



## wwPDB EM Validation Summary Report ⓘ

Jan 1, 2025 – 11:55 AM EST

PDB ID : 8TW2  
EMDB ID : EMD-41657  
Title : Acinetobacter phage AP205 T=4 VLP  
Authors : Meng, R.; Xing, Z.; Zhang, J.  
Deposited on : 2023-08-19  
Resolution : 3.39 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 ⓘ 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.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

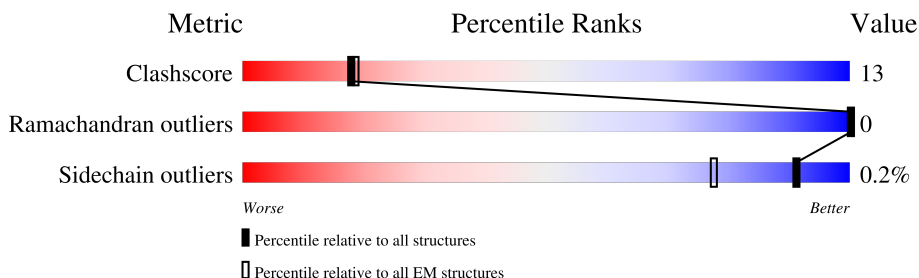
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.39 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.









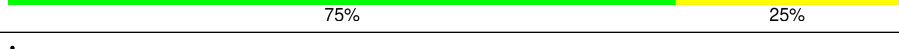
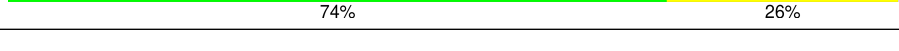
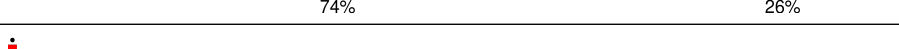
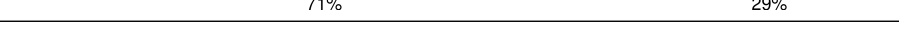
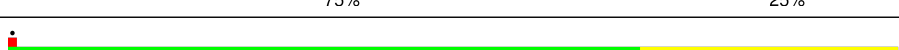

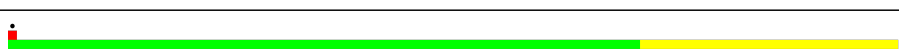

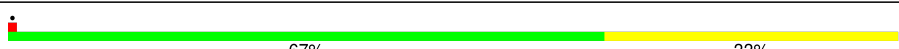





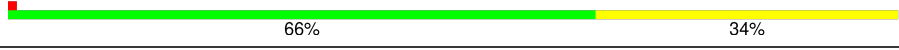
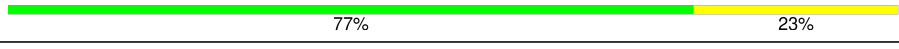



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	AA	129	74% 26%
1	AB	129	65% 35%
1	AC	129	77% 23%
1	AD	129	64% 36%
1	AE	129	67% 33%
1	AF	129	68% 32%
1	AG	129	78% 22%
1	AH	129	67% 33%



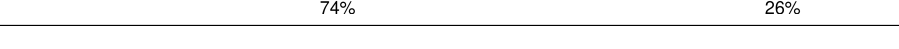
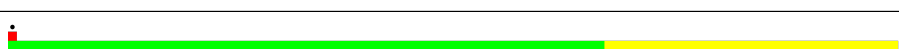



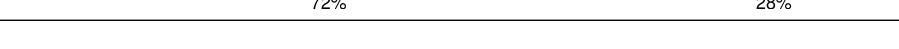



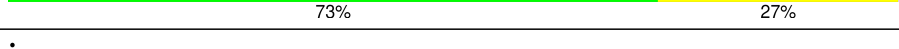

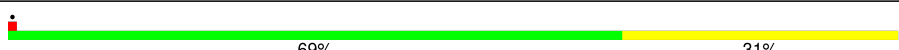


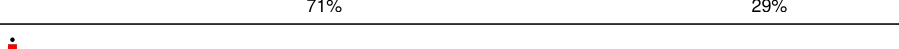







Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	AI	129	
1	AJ	129	
1	AK	129	
1	AL	129	
1	AM	129	
1	AN	129	
1	AO	129	
1	AP	129	
1	AQ	129	
1	AR	129	
1	AS	129	
1	AT	129	
1	AU	129	
1	AV	129	
1	AW	129	
1	AX	129	
1	AY	129	
1	AZ	129	
1	BA	129	
1	BB	129	
1	BC	129	
1	BD	129	
1	BE	129	
1	BF	129	
1	BG	129	





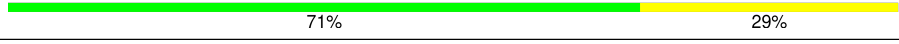


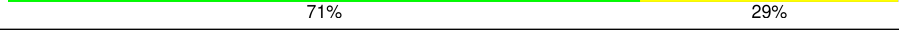
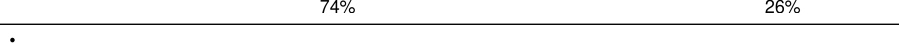
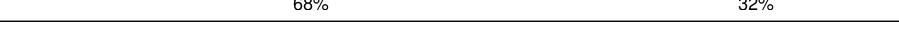
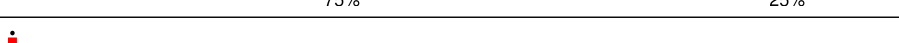











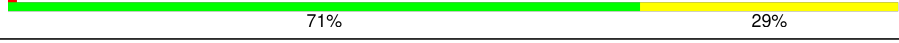


*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	BH	129	
1	BI	129	
1	BJ	129	
1	BK	129	
1	BL	129	
1	BM	129	
1	BN	129	
1	BO	129	
1	BP	129	
1	BQ	129	
1	BR	129	
1	BS	129	
1	BT	129	
1	BU	129	
1	BV	129	
1	BW	129	
1	BX	129	
1	BY	129	
1	BZ	129	
1	CA	129	
1	CB	129	
1	CC	129	
1	CD	129	
1	CE	129	
1	CF	129	



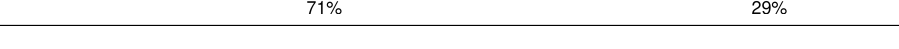
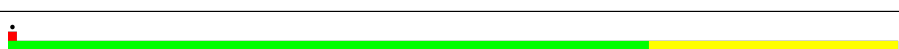



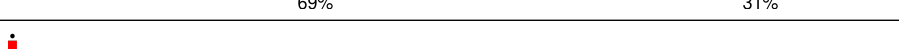



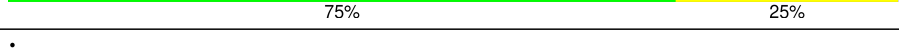

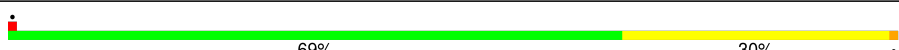


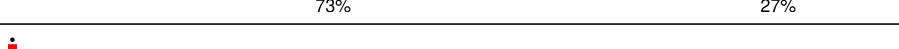







*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	CG	129	 74%26%
1	CH	129	 73%27%
1	CI	129	 68%32%
1	CJ	129	 69%31%
1	CK	129	 71%29%
1	CL	129	 70%30%
1	CM	129	 69%31%
1	CN	129	 71%29%
1	CO	129	 74%26%
1	CP	129	 68%32%
1	CQ	129	 75%25%
1	CR	129	 73%27%
1	CS	129	 76%24%
1	CT	129	 70%30%
1	CU	129	 72%28%
1	CV	129	 69%31%
1	CW	129	 76%24%
1	CX	129	 75%25%
1	CY	129	 73%27%
1	CZ	129	 70%29%
1	DA	129	 74%26%
1	DB	129	 65%35%
1	DC	129	 73%27%
1	DE	129	 71%29%
1	DF	129	 71%29%


























*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	DG	129	
1	DH	129	
1	DI	129	
1	DJ	129	
1	DK	129	
1	DL	129	
1	DM	129	
1	DN	129	
1	DO	129	
1	DP	129	
1	DQ	129	
1	DR	129	
1	DS	129	
1	DT	129	
1	DU	129	
1	DV	129	
1	DW	129	
1	DX	129	
1	DY	129	
1	DZ	129	
1	EA	129	
1	EB	129	
1	EC	129	
1	ED	129	
1	EE	129	











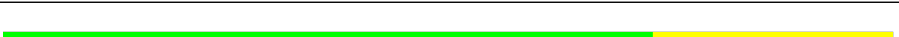


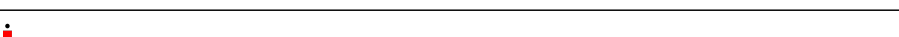
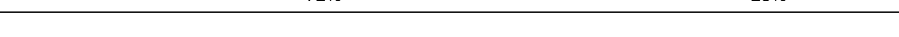
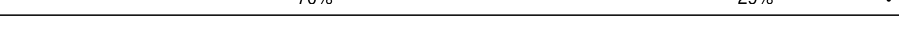



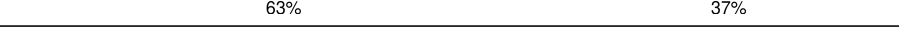





*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	EF	129	
1	EG	129	
1	EH	129	
1	EI	129	
1	EJ	129	
1	EK	129	
1	EL	129	
1	EM	129	
1	EN	129	
1	EO	129	
1	EP	129	
1	EQ	129	
1	ER	129	
1	ES	129	
1	ET	129	
1	EU	129	
1	EV	129	
1	EW	129	
1	EX	129	
1	EY	129	
1	EZ	129	
1	FA	129	
1	FB	129	
1	FC	129	
1	FD	129	

*Continued on next page...*












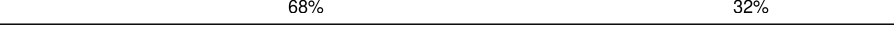







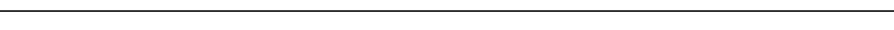

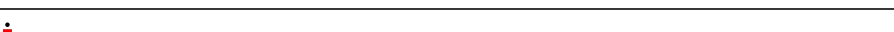
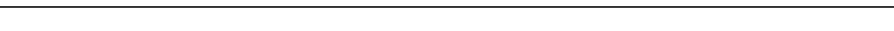


Continued from previous page...

Mol	Chain	Length	Quality of chain
1	FE	129	
1	FF	129	
1	FG	129	
1	FH	129	
1	FI	129	
1	FJ	129	
1	FK	129	
1	FL	129	
1	FM	129	
1	FN	129	
1	FO	129	
1	FP	129	
1	FQ	129	
1	FR	129	
1	FS	129	
1	FT	129	
1	FU	129	
1	FV	129	
1	FW	129	
1	FX	129	
1	FY	129	
1	FZ	129	
1	GA	129	
1	GB	129	
1	GC	129	

Continued on next page...













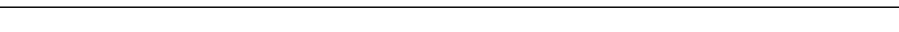

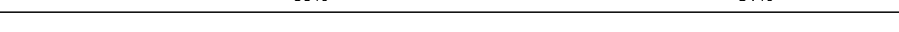

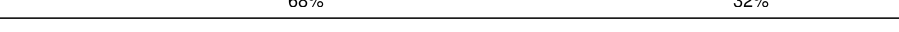










Continued from previous page...

Mol	Chain	Length	Quality of chain
1	GD	129	
1	GE	129	
1	GF	129	
1	GG	129	
1	GH	129	
1	GI	129	
1	GK	129	
1	GL	129	
1	GM	129	
1	GN	129	
1	GO	129	
1	GP	129	
1	GQ	129	
1	GR	129	
1	GS	129	
1	GT	129	
1	GU	129	
1	GV	129	
1	GW	129	
1	GX	129	
1	GY	129	
1	GZ	129	
1	HA	129	
1	HB	129	
1	HC	129	



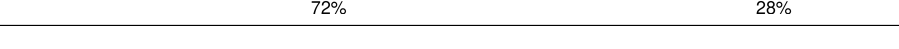
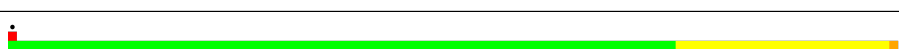



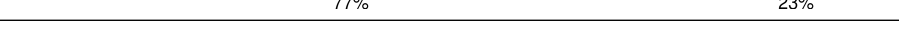



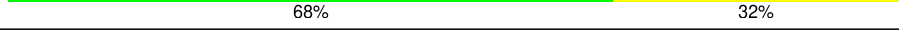

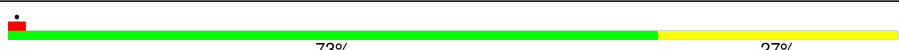


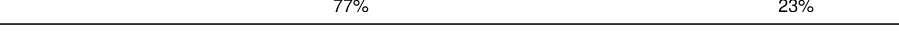







Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	HD	129	
1	HE	129	
1	HF	129	
1	HG	129	
1	HI	129	
1	HJ	129	
1	HK	129	
1	HL	129	
1	HM	129	
1	HN	129	
1	HO	129	
1	HP	129	
1	HQ	129	
1	HR	129	
1	HS	129	
1	HT	129	
1	HU	129	
1	HV	129	
1	HW	129	
1	HX	129	
1	HY	129	
1	HZ	129	
1	IA	129	
1	IB	129	
1	IC	129	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	ID	129	
1	IE	129	
1	IF	129	
1	IG	129	
1	IH	129	
1	II	129	
1	IJ	129	
1	IK	129	
1	IL	129	
1	IM	129	
1	IN	129	
1	IO	129	
1	IP	129	
1	IQ	129	
1	IR	129	
1	IS	129	
1	IT	129	
1	IU	129	
1	IV	129	
1	IW	129	
1	IX	129	
1	IZ	129	
1	JA	129	
1	JB	129	
1	JC	129	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	JD	129	 71%29%
1	JE	129	 73%27%
1	JF	129	 66%34%
1	JG	129	 77%23%
1	JH	129	 74%26%
1	JI	129	 71%29%
1	JJ	129	 71%29%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 232320 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 Coat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AB	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AC	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AD	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AE	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AF	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AG	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AH	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AI	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AJ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AK	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AL	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AM	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AN	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AO	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AP	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AQ	129	Total 968	C 602	N 171	O 191	S 4	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AR	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AS	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AT	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AU	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AV	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AW	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AX	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AY	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	AZ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BA	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BB	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BC	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BD	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BE	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BF	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BG	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BH	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BI	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BJ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BK	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BL	129	Total 968	C 602	N 171	O 191	S 4	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BM	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BN	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BO	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BP	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BQ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BR	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BS	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BT	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BU	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BV	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BW	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BX	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BY	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	BZ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CA	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CB	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CC	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CD	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CE	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CF	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CG	129	Total 968	C 602	N 171	O 191	S 4	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
1	CH	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CI	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CJ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CK	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CL	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CM	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CN	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CO	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CP	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CQ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CR	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CS	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CT	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CU	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CV	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CW	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CX	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CY	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	CZ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DA	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DB	129	Total 968	C 602	N 171	O 191	S 4	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
1	DC	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DE	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DF	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DG	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DH	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DI	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DJ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DK	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DL	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DM	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DN	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DO	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DP	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DQ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DR	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DS	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DT	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DU	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DV	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DW	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DX	129	Total 968	C 602	N 171	O 191	S 4	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
1	DY	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	DZ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EA	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EB	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EC	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	ED	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EE	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EF	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EG	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EH	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EI	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EJ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EK	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EL	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EM	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EN	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EO	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EP	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EQ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	ER	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	ES	129	Total 968	C 602	N 171	O 191	S 4	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
1	ET	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EU	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EV	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EW	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EX	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EY	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	EZ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FA	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FB	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FC	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FD	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FE	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FF	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FG	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FH	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FI	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FJ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FK	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FL	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FM	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FN	129	Total 968	C 602	N 171	O 191	S 4	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
1	FO	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FP	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FQ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FR	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FS	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FT	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FU	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FV	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FW	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FX	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FY	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	FZ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GA	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GB	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GC	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GD	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GE	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GF	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GG	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GH	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GI	129	Total 968	C 602	N 171	O 191	S 4	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
1	GK	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GL	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GM	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GN	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GO	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GP	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GQ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GR	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GS	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GT	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GU	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GV	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GW	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GX	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GY	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	GZ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HA	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HB	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HC	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HD	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HE	129	Total 968	C 602	N 171	O 191	S 4	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
1	HF	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HG	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HI	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HJ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HK	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HL	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HM	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HN	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HO	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HP	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HQ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HR	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HS	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HT	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HU	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HV	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HW	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HX	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HY	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	HZ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	IA	129	Total 968	C 602	N 171	O 191	S 4	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
1	IB	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	IC	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	ID	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	IE	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	IF	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	IG	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	IH	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	II	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	IJ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	IK	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	IL	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	IM	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	IN	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	IO	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	IP	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	IQ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	IR	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	IS	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	IT	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	IU	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	IV	129	Total 968	C 602	N 171	O 191	S 4	0	0

*Continued on next page...*

*Continued from previous page...*


Mol	Chain	Residues	Atoms					AltConf	Trace
1	IW	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	IX	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	IZ	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	JA	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	JB	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	JC	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	JD	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	JE	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	JF	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	JG	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	JH	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	JI	129	Total 968	C 602	N 171	O 191	S 4	0	0
1	JJ	129	Total 968	C 602	N 171	O 191	S 4	0	0

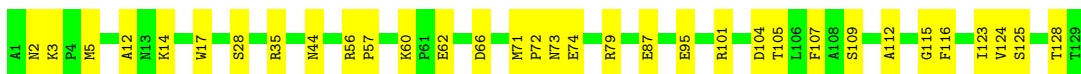


### 3 Residue-property plots

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

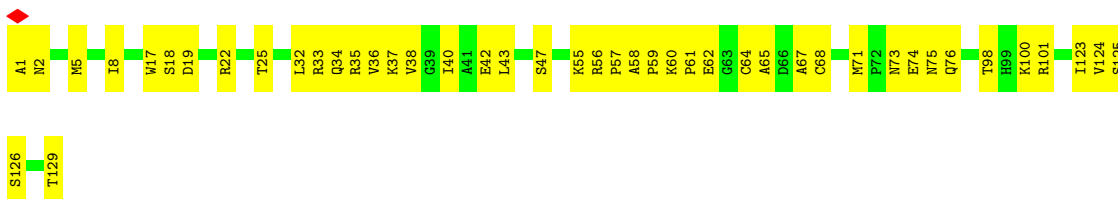
- Molecule 1: Coat protein

Chain AA:  74% 26%




- Molecule 1: Coat protein

Chain AB:  65% 35%



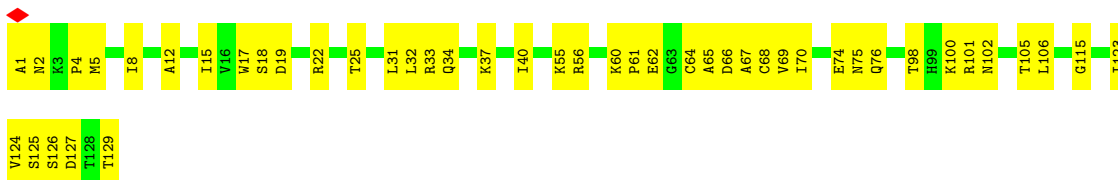
- Molecule 1: Coat protein

Chain AC:  77% 23%



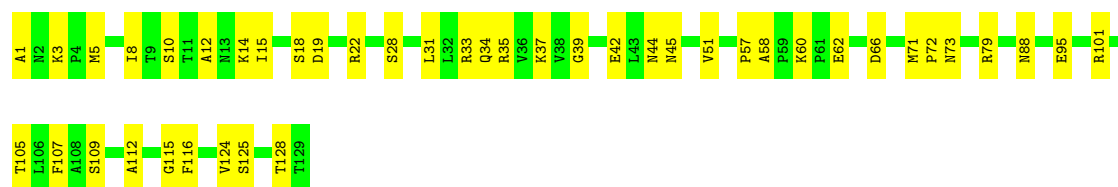
- Molecule 1: Coat protein

Chain AD:  64% 36%



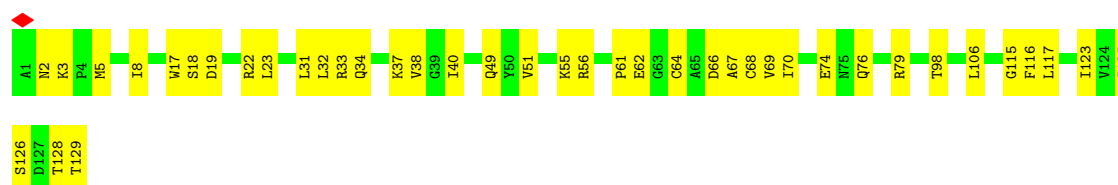
- Molecule 1: Coat protein

Chain AE:  67% 33%




- Molecule 1: Coat protein

Chain AF:  68% 32%



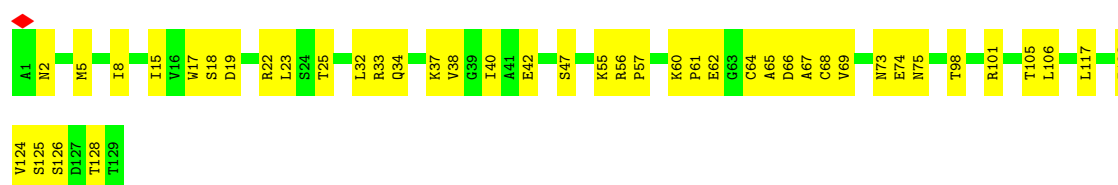
- Molecule 1: Coat protein

Chain AG:  78% 22%



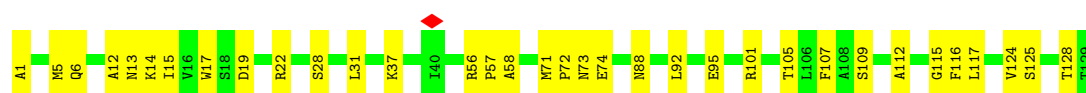
- Molecule 1: Coat protein

Chain AH:  67% 33%



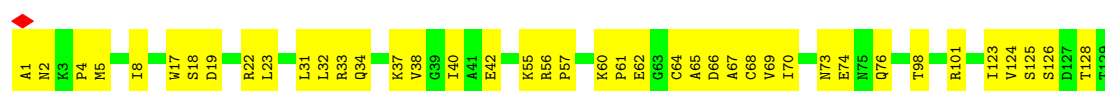
- Molecule 1: Coat protein

Chain AI:  74% 26%




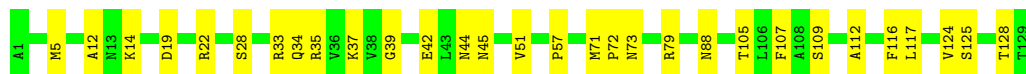
- Molecule 1: Coat protein

Chain AJ:  68% 32%



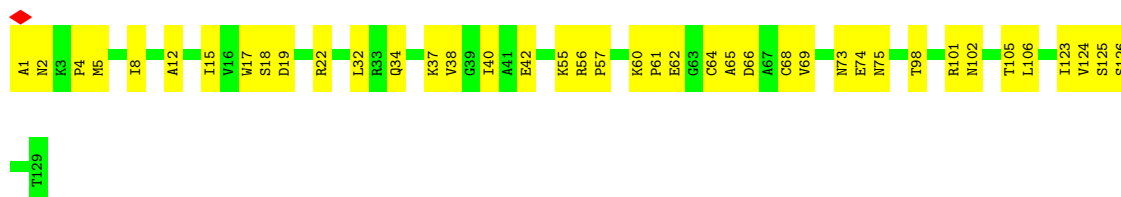
- Molecule 1: Coat protein

Chain AK:  77% 23%



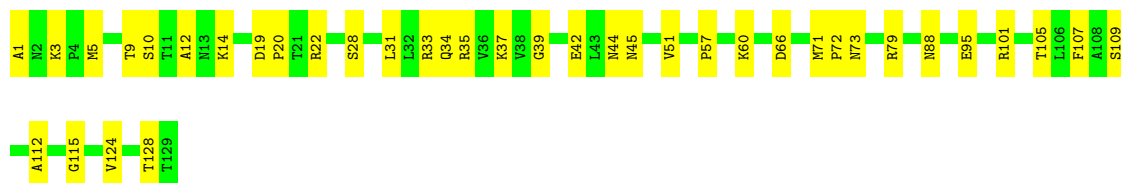
- Molecule 1: Coat protein

Chain AL:  69% 31%



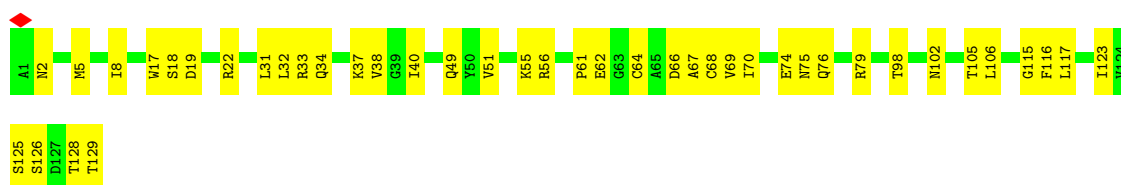
- Molecule 1: Coat protein

Chain AM:  71% 29%




- Molecule 1: Coat protein

Chain AN:  67% 33%



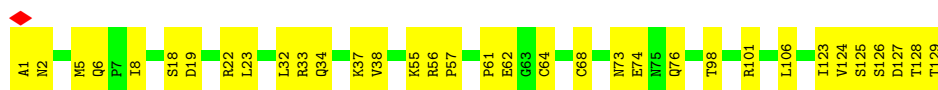
- Molecule 1: Coat protein

Chain AO:  75% 25%

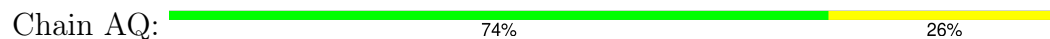


- Molecule 1: Coat protein

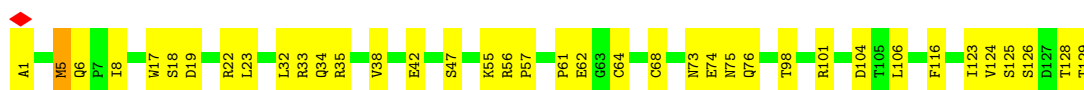
Chain AP:  74% 26%



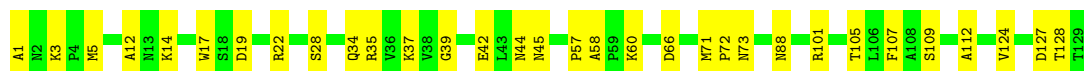
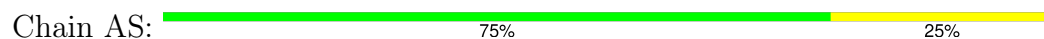
- Molecule 1: Coat protein



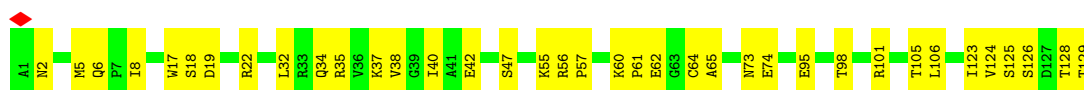
- Molecule 1: Coat protein



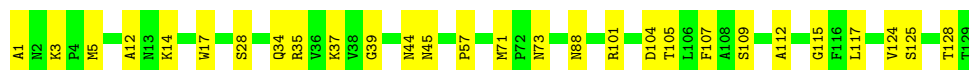
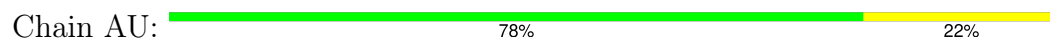
- Molecule 1: Coat protein



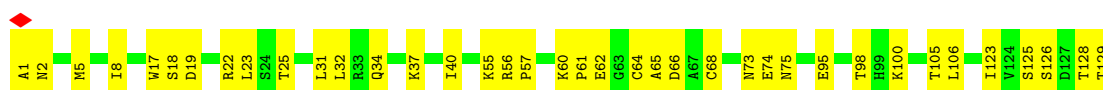
- Molecule 1: Coat protein




- Molecule 1: Coat protein



- Molecule 1: Coat protein



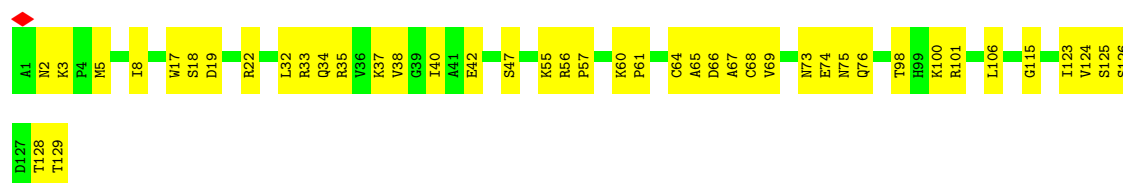
- Molecule 1: Coat protein

Chain AW:  77% 23%



- Molecule 1: Coat protein

Chain AX:  67% 33%



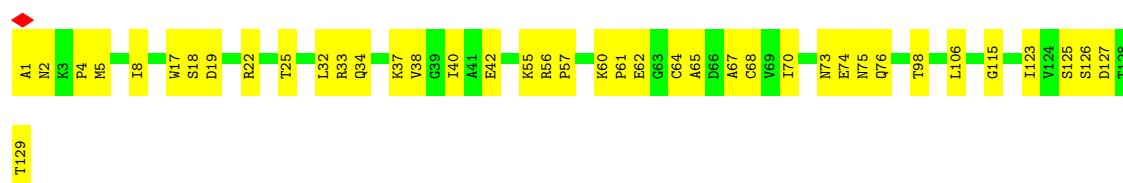
- Molecule 1: Coat protein

Chain AY:  74% 26%




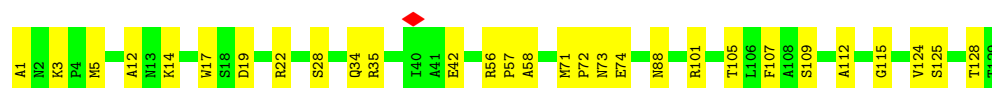
- Molecule 1: Coat protein

Chain AZ:  69% 31%



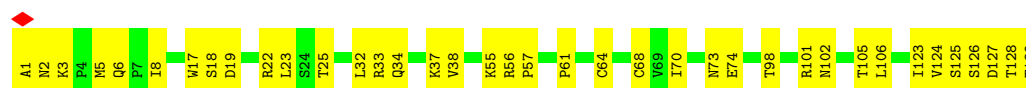
- Molecule 1: Coat protein

Chain BA:  78% 22%



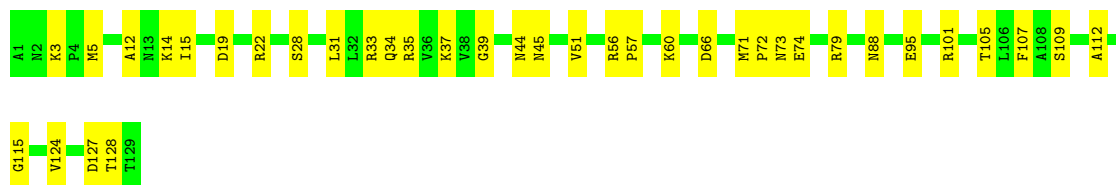
- Molecule 1: Coat protein

Chain BB:  71% 29%



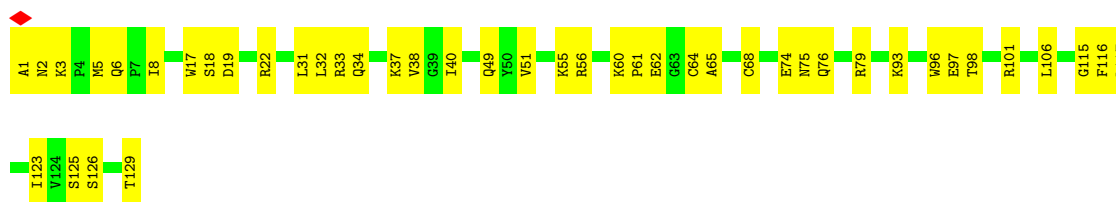
- Molecule 1: Coat protein

Chain BC:  71% 29%




- Molecule 1: Coat protein

Chain BD:  66% 34%



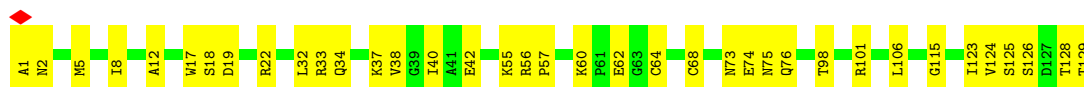
- Molecule 1: Coat protein

Chain BE:  77% 23%



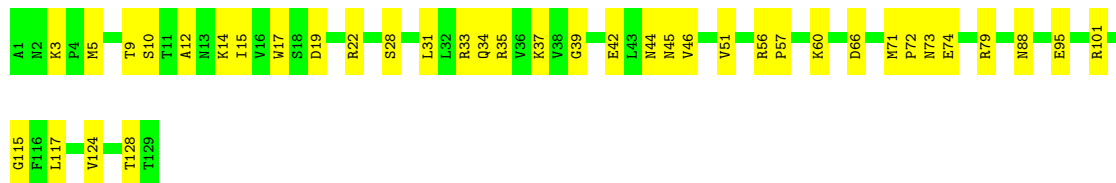
- Molecule 1: Coat protein

Chain BF:  71% 29%



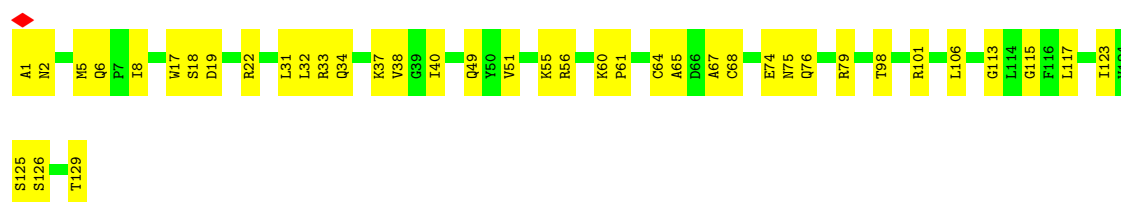
- Molecule 1: Coat protein

Chain BG:  71% 29%



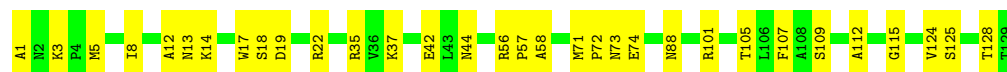
- Molecule 1: Coat protein

Chain BH:  69% 31%



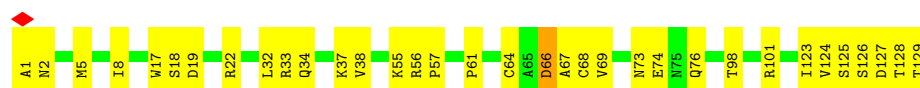
- Molecule 1: Coat protein

Chain BI: 75% 25%



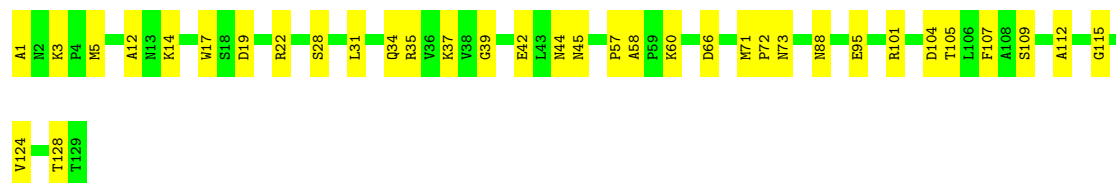
- Molecule 1: Coat protein

Chain BJ: 74% 26%



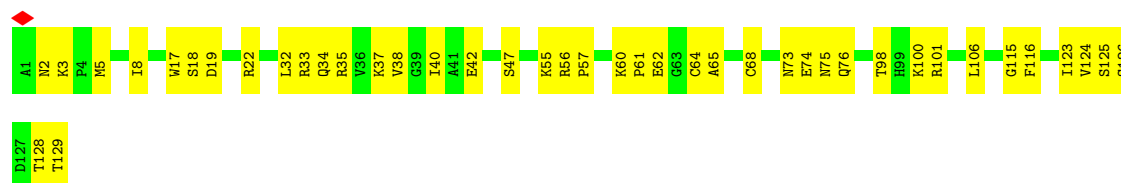
- Molecule 1: Coat protein

Chain BK: 73% 27%



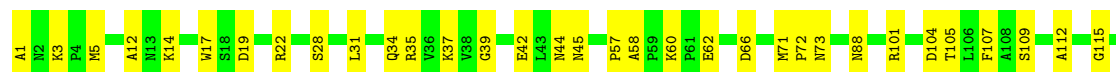
- Molecule 1: Coat protein

Chain BL: 67% 33%



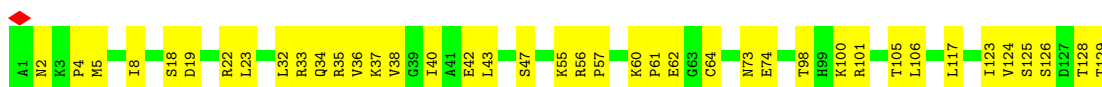
- Molecule 1: Coat protein

Chain BM: 71% 29%

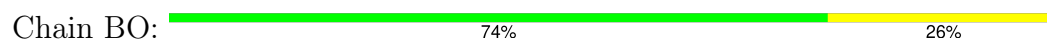




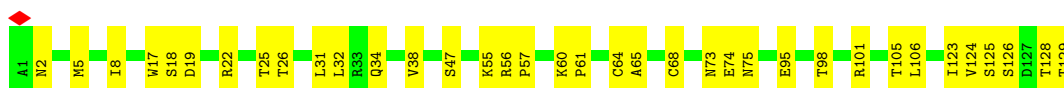
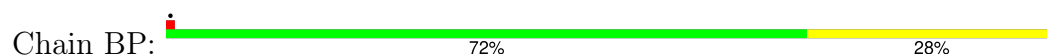
- Molecule 1: Coat protein



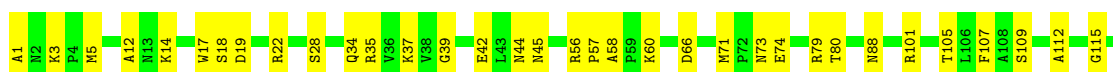
- Molecule 1: Coat protein



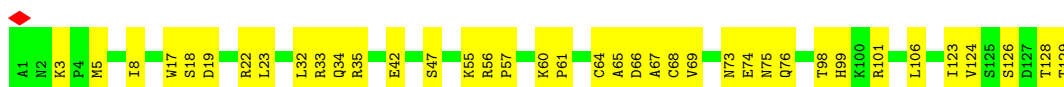
- Molecule 1: Coat protein



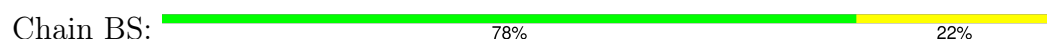
- Molecule 1: Coat protein



- Molecule 1: Coat protein



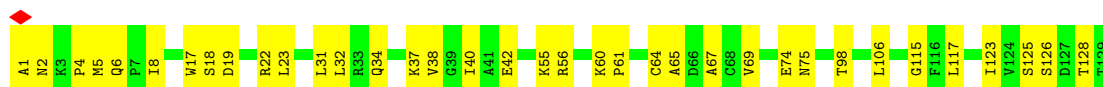
- Molecule 1: Coat protein



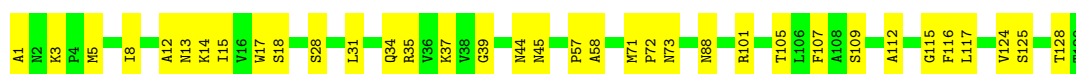




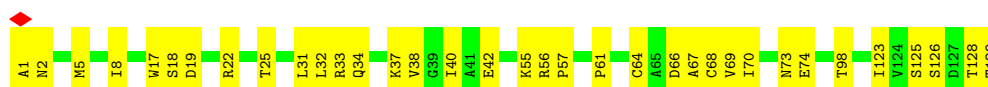
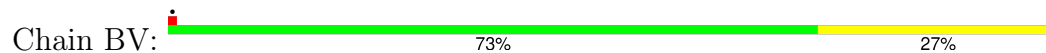
- Molecule 1: Coat protein



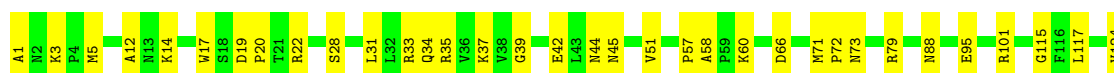
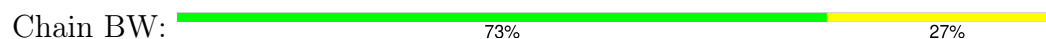
- Molecule 1: Coat protein



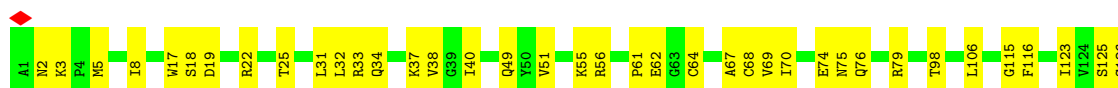
- Molecule 1: Coat protein



- Molecule 1: Coat protein

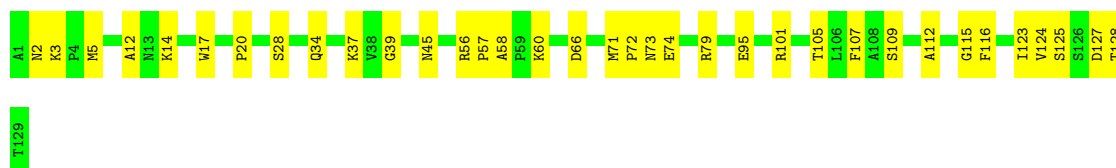


- Molecule 1: Coat protein

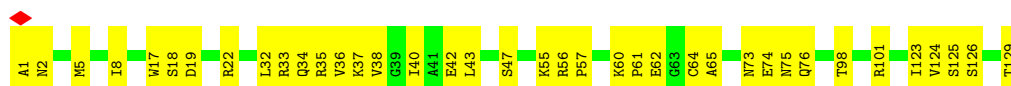


- Molecule 1: Coat protein





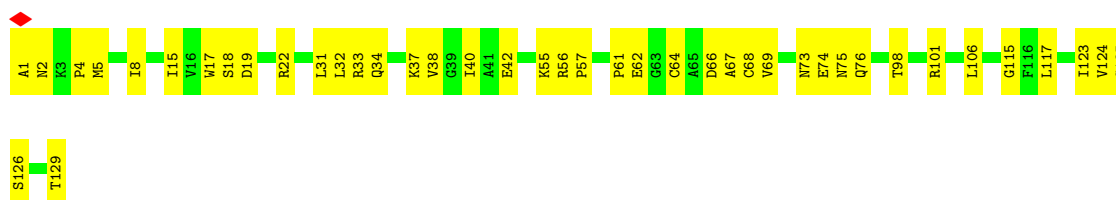
- Molecule 1: Coat protein



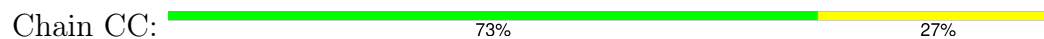
- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein

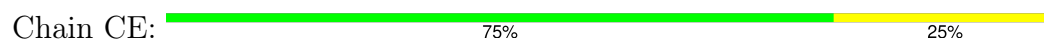


- Molecule 1: Coat protein

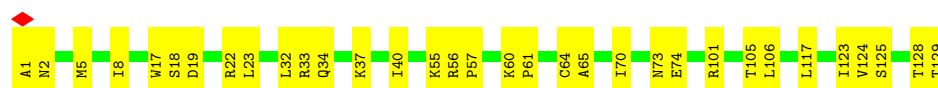




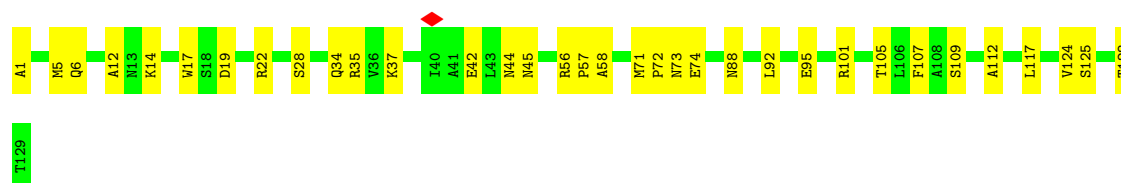
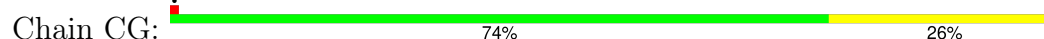
- Molecule 1: Coat protein



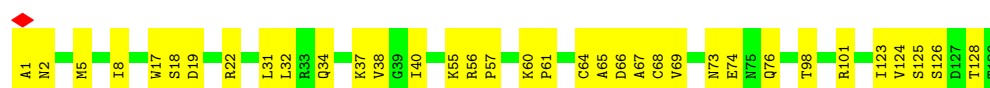
- Molecule 1: Coat protein



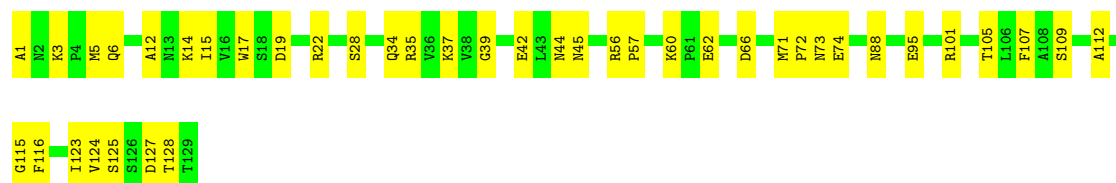
- Molecule 1: Coat protein



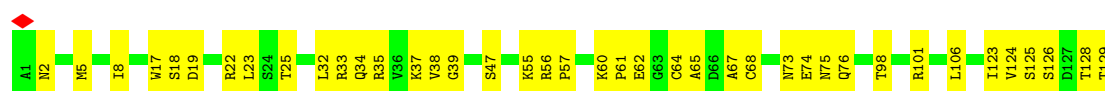
- Molecule 1: Coat protein



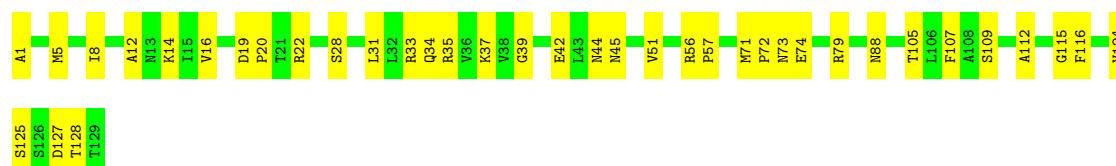
- Molecule 1: Coat protein



- Molecule 1: Coat protein



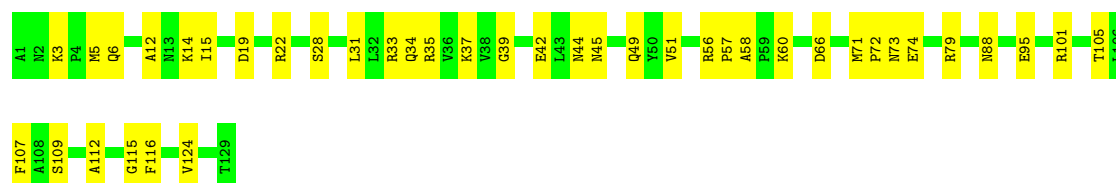
- Molecule 1: Coat protein



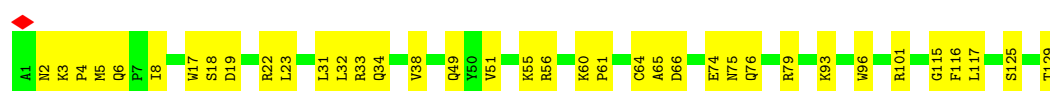
- Molecule 1: Coat protein



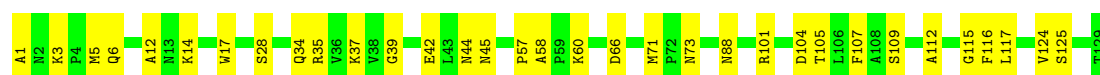
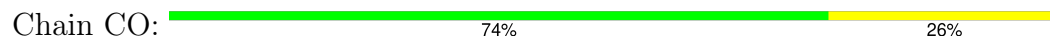
- Molecule 1: Coat protein



- Molecule 1: Coat protein



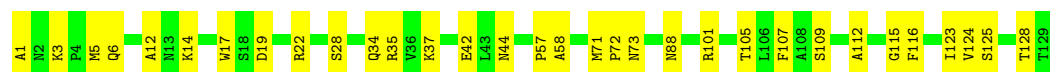
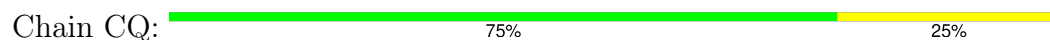
- Molecule 1: Coat protein



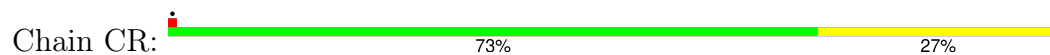
- Molecule 1: Coat protein



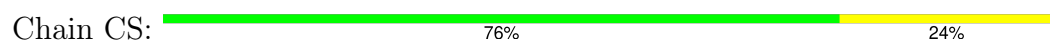
- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein

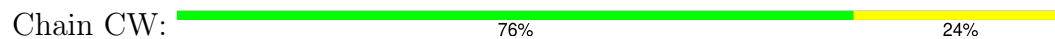


- Molecule 1: Coat protein

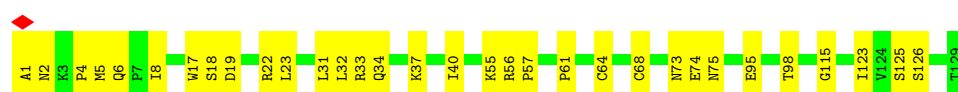
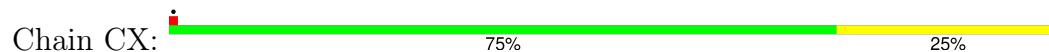




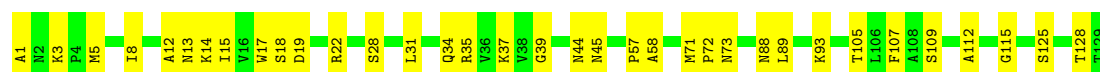
- Molecule 1: Coat protein



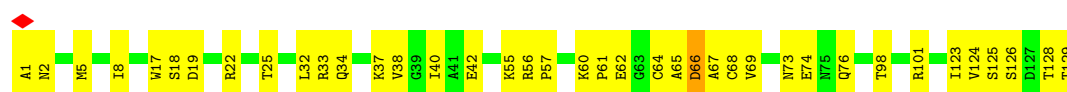
- Molecule 1: Coat protein



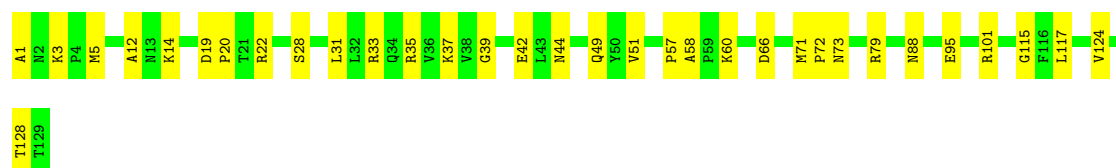
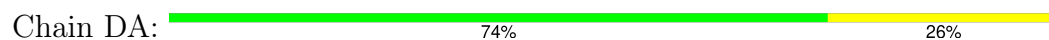
- Molecule 1: Coat protein



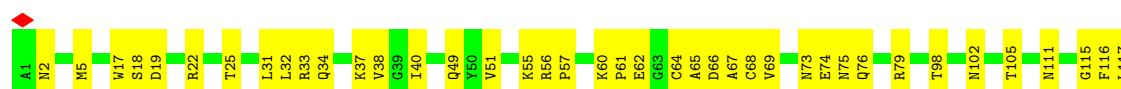
- Molecule 1: Coat protein



- Molecule 1: Coat protein



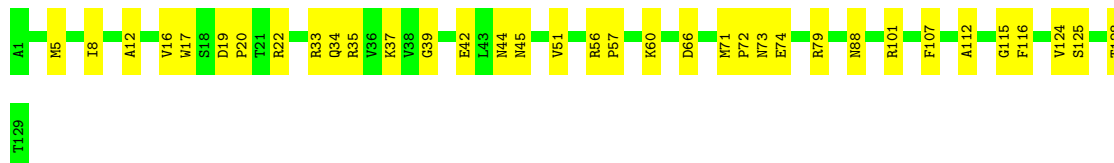
- Molecule 1: Coat protein





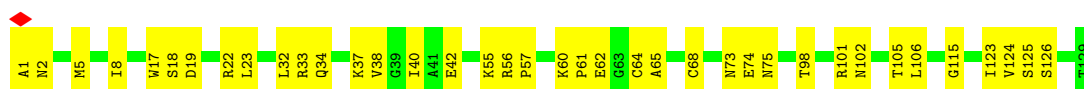
- Molecule 1: Coat protein

Chain DC: 73% 27%



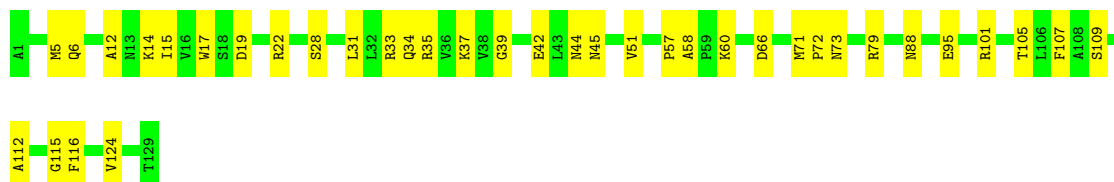
- Molecule 1: Coat protein

Chain DE: 71% 29%



- Molecule 1: Coat protein

Chain DF: 71% 29%



- Molecule 1: Coat protein

Chain DG: 69% 31%



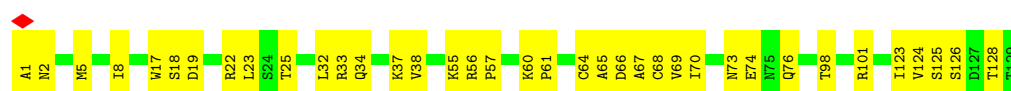
- Molecule 1: Coat protein

Chain DH: 76% 24%



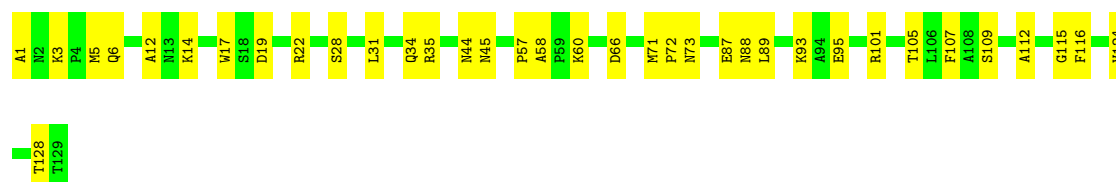
- Molecule 1: Coat protein

Chain DI:  71% 29%




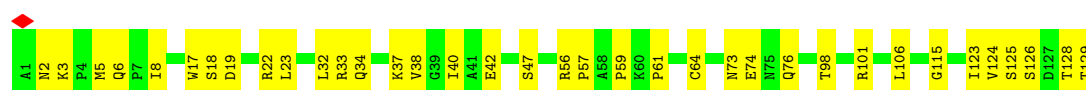
- Molecule 1: Coat protein

Chain DJ:  72% 28%




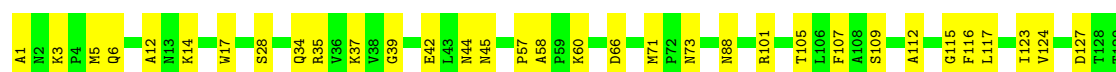
- Molecule 1: Coat protein

Chain DK:  72% 28%




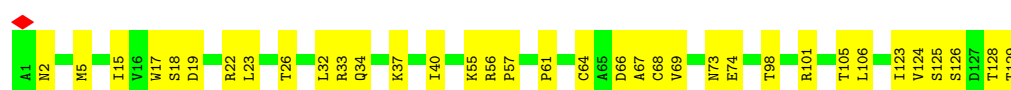
- Molecule 1: Coat protein

Chain DL:  74% 26%



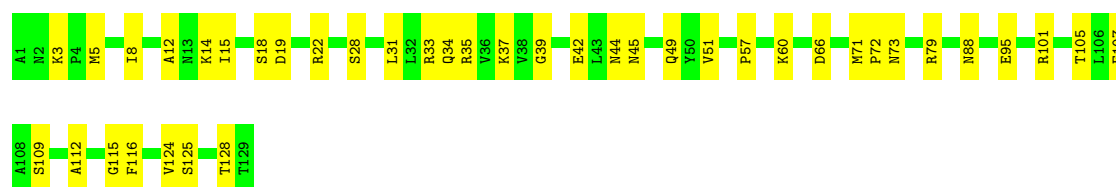
- Molecule 1: Coat protein

Chain DM:  73% 27%



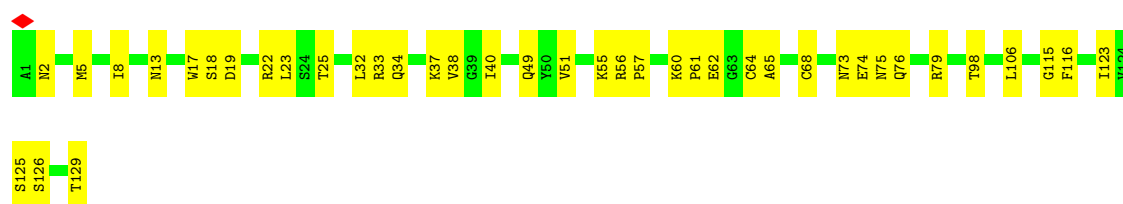
- Molecule 1: Coat protein

Chain DN:  69% 31%

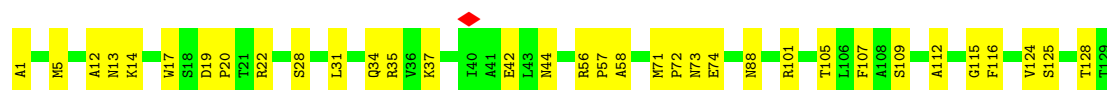


- Molecule 1: Coat protein

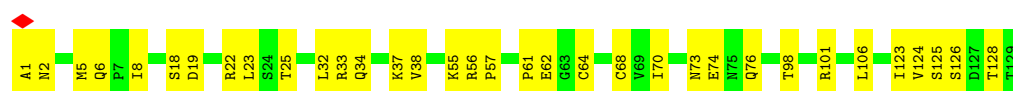
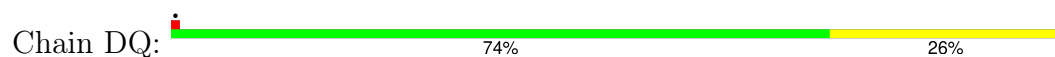




- Molecule 1: Coat protein



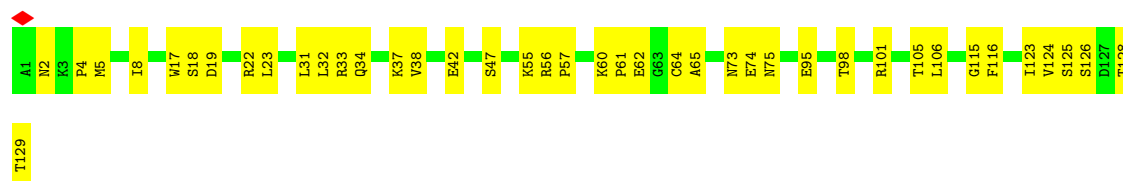
- Molecule 1: Coat protein



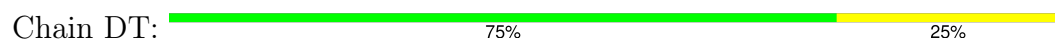
- Molecule 1: Coat protein



- Molecule 1: Coat protein

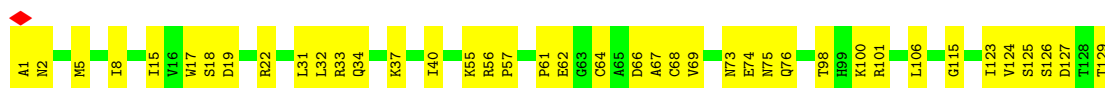


- Molecule 1: Coat protein

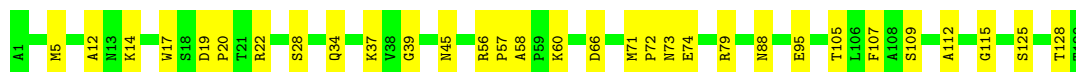
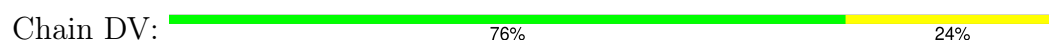




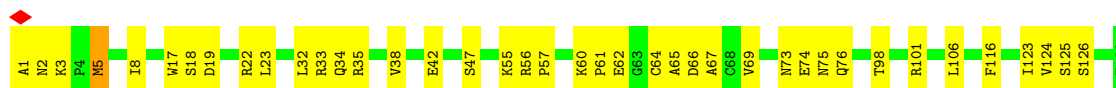
- Molecule 1: Coat protein



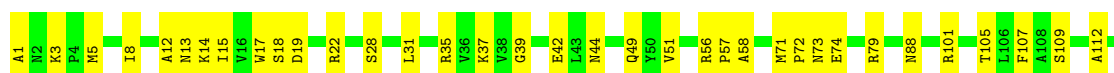
- Molecule 1: Coat protein



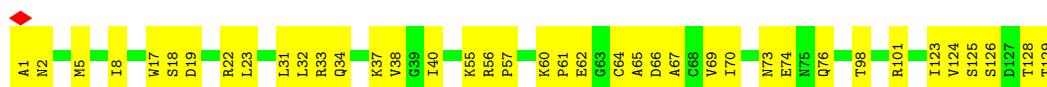
- Molecule 1: Coat protein



- Molecule 1: Coat protein

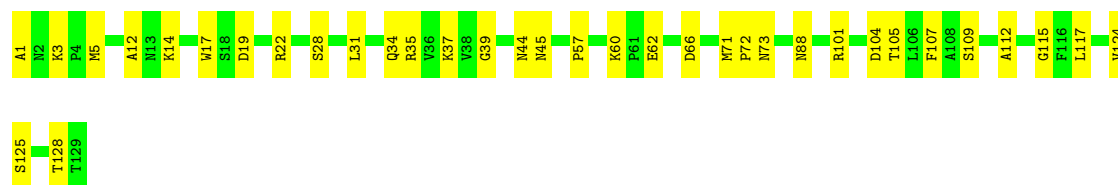


- Molecule 1: Coat protein

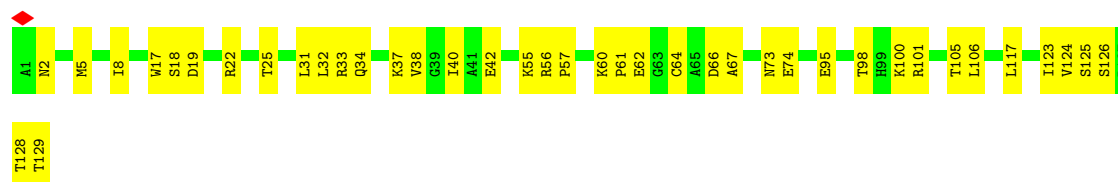


- Molecule 1: Coat protein

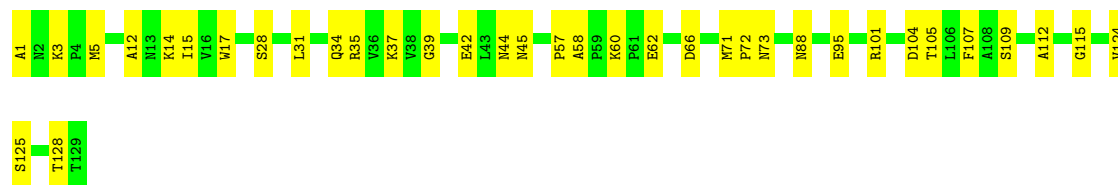




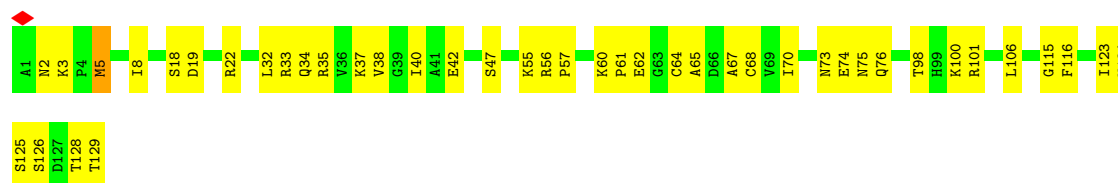
- Molecule 1: Coat protein



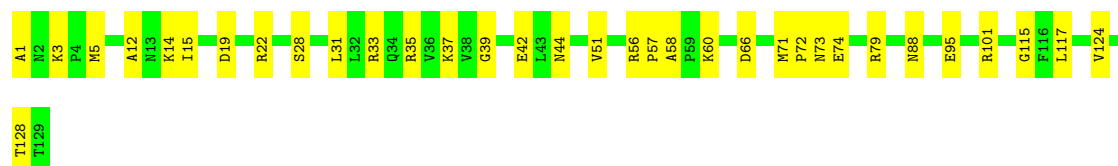
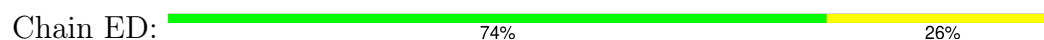
- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein





- Molecule 1: Coat protein

Chain EF: 77% 23%



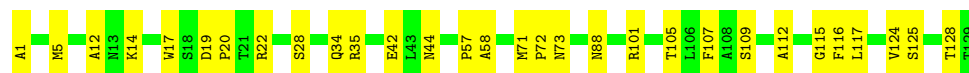
- Molecule 1: Coat protein

Chain EG: 69% 31%



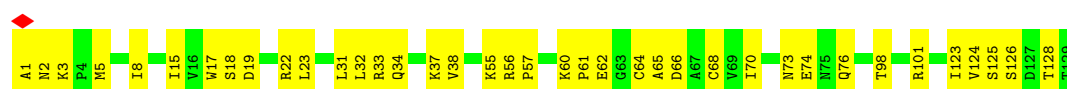
- Molecule 1: Coat protein

Chain EH: 77% 23%



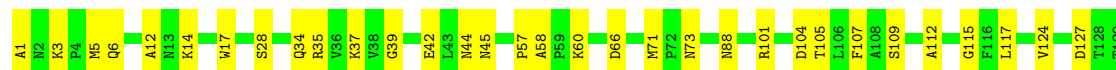
- Molecule 1: Coat protein

Chain EI: 71% 29%



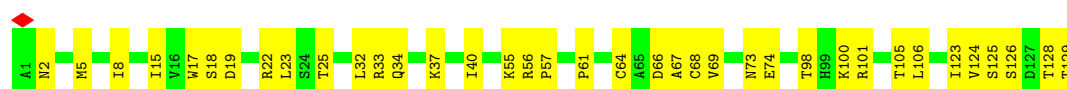
- Molecule 1: Coat protein

Chain EJ: 75% 25%

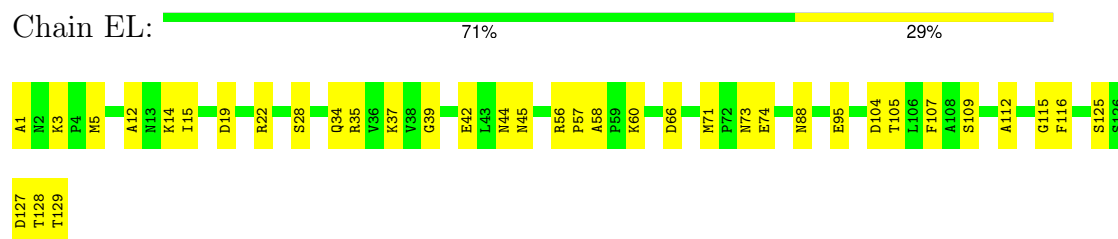


- Molecule 1: Coat protein

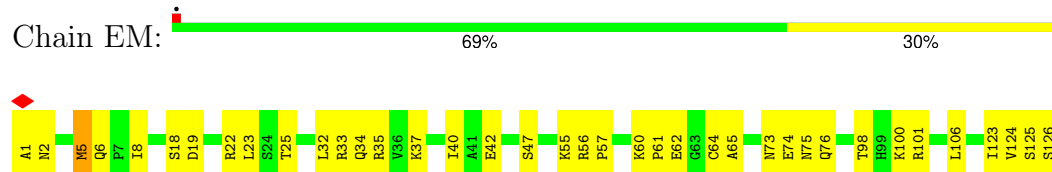
Chain EK: 71% 29%



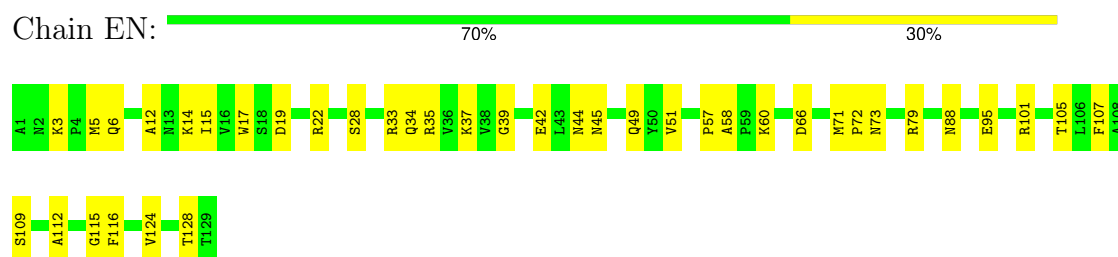
- Molecule 1: Coat protein



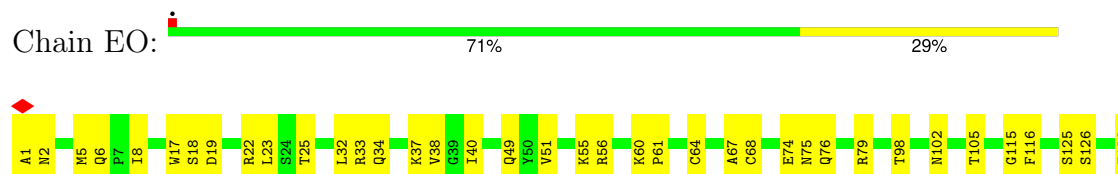
- Molecule 1: Coat protein



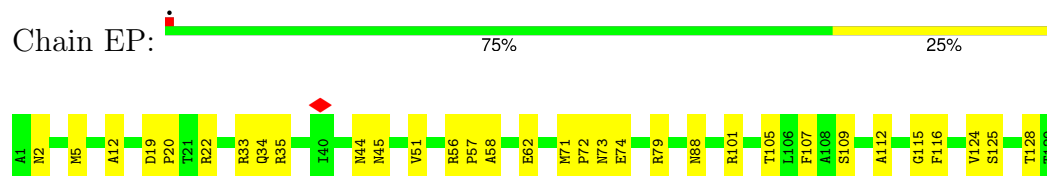
- Molecule 1: Coat protein



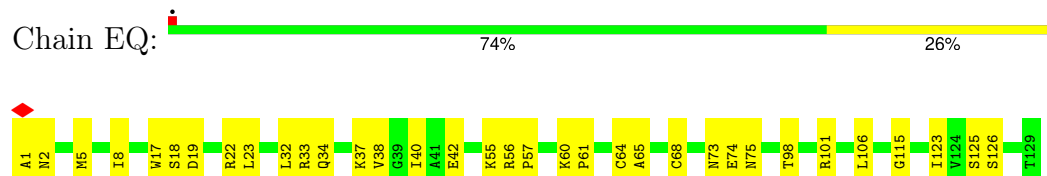
- Molecule 1: Coat protein



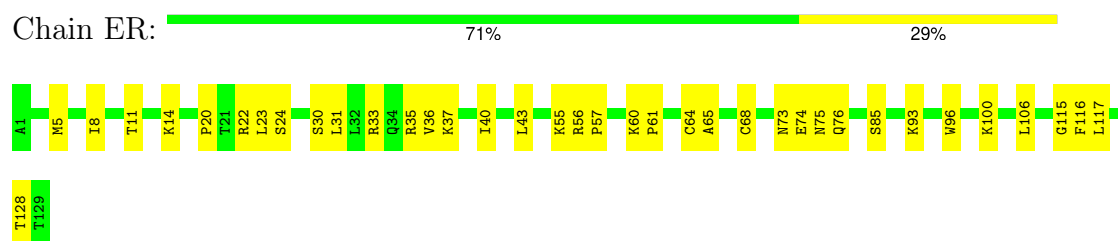
- Molecule 1: Coat protein



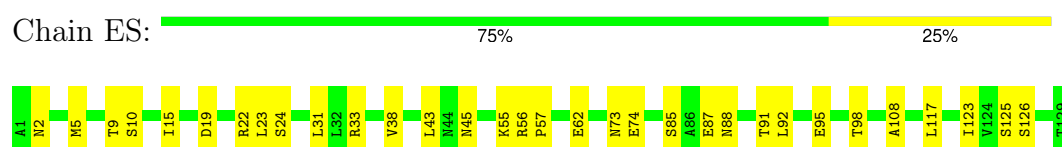
- Molecule 1: Coat protein



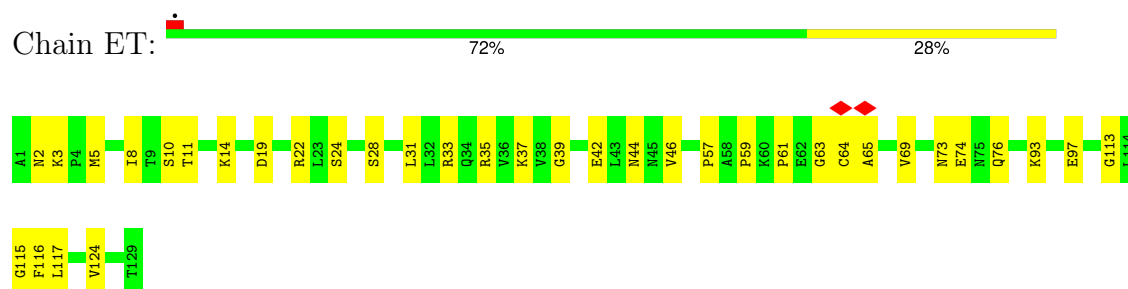
- Molecule 1: Coat protein



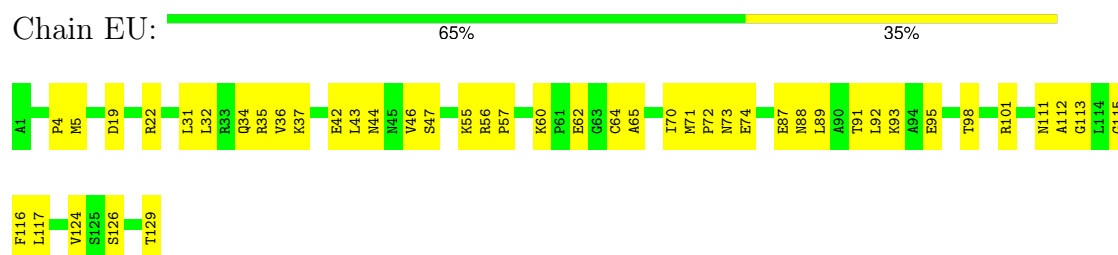
- Molecule 1: Coat protein



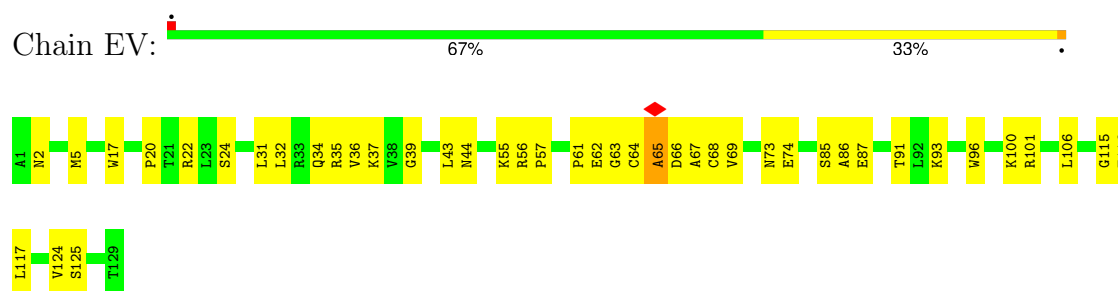
- Molecule 1: Coat protein



- Molecule 1: Coat protein

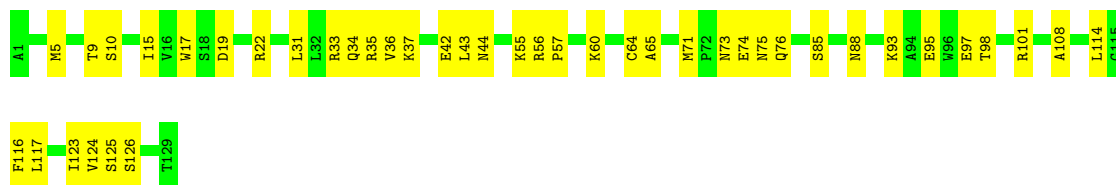


- Molecule 1: Coat protein



- Molecule 1: Coat protein

Chain EW:  67% 33%




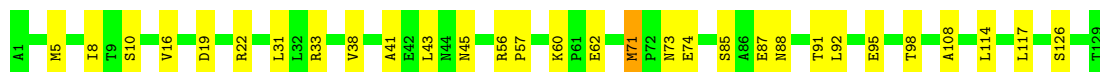
- Molecule 1: Coat protein

Chain EX:  72% 28%



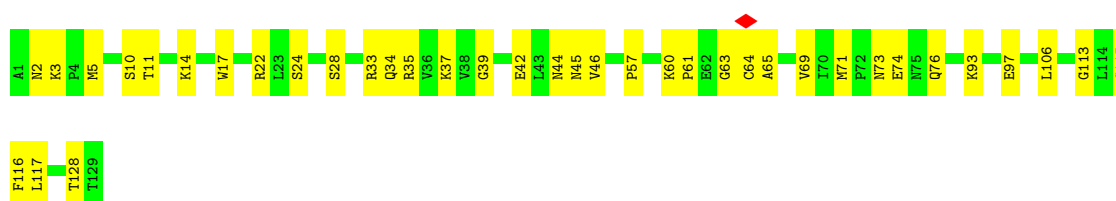
- Molecule 1: Coat protein

Chain EY:  77% 22%



- Molecule 1: Coat protein

Chain EZ:  71% 29%



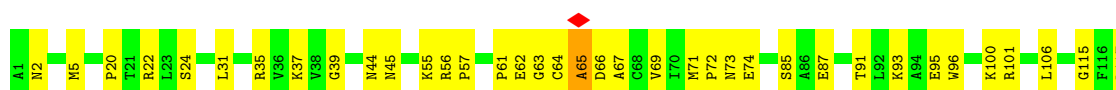
- Molecule 1: Coat protein

Chain FA:  71% 29%



- Molecule 1: Coat protein

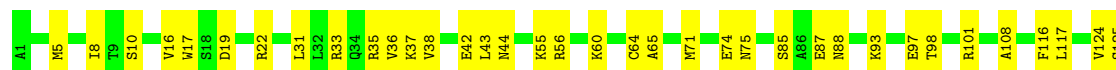
Chain FB:  70% 29%





- Molecule 1: Coat protein

Chain FC: 71% 29%



- Molecule 1: Coat protein

Chain FD: 72% 28%



- Molecule 1: Coat protein

Chain FE: 80% 19%



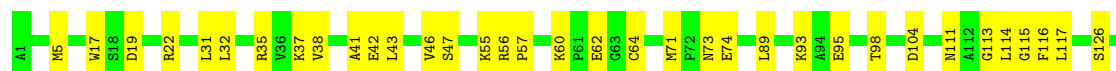
- Molecule 1: Coat protein

Chain FF: 71% 28%



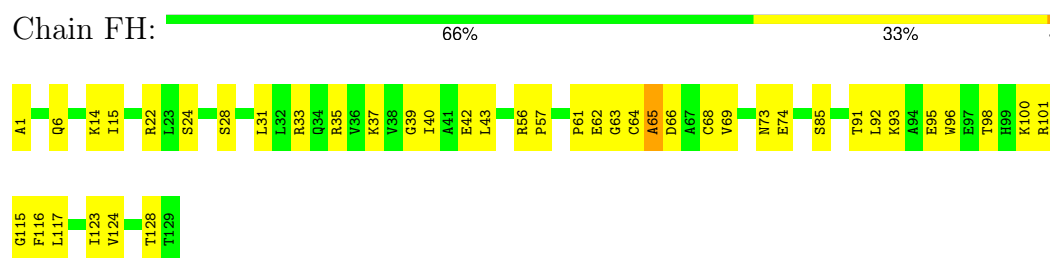
- Molecule 1: Coat protein

Chain FG: 73% 27%

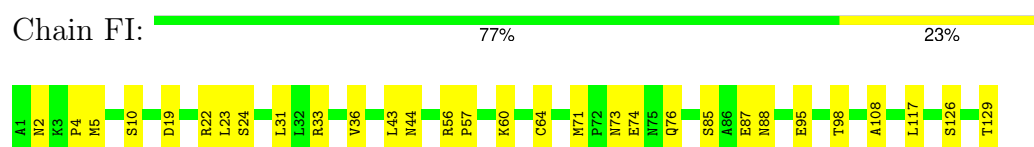




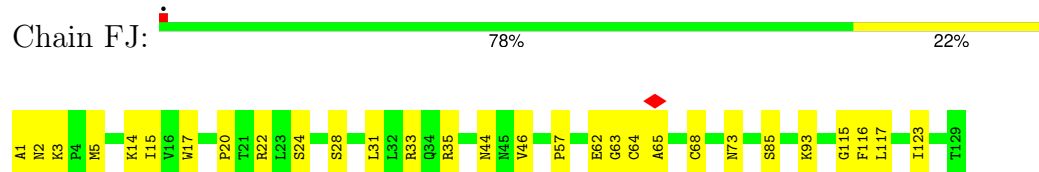
- Molecule 1: Coat protein



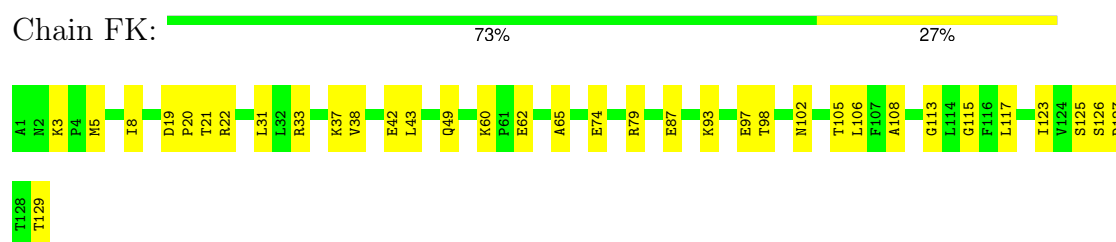
- Molecule 1: Coat protein



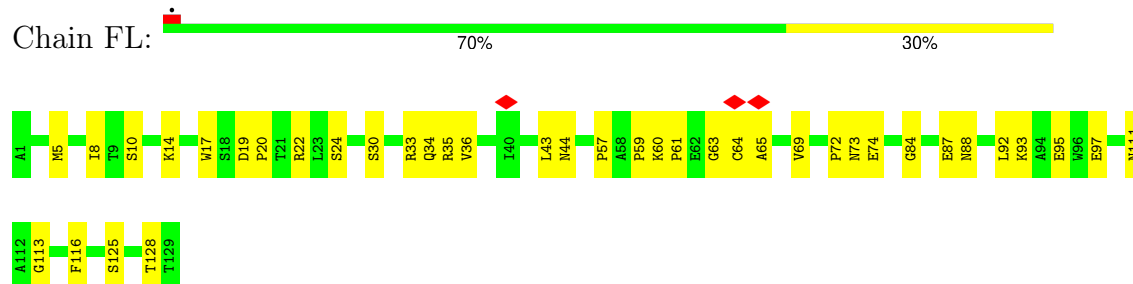
- Molecule 1: Coat protein



- Molecule 1: Coat protein

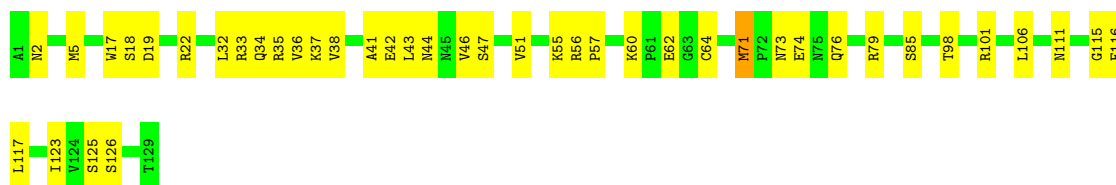


- Molecule 1: Coat protein



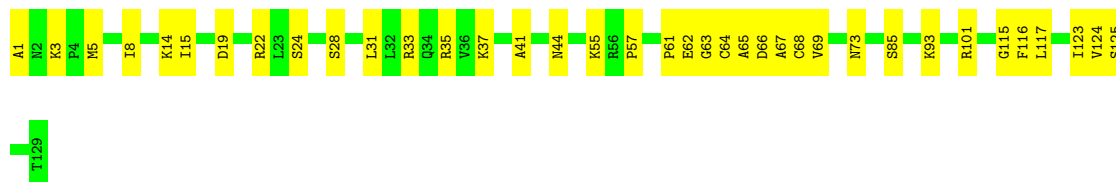
- Molecule 1: Coat protein





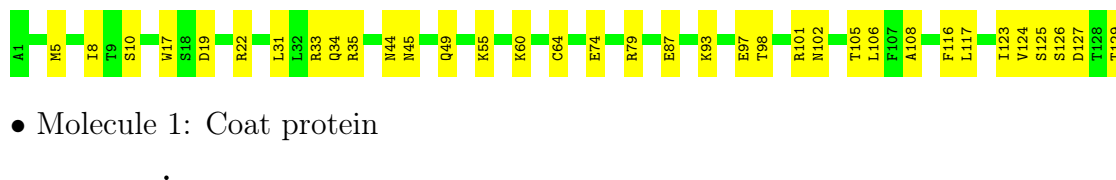
- Molecule 1: Coat protein

Chain FN: 71% 29%



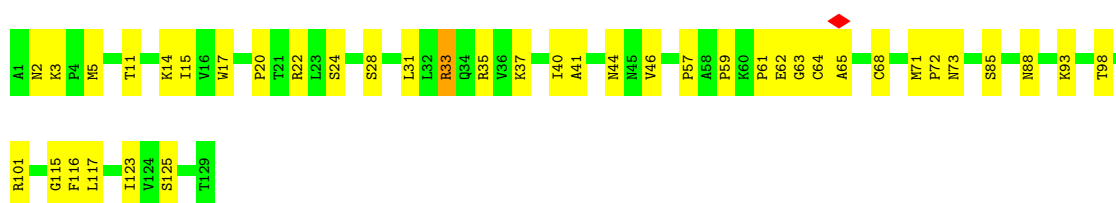
- Molecule 1: Coat protein

Chain FO: 73% 27%



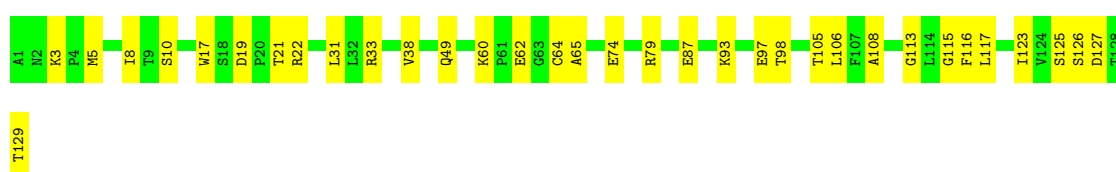
- Molecule 1: Coat protein

Chain FP: 69% 30%



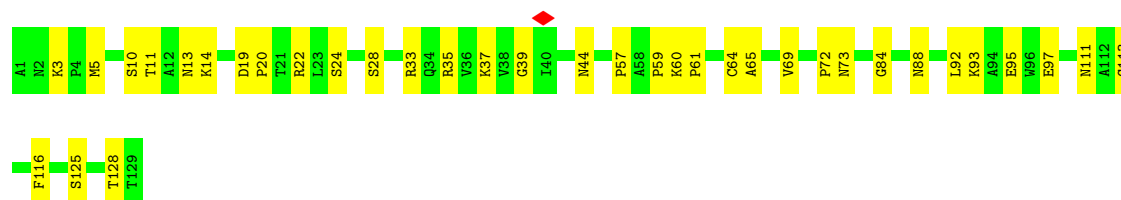
- Molecule 1: Coat protein

Chain FQ: 74% 26%



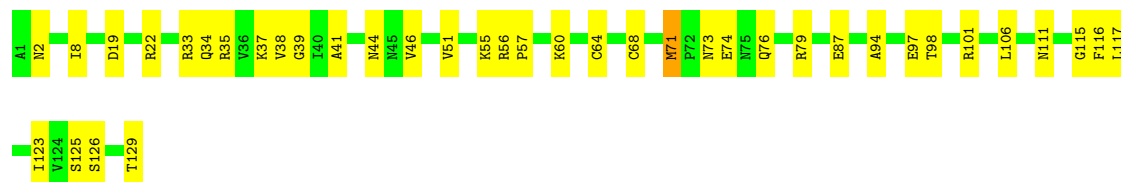
- Molecule 1: Coat protein

Chain FR: 72% 28%



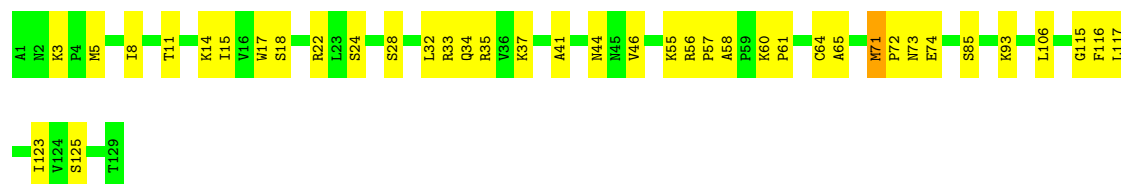
- Molecule 1: Coat protein

Chain FS: 70% 29% .



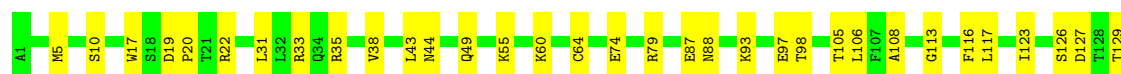
- Molecule 1: Coat protein

Chain FT: 70% 29% .



- Molecule 1: Coat protein

Chain FU: 74% 26%



- Molecule 1: Coat protein

Chain FV: 74% 26%



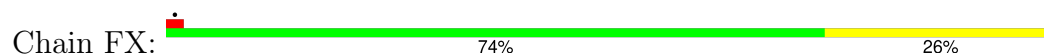
- Molecule 1: Coat protein

Chain FW: 63% 37%

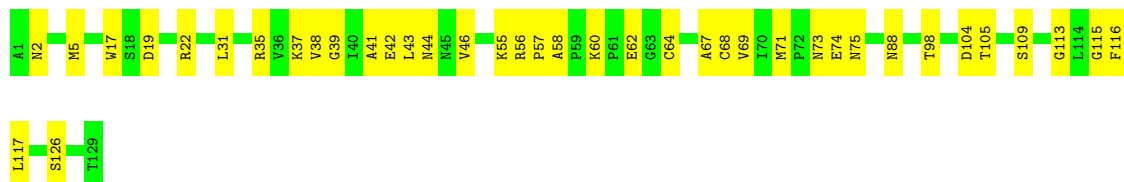




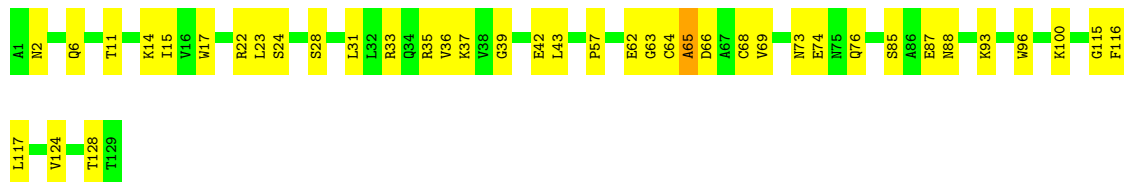
- Molecule 1: Coat protein



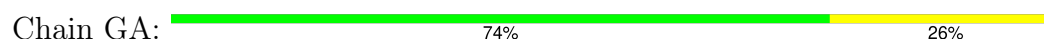
- Molecule 1: Coat protein



- Molecule 1: Coat protein




- Molecule 1: Coat protein



- Molecule 1: Coat protein




- Molecule 1: Coat protein

Chain GC:  84% 16%



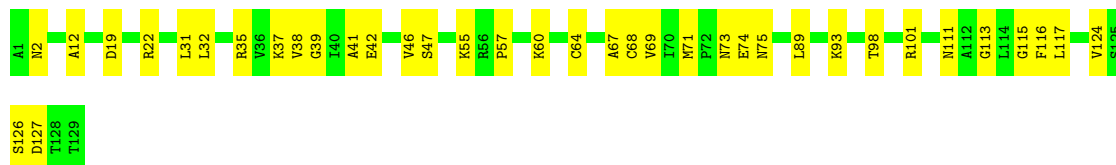
- Molecule 1: Coat protein

Chain GD:  74% 26%



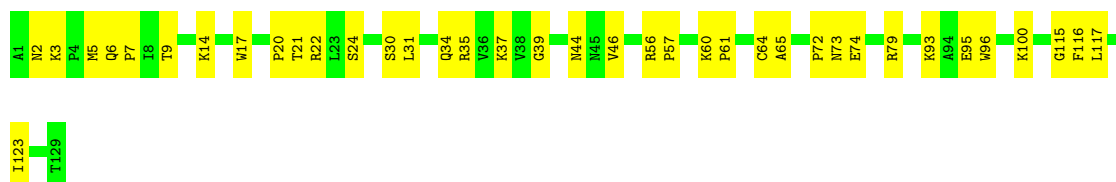
- Molecule 1: Coat protein

Chain GE:  71% 29%



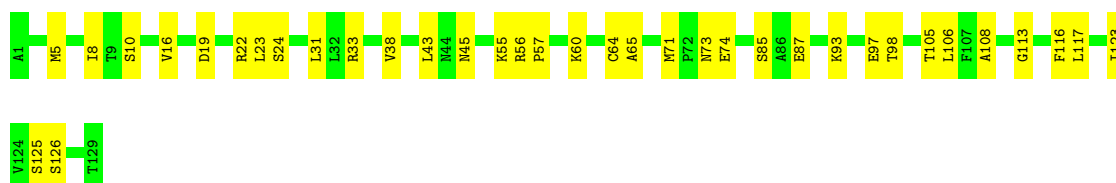
- Molecule 1: Coat protein

Chain GF:  71% 29%




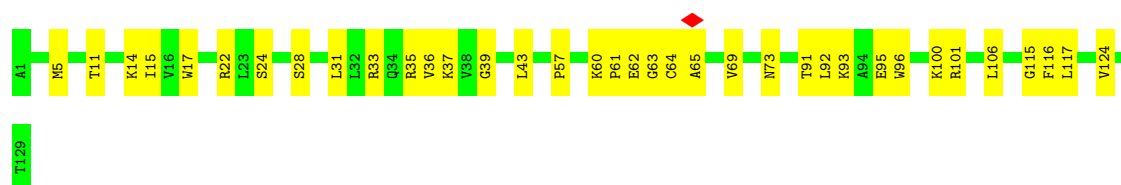
- Molecule 1: Coat protein

Chain GG:  72% 28%

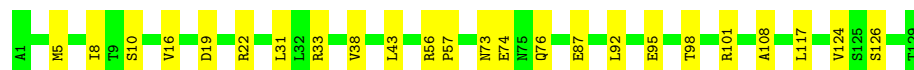
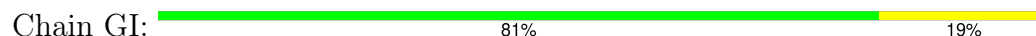


- Molecule 1: Coat protein

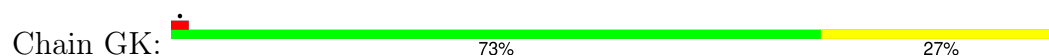
Chain GH:  72% 28%



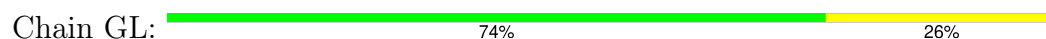
- Molecule 1: Coat protein



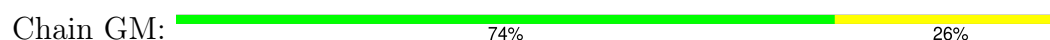
- Molecule 1: Coat protein



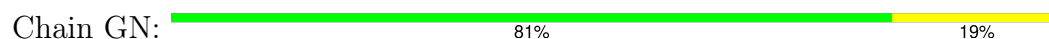
- Molecule 1: Coat protein



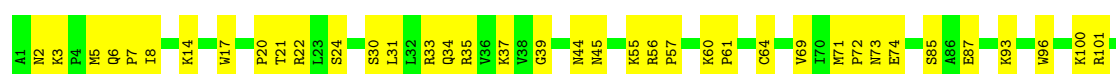
- Molecule 1: Coat protein



- Molecule 1: Coat protein



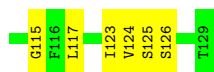
- Molecule 1: Coat protein





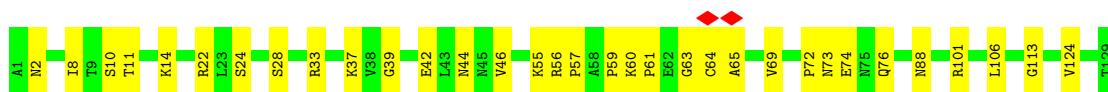
- Molecule 1: Coat protein

Chain GP: 68% 32%



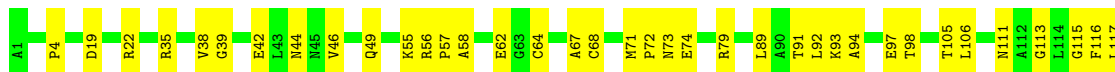
- Molecule 1: Coat protein

Chain GQ: 74% 26%



- Molecule 1: Coat protein

Chain GR: 70% 30%



- Molecule 1: Coat protein

Chain GS: 77% 22%

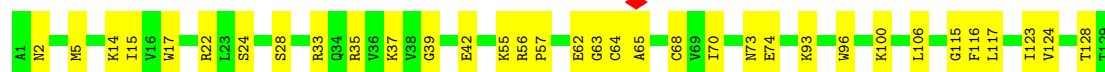
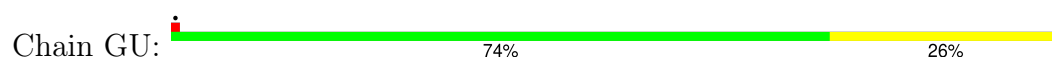


- Molecule 1: Coat protein

Chain GT: 71% 29%



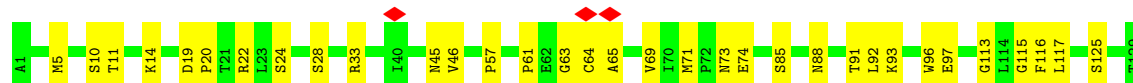
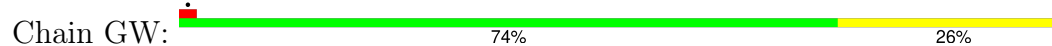
- Molecule 1: Coat protein



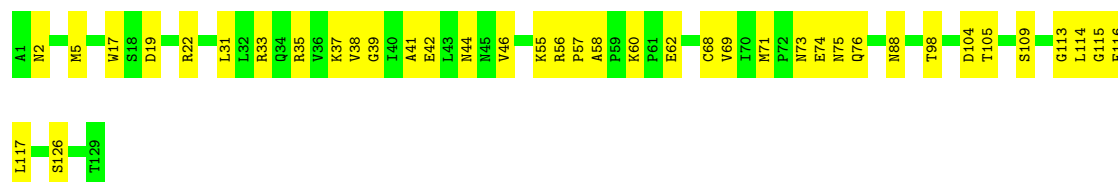
- Molecule 1: Coat protein



- Molecule 1: Coat protein



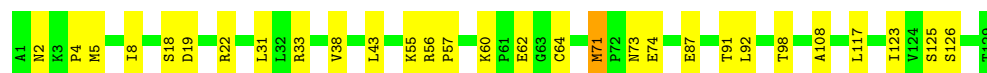
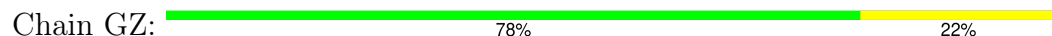
- Molecule 1: Coat protein



- Molecule 1: Coat protein

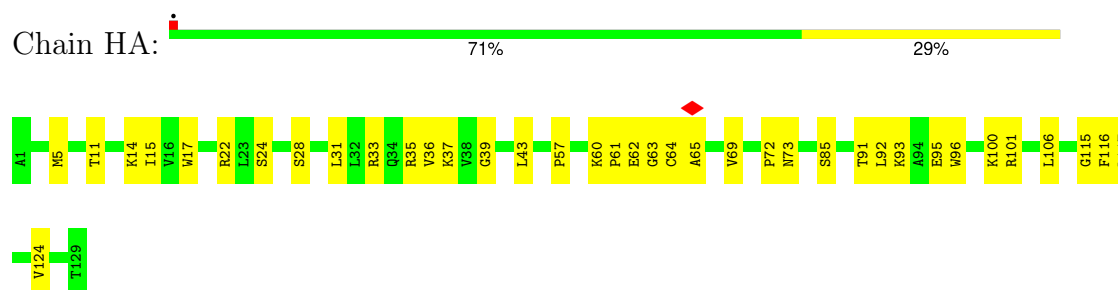


- Molecule 1: Coat protein

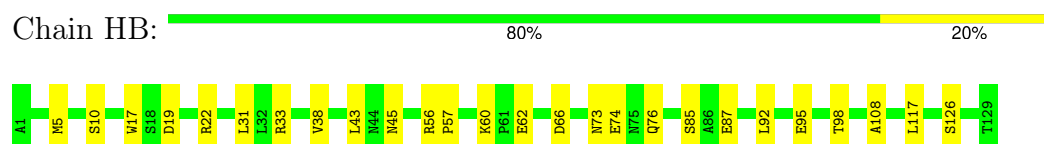




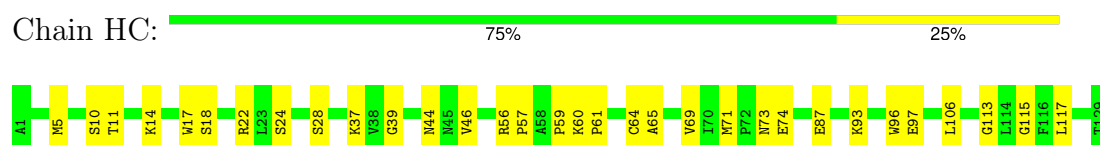
- Molecule 1: Coat protein



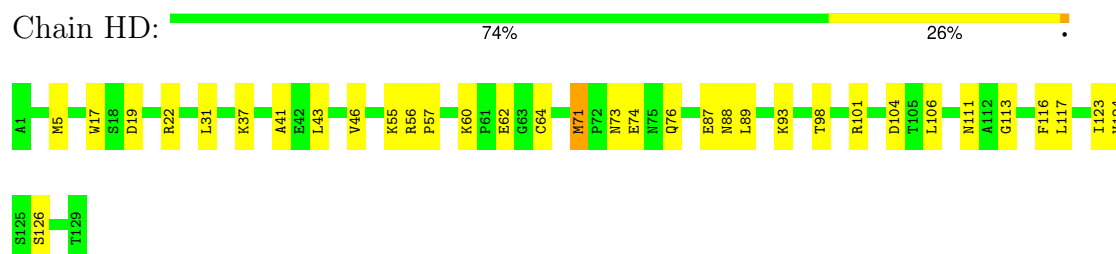
- Molecule 1: Coat protein



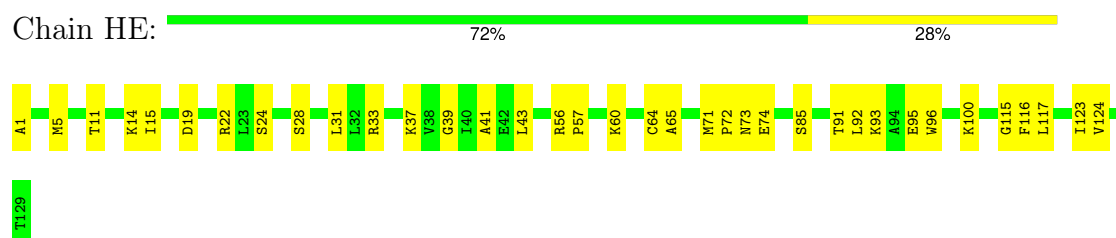
- Molecule 1: Coat protein



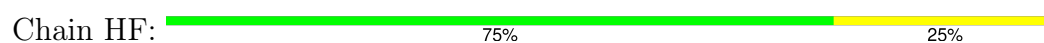
- Molecule 1: Coat protein

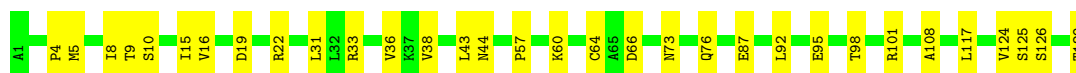


- Molecule 1: Coat protein

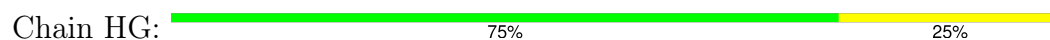


- Molecule 1: Coat protein

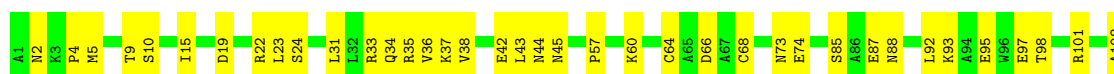




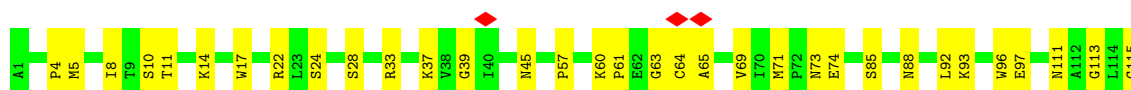
- Molecule 1: Coat protein



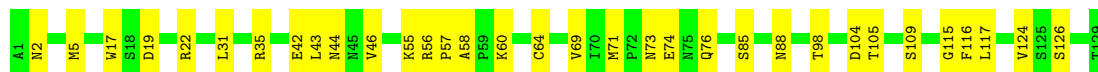
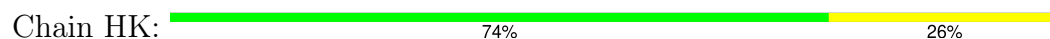
- Molecule 1: Coat protein



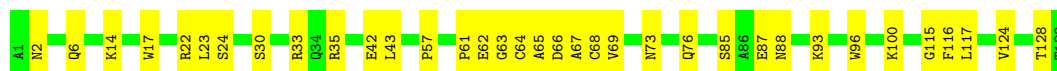
- Molecule 1: Coat protein



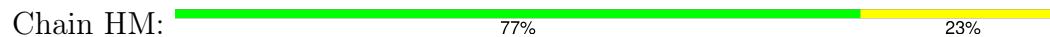
- Molecule 1: Coat protein



- Molecule 1: Coat protein

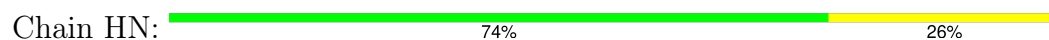


- Molecule 1: Coat protein

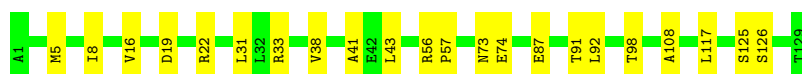
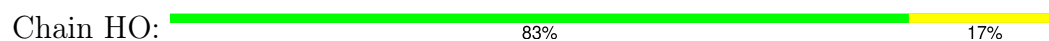




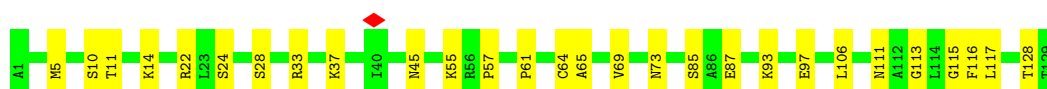
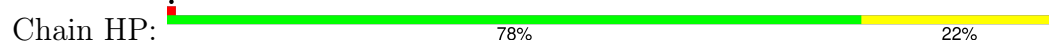
- Molecule 1: Coat protein



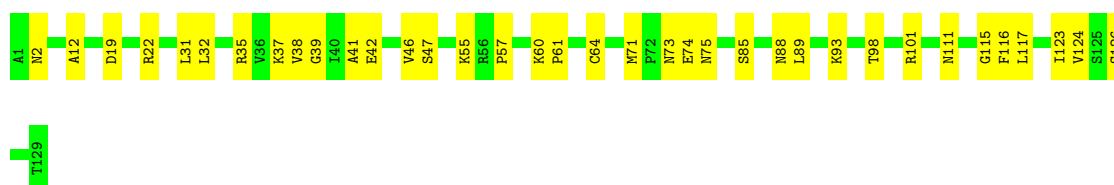
- Molecule 1: Coat protein



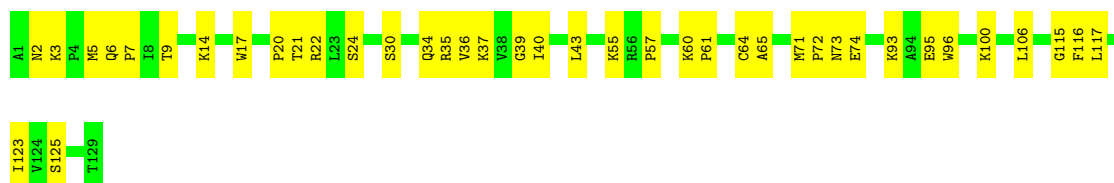
- Molecule 1: Coat protein



- Molecule 1: Coat protein

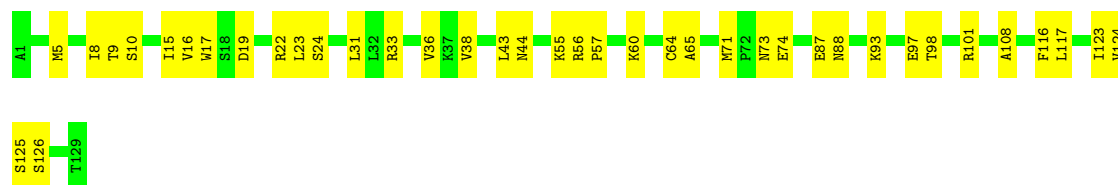


- Molecule 1: Coat protein



- Molecule 1: Coat protein





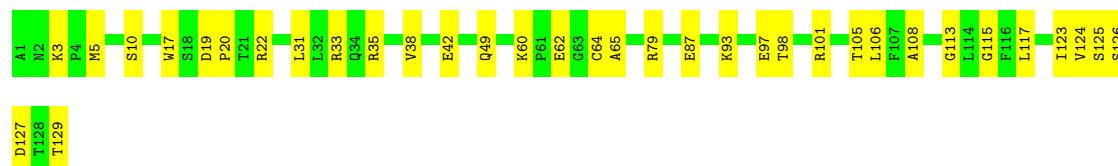
- Molecule 1: Coat protein

Chain HT: 68% 32%



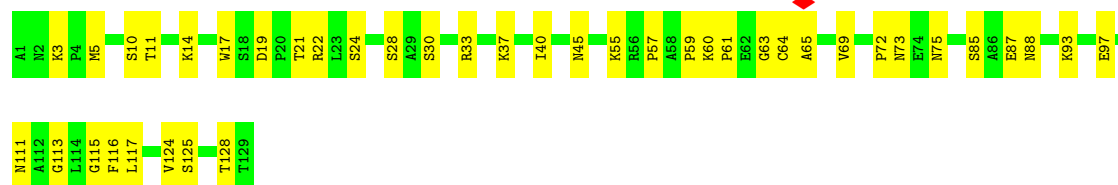
- Molecule 1: Coat protein

Chain HU: 73% 27%



- Molecule 1: Coat protein

Chain HV: 68% 32%



- Molecule 1: Coat protein

Chain HW: 72% 28%




- Molecule 1: Coat protein

Chain HX: 73% 27%



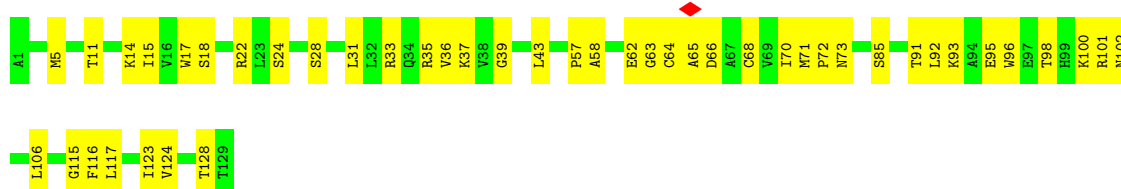
- Molecule 1: Coat protein

Chain HY:  78% 22%




- Molecule 1: Coat protein

Chain HZ:  65% 35%



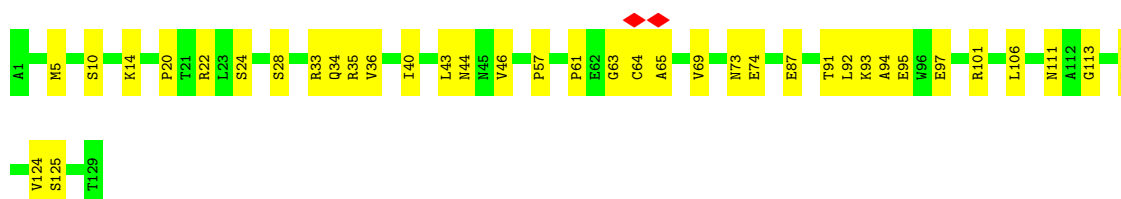
- Molecule 1: Coat protein

Chain IA:  77% 23%



- Molecule 1: Coat protein

Chain IB:  71% 29%



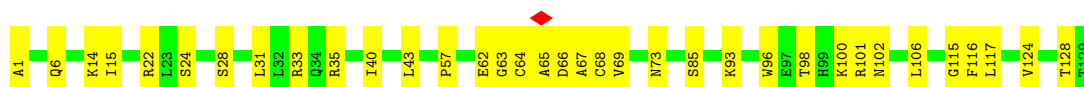
- Molecule 1: Coat protein

Chain IC:  74% 26%




- Molecule 1: Coat protein

Chain ID:  73% 27%



- Molecule 1: Coat protein

Chain IE:  78% 22%



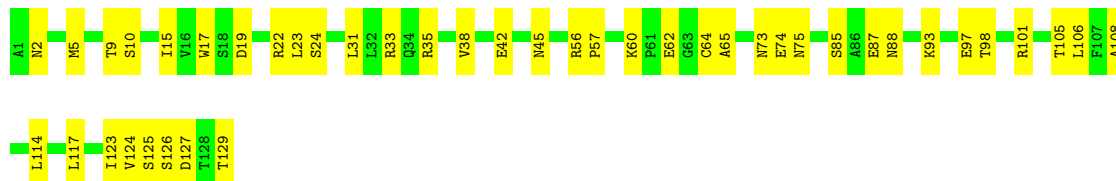
- Molecule 1: Coat protein

Chain IF:  72% 28%




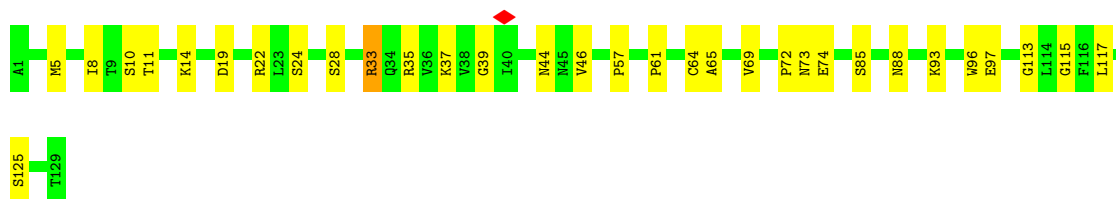
- Molecule 1: Coat protein

Chain IG:  67% 33%



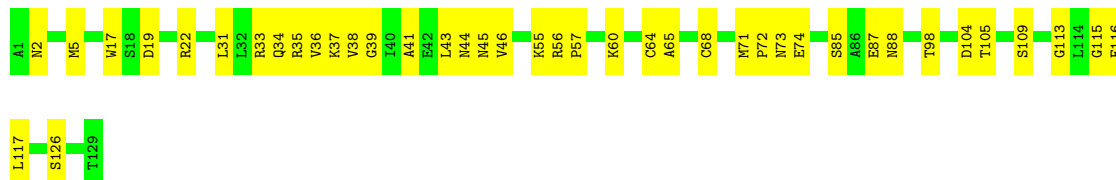
- Molecule 1: Coat protein

Chain IH:  75% 24%



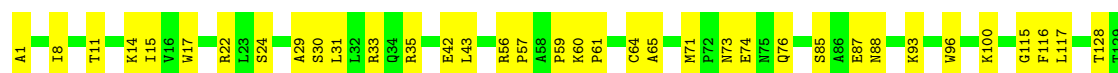
- Molecule 1: Coat protein

Chain II:  68% 32%




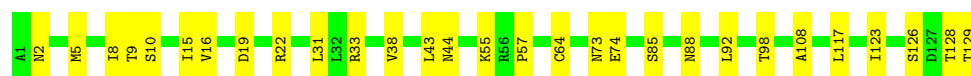
- Molecule 1: Coat protein

Chain IJ:  72% 28%




- Molecule 1: Coat protein

Chain IK:  78% 22%



- Molecule 1: Coat protein

Chain IL:  77% 23%



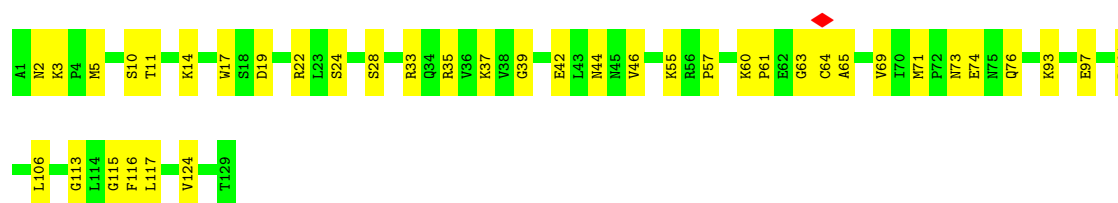
- Molecule 1: Coat protein

Chain IM:  73% 27%



- Molecule 1: Coat protein

Chain IN:  70% 30%



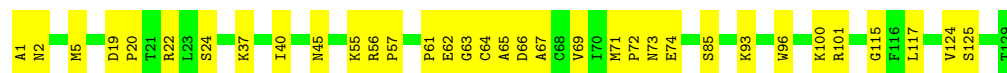
- Molecule 1: Coat protein

Chain IO:  74% 26%



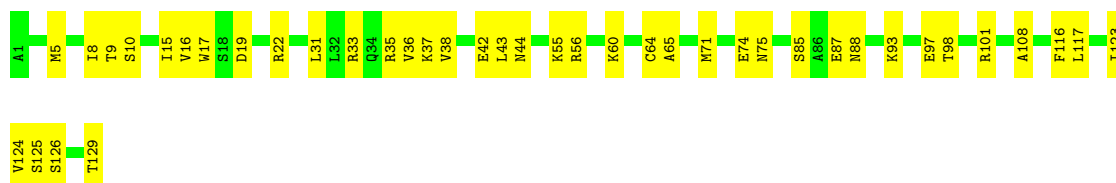
- Molecule 1: Coat protein

Chain IP:  74% 26%



- Molecule 1: Coat protein

Chain IQ:  68% 32%



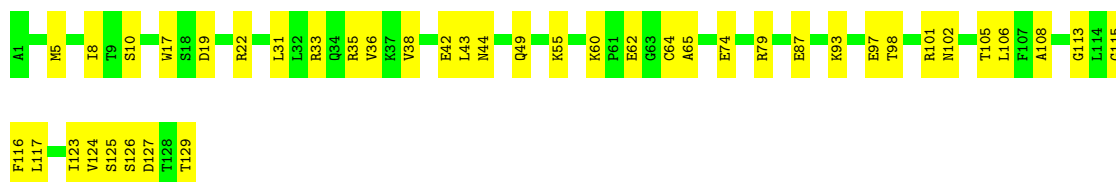
- Molecule 1: Coat protein

Chain IR:  67% 32% .



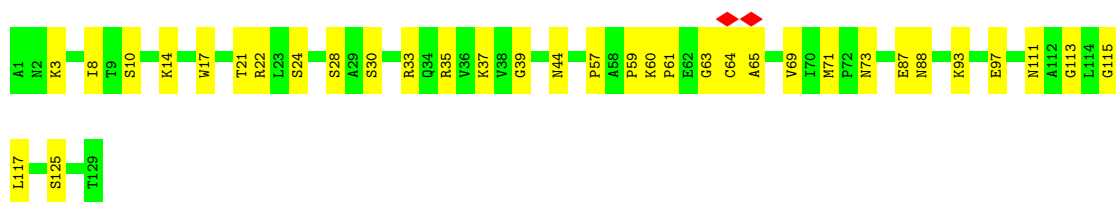
- Molecule 1: Coat protein

Chain IS:  68% 32%



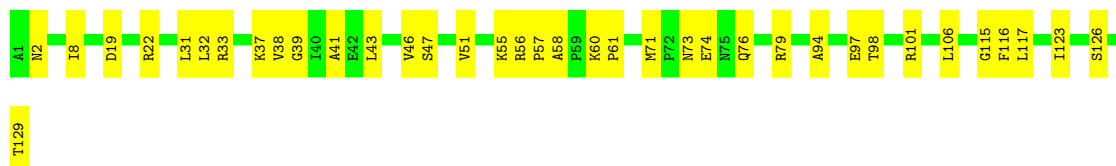
- Molecule 1: Coat protein

Chain IT:  73% 27%



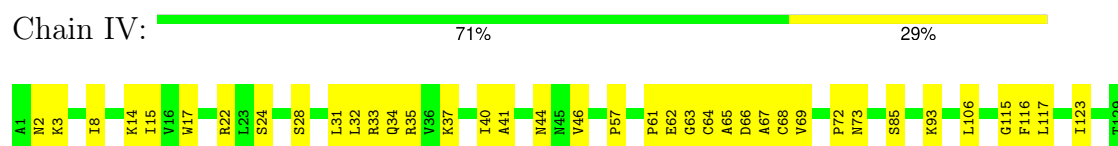
- Molecule 1: Coat protein

Chain IU:  71% 29%

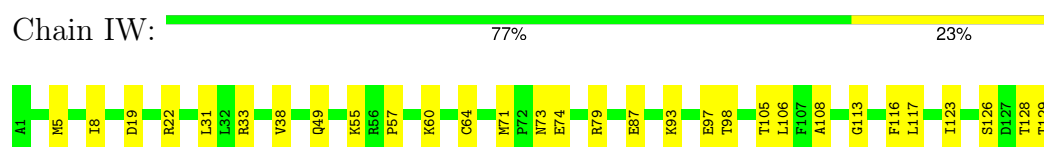




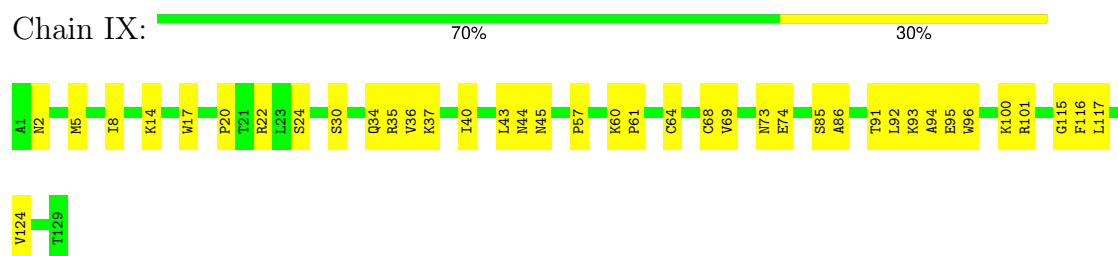
- Molecule 1: Coat protein



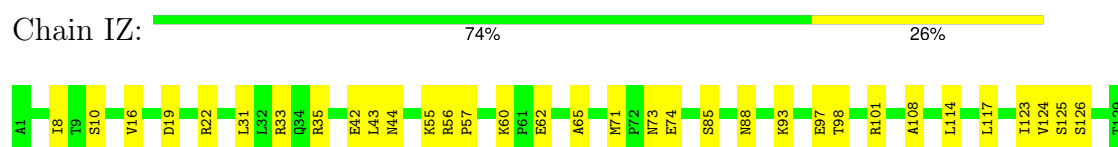
- Molecule 1: Coat protein



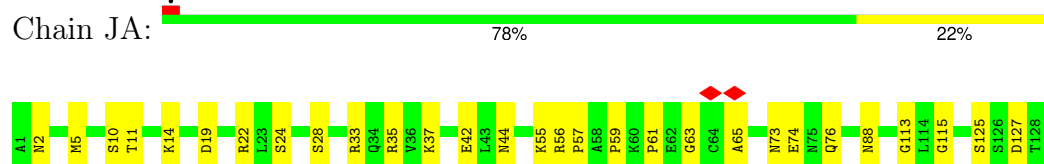
- Molecule 1: Coat protein



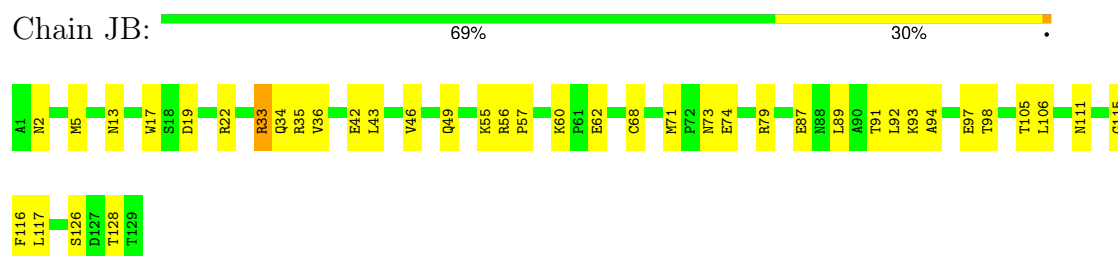
- Molecule 1: Coat protein




- Molecule 1: Coat protein

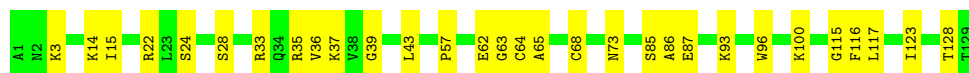


- Molecule 1: Coat protein



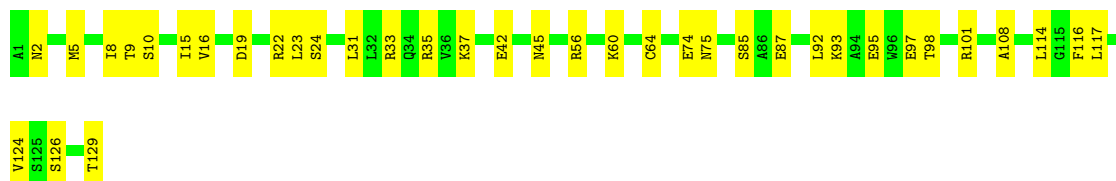
- Molecule 1: Coat protein

Chain JC:  77% 23%



- Molecule 1: Coat protein

Chain JD:  71% 29%



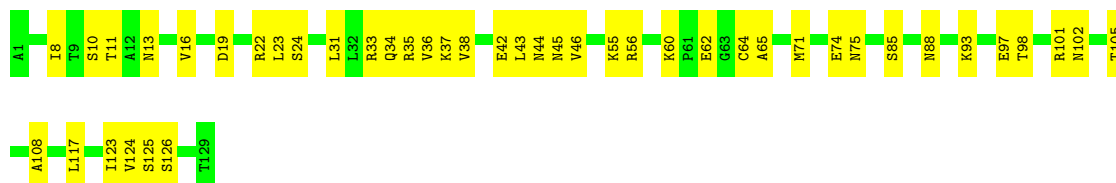
- Molecule 1: Coat protein

Chain JE:  73% 27%




- Molecule 1: Coat protein

Chain JF:  66% 34%



- Molecule 1: Coat protein

Chain JG:  77% 23%

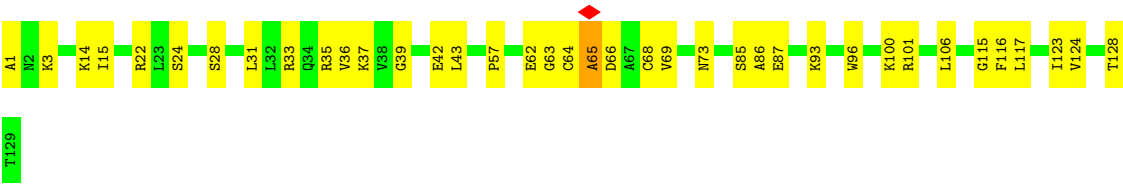


- Molecule 1: Coat protein

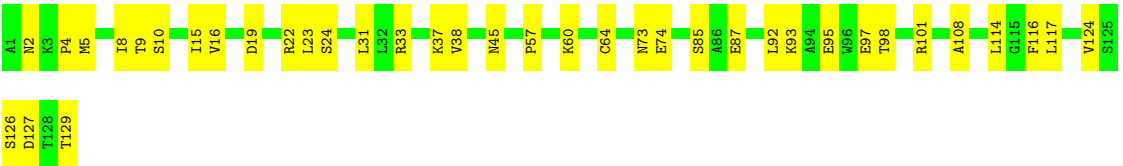
Chain JH:  74% 26%



- Molecule 1: Coat protein



● Molecule 1: Coat protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.039	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	Depositor
Map size ( $\text{\AA}$ )	457.91998, 457.91998, 457.91998	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.06, 1.06, 1.06	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	AA	0.32	0/985	0.50	0/1342
1	AB	0.33	0/985	0.53	0/1342
1	AC	0.32	0/985	0.49	0/1342
1	AD	0.33	0/985	0.55	0/1342
1	AE	0.32	0/985	0.49	0/1342
1	AF	0.34	0/985	0.55	0/1342
1	AG	0.32	0/985	0.49	0/1342
1	AH	0.33	0/985	0.55	0/1342
1	AI	0.33	0/985	0.50	0/1342
1	AJ	0.33	0/985	0.56	0/1342
1	AK	0.32	0/985	0.49	0/1342
1	AL	0.33	0/985	0.56	0/1342
1	AM	0.32	0/985	0.49	0/1342
1	AN	0.34	0/985	0.56	0/1342
1	AO	0.32	0/985	0.50	0/1342
1	AP	0.34	0/985	0.52	0/1342
1	AQ	0.33	0/985	0.50	0/1342
1	AR	0.34	0/985	0.52	0/1342
1	AS	0.32	0/985	0.49	0/1342
1	AT	0.33	0/985	0.52	0/1342
1	AU	0.32	0/985	0.49	0/1342
1	AV	0.33	0/985	0.54	0/1342
1	AW	0.32	0/985	0.50	0/1342
1	AX	0.34	0/985	0.56	0/1342
1	AY	0.32	0/985	0.49	0/1342
1	AZ	0.33	0/985	0.53	0/1342
1	BA	0.32	0/985	0.50	0/1342
1	BB	0.34	0/985	0.53	0/1342
1	BC	0.32	0/985	0.49	0/1342
1	BD	0.35	0/985	0.53	0/1342
1	BE	0.32	0/985	0.48	0/1342
1	BF	0.34	0/985	0.54	0/1342
1	BG	0.32	0/985	0.50	0/1342
1	BH	0.33	0/985	0.52	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	BI	0.32	0/985	0.50	0/1342
1	BJ	0.33	0/985	0.57	0/1342
1	BK	0.33	0/985	0.50	0/1342
1	BL	0.33	0/985	0.53	0/1342
1	BM	0.32	0/985	0.49	0/1342
1	BN	0.33	0/985	0.52	0/1342
1	BO	0.32	0/985	0.49	0/1342
1	BP	0.33	0/985	0.54	0/1342
1	BQ	0.33	0/985	0.50	0/1342
1	BR	0.34	0/985	0.57	0/1342
1	BS	0.32	0/985	0.49	0/1342
1	BT	0.33	0/985	0.53	0/1342
1	BU	0.32	0/985	0.49	0/1342
1	BV	0.33	0/985	0.55	0/1342
1	BW	0.32	0/985	0.49	0/1342
1	BX	0.33	0/985	0.54	0/1342
1	BY	0.32	0/985	0.50	0/1342
1	BZ	0.33	0/985	0.53	0/1342
1	CA	0.32	0/985	0.50	0/1342
1	CB	0.33	0/985	0.56	0/1342
1	CC	0.32	0/985	0.49	0/1342
1	CD	0.33	0/985	0.52	0/1342
1	CE	0.32	0/985	0.49	0/1342
1	CF	0.33	0/985	0.54	0/1342
1	CG	0.32	0/985	0.50	0/1342
1	CH	0.33	0/985	0.55	0/1342
1	CI	0.32	0/985	0.50	0/1342
1	CJ	0.33	0/985	0.52	0/1342
1	CK	0.32	0/985	0.49	0/1342
1	CL	0.33	0/985	0.55	0/1342
1	CM	0.32	0/985	0.49	0/1342
1	CN	0.34	0/985	0.54	0/1342
1	CO	0.32	0/985	0.49	0/1342
1	CP	0.33	0/985	0.54	0/1342
1	CQ	0.32	0/985	0.49	0/1342
1	CR	0.34	0/985	0.52	0/1342
1	CS	0.32	0/985	0.48	0/1342
1	CT	0.34	0/985	0.54	0/1342
1	CU	0.32	0/985	0.51	0/1342
1	CV	0.33	0/985	0.56	0/1342
1	CW	0.32	0/985	0.49	0/1342
1	CX	0.34	0/985	0.54	0/1342
1	CY	0.32	0/985	0.49	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	CZ	0.33	0/985	0.56	0/1342
1	DA	0.32	0/985	0.49	0/1342
1	DB	0.33	0/985	0.52	0/1342
1	DC	0.32	0/985	0.48	0/1342
1	DE	0.33	0/985	0.53	0/1342
1	DF	0.32	0/985	0.49	0/1342
1	DG	0.34	0/985	0.53	0/1342
1	DH	0.32	0/985	0.49	0/1342
1	DI	0.33	0/985	0.55	0/1342
1	DJ	0.32	0/985	0.50	0/1342
1	DK	0.34	0/985	0.53	0/1342
1	DL	0.32	0/985	0.49	0/1342
1	DM	0.33	0/985	0.55	0/1342
1	DN	0.32	0/985	0.50	0/1342
1	DO	0.33	0/985	0.52	0/1342
1	DP	0.32	0/985	0.49	0/1342
1	DQ	0.34	0/985	0.53	0/1342
1	DR	0.32	0/985	0.49	0/1342
1	DS	0.33	0/985	0.53	0/1342
1	DT	0.32	0/985	0.49	0/1342
1	DU	0.33	0/985	0.55	0/1342
1	DV	0.32	0/985	0.50	0/1342
1	DW	0.35	0/985	0.54	0/1342
1	DX	0.32	0/985	0.49	0/1342
1	DY	0.33	0/985	0.53	0/1342
1	DZ	0.32	0/985	0.49	0/1342
1	EA	0.33	0/985	0.52	0/1342
1	EB	0.32	0/985	0.50	0/1342
1	EC	0.33	0/985	0.52	0/1342
1	ED	0.32	0/985	0.50	0/1342
1	EE	0.34	0/985	0.57	0/1342
1	EF	0.32	0/985	0.49	0/1342
1	EG	0.33	0/985	0.56	0/1342
1	EH	0.32	0/985	0.49	0/1342
1	EI	0.33	0/985	0.54	0/1342
1	EJ	0.32	0/985	0.49	0/1342
1	EK	0.33	0/985	0.55	0/1342
1	EL	0.32	0/985	0.50	0/1342
1	EM	0.33	0/985	0.53	0/1342
1	EN	0.32	0/985	0.49	0/1342
1	EO	0.33	0/985	0.53	0/1342
1	EP	0.32	0/985	0.49	0/1342
1	EQ	0.34	0/985	0.54	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	ER	0.33	0/985	0.51	0/1342
1	ES	0.33	0/985	0.53	0/1342
1	ET	0.33	0/985	0.50	0/1342
1	EU	0.33	0/985	0.53	0/1342
1	EV	0.33	0/985	0.54	0/1342
1	EW	0.33	0/985	0.53	0/1342
1	EX	0.33	0/985	0.52	0/1342
1	EY	0.33	0/985	0.53	0/1342
1	EZ	0.32	0/985	0.50	0/1342
1	FA	0.33	0/985	0.53	0/1342
1	FB	0.34	0/985	0.53	0/1342
1	FC	0.32	0/985	0.53	0/1342
1	FD	0.33	0/985	0.51	0/1342
1	FE	0.33	0/985	0.54	0/1342
1	FF	0.33	0/985	0.51	0/1342
1	FG	0.34	0/985	0.53	0/1342
1	FH	0.34	0/985	0.54	0/1342
1	FI	0.33	0/985	0.52	0/1342
1	FJ	0.33	0/985	0.52	0/1342
1	FK	0.33	0/985	0.54	0/1342
1	FL	0.32	0/985	0.51	0/1342
1	FM	0.33	0/985	0.54	0/1342
1	FN	0.35	0/985	0.53	0/1342
1	FO	0.33	0/985	0.54	0/1342
1	FP	0.33	0/985	0.51	0/1342
1	FQ	0.33	0/985	0.54	0/1342
1	FR	0.32	0/985	0.52	0/1342
1	FS	0.34	0/985	0.53	0/1342
1	FT	0.32	0/985	0.51	0/1342
1	FU	0.33	0/985	0.52	0/1342
1	FV	0.33	0/985	0.52	0/1342
1	FW	0.33	0/985	0.53	0/1342
1	FX	0.32	0/985	0.50	0/1342
1	FY	0.33	0/985	0.53	0/1342
1	FZ	0.34	0/985	0.54	0/1342
1	GA	0.33	0/985	0.55	0/1342
1	GB	0.33	0/985	0.51	0/1342
1	GC	0.32	0/985	0.53	0/1342
1	GD	0.32	0/985	0.50	0/1342
1	GE	0.33	0/985	0.52	0/1342
1	GF	0.33	0/985	0.55	0/1342
1	GG	0.33	0/985	0.54	0/1342
1	GH	0.33	0/985	0.53	0/1342



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	GI	0.33	0/985	0.54	0/1342
1	GK	0.33	0/985	0.51	0/1342
1	GL	0.34	0/985	0.54	0/1342
1	GM	0.34	0/985	0.54	0/1342
1	GN	0.32	0/985	0.54	0/1342
1	GO	0.32	0/985	0.53	0/1342
1	GP	0.33	0/985	0.54	0/1342
1	GQ	0.33	0/985	0.51	0/1342
1	GR	0.33	0/985	0.54	0/1342
1	GS	0.34	0/985	0.55	0/1342
1	GT	0.33	0/985	0.54	0/1342
1	GU	0.33	0/985	0.52	0/1342
1	GV	0.33	0/985	0.52	0/1342
1	GW	0.32	0/985	0.50	0/1342
1	GX	0.33	0/985	0.55	0/1342
1	GY	0.34	0/985	0.54	0/1342
1	GZ	0.32	0/985	0.54	0/1342
1	HA	0.33	0/985	0.53	0/1342
1	HB	0.33	0/985	0.55	0/1342
1	HC	0.33	0/985	0.50	0/1342
1	HD	0.34	0/985	0.54	0/1342
1	HE	0.33	0/985	0.51	0/1342
1	HF	0.33	0/985	0.54	0/1342
1	HG	0.33	0/985	0.52	0/1342
1	HI	0.33	0/985	0.53	0/1342
1	HJ	0.32	0/985	0.51	0/1342
1	HK	0.33	0/985	0.54	0/1342
1	HL	0.34	0/985	0.53	0/1342
1	HM	0.33	0/985	0.54	0/1342
1	HN	0.33	0/985	0.51	0/1342
1	HO	0.32	0/985	0.53	0/1342
1	HP	0.32	0/985	0.50	0/1342
1	HQ	0.34	0/985	0.52	0/1342
1	HR	0.33	0/985	0.53	0/1342
1	HS	0.32	0/985	0.53	0/1342
1	HT	0.33	0/985	0.51	0/1342
1	HU	0.33	0/985	0.55	0/1342
1	HV	0.33	0/985	0.51	0/1342
1	HW	0.34	0/985	0.53	0/1342
1	HX	0.34	0/985	0.53	0/1342
1	HY	0.34	0/985	0.54	0/1342
1	HZ	0.34	0/985	0.54	0/1342
1	IA	0.33	0/985	0.53	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	IB	0.33	0/985	0.51	0/1342
1	IC	0.34	0/985	0.53	0/1342
1	ID	0.34	0/985	0.53	0/1342
1	IE	0.33	0/985	0.54	0/1342
1	IF	0.33	0/985	0.52	0/1342
1	IG	0.33	0/985	0.54	0/1342
1	IH	0.32	0/985	0.50	0/1342
1	II	0.34	0/985	0.55	0/1342
1	IJ	0.33	0/985	0.50	0/1342
1	IK	0.32	0/985	0.53	0/1342
1	IL	0.33	0/985	0.51	0/1342
1	IM	0.33	0/985	0.55	0/1342
1	IN	0.32	0/985	0.50	0/1342
1	IO	0.33	0/985	0.54	0/1342
1	IP	0.34	0/985	0.53	0/1342
1	IQ	0.33	0/985	0.54	0/1342
1	IR	0.33	0/985	0.51	0/1342
1	IS	0.33	0/985	0.55	0/1342
1	IT	0.33	0/985	0.51	0/1342
1	IU	0.34	0/985	0.52	0/1342
1	IV	0.34	0/985	0.53	0/1342
1	IW	0.33	0/985	0.53	0/1342
1	IX	0.33	0/985	0.52	0/1342
1	IZ	0.33	0/985	0.53	0/1342
1	JA	0.32	0/985	0.51	0/1342
1	JB	0.33	0/985	0.54	0/1342
1	JC	0.34	0/985	0.56	0/1342
1	JD	0.33	0/985	0.53	0/1342
1	JE	0.33	0/985	0.52	0/1342
1	JF	0.33	0/985	0.54	0/1342
1	JG	0.32	0/985	0.51	0/1342
1	JH	0.33	0/985	0.55	0/1342
1	JI	0.34	0/985	0.55	0/1342
1	JJ	0.33	0/985	0.52	0/1342
All	All	0.33	0/236400	0.52	0/322080

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	AF	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AN	0	1
1	BJ	0	1
1	CB	0	1
1	CZ	0	1
1	EV	0	1
1	FB	0	1
1	FH	0	1
1	FZ	0	1
1	GY	0	1
1	JI	0	1
All	All	0	11

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AF	66	ASP	Peptide
1	AN	66	ASP	Peptide
1	BJ	66	ASP	Peptide
1	CB	66	ASP	Peptide
1	CZ	66	ASP	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	968	0	975	28	0
1	AB	968	0	975	36	0
1	AC	968	0	975	33	0
1	AD	968	0	975	60	0
1	AE	968	0	975	37	0
1	AF	968	0	975	48	0
1	AG	968	0	975	27	0
1	AH	968	0	975	48	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AI	968	0	975	32	0
1	AJ	968	0	975	55	0
1	AK	968	0	975	24	0
1	AL	968	0	975	33	0
1	AM	968	0	975	34	0
1	AN	968	0	975	52	0
1	AO	968	0	975	30	0
1	AP	968	0	974	30	0
1	AQ	968	0	975	26	0
1	AR	968	0	974	31	0
1	AS	968	0	975	26	0
1	AT	968	0	974	29	0
1	AU	968	0	975	24	0
1	AV	968	0	975	36	0
1	AW	968	0	975	27	0
1	AX	968	0	975	50	0
1	AY	968	0	975	28	0
1	AZ	968	0	975	36	0
1	BA	968	0	975	25	0
1	BB	968	0	974	32	0
1	BC	968	0	975	31	0
1	BD	968	0	974	37	0
1	BE	968	0	975	23	0
1	BF	968	0	974	33	0
1	BG	968	0	975	32	0
1	BH	968	0	974	35	0
1	BI	968	0	975	28	0
1	BJ	968	0	975	46	0
1	BK	968	0	975	29	0
1	BL	968	0	975	36	0
1	BM	968	0	975	31	0
1	BN	968	0	974	32	0
1	BO	968	0	975	29	0
1	BP	968	0	975	33	0
1	BQ	968	0	975	27	0
1	BR	968	0	975	51	0
1	BS	968	0	975	20	0
1	BT	968	0	974	30	0
1	BU	968	0	975	31	0
1	BV	968	0	975	50	0
1	BW	968	0	975	32	0
1	BX	968	0	975	54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BY	968	0	975	30	0
1	BZ	968	0	975	31	0
1	CA	968	0	975	39	0
1	CB	968	0	975	52	0
1	CC	968	0	975	29	0
1	CD	968	0	975	37	0
1	CE	968	0	975	27	0
1	CF	968	0	975	29	0
1	CG	968	0	975	27	0
1	CH	968	0	975	48	0
1	CI	968	0	975	36	0
1	CJ	968	0	975	36	0
1	CK	968	0	975	31	0
1	CL	968	0	975	51	0
1	CM	968	0	975	34	0
1	CN	968	0	974	32	0
1	CO	968	0	975	31	0
1	CP	968	0	975	52	0
1	CQ	968	0	975	28	0
1	CR	968	0	974	31	0
1	CS	968	0	975	25	0
1	CT	968	0	975	36	0
1	CU	968	0	975	28	0
1	CV	968	0	975	52	0
1	CW	968	0	975	24	0
1	CX	968	0	974	25	0
1	CY	968	0	975	27	0
1	CZ	968	0	975	56	0
1	DA	968	0	975	29	0
1	DB	968	0	975	39	0
1	DC	968	0	975	26	0
1	DE	968	0	975	30	0
1	DF	968	0	975	30	0
1	DG	968	0	974	32	0
1	DH	968	0	975	27	0
1	DI	968	0	975	47	0
1	DJ	968	0	975	34	0
1	DK	968	0	974	32	0
1	DL	968	0	975	29	0
1	DM	968	0	975	47	0
1	DN	968	0	975	32	0
1	DO	968	0	975	36	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DP	968	0	975	30	0
1	DQ	968	0	974	29	0
1	DR	968	0	975	39	0
1	DS	968	0	974	37	0
1	DT	968	0	975	31	0
1	DU	968	0	975	52	0
1	DV	968	0	975	25	0
1	DW	968	0	975	32	0
1	DX	968	0	975	31	0
1	DY	968	0	975	35	0
1	DZ	968	0	975	34	0
1	EA	968	0	974	36	0
1	EB	968	0	975	31	0
1	EC	968	0	975	37	0
1	ED	968	0	975	33	0
1	EE	968	0	975	55	0
1	EF	968	0	975	23	0
1	EG	968	0	975	52	0
1	EH	968	0	975	27	0
1	EI	968	0	975	36	0
1	EJ	968	0	975	27	0
1	EK	968	0	975	50	0
1	EL	968	0	975	31	0
1	EM	968	0	974	34	0
1	EN	968	0	975	33	0
1	EO	968	0	974	30	0
1	EP	968	0	975	25	0
1	EQ	968	0	974	28	0
1	ER	968	0	974	35	0
1	ES	968	0	975	28	0
1	ET	968	0	975	32	0
1	EU	968	0	974	41	0
1	EV	968	0	975	62	0
1	EW	968	0	974	40	0
1	EX	968	0	974	36	0
1	EY	968	0	975	25	0
1	EZ	968	0	975	32	0
1	FA	968	0	974	36	0
1	FB	968	0	975	54	0
1	FC	968	0	974	37	0
1	FD	968	0	974	33	0
1	FE	968	0	975	24	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	FF	968	0	975	35	0
1	FG	968	0	974	29	0
1	FH	968	0	975	56	0
1	FI	968	0	974	28	0
1	FJ	968	0	974	40	0
1	FK	968	0	975	32	0
1	FL	968	0	975	35	0
1	FM	968	0	974	45	0
1	FN	968	0	975	53	0
1	FO	968	0	974	33	0
1	FP	968	0	974	54	0
1	FQ	968	0	975	35	0
1	FR	968	0	975	36	0
1	FS	968	0	974	42	0
1	FT	968	0	975	37	0
1	FU	968	0	974	32	0
1	FV	968	0	974	31	0
1	FW	968	0	975	41	0
1	FX	968	0	975	30	0
1	FY	968	0	974	34	0
1	FZ	968	0	975	56	0
1	GA	968	0	974	30	0
1	GB	968	0	974	31	0
1	GC	968	0	975	19	0
1	GD	968	0	975	26	0
1	GE	968	0	974	33	0
1	GF	968	0	975	30	0
1	GG	968	0	974	31	0
1	GH	968	0	974	43	0
1	GI	968	0	975	19	0
1	GK	968	0	975	29	0
1	GL	968	0	974	26	0
1	GM	968	0	975	48	0
1	GN	968	0	974	22	0
1	GO	968	0	974	43	0
1	GP	968	0	975	45	0
1	GQ	968	0	975	29	0
1	GR	968	0	974	30	0
1	GS	968	0	975	32	0
1	GT	968	0	974	33	0
1	GU	968	0	974	48	0
1	GV	968	0	975	29	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	GW	968	0	975	31	0
1	GX	968	0	974	34	0
1	GY	968	0	975	56	0
1	GZ	968	0	974	26	0
1	HA	968	0	974	47	0
1	HB	968	0	975	23	0
1	HC	968	0	975	26	0
1	HD	968	0	974	30	0
1	HE	968	0	975	28	0
1	HF	968	0	974	29	0
1	HG	968	0	974	32	0
1	HI	968	0	975	35	0
1	HJ	968	0	975	32	0
1	HK	968	0	974	33	0
1	HL	968	0	975	53	0
1	HM	968	0	974	28	0
1	HN	968	0	974	31	0
1	HO	968	0	975	20	0
1	HP	968	0	975	23	0
1	HQ	968	0	974	29	0
1	HR	968	0	975	36	0
1	HS	968	0	974	34	0
1	HT	968	0	974	41	0
1	HU	968	0	975	34	0
1	HV	968	0	975	36	0
1	HW	968	0	974	33	0
1	HX	968	0	975	51	0
1	HY	968	0	974	26	0
1	HZ	968	0	974	59	0
1	IA	968	0	975	27	0
1	IB	968	0	975	29	0
1	IC	968	0	974	28	0
1	ID	968	0	975	50	0
1	IE	968	0	974	25	0
1	IF	968	0	974	36	0
1	IG	968	0	975	37	0
1	IH	968	0	975	28	0
1	II	968	0	974	38	0
1	IJ	968	0	975	36	0
1	IK	968	0	974	27	0
1	IL	968	0	974	30	0
1	IM	968	0	975	30	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	IN	968	0	975	35	0
1	IO	968	0	974	31	0
1	IP	968	0	975	48	0
1	IQ	968	0	974	39	0
1	IR	968	0	974	40	0
1	IS	968	0	975	38	0
1	IT	968	0	975	28	0
1	IU	968	0	974	32	0
1	IV	968	0	975	50	0
1	IW	968	0	974	28	0
1	IX	968	0	974	32	0
1	IZ	968	0	975	31	0
1	JA	968	0	975	27	0
1	JB	968	0	974	33	0
1	JC	968	0	975	43	0
1	JD	968	0	974	32	0
1	JE	968	0	974	44	0
1	JF	968	0	975	39	0
1	JG	968	0	975	26	0
1	JH	968	0	974	27	0
1	JI	968	0	975	55	0
1	JJ	968	0	974	36	0
All	All	232320	0	233920	6106	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 6106 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EG:68:CYS:H	1:HX:64:CYS:H	1.07	1.00
1:AD:68:CYS:H	1:IV:64:CYS:H	1.08	1.00
1:CL:68:CYS:H	1:FN:64:CYS:H	1.07	1.00
1:DI:68:CYS:H	1:FH:64:CYS:H	1.10	0.96
1:CP:68:CYS:H	1:IP:64:CYS:H	1.09	0.96

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
1	AB	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	AC	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AD	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AE	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	AF	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	AG	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AH	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	AI	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AJ	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AK	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AL	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AM	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	AN	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	AO	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AP	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	AQ	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	AR	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	AS	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
1	AT	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	AU	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	AV	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	AW	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	AX	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AY	127/129 (98%)	123 (97%)	4 (3%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AZ	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	BA	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	BB	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	BC	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	BD	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	BE	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	BF	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	BG	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	BH	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	BI	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	BJ	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	BK	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	BL	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	BM	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	BN	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	BO	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
1	BP	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	BQ	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	BR	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	BS	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	BT	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	BU	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	BV	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	BW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	BX	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	BY	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	BZ	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	CA	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CB	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	CC	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	CD	127/129 (98%)	125 (98%)	2 (2%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CE	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	CF	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	CG	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	CH	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	CI	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	CJ	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	CK	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CL	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CM	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CN	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	CO	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	CP	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	CQ	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	CR	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	CS	127/129 (98%)	127 (100%)	0	0	100	100
1	CT	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	CU	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	CV	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	CX	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	CY	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CZ	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	DA	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	DB	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	DC	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	DE	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	DF	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	DG	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
1	DH	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	DI	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	DJ	127/129 (98%)	125 (98%)	2 (2%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DK	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	DL	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	DM	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	DN	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	DO	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	DP	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	DQ	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	DR	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
1	DS	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	DT	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	DU	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	DV	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	DW	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	DX	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	DY	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	DZ	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
1	EA	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	EB	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	EC	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	ED	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	EE	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	EF	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	EG	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	EH	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	EI	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	EJ	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	EK	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	EL	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	EM	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
1	EN	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	EO	127/129 (98%)	126 (99%)	1 (1%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EP	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	EQ	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	ER	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	ES	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	ET	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	EU	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
1	EV	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	EW	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
1	EX	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	EY	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
1	EZ	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	FA	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
1	FB	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	FC	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	FD	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	FE	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
1	FF	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	FG	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	FH	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	FI	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	FJ	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	FK	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	FL	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	FM	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
1	FN	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	FO	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	FP	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	FQ	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	FR	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
1	FS	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
1	FT	127/129 (98%)	125 (98%)	2 (2%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	FU	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	FV	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	FW	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
1	FX	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	FY	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	FZ	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	GA	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
1	GB	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	GC	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
1	GD	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
1	GE	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	GF	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	GG	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
1	GH	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	GI	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
1	GK	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	GL	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
1	GM	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	GN	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
1	GO	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	GP	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	GQ	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	GR	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
1	GS	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
1	GT	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	GU	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	GV	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	GW	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	GX	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
1	GY	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
1	GZ	127/129 (98%)	119 (94%)	8 (6%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	HA	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	HB	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
1	HC	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
1	HD	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
1	HE	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	HF	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	HG	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	HI	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
1	HJ	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
1	HK	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	HL	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	HM	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
1	HN	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	HO	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	HP	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
1	HQ	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
1	HR	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	HS	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
1	HT	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	HU	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	HV	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	HW	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	HX	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	HY	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	HZ	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	IA	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	IB	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
1	IC	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
1	ID	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	IE	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
1	IF	127/129 (98%)	122 (96%)	5 (4%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	IG	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
1	IH	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
1	II	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	IJ	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	IK	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	IL	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	IM	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
1	IN	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
1	IO	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
1	IP	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	IQ	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	IR	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	IS	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	IT	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	IU	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
1	IV	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	IW	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	IX	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	IZ	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	JA	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	JB	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
1	JC	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	JD	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
1	JE	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	JF	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
1	JG	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	JH	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	JI	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	JJ	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
All	All	30480/30960 (98%)	29335 (96%)	1145 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	108/108 (100%)	108 (100%)	0	100	100
1	AB	108/108 (100%)	108 (100%)	0	100	100
1	AC	108/108 (100%)	108 (100%)	0	100	100
1	AD	108/108 (100%)	108 (100%)	0	100	100
1	AE	108/108 (100%)	108 (100%)	0	100	100
1	AF	108/108 (100%)	108 (100%)	0	100	100
1	AG	108/108 (100%)	108 (100%)	0	100	100
1	AH	108/108 (100%)	108 (100%)	0	100	100
1	AI	108/108 (100%)	108 (100%)	0	100	100
1	AJ	108/108 (100%)	108 (100%)	0	100	100
1	AK	108/108 (100%)	108 (100%)	0	100	100
1	AL	108/108 (100%)	108 (100%)	0	100	100
1	AM	108/108 (100%)	108 (100%)	0	100	100
1	AN	108/108 (100%)	108 (100%)	0	100	100
1	AO	108/108 (100%)	108 (100%)	0	100	100
1	AP	108/108 (100%)	108 (100%)	0	100	100
1	AQ	108/108 (100%)	108 (100%)	0	100	100
1	AR	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	AS	108/108 (100%)	108 (100%)	0	100	100
1	AT	108/108 (100%)	108 (100%)	0	100	100
1	AU	108/108 (100%)	108 (100%)	0	100	100
1	AV	108/108 (100%)	108 (100%)	0	100	100
1	AW	108/108 (100%)	108 (100%)	0	100	100
1	AX	108/108 (100%)	108 (100%)	0	100	100
1	AY	108/108 (100%)	108 (100%)	0	100	100
1	AZ	108/108 (100%)	108 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BA	108/108 (100%)	108 (100%)	0	100	100
1	BB	108/108 (100%)	108 (100%)	0	100	100
1	BC	108/108 (100%)	108 (100%)	0	100	100
1	BD	108/108 (100%)	108 (100%)	0	100	100
1	BE	108/108 (100%)	108 (100%)	0	100	100
1	BF	108/108 (100%)	108 (100%)	0	100	100
1	BG	108/108 (100%)	108 (100%)	0	100	100
1	BH	108/108 (100%)	108 (100%)	0	100	100
1	BI	108/108 (100%)	108 (100%)	0	100	100
1	BJ	108/108 (100%)	108 (100%)	0	100	100
1	BK	108/108 (100%)	108 (100%)	0	100	100
1	BL	108/108 (100%)	108 (100%)	0	100	100
1	BM	108/108 (100%)	108 (100%)	0	100	100
1	BN	108/108 (100%)	108 (100%)	0	100	100
1	BO	108/108 (100%)	108 (100%)	0	100	100
1	BP	108/108 (100%)	108 (100%)	0	100	100
1	BQ	108/108 (100%)	108 (100%)	0	100	100
1	BR	108/108 (100%)	108 (100%)	0	100	100
1	BS	108/108 (100%)	108 (100%)	0	100	100
1	BT	108/108 (100%)	108 (100%)	0	100	100
1	BU	108/108 (100%)	108 (100%)	0	100	100
1	BV	108/108 (100%)	108 (100%)	0	100	100
1	BW	108/108 (100%)	108 (100%)	0	100	100
1	BX	108/108 (100%)	108 (100%)	0	100	100
1	BY	108/108 (100%)	108 (100%)	0	100	100
1	BZ	108/108 (100%)	108 (100%)	0	100	100
1	CA	108/108 (100%)	108 (100%)	0	100	100
1	CB	108/108 (100%)	108 (100%)	0	100	100
1	CC	108/108 (100%)	108 (100%)	0	100	100
1	CD	108/108 (100%)	108 (100%)	0	100	100
1	CE	108/108 (100%)	108 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CF	108/108 (100%)	108 (100%)	0	100	100
1	CG	108/108 (100%)	108 (100%)	0	100	100
1	CH	108/108 (100%)	108 (100%)	0	100	100
1	CI	108/108 (100%)	108 (100%)	0	100	100
1	CJ	108/108 (100%)	108 (100%)	0	100	100
1	CK	108/108 (100%)	108 (100%)	0	100	100
1	CL	108/108 (100%)	108 (100%)	0	100	100
1	CM	108/108 (100%)	108 (100%)	0	100	100
1	CN	108/108 (100%)	108 (100%)	0	100	100
1	CO	108/108 (100%)	108 (100%)	0	100	100
1	CP	108/108 (100%)	108 (100%)	0	100	100
1	CQ	108/108 (100%)	108 (100%)	0	100	100
1	CR	108/108 (100%)	108 (100%)	0	100	100
1	CS	108/108 (100%)	108 (100%)	0	100	100
1	CT	108/108 (100%)	108 (100%)	0	100	100
1	CU	108/108 (100%)	108 (100%)	0	100	100
1	CV	108/108 (100%)	108 (100%)	0	100	100
1	CW	108/108 (100%)	108 (100%)	0	100	100
1	CX	108/108 (100%)	108 (100%)	0	100	100
1	CY	108/108 (100%)	108 (100%)	0	100	100
1	CZ	108/108 (100%)	108 (100%)	0	100	100
1	DA	108/108 (100%)	108 (100%)	0	100	100
1	DB	108/108 (100%)	108 (100%)	0	100	100
1	DC	108/108 (100%)	108 (100%)	0	100	100
1	DE	108/108 (100%)	108 (100%)	0	100	100
1	DF	108/108 (100%)	108 (100%)	0	100	100
1	DG	108/108 (100%)	108 (100%)	0	100	100
1	DH	108/108 (100%)	108 (100%)	0	100	100
1	DI	108/108 (100%)	108 (100%)	0	100	100
1	DJ	108/108 (100%)	108 (100%)	0	100	100
1	DK	108/108 (100%)	108 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DL	108/108 (100%)	108 (100%)	0	100	100
1	DM	108/108 (100%)	108 (100%)	0	100	100
1	DN	108/108 (100%)	108 (100%)	0	100	100
1	DO	108/108 (100%)	108 (100%)	0	100	100
1	DP	108/108 (100%)	108 (100%)	0	100	100
1	DQ	108/108 (100%)	108 (100%)	0	100	100
1	DR	108/108 (100%)	108 (100%)	0	100	100
1	DS	108/108 (100%)	108 (100%)	0	100	100
1	DT	108/108 (100%)	108 (100%)	0	100	100
1	DU	108/108 (100%)	108 (100%)	0	100	100
1	DV	108/108 (100%)	108 (100%)	0	100	100
1	DW	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	DX	108/108 (100%)	108 (100%)	0	100	100
1	DY	108/108 (100%)	108 (100%)	0	100	100
1	DZ	108/108 (100%)	108 (100%)	0	100	100
1	EA	108/108 (100%)	108 (100%)	0	100	100
1	EB	108/108 (100%)	108 (100%)	0	100	100
1	EC	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	ED	108/108 (100%)	108 (100%)	0	100	100
1	EE	108/108 (100%)	108 (100%)	0	100	100
1	EF	108/108 (100%)	108 (100%)	0	100	100
1	EG	108/108 (100%)	108 (100%)	0	100	100
1	EH	108/108 (100%)	108 (100%)	0	100	100
1	EI	108/108 (100%)	108 (100%)	0	100	100
1	EJ	108/108 (100%)	108 (100%)	0	100	100
1	EK	108/108 (100%)	108 (100%)	0	100	100
1	EL	108/108 (100%)	108 (100%)	0	100	100
1	EM	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	EN	108/108 (100%)	108 (100%)	0	100	100
1	EO	108/108 (100%)	108 (100%)	0	100	100
1	EP	108/108 (100%)	108 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	EQ	108/108 (100%)	108 (100%)	0	100	100
1	ER	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	ES	108/108 (100%)	108 (100%)	0	100	100
1	ET	108/108 (100%)	108 (100%)	0	100	100
1	EU	108/108 (100%)	108 (100%)	0	100	100
1	EV	108/108 (100%)	108 (100%)	0	100	100
1	EW	108/108 (100%)	108 (100%)	0	100	100
1	EX	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	EY	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	EZ	108/108 (100%)	108 (100%)	0	100	100
1	FA	108/108 (100%)	108 (100%)	0	100	100
1	FB	108/108 (100%)	108 (100%)	0	100	100
1	FC	108/108 (100%)	108 (100%)	0	100	100
1	FD	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	FE	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	FF	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	FG	108/108 (100%)	108 (100%)	0	100	100
1	FH	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	FI	108/108 (100%)	108 (100%)	0	100	100
1	FJ	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	FK	108/108 (100%)	108 (100%)	0	100	100
1	FL	108/108 (100%)	108 (100%)	0	100	100
1	FM	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	FN	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	FO	108/108 (100%)	108 (100%)	0	100	100
1	FP	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	FQ	108/108 (100%)	108 (100%)	0	100	100
1	FR	108/108 (100%)	108 (100%)	0	100	100
1	FS	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	FT	108/108 (100%)	106 (98%)	2 (2%)	52	71
1	FU	108/108 (100%)	108 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	FV	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	FW	108/108 (100%)	108 (100%)	0	100	100
1	FX	108/108 (100%)	108 (100%)	0	100	100
1	FY	108/108 (100%)	108 (100%)	0	100	100
1	FZ	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	GA	108/108 (100%)	108 (100%)	0	100	100
1	GB	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	GC	108/108 (100%)	108 (100%)	0	100	100
1	GD	108/108 (100%)	108 (100%)	0	100	100
1	GE	108/108 (100%)	108 (100%)	0	100	100
1	GF	108/108 (100%)	108 (100%)	0	100	100
1	GG	108/108 (100%)	108 (100%)	0	100	100
1	GH	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	GI	108/108 (100%)	108 (100%)	0	100	100
1	GK	108/108 (100%)	108 (100%)	0	100	100
1	GL	108/108 (100%)	108 (100%)	0	100	100
1	GM	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	GN	108/108 (100%)	108 (100%)	0	100	100
1	GO	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	GP	108/108 (100%)	108 (100%)	0	100	100
1	GQ	108/108 (100%)	108 (100%)	0	100	100
1	GR	108/108 (100%)	108 (100%)	0	100	100
1	GS	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	GT	108/108 (100%)	108 (100%)	0	100	100
1	GU	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	GV	108/108 (100%)	108 (100%)	0	100	100
1	GW	108/108 (100%)	108 (100%)	0	100	100
1	GX	108/108 (100%)	108 (100%)	0	100	100
1	GY	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	GZ	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	HA	108/108 (100%)	107 (99%)	1 (1%)	75	86

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	HB	108/108 (100%)	108 (100%)	0	100	100
1	HC	108/108 (100%)	108 (100%)	0	100	100
1	HD	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	HE	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	HF	108/108 (100%)	108 (100%)	0	100	100
1	HG	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	HI	108/108 (100%)	108 (100%)	0	100	100
1	HJ	108/108 (100%)	108 (100%)	0	100	100
1	HK	108/108 (100%)	108 (100%)	0	100	100
1	HL	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	HM	108/108 (100%)	108 (100%)	0	100	100
1	HN	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	HO	108/108 (100%)	108 (100%)	0	100	100
1	HP	108/108 (100%)	108 (100%)	0	100	100
1	HQ	108/108 (100%)	108 (100%)	0	100	100
1	HR	108/108 (100%)	108 (100%)	0	100	100
1	HS	108/108 (100%)	108 (100%)	0	100	100
1	HT	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	HU	108/108 (100%)	108 (100%)	0	100	100
1	HV	108/108 (100%)	108 (100%)	0	100	100
1	HW	108/108 (100%)	108 (100%)	0	100	100
1	HX	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	HY	108/108 (100%)	108 (100%)	0	100	100
1	HZ	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	IA	108/108 (100%)	108 (100%)	0	100	100
1	IB	108/108 (100%)	108 (100%)	0	100	100
1	IC	108/108 (100%)	108 (100%)	0	100	100
1	ID	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	IE	108/108 (100%)	108 (100%)	0	100	100
1	IF	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	IG	108/108 (100%)	108 (100%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	IH	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	II	108/108 (100%)	108 (100%)	0	100	100
1	IJ	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	IK	108/108 (100%)	108 (100%)	0	100	100
1	IL	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	IM	108/108 (100%)	108 (100%)	0	100	100
1	IN	108/108 (100%)	108 (100%)	0	100	100
1	IO	108/108 (100%)	108 (100%)	0	100	100
1	IP	108/108 (100%)	108 (100%)	0	100	100
1	IQ	108/108 (100%)	108 (100%)	0	100	100
1	IR	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	IS	108/108 (100%)	108 (100%)	0	100	100
1	IT	108/108 (100%)	108 (100%)	0	100	100
1	IU	108/108 (100%)	108 (100%)	0	100	100
1	IV	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	IW	108/108 (100%)	108 (100%)	0	100	100
1	IX	108/108 (100%)	108 (100%)	0	100	100
1	IZ	108/108 (100%)	108 (100%)	0	100	100
1	JA	108/108 (100%)	108 (100%)	0	100	100
1	JB	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	JC	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	JD	108/108 (100%)	108 (100%)	0	100	100
1	JE	108/108 (100%)	108 (100%)	0	100	100
1	JF	108/108 (100%)	108 (100%)	0	100	100
1	JG	108/108 (100%)	108 (100%)	0	100	100
1	JH	108/108 (100%)	108 (100%)	0	100	100
1	JI	108/108 (100%)	107 (99%)	1 (1%)	75	86
1	JJ	108/108 (100%)	108 (100%)	0	100	100
All	All	25920/25920 (100%)	25873 (100%)	47 (0%)	91	96

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	HA	33	ARG
1	HX	33	ARG
1	HD	71	MET
1	HL	33	ARG
1	ID	33	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	DI	34	GLN
1	IT	88	ASN
1	EA	34	GLN
1	IR	2	ASN
1	GR	111	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 oligosaccharides 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.

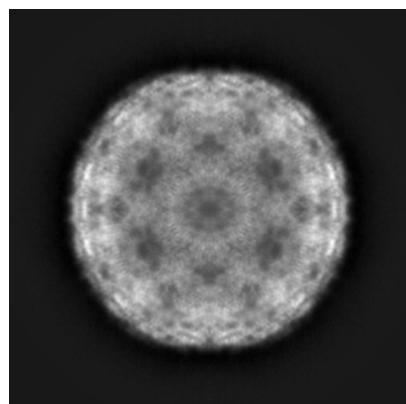
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41657. These allow visual inspection of the internal detail of the map and identification of artifacts.

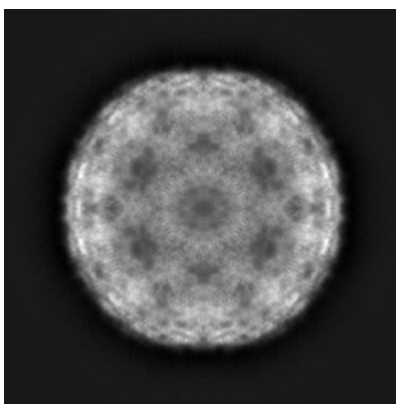
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

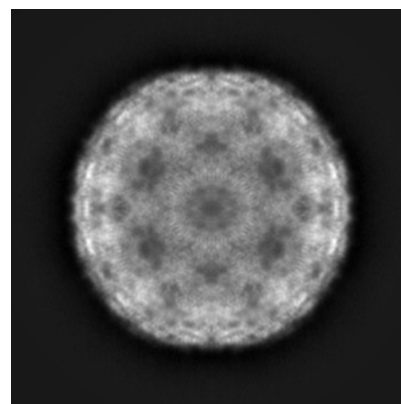
#### 6.1.1 Primary map



X

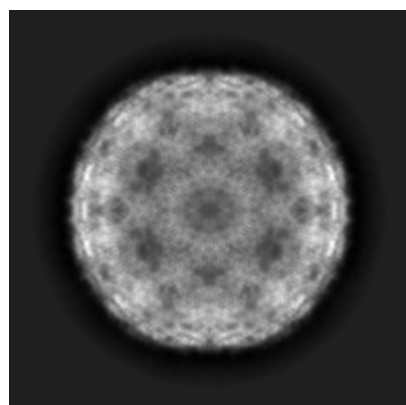


Y

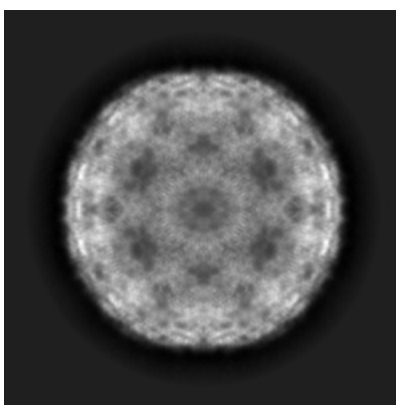


Z

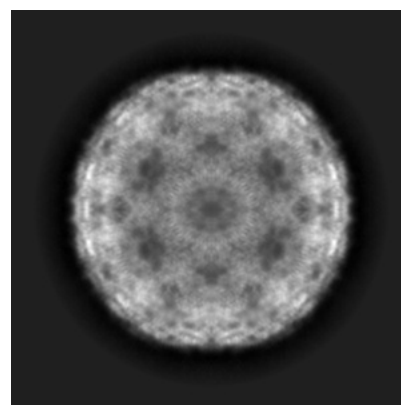
#### 6.1.2 Raw map



X



Y

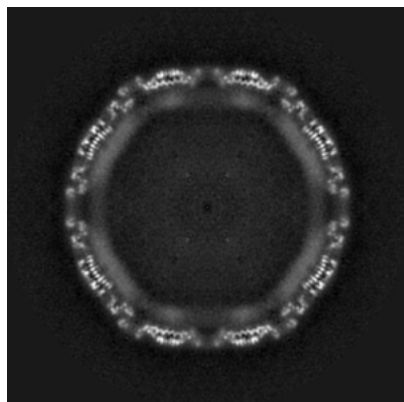


Z

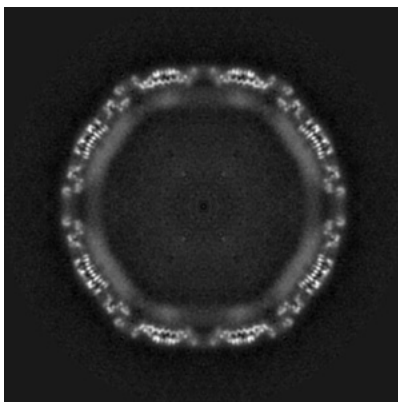
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

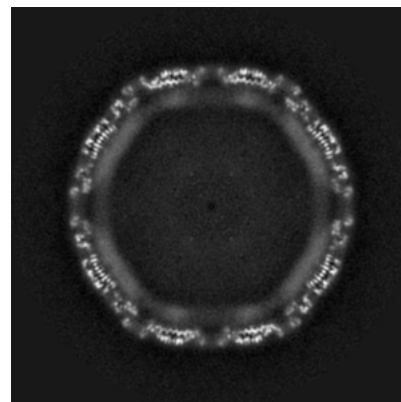
### 6.2.1 Primary map



X Index: 216

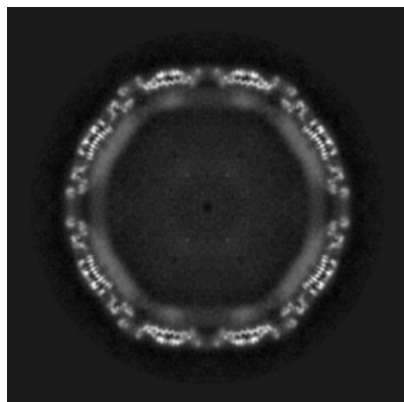


Y Index: 216

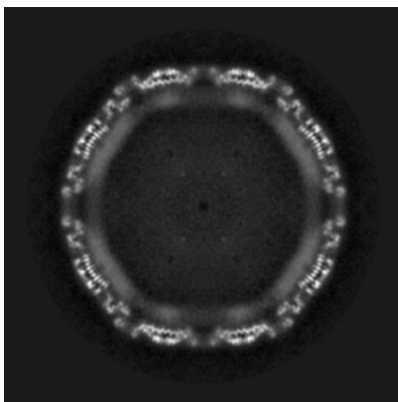


Z Index: 216

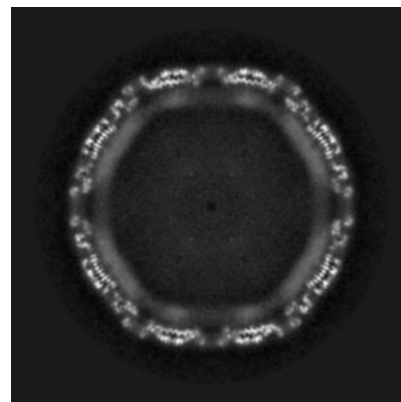
### 6.2.2 Raw map



X Index: 216



Y Index: 216

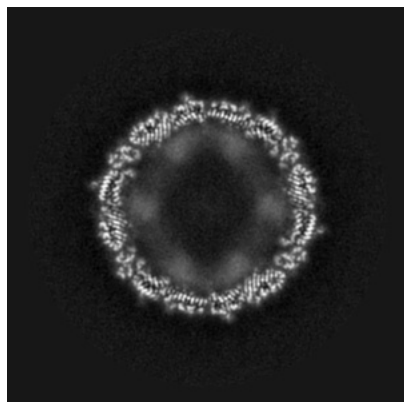


Z Index: 216

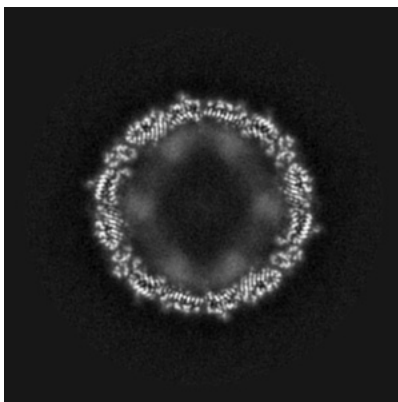
The images above show central slices of the map in three orthogonal directions.

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

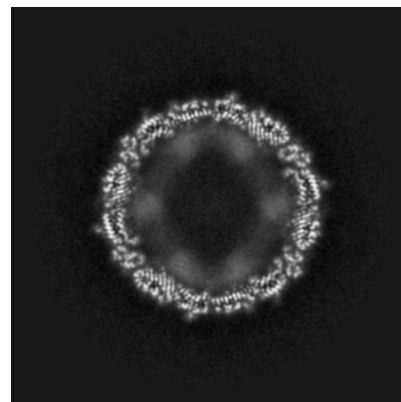
### 6.3.1 Primary map



X Index: 117

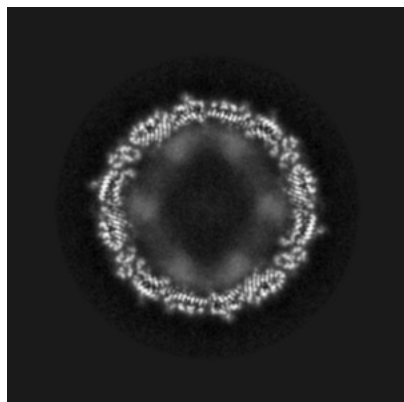


Y Index: 117

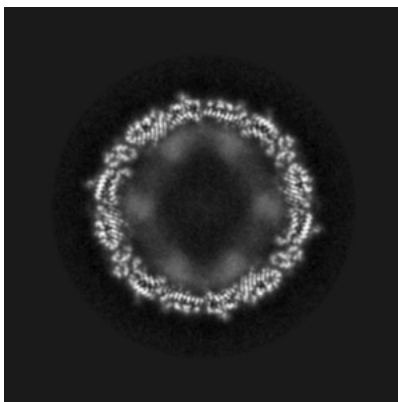


Z Index: 314

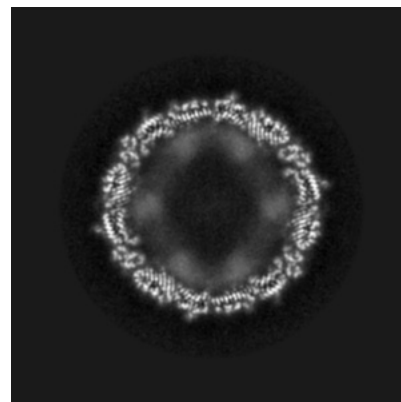
### 6.3.2 Raw map



X Index: 117



Y Index: 117

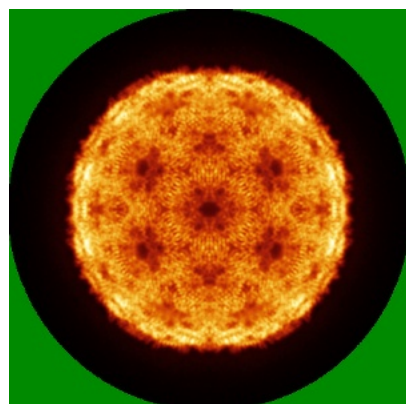


Z Index: 314

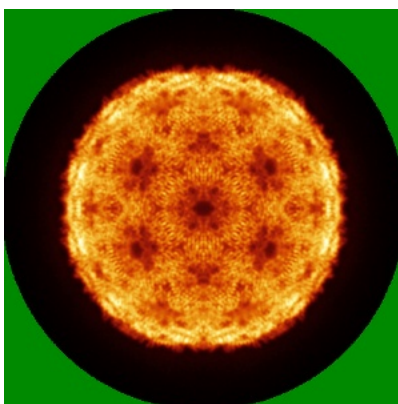
The images above show the largest variance slices of the map in three orthogonal directions.

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

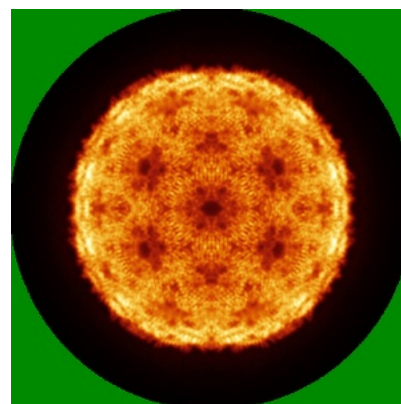
### 6.4.1 Primary map



X

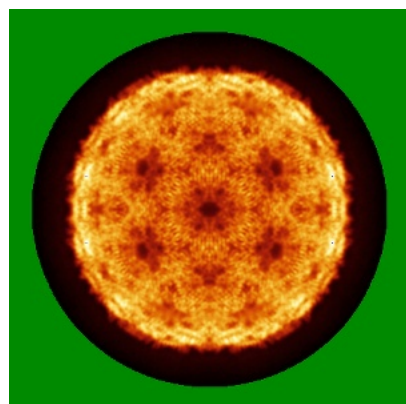


Y

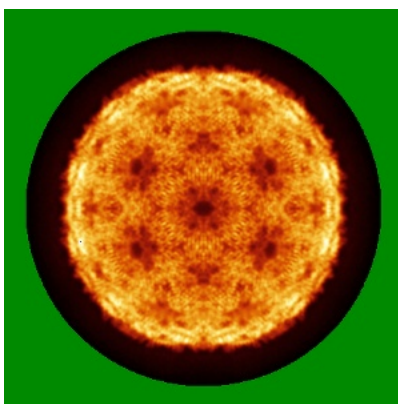


Z

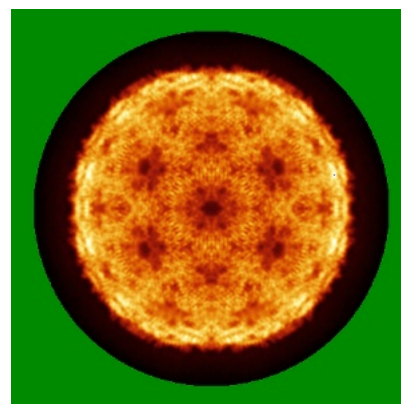
### 6.4.2 Raw map



X



Y



Z

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



## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



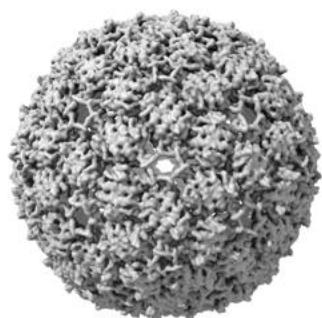
Y



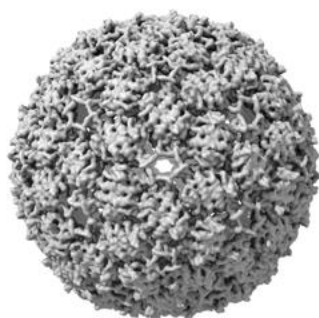
Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

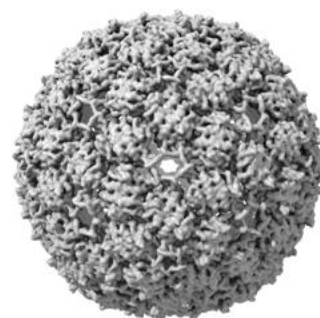
### 6.5.2 Raw map



X



Y



Z

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

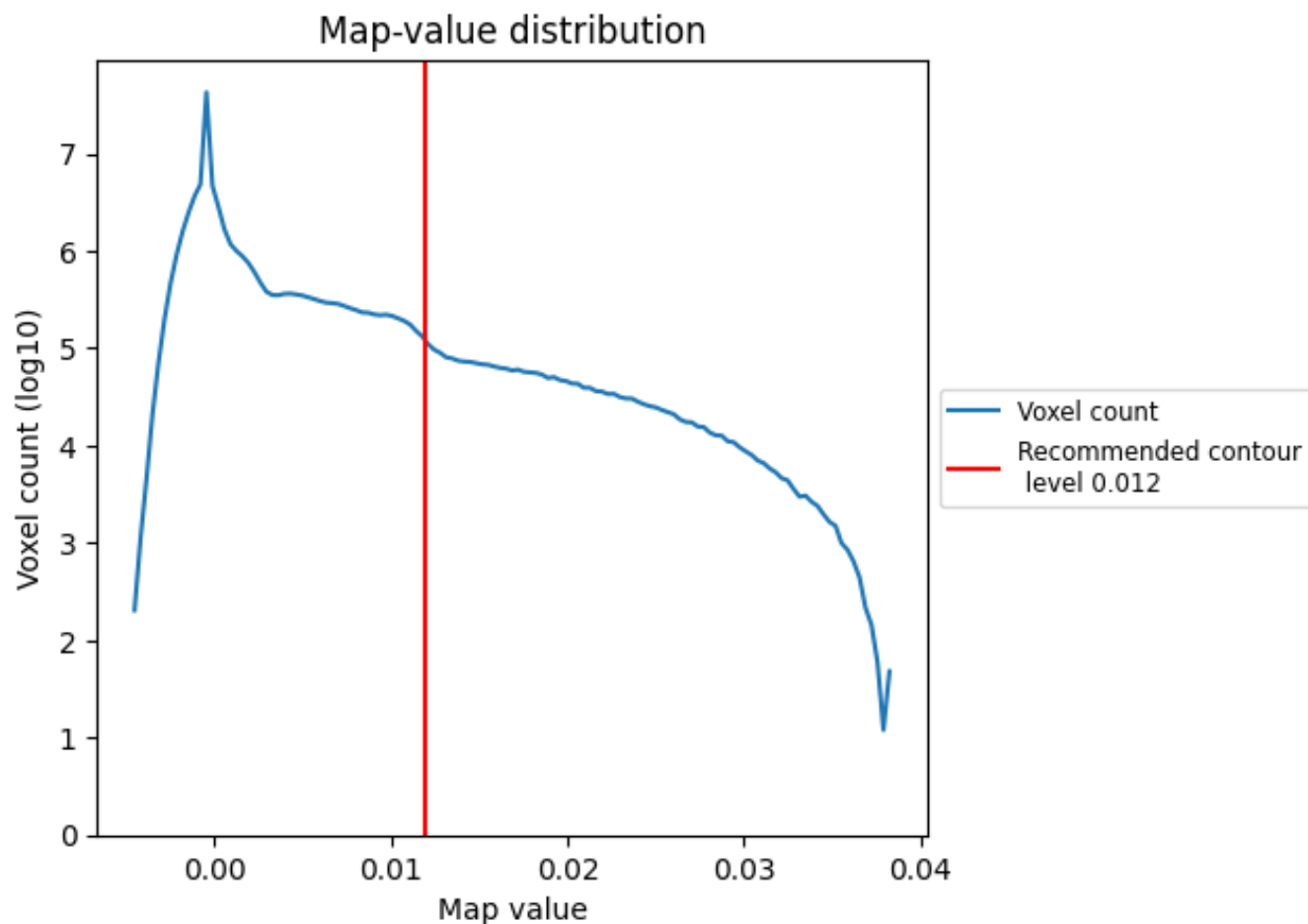
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

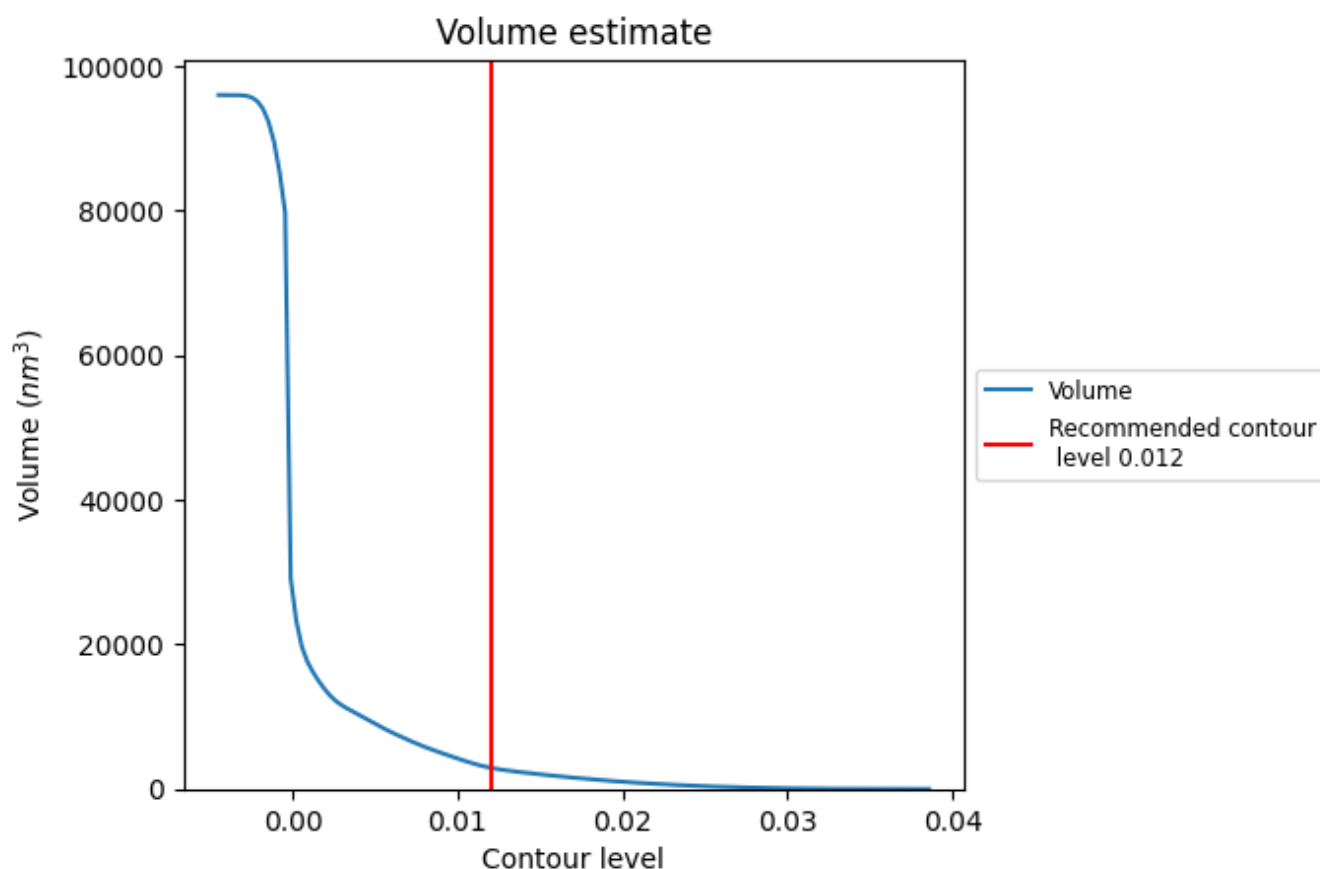
### 7.1 Map-value distribution [i](#)



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.



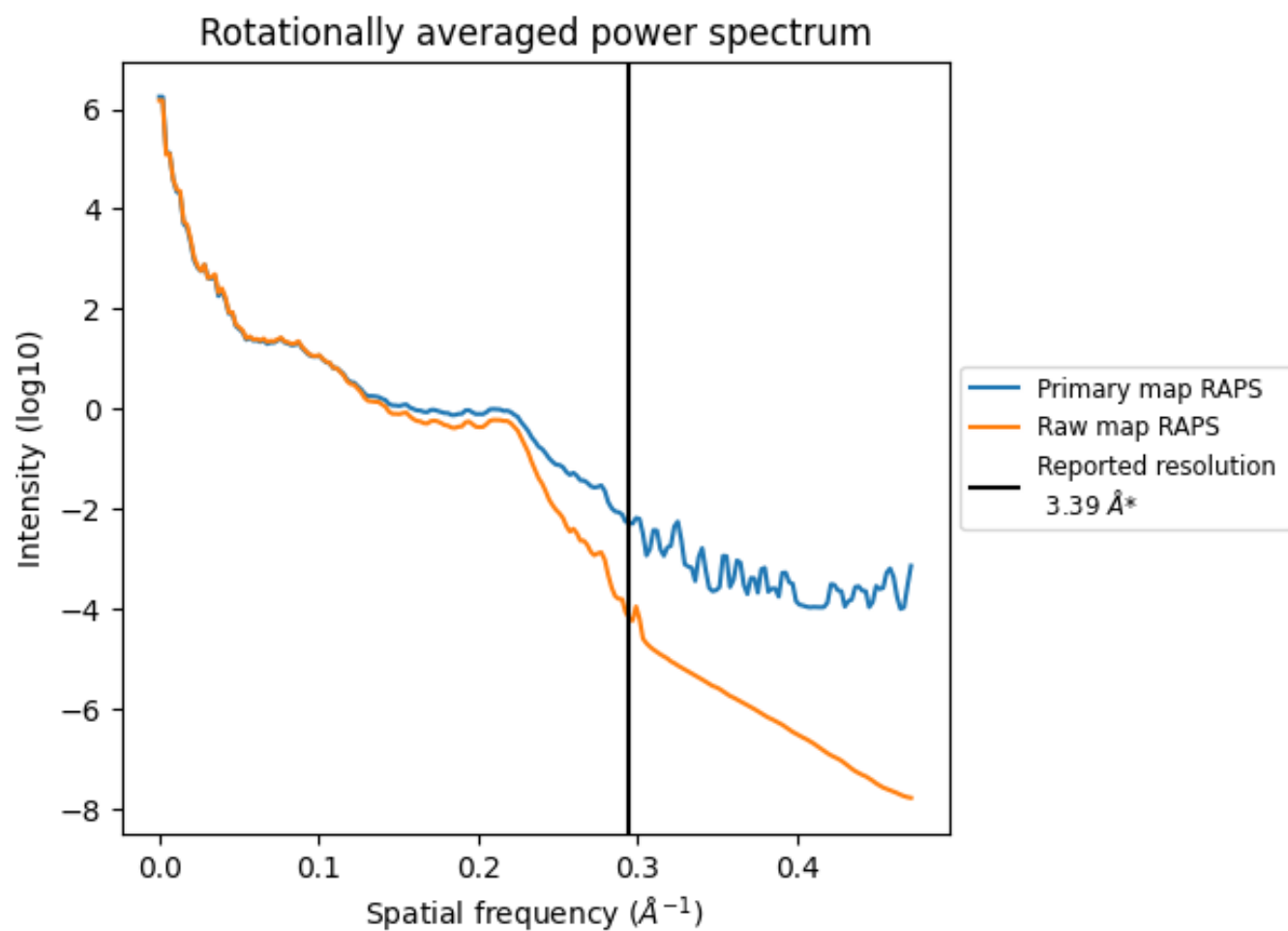
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2923 nm<sup>3</sup>; this corresponds to an approximate mass of 2640 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

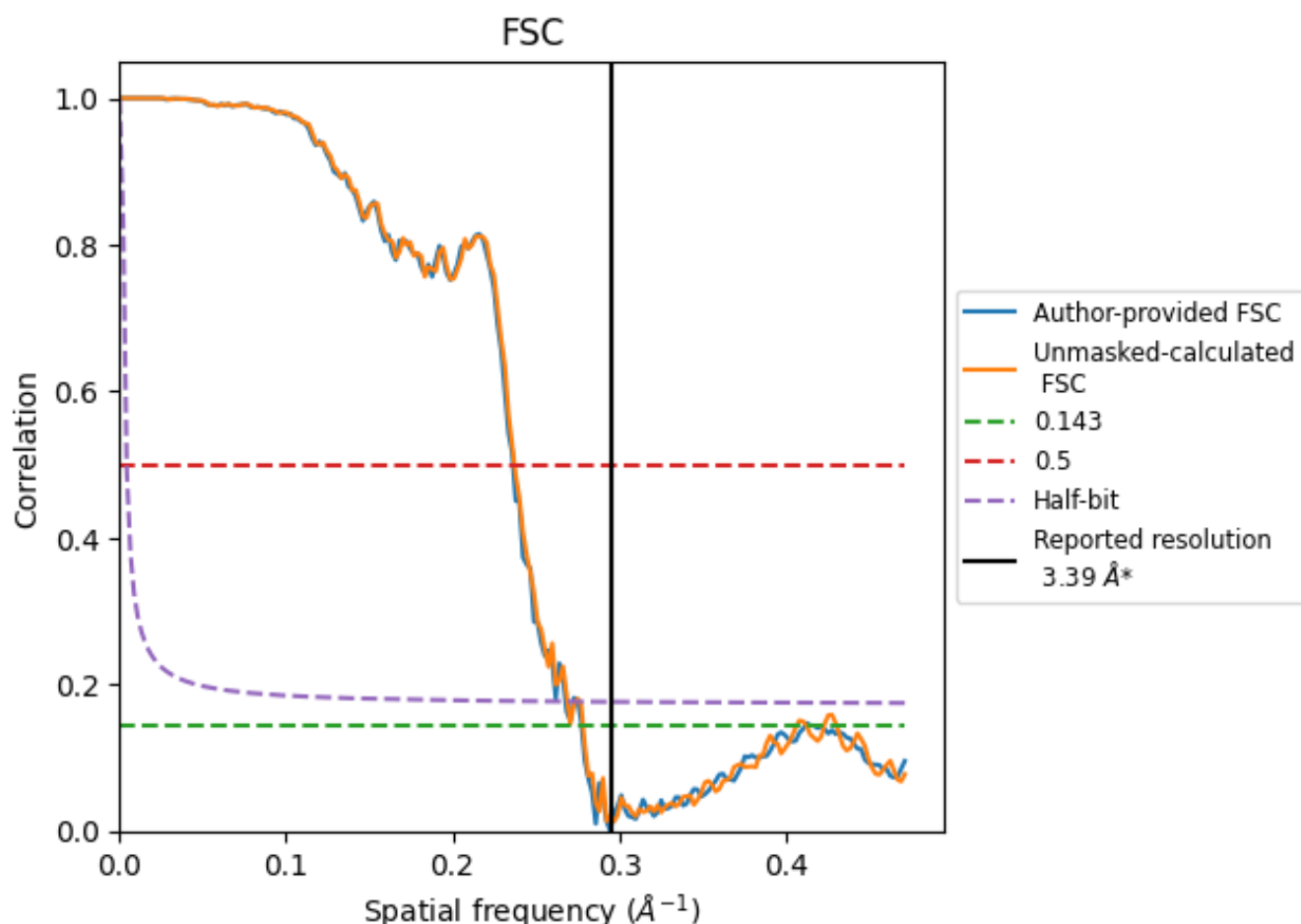


\*Reported resolution corresponds to spatial frequency of 0.295 Å<sup>-1</sup>

## 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 0.295 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

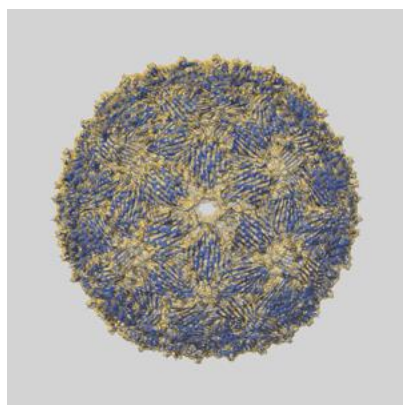
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.39	-	-
Author-provided FSC curve	3.60	4.23	3.73
Unmasked-calculated*	3.59	4.21	3.72

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

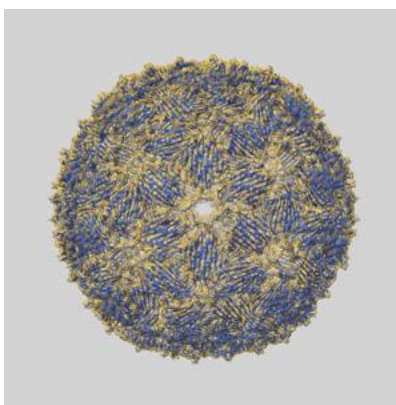
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41657 and PDB model 8TW2. Per-residue inclusion information can be found in section [3](#) on page [25](#).

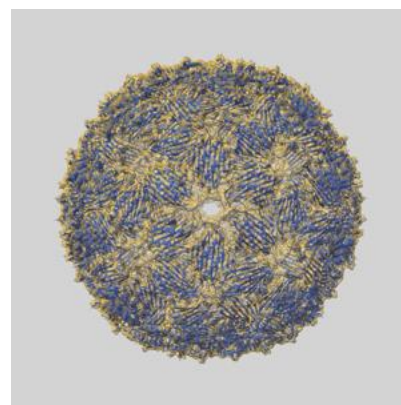
### 9.1 Map-model overlay [i](#)



X



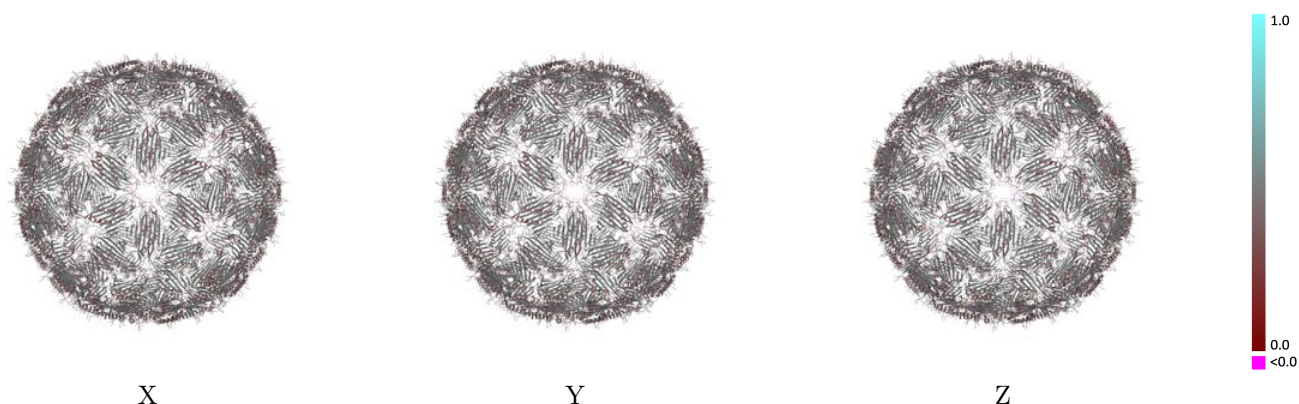
Y



Z

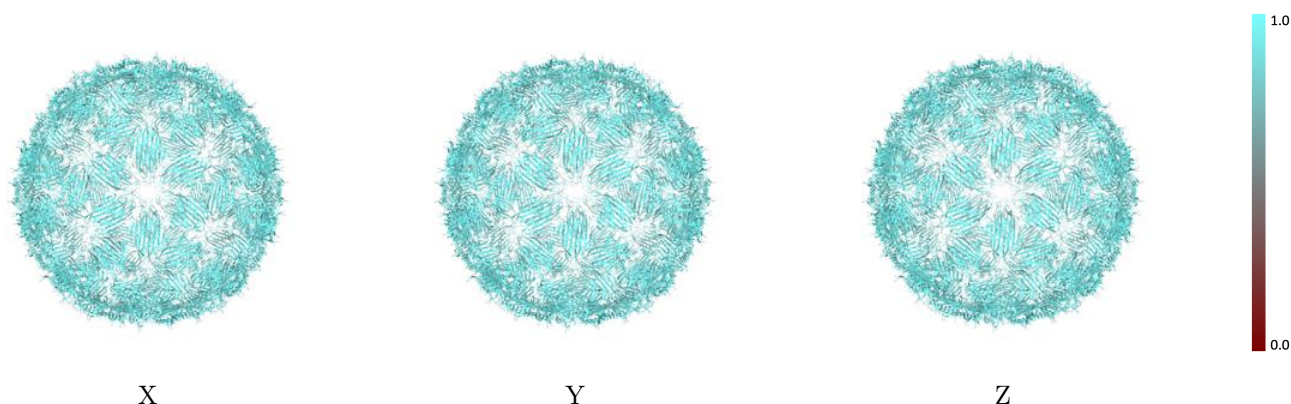
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



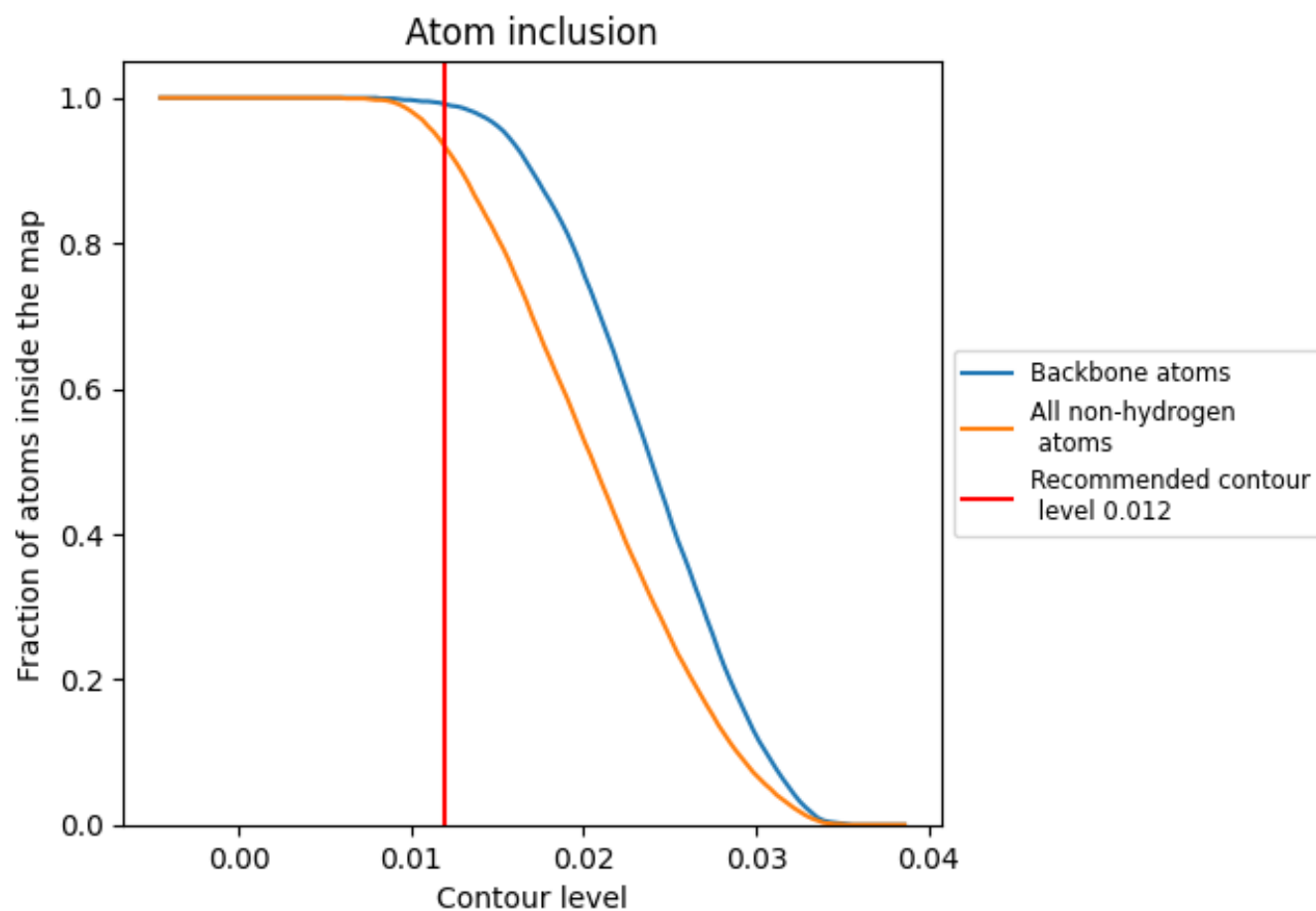
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 93% 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 (0.012) and Q-score for the entire model and for each chain.





















































































Chain	Atom inclusion	Q-score
All	 0.9320	 0.4320
AA	 0.9300	 0.4360
AB	 0.9310	 0.4380
AC	 0.9290	 0.4380
AD	 0.9260	 0.4340
AE	 0.9320	 0.4380
AF	 0.9320	 0.4370
AG	 0.9320	 0.4390
AH	 0.9320	 0.4350
AI	 0.9300	 0.4360
AJ	 0.9340	 0.4360
AK	 0.9260	 0.4360
AL	 0.9300	 0.4330
AM	 0.9290	 0.4370
AN	 0.9300	 0.4350
AO	 0.9220	 0.4360
AP	 0.9420	 0.4380
AQ	 0.9270	 0.4370
AR	 0.9300	 0.4370
AS	 0.9340	 0.4370
AT	 0.9360	 0.4380
AU	 0.9330	 0.4390
AV	 0.9340	 0.4370
AW	 0.9290	 0.4300
AX	 0.9240	 0.4380
AY	 0.9310	 0.4370
AZ	 0.9330	 0.4340
BA	 0.9250	 0.4340
BB	 0.9410	 0.4380
BC	 0.9290	 0.4370
BD	 0.9420	 0.4360
BE	 0.9260	 0.4340
BF	 0.9380	 0.4340
BG	 0.9340	 0.4390
BH	 0.9410	 0.4400



*Continued on next page...*





















































































*Continued from previous page...*

Chain	Atom inclusion	Q-score
BI	 0.9300	 0.4390
BJ	 0.9320	 0.4380
BK	 0.9320	 0.4340
BL	 0.9300	 0.4420
BM	 0.9300	 0.4370
BN	 0.9320	 0.4390
BO	 0.9320	 0.4370
BP	 0.9380	 0.4380
BQ	 0.9300	 0.4370
BR	 0.9240	 0.4400
BS	 0.9310	 0.4370
BT	 0.9340	 0.4360
BU	 0.9320	 0.4360
BV	 0.9330	 0.4350
BW	 0.9290	 0.4370
BX	 0.9310	 0.4380
BY	 0.9310	 0.4370
BZ	 0.9290	 0.4410
CA	 0.9240	 0.4320
CB	 0.9290	 0.4340
CC	 0.9330	 0.4370
CD	 0.9340	 0.4370
CE	 0.9310	 0.4410
CF	 0.9300	 0.4350
CG	 0.9220	 0.4390
CH	 0.9320	 0.4330
CI	 0.9310	 0.4320
CJ	 0.9300	 0.4390
CK	 0.9270	 0.4390
CL	 0.9240	 0.4330
CM	 0.9270	 0.4330
CN	 0.9410	 0.4340
CO	 0.9330	 0.4380
CP	 0.9250	 0.4340
CQ	 0.9330	 0.4360
CR	 0.9440	 0.4360
CS	 0.9320	 0.4380
CT	 0.9330	 0.4380
CU	 0.9270	 0.4350
CV	 0.9240	 0.4370
CW	 0.9300	 0.4370
CX	 0.9320	 0.4330





















































































*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
CY	 0.9320	 0.4380
CZ	 0.9330	 0.4360
DA	 0.9290	 0.4350
DB	 0.9340	 0.4380
DC	 0.9250	 0.4410
DE	 0.9320	 0.4340
DF	 0.9300	 0.4380
DG	 0.9430	 0.4360
DH	 0.9330	 0.4360
DI	 0.9330	 0.4350
DJ	 0.9270	 0.4340
DK	 0.9360	 0.4410
DL	 0.9320	 0.4380
DM	 0.9300	 0.4340
DN	 0.9270	 0.4380
DO	 0.9310	 0.4360
DP	 0.9210	 0.4370
DQ	 0.9410	 0.4380
DR	 0.9350	 0.4380
DS	 0.9420	 0.4390
DT	 0.9240	 0.4350
DU	 0.9290	 0.4300
DV	 0.9300	 0.4350
DW	 0.9310	 0.4370
DX	 0.9230	 0.4360
DY	 0.9420	 0.4370
DZ	 0.9330	 0.4380
EA	 0.9390	 0.4390
EB	 0.9340	 0.4340
EC	 0.9320	 0.4390
ED	 0.9310	 0.4360
EE	 0.9310	 0.4360
EF	 0.9270	 0.4330
EG	 0.9250	 0.4360
EH	 0.9310	 0.4360
EI	 0.9370	 0.4360
EJ	 0.9310	 0.4390
EK	 0.9270	 0.4340
EL	 0.9320	 0.4370
EM	 0.9370	 0.4420
EN	 0.9330	 0.4390
EO	 0.9380	 0.4370





















































































*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
EP	 0.9240	 0.4380
EQ	 0.9330	 0.4310
ER	 0.9340	 0.4240
ES	 0.9350	 0.4300
ET	 0.9290	 0.4260
EU	 0.9310	 0.4280
EV	 0.9250	 0.4230
EW	 0.9400	 0.4290
EX	 0.9400	 0.4230
EY	 0.9340	 0.4320
EZ	 0.9300	 0.4230
FA	 0.9350	 0.4270
FB	 0.9240	 0.4260
FC	 0.9380	 0.4340
FD	 0.9350	 0.4250
FE	 0.9340	 0.4330
FF	 0.9230	 0.4210
FG	 0.9340	 0.4300
FH	 0.9240	 0.4160
FI	 0.9340	 0.4350
FJ	 0.9290	 0.4240
FK	 0.9320	 0.4380
FL	 0.9310	 0.4220
FM	 0.9380	 0.4330
FN	 0.9270	 0.4220
FO	 0.9360	 0.4370
FP	 0.9300	 0.4210
FQ	 0.9370	 0.4360
FR	 0.9380	 0.4230
FS	 0.9350	 0.4320
FT	 0.9360	 0.4230
FU	 0.9350	 0.4330
FV	 0.9360	 0.4270
FW	 0.9360	 0.4250
FX	 0.9370	 0.4250
FY	 0.9370	 0.4360
FZ	 0.9300	 0.4230
GA	 0.9320	 0.4290
GB	 0.9380	 0.4250
GC	 0.9330	 0.4320
GD	 0.9360	 0.4260
GE	 0.9310	 0.4310













































































*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
GF	 0.9340	 0.4260
GG	 0.9390	 0.4360
GH	 0.9250	 0.4230
GI	 0.9350	 0.4340
GK	 0.9270	 0.4250
GL	 0.9240	 0.4310
GM	 0.9250	 0.4210
GN	 0.9340	 0.4360
GO	 0.9370	 0.4260
GP	 0.9380	 0.4330
GQ	 0.9170	 0.4160
GR	 0.9390	 0.4330
GS	 0.9230	 0.4250
GT	 0.9330	 0.4320
GU	 0.9230	 0.4270
GV	 0.9340	 0.4290
GW	 0.9340	 0.4240
GX	 0.9410	 0.4300
GY	 0.9310	 0.4230
GZ	 0.9330	 0.4300
HA	 0.9270	 0.4260
HB	 0.9370	 0.4340
HC	 0.9310	 0.4260
HD	 0.9290	 0.4260
HE	 0.9320	 0.4230
HF	 0.9330	 0.4350
HG	 0.9370	 0.4280
HI	 0.9340	 0.4270
HJ	 0.9320	 0.4240
HK	 0.9350	 0.4330
HL	 0.9300	 0.4260
HM	 0.9350	 0.4320
HN	 0.9330	 0.4300
HO	 0.9310	 0.4360
HP	 0.9300	 0.4250
HQ	 0.9320	 0.4310
HR	 0.9320	 0.4250
HS	 0.9360	 0.4340
HT	 0.9380	 0.4240
HU	 0.9340	 0.4350
HV	 0.9340	 0.4220
HW	 0.9400	 0.4350

*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
HX	 0.9260	 0.4220
HY	 0.9370	 0.4330
HZ	 0.9310	 0.4210
IA	 0.9360	 0.4350
IB	 0.9290	 0.4290
IC	 0.9350	 0.4270
ID	 0.9230	 0.4190
IE	 0.9320	 0.4330
IF	 0.9360	 0.4260
IG	 0.9370	 0.4310
IH	 0.9330	 0.4240
II	 0.9370	 0.4250
IJ	 0.9360	 0.4290
IK	 0.9290	 0.4250
IL	 0.9390	 0.4220
IM	 0.9310	 0.4280
IN	 0.9320	 0.4240
IO	 0.9320	 0.4290
IP	 0.9210	 0.4230
IQ	 0.9380	 0.4290
IR	 0.9380	 0.4250
IS	 0.9320	 0.4360
IT	 0.9330	 0.4250
IU	 0.9400	 0.4320
IV	 0.9260	 0.4210
IW	 0.9370	 0.4370
IX	 0.9380	 0.4270
IZ	 0.9410	 0.4330
JA	 0.9190	 0.4170
JB	 0.9390	 0.4300
JC	 0.9300	 0.4220
JD	 0.9350	 0.4310
JE	 0.9290	 0.4280
JF	 0.9380	 0.4330
JG	 0.9180	 0.4180
JH	 0.9380	 0.4320
JI	 0.9270	 0.4180
JJ	 0.9380	 0.4330