



# Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 08:44 pm GMT

PDB ID : 6EK5  
EMDB ID : EMD-3521  
Title : Near-atomic resolution structure of a plant geminivirus determined by electron cryo-microscopy.  
Authors : Grimm, C.; Bottcher, B.; Hipp, K.; Jeske, H.  
Deposited on : 2017-09-25  
Resolution : 4.20 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the (i) symbol.

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

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

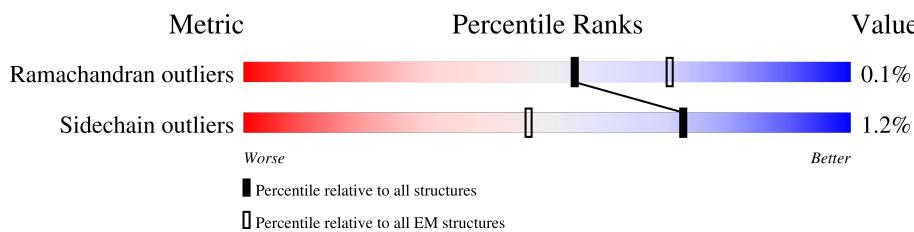
EMDB validation analysis : 0.0.1.dev43  
MolProbitY : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP)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

# 1 Overall quality at a glance

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

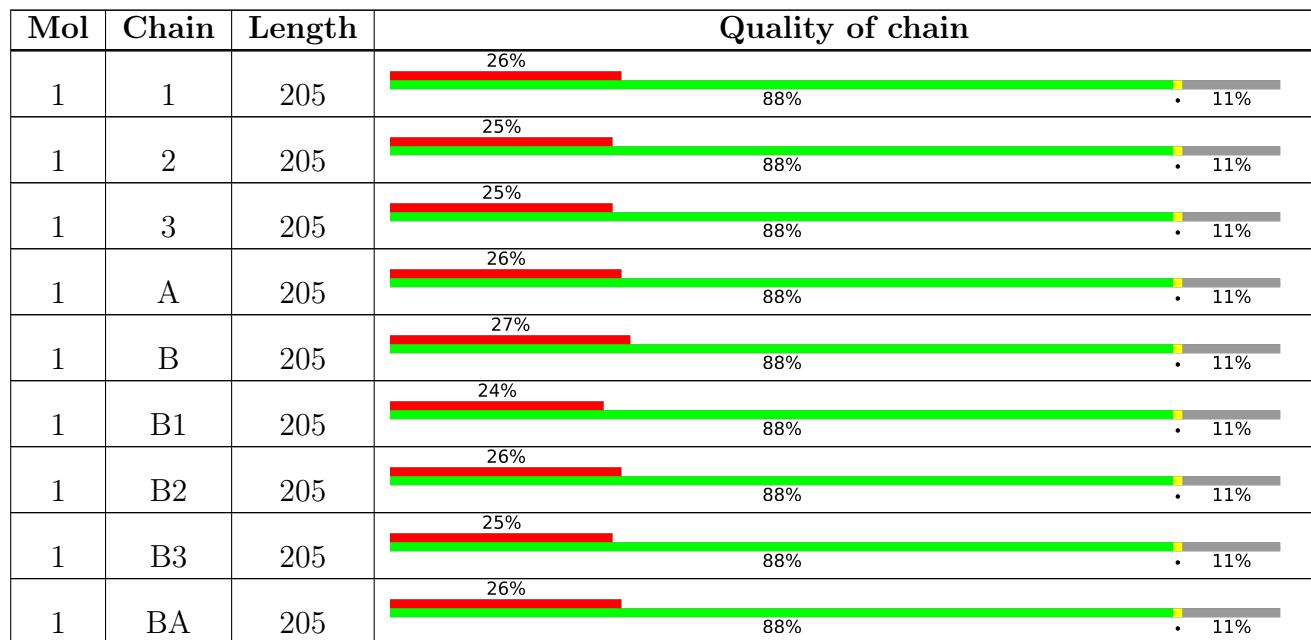
The reported resolution of this entry is 4.20 Å.

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.



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Mol	Chain	Length	Quality of chain		
1	BB	205	26%	88%	• 11%
1	BC	205	28%	88%	• 11%
1	BD	205	26%	88%	• 11%
1	BE	205	27%	88%	• 11%
1	BF	205	22%	88%	• 11%
1	BG	205	20%	88%	• 11%
1	BH	205	18%	94%	..
1	BI	205	19%	89%	• 10%
1	BJ	205	19%	88%	• 11%
1	BK	205	29%	88%	• 11%
1	BL	205	28%	88%	• 11%
1	BM	205	28%	88%	• 11%
1	BN	205	27%	88%	• 11%
1	BO	205	28%	88%	• 11%
1	BP	205	20%	86%	• 11%
1	BQ	205	21%	94%	..
1	BR	205	22%	89%	• 10%
1	BS	205	22%	88%	• 11%
1	BT	205	18%	88%	• 11%
1	BU	205	19%	88%	• 11%
1	BV	205	20%	94%	..
1	BW	205	27%	88%	• 10%
1	BX	205	21%	88%	• 11%
1	BY	205	18%	88%	• 11%
1	BZ	205	25%	88%	• 11%

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Mol	Chain	Length	Quality of chain		
1	Ba	205	27%	88%	• 11%
1	Bb	205	25%	88%	• 11%
1	Bc	205	27%	88%	• 11%
1	Bd	205	26%	88%	• 11%
1	Be	205	27%	88%	• 11%
1	Bf	205	25%	88%	• 11%
1	Bg	205	25%	88%	• 11%
1	Bh	205	24%	88%	• 11%
1	Bi	205	26%	88%	• 11%
1	Bj	205	17%	88%	• 11%
1	Bk	205	20%	94%	• •
1	Bl	205	21%	89%	• 10%
1	Bm	205	20%	88%	• 11%
1	Bn	205	19%	88%	• 11%
1	Bo	205	27%	88%	• 11%
1	Bp	205	25%	88%	• 11%
1	Bq	205	25%	88%	• 11%
1	Br	205	25%	88%	• 11%
1	Bs	205	25%	88%	• 11%
1	Bt	205	20%	88%	• 11%
1	Bu	205	18%	88%	• 11%
1	Bv	205	22%	88%	• 10%
1	Bw	205	19%	94%	• •
1	Bx	205	20%	88%	• 11%
1	By	205	25%	88%	• 11%

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Mol	Chain	Length	Quality of chain		
1	Bz	205	26%	88%	• 11%
1	C	205	28%	88%	• 11%
1	D	205	26%	88%	• 11%
1	E	205	27%	88%	• 11%
1	F	205	22%	88%	• 11%
1	G	205	18%	88%	• 11%
1	H	205	20%	94%	..
1	I	205	20%	89%	• 10%
1	J	205	19%	88%	• 11%
1	K	205	28%	88%	• 11%
1	L	205	28%	88%	• 11%
1	M	205	27%	88%	• 11%
1	N	205	28%	88%	• 11%
1	O	205	30%	88%	• 11%
1	P	205	19%	88%	• 11%
1	Q	205	21%	94%	..
1	R	205	22%	88%	• 10%
1	S	205	20%	88%	• 11%
1	T	205	19%	88%	• 11%
1	U	205	19%	88%	• 11%
1	V	205	21%	94%	..
1	W	205	18%	89%	• 10%
1	X	205	20%	88%	• 11%
1	Y	205	19%	88%	• 11%
1	Z	205	25%	88%	• 11%

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Mol	Chain	Length	Quality of chain		
1	a	205	26%	88%	• 11%
1	b	205	26%	88%	• 11%
1	c	205	27%	88%	• 11%
1	d	205	25%	88%	• 11%
1	e	205	26%	88%	• 11%
1	f	205	26%	88%	• 11%
1	g	205	25%	88%	• 11%
1	h	205	25%	88%	• 11%
1	i	205	26%	88%	• 11%
1	j	205	20%	88%	• 11%
1	k	205	20%	94%	• •
1	l	205	21%	89%	• 10%
1	m	205	19%	88%	• 11%
1	n	205	18%	88%	• 11%
1	o	205	26%	88%	• 11%
1	p	205	24%	88%	• 11%
1	q	205	26%	88%	• 11%
1	r	205	24%	88%	• 11%
1	s	205	26%	88%	• 11%
1	t	205	21%	88%	• 11%
1	u	205	19%	88%	• 11%
1	v	205	20%	89%	• 10%
1	w	205	19%	94%	• •
1	x	205	18%	88%	• 11%
1	y	205	27%	88%	• 11%

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Mol	Chain	Length	Quality of chain		
1	z	205	23%	88%	• 11%

## 2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 165959 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	183	1495	956	270	260	9	0	0
1	B	183	1495	956	270	260	9	0	0
1	C	183	1495	956	270	260	9	0	0
1	D	183	1495	956	270	260	9	0	0
1	E	183	1495	956	270	260	9	0	0
1	F	183	1495	956	270	260	9	0	0
1	G	183	1495	956	270	260	9	0	0
1	H	198	1629	1042	295	280	12	0	0
1	I	185	1512	965	275	263	9	0	0
1	J	183	1495	956	270	260	9	0	0
1	K	183	1495	956	270	260	9	0	0
1	L	183	1495	956	270	260	9	0	0
1	M	183	1495	956	270	260	9	0	0
1	N	183	1495	956	270	260	9	0	0
1	O	183	1495	956	270	260	9	0	0
1	P	183	1495	956	270	260	9	0	0
1	Q	198	1629	1042	295	280	12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	185	Total	C	N	O	S		
			1512	965	275	263	9	0	0
1	S	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	T	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	U	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	V	198	Total	C	N	O	S		
			1629	1042	295	280	12	0	0
1	W	185	Total	C	N	O	S		
			1512	965	275	263	9	0	0
1	X	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Y	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Z	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	BA	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	BB	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	BC	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	BD	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	a	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	b	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	c	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	d	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	e	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	f	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	g	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	h	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	i	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	j	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	m	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	n	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	o	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	p	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	q	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	r	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	s	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	t	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	u	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	x	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	y	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	z	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	3	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	1	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	2	183	Total	C	N	O	S	0	0
			1495	956	270	260	9		
1	k	198	Total	C	N	O	S	0	0
			1629	1042	295	280	12		
1	w	198	Total	C	N	O	S	0	0
			1629	1042	295	280	12		
1	l	185	Total	C	N	O	S	0	0
			1512	965	275	263	9		
1	v	185	Total	C	N	O	S	0	0
			1512	965	275	263	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	BE	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	BF	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	BG	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	BJ	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	BP	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	BS	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	BT	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	BU	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	BX	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	BY	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	BZ	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Ba	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Bb	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Bc	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Bd	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	BK	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	BL	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	BM	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	BN	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	BO	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Be	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Bf	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Bg	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Bh	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Bi	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Bj	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Bm	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Bn	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Bo	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Bp	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Bq	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Br	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Bs	183	Total	C	N	O	S		
			1494	955	270	260	9	0	0
1	Bt	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Bu	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Bx	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	By	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Bz	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	B3	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	B1	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	B2	183	Total	C	N	O	S		
			1495	956	270	260	9	0	0
1	Bw	198	Total	C	N	O	S		
			1629	1042	295	280	12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	BH	198	Total	C	N	O	S		
			1629	1042	295	280	12	0	0
1	BQ	198	Total	C	N	O	S		
			1629	1042	295	280	12	0	0
1	BV	198	Total	C	N	O	S		
			1629	1042	295	280	12	0	0
1	Bk	198	Total	C	N	O	S		
			1629	1042	295	280	12	0	0
1	Bv	185	Total	C	N	O	S		
			1512	965	275	263	9	0	0
1	BI	185	Total	C	N	O	S		
			1512	965	275	263	9	0	0
1	BR	185	Total	C	N	O	S		
			1512	965	275	263	9	0	0
1	BW	185	Total	C	N	O	S		
			1512	965	275	263	9	0	0
1	Bl	185	Total	C	N	O	S		
			1512	965	275	263	9	0	0

There are 330 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	ALA	ARG	conflict	UNP P03561
A	192	LEU	PRO	conflict	UNP P03561
A	194	CYS	GLY	conflict	UNP P03561
B	48	ALA	ARG	conflict	UNP P03561
B	192	LEU	PRO	conflict	UNP P03561
B	194	CYS	GLY	conflict	UNP P03561
C	48	ALA	ARG	conflict	UNP P03561
C	192	LEU	PRO	conflict	UNP P03561
C	194	CYS	GLY	conflict	UNP P03561
D	48	ALA	ARG	conflict	UNP P03561
D	192	LEU	PRO	conflict	UNP P03561
D	194	CYS	GLY	conflict	UNP P03561
E	48	ALA	ARG	conflict	UNP P03561
E	192	LEU	PRO	conflict	UNP P03561
E	194	CYS	GLY	conflict	UNP P03561
F	48	ALA	ARG	conflict	UNP P03561
F	192	LEU	PRO	conflict	UNP P03561
F	194	CYS	GLY	conflict	UNP P03561
G	48	ALA	ARG	conflict	UNP P03561
G	192	LEU	PRO	conflict	UNP P03561
G	194	CYS	GLY	conflict	UNP P03561

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Chain	Residue	Modelled	Actual	Comment	Reference
H	48	ALA	ARG	conflict	UNP P03561
H	192	LEU	PRO	conflict	UNP P03561
H	194	CYS	GLY	conflict	UNP P03561
I	48	ALA	ARG	conflict	UNP P03561
I	192	LEU	PRO	conflict	UNP P03561
I	194	CYS	GLY	conflict	UNP P03561
J	48	ALA	ARG	conflict	UNP P03561
J	192	LEU	PRO	conflict	UNP P03561
J	194	CYS	GLY	conflict	UNP P03561
K	48	ALA	ARG	conflict	UNP P03561
K	192	LEU	PRO	conflict	UNP P03561
K	194	CYS	GLY	conflict	UNP P03561
L	48	ALA	ARG	conflict	UNP P03561
L	192	LEU	PRO	conflict	UNP P03561
L	194	CYS	GLY	conflict	UNP P03561
M	48	ALA	ARG	conflict	UNP P03561
M	192	LEU	PRO	conflict	UNP P03561
M	194	CYS	GLY	conflict	UNP P03561
N	48	ALA	ARG	conflict	UNP P03561
N	192	LEU	PRO	conflict	UNP P03561
N	194	CYS	GLY	conflict	UNP P03561
O	48	ALA	ARG	conflict	UNP P03561
O	192	LEU	PRO	conflict	UNP P03561
O	194	CYS	GLY	conflict	UNP P03561
P	48	ALA	ARG	conflict	UNP P03561
P	192	LEU	PRO	conflict	UNP P03561
P	194	CYS	GLY	conflict	UNP P03561
Q	48	ALA	ARG	conflict	UNP P03561
Q	192	LEU	PRO	conflict	UNP P03561
Q	194	CYS	GLY	conflict	UNP P03561
R	48	ALA	ARG	conflict	UNP P03561
R	192	LEU	PRO	conflict	UNP P03561
R	194	CYS	GLY	conflict	UNP P03561
S	48	ALA	ARG	conflict	UNP P03561
S	192	LEU	PRO	conflict	UNP P03561
S	194	CYS	GLY	conflict	UNP P03561
T	48	ALA	ARG	conflict	UNP P03561
T	192	LEU	PRO	conflict	UNP P03561
T	194	CYS	GLY	conflict	UNP P03561
U	48	ALA	ARG	conflict	UNP P03561
U	192	LEU	PRO	conflict	UNP P03561
U	194	CYS	GLY	conflict	UNP P03561

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Chain	Residue	Modelled	Actual	Comment	Reference
V	48	ALA	ARG	conflict	UNP P03561
V	192	LEU	PRO	conflict	UNP P03561
V	194	CYS	GLY	conflict	UNP P03561
W	48	ALA	ARG	conflict	UNP P03561
W	192	LEU	PRO	conflict	UNP P03561
W	194	CYS	GLY	conflict	UNP P03561
X	48	ALA	ARG	conflict	UNP P03561
X	192	LEU	PRO	conflict	UNP P03561
X	194	CYS	GLY	conflict	UNP P03561
Y	48	ALA	ARG	conflict	UNP P03561
Y	192	LEU	PRO	conflict	UNP P03561
Y	194	CYS	GLY	conflict	UNP P03561
Z	48	ALA	ARG	conflict	UNP P03561
Z	192	LEU	PRO	conflict	UNP P03561
Z	194	CYS	GLY	conflict	UNP P03561
BA	48	ALA	ARG	conflict	UNP P03561
BA	192	LEU	PRO	conflict	UNP P03561
BA	194	CYS	GLY	conflict	UNP P03561
BB	48	ALA	ARG	conflict	UNP P03561
BB	192	LEU	PRO	conflict	UNP P03561
BB	194	CYS	GLY	conflict	UNP P03561
BC	48	ALA	ARG	conflict	UNP P03561
BC	192	LEU	PRO	conflict	UNP P03561
BC	194	CYS	GLY	conflict	UNP P03561
BD	48	ALA	ARG	conflict	UNP P03561
BD	192	LEU	PRO	conflict	UNP P03561
BD	194	CYS	GLY	conflict	UNP P03561
a	48	ALA	ARG	conflict	UNP P03561
a	192	LEU	PRO	conflict	UNP P03561
a	194	CYS	GLY	conflict	UNP P03561
b	48	ALA	ARG	conflict	UNP P03561
b	192	LEU	PRO	conflict	UNP P03561
b	194	CYS	GLY	conflict	UNP P03561
c	48	ALA	ARG	conflict	UNP P03561
c	192	LEU	PRO	conflict	UNP P03561
c	194	CYS	GLY	conflict	UNP P03561
d	48	ALA	ARG	conflict	UNP P03561
d	192	LEU	PRO	conflict	UNP P03561
d	194	CYS	GLY	conflict	UNP P03561
e	48	ALA	ARG	conflict	UNP P03561
e	192	LEU	PRO	conflict	UNP P03561
e	194	CYS	GLY	conflict	UNP P03561

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Chain	Residue	Modelled	Actual	Comment	Reference
f	48	ALA	ARG	conflict	UNP P03561
f	192	LEU	PRO	conflict	UNP P03561
f	194	CYS	GLY	conflict	UNP P03561
g	48	ALA	ARG	conflict	UNP P03561
g	192	LEU	PRO	conflict	UNP P03561
g	194	CYS	GLY	conflict	UNP P03561
h	48	ALA	ARG	conflict	UNP P03561
h	192	LEU	PRO	conflict	UNP P03561
h	194	CYS	GLY	conflict	UNP P03561
i	48	ALA	ARG	conflict	UNP P03561
i	192	LEU	PRO	conflict	UNP P03561
i	194	CYS	GLY	conflict	UNP P03561
j	48	ALA	ARG	conflict	UNP P03561
j	192	LEU	PRO	conflict	UNP P03561
j	194	CYS	GLY	conflict	UNP P03561
m	48	ALA	ARG	conflict	UNP P03561
m	192	LEU	PRO	conflict	UNP P03561
m	194	CYS	GLY	conflict	UNP P03561
n	48	ALA	ARG	conflict	UNP P03561
n	192	LEU	PRO	conflict	UNP P03561
n	194	CYS	GLY	conflict	UNP P03561
o	48	ALA	ARG	conflict	UNP P03561
o	192	LEU	PRO	conflict	UNP P03561
o	194	CYS	GLY	conflict	UNP P03561
p	48	ALA	ARG	conflict	UNP P03561
p	192	LEU	PRO	conflict	UNP P03561
p	194	CYS	GLY	conflict	UNP P03561
q	48	ALA	ARG	conflict	UNP P03561
q	192	LEU	PRO	conflict	UNP P03561
q	194	CYS	GLY	conflict	UNP P03561
r	48	ALA	ARG	conflict	UNP P03561
r	192	LEU	PRO	conflict	UNP P03561
r	194	CYS	GLY	conflict	UNP P03561
s	48	ALA	ARG	conflict	UNP P03561
s	192	LEU	PRO	conflict	UNP P03561
s	194	CYS	GLY	conflict	UNP P03561
t	48	ALA	ARG	conflict	UNP P03561
t	192	LEU	PRO	conflict	UNP P03561
t	194	CYS	GLY	conflict	UNP P03561
u	48	ALA	ARG	conflict	UNP P03561
u	192	LEU	PRO	conflict	UNP P03561
u	194	CYS	GLY	conflict	UNP P03561

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Chain	Residue	Modelled	Actual	Comment	Reference
x	48	ALA	ARG	conflict	UNP P03561
x	192	LEU	PRO	conflict	UNP P03561
x	194	CYS	GLY	conflict	UNP P03561
y	48	ALA	ARG	conflict	UNP P03561
y	192	LEU	PRO	conflict	UNP P03561
y	194	CYS	GLY	conflict	UNP P03561
z	48	ALA	ARG	conflict	UNP P03561
z	192	LEU	PRO	conflict	UNP P03561
z	194	CYS	GLY	conflict	UNP P03561
3	48	ALA	ARG	conflict	UNP P03561
3	192	LEU	PRO	conflict	UNP P03561
3	194	CYS	GLY	conflict	UNP P03561
1	48	ALA	ARG	conflict	UNP P03561
1	192	LEU	PRO	conflict	UNP P03561
1	194	CYS	GLY	conflict	UNP P03561
2	48	ALA	ARG	conflict	UNP P03561
2	192	LEU	PRO	conflict	UNP P03561
2	194	CYS	GLY	conflict	UNP P03561
k	48	ALA	ARG	conflict	UNP P03561
k	192	LEU	PRO	conflict	UNP P03561
k	194	CYS	GLY	conflict	UNP P03561
w	48	ALA	ARG	conflict	UNP P03561
w	192	LEU	PRO	conflict	UNP P03561
w	194	CYS	GLY	conflict	UNP P03561
l	48	ALA	ARG	conflict	UNP P03561
l	192	LEU	PRO	conflict	UNP P03561
l	194	CYS	GLY	conflict	UNP P03561
v	48	ALA	ARG	conflict	UNP P03561
v	192	LEU	PRO	conflict	UNP P03561
v	194	CYS	GLY	conflict	UNP P03561
BE	48	ALA	ARG	conflict	UNP P03561
BE	192	LEU	PRO	conflict	UNP P03561
BE	194	CYS	GLY	conflict	UNP P03561
BF	48	ALA	ARG	conflict	UNP P03561
BF	192	LEU	PRO	conflict	UNP P03561
BF	194	CYS	GLY	conflict	UNP P03561
BG	48	ALA	ARG	conflict	UNP P03561
BG	192	LEU	PRO	conflict	UNP P03561
BG	194	CYS	GLY	conflict	UNP P03561
BJ	48	ALA	ARG	conflict	UNP P03561
BJ	192	LEU	PRO	conflict	UNP P03561
BJ	194	CYS	GLY	conflict	UNP P03561

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Chain	Residue	Modelled	Actual	Comment	Reference
BP	48	ALA	ARG	conflict	UNP P03561
BP	192	LEU	PRO	conflict	UNP P03561
BP	194	CYS	GLY	conflict	UNP P03561
BS	48	ALA	ARG	conflict	UNP P03561
BS	192	LEU	PRO	conflict	UNP P03561
BS	194	CYS	GLY	conflict	UNP P03561
BT	48	ALA	ARG	conflict	UNP P03561
BT	192	LEU	PRO	conflict	UNP P03561
BT	194	CYS	GLY	conflict	UNP P03561
BU	48	ALA	ARG	conflict	UNP P03561
BU	192	LEU	PRO	conflict	UNP P03561
BU	194	CYS	GLY	conflict	UNP P03561
BX	48	ALA	ARG	conflict	UNP P03561
BX	192	LEU	PRO	conflict	UNP P03561
BX	194	CYS	GLY	conflict	UNP P03561
BY	48	ALA	ARG	conflict	UNP P03561
BY	192	LEU	PRO	conflict	UNP P03561
BY	194	CYS	GLY	conflict	UNP P03561
BZ	48	ALA	ARG	conflict	UNP P03561
BZ	192	LEU	PRO	conflict	UNP P03561
BZ	194	CYS	GLY	conflict	UNP P03561
Ba	48	ALA	ARG	conflict	UNP P03561
Ba	192	LEU	PRO	conflict	UNP P03561
Ba	194	CYS	GLY	conflict	UNP P03561
Bb	48	ALA	ARG	conflict	UNP P03561
Bb	192	LEU	PRO	conflict	UNP P03561
Bb	194	CYS	GLY	conflict	UNP P03561
Bc	48	ALA	ARG	conflict	UNP P03561
Bc	192	LEU	PRO	conflict	UNP P03561
Bc	194	CYS	GLY	conflict	UNP P03561
Bd	48	ALA	ARG	conflict	UNP P03561
Bd	192	LEU	PRO	conflict	UNP P03561
Bd	194	CYS	GLY	conflict	UNP P03561
BK	48	ALA	ARG	conflict	UNP P03561
BK	192	LEU	PRO	conflict	UNP P03561
BK	194	CYS	GLY	conflict	UNP P03561
BL	48	ALA	ARG	conflict	UNP P03561
BL	192	LEU	PRO	conflict	UNP P03561
BL	194	CYS	GLY	conflict	UNP P03561
BM	48	ALA	ARG	conflict	UNP P03561
BM	192	LEU	PRO	conflict	UNP P03561
BM	194	CYS	GLY	conflict	UNP P03561

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Chain	Residue	Modelled	Actual	Comment	Reference
BN	48	ALA	ARG	conflict	UNP P03561
BN	192	LEU	PRO	conflict	UNP P03561
BN	194	CYS	GLY	conflict	UNP P03561
BO	48	ALA	ARG	conflict	UNP P03561
BO	192	LEU	PRO	conflict	UNP P03561
BO	194	CYS	GLY	conflict	UNP P03561
Be	48	ALA	ARG	conflict	UNP P03561
Be	192	LEU	PRO	conflict	UNP P03561
Be	194	CYS	GLY	conflict	UNP P03561
Bf	48	ALA	ARG	conflict	UNP P03561
Bf	192	LEU	PRO	conflict	UNP P03561
Bf	194	CYS	GLY	conflict	UNP P03561
Bg	48	ALA	ARG	conflict	UNP P03561
Bg	192	LEU	PRO	conflict	UNP P03561
Bg	194	CYS	GLY	conflict	UNP P03561
Bh	48	ALA	ARG	conflict	UNP P03561
Bh	192	LEU	PRO	conflict	UNP P03561
Bh	194	CYS	GLY	conflict	UNP P03561
Bi	48	ALA	ARG	conflict	UNP P03561
Bi	192	LEU	PRO	conflict	UNP P03561
Bi	194	CYS	GLY	conflict	UNP P03561
Bj	48	ALA	ARG	conflict	UNP P03561
Bj	192	LEU	PRO	conflict	UNP P03561
Bj	194	CYS	GLY	conflict	UNP P03561
Bm	48	ALA	ARG	conflict	UNP P03561
Bm	192	LEU	PRO	conflict	UNP P03561
Bm	194	CYS	GLY	conflict	UNP P03561
Bn	48	ALA	ARG	conflict	UNP P03561
Bn	192	LEU	PRO	conflict	UNP P03561
Bn	194	CYS	GLY	conflict	UNP P03561
Bo	48	ALA	ARG	conflict	UNP P03561
Bo	192	LEU	PRO	conflict	UNP P03561
Bo	194	CYS	GLY	conflict	UNP P03561
Bp	48	ALA	ARG	conflict	UNP P03561
Bp	192	LEU	PRO	conflict	UNP P03561
Bp	194	CYS	GLY	conflict	UNP P03561
Bq	48	ALA	ARG	conflict	UNP P03561
Bq	192	LEU	PRO	conflict	UNP P03561
Bq	194	CYS	GLY	conflict	UNP P03561
Br	48	ALA	ARG	conflict	UNP P03561
Br	192	LEU	PRO	conflict	UNP P03561
Br	194	CYS	GLY	conflict	UNP P03561

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Chain	Residue	Modelled	Actual	Comment	Reference
Bs	48	ALA	ARG	conflict	UNP P03561
Bs	192	LEU	PRO	conflict	UNP P03561
Bs	194	CYS	GLY	conflict	UNP P03561
Bt	48	ALA	ARG	conflict	UNP P03561
Bt	192	LEU	PRO	conflict	UNP P03561
Bt	194	CYS	GLY	conflict	UNP P03561
Bu	48	ALA	ARG	conflict	UNP P03561
Bu	192	LEU	PRO	conflict	UNP P03561
Bu	194	CYS	GLY	conflict	UNP P03561
Bx	48	ALA	ARG	conflict	UNP P03561
Bx	192	LEU	PRO	conflict	UNP P03561
Bx	194	CYS	GLY	conflict	UNP P03561
By	48	ALA	ARG	conflict	UNP P03561
By	192	LEU	PRO	conflict	UNP P03561
By	194	CYS	GLY	conflict	UNP P03561
Bz	48	ALA	ARG	conflict	UNP P03561
Bz	192	LEU	PRO	conflict	UNP P03561
Bz	194	CYS	GLY	conflict	UNP P03561
B3	48	ALA	ARG	conflict	UNP P03561
B3	192	LEU	PRO	conflict	UNP P03561
B3	194	CYS	GLY	conflict	UNP P03561
B1	48	ALA	ARG	conflict	UNP P03561
B1	192	LEU	PRO	conflict	UNP P03561
B1	194	CYS	GLY	conflict	UNP P03561
B2	48	ALA	ARG	conflict	UNP P03561
B2	192	LEU	PRO	conflict	UNP P03561
B2	194	CYS	GLY	conflict	UNP P03561
Bw	48	ALA	ARG	conflict	UNP P03561
Bw	192	LEU	PRO	conflict	UNP P03561
Bw	194	CYS	GLY	conflict	UNP P03561
BH	48	ALA	ARG	conflict	UNP P03561
BH	192	LEU	PRO	conflict	UNP P03561
BH	194	CYS	GLY	conflict	UNP P03561
BQ	48	ALA	ARG	conflict	UNP P03561
BQ	192	LEU	PRO	conflict	UNP P03561
BQ	194	CYS	GLY	conflict	UNP P03561
BV	48	ALA	ARG	conflict	UNP P03561
BV	192	LEU	PRO	conflict	UNP P03561
BV	194	CYS	GLY	conflict	UNP P03561
Bk	48	ALA	ARG	conflict	UNP P03561
Bk	192	LEU	PRO	conflict	UNP P03561
Bk	194	CYS	GLY	conflict	UNP P03561

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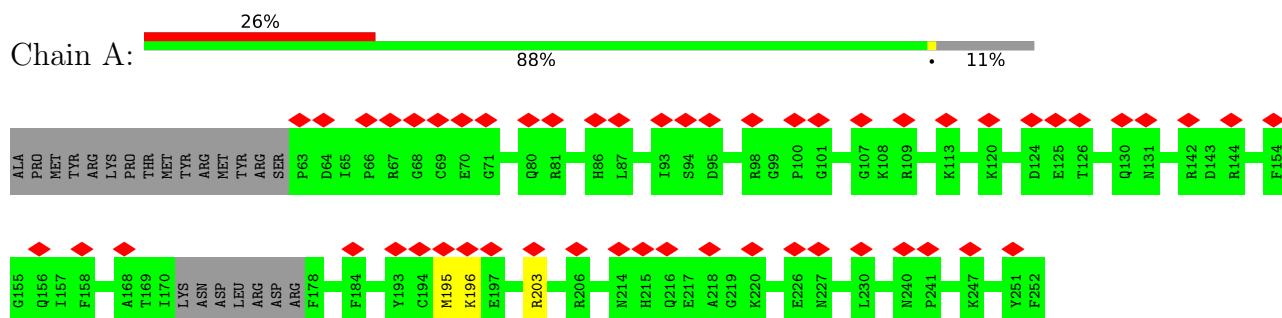
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Chain	Residue	Modelled	Actual	Comment	Reference
Bv	48	ALA	ARG	conflict	UNP P03561
Bv	192	LEU	PRO	conflict	UNP P03561
Bv	194	CYS	GLY	conflict	UNP P03561
BI	48	ALA	ARG	conflict	UNP P03561
BI	192	LEU	PRO	conflict	UNP P03561
BI	194	CYS	GLY	conflict	UNP P03561
BR	48	ALA	ARG	conflict	UNP P03561
BR	192	LEU	PRO	conflict	UNP P03561
BR	194	CYS	GLY	conflict	UNP P03561
BW	48	ALA	ARG	conflict	UNP P03561
BW	192	LEU	PRO	conflict	UNP P03561
BW	194	CYS	GLY	conflict	UNP P03561
Bl	48	ALA	ARG	conflict	UNP P03561
Bl	192	LEU	PRO	conflict	UNP P03561
Bl	194	CYS	GLY	conflict	UNP P03561

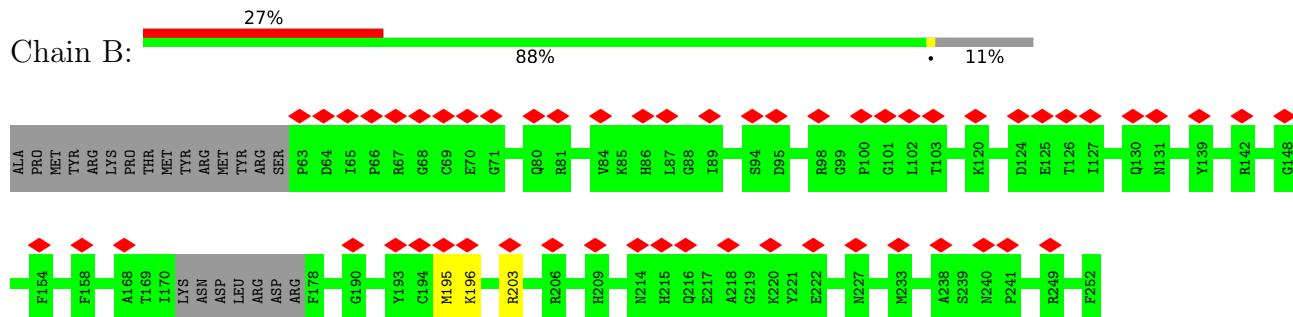
### 3 Residue-property plots

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

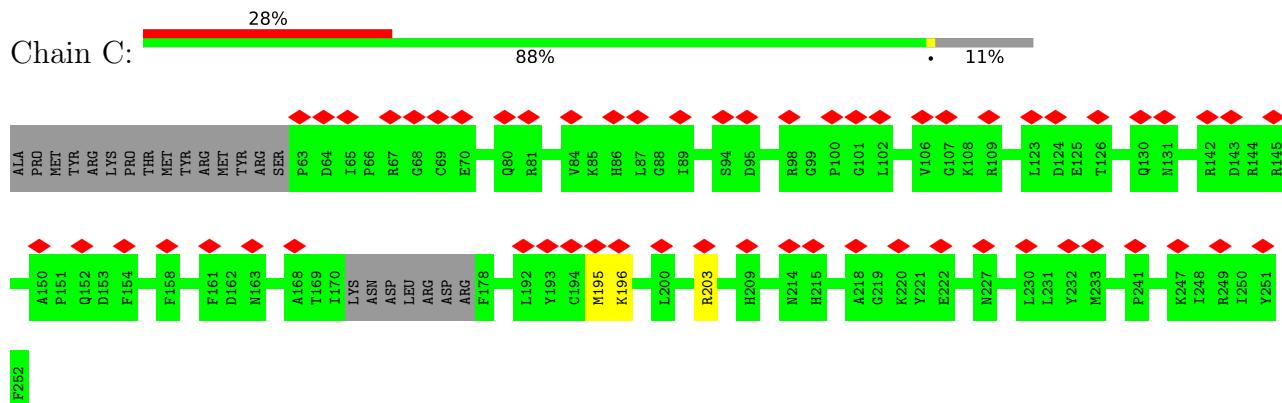
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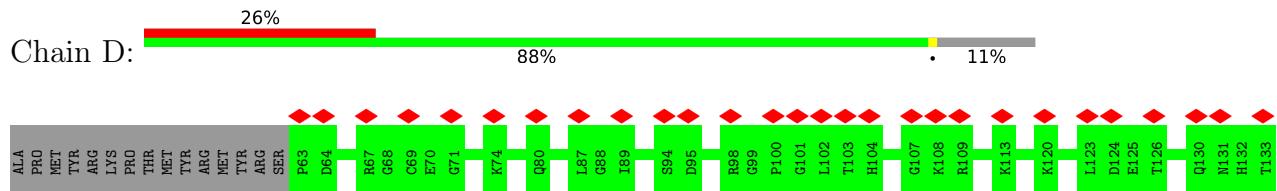
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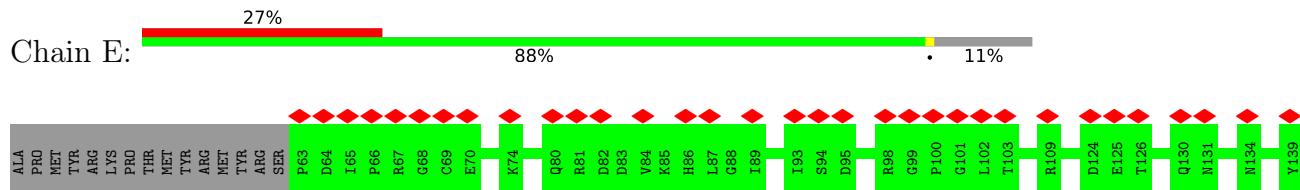
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



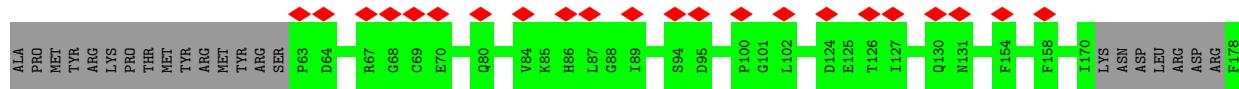
- Molecule 1: Capsid protein



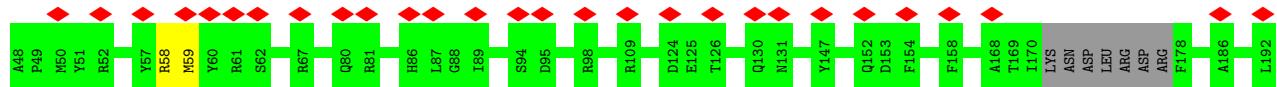
- Molecule 1: Capsid protein

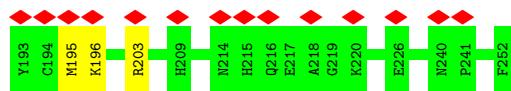


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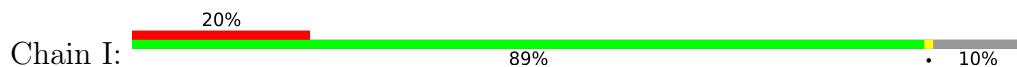


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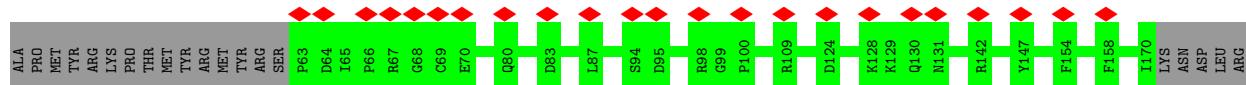
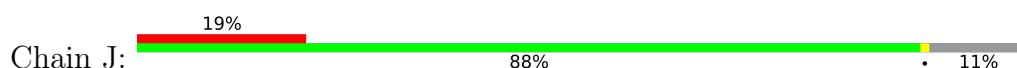




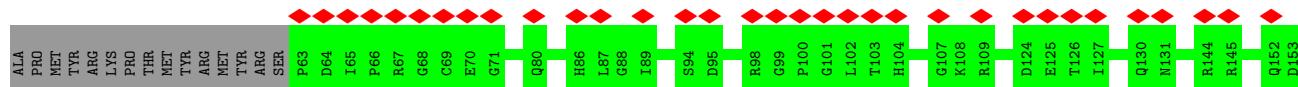
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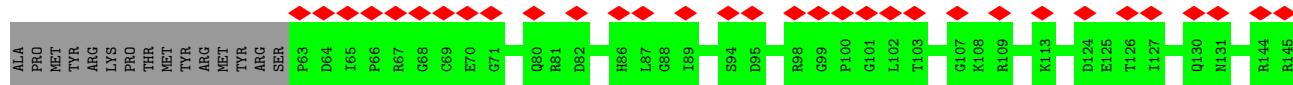
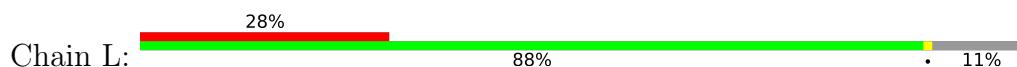
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

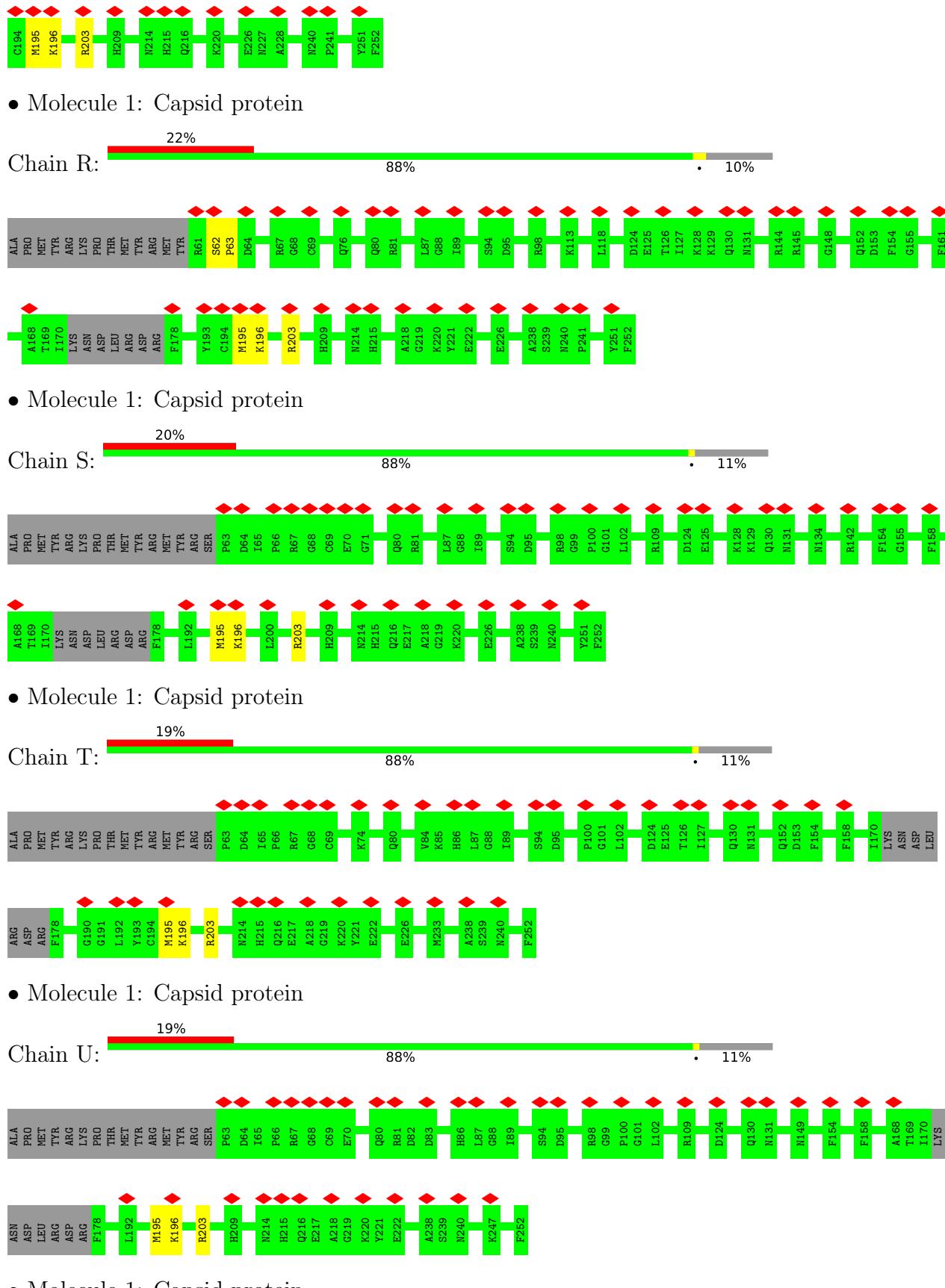


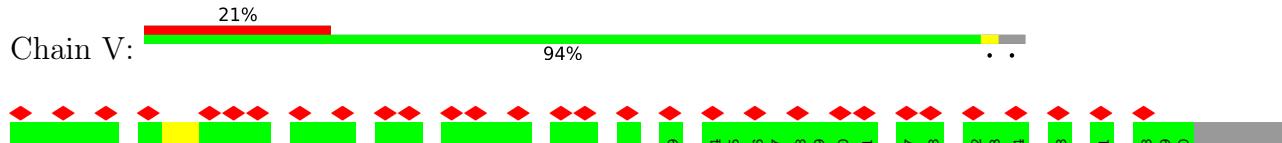
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



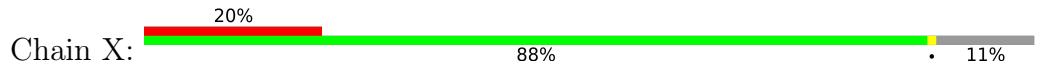




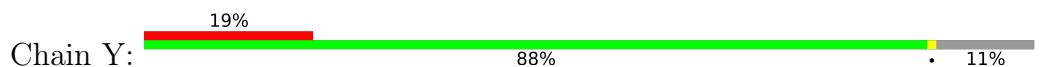
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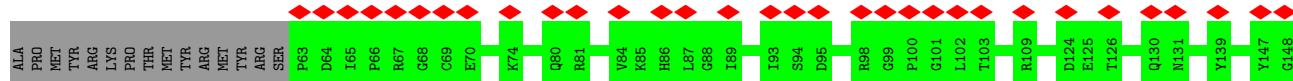
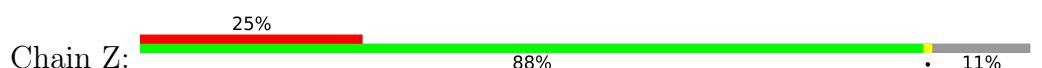
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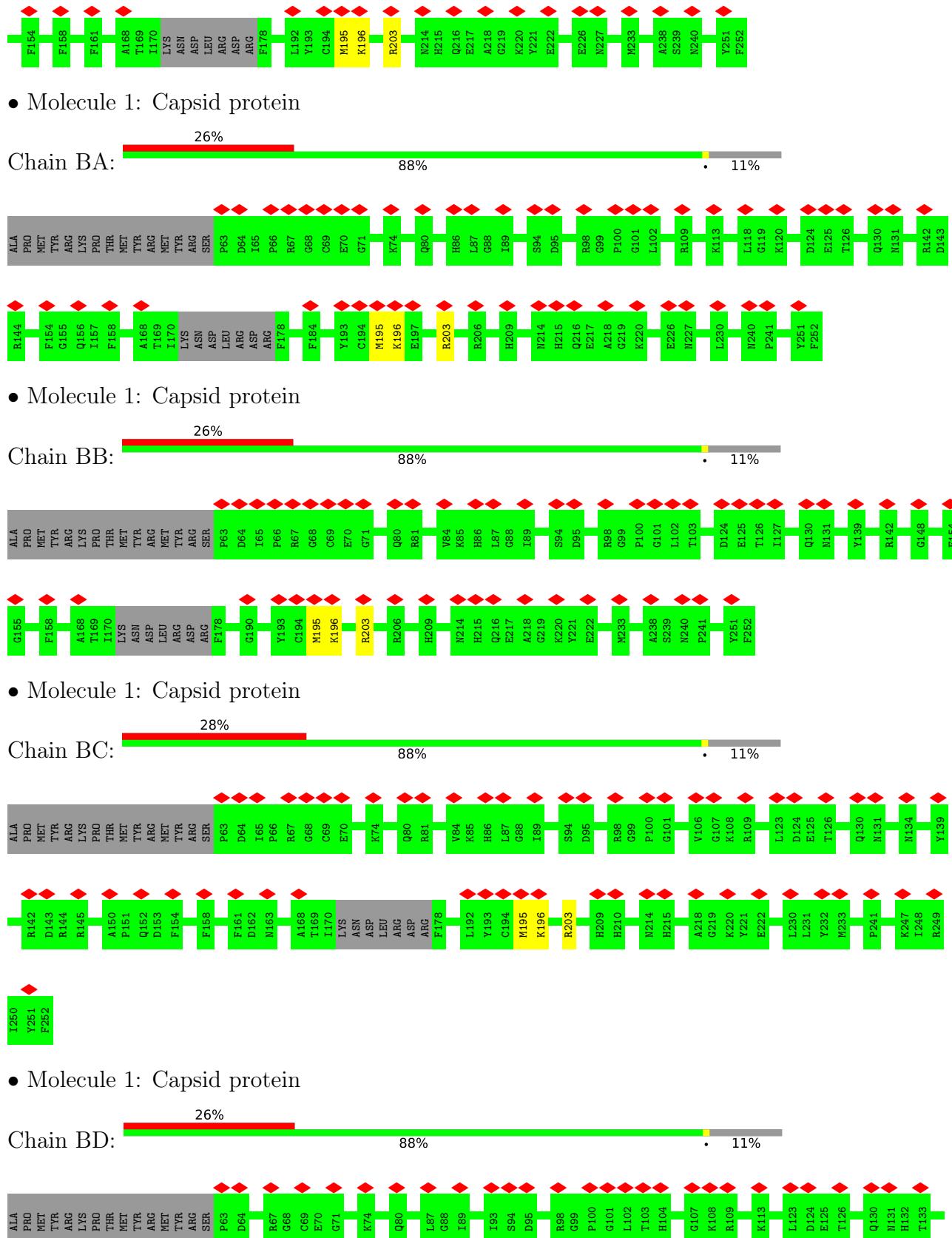


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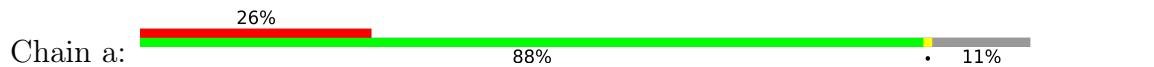


- Molecule 1: Capsid protein

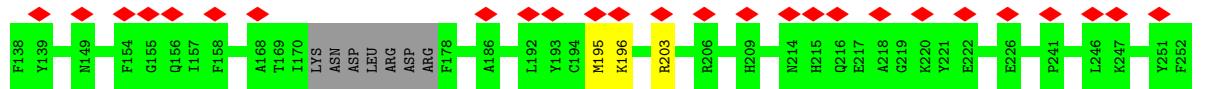
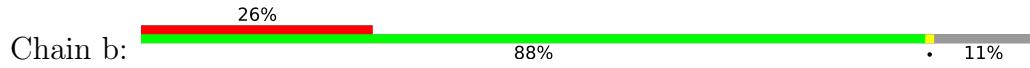




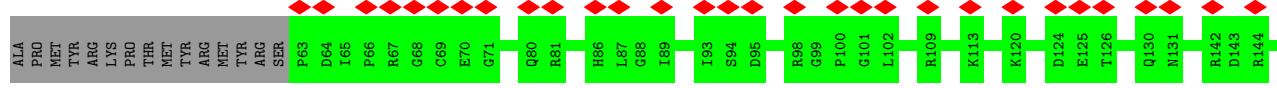
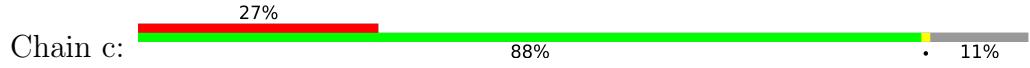
- Molecule 1: Capsid protein



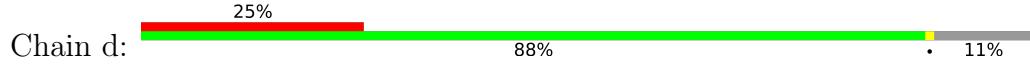
- Molecule 1: Capsid protein



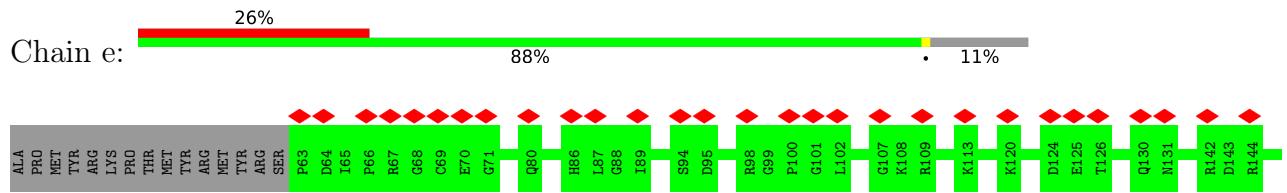
- Molecule 1: Capsid protein



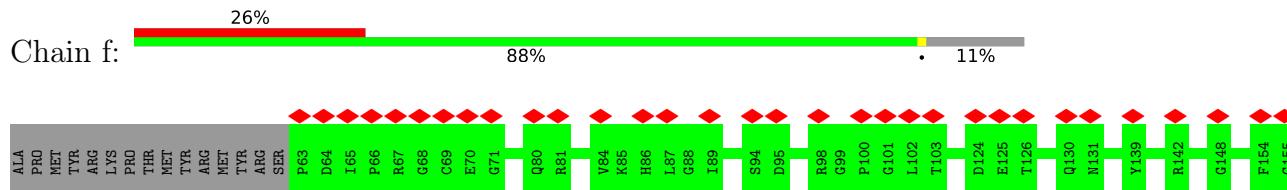
- Molecule 1: Capsid protein



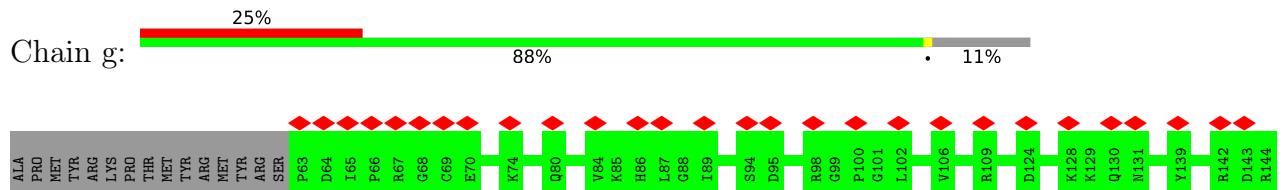
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



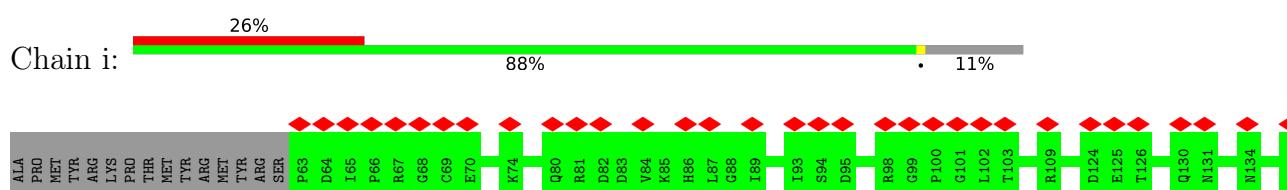
- Molecule 1: Capsid protein

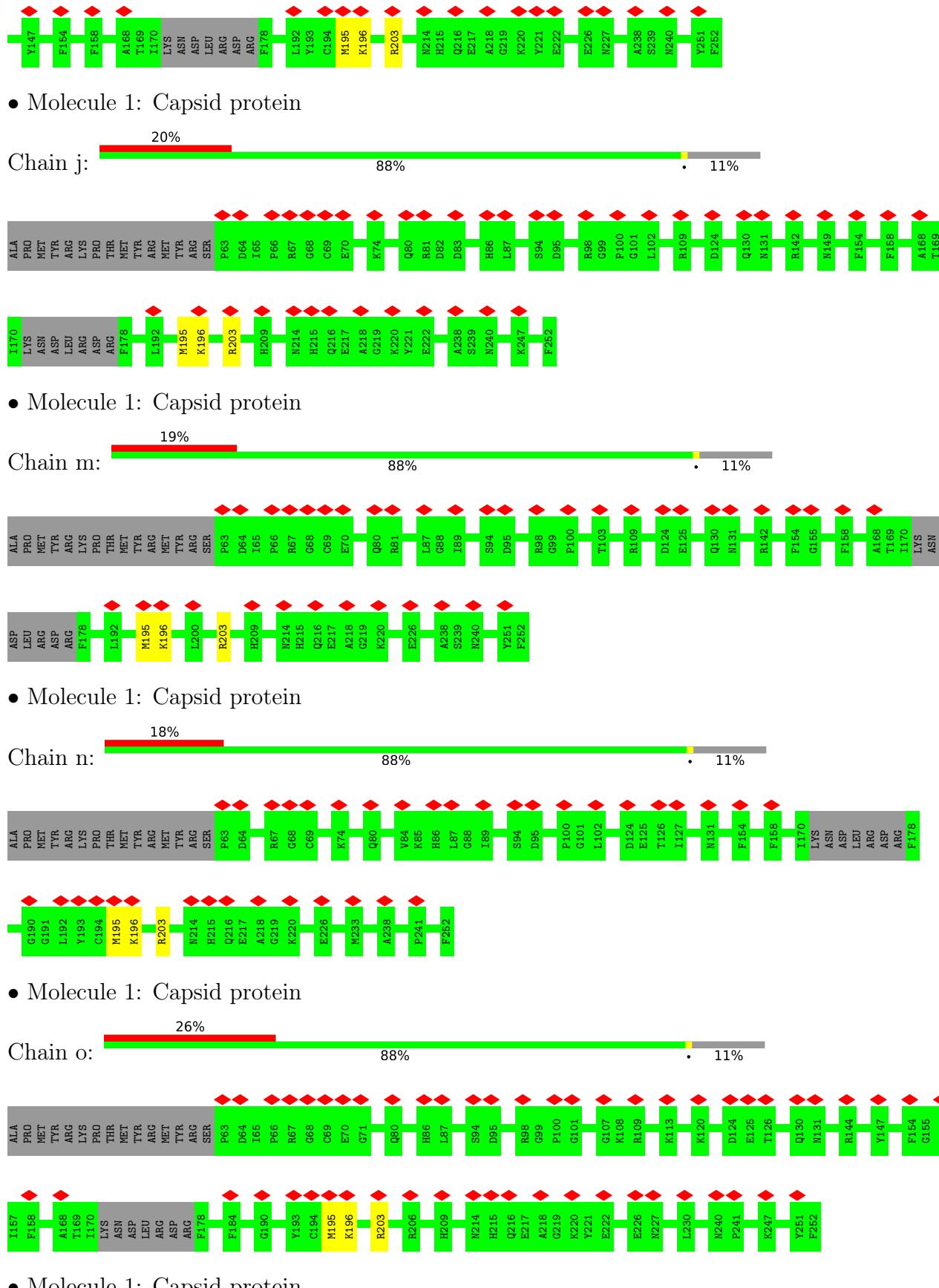


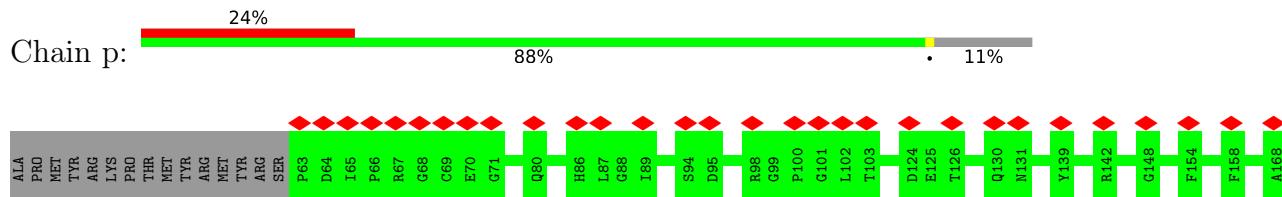
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



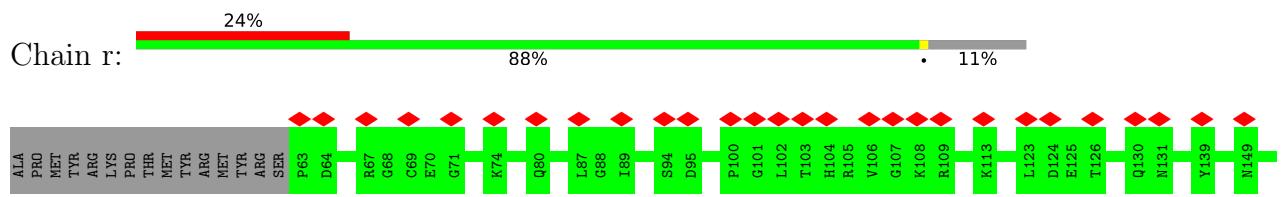




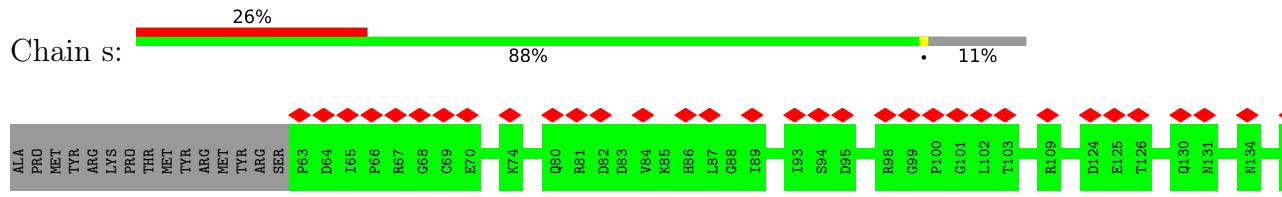
- Molecule 1: Capsid protein



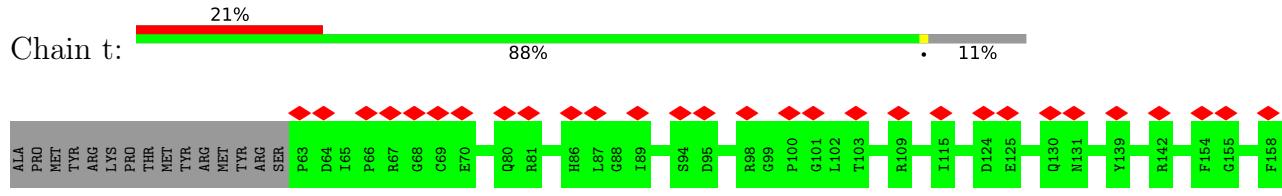
- Molecule 1: Capsid protein

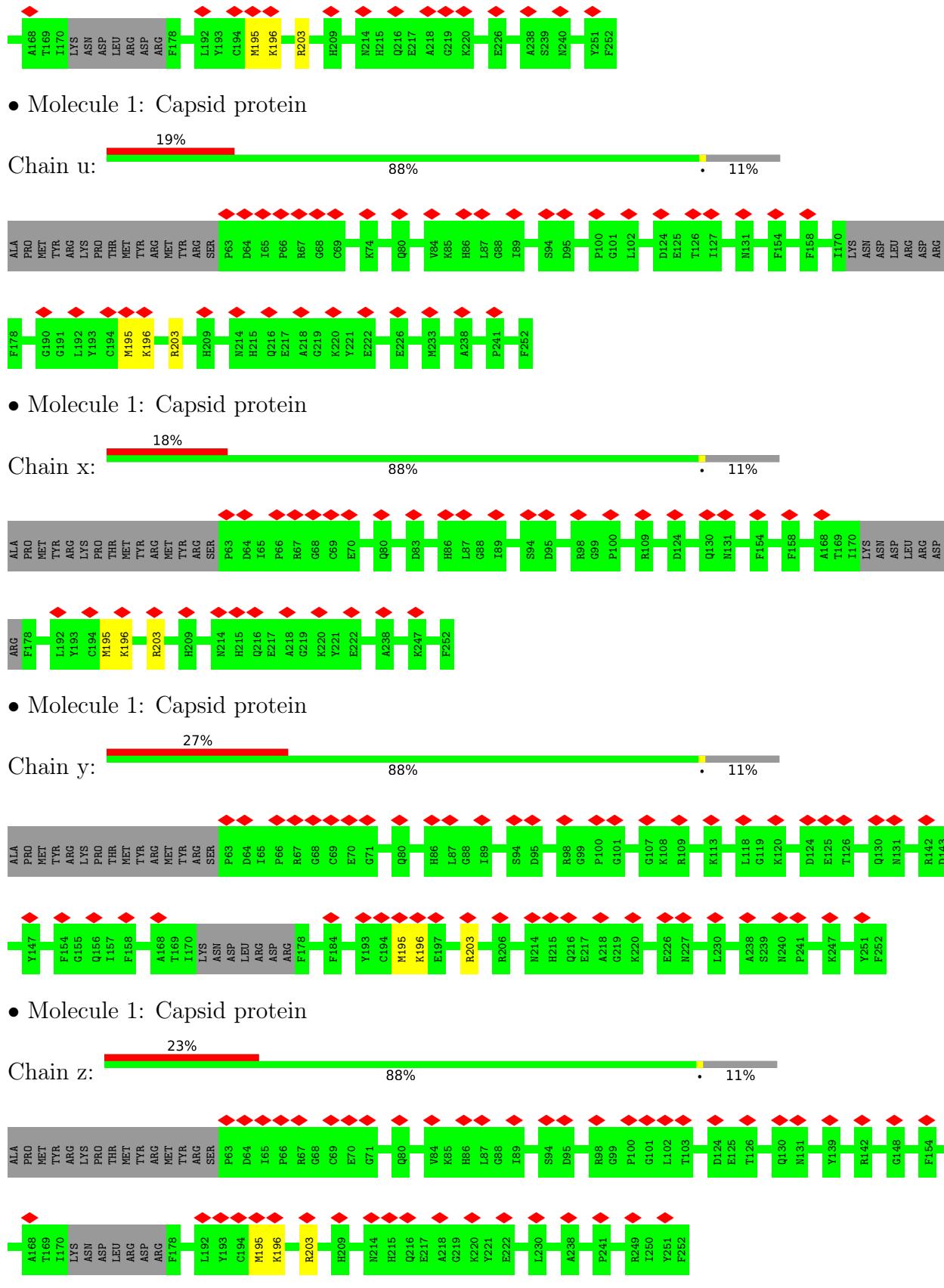


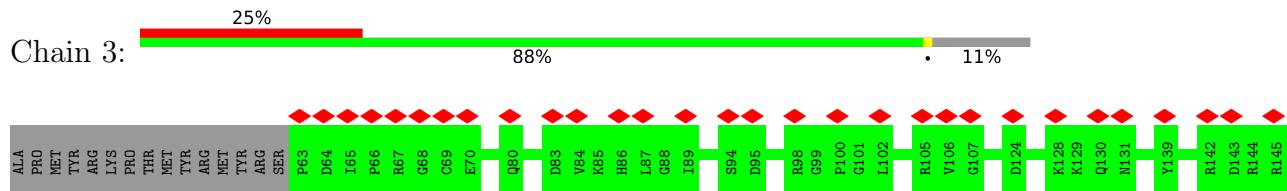
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



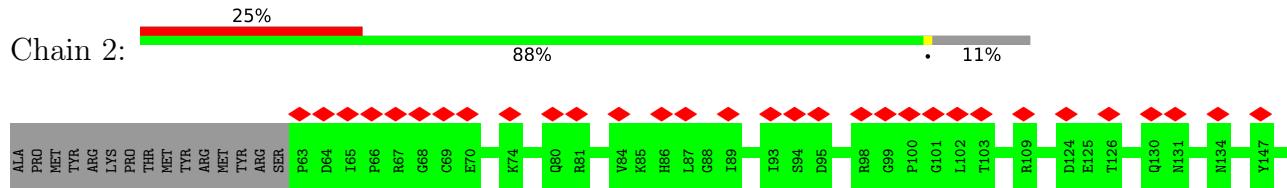




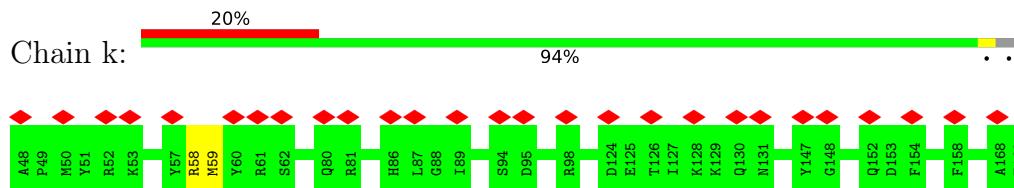
- Molecule 1: Capsid protein



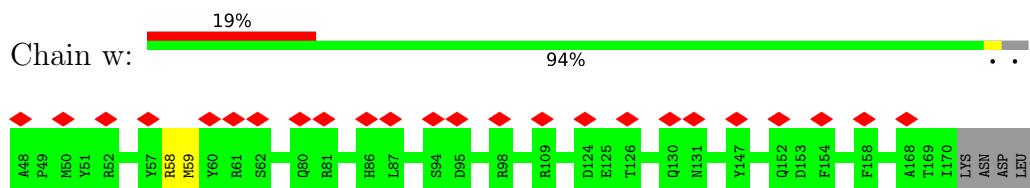
- Molecule 1: Capsid protein

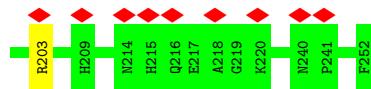


- Molecule 1: Capsid protein

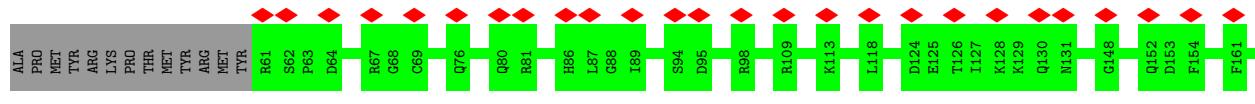
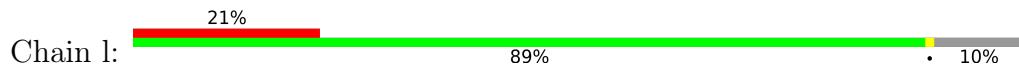


- Molecule 1: Capsid protein





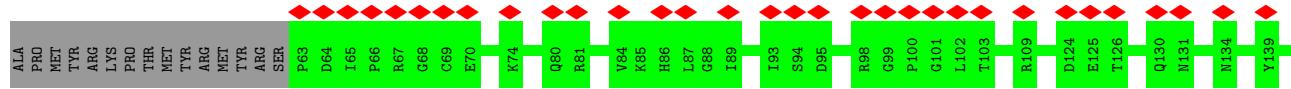
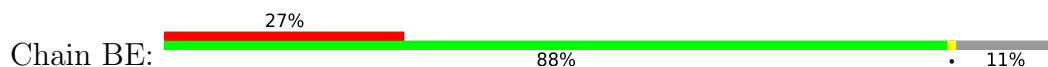
- Molecule 1: Capsid protein



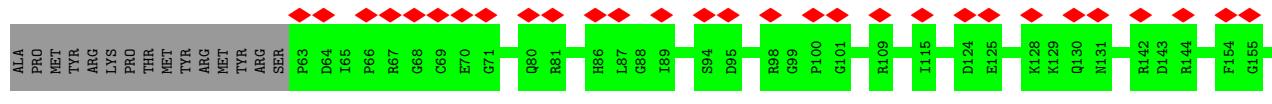
- Molecule 1: Capsid protein



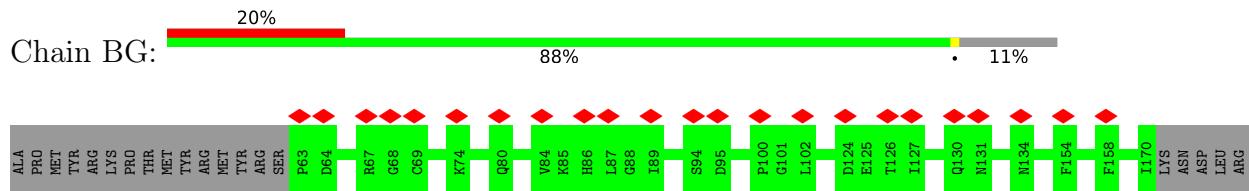
- Molecule 1: Capsid protein



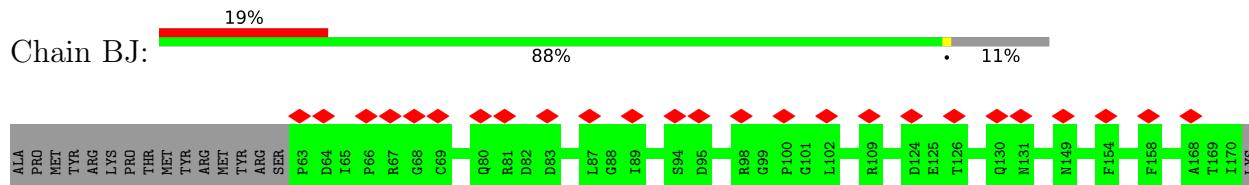
- Molecule 1: Capsid protein



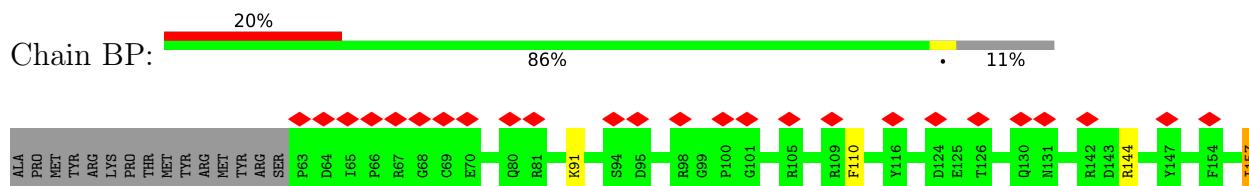
- Molecule 1: Capsid protein



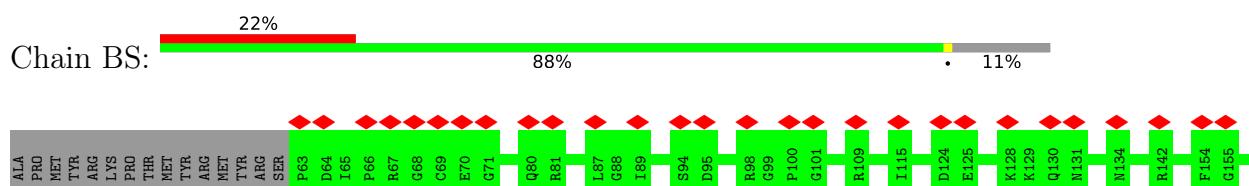
- Molecule 1: Capsid protein



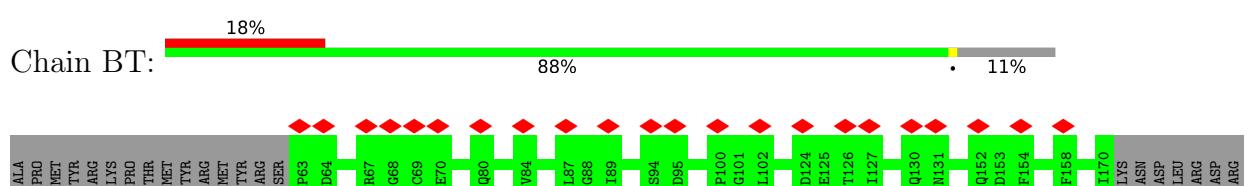
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- #### • Molecule 1: Capsid protein





- Molecule 1: Capsid protein

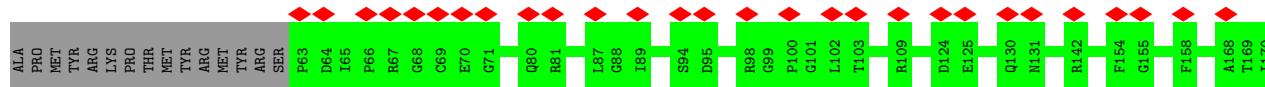
A horizontal bar chart illustrating the composition of Chain BU. The total length of the bar is 100%, divided into three segments: a red segment at 19%, a green segment at 88%, and a yellow segment at 11%.

Component	Percentage
Red	19%
Green	88%
Yellow	11%



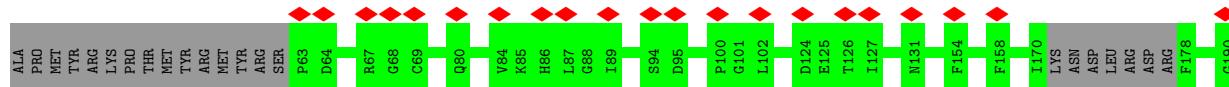
- Molecule 1: Capsid protein

Chain BX:  21% 88% 11%



- Molecule 1: Capsid protein

Chain BY: 18% 88% 11%

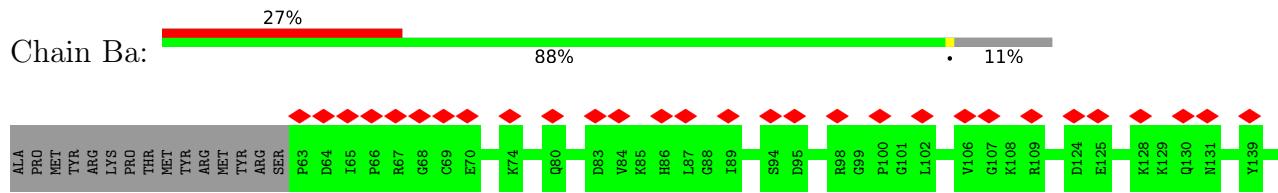


- Molecule 1: Capsid protein

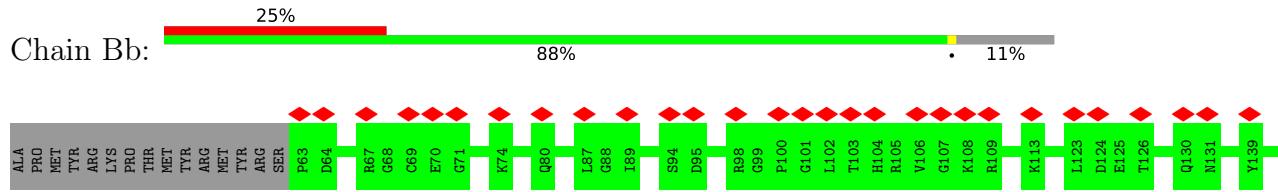
Chain BZ: 25% 88% 11%



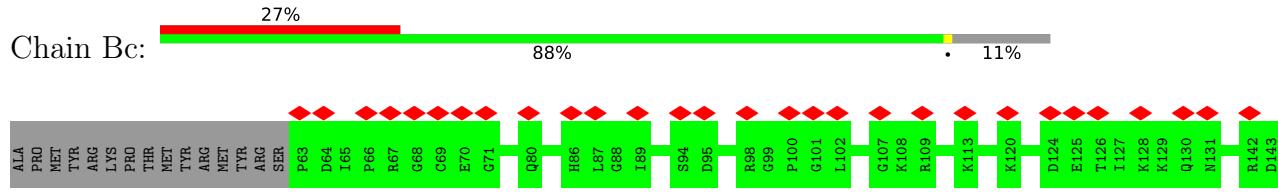
- Molecule 1: Capsid protein



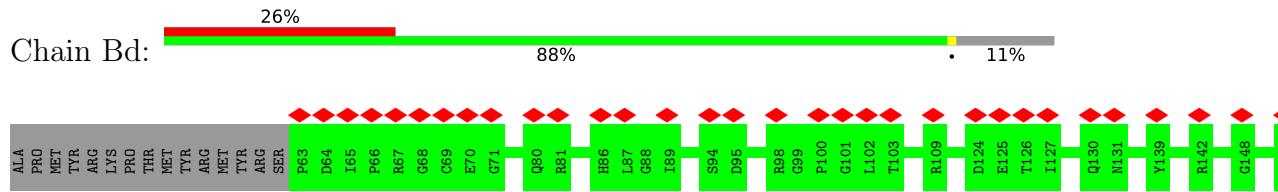
- Molecule 1: Capsid protein



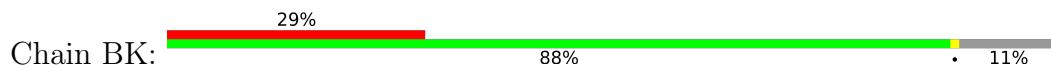
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



- Molecule 1: Capsid protein





- Molecule 1: Capsid protein



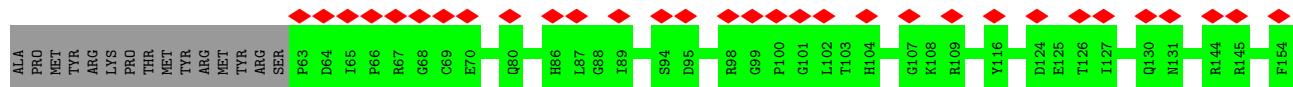
Chain BL: 28% • 88% • 11%

A horizontal bar chart with three segments. The first segment is red and labeled '28%'. The second segment is green and labeled '88%'. The third segment is yellow and labeled '11%'. The bars are separated by small black dots.



- Molecule 1: Capsid protein

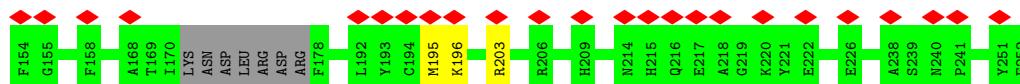
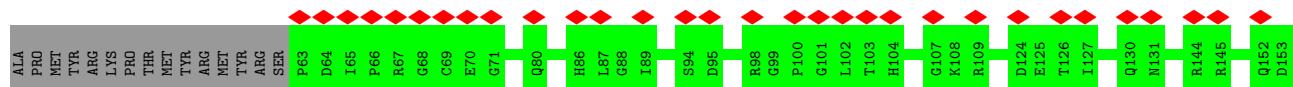
Chain BM: 28% 88% 11%



- Molecule 1: Capsid protein

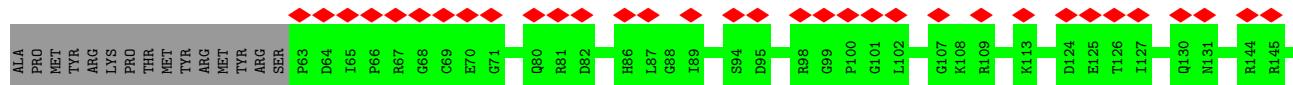
Chain BN: 27%

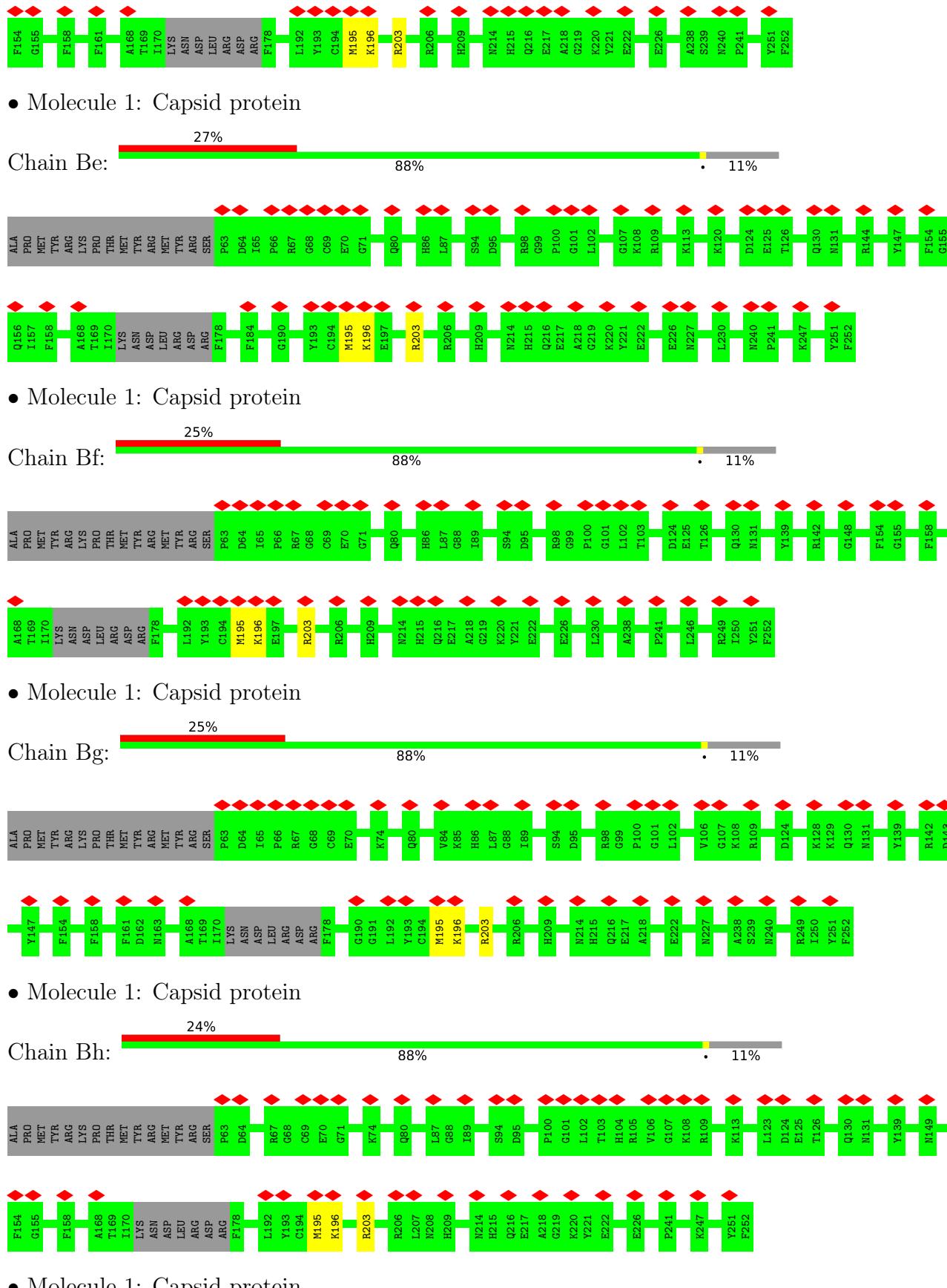
The progress bar consists of a red segment at the left end labeled '27%', followed by a long green segment labeled '88%', and a small grey segment at the right end labeled '11%'.

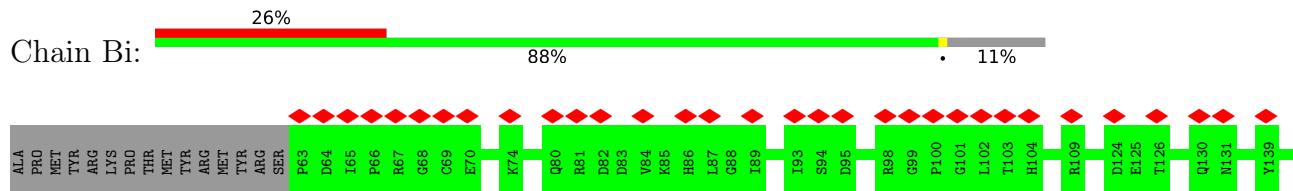


- Molecule 1: Capsid protein

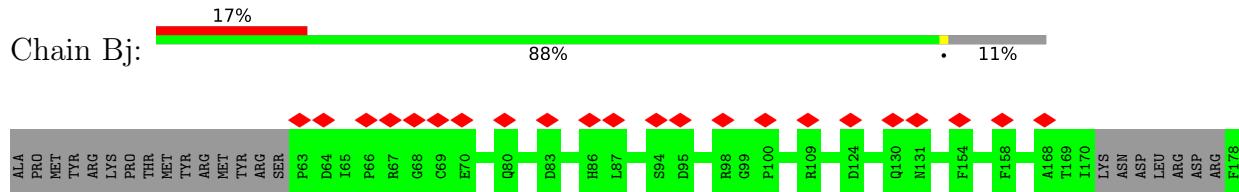
Chain BO: 28% 88% 1% 1%



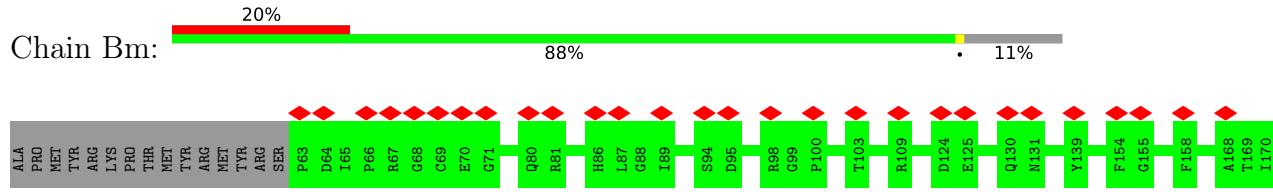




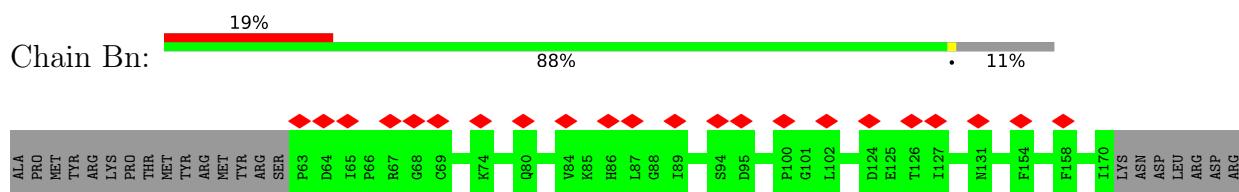
- Molecule 1: Capsid protein



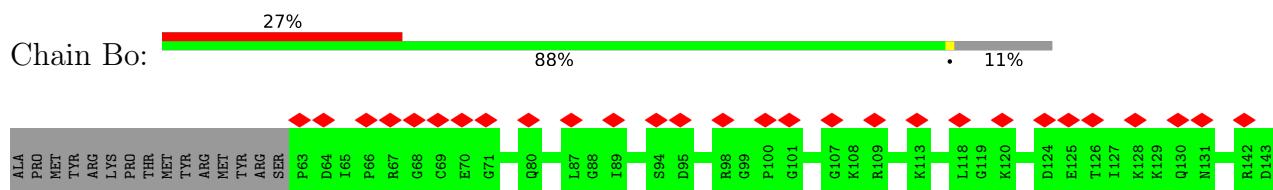
- Molecule 1: Capsid protein

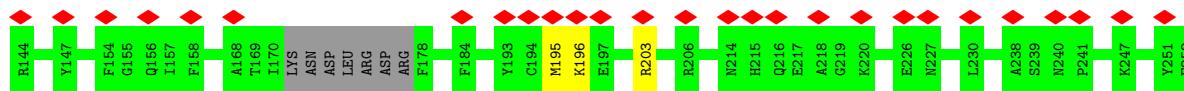


- Molecule 1: Capsid protein

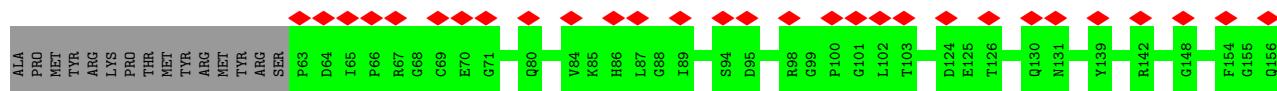
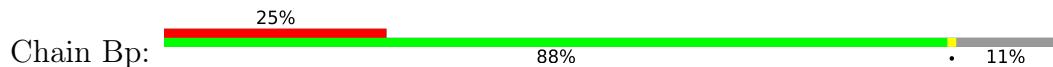


- Molecule 1: Capsid protein

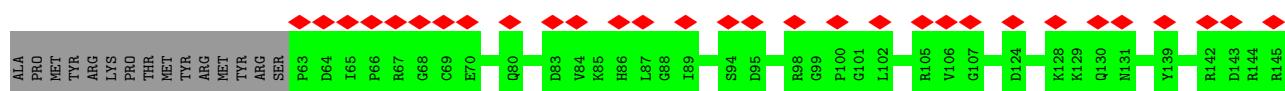




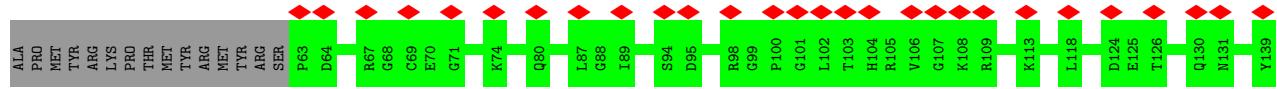
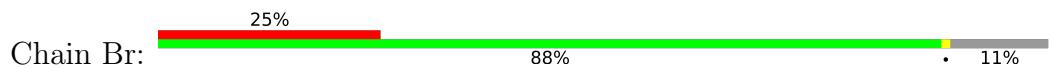
- Molecule 1: Capsid protein



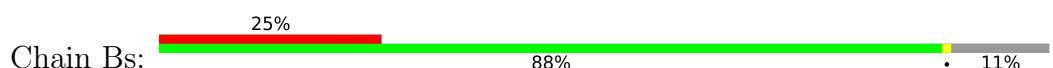
- Molecule 1: Capsid protein



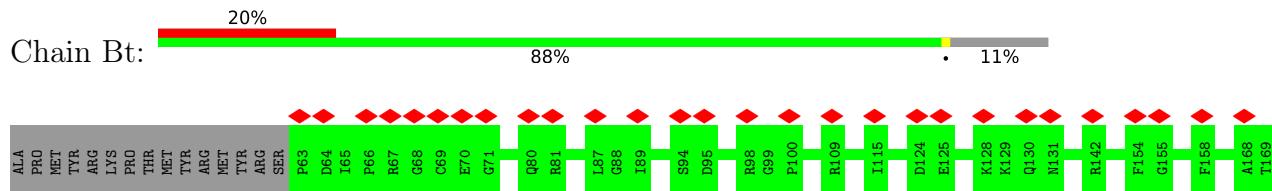
- Molecule 1: Capsid protein



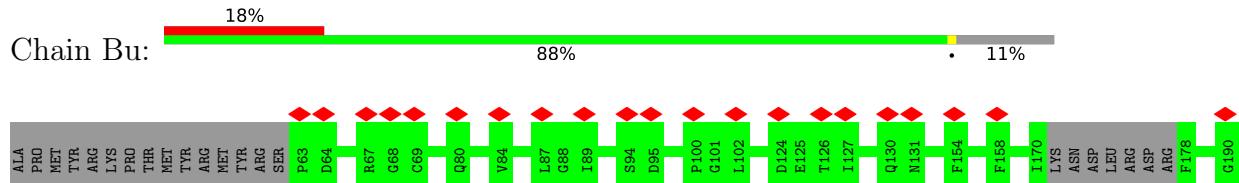
- Molecule 1: Capsid protein



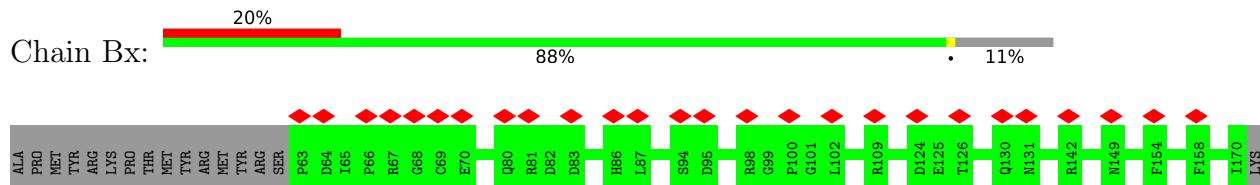
- #### • Molecule 1: Capsid protein



- Molecule 1: Capsid protein



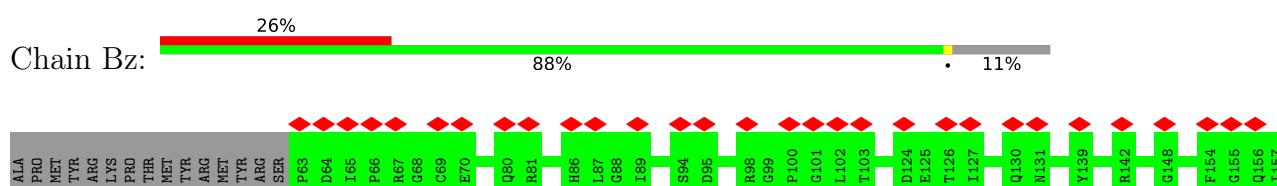
- Molecule 1: Capsid protein

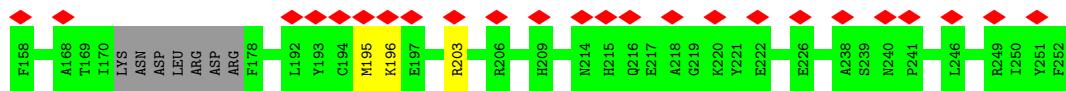


- Molecule 1: Capsid protein

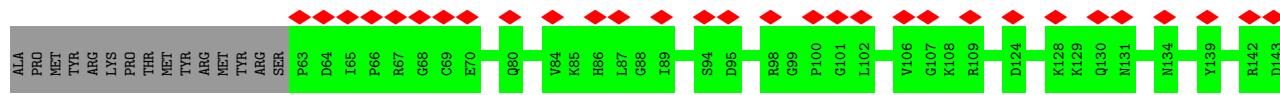
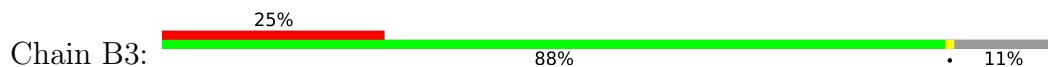


- Molecule 1: Capsid protein

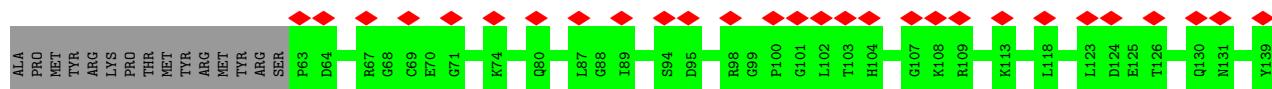




- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



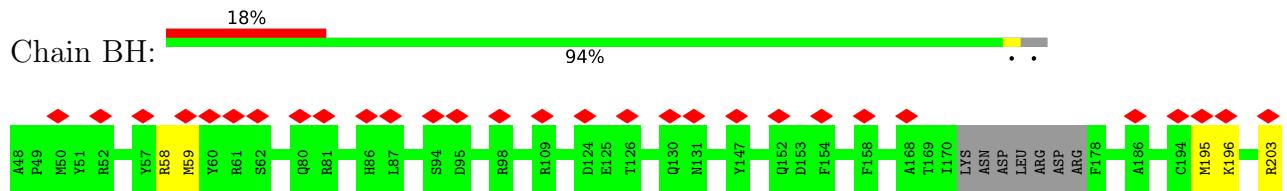
- Molecule 1: Capsid protein



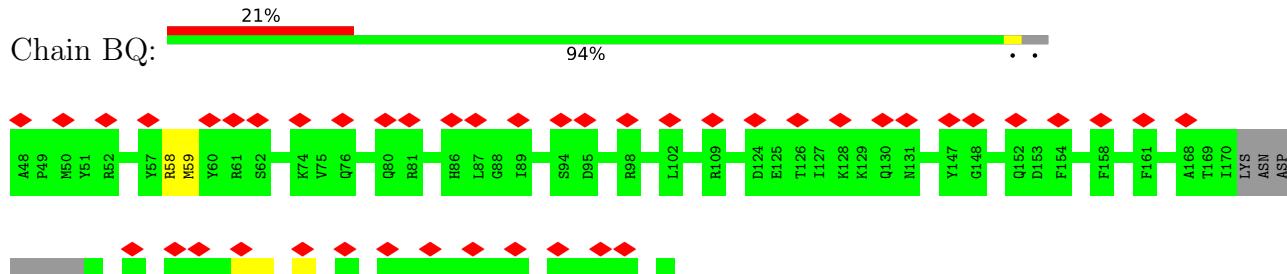
- Molecule 1: Capsid protein



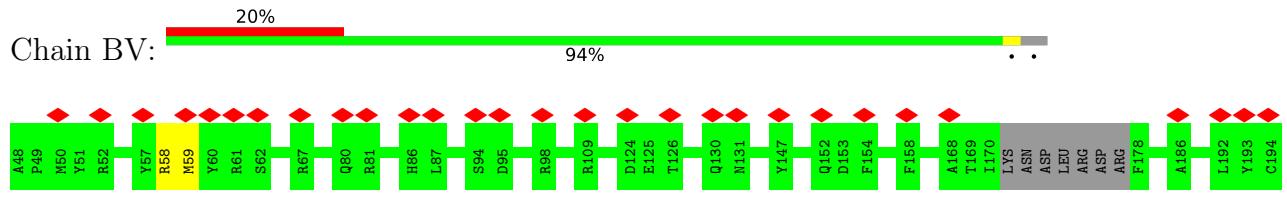
- Molecule 1: Capsid protein



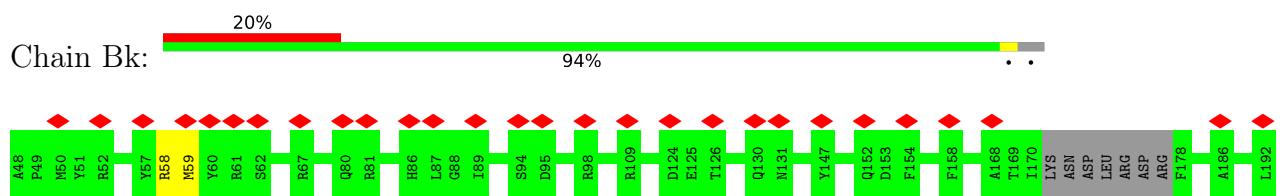
- Molecule 1: Capsid protein



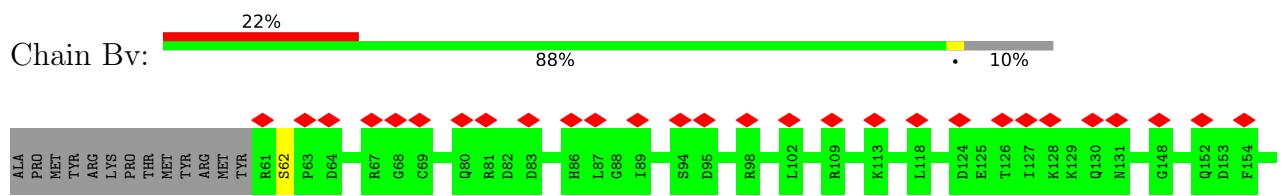
- Molecule 1: Capsid protein

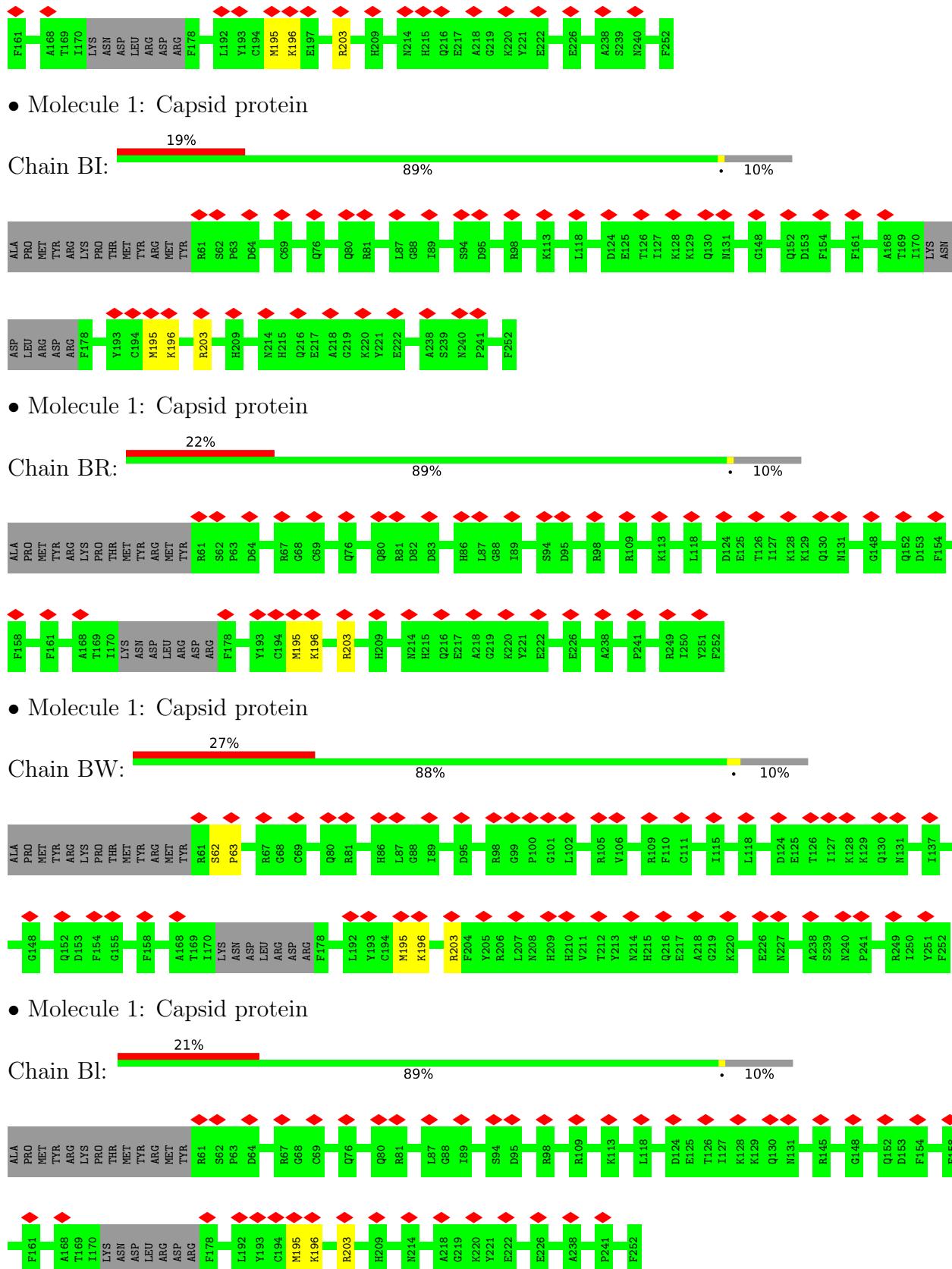


- Molecule 1: Capsid protein



- Molecule 1: Capsid protein





## 4 Experimental information i

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D5	Depositor
Number of particles used	24451	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	780	Depositor
Maximum defocus (nm)	5600	Depositor
Magnification	94000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.490	Depositor
Minimum map value	-0.317	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	471.00003, 471.00003, 471.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.57, 1.57, 1.57	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	0.28	0/1532	0.65	0/2067
1	2	0.28	0/1532	0.66	0/2067
1	3	0.28	0/1532	0.65	0/2067
1	A	0.28	0/1532	0.66	0/2067
1	B	0.28	0/1532	0.65	0/2067
1	B1	0.28	0/1532	0.65	0/2067
1	B2	0.28	0/1532	0.66	0/2067
1	B3	0.28	0/1532	0.65	0/2067
1	BA	0.28	0/1532	0.65	0/2067
1	BB	0.28	0/1532	0.65	0/2067
1	BC	0.33	0/1532	0.72	0/2067
1	BD	0.28	0/1532	0.66	0/2067
1	BE	0.28	0/1532	0.65	0/2067
1	BF	0.28	0/1532	0.66	0/2067
1	BG	0.28	0/1532	0.66	0/2067
1	BH	0.32	0/1671	0.72	0/2254
1	BI	0.33	0/1549	0.72	0/2090
1	BJ	0.28	0/1532	0.65	0/2067
1	BK	0.28	0/1532	0.66	0/2067
1	BL	0.28	0/1532	0.66	0/2067
1	BM	0.28	0/1532	0.66	0/2067
1	BN	0.28	0/1532	0.66	0/2067
1	BO	0.28	0/1532	0.66	0/2067
1	BP	0.45	3/1532 (0.2%)	0.75	4/2067 (0.2%)
1	BQ	0.33	0/1671	0.72	0/2254
1	BR	0.33	0/1549	0.72	0/2090
1	BS	0.28	0/1532	0.66	0/2067
1	BT	0.29	0/1532	0.66	0/2067
1	BU	0.28	0/1532	0.66	0/2067
1	BV	0.32	0/1671	0.72	0/2254
1	BW	0.38	0/1549	0.75	1/2090 (0.0%)
1	BX	0.28	0/1532	0.65	0/2067
1	BY	0.28	0/1532	0.66	0/2067
1	BZ	0.28	0/1532	0.66	0/2067

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	Ba	0.28	0/1532	0.65	0/2067
1	Bb	0.28	0/1532	0.66	0/2067
1	Bc	0.28	0/1532	0.66	0/2067
1	Bd	0.28	0/1532	0.65	0/2067
1	Be	0.28	0/1532	0.65	0/2067
1	Bf	0.28	0/1532	0.66	0/2067
1	Bg	0.28	0/1532	0.65	0/2067
1	Bh	0.28	0/1532	0.66	0/2067
1	Bi	0.28	0/1532	0.66	0/2067
1	Bj	0.28	0/1532	0.65	0/2067
1	Bk	0.33	0/1671	0.72	0/2254
1	Bl	0.33	0/1549	0.72	0/2090
1	Bm	0.28	0/1532	0.65	0/2067
1	Bn	0.28	0/1532	0.66	0/2067
1	Bo	0.28	0/1532	0.66	0/2067
1	Bp	0.28	0/1532	0.66	0/2067
1	Bq	0.28	0/1532	0.66	0/2067
1	Br	0.28	0/1532	0.65	0/2067
1	Bs	0.28	0/1531	0.66	0/2065
1	Bt	0.28	0/1532	0.65	0/2067
1	Bu	0.28	0/1532	0.65	0/2067
1	Bv	0.31	0/1549	0.73	2/2090 (0.1%)
1	Bw	0.32	0/1671	0.72	0/2254
1	Bx	0.28	0/1532	0.65	0/2067
1	By	0.28	0/1532	0.66	0/2067
1	Bz	0.28	0/1532	0.65	0/2067
1	C	0.33	0/1532	0.72	0/2067
1	D	0.28	0/1532	0.65	0/2067
1	E	0.28	0/1532	0.65	0/2067
1	F	0.28	0/1532	0.65	0/2067
1	G	0.28	0/1532	0.66	0/2067
1	H	0.32	0/1671	0.72	0/2254
1	I	0.33	0/1549	0.72	0/2090
1	J	0.28	0/1532	0.66	0/2067
1	K	0.28	0/1532	0.65	0/2067
1	L	0.28	0/1532	0.66	0/2067
1	M	0.28	0/1532	0.66	0/2067
1	N	0.28	0/1532	0.66	0/2067
1	O	0.28	0/1532	0.66	0/2067
1	P	0.28	0/1532	0.68	0/2067
1	Q	0.33	0/1671	0.72	0/2254
1	R	0.33	0/1549	0.72	0/2090
1	S	0.28	0/1532	0.65	0/2067

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	T	0.29	0/1532	0.66	0/2067
1	U	0.28	0/1532	0.65	0/2067
1	V	0.33	0/1671	0.73	0/2254
1	W	0.37	0/1549	0.73	0/2090
1	X	0.28	0/1532	0.65	0/2067
1	Y	0.28	0/1532	0.66	0/2067
1	Z	0.28	0/1532	0.66	0/2067
1	a	0.28	0/1532	0.65	0/2067
1	b	0.28	0/1532	0.66	0/2067
1	c	0.28	0/1532	0.65	0/2067
1	d	0.28	0/1532	0.66	0/2067
1	e	0.28	0/1532	0.65	0/2067
1	f	0.28	0/1532	0.66	0/2067
1	g	0.28	0/1532	0.66	0/2067
1	h	0.28	0/1532	0.66	0/2067
1	i	0.28	0/1532	0.66	0/2067
1	j	0.28	0/1532	0.66	0/2067
1	k	0.33	0/1671	0.72	0/2254
1	l	0.33	0/1549	0.72	0/2090
1	m	0.28	0/1532	0.65	0/2067
1	n	0.29	0/1532	0.65	0/2067
1	o	0.28	0/1532	0.65	0/2067
1	p	0.28	0/1532	0.66	0/2067
1	q	0.28	0/1532	0.66	0/2067
1	r	0.28	0/1532	0.66	0/2067
1	s	0.28	0/1532	0.66	0/2067
1	t	0.28	0/1532	0.65	0/2067
1	u	0.28	0/1532	0.66	0/2067
1	v	0.30	0/1549	0.66	0/2090
1	w	0.32	0/1671	0.72	0/2254
1	x	0.28	0/1532	0.65	0/2067
1	y	0.28	0/1532	0.65	0/2067
1	z	0.28	0/1532	0.66	0/2067
All	All	0.29	3/170079 (0.0%)	0.67	7/229468 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	0	1
1	3	0	1
1	A	0	1
1	B	0	1
1	B1	0	1
1	B2	0	1
1	B3	0	1
1	BA	0	1
1	BB	0	1
1	BC	0	1
1	BD	0	1
1	BE	0	1
1	BF	0	1
1	BG	0	1
1	BH	0	2
1	BI	0	1
1	BJ	0	1
1	BK	0	1
1	BL	0	1
1	BM	0	1
1	BN	0	1
1	BO	0	1
1	BP	0	2
1	BQ	0	2
1	BR	0	1
1	BS	0	1
1	BT	0	1
1	BU	0	1
1	BV	0	2
1	BW	0	1
1	BX	0	1
1	BY	0	1
1	BZ	0	1
1	Ba	0	1
1	Bb	0	1
1	Bc	0	1
1	Bd	0	1
1	Be	0	1
1	Bf	0	1
1	Bg	0	1
1	Bh	0	1
1	Bi	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	Bj	0	1
1	Bk	0	2
1	Bl	0	1
1	Bm	0	1
1	Bn	0	1
1	Bo	0	1
1	Bp	0	1
1	Bq	0	1
1	Br	0	1
1	Bs	0	1
1	Bt	0	1
1	Bu	0	1
1	Bv	0	1
1	Bw	0	2
1	Bx	0	1
1	By	0	1
1	Bz	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	2
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
1	O	0	1
1	P	0	1
1	Q	0	2
1	R	0	2
1	S	0	1
1	T	0	1
1	U	0	1
1	V	0	2
1	W	0	1
1	X	0	1
1	Y	0	1
1	Z	0	1
1	a	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	b	0	1
1	c	0	1
1	d	0	1
1	e	0	1
1	f	0	1
1	g	0	1
1	h	0	1
1	i	0	1
1	j	0	1
1	k	0	2
1	l	0	1
1	m	0	1
1	n	0	1
1	o	0	1
1	p	0	1
1	q	0	1
1	r	0	1
1	s	0	1
1	t	0	1
1	u	0	1
1	v	0	1
1	w	0	2
1	x	0	1
1	y	0	1
1	z	0	1
All	All	0	122

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BP	91	LYS	C-N	8.92	1.54	1.34
1	BP	110	PHE	C-N	7.54	1.51	1.34
1	BP	144	ARG	C-N	5.64	1.47	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bv	62	SER	C-N-CD	-11.97	94.26	120.60
1	BP	157	ILE	O-C-N	-8.56	109.00	122.70
1	BP	144	ARG	O-C-N	8.06	135.60	122.70
1	BP	157	ILE	C-N-CA	6.85	138.82	121.70
1	Bv	62	SER	C-N-CA	6.30	148.46	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	BW	62	SER	C-N-CD	-5.82	107.79	120.60
1	BP	144	ARG	CA-C-N	-5.38	105.36	117.20

There are no chirality outliers.

All (122) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	196	LYS	Peptide
1	2	196	LYS	Peptide
1	3	196	LYS	Peptide
1	A	196	LYS	Peptide
1	B	196	LYS	Peptide
1	B1	196	LYS	Peptide
1	B2	196	LYS	Peptide
1	B3	196	LYS	Peptide
1	BA	196	LYS	Peptide
1	BB	196	LYS	Peptide
1	BC	196	LYS	Peptide
1	BD	196	LYS	Peptide
1	BE	196	LYS	Peptide
1	BF	196	LYS	Peptide
1	BG	196	LYS	Peptide
1	BH	196	LYS	Peptide
1	BH	58	ARG	Peptide
1	BI	196	LYS	Peptide
1	BJ	196	LYS	Peptide
1	BK	196	LYS	Peptide
1	BL	196	LYS	Peptide
1	BM	196	LYS	Peptide
1	BN	196	LYS	Peptide
1	BO	196	LYS	Peptide
1	BP	157	ILE	Mainchain
1	BP	196	LYS	Peptide
1	BQ	196	LYS	Peptide
1	BQ	58	ARG	Peptide
1	BR	196	LYS	Peptide
1	BS	196	LYS	Peptide
1	BT	196	LYS	Peptide
1	BU	196	LYS	Peptide
1	BV	196	LYS	Peptide
1	BV	58	ARG	Peptide
1	BW	196	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	BX	196	LYS	Peptide
1	BY	196	LYS	Peptide
1	BZ	196	LYS	Peptide
1	Ba	196	LYS	Peptide
1	Bb	196	LYS	Peptide
1	Bc	196	LYS	Peptide
1	Bd	196	LYS	Peptide
1	Be	196	LYS	Peptide
1	Bf	196	LYS	Peptide
1	Bg	196	LYS	Peptide
1	Bh	196	LYS	Peptide
1	Bi	196	LYS	Peptide
1	Bj	196	LYS	Peptide
1	Bk	196	LYS	Peptide
1	Bk	58	ARG	Peptide
1	Bl	196	LYS	Peptide
1	Bm	196	LYS	Peptide
1	Bn	196	LYS	Peptide
1	Bo	196	LYS	Peptide
1	Bp	196	LYS	Peptide
1	Bq	196	LYS	Peptide
1	Br	196	LYS	Peptide
1	Bs	196	LYS	Peptide
1	Bt	196	LYS	Peptide
1	Bu	196	LYS	Peptide
1	Bv	196	LYS	Peptide
1	Bw	196	LYS	Peptide
1	Bw	58	ARG	Peptide
1	Bx	196	LYS	Peptide
1	By	196	LYS	Peptide
1	Bz	196	LYS	Peptide
1	C	196	LYS	Peptide
1	D	196	LYS	Peptide
1	E	196	LYS	Peptide
1	F	196	LYS	Peptide
1	G	196	LYS	Peptide
1	H	196	LYS	Peptide
1	H	58	ARG	Peptide
1	I	196	LYS	Peptide
1	J	196	LYS	Peptide
1	K	196	LYS	Peptide
1	L	196	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	M	196	LYS	Peptide
1	N	196	LYS	Peptide
1	O	196	LYS	Peptide
1	P	196	LYS	Peptide
1	Q	196	LYS	Peptide
1	Q	58	ARG	Peptide
1	R	196	LYS	Peptide
1	R	62	SER	Peptide
1	S	196	LYS	Peptide
1	T	196	LYS	Peptide
1	U	196	LYS	Peptide
1	V	196	LYS	Peptide
1	V	58	ARG	Peptide
1	W	196	LYS	Peptide
1	X	196	LYS	Peptide
1	Y	196	LYS	Peptide
1	Z	196	LYS	Peptide
1	a	196	LYS	Peptide
1	b	196	LYS	Peptide
1	c	196	LYS	Peptide
1	d	196	LYS	Peptide
1	e	196	LYS	Peptide
1	f	196	LYS	Peptide
1	g	196	LYS	Peptide
1	h	196	LYS	Peptide
1	i	196	LYS	Peptide
1	j	196	LYS	Peptide
1	k	196	LYS	Peptide
1	k	58	ARG	Peptide
1	l	196	LYS	Peptide
1	m	196	LYS	Peptide
1	n	196	LYS	Peptide
1	o	196	LYS	Peptide
1	p	196	LYS	Peptide
1	q	196	LYS	Peptide
1	r	196	LYS	Peptide
1	s	196	LYS	Peptide
1	t	196	LYS	Peptide
1	u	196	LYS	Peptide
1	v	196	LYS	Peptide
1	w	196	LYS	Peptide
1	w	58	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	x	196	LYS	Peptide
1	y	196	LYS	Peptide
1	z	196	LYS	Peptide

## 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	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	2	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	3	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	A	179/205 (87%)	144 (80%)	35 (20%)	0	100 100
1	B	179/205 (87%)	144 (80%)	35 (20%)	0	100 100
1	B1	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	B2	179/205 (87%)	144 (80%)	35 (20%)	0	100 100
1	B3	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	BA	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	BB	179/205 (87%)	144 (80%)	35 (20%)	0	100 100
1	BC	179/205 (87%)	144 (80%)	35 (20%)	0	100 100
1	BD	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	BE	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	BF	179/205 (87%)	144 (80%)	35 (20%)	0	100 100
1	BG	179/205 (87%)	144 (80%)	35 (20%)	0	100 100
1	BH	194/205 (95%)	153 (79%)	40 (21%)	1 (0%)	29 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	BI	181/205 (88%)	145 (80%)	36 (20%)	0	100 100
1	BJ	179/205 (87%)	144 (80%)	35 (20%)	0	100 100
1	BK	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	BL	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	BM	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	BN	179/205 (87%)	144 (80%)	35 (20%)	0	100 100
1	BO	179/205 (87%)	144 (80%)	35 (20%)	0	100 100
1	BP	179/205 (87%)	146 (82%)	33 (18%)	0	100 100
1	BQ	194/205 (95%)	153 (79%)	40 (21%)	1 (0%)	29 68
1	BR	181/205 (88%)	145 (80%)	36 (20%)	0	100 100
1	BS	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	BT	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	BU	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	BV	194/205 (95%)	153 (79%)	40 (21%)	1 (0%)	29 68
1	BW	181/205 (88%)	143 (79%)	37 (20%)	1 (1%)	25 64
1	BX	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	BY	179/205 (87%)	146 (82%)	33 (18%)	0	100 100
1	BZ	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	Ba	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	Bb	179/205 (87%)	144 (80%)	35 (20%)	0	100 100
1	Bc	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	Bd	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	Be	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	Bf	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	Bg	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	Bh	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	Bi	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	Bj	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	Bk	194/205 (95%)	153 (79%)	40 (21%)	1 (0%)	29 68
1	Bl	181/205 (88%)	145 (80%)	36 (20%)	0	100 100
1	Bm	179/205 (87%)	144 (80%)	35 (20%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	Bn	179/205 (87%)	144 (80%)	35 (20%)	0	100 100
1	Bo	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	Bp	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	Bq	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	Br	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	Bs	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	Bt	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	Bu	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	Bv	181/205 (88%)	145 (80%)	36 (20%)	0	100 100
1	Bw	194/205 (95%)	153 (79%)	40 (21%)	1 (0%)	29 68
1	Bx	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	By	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	Bz	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	C	179/205 (87%)	144 (80%)	35 (20%)	0	100 100
1	D	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	E	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	F	179/205 (87%)	144 (80%)	35 (20%)	0	100 100
1	G	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	H	194/205 (95%)	153 (79%)	40 (21%)	1 (0%)	29 68
1	I	181/205 (88%)	145 (80%)	36 (20%)	0	100 100
1	J	179/205 (87%)	144 (80%)	35 (20%)	0	100 100
1	K	179/205 (87%)	144 (80%)	35 (20%)	0	100 100
1	L	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	M	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	N	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	O	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	P	179/205 (87%)	146 (82%)	33 (18%)	0	100 100
1	Q	194/205 (95%)	154 (79%)	39 (20%)	1 (0%)	29 68
1	R	181/205 (88%)	145 (80%)	35 (19%)	1 (1%)	25 64
1	S	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	T	179/205 (87%)	145 (81%)	34 (19%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	U	179/205 (87%)	144 (80%)	35 (20%)	0	100 100
1	V	194/205 (95%)	153 (79%)	40 (21%)	1 (0%)	29 68
1	W	181/205 (88%)	145 (80%)	36 (20%)	0	100 100
1	X	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	Y	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	Z	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	a	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	b	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	c	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	d	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	e	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	f	179/205 (87%)	144 (80%)	35 (20%)	0	100 100
1	g	179/205 (87%)	144 (80%)	35 (20%)	0	100 100
1	h	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	i	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	j	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	k	194/205 (95%)	154 (79%)	39 (20%)	1 (0%)	29 68
1	l	181/205 (88%)	145 (80%)	36 (20%)	0	100 100
1	m	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	n	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	o	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	p	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	q	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	r	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	s	179/205 (87%)	144 (80%)	35 (20%)	0	100 100
1	t	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	u	179/205 (87%)	144 (80%)	35 (20%)	0	100 100
1	v	181/205 (88%)	146 (81%)	35 (19%)	0	100 100
1	w	194/205 (95%)	153 (79%)	40 (21%)	1 (0%)	29 68
1	x	179/205 (87%)	145 (81%)	34 (19%)	0	100 100
1	y	179/205 (87%)	145 (81%)	34 (19%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	z	179/205 (87%)	145 (81%)	34 (19%)	0	100   100
All	All	19860/22550 (88%)	16012 (81%)	3836 (19%)	12 (0%)	54   85

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BW	63	PRO
1	H	59	MET
1	Q	59	MET
1	V	59	MET
1	k	59	MET
1	w	59	MET
1	Bw	59	MET
1	BH	59	MET
1	BQ	59	MET
1	BV	59	MET
1	Bk	59	MET
1	R	63	PRO

### 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	162/183 (88%)	160 (99%)	2 (1%)	71   83
1	2	162/183 (88%)	160 (99%)	2 (1%)	71   83
1	3	162/183 (88%)	160 (99%)	2 (1%)	71   83
1	A	162/183 (88%)	160 (99%)	2 (1%)	71   83
1	B	162/183 (88%)	160 (99%)	2 (1%)	71   83
1	B1	162/183 (88%)	160 (99%)	2 (1%)	71   83
1	B2	162/183 (88%)	160 (99%)	2 (1%)	71   83
1	B3	162/183 (88%)	160 (99%)	2 (1%)	71   83
1	BA	162/183 (88%)	160 (99%)	2 (1%)	71   83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	BB	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	BC	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	BD	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	BE	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	BF	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	BG	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	BH	176/183 (96%)	174 (99%)	2 (1%)	73 84
1	BI	164/183 (90%)	162 (99%)	2 (1%)	71 83
1	BJ	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	BK	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	BL	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	BM	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	BN	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	BO	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	BP	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	BQ	176/183 (96%)	174 (99%)	2 (1%)	73 84
1	BR	164/183 (90%)	162 (99%)	2 (1%)	71 83
1	BS	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	BT	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	BU	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	BV	176/183 (96%)	174 (99%)	2 (1%)	73 84
1	BW	164/183 (90%)	162 (99%)	2 (1%)	71 83
1	BX	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	BY	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	BZ	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Ba	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Bb	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Bc	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Bd	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Be	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Bf	162/183 (88%)	160 (99%)	2 (1%)	71 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Bg	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Bh	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Bi	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Bj	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Bk	176/183 (96%)	174 (99%)	2 (1%)	73 84
1	Bl	164/183 (90%)	162 (99%)	2 (1%)	71 83
1	Bm	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Bn	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Bo	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Bp	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Bq	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Br	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Bs	161/183 (88%)	159 (99%)	2 (1%)	71 83
1	Bt	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Bu	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Bv	164/183 (90%)	162 (99%)	2 (1%)	71 83
1	Bw	176/183 (96%)	174 (99%)	2 (1%)	73 84
1	Bx	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	By	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Bz	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	C	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	D	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	E	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	F	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	G	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	H	176/183 (96%)	174 (99%)	2 (1%)	73 84
1	I	164/183 (90%)	162 (99%)	2 (1%)	71 83
1	J	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	K	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	L	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	M	162/183 (88%)	160 (99%)	2 (1%)	71 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	O	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	P	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Q	176/183 (96%)	174 (99%)	2 (1%)	73 84
1	R	164/183 (90%)	162 (99%)	2 (1%)	71 83
1	S	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	T	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	U	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	V	176/183 (96%)	174 (99%)	2 (1%)	73 84
1	W	164/183 (90%)	162 (99%)	2 (1%)	71 83
1	X	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Y	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	Z	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	a	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	b	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	c	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	d	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	e	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	f	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	g	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	h	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	i	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	j	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	k	176/183 (96%)	174 (99%)	2 (1%)	73 84
1	l	164/183 (90%)	162 (99%)	2 (1%)	71 83
1	m	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	n	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	o	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	p	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	q	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	r	162/183 (88%)	160 (99%)	2 (1%)	71 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	s	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	t	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	u	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	v	164/183 (90%)	162 (99%)	2 (1%)	71 83
1	w	176/183 (96%)	174 (99%)	2 (1%)	73 84
1	x	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	y	162/183 (88%)	160 (99%)	2 (1%)	71 83
1	z	162/183 (88%)	160 (99%)	2 (1%)	71 83
All	All	17979/20130 (89%)	17759 (99%)	220 (1%)	72 83

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	MET
1	A	203	ARG
1	B	195	MET
1	B	203	ARG
1	C	195	MET
1	C	203	ARG
1	D	195	MET
1	D	203	ARG
1	E	195	MET
1	E	203	ARG
1	F	195	MET
1	F	203	ARG
1	G	195	MET
1	G	203	ARG
1	H	195	MET
1	H	203	ARG
1	I	195	MET
1	I	203	ARG
1	J	195	MET
1	J	203	ARG
1	K	195	MET
1	K	203	ARG
1	L	195	MET
1	L	203	ARG
1	M	195	MET
1	M	203	ARG

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Mol	Chain	Res	Type
1	N	195	MET
1	N	203	ARG
1	O	195	MET
1	O	203	ARG
1	P	195	MET
1	P	203	ARG
1	Q	195	MET
1	Q	203	ARG
1	R	195	MET
1	R	203	ARG
1	S	195	MET
1	S	203	ARG
1	T	195	MET
1	T	203	ARG
1	U	195	MET
1	U	203	ARG
1	V	195	MET
1	V	203	ARG
1	W	195	MET
1	W	203	ARG
1	X	195	MET
1	X	203	ARG
1	Y	195	MET
1	Y	203	ARG
1	Z	195	MET
1	Z	203	ARG
1	BA	195	MET
1	BA	203	ARG
1	BB	195	MET
1	BB	203	ARG
1	BC	195	MET
1	BC	203	ARG
1	BD	195	MET
1	BD	203	ARG
1	a	195	MET
1	a	203	ARG
1	b	195	MET
1	b	203	ARG
1	c	195	MET
1	c	203	ARG
1	d	195	MET
1	d	203	ARG

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Mol	Chain	Res	Type
1	e	195	MET
1	e	203	ARG
1	f	195	MET
1	f	203	ARG
1	g	195	MET
1	g	203	ARG
1	h	195	MET
1	h	203	ARG
1	i	195	MET
1	i	203	ARG
1	j	195	MET
1	j	203	ARG
1	m	195	MET
1	m	203	ARG
1	n	195	MET
1	n	203	ARG
1	o	195	MET
1	o	203	ARG
1	p	195	MET
1	p	203	ARG
1	q	195	MET
1	q	203	ARG
1	r	195	MET
1	r	203	ARG
1	s	195	MET
1	s	203	ARG
1	t	195	MET
1	t	203	ARG
1	u	195	MET
1	u	203	ARG
1	x	195	MET
1	x	203	ARG
1	y	195	MET
1	y	203	ARG
1	z	195	MET
1	z	203	ARG
1	3	195	MET
1	3	203	ARG
1	1	195	MET
1	1	203	ARG
1	2	195	MET
1	2	203	ARG

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Mol	Chain	Res	Type
1	k	195	MET
1	k	203	ARG
1	w	195	MET
1	w	203	ARG
1	l	195	MET
1	l	203	ARG
1	v	195	MET
1	v	203	ARG
1	BE	195	MET
1	BE	203	ARG
1	BF	195	MET
1	BF	203	ARG
1	BG	195	MET
1	BG	203	ARG
1	BJ	195	MET
1	BJ	203	ARG
1	BP	195	MET
1	BP	203	ARG
1	BS	195	MET
1	BS	203	ARG
1	BT	195	MET
1	BT	203	ARG
1	BU	195	MET
1	BU	203	ARG
1	BX	195	MET
1	BX	203	ARG
1	BY	195	MET
1	BY	203	ARG
1	BZ	195	MET
1	BZ	203	ARG
1	Ba	195	MET
1	Ba	203	ARG
1	Bb	195	MET
1	Bb	203	ARG
1	Bc	195	MET
1	Bc	203	ARG
1	Bd	195	MET
1	Bd	203	ARG
1	BK	195	MET
1	BK	203	ARG
1	BL	195	MET
1	BL	203	ARG

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Mol	Chain	Res	Type
1	BM	195	MET
1	BM	203	ARG
1	BN	195	MET
1	BN	203	ARG
1	BO	195	MET
1	BO	203	ARG
1	Be	195	MET
1	Be	203	ARG
1	Bf	195	MET
1	Bf	203	ARG
1	Bg	195	MET
1	Bg	203	ARG
1	Bh	195	MET
1	Bh	203	ARG
1	Bi	195	MET
1	Bi	203	ARG
1	Bj	195	MET
1	Bj	203	ARG
1	Bm	195	MET
1	Bm	203	ARG
1	Bn	195	MET
1	Bn	203	ARG
1	Bo	195	MET
1	Bo	203	ARG
1	Bp	195	MET
1	Bp	203	ARG
1	Bq	195	MET
1	Bq	203	ARG
1	Br	195	MET
1	Br	203	ARG
1	Bs	195	MET
1	Bs	203	ARG
1	Bt	195	MET
1	Bt	203	ARG
1	Bu	195	MET
1	Bu	203	ARG
1	Bx	195	MET
1	Bx	203	ARG
1	By	195	MET
1	By	203	ARG
1	Bz	195	MET
1	Bz	203	ARG

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Mol	Chain	Res	Type
1	B3	195	MET
1	B3	203	ARG
1	B1	195	MET
1	B1	203	ARG
1	B2	195	MET
1	B2	203	ARG
1	Bw	195	MET
1	Bw	203	ARG
1	BH	195	MET
1	BH	203	ARG
1	BQ	195	MET
1	BQ	203	ARG
1	BV	195	MET
1	BV	203	ARG
1	Bk	195	MET
1	Bk	203	ARG
1	Bv	195	MET
1	Bv	203	ARG
1	BI	195	MET
1	BI	203	ARG
1	BR	195	MET
1	BR	203	ARG
1	BW	195	MET
1	BW	203	ARG
1	Bl	195	MET
1	Bl	203	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	185	HIS
1	H	163	ASN
1	Q	163	ASN
1	R	215	HIS
1	V	163	ASN
1	BB	185	HIS
1	n	216	GLN
1	k	163	ASN
1	k	185	HIS
1	w	163	ASN
1	BS	185	HIS
1	BX	185	HIS

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Mol	Chain	Res	Type
1	Bw	163	ASN
1	BH	163	ASN
1	BQ	163	ASN
1	Bk	163	ASN
1	Bk	185	HIS
1	BR	216	GLN
1	BW	163	ASN
1	BW	185	HIS

### 5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

### 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

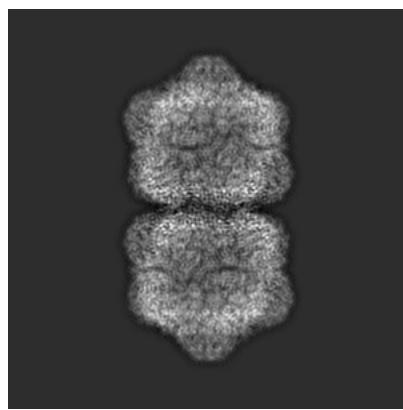
## 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3521. These allow visual inspection of the internal detail of the map and identification of artifacts.

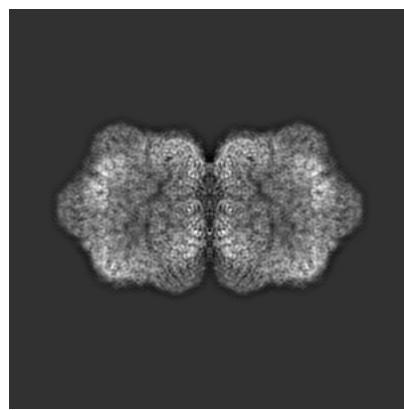
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections (i)

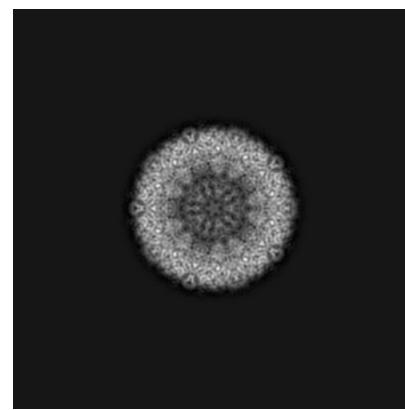
#### 6.1.1 Primary map



X

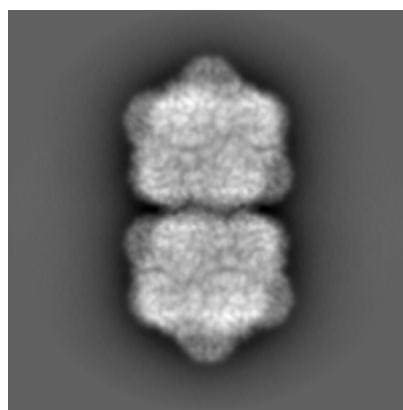


Y

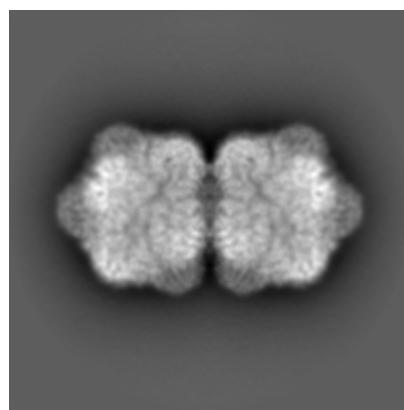


Z

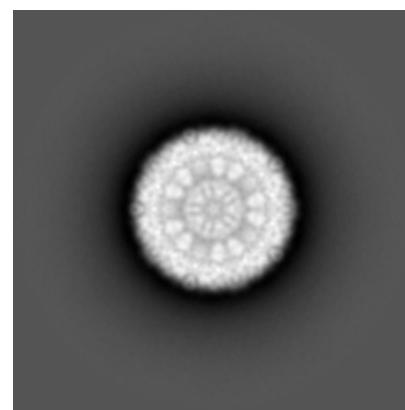
#### 6.1.2 Raw map



X



Y

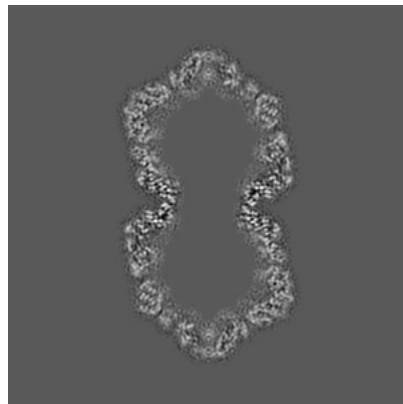


Z

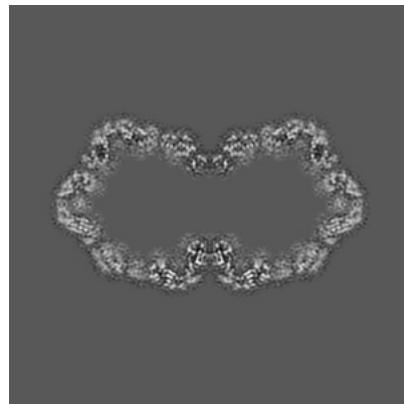
The images above show the map projected in three orthogonal directions.

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

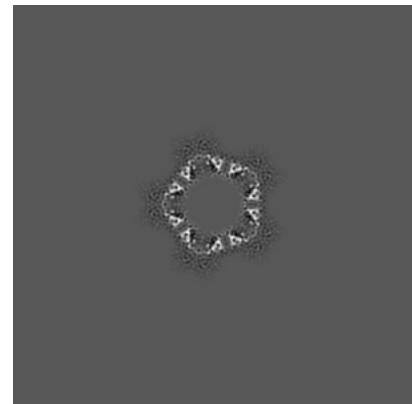
### 6.2.1 Primary map



X Index: 150

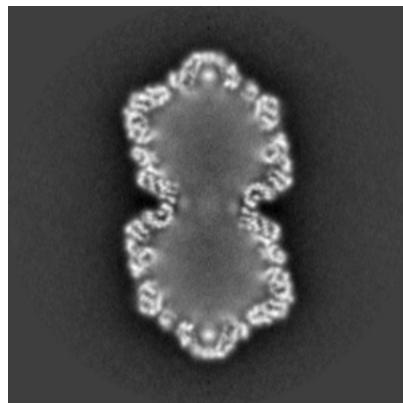


Y Index: 150

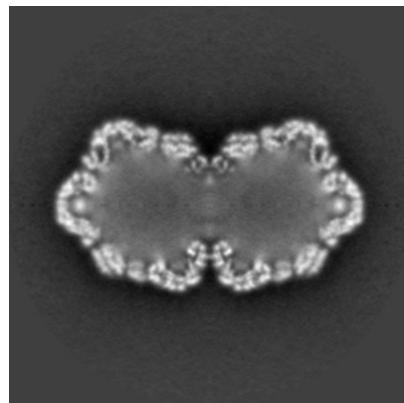


Z Index: 150

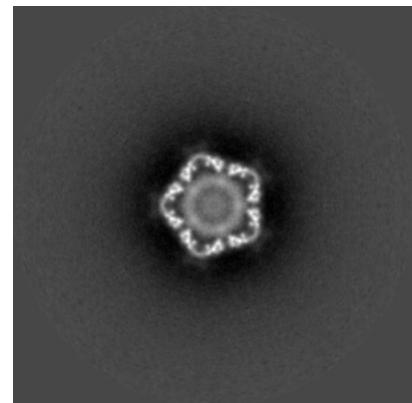
### 6.2.2 Raw map



X Index: 150



Y Index: 150

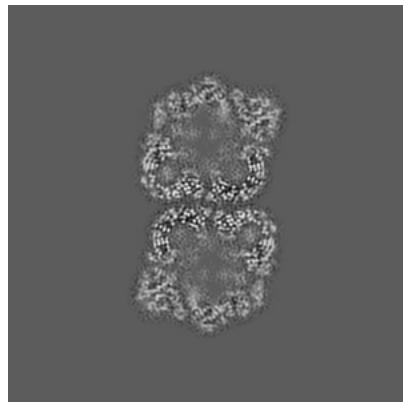


Z Index: 150

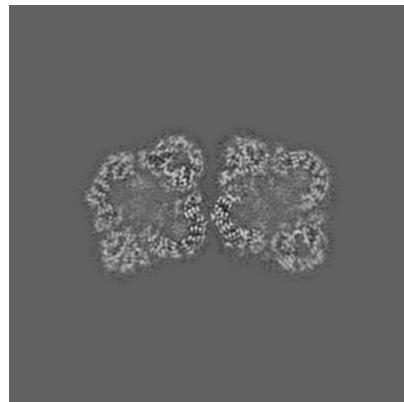
The images above show central slices of the map in three orthogonal directions.

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

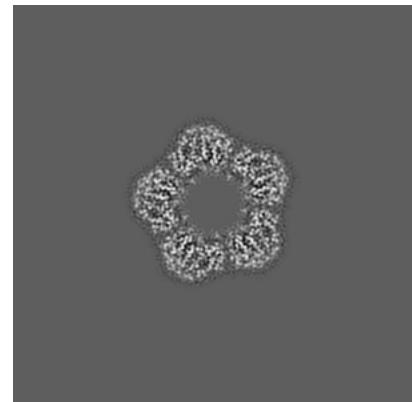
### 6.3.1 Primary map



X Index: 185

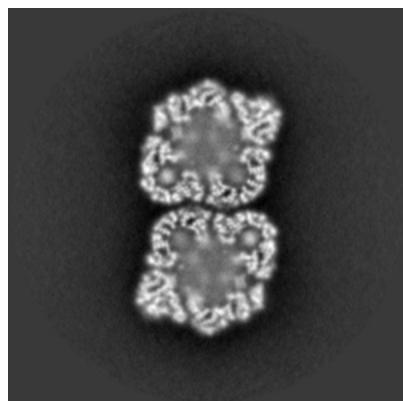


Y Index: 188

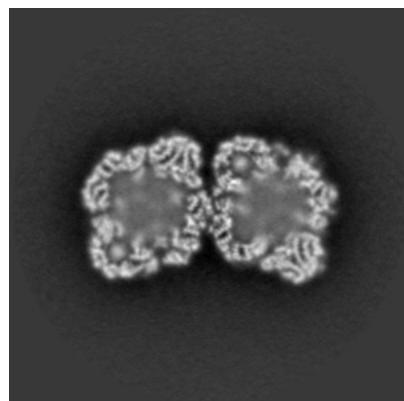


Z Index: 163

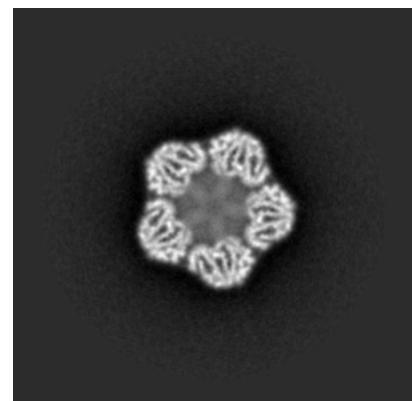
### 6.3.2 Raw map



X Index: 185



Y Index: 117

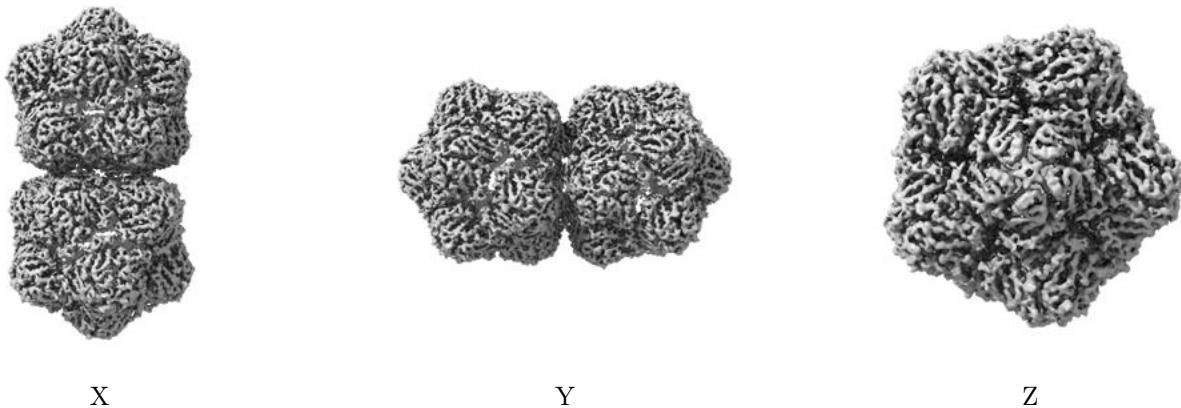


Z Index: 229

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

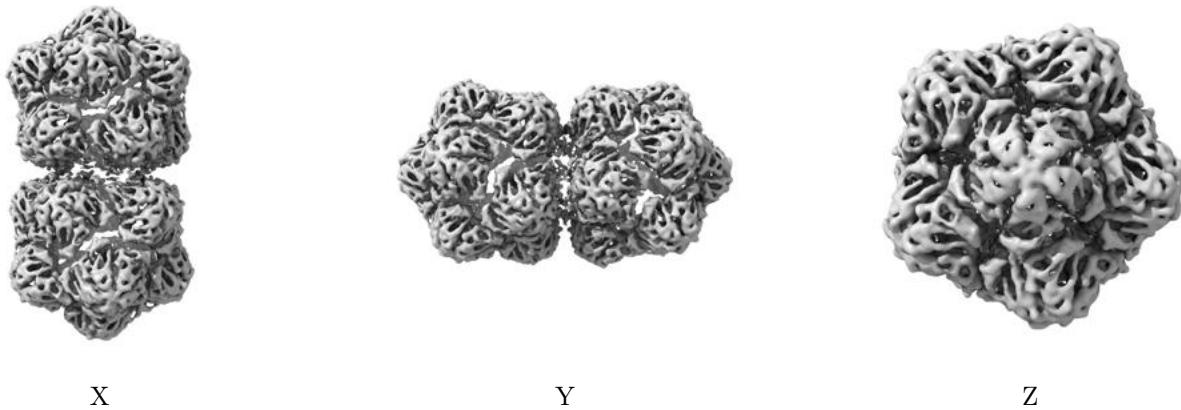
## 6.4 Orthogonal surface views [\(i\)](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

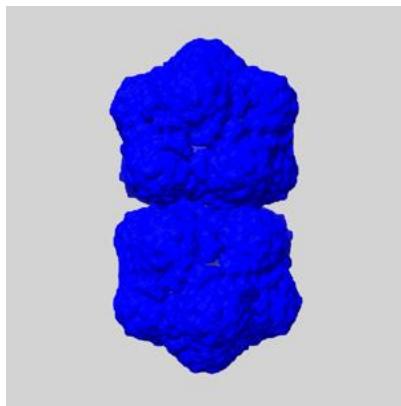
## 6.5 Mask visualisation [\(i\)](#)

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

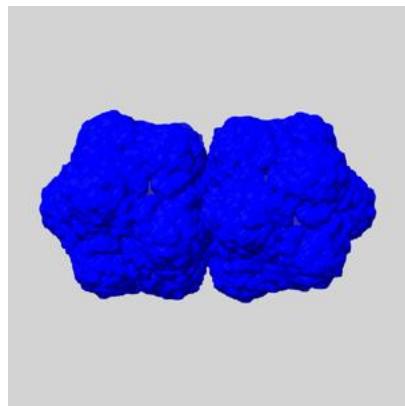
A mask typically either:

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

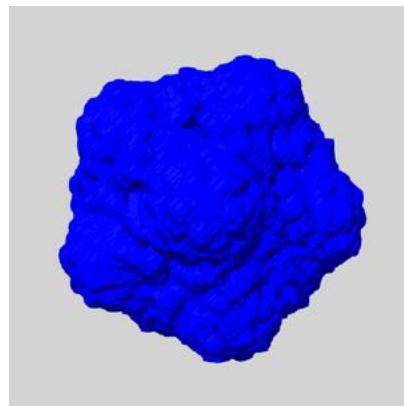
### 6.5.1 emd\_3521\_msk\_1.map [\(i\)](#)



X



Y

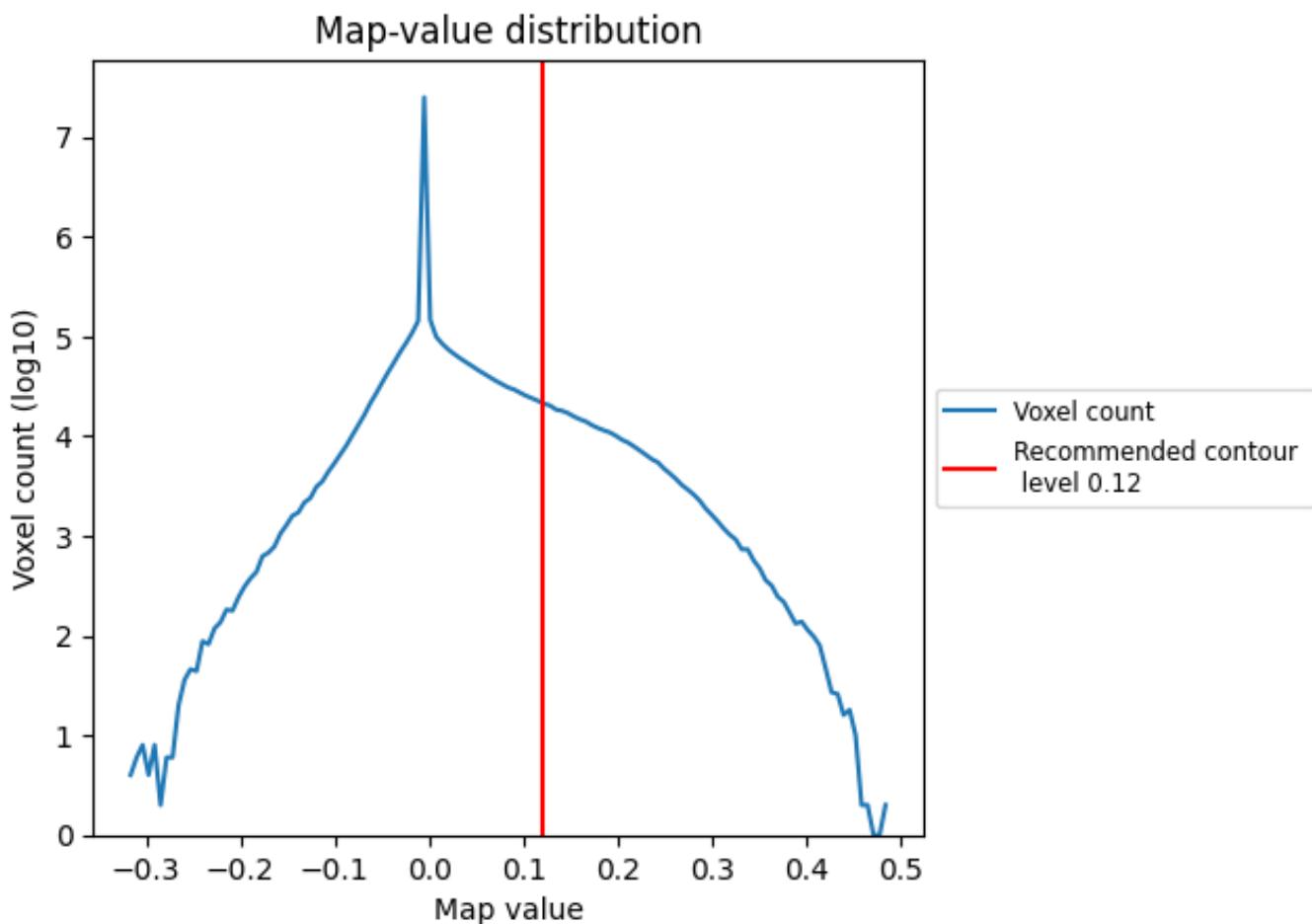


Z

## 7 Map analysis (i)

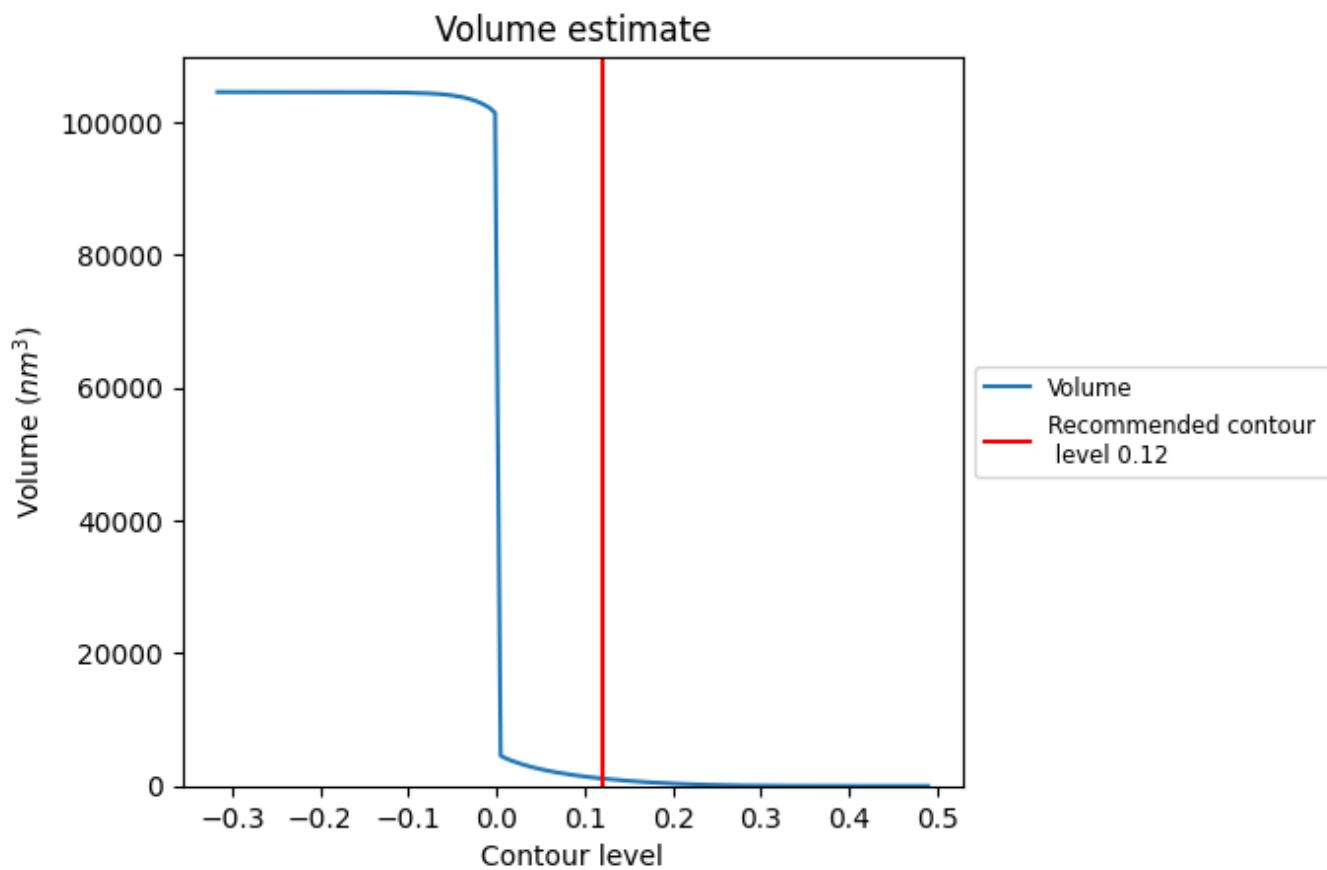
This section contains the results of statistical analysis of the map.

### 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.

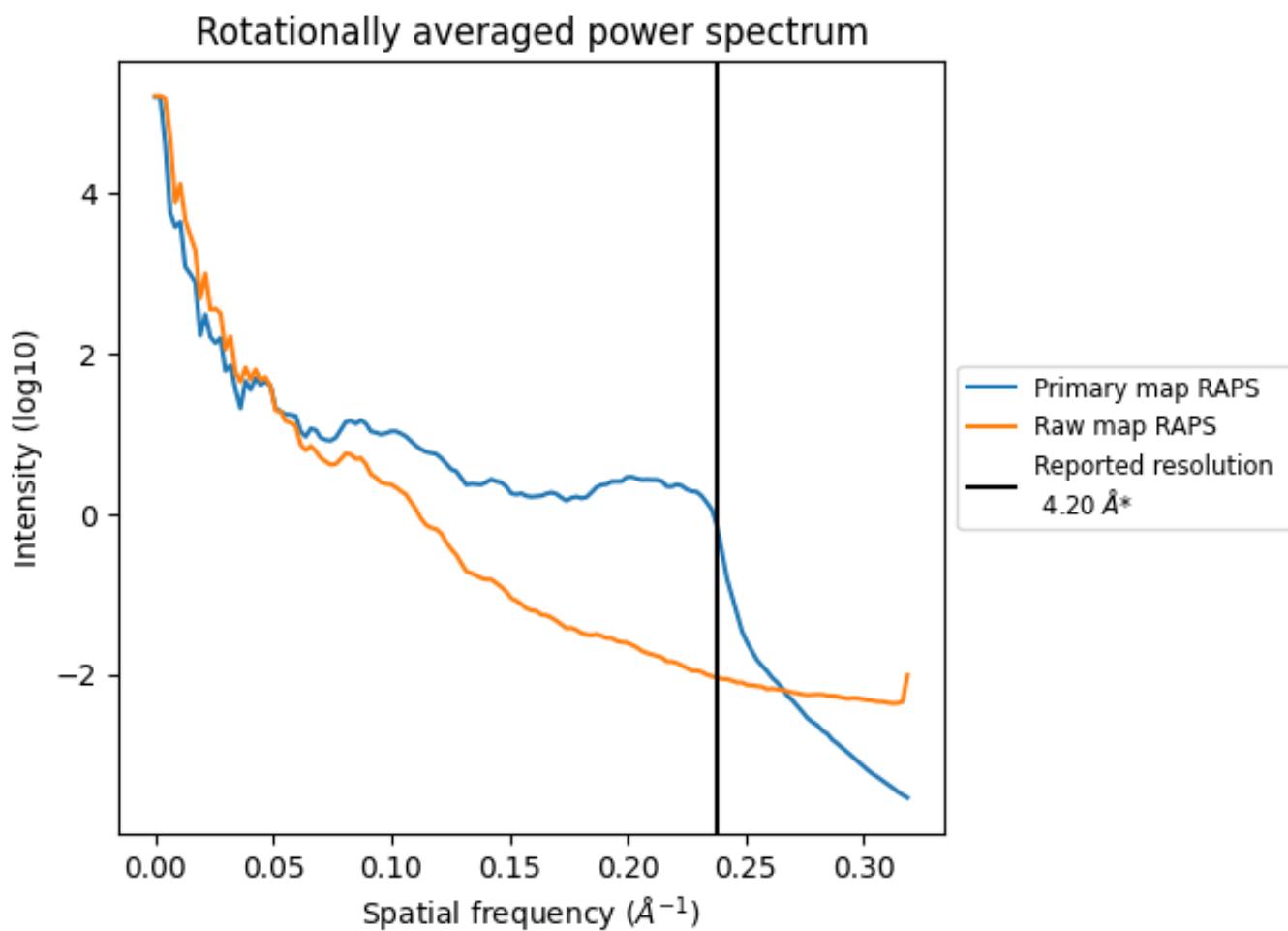
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1121 nm<sup>3</sup>; this corresponds to an approximate mass of 1013 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 [\(i\)](#)

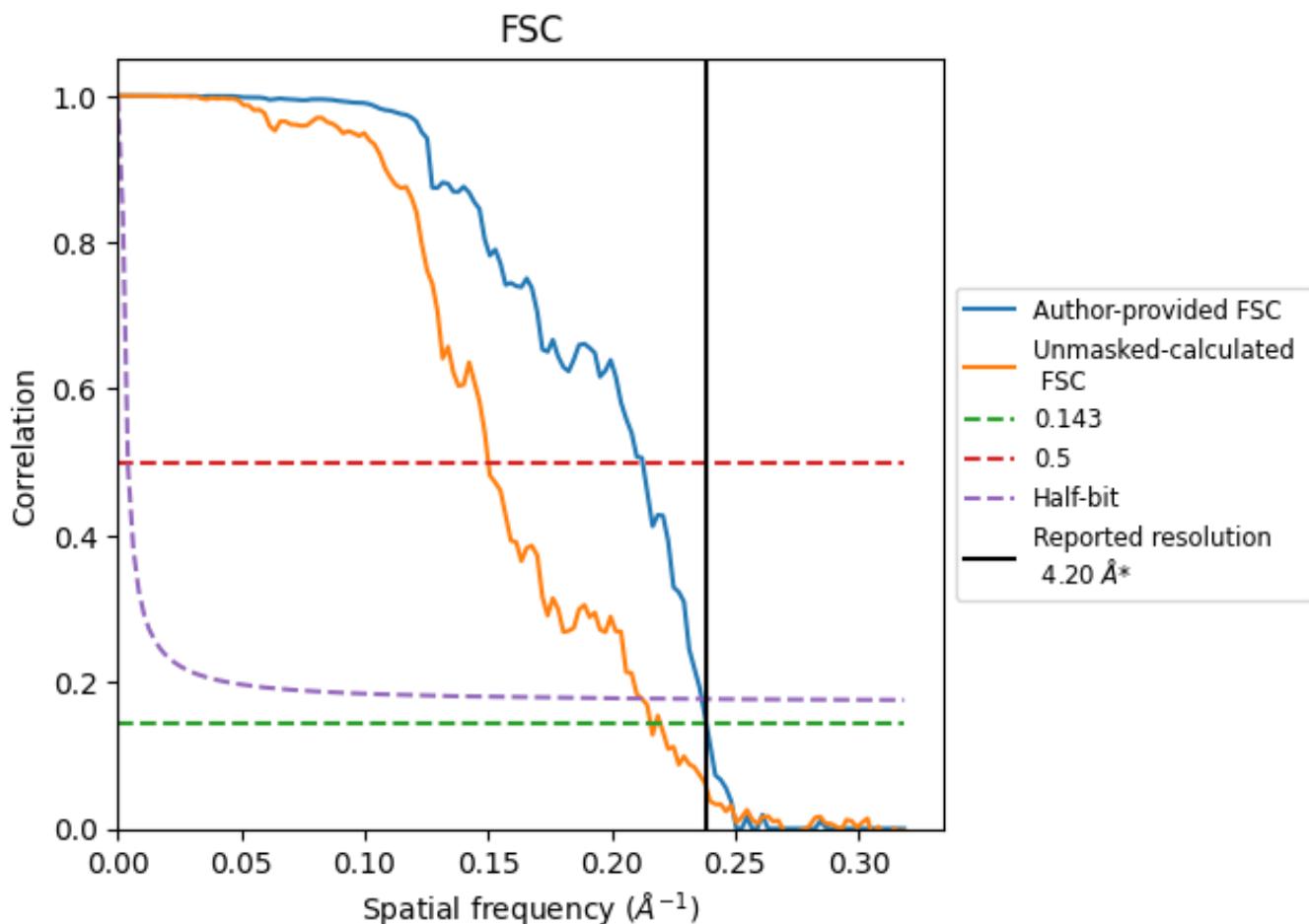


\*Reported resolution corresponds to spatial frequency of  $0.238 \text{ \AA}^{-1}$

## 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  $0.238 \text{\AA}^{-1}$

## 8.2 Resolution estimates [\(i\)](#)

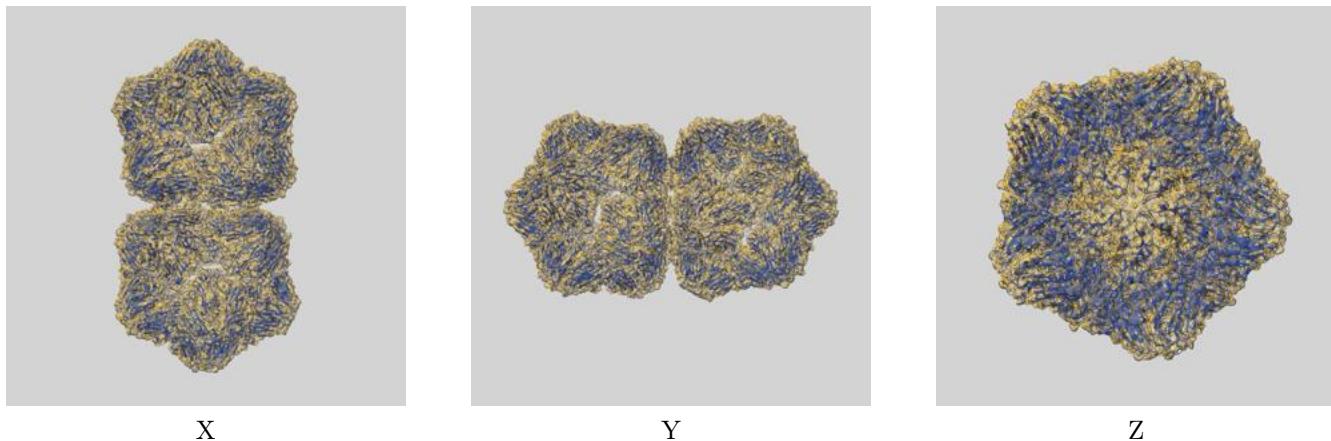
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.19	4.70	4.23
Unmasked-calculated*	4.63	6.66	4.71

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.63 differs from the reported value 4.2 by more than 10 %

## 9 Map-model fit i

This section contains information regarding the fit between EMDB map EMD-3521 and PDB model 6EK5. Per-residue inclusion information can be found in section 3 on page 22.

### 9.1 Map-model overlay i

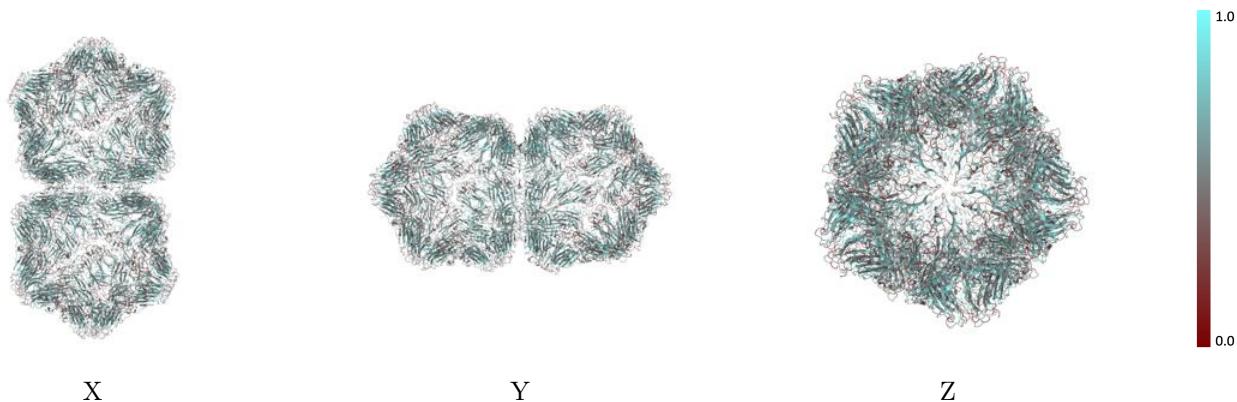


The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

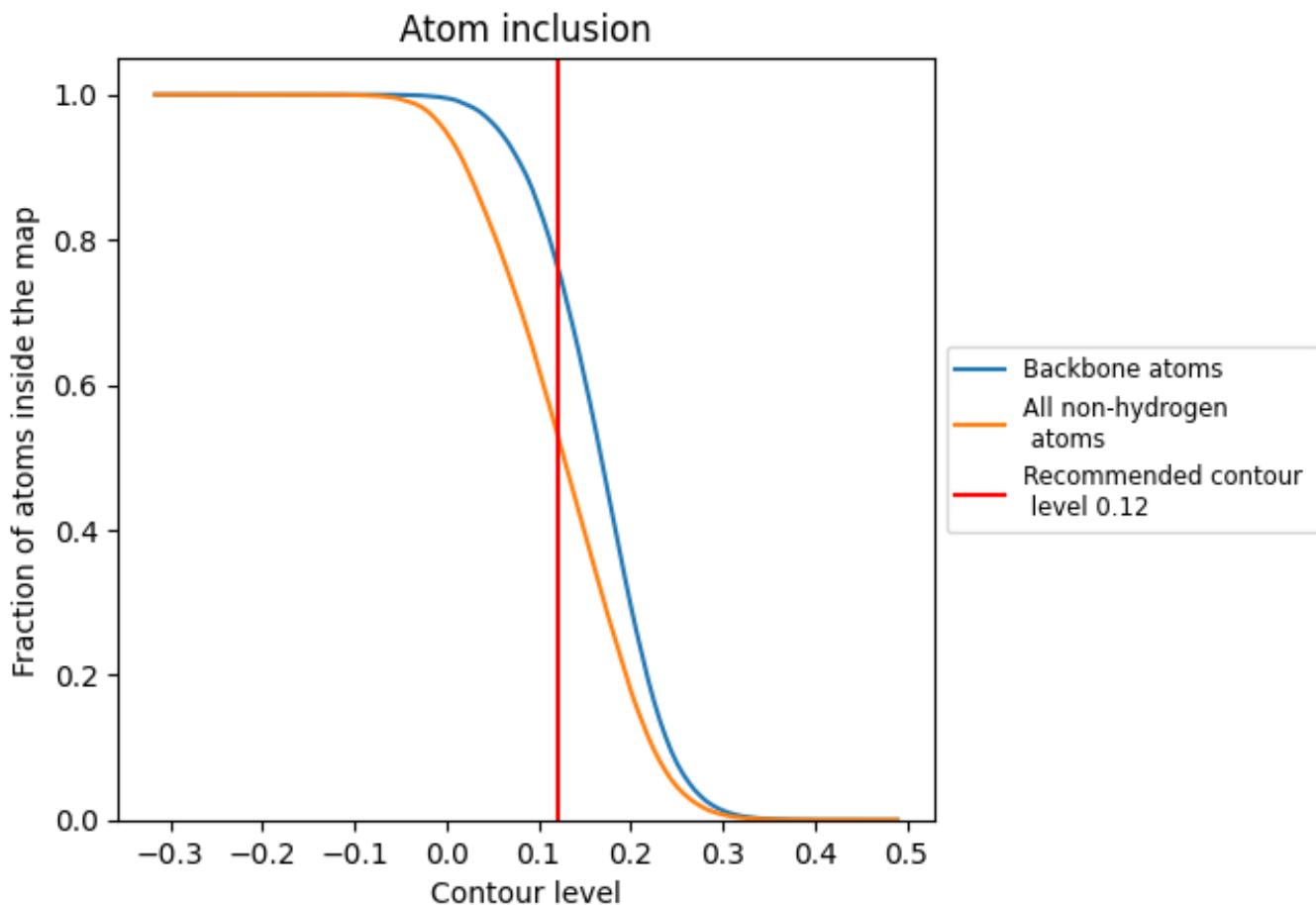
This section was not generated.

## 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 (0.12).

## 9.4 Atom inclusion [\(i\)](#)

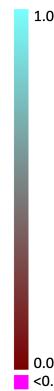


At the recommended contour level, 77% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.5333
1	0.5205
2	0.5212
3	0.5096
A	0.5096
B	0.5089
B1	0.5267
B2	0.5158
B3	0.5062
BA	0.5185
BB	0.5048
BC	0.5041
BD	0.5205
BE	0.5151
BF	0.5397
BG	0.5486
BH	0.5748
BI	0.5722
BJ	0.5432
BK	0.5089
BL	0.5055
BM	0.5014
BN	0.5068
BO	0.5082
BP	0.5507
BQ	0.5685
BR	0.5695
BS	0.5390
BT	0.5582
BU	0.5404
BV	0.5754
BW	0.5207
BX	0.5432
BY	0.5486
BZ	0.5205



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Chain	Atom inclusion
Ba	0.5007
Bb	0.5240
Bc	0.5199
Bd	0.5158
Be	0.5212
Bf	0.5089
Bg	0.5068
Bh	0.5247
Bi	0.5171
Bj	0.5493
Bk	0.5659
Bl	0.5688
Bm	0.5521
Bn	0.5541
Bo	0.5178
Bp	0.5130
Bq	0.5096
Br	0.5219
Bs	0.5195
Bt	0.5514
Bu	0.5568
Bv	0.5525
Bw	0.5741
Bx	0.5473
By	0.5137
Bz	0.5123
C	0.5014
D	0.5260
E	0.5089
F	0.5425
G	0.5534
H	0.5735
I	0.5729
J	0.5452
K	0.5034
L	0.5082
M	0.5062
N	0.5007
O	0.5062
P	0.5507
Q	0.5886
R	0.5668

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Chain	Atom inclusion
S	0.5486
T	0.5610
U	0.5404
V	0.5710
W	0.5736
X	0.5479
Y	0.5500
Z	0.5274
a	0.5027
b	0.5233
c	0.5158
d	0.5123
e	0.5199
f	0.5123
g	0.5007
h	0.5247
i	0.5240
j	0.5459
k	0.5603
l	0.5641
m	0.5459
n	0.5514
o	0.5219
p	0.5164
q	0.5075
r	0.5253
s	0.5205
t	0.5514
u	0.5507
v	0.5573
w	0.5785
x	0.5479
y	0.5164
z	0.5137