110.60
1	U	518	ASN	N-CA-CB	-5.27	101.12	110.60
1	x	518	ASN	N-CA-CB	-5.27	101.12	110.60
1	X	518	ASN	N-CA-CB	-5.27	101.12	110.60
1	k	518	ASN	N-CA-CB	-5.27	101.12	110.60
1	8	518	ASN	N-CA-CB	-5.27	101.12	110.60
1	W	518	ASN	N-CA-CB	-5.26	101.12	110.60
1	D	518	ASN	N-CA-CB	-5.26	101.13	110.60
1	7	518	ASN	N-CA-CB	-5.26	101.13	110.60
1	F	518	ASN	N-CA-CB	-5.26	101.13	110.60
1	l	518	ASN	N-CA-CB	-5.26	101.13	110.60
1	Z	518	ASN	N-CA-CB	-5.26	101.13	110.60
1	s	518	ASN	N-CA-CB	-5.26	101.14	110.60
1	T	518	ASN	N-CA-CB	-5.26	101.14	110.60
1	h	518	ASN	N-CA-CB	-5.26	101.14	110.60
1	i	518	ASN	N-CA-CB	-5.26	101.14	110.60
1	r	518	ASN	N-CA-CB	-5.26	101.14	110.60
1	E	518	ASN	N-CA-CB	-5.25	101.14	110.60
1	N	518	ASN	N-CA-CB	-5.25	101.14	110.60
1	t	518	ASN	N-CA-CB	-5.25	101.14	110.60
1	y	518	ASN	N-CA-CB	-5.25	101.15	110.60
1	G	518	ASN	N-CA-CB	-5.24	101.17	110.60

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	1	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	2	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	3	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	4	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	5	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	6	508/735 (69%)	501 (99%)	7 (1%)	0	100	100
1	7	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	8	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	A	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	B	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	C	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	D	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	E	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	F	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	G	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	H	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	I	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	J	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	K	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	L	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	M	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	N	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	O	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	P	508/735 (69%)	501 (99%)	7 (1%)	0	100	100
1	Q	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	R	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	S	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	T	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	U	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	V	508/735 (69%)	502 (99%)	6 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	508/735 (69%)	501 (99%)	7 (1%)	0	100	100
1	X	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	Y	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	Z	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	a	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	b	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	c	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	d	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	e	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	f	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	g	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	h	508/735 (69%)	501 (99%)	7 (1%)	0	100	100
1	i	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	j	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	k	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	l	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	m	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	n	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	o	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	p	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	q	508/735 (69%)	501 (99%)	7 (1%)	0	100	100
1	r	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	s	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	t	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	u	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	v	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	w	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	x	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	y	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
1	z	508/735 (69%)	502 (99%)	6 (1%)	0	100	100
All	All	30480/44100 (69%)	30115 (99%)	365 (1%)	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	1	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	2	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	3	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	4	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	5	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	6	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	7	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	8	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	A	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	B	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	C	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	D	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	E	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	F	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	G	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	H	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	I	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	J	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	K	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	L	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	M	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	N	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	O	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	P	454/630 (72%)	446 (98%)	8 (2%)	59	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	R	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	S	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	T	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	U	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	V	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	W	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	X	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	Y	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	Z	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	a	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	b	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	c	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	d	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	e	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	f	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	g	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	h	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	i	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	j	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	k	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	l	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	m	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	n	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	o	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	p	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	q	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	r	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	s	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	t	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	u	454/630 (72%)	446 (98%)	8 (2%)	59	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	v	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	w	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	x	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	y	454/630 (72%)	446 (98%)	8 (2%)	59	45
1	z	454/630 (72%)	446 (98%)	8 (2%)	59	45
All	All	27240/37800 (72%)	26760 (98%)	480 (2%)	61	45

All (480) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	MET
1	A	288	HIS
1	A	482	CYS
1	A	597	THR
1	A	666	PHE
1	A	688	LYS
1	A	691	SER
1	A	693	ARG
1	B	235	MET
1	B	288	HIS
1	B	482	CYS
1	B	597	THR
1	B	666	PHE
1	B	688	LYS
1	B	691	SER
1	B	693	ARG
1	C	235	MET
1	C	288	HIS
1	C	482	CYS
1	C	597	THR
1	C	666	PHE
1	C	688	LYS
1	C	691	SER
1	C	693	ARG
1	D	235	MET
1	D	288	HIS
1	D	482	CYS
1	D	597	THR
1	D	666	PHE
1	D	688	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	691	SER
1	D	693	ARG
1	E	235	MET
1	E	288	HIS
1	E	482	CYS
1	E	597	THR
1	E	666	PHE
1	E	688	LYS
1	E	691	SER
1	E	693	ARG
1	F	235	MET
1	F	288	HIS
1	F	482	CYS
1	F	597	THR
1	F	666	PHE
1	F	688	LYS
1	F	691	SER
1	F	693	ARG
1	G	235	MET
1	G	288	HIS
1	G	482	CYS
1	G	597	THR
1	G	666	PHE
1	G	688	LYS
1	G	691	SER
1	G	693	ARG
1	H	235	MET
1	H	288	HIS
1	H	482	CYS
1	H	597	THR
1	H	666	PHE
1	H	688	LYS
1	H	691	SER
1	H	693	ARG
1	I	235	MET
1	I	288	HIS
1	I	482	CYS
1	I	597	THR
1	I	666	PHE
1	I	688	LYS
1	I	691	SER
1	I	693	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	235	MET
1	J	288	HIS
1	J	482	CYS
1	J	597	THR
1	J	666	PHE
1	J	688	LYS
1	J	691	SER
1	J	693	ARG
1	K	235	MET
1	K	288	HIS
1	K	482	CYS
1	K	597	THR
1	K	666	PHE
1	K	688	LYS
1	K	691	SER
1	K	693	ARG
1	L	235	MET
1	L	288	HIS
1	L	482	CYS
1	L	597	THR
1	L	666	PHE
1	L	688	LYS
1	L	691	SER
1	L	693	ARG
1	M	235	MET
1	M	288	HIS
1	M	482	CYS
1	M	597	THR
1	M	666	PHE
1	M	688	LYS
1	M	691	SER
1	M	693	ARG
1	N	235	MET
1	N	288	HIS
1	N	482	CYS
1	N	597	THR
1	N	666	PHE
1	N	688	LYS
1	N	691	SER
1	N	693	ARG
1	O	235	MET
1	O	288	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	482	CYS
1	O	597	THR
1	O	666	PHE
1	O	688	LYS
1	O	691	SER
1	O	693	ARG
1	P	235	MET
1	P	288	HIS
1	P	482	CYS
1	P	597	THR
1	P	666	PHE
1	P	688	LYS
1	P	691	SER
1	P	693	ARG
1	Q	235	MET
1	Q	288	HIS
1	Q	482	CYS
1	Q	597	THR
1	Q	666	PHE
1	Q	688	LYS
1	Q	691	SER
1	Q	693	ARG
1	R	235	MET
1	R	288	HIS
1	R	482	CYS
1	R	597	THR
1	R	666	PHE
1	R	688	LYS
1	R	691	SER
1	R	693	ARG
1	S	235	MET
1	S	288	HIS
1	S	482	CYS
1	S	597	THR
1	S	666	PHE
1	S	688	LYS
1	S	691	SER
1	S	693	ARG
1	T	235	MET
1	T	288	HIS
1	T	482	CYS
1	T	597	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	666	PHE
1	T	688	LYS
1	T	691	SER
1	T	693	ARG
1	U	235	MET
1	U	288	HIS
1	U	482	CYS
1	U	597	THR
1	U	666	PHE
1	U	688	LYS
1	U	691	SER
1	U	693	ARG
1	V	235	MET
1	V	288	HIS
1	V	482	CYS
1	V	597	THR
1	V	666	PHE
1	V	688	LYS
1	V	691	SER
1	V	693	ARG
1	W	235	MET
1	W	288	HIS
1	W	482	CYS
1	W	597	THR
1	W	666	PHE
1	W	688	LYS
1	W	691	SER
1	W	693	ARG
1	X	235	MET
1	X	288	HIS
1	X	482	CYS
1	X	597	THR
1	X	666	PHE
1	X	688	LYS
1	X	691	SER
1	X	693	ARG
1	Y	235	MET
1	Y	288	HIS
1	Y	482	CYS
1	Y	597	THR
1	Y	666	PHE
1	Y	688	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Y	691	SER
1	Y	693	ARG
1	Z	235	MET
1	Z	288	HIS
1	Z	482	CYS
1	Z	597	THR
1	Z	666	PHE
1	Z	688	LYS
1	Z	691	SER
1	Z	693	ARG
1	1	235	MET
1	1	288	HIS
1	1	482	CYS
1	1	597	THR
1	1	666	PHE
1	1	688	LYS
1	1	691	SER
1	1	693	ARG
1	2	235	MET
1	2	288	HIS
1	2	482	CYS
1	2	597	THR
1	2	666	PHE
1	2	688	LYS
1	2	691	SER
1	2	693	ARG
1	3	235	MET
1	3	288	HIS
1	3	482	CYS
1	3	597	THR
1	3	666	PHE
1	3	688	LYS
1	3	691	SER
1	3	693	ARG
1	4	235	MET
1	4	288	HIS
1	4	482	CYS
1	4	597	THR
1	4	666	PHE
1	4	688	LYS
1	4	691	SER
1	4	693	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	235	MET
1	5	288	HIS
1	5	482	CYS
1	5	597	THR
1	5	666	PHE
1	5	688	LYS
1	5	691	SER
1	5	693	ARG
1	6	235	MET
1	6	288	HIS
1	6	482	CYS
1	6	597	THR
1	6	666	PHE
1	6	688	LYS
1	6	691	SER
1	6	693	ARG
1	a	235	MET
1	a	288	HIS
1	a	482	CYS
1	a	597	THR
1	a	666	PHE
1	a	688	LYS
1	a	691	SER
1	a	693	ARG
1	b	235	MET
1	b	288	HIS
1	b	482	CYS
1	b	597	THR
1	b	666	PHE
1	b	688	LYS
1	b	691	SER
1	b	693	ARG
1	c	235	MET
1	c	288	HIS
1	c	482	CYS
1	c	597	THR
1	c	666	PHE
1	c	688	LYS
1	c	691	SER
1	c	693	ARG
1	d	235	MET
1	d	288	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	d	482	CYS
1	d	597	THR
1	d	666	PHE
1	d	688	LYS
1	d	691	SER
1	d	693	ARG
1	e	235	MET
1	e	288	HIS
1	e	482	CYS
1	e	597	THR
1	e	666	PHE
1	e	688	LYS
1	e	691	SER
1	e	693	ARG
1	f	235	MET
1	f	288	HIS
1	f	482	CYS
1	f	597	THR
1	f	666	PHE
1	f	688	LYS
1	f	691	SER
1	f	693	ARG
1	g	235	MET
1	g	288	HIS
1	g	482	CYS
1	g	597	THR
1	g	666	PHE
1	g	688	LYS
1	g	691	SER
1	g	693	ARG
1	h	235	MET
1	h	288	HIS
1	h	482	CYS
1	h	597	THR
1	h	666	PHE
1	h	688	LYS
1	h	691	SER
1	h	693	ARG
1	i	235	MET
1	i	288	HIS
1	i	482	CYS
1	i	597	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	i	666	PHE
1	i	688	LYS
1	i	691	SER
1	i	693	ARG
1	j	235	MET
1	j	288	HIS
1	j	482	CYS
1	j	597	THR
1	j	666	PHE
1	j	688	LYS
1	j	691	SER
1	j	693	ARG
1	k	235	MET
1	k	288	HIS
1	k	482	CYS
1	k	597	THR
1	k	666	PHE
1	k	688	LYS
1	k	691	SER
1	k	693	ARG
1	l	235	MET
1	l	288	HIS
1	l	482	CYS
1	l	597	THR
1	l	666	PHE
1	l	688	LYS
1	l	691	SER
1	l	693	ARG
1	m	235	MET
1	m	288	HIS
1	m	482	CYS
1	m	597	THR
1	m	666	PHE
1	m	688	LYS
1	m	691	SER
1	m	693	ARG
1	n	235	MET
1	n	288	HIS
1	n	482	CYS
1	n	597	THR
1	n	666	PHE
1	n	688	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	n	691	SER
1	n	693	ARG
1	o	235	MET
1	o	288	HIS
1	o	482	CYS
1	o	597	THR
1	o	666	PHE
1	o	688	LYS
1	o	691	SER
1	o	693	ARG
1	p	235	MET
1	p	288	HIS
1	p	482	CYS
1	p	597	THR
1	p	666	PHE
1	p	688	LYS
1	p	691	SER
1	p	693	ARG
1	q	235	MET
1	q	288	HIS
1	q	482	CYS
1	q	597	THR
1	q	666	PHE
1	q	688	LYS
1	q	691	SER
1	q	693	ARG
1	r	235	MET
1	r	288	HIS
1	r	482	CYS
1	r	597	THR
1	r	666	PHE
1	r	688	LYS
1	r	691	SER
1	r	693	ARG
1	s	235	MET
1	s	288	HIS
1	s	482	CYS
1	s	597	THR
1	s	666	PHE
1	s	688	LYS
1	s	691	SER
1	s	693	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	t	235	MET
1	t	288	HIS
1	t	482	CYS
1	t	597	THR
1	t	666	PHE
1	t	688	LYS
1	t	691	SER
1	t	693	ARG
1	u	235	MET
1	u	288	HIS
1	u	482	CYS
1	u	597	THR
1	u	666	PHE
1	u	688	LYS
1	u	691	SER
1	u	693	ARG
1	v	235	MET
1	v	288	HIS
1	v	482	CYS
1	v	597	THR
1	v	666	PHE
1	v	688	LYS
1	v	691	SER
1	v	693	ARG
1	w	235	MET
1	w	288	HIS
1	w	482	CYS
1	w	597	THR
1	w	666	PHE
1	w	688	LYS
1	w	691	SER
1	w	693	ARG
1	x	235	MET
1	x	288	HIS
1	x	482	CYS
1	x	597	THR
1	x	666	PHE
1	x	688	LYS
1	x	691	SER
1	x	693	ARG
1	y	235	MET
1	y	288	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	y	482	CYS
1	y	597	THR
1	y	666	PHE
1	y	688	LYS
1	y	691	SER
1	y	693	ARG
1	z	235	MET
1	z	288	HIS
1	z	482	CYS
1	z	597	THR
1	z	666	PHE
1	z	688	LYS
1	z	691	SER
1	z	693	ARG
1	7	235	MET
1	7	288	HIS
1	7	482	CYS
1	7	597	THR
1	7	666	PHE
1	7	688	LYS
1	7	691	SER
1	7	693	ARG
1	8	235	MET
1	8	288	HIS
1	8	482	CYS
1	8	597	THR
1	8	666	PHE
1	8	688	LYS
1	8	691	SER
1	8	693	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (517) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	ASN
1	A	288	HIS
1	A	303	ASN
1	A	325	GLN
1	A	341	GLN
1	A	349	GLN
1	A	457	GLN
1	A	518	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	717	ASN
1	B	270	ASN
1	B	288	HIS
1	B	303	ASN
1	B	325	GLN
1	B	341	GLN
1	B	349	GLN
1	B	457	GLN
1	B	518	ASN
1	B	717	ASN
1	C	270	ASN
1	C	288	HIS
1	C	303	ASN
1	C	325	GLN
1	C	341	GLN
1	C	349	GLN
1	C	457	GLN
1	C	518	ASN
1	D	270	ASN
1	D	288	HIS
1	D	303	ASN
1	D	325	GLN
1	D	341	GLN
1	D	349	GLN
1	D	457	GLN
1	D	518	ASN
1	E	270	ASN
1	E	288	HIS
1	E	303	ASN
1	E	325	GLN
1	E	341	GLN
1	E	349	GLN
1	E	457	GLN
1	E	518	ASN
1	F	270	ASN
1	F	288	HIS
1	F	303	ASN
1	F	325	GLN
1	F	341	GLN
1	F	349	GLN
1	F	457	GLN
1	F	518	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	717	ASN
1	G	270	ASN
1	G	288	HIS
1	G	303	ASN
1	G	325	GLN
1	G	341	GLN
1	G	349	GLN
1	G	457	GLN
1	G	518	ASN
1	G	717	ASN
1	H	270	ASN
1	H	288	HIS
1	H	303	ASN
1	H	325	GLN
1	H	341	GLN
1	H	349	GLN
1	H	457	GLN
1	H	518	ASN
1	I	270	ASN
1	I	288	HIS
1	I	303	ASN
1	I	325	GLN
1	I	341	GLN
1	I	349	GLN
1	I	457	GLN
1	I	518	ASN
1	J	270	ASN
1	J	288	HIS
1	J	303	ASN
1	J	325	GLN
1	J	341	GLN
1	J	349	GLN
1	J	457	GLN
1	J	518	ASN
1	K	270	ASN
1	K	288	HIS
1	K	303	ASN
1	K	325	GLN
1	K	341	GLN
1	K	349	GLN
1	K	457	GLN
1	K	518	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	270	ASN
1	L	288	HIS
1	L	303	ASN
1	L	325	GLN
1	L	341	GLN
1	L	349	GLN
1	L	457	GLN
1	L	518	ASN
1	L	717	ASN
1	M	270	ASN
1	M	288	HIS
1	M	303	ASN
1	M	325	GLN
1	M	341	GLN
1	M	349	GLN
1	M	457	GLN
1	M	518	ASN
1	N	270	ASN
1	N	288	HIS
1	N	303	ASN
1	N	325	GLN
1	N	341	GLN
1	N	349	GLN
1	N	457	GLN
1	N	518	ASN
1	N	717	ASN
1	O	270	ASN
1	O	288	HIS
1	O	303	ASN
1	O	325	GLN
1	O	341	GLN
1	O	349	GLN
1	O	457	GLN
1	O	518	ASN
1	O	717	ASN
1	P	270	ASN
1	P	288	HIS
1	P	303	ASN
1	P	325	GLN
1	P	341	GLN
1	P	349	GLN
1	P	457	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	518	ASN
1	P	717	ASN
1	Q	270	ASN
1	Q	288	HIS
1	Q	303	ASN
1	Q	325	GLN
1	Q	341	GLN
1	Q	349	GLN
1	Q	457	GLN
1	Q	518	ASN
1	Q	717	ASN
1	R	270	ASN
1	R	288	HIS
1	R	303	ASN
1	R	325	GLN
1	R	341	GLN
1	R	349	GLN
1	R	457	GLN
1	R	518	ASN
1	R	717	ASN
1	S	270	ASN
1	S	288	HIS
1	S	303	ASN
1	S	325	GLN
1	S	341	GLN
1	S	349	GLN
1	S	457	GLN
1	S	518	ASN
1	T	270	ASN
1	T	288	HIS
1	T	303	ASN
1	T	325	GLN
1	T	341	GLN
1	T	349	GLN
1	T	457	GLN
1	T	518	ASN
1	T	717	ASN
1	U	270	ASN
1	U	288	HIS
1	U	303	ASN
1	U	325	GLN
1	U	341	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	U	349	GLN
1	U	457	GLN
1	U	518	ASN
1	U	717	ASN
1	V	270	ASN
1	V	288	HIS
1	V	303	ASN
1	V	325	GLN
1	V	341	GLN
1	V	349	GLN
1	V	457	GLN
1	V	518	ASN
1	W	270	ASN
1	W	288	HIS
1	W	303	ASN
1	W	325	GLN
1	W	341	GLN
1	W	349	GLN
1	W	457	GLN
1	W	518	ASN
1	W	717	ASN
1	X	270	ASN
1	X	288	HIS
1	X	303	ASN
1	X	325	GLN
1	X	341	GLN
1	X	349	GLN
1	X	457	GLN
1	X	518	ASN
1	X	717	ASN
1	Y	270	ASN
1	Y	288	HIS
1	Y	303	ASN
1	Y	325	GLN
1	Y	341	GLN
1	Y	349	GLN
1	Y	457	GLN
1	Y	518	ASN
1	Y	717	ASN
1	Z	270	ASN
1	Z	288	HIS
1	Z	303	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Z	325	GLN
1	Z	341	GLN
1	Z	349	GLN
1	Z	457	GLN
1	Z	518	ASN
1	1	270	ASN
1	1	288	HIS
1	1	303	ASN
1	1	325	GLN
1	1	341	GLN
1	1	349	GLN
1	1	457	GLN
1	1	518	ASN
1	1	717	ASN
1	2	270	ASN
1	2	288	HIS
1	2	303	ASN
1	2	325	GLN
1	2	341	GLN
1	2	349	GLN
1	2	457	GLN
1	2	518	ASN
1	2	717	ASN
1	3	270	ASN
1	3	288	HIS
1	3	303	ASN
1	3	325	GLN
1	3	341	GLN
1	3	349	GLN
1	3	457	GLN
1	3	518	ASN
1	4	270	ASN
1	4	288	HIS
1	4	303	ASN
1	4	325	GLN
1	4	341	GLN
1	4	349	GLN
1	4	457	GLN
1	4	518	ASN
1	5	270	ASN
1	5	288	HIS
1	5	303	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	325	GLN
1	5	341	GLN
1	5	349	GLN
1	5	457	GLN
1	5	518	ASN
1	5	717	ASN
1	6	270	ASN
1	6	288	HIS
1	6	303	ASN
1	6	325	GLN
1	6	341	GLN
1	6	349	GLN
1	6	457	GLN
1	6	518	ASN
1	6	717	ASN
1	a	270	ASN
1	a	288	HIS
1	a	303	ASN
1	a	325	GLN
1	a	341	GLN
1	a	349	GLN
1	a	457	GLN
1	a	518	ASN
1	a	717	ASN
1	b	270	ASN
1	b	288	HIS
1	b	303	ASN
1	b	325	GLN
1	b	341	GLN
1	b	349	GLN
1	b	457	GLN
1	b	518	ASN
1	b	717	ASN
1	c	270	ASN
1	c	288	HIS
1	c	303	ASN
1	c	325	GLN
1	c	341	GLN
1	c	349	GLN
1	c	457	GLN
1	c	518	ASN
1	c	717	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	d	270	ASN
1	d	288	HIS
1	d	303	ASN
1	d	325	GLN
1	d	341	GLN
1	d	349	GLN
1	d	457	GLN
1	d	518	ASN
1	d	717	ASN
1	e	270	ASN
1	e	288	HIS
1	e	303	ASN
1	e	325	GLN
1	e	341	GLN
1	e	349	GLN
1	e	457	GLN
1	e	518	ASN
1	e	717	ASN
1	f	270	ASN
1	f	288	HIS
1	f	303	ASN
1	f	325	GLN
1	f	341	GLN
1	f	349	GLN
1	f	457	GLN
1	f	518	ASN
1	g	270	ASN
1	g	288	HIS
1	g	303	ASN
1	g	325	GLN
1	g	341	GLN
1	g	349	GLN
1	g	457	GLN
1	g	518	ASN
1	h	270	ASN
1	h	288	HIS
1	h	303	ASN
1	h	325	GLN
1	h	341	GLN
1	h	349	GLN
1	h	457	GLN
1	h	518	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	i	270	ASN
1	i	288	HIS
1	i	303	ASN
1	i	325	GLN
1	i	341	GLN
1	i	349	GLN
1	i	457	GLN
1	i	518	ASN
1	i	717	ASN
1	j	270	ASN
1	j	288	HIS
1	j	303	ASN
1	j	325	GLN
1	j	341	GLN
1	j	349	GLN
1	j	457	GLN
1	j	518	ASN
1	j	717	ASN
1	k	270	ASN
1	k	288	HIS
1	k	303	ASN
1	k	325	GLN
1	k	341	GLN
1	k	349	GLN
1	k	457	GLN
1	k	518	ASN
1	k	717	ASN
1	l	270	ASN
1	l	288	HIS
1	l	303	ASN
1	l	325	GLN
1	l	341	GLN
1	l	349	GLN
1	l	457	GLN
1	l	518	ASN
1	l	717	ASN
1	m	270	ASN
1	m	288	HIS
1	m	303	ASN
1	m	325	GLN
1	m	341	GLN
1	m	349	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	m	457	GLN
1	m	518	ASN
1	n	270	ASN
1	n	288	HIS
1	n	303	ASN
1	n	325	GLN
1	n	341	GLN
1	n	349	GLN
1	n	457	GLN
1	n	518	ASN
1	n	717	ASN
1	o	270	ASN
1	o	288	HIS
1	o	303	ASN
1	o	325	GLN
1	o	341	GLN
1	o	349	GLN
1	o	457	GLN
1	o	518	ASN
1	p	270	ASN
1	p	288	HIS
1	p	303	ASN
1	p	325	GLN
1	p	341	GLN
1	p	349	GLN
1	p	457	GLN
1	p	518	ASN
1	p	717	ASN
1	q	270	ASN
1	q	288	HIS
1	q	303	ASN
1	q	325	GLN
1	q	341	GLN
1	q	349	GLN
1	q	457	GLN
1	q	518	ASN
1	q	717	ASN
1	r	270	ASN
1	r	288	HIS
1	r	303	ASN
1	r	325	GLN
1	r	341	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	r	349	GLN
1	r	457	GLN
1	r	518	ASN
1	r	717	ASN
1	s	270	ASN
1	s	288	HIS
1	s	303	ASN
1	s	325	GLN
1	s	341	GLN
1	s	349	GLN
1	s	457	GLN
1	s	518	ASN
1	t	270	ASN
1	t	288	HIS
1	t	303	ASN
1	t	325	GLN
1	t	341	GLN
1	t	349	GLN
1	t	457	GLN
1	t	518	ASN
1	u	270	ASN
1	u	288	HIS
1	u	303	ASN
1	u	325	GLN
1	u	341	GLN
1	u	349	GLN
1	u	457	GLN
1	u	518	ASN
1	u	717	ASN
1	v	270	ASN
1	v	288	HIS
1	v	303	ASN
1	v	325	GLN
1	v	341	GLN
1	v	349	GLN
1	v	457	GLN
1	v	518	ASN
1	w	270	ASN
1	w	288	HIS
1	w	303	ASN
1	w	325	GLN
1	w	341	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	w	349	GLN
1	w	457	GLN
1	w	518	ASN
1	w	717	ASN
1	x	270	ASN
1	x	288	HIS
1	x	303	ASN
1	x	325	GLN
1	x	341	GLN
1	x	349	GLN
1	x	457	GLN
1	x	518	ASN
1	y	270	ASN
1	y	288	HIS
1	y	303	ASN
1	y	325	GLN
1	y	341	GLN
1	y	349	GLN
1	y	457	GLN
1	y	518	ASN
1	y	717	ASN
1	z	270	ASN
1	z	288	HIS
1	z	303	ASN
1	z	325	GLN
1	z	341	GLN
1	z	349	GLN
1	z	457	GLN
1	z	518	ASN
1	z	717	ASN
1	7	270	ASN
1	7	288	HIS
1	7	303	ASN
1	7	325	GLN
1	7	341	GLN
1	7	349	GLN
1	7	457	GLN
1	7	518	ASN
1	8	270	ASN
1	8	288	HIS
1	8	303	ASN
1	8	325	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8	341	GLN
1	8	349	GLN
1	8	457	GLN
1	8	518	ASN
1	8	717	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

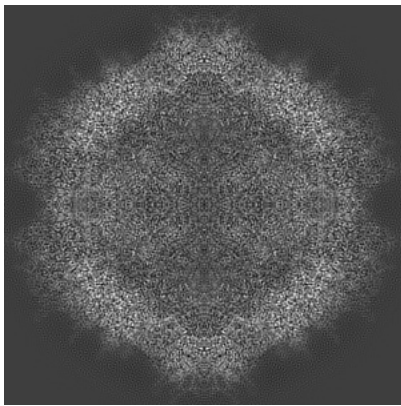
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9012. These allow visual inspection of the internal detail of the map and identification of artifacts.

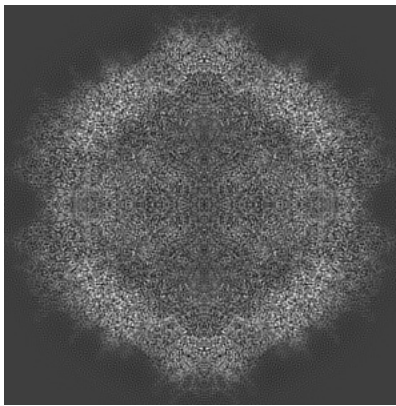
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

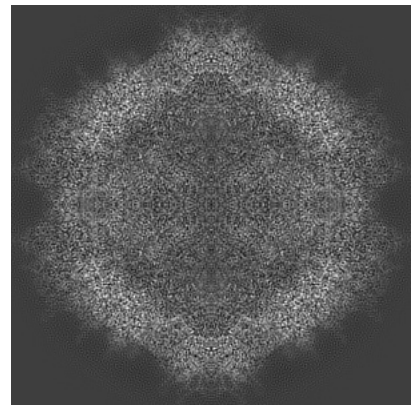
6.1.1 Primary map



X

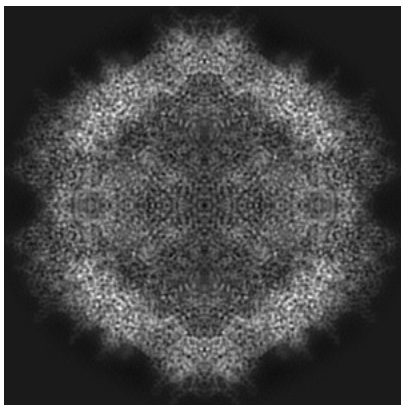


Y

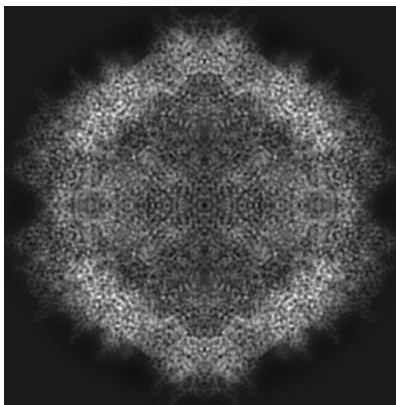


Z

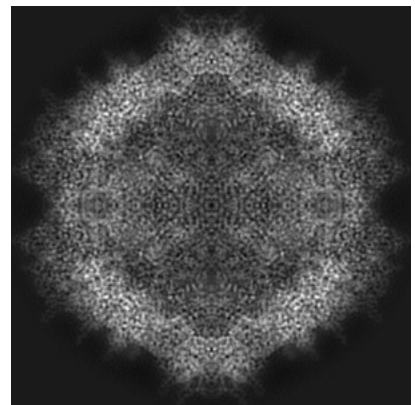
6.1.2 Raw map



X



Y

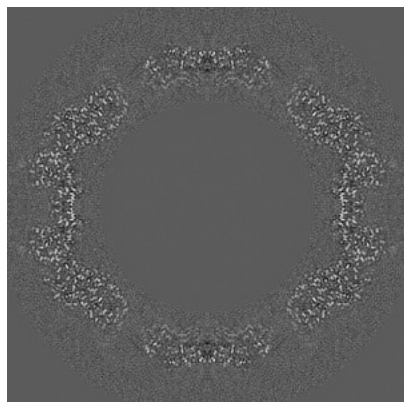


Z

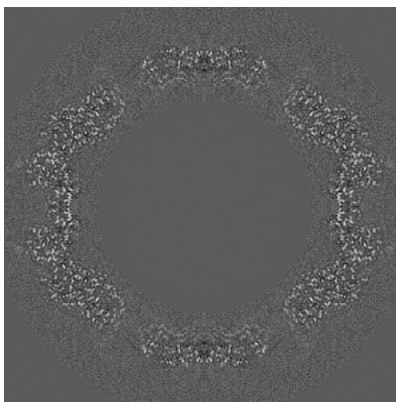
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

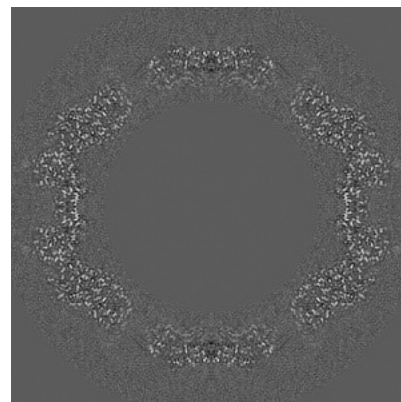
6.2.1 Primary map



X Index: 360

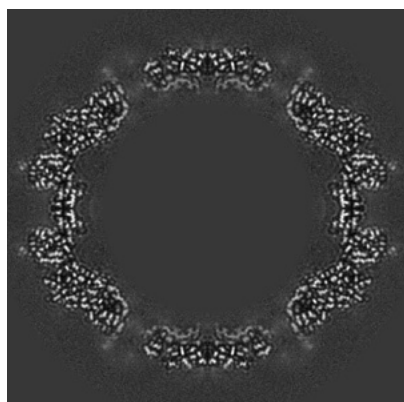


Y Index: 360

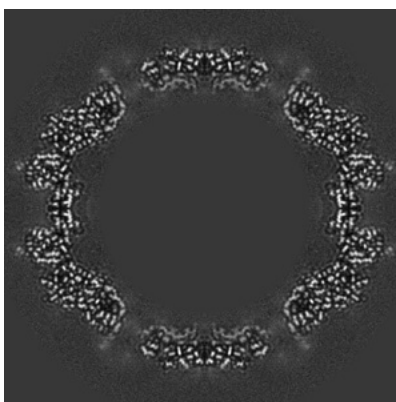


Z Index: 360

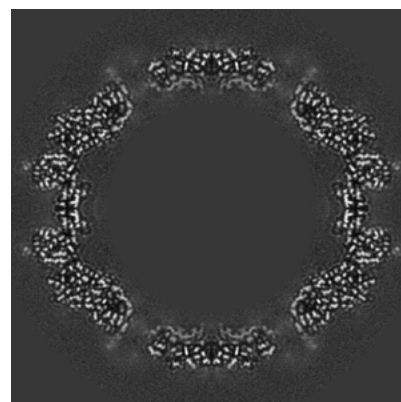
6.2.2 Raw map



X Index: 180



Y Index: 180

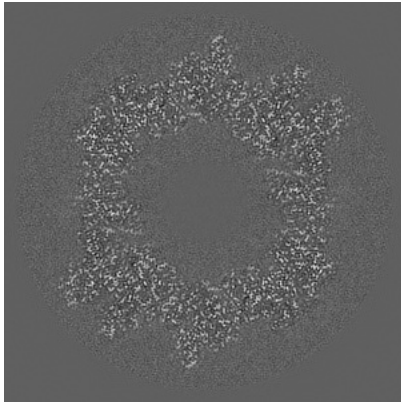


Z Index: 180

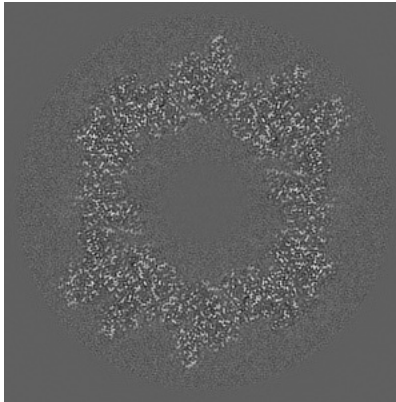
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

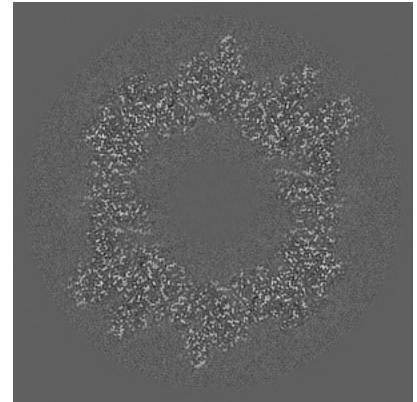
6.3.1 Primary map



X Index: 534

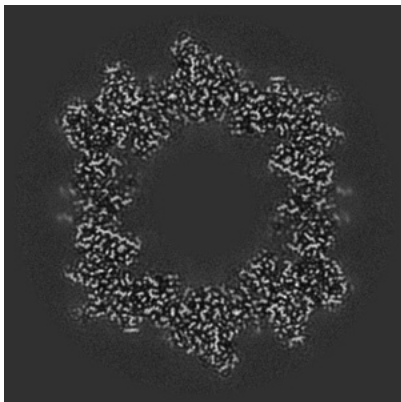


Y Index: 534

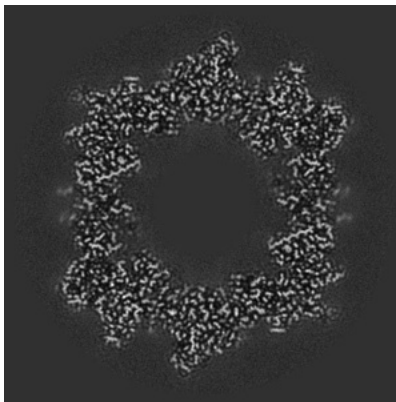


Z Index: 534

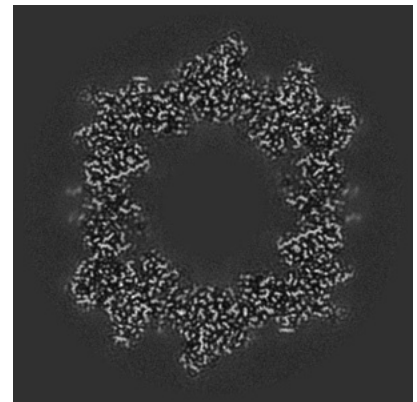
6.3.2 Raw map



X Index: 97



Y Index: 263

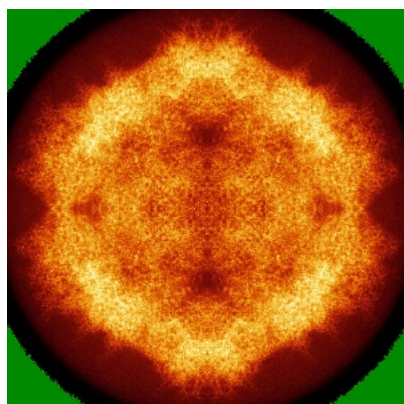


Z Index: 263

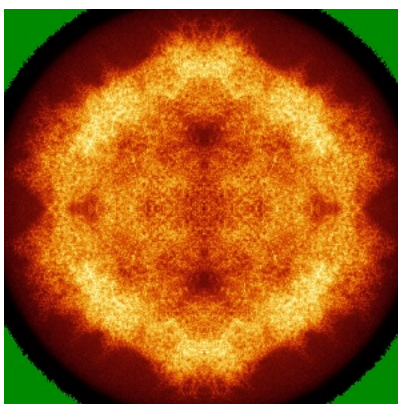
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

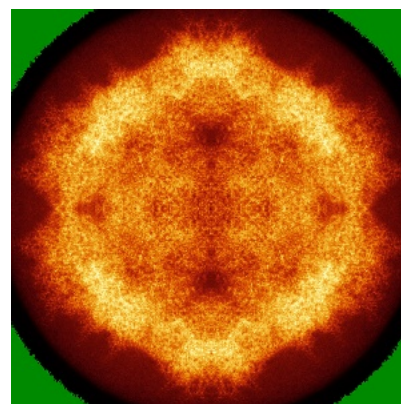
6.4.1 Primary map



X

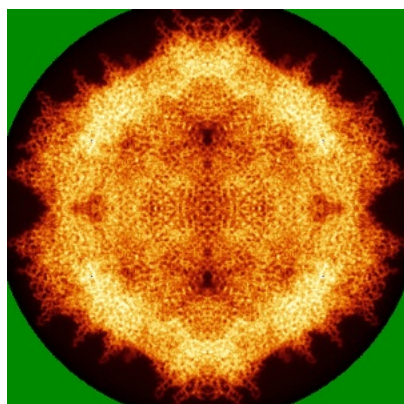


Y

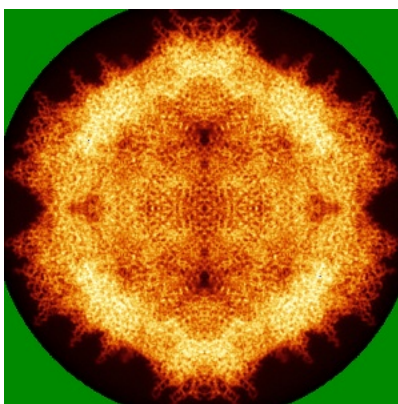


Z

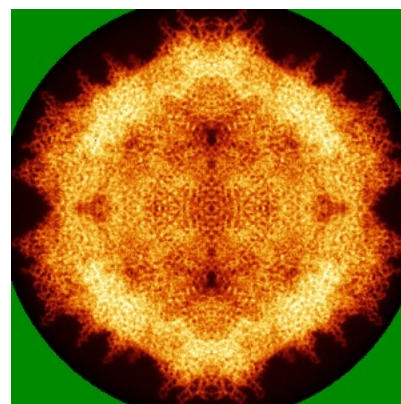
6.4.2 Raw map



X



Y

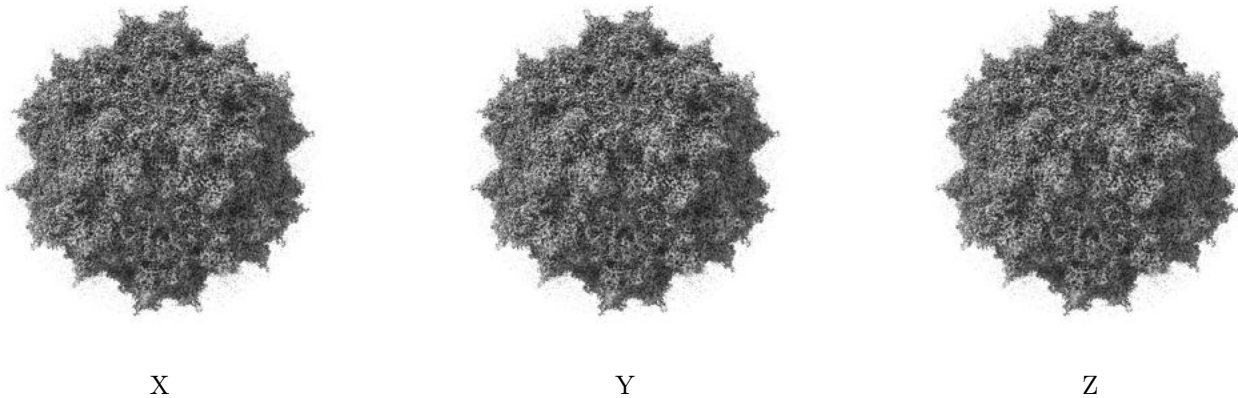


Z

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.

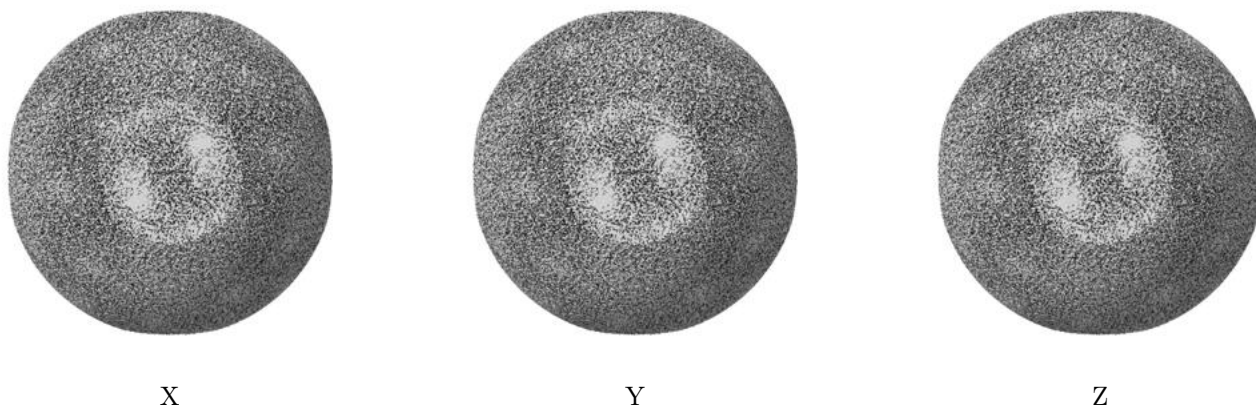
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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



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.

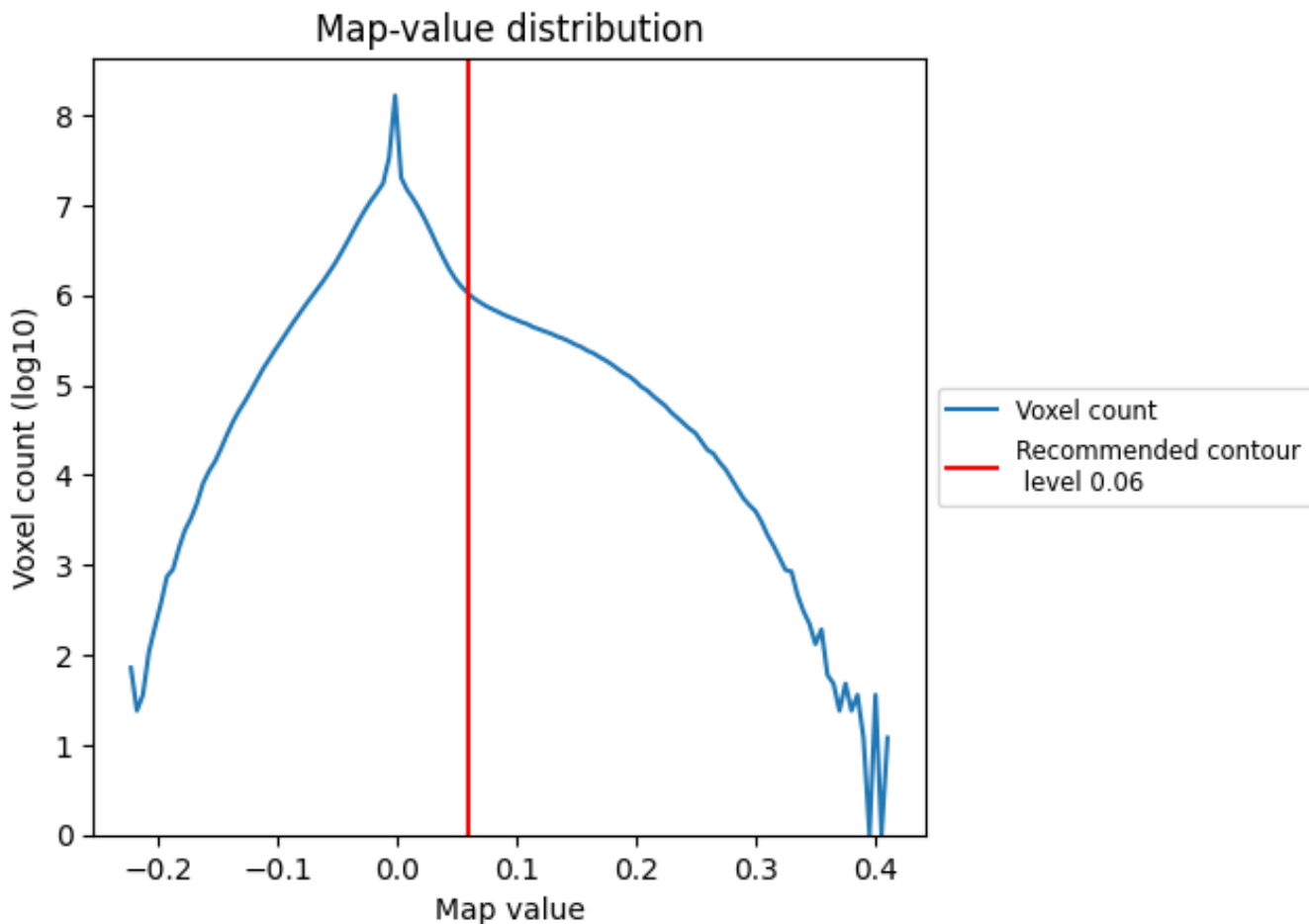
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

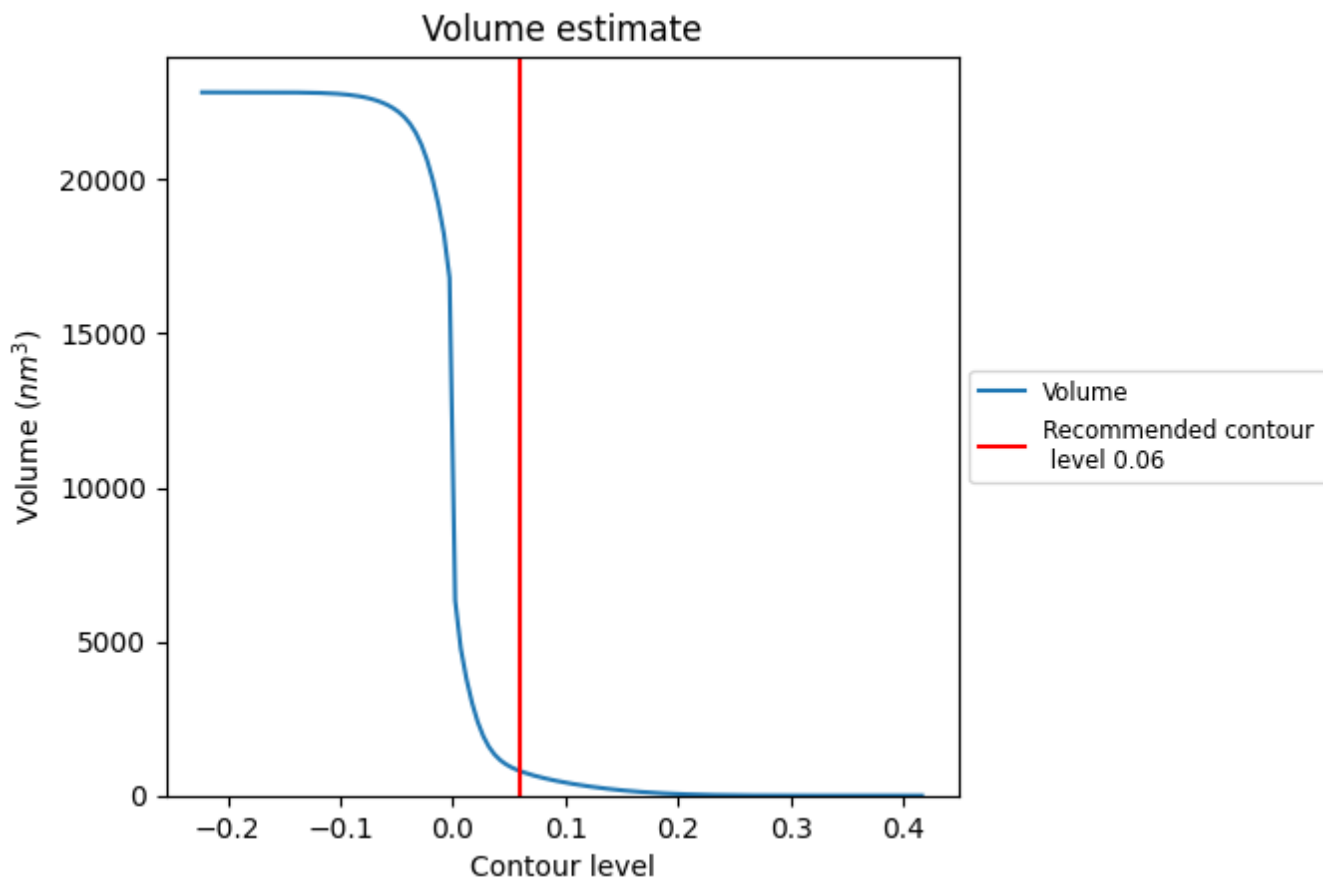
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

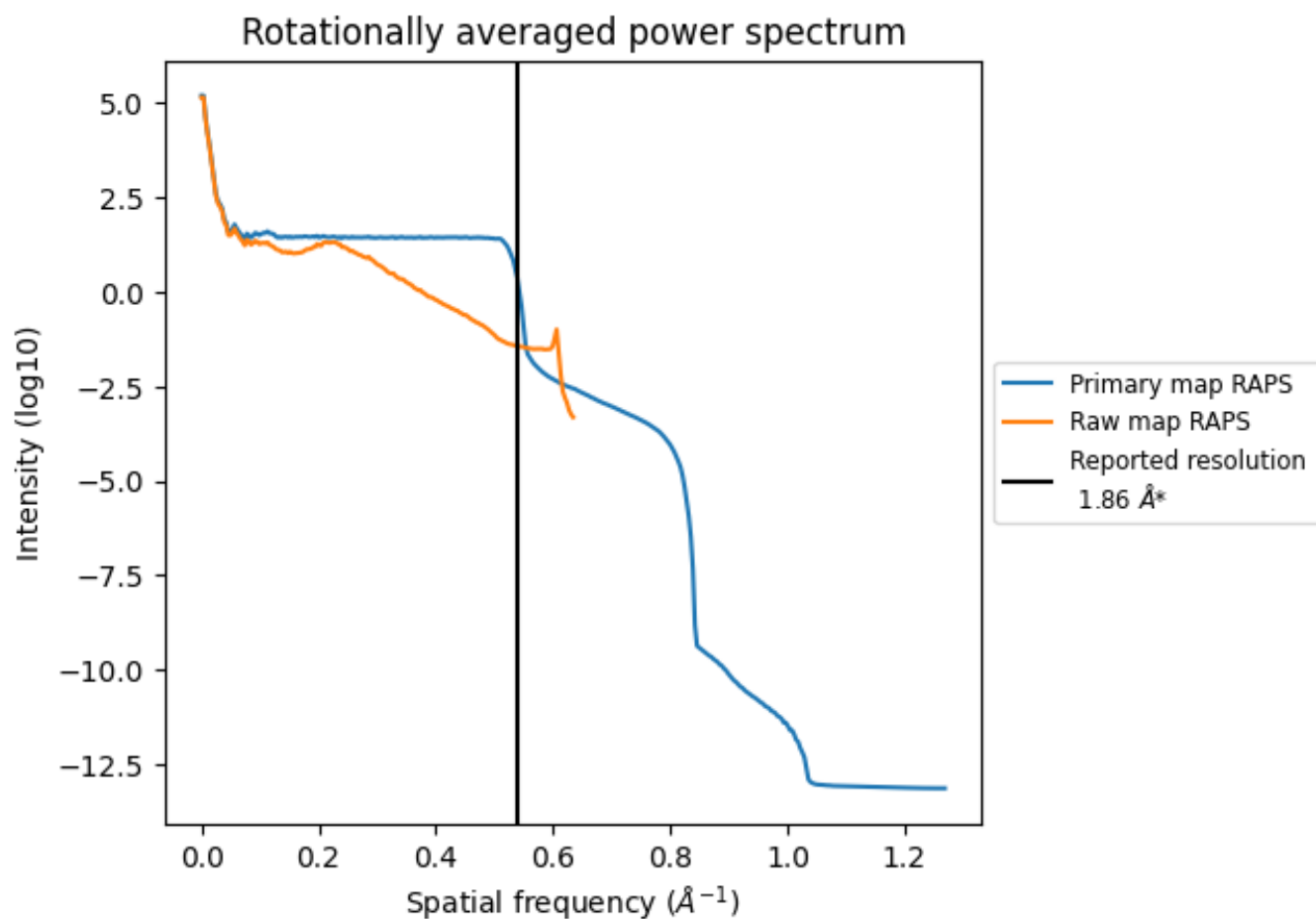
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 790 nm³; this corresponds to an approximate mass of 714 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](#)

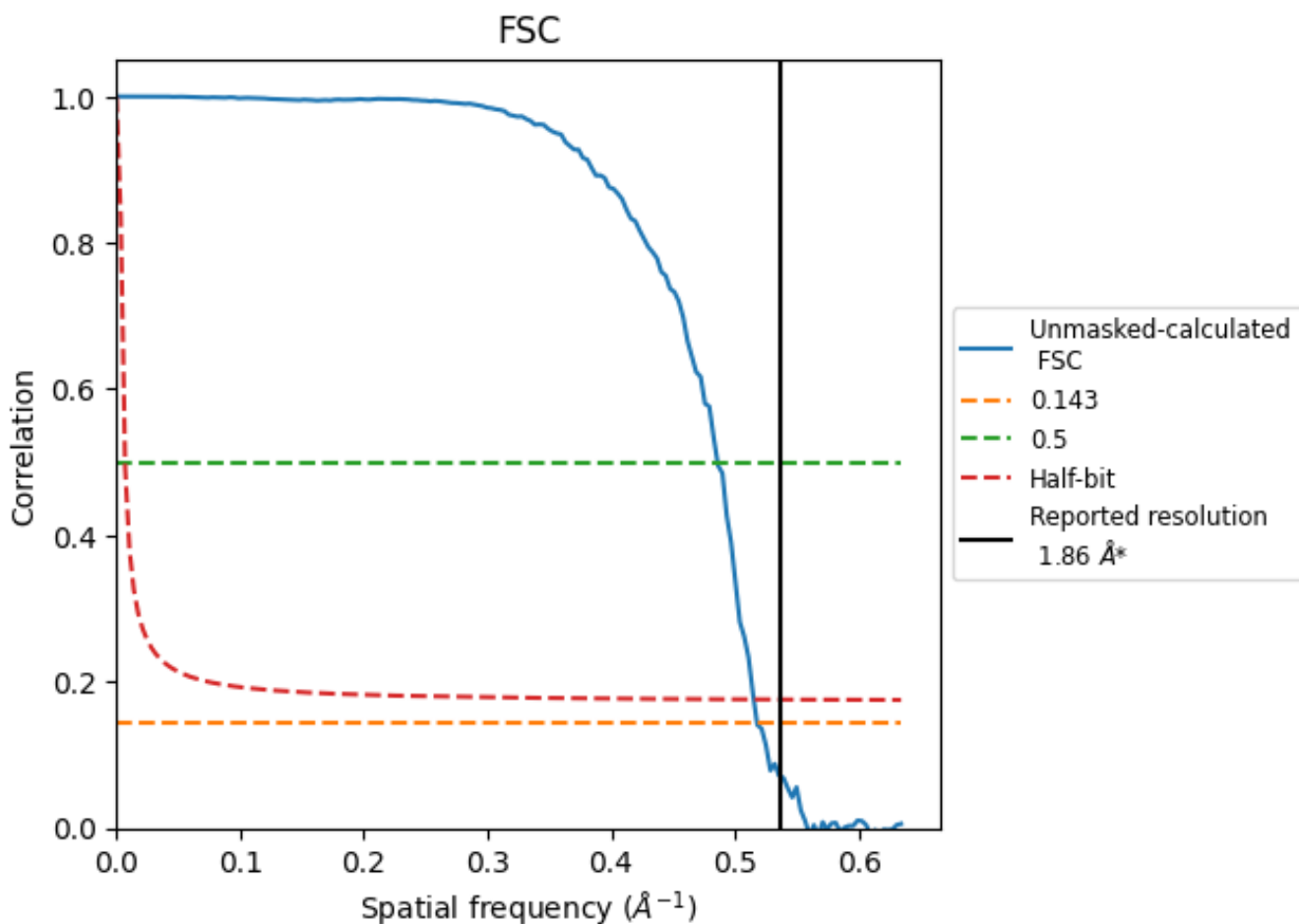


*Reported resolution corresponds to spatial frequency of 0.538 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.538 \AA^{-1}

8.2 Resolution estimates [i](#)

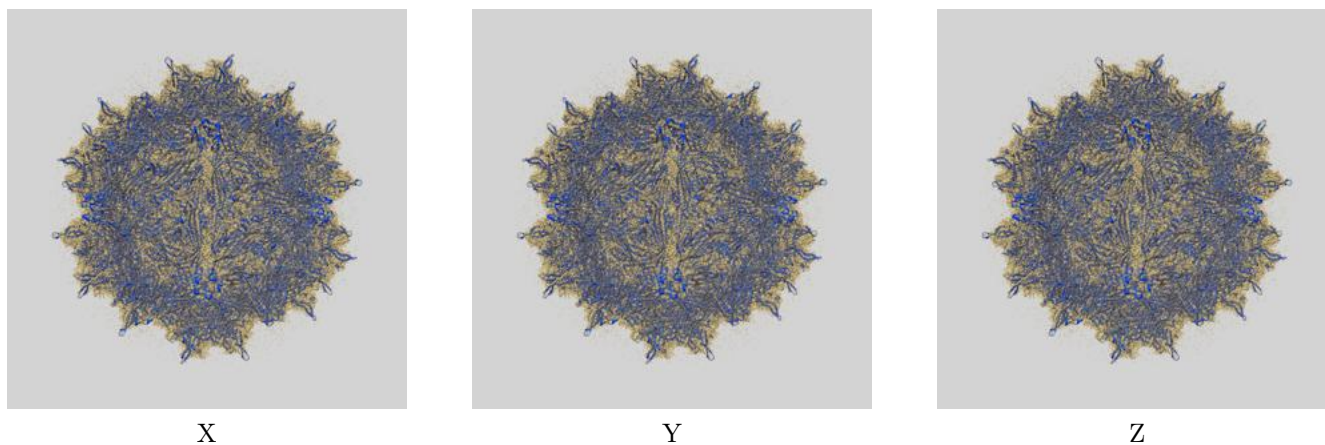
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.86	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	1.93	2.06	1.94

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

9 Map-model fit [i](#)

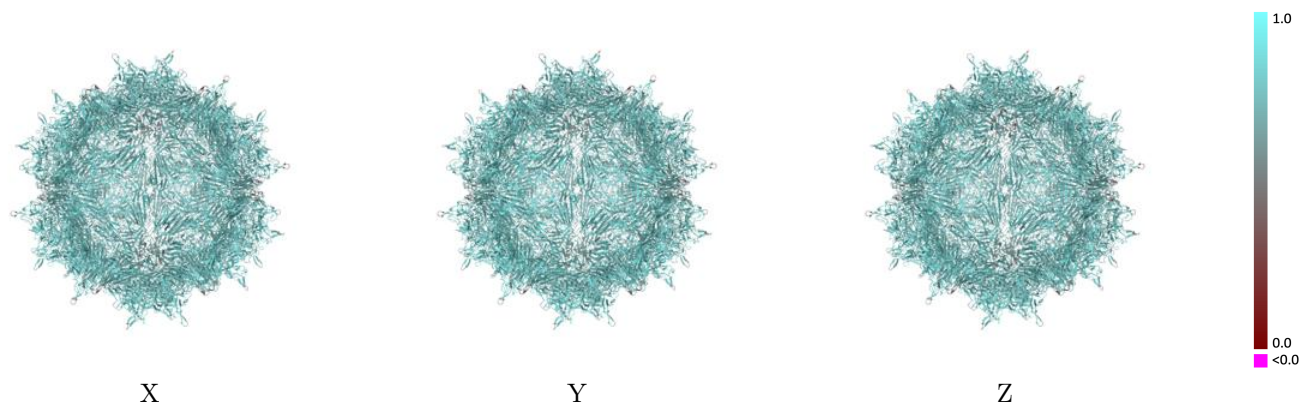
This section contains information regarding the fit between EMDB map EMD-9012 and PDB model 6E9D. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



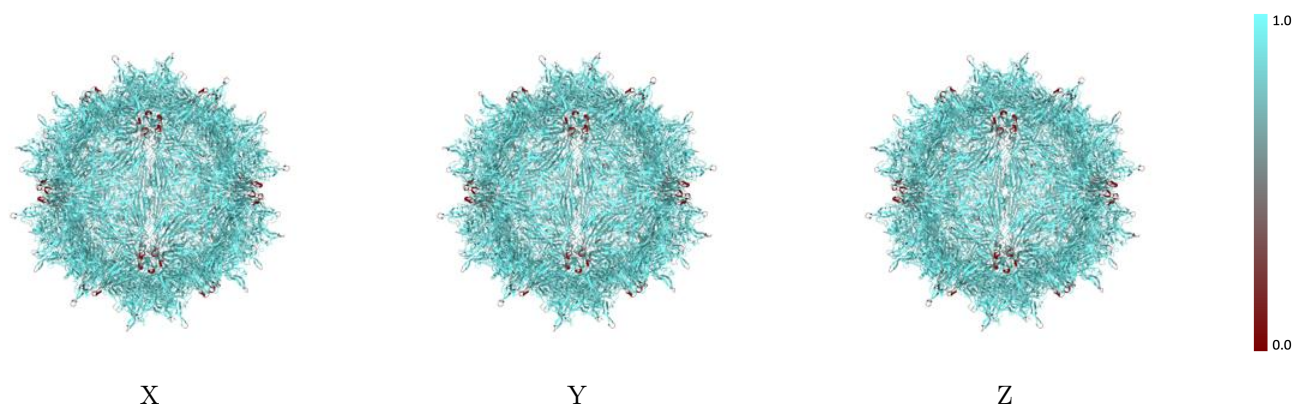
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



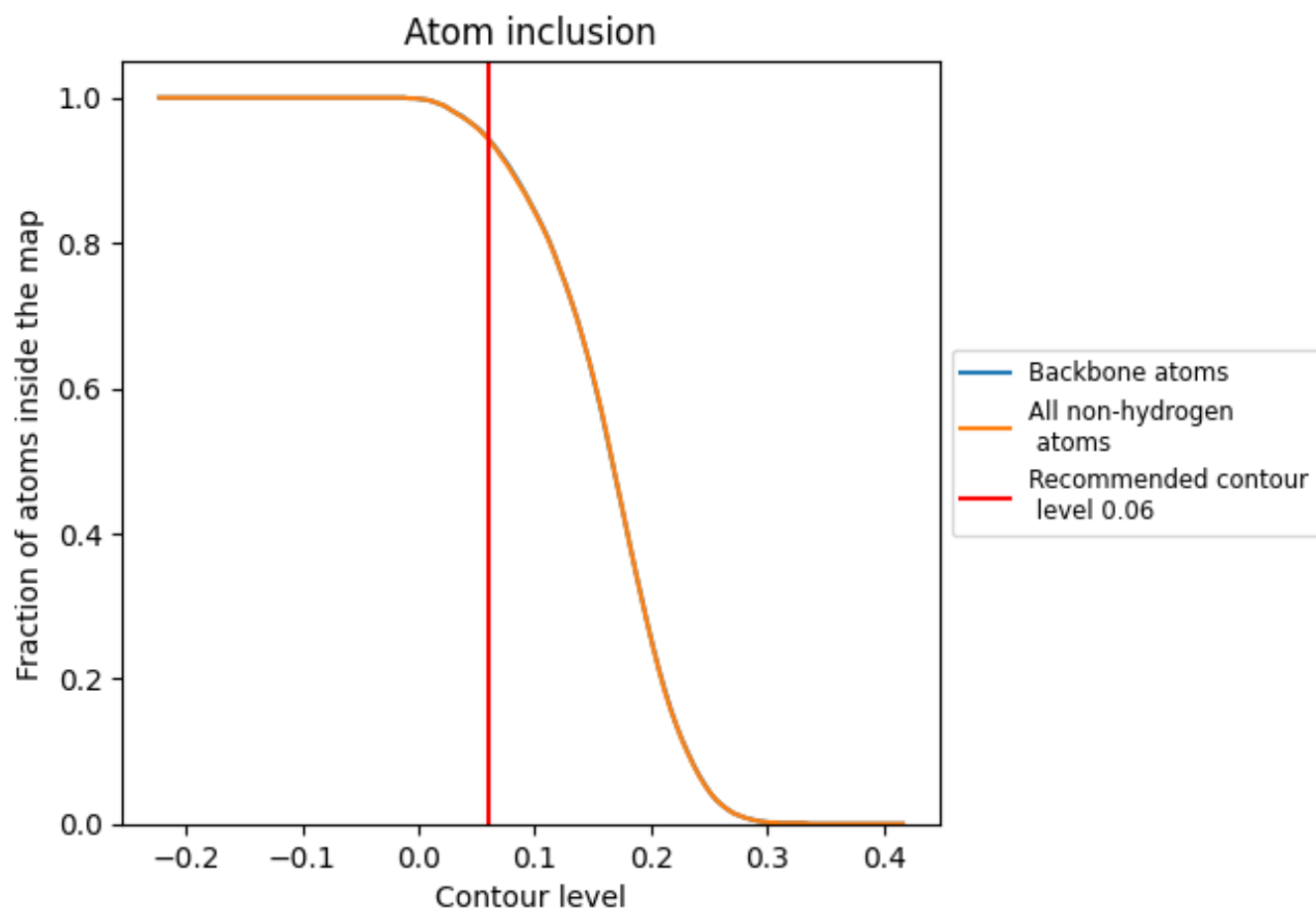
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9430	 0.8010
1	 0.9450	 0.8040
2	 0.9470	 0.8080
3	 0.9440	 0.8050
4	 0.9480	 0.8040
5	 0.9450	 0.8000
6	 0.9450	 0.7910
7	 0.9420	 0.7900
8	 0.9420	 0.7950
A	 0.9510	 0.8190
B	 0.9490	 0.8140
C	 0.9490	 0.8130
D	 0.9510	 0.8180
E	 0.9500	 0.8180
F	 0.9490	 0.8170
G	 0.9490	 0.8190
H	 0.9490	 0.8160
I	 0.9490	 0.8170
J	 0.9480	 0.8100
K	 0.9430	 0.8020
L	 0.9460	 0.8100
M	 0.9480	 0.8140
N	 0.9510	 0.8170
O	 0.9480	 0.8130
P	 0.9500	 0.8180
Q	 0.9500	 0.8170
R	 0.9490	 0.8110
S	 0.9470	 0.8080
T	 0.9450	 0.7990
U	 0.9470	 0.8030
V	 0.9470	 0.8080
W	 0.9500	 0.8150
X	 0.9480	 0.8050
Y	 0.9450	 0.8110
Z	 0.9480	 0.8070



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	 0.9400	 0.7820
b	 0.9420	 0.7880
c	 0.9400	 0.7870
d	 0.9420	 0.7830
e	 0.9400	 0.7780
f	 0.9440	 0.7950
g	 0.9500	 0.8100
h	 0.9450	 0.8060
i	 0.9430	 0.7960
j	 0.9430	 0.7970
k	 0.9420	 0.7910
l	 0.9440	 0.8000
m	 0.9450	 0.8030
n	 0.9380	 0.7780
o	 0.9380	 0.7770
p	 0.9380	 0.7760
q	 0.9400	 0.7780
r	 0.9430	 0.7850
s	 0.9380	 0.7780
t	 0.9410	 0.7910
u	 0.9400	 0.7810
v	 0.9390	 0.7870
w	 0.9430	 0.7990
x	 0.9450	 0.8020
y	 0.9380	 0.7850
z	 0.9430	 0.7870