



# wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 04:51 PM UTC

PDB ID : 8TOC / pdb\_00008toc  
EMDB ID : EMD-41443  
Title : Acinetobacter phage AP205  
Authors : Meng, R.; Xing, Z.; Chang, J.; Zhang, J.  
Deposited on : 2023-08-03  
Resolution : 3.11 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>.

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

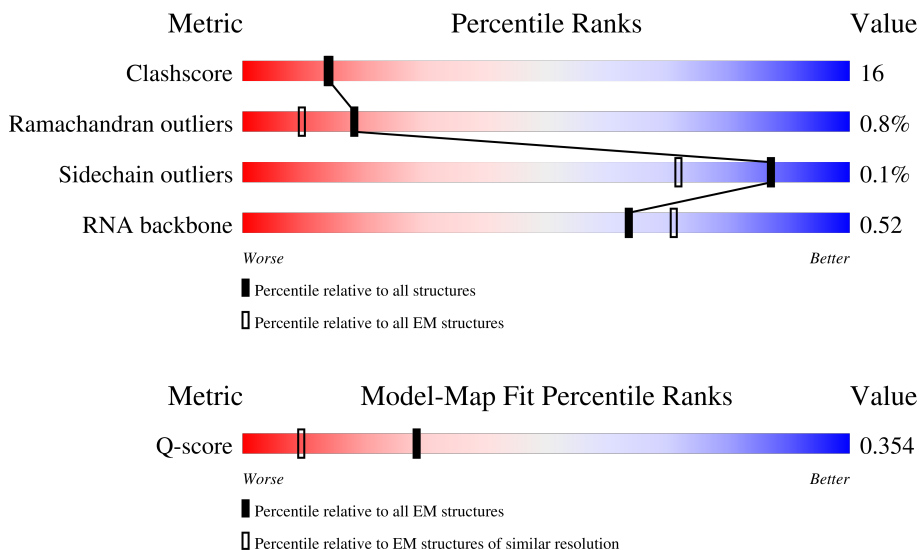
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 3.11 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14465 ( 2.61 - 3.61 )

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	R	4269	
2	a	534	
2	b	534	

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Mol	Chain	Length	Quality of chain
3	AB	129	61% 39%
3	AC	129	62% 37%
3	AE	129	71% 27%
3	AF	129	74% 26%
3	AG	129	66% 34%
3	AH	129	69% 31%
3	AI	129	66% 34%
3	AJ	129	71% 28%
3	AK	129	78% 22%
3	AL	129	65% 35%
3	AM	129	73% 26%
3	AN	129	66% 34%
3	AO	129	64% 36%
3	AP	129	64% 36%
3	AQ	129	73% 26%
3	AS	129	68% 31%
3	AT	129	70% 29%
3	AU	129	69% 31%
3	AV	129	68% 31%
3	AW	129	71% 29%
3	AX	129	63% 37%
3	AY	129	74% 26%
3	AZ	129	68% 28%
3	Ac	129	65% 35%
3	BA	129	67% 33%

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Mol	Chain	Length	Quality of chain	
3	BB	129	78%	22%
3	BC	129	73%	26%
3	BD	129	68%	31%
3	BE	129	70%	29%
3	BF	129	71%	29%
3	BG	129	64%	36%
3	BH	129	70%	29%
3	BI	129	70%	30%
3	BJ	129	68%	32%
3	BK	129	66%	34%
3	BL	129	72%	28%
3	BM	129	67%	33%
3	BN	129	63%	34%
3	BO	129	70%	29%
3	BP	129	74%	25%
3	BQ	129	67%	33%
3	BS	129	66%	34%
3	BT	129	67%	32%
3	BU	129	62%	37%
3	BV	129	71%	27%
3	BW	129	58%	42%
3	BX	129	71%	29%
3	BY	129	73%	27%
3	BZ	129	72%	28%
3	Bc	129	71%	29%

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Mol	Chain	Length	Quality of chain	
3	CA	129	71%	29%
3	CB	129	72%	28%
3	CC	129	66%	33%
3	CD	129	83%	17%
3	CE	129	66%	33%
3	CF	129	74%	26%
3	CG	129	71%	28%
3	CH	129	71%	29%
3	CI	129	67%	33%
3	CJ	129	75%	25%
3	CK	129	64%	36%
3	CL	129	73%	27%
3	CM	129	55%	44%
3	CN	129	56%	43%
3	CO	129	57%	43%
3	CP	129	71%	29%
3	CQ	129	73%	26%
3	CS	129	69%	31%
3	CT	129	78%	22%
3	CU	129	73%	27%
3	CV	129	64%	35%
3	CW	129	72%	27%
3	CX	129	67%	33%
3	CY	129	73%	27%
3	CZ	129	67%	33%

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Mol	Chain	Length	Quality of chain	
3	Cc	129	63%	37%
3	DA	129	71%	29%
3	DB	129	70%	30%
3	DC	129	69%	31%
3	DD	129	69%	30%
3	DE	129	74%	26%
3	DF	129	70%	30%
3	DG	129	74%	26%
3	DH	129	64%	36%
3	DI	129	70%	30%
3	DJ	129	64%	36%
3	DK	129	67%	33%
3	DL	129	66%	34%
3	DM	129	76%	23%
3	DN	129	58%	42%
3	DO	129	57%	43%
3	DQ	129	74%	26%
3	DS	129	71%	29%
3	DT	129	77%	22%
3	DU	129	69%	31%
3	DV	129	67%	32%
3	DW	129	77%	23%
3	DX	129	77%	23%
3	DY	129	72%	28%
3	DZ	129	67%	33%

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Mol	Chain	Length	Quality of chain	
3	Dc	129	64%	36%
3	EA	129	71%	29%
3	EB	129	83%	17%
3	EC	129	74%	26%
3	ED	129	64%	36%
3	EE	129	62%	35%
3	EF	129	67%	33%
3	EG	129	67%	31%
3	EH	129	63%	37%
3	EI	129	70%	30%
3	EJ	129	64%	36%
3	EK	129	67%	33%
3	EL	129	67%	33%
3	EM	129	70%	30%
3	EN	129	73%	26%
3	EO	129	67%	33%
3	EP	129	72%	26%
3	EQ	129	71%	29%
3	ES	129	74%	26%
3	ET	129	64%	34%
3	EU	129	63%	37%
3	EV	129	63%	37%
3	EW	129	67%	33%
3	EX	129	71%	28%
3	EY	129	73%	27%

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Mol	Chain	Length	Quality of chain	
3	EZ	129	71%	29%
3	Ec	129	60%	40%
3	FA	129	64%	36%
3	FB	129	60%	39%
3	FC	129	71%	28%
3	FD	129	64%	36%
3	FE	129	76%	24%
3	FF	129	67%	33%
3	FG	129	64%	36%
3	FH	129	74%	26%
3	FI	129	57%	43%
3	FJ	129	72%	28%
3	FK	129	68%	32%
3	FL	129	73%	27%
3	FM	129	69%	31%
3	FN	129	67%	33%
3	FO	129	71%	29%
3	FP	129	71%	29%
3	FQ	129	70%	30%
3	FS	129	72%	28%
3	FT	129	74%	26%
3	FU	129	68%	32%
3	FV	129	77%	23%
3	FW	129	65%	32%
3	FX	129	59%	40%




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Mol	Chain	Length	Quality of chain
3	FY	129	71% 29%
3	FZ	129	64% 34% 2%
3	Fc	129	74% 26% 1%
3	GA	129	50% 50% 1%
3	GB	129	74% 26%
3	GC	129	61% 34% 5%
3	GD	129	71% 29%
3	GE	129	58% 40% 2%
3	GF	129	68% 31% 1%
3	GG	129	78% 22% 1%
3	GH	129	64% 36%
3	GI	129	73% 26% 1%
3	GJ	129	70% 30%
3	GK	129	81% 19%
3	GL	129	69% 31%
3	GM	129	73% 27%
3	GN	129	69% 30% 1%
3	GO	129	82% 17% 1%
3	GP	129	69% 31%
3	GQ	129	72% 28%
3	GS	129	73% 27%
3	GT	129	71% 28% 1%
3	GU	129	70% 29% 1%
3	GV	129	62% 37% 1%
3	GW	129	77% 23%

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Mol	Chain	Length	Quality of chain
3	GX	129	 62% 32% 5% •
3	GY	129	 67% 32% •
3	Gc	129	 67% 33%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 271353 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 RNA chain called RNA (4269-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	R	4269	90441	40490	15694	29988	4269	0	0

- Molecule 2 is a protein called Maturation protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	a	534	4304	2746	765	776	17	0	0
2	b	534	4304	2746	765	776	17	0	0

- Molecule 3 is a protein called Coat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AB	129	968	602	171	191	4	0	0
3	AC	129	968	602	171	191	4	0	0
3	AE	129	968	602	171	191	4	0	0
3	AF	129	968	602	171	191	4	0	0
3	AG	129	968	602	171	191	4	0	0
3	AH	129	968	602	171	191	4	0	0
3	AI	129	968	602	171	191	4	0	0
3	AJ	129	968	602	171	191	4	0	0
3	AK	129	968	602	171	191	4	0	0
3	AL	129	968	602	171	191	4	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace	
3	AM	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	AN	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	AO	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	AP	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	AQ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	Ac	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	AS	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	AT	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	AU	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	AV	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	AW	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	AX	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	AY	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	AZ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BA	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BB	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BC	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BD	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BE	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BF	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BG	129	Total 968	C 602	N 171	O 191	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	BH	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BI	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BJ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BK	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BL	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BM	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BN	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BO	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BP	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BQ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	Bc	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BS	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BT	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BU	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BV	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BW	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BX	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BY	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BZ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CA	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CB	129	Total 968	C 602	N 171	O 191	S 4	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace	
3	CC	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CD	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CE	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CF	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CG	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CH	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CI	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CJ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CK	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CL	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CM	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CN	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CO	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CP	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CQ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	Cc	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CS	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CT	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CU	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CV	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CW	129	Total 968	C 602	N 171	O 191	S 4	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace	
3	CX	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CY	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CZ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DA	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DB	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DC	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DD	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DE	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DF	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DG	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DH	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DI	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DJ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DK	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DL	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DM	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DN	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DO	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DQ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	Dc	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DS	129	Total 968	C 602	N 171	O 191	S 4	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace	
3	DT	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DU	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DV	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DW	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DX	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DY	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DZ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EA	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EB	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EC	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	ED	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EE	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EF	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EG	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EH	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EI	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EJ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EK	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EL	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EM	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EN	129	Total 968	C 602	N 171	O 191	S 4	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace	
3	EO	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EP	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EQ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	Ec	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	ES	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	ET	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EU	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EV	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EW	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EX	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EY	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EZ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FA	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FB	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FC	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FD	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FE	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FF	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FG	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FH	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FI	129	Total 968	C 602	N 171	O 191	S 4	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace	
3	FJ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FK	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FL	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FM	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FN	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FO	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FP	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FQ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	Fc	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FS	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FT	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FU	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FV	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FW	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FX	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FY	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FZ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GA	129	Total 968	C 602	N 171	O 191	S 4	0	0
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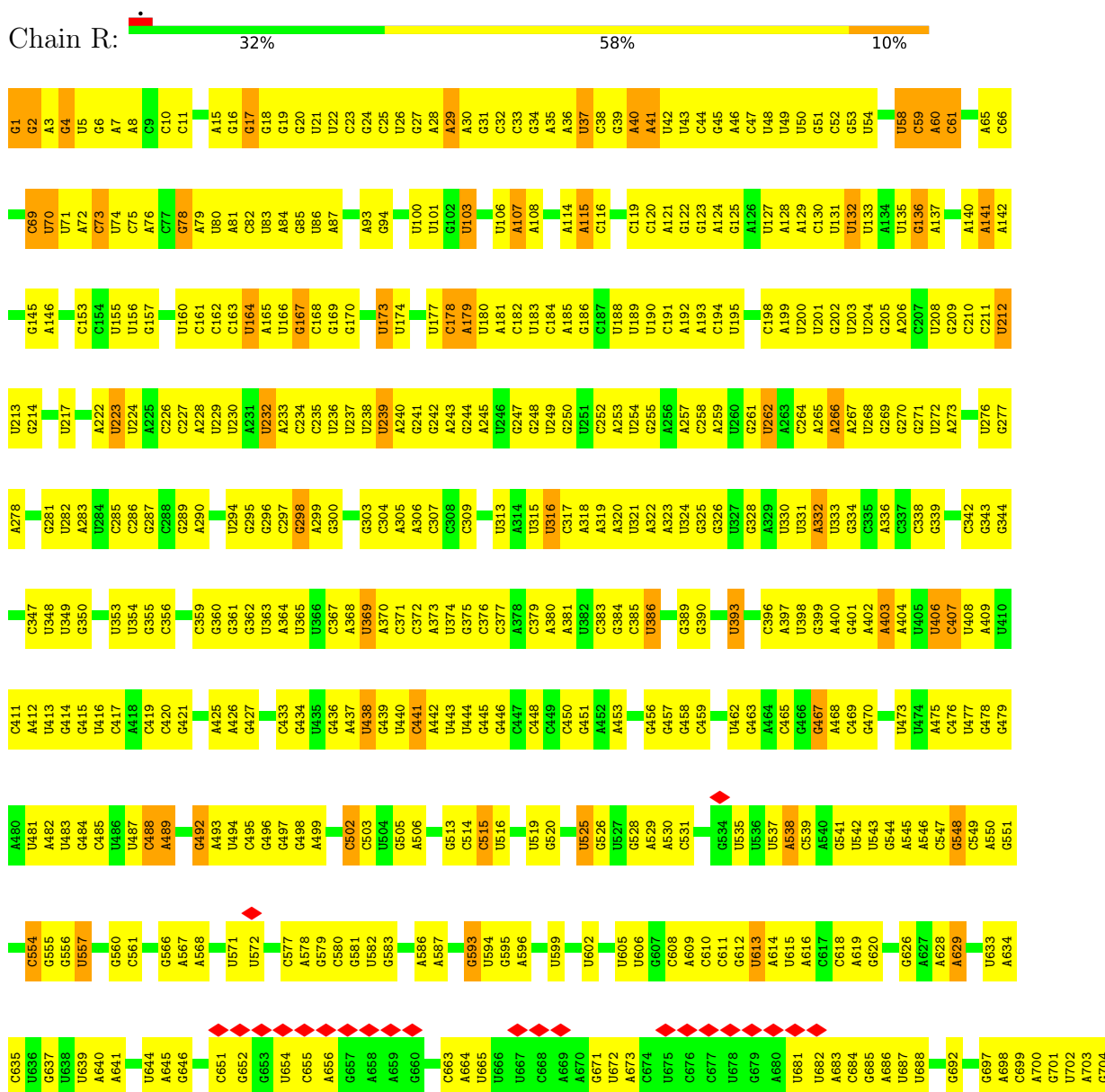
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3	GY	129	Total 968	C 602	N 171	O 191	S 4	0	0

### 3 Residue-property plots [i](#)

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

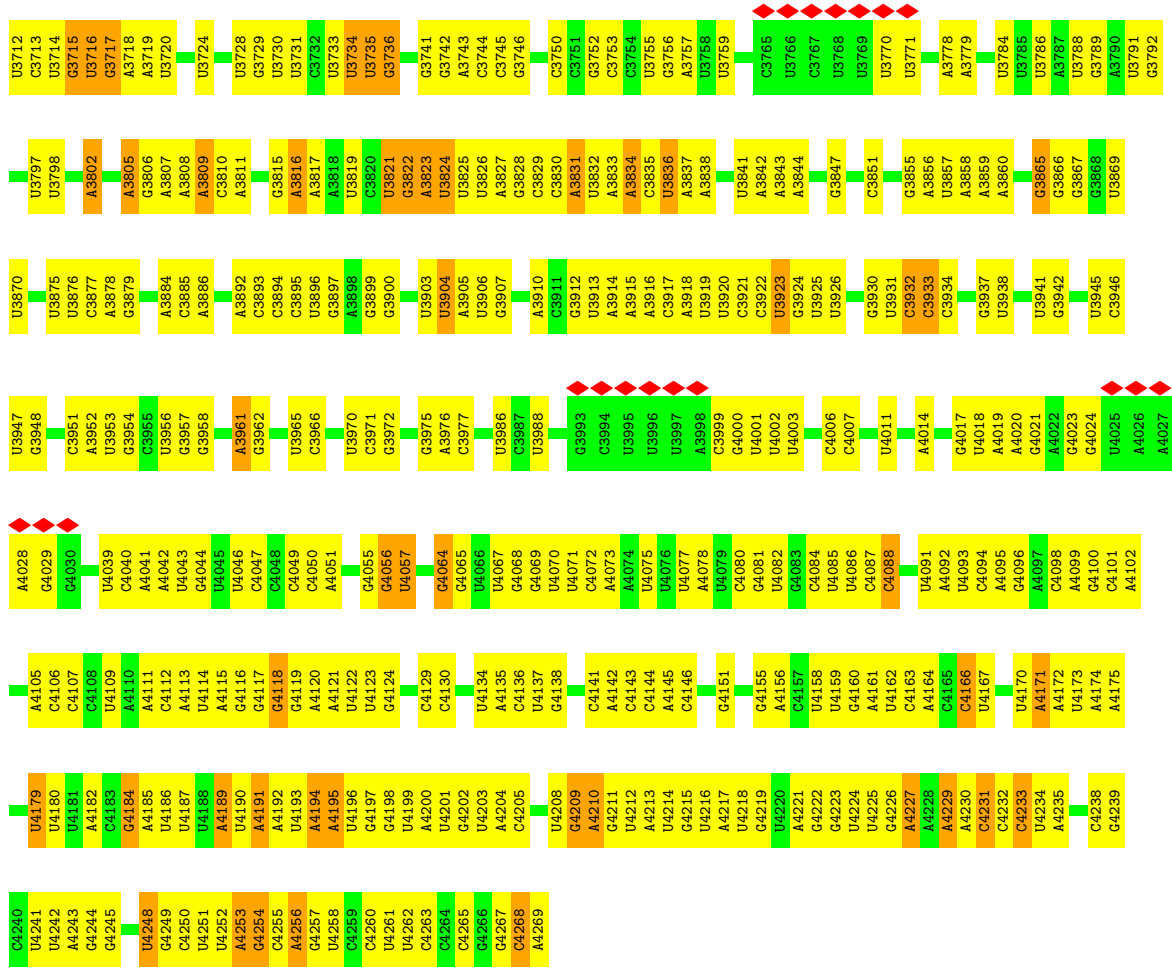
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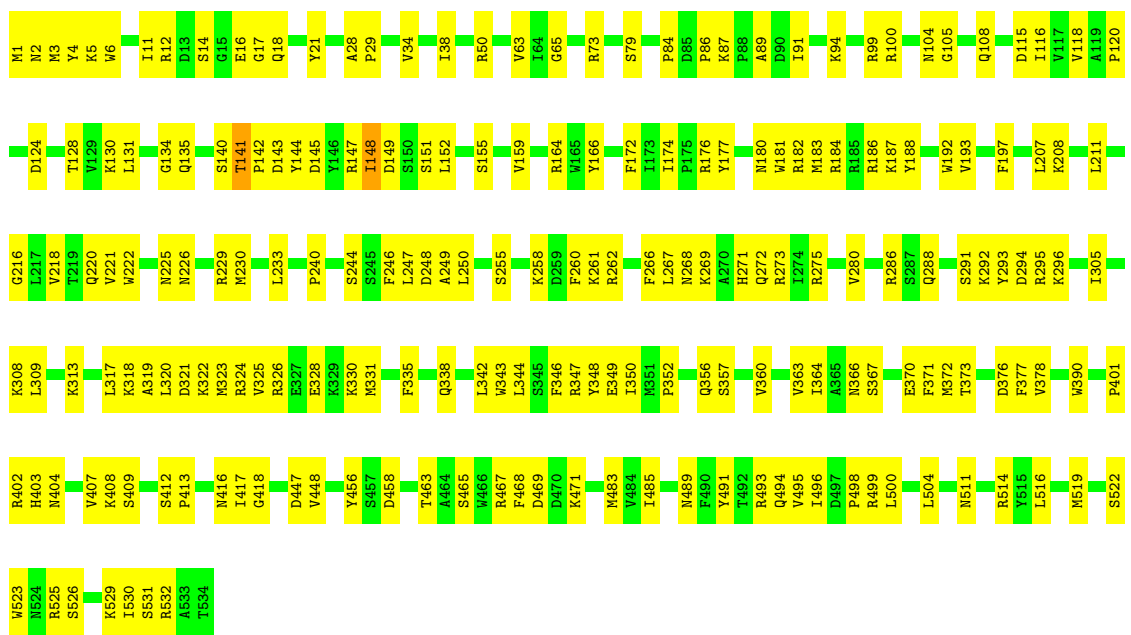


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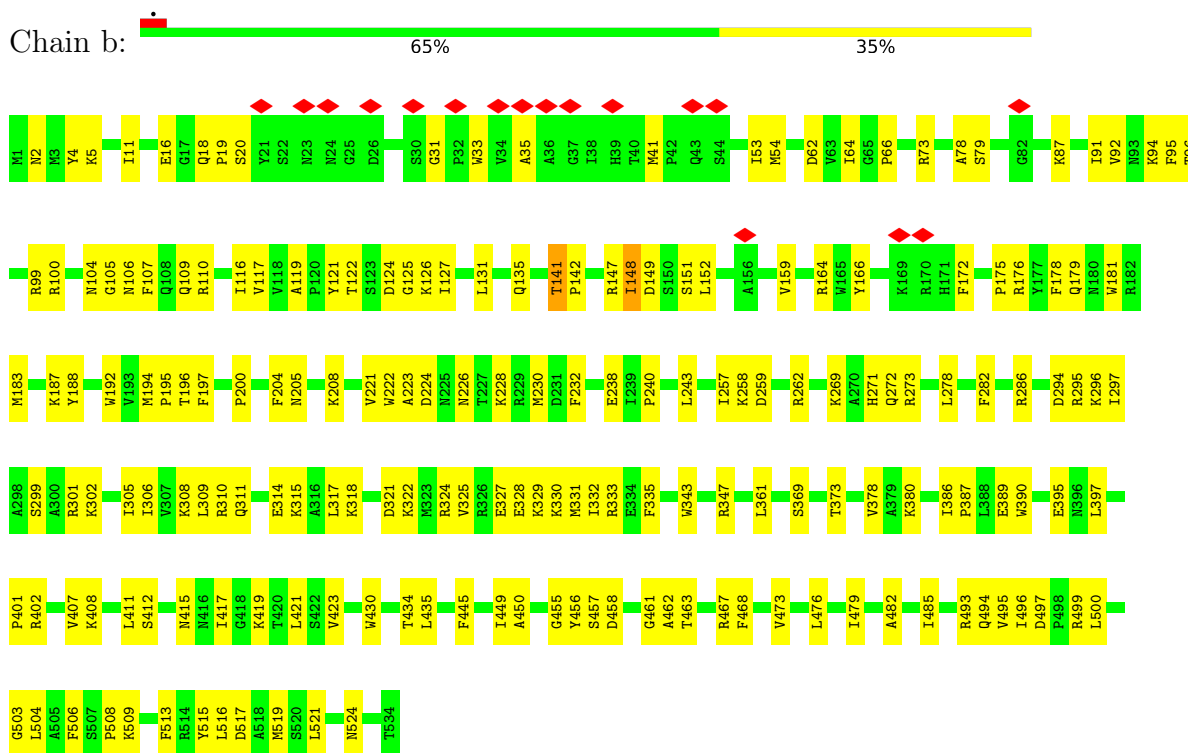
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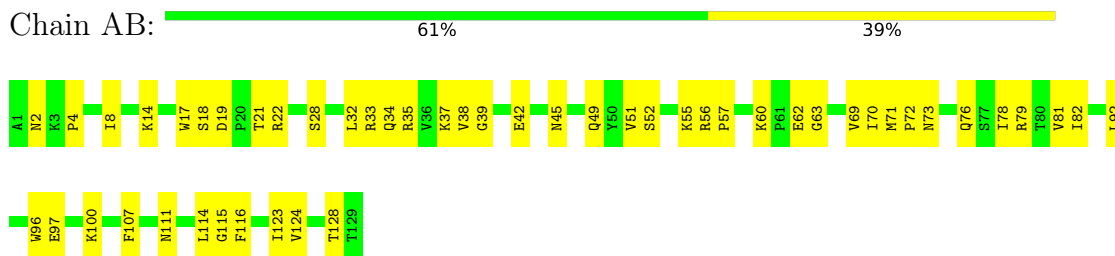
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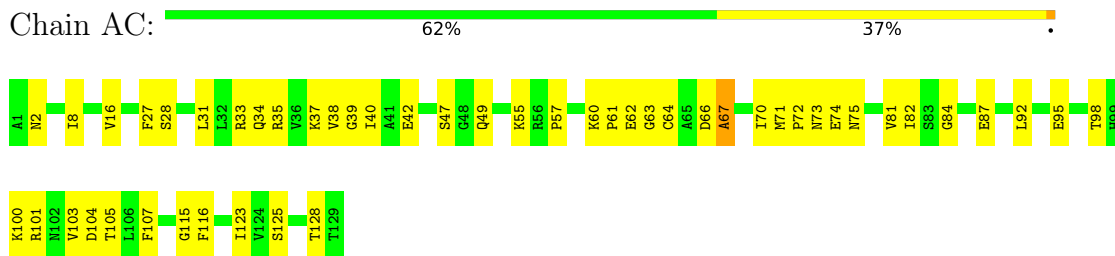
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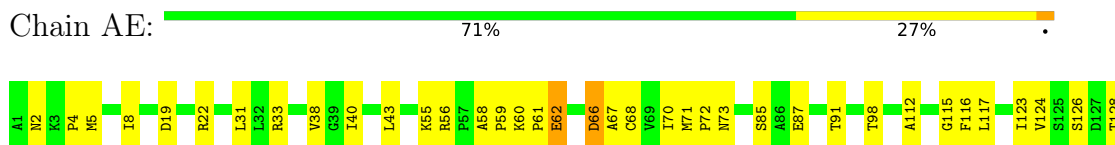
• Molecule 3: Coat protein



• Molecule 3: Coat protein

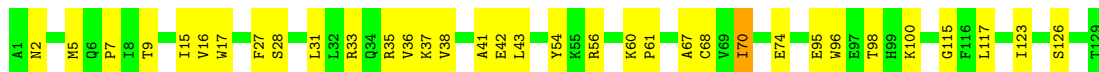
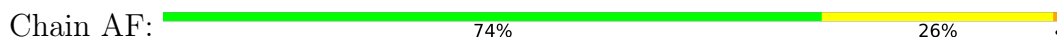


• Molecule 3: Coat protein



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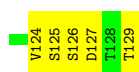
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• Molecule 3: Coat protein



• Molecule 3: Coat protein



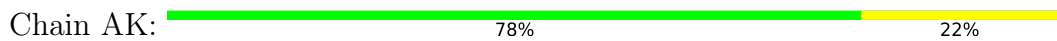
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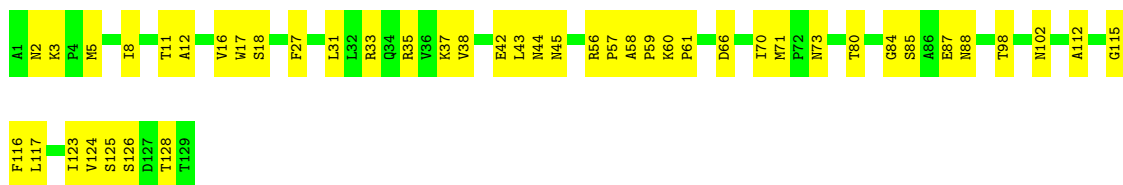
• Molecule 3: Coat protein



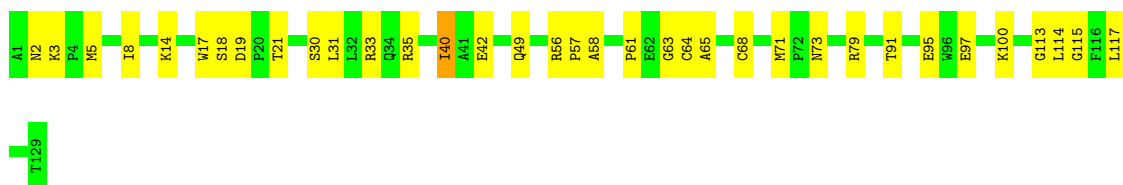
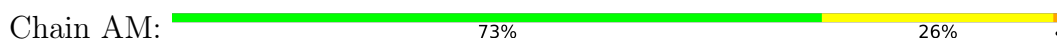
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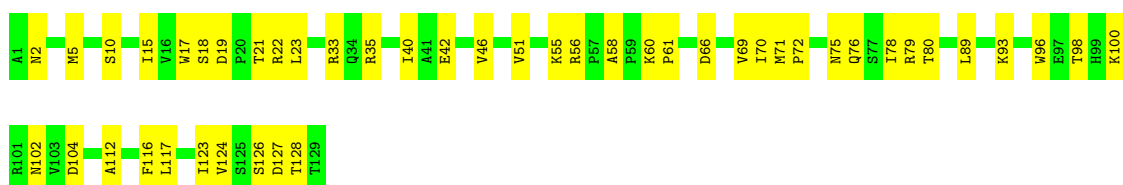
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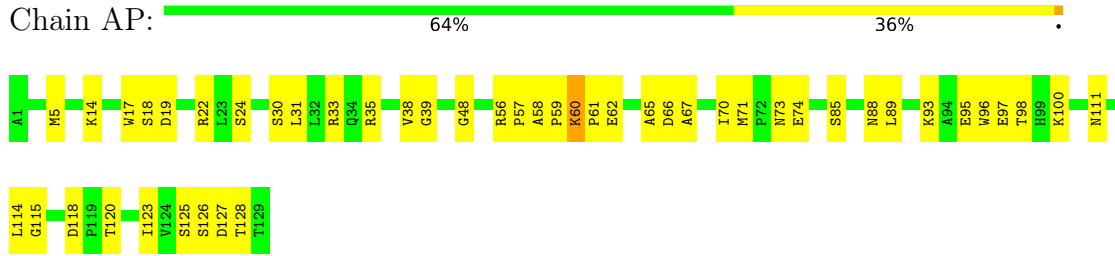
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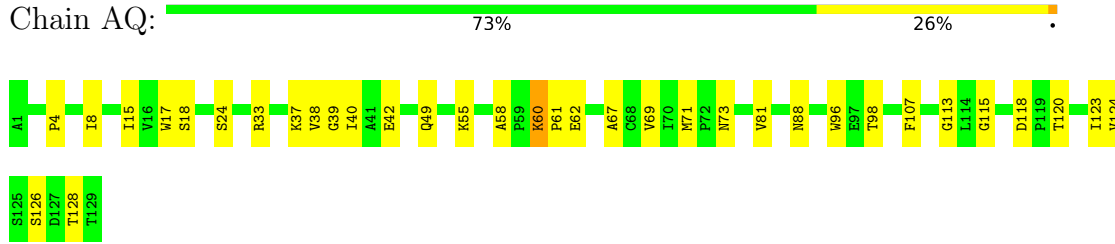
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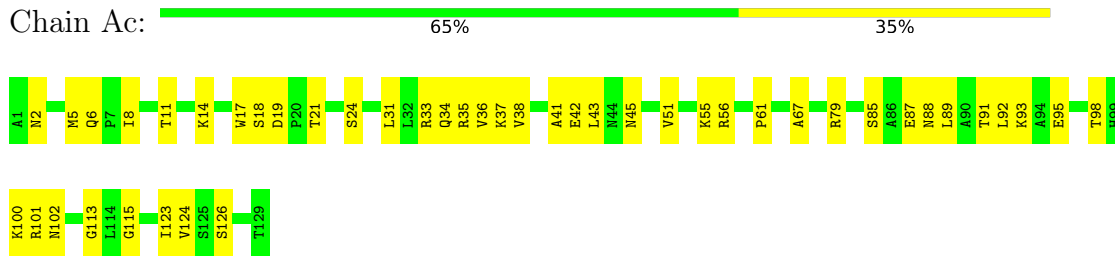
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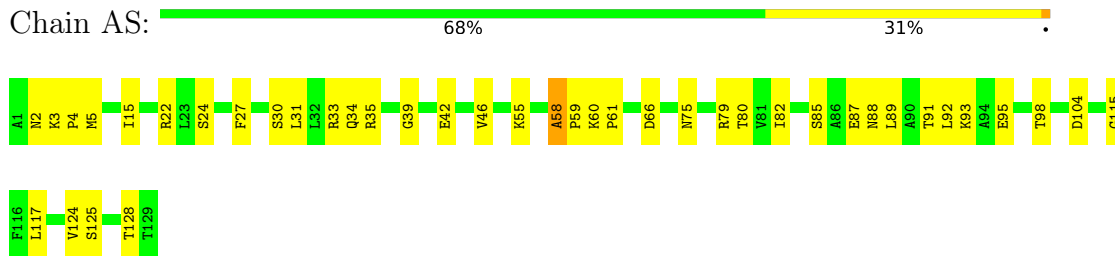
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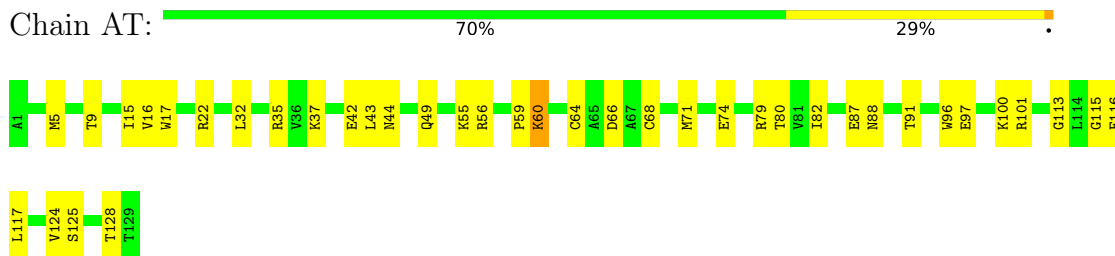
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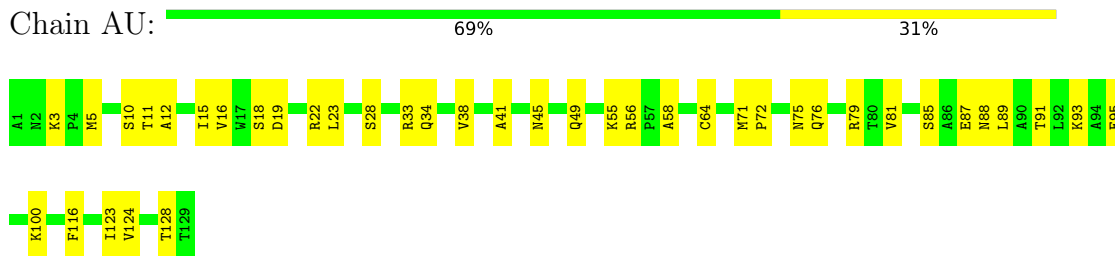
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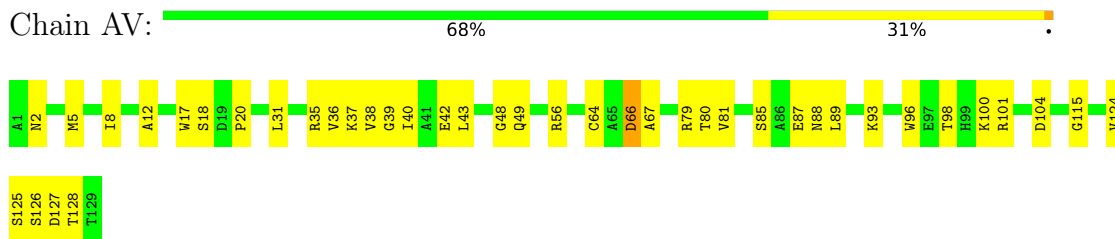
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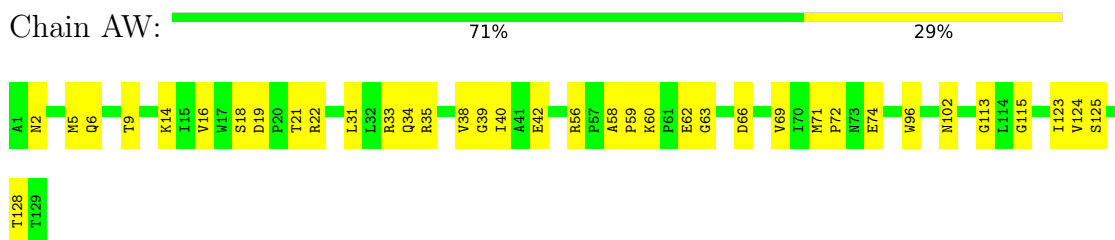
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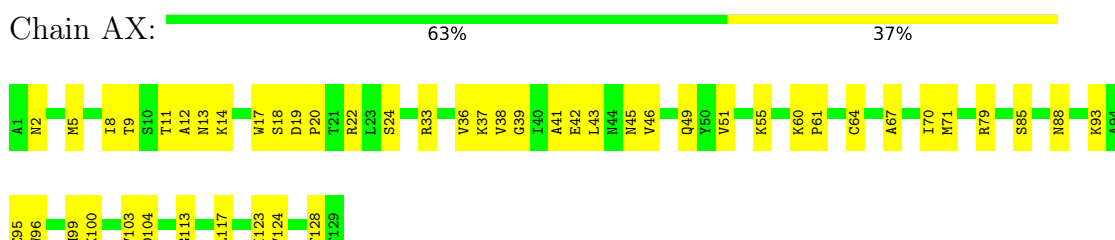
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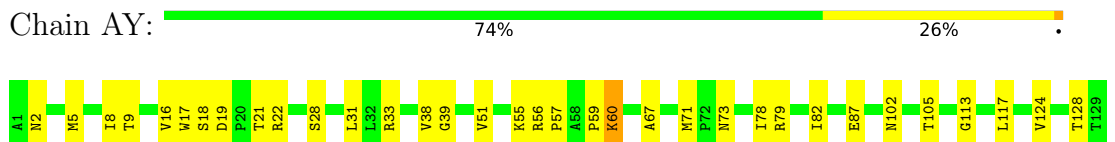
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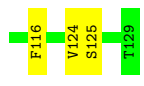


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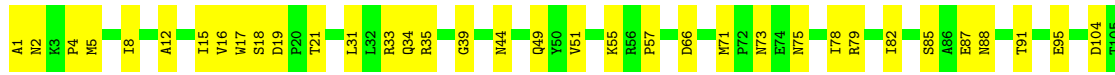


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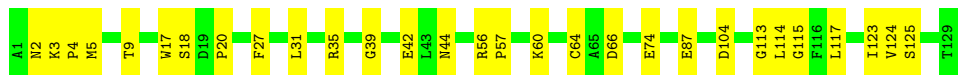
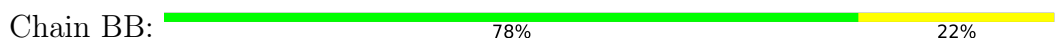




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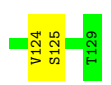
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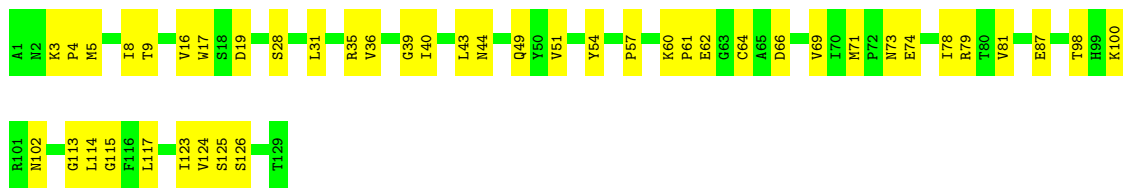


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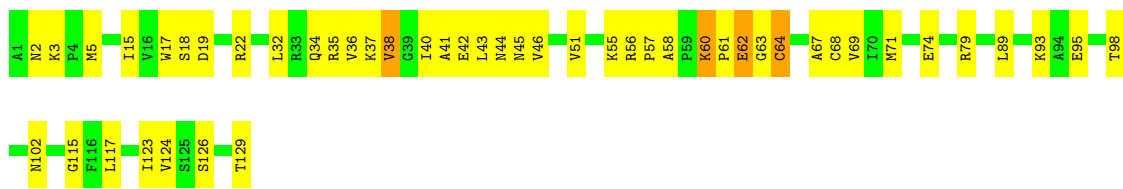
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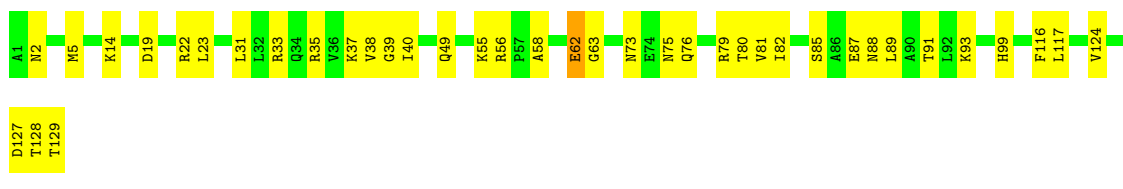
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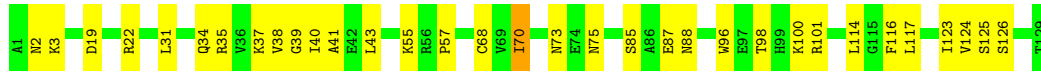


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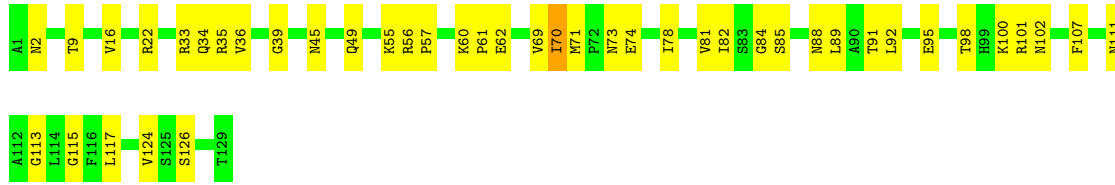


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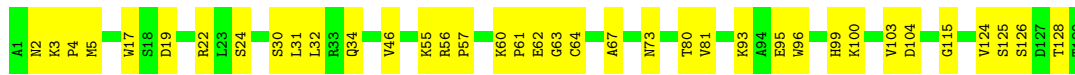




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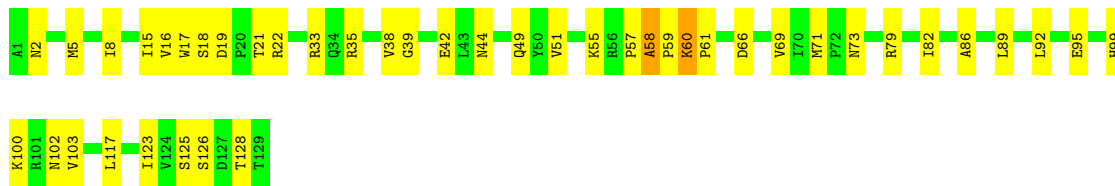
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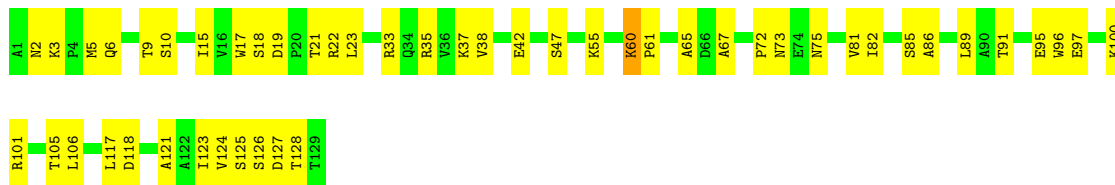
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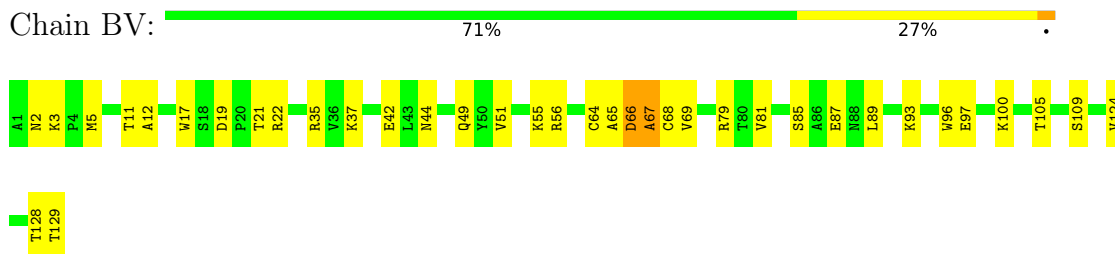
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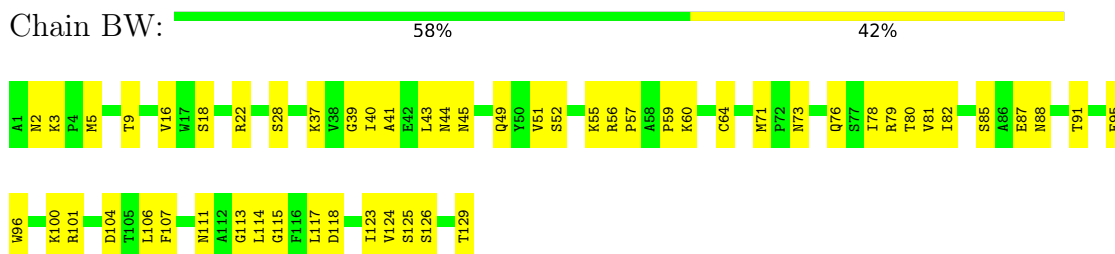
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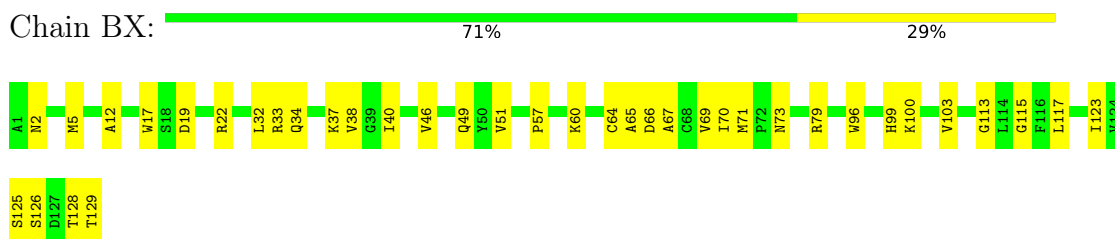
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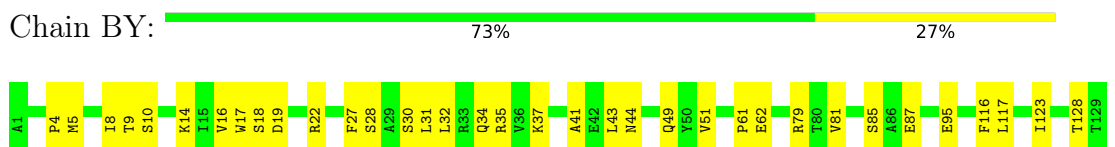
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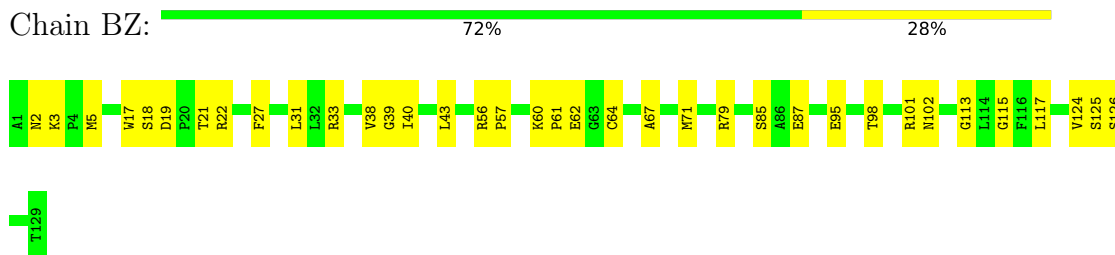
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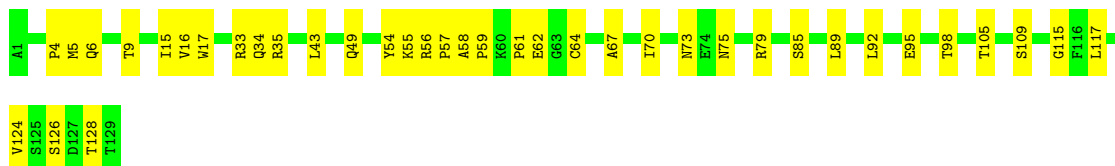


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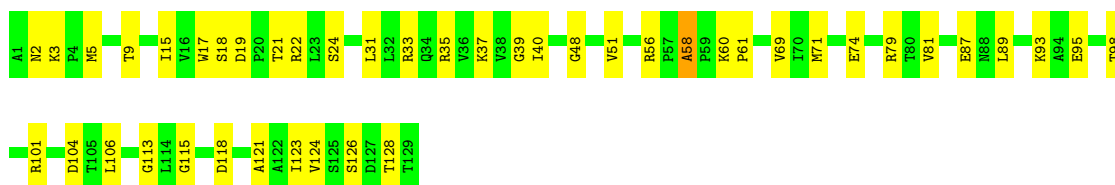




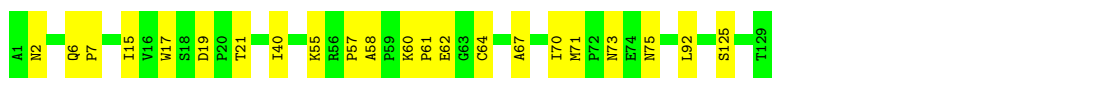
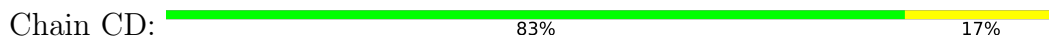
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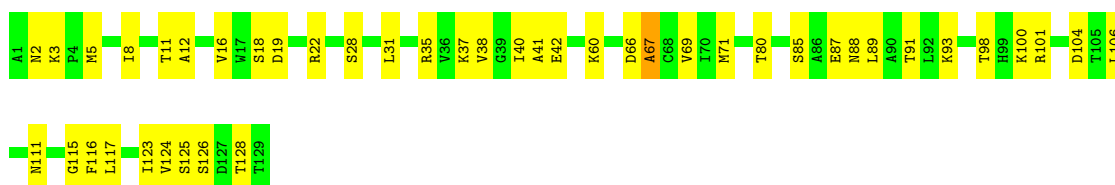
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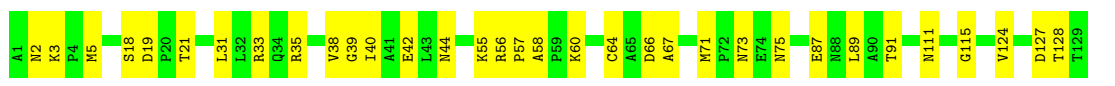
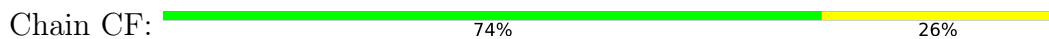
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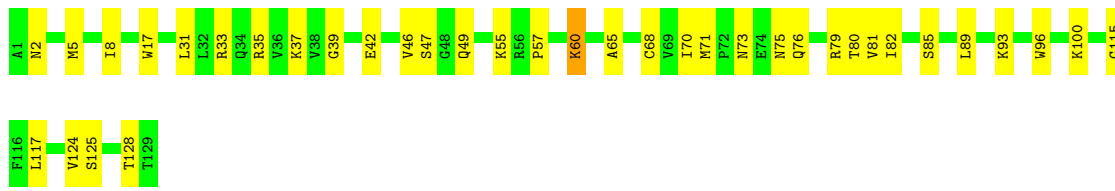
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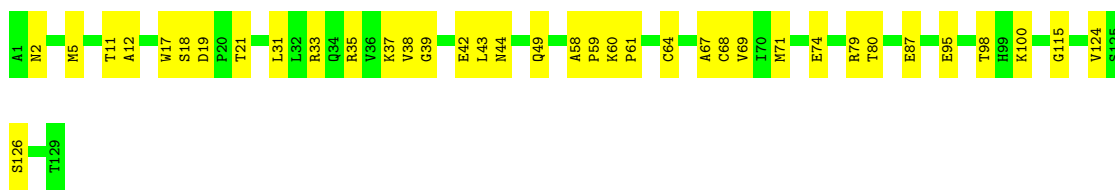
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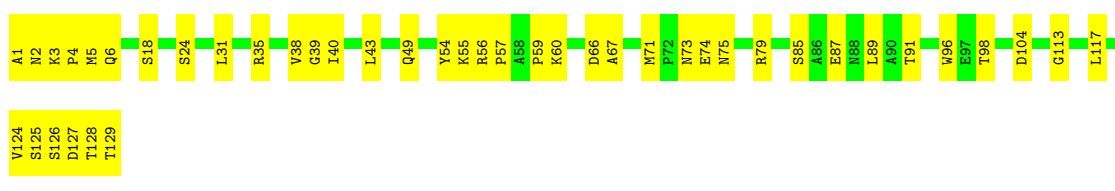
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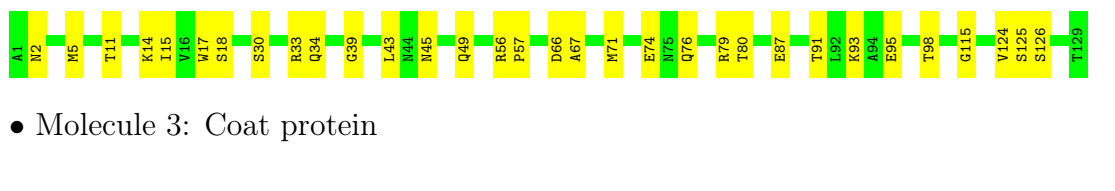
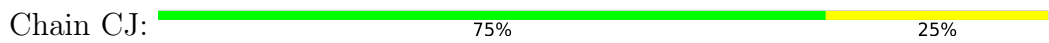
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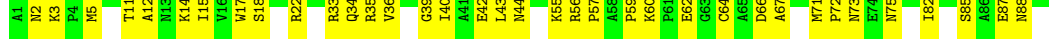
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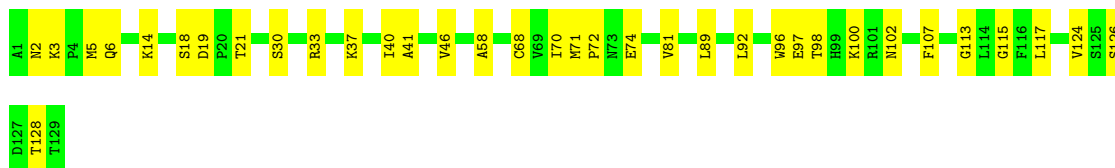


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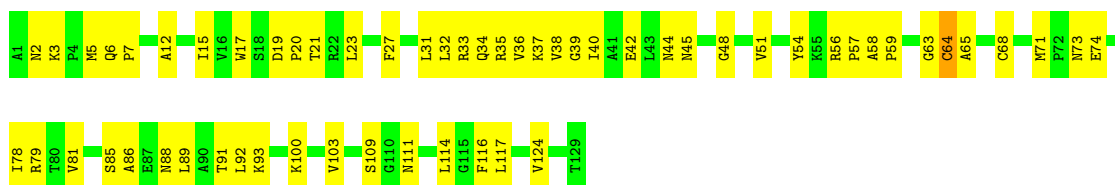


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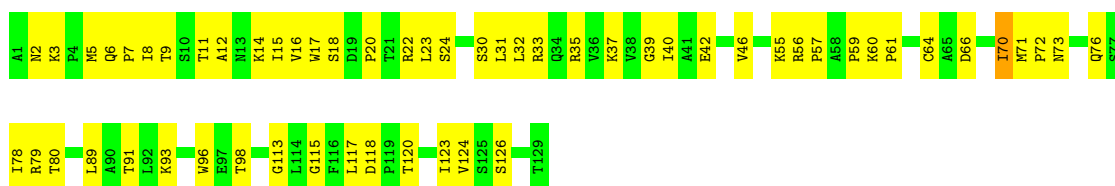




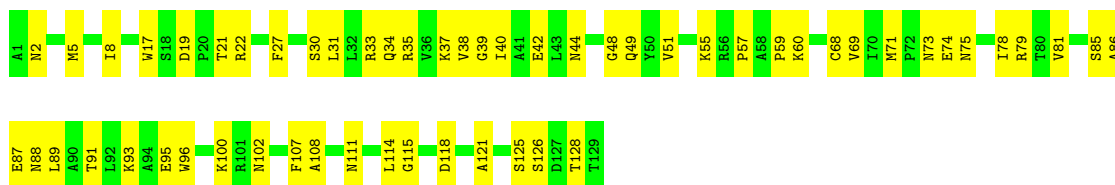
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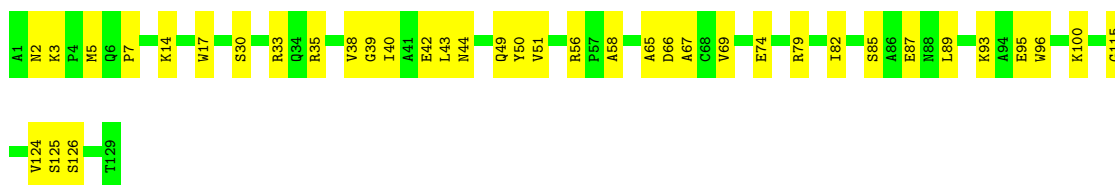
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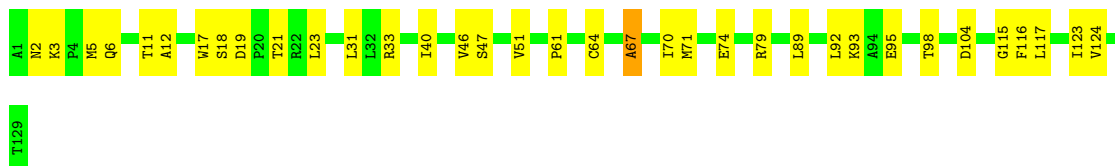


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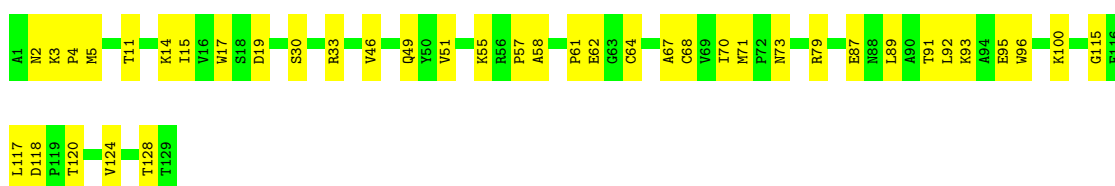




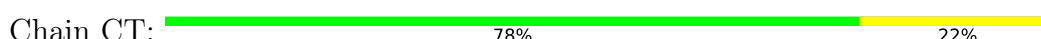
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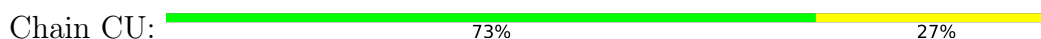
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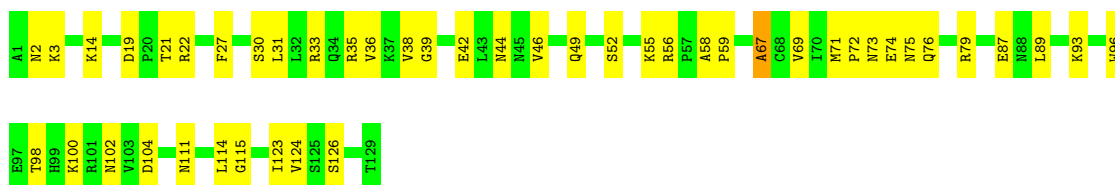
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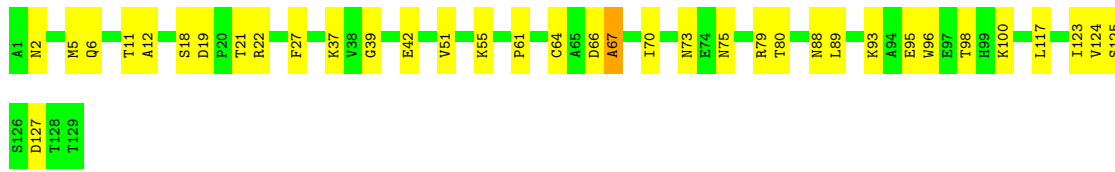
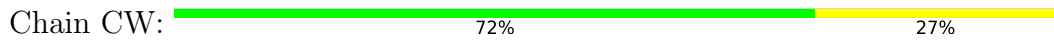
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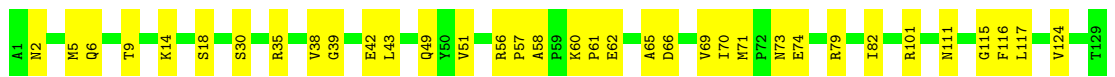
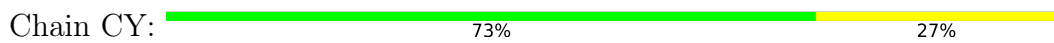
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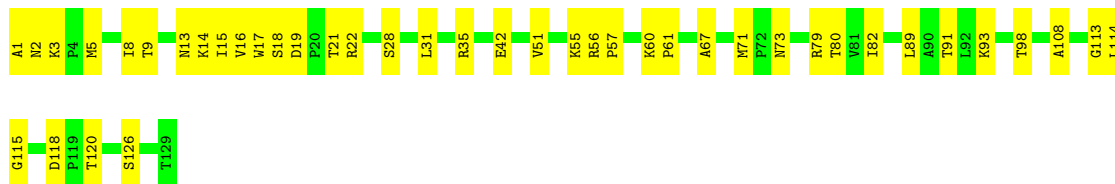
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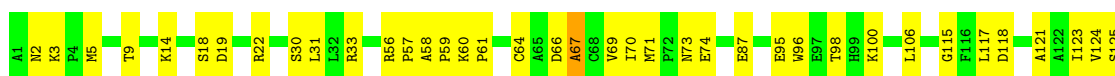




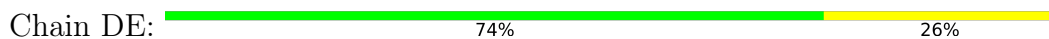
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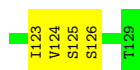
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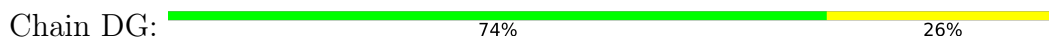
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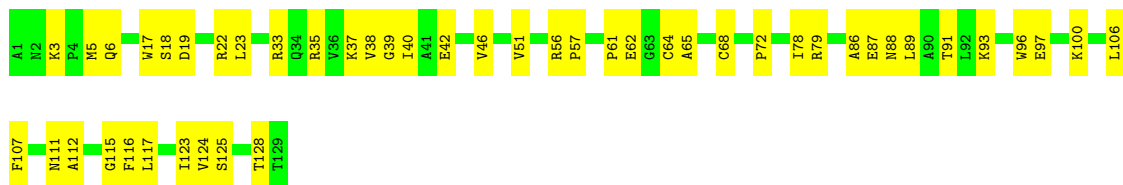
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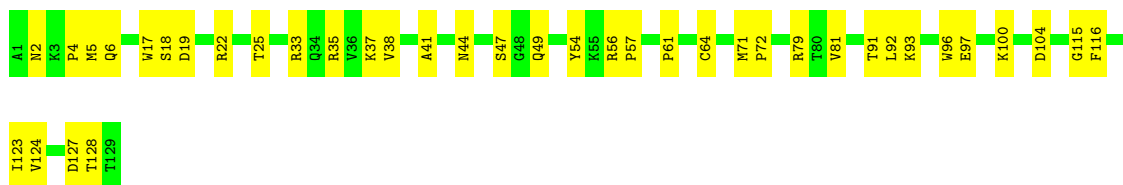
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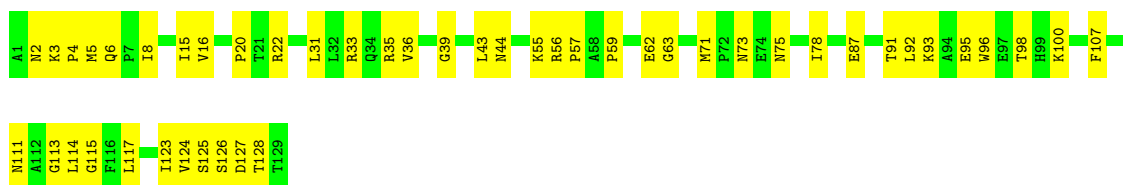
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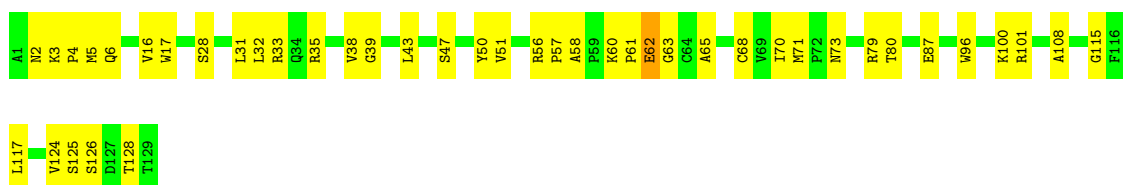
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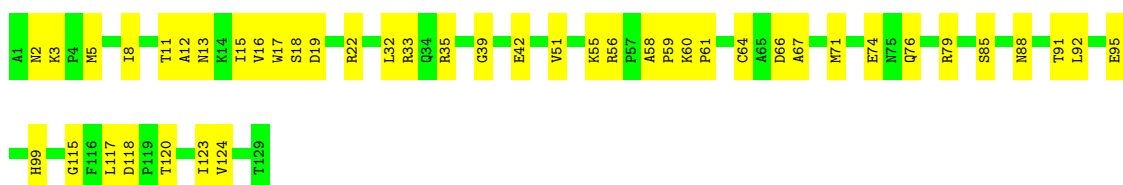
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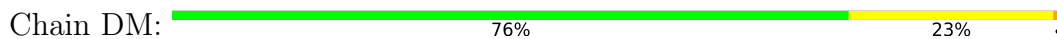
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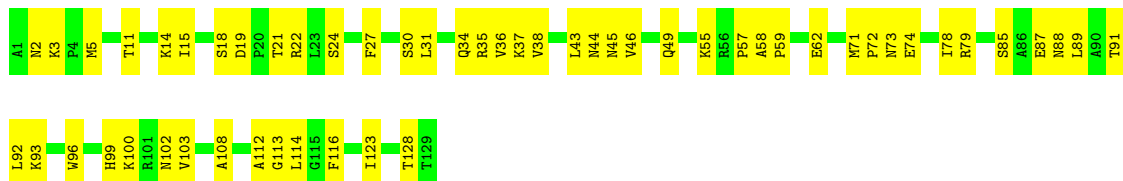
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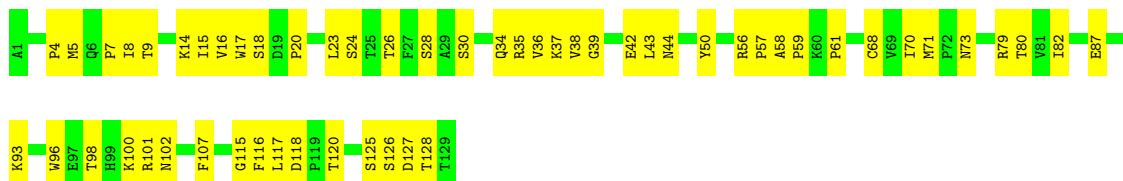
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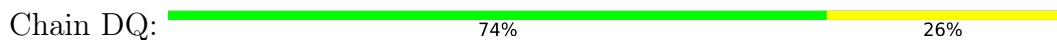
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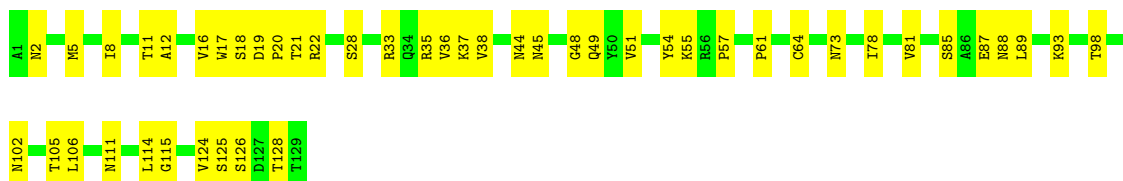
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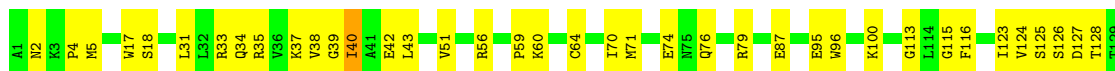


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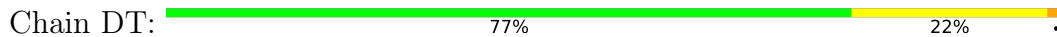


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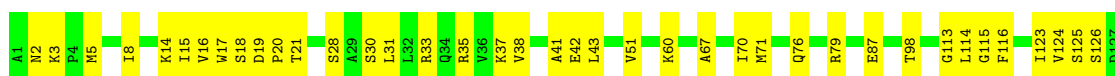




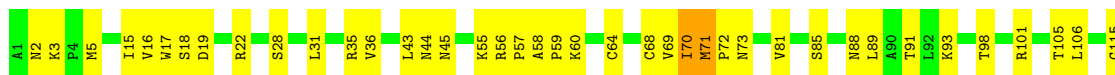
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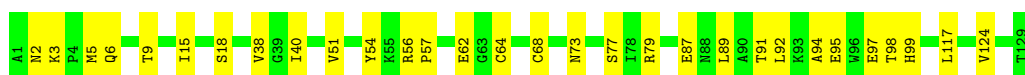
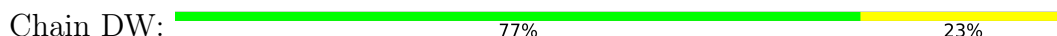
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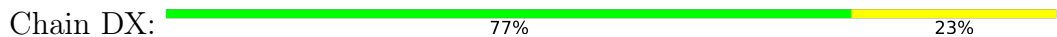
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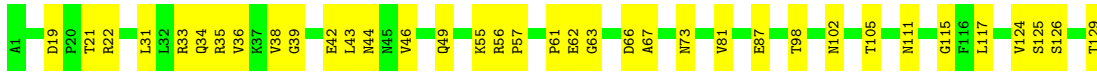


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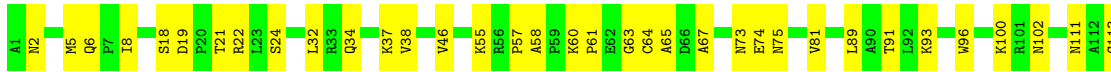


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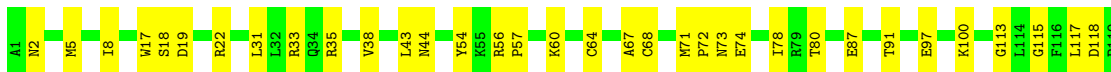




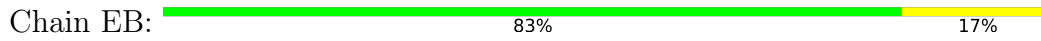
• Molecule 3: Coat protein



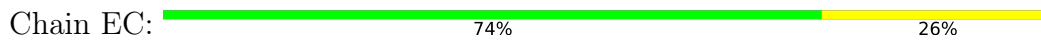
• Molecule 3: Coat protein



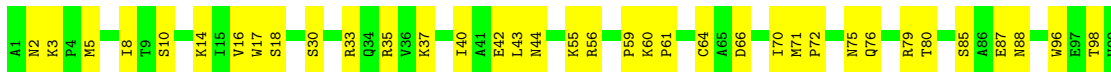
• Molecule 3: Coat protein



• Molecule 3: Coat protein

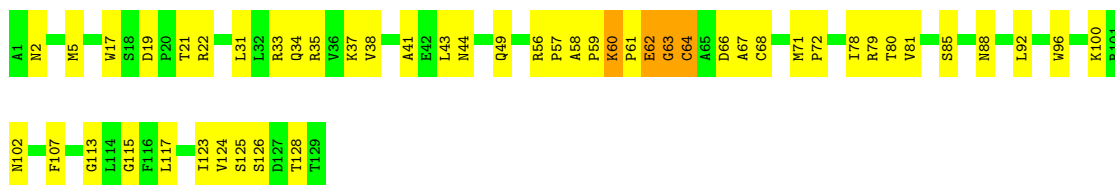


• Molecule 3: Coat protein



• Molecule 3: Coat protein

Chain EE:  62% 35%



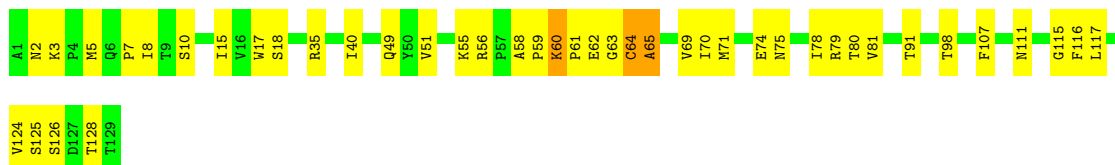
• Molecule 3: Coat protein

Chain EF:  67% 33%



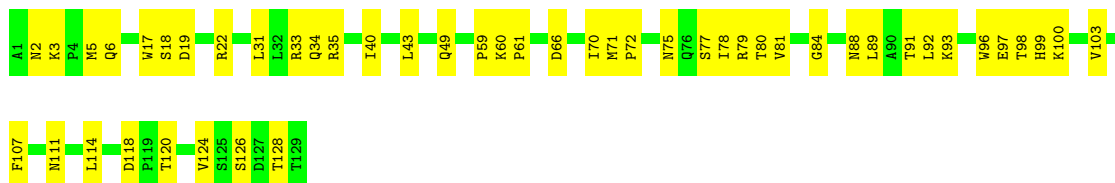
• Molecule 3: Coat protein

Chain EG:  67% 31%



• Molecule 3: Coat protein

Chain EH:  63% 37%



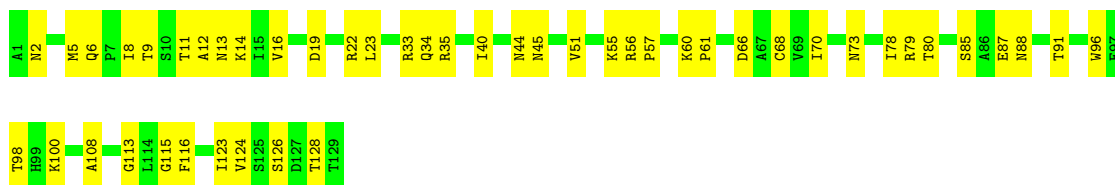
• Molecule 3: Coat protein

Chain EI:  70% 30%



• Molecule 3: Coat protein

Chain EJ:  64% 36%



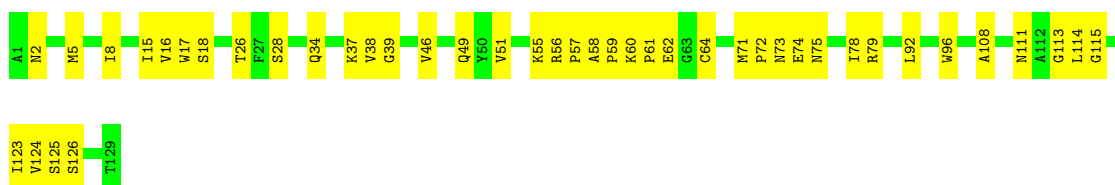
• Molecule 3: Coat protein

Chain EK:  67% 33%



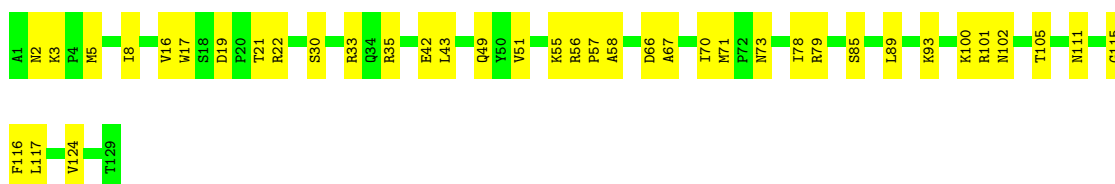
• Molecule 3: Coat protein

Chain EL:  67% 33%



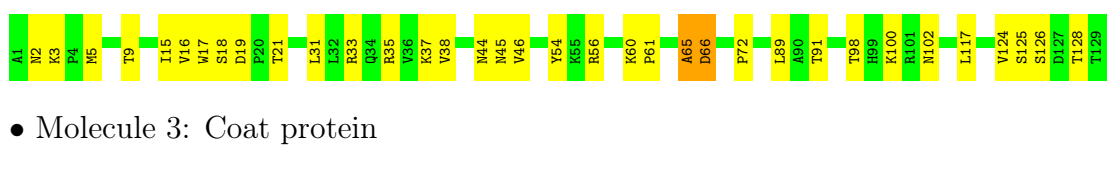
• Molecule 3: Coat protein

Chain EM:  70% 30%



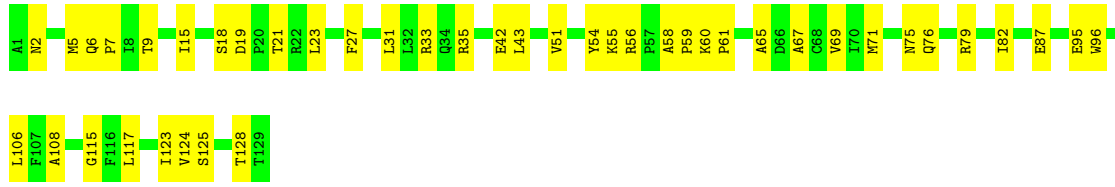
• Molecule 3: Coat protein

Chain EN:  73% 26%

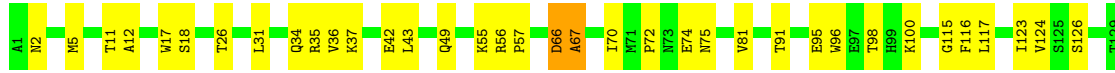


• Molecule 3: Coat protein

Chain EO:  67% 33%



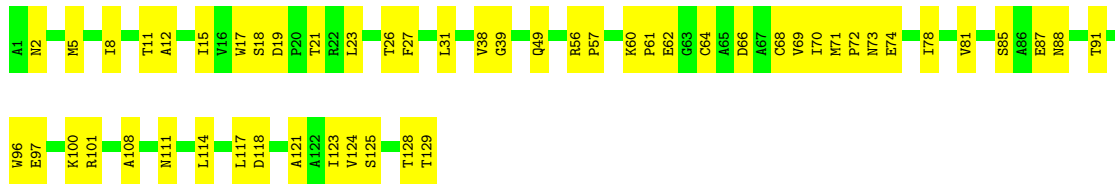
• Molecule 3: Coat protein



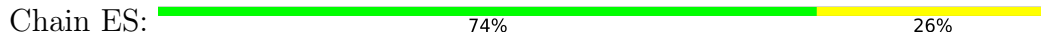
• Molecule 3: Coat protein



• Molecule 3: Coat protein



• Molecule 3: Coat protein

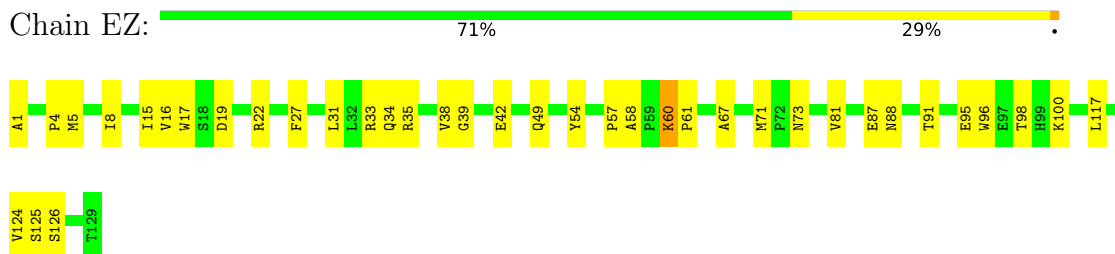


• Molecule 3: Coat protein

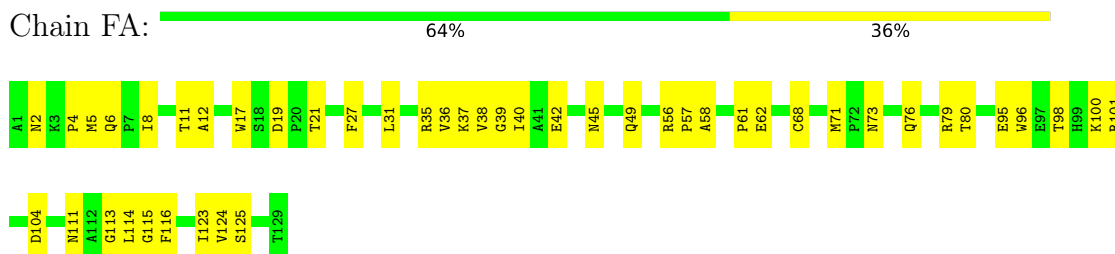




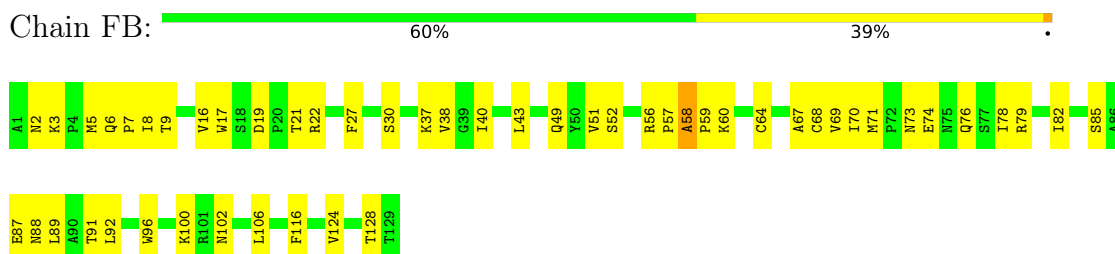
• Molecule 3: Coat protein



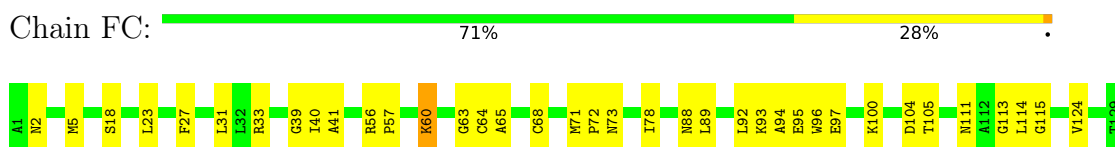
• Molecule 3: Coat protein



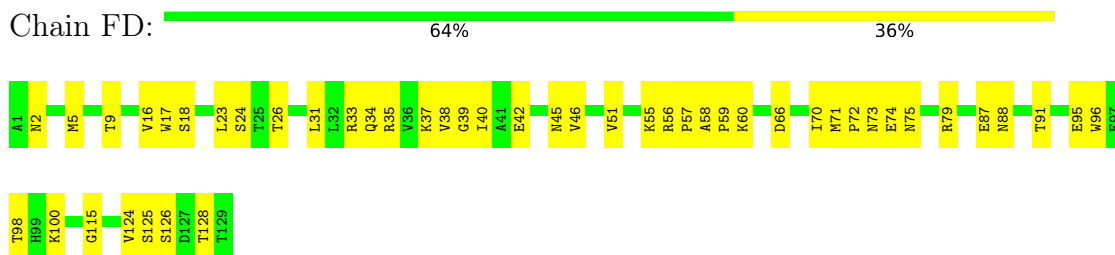
• Molecule 3: Coat protein




• Molecule 3: Coat protein



• Molecule 3: Coat protein



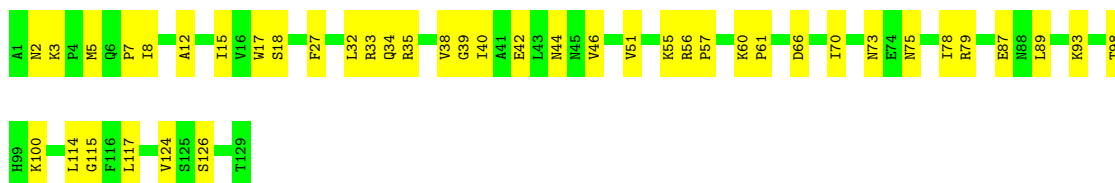
• Molecule 3: Coat protein

Chain FE:  76% 24%



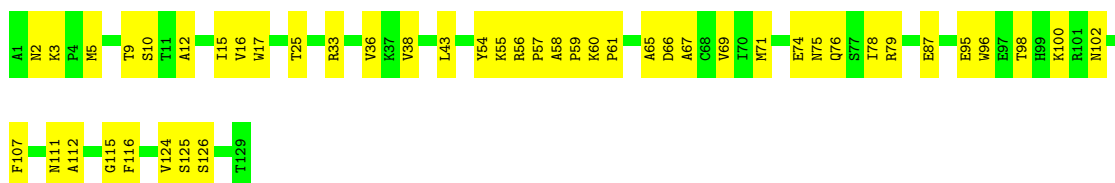
• Molecule 3: Coat protein

Chain FF:  67% 33%




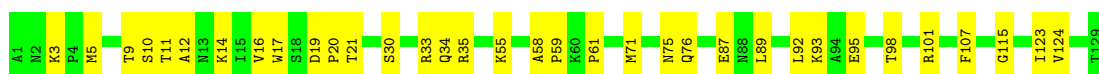
• Molecule 3: Coat protein

Chain FG:  64% 36%



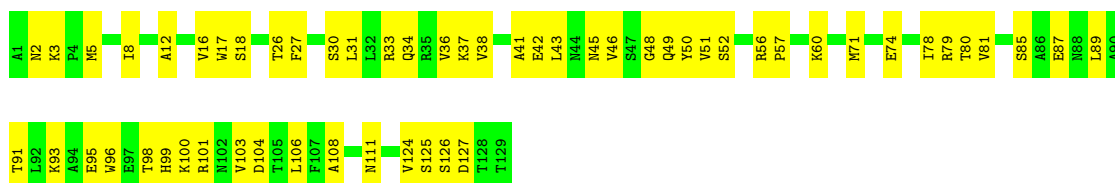
• Molecule 3: Coat protein

Chain FH:  74% 26%



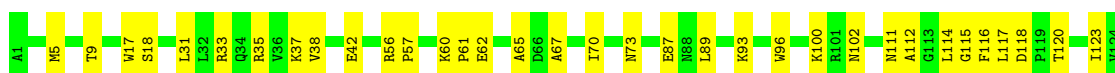
• Molecule 3: Coat protein

Chain FI:  57% 43%



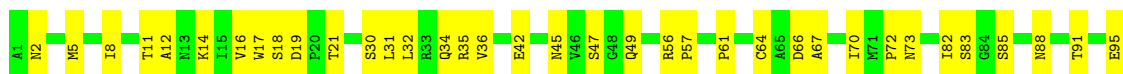
• Molecule 3: Coat protein

Chain FJ:  72% 28%

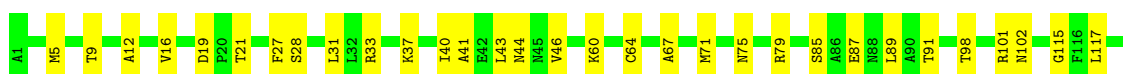




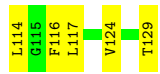
• Molecule 3: Coat protein



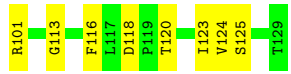
• Molecule 3: Coat protein



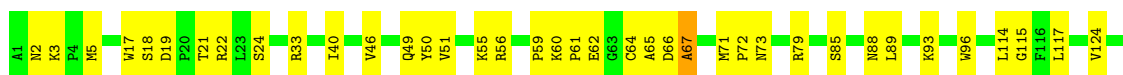
• Molecule 3: Coat protein



• Molecule 3: Coat protein

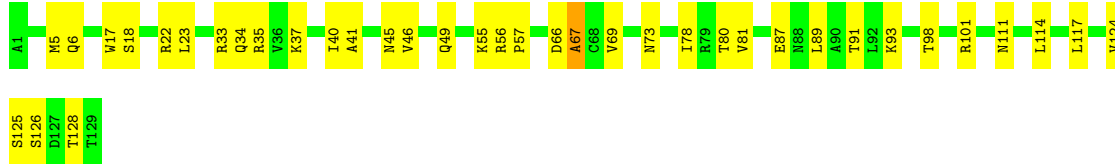


• Molecule 3: Coat protein

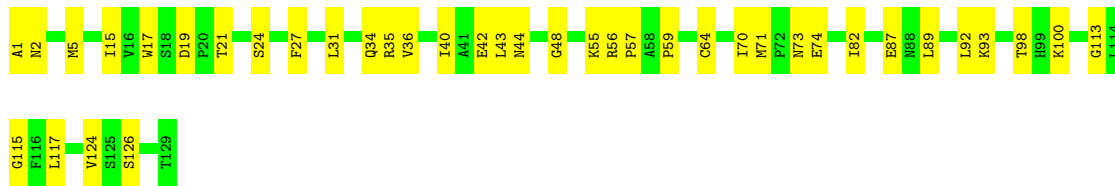


T129

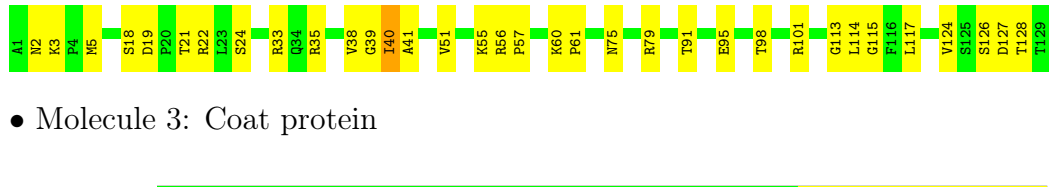
• Molecule 3: Coat protein



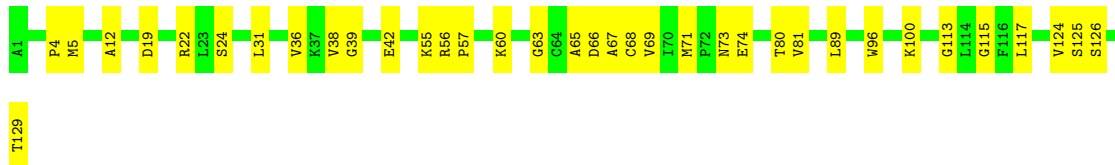
• Molecule 3: Coat protein



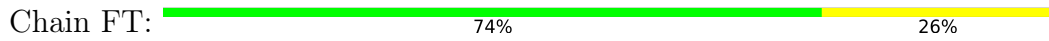
• Molecule 3: Coat protein



• Molecule 3: Coat protein

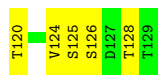
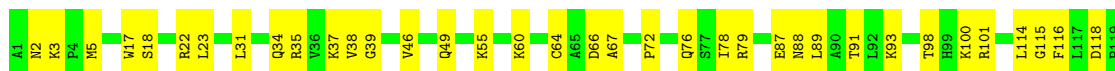


• Molecule 3: Coat protein

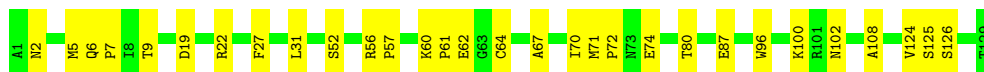
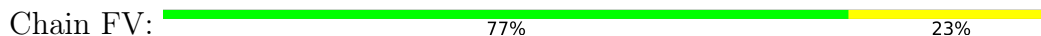


• Molecule 3: Coat protein





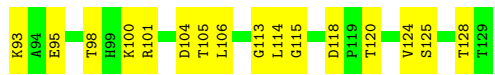
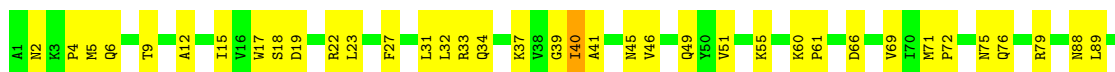
• Molecule 3: Coat protein



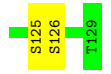
• Molecule 3: Coat protein



• Molecule 3: Coat protein



• Molecule 3: Coat protein

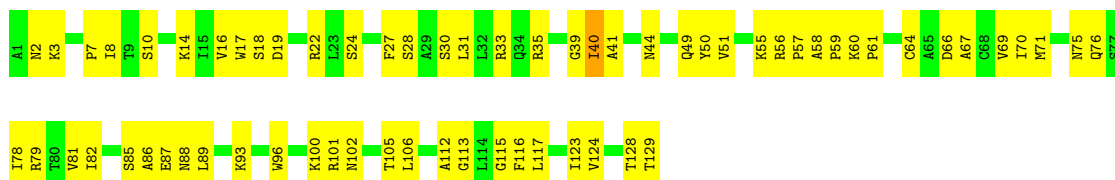


• Molecule 3: Coat protein

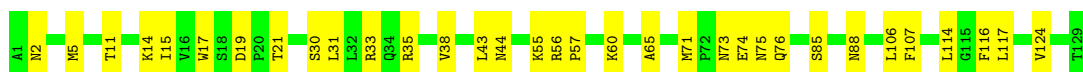
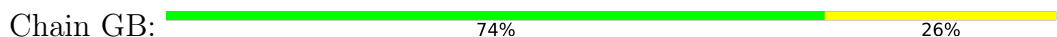




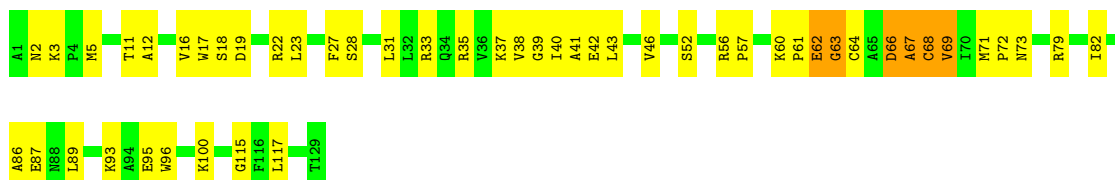
• Molecule 3: Coat protein



• Molecule 3: Coat protein



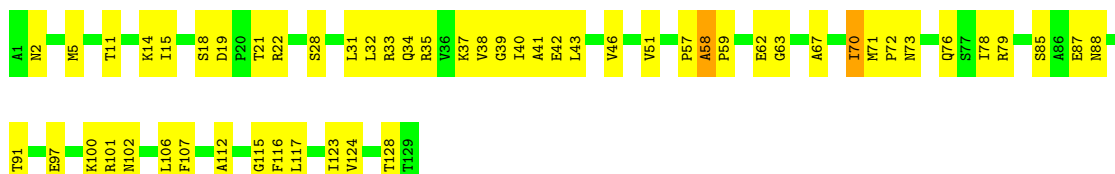
• Molecule 3: Coat protein



• Molecule 3: Coat protein

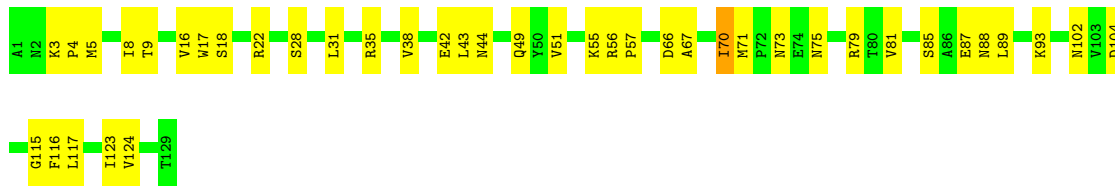


• Molecule 3: Coat protein




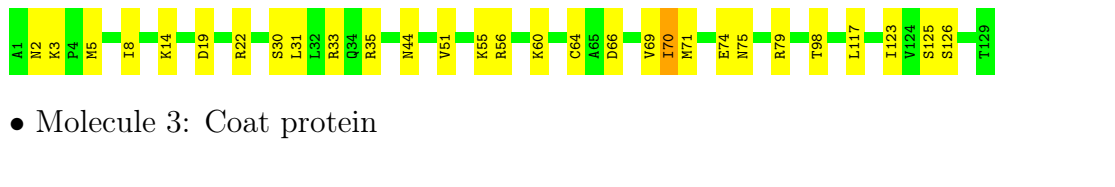
• Molecule 3: Coat protein

Chain GF:  68% 31%



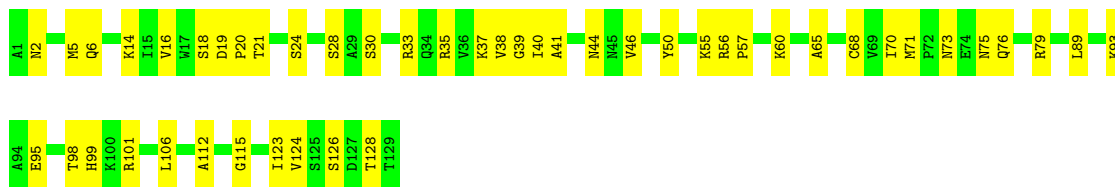
• Molecule 3: Coat protein

Chain GG:  78% 22%



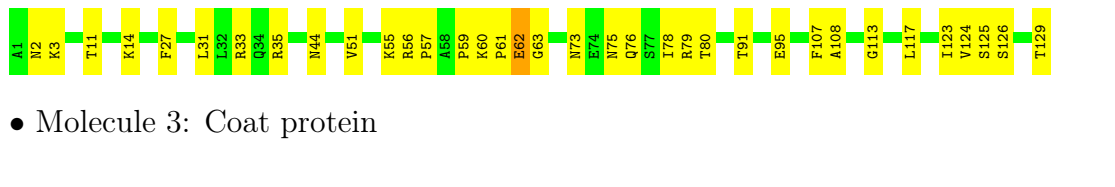
• Molecule 3: Coat protein

Chain GH:  64% 36%



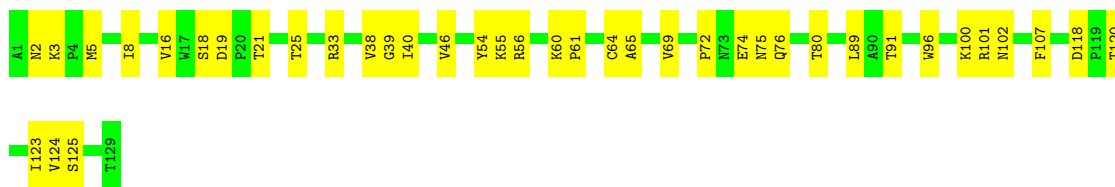
• Molecule 3: Coat protein

Chain GI:  73% 26%




• Molecule 3: Coat protein

Chain GJ:  70% 30%

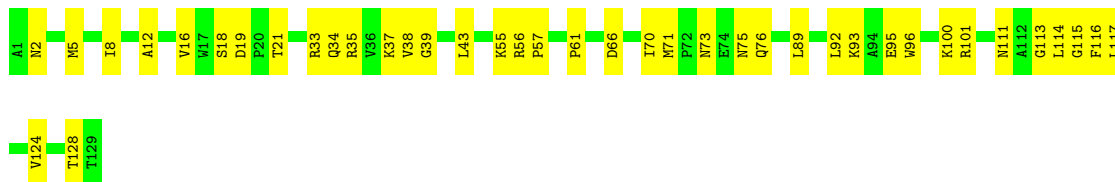


• Molecule 3: Coat protein

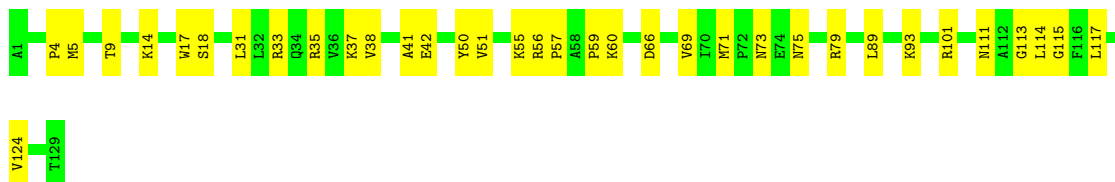
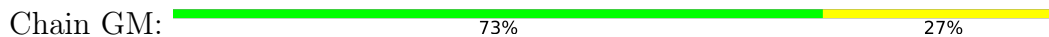
Chain GK:  81% 19%



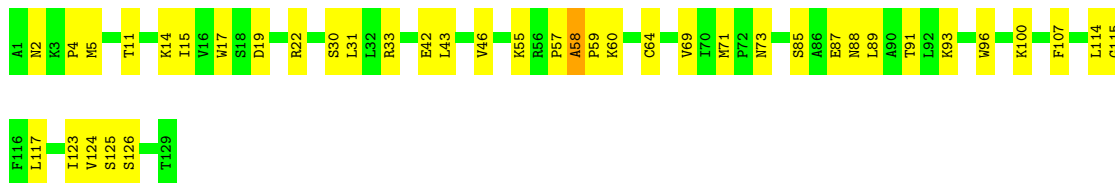
• Molecule 3: Coat protein



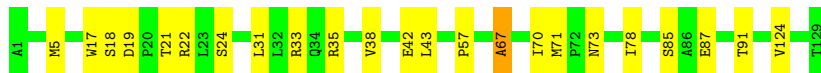
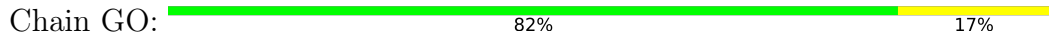
• Molecule 3: Coat protein



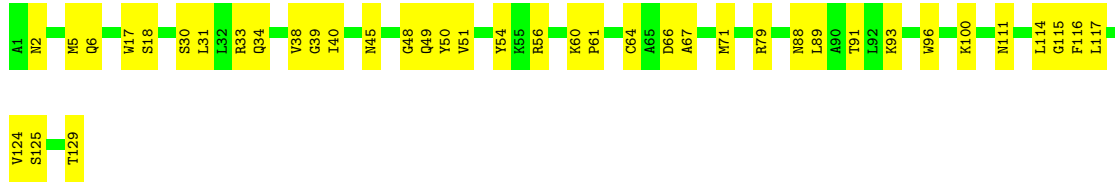
• Molecule 3: Coat protein



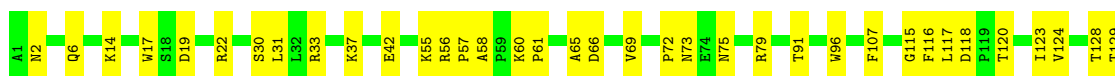
• Molecule 3: Coat protein



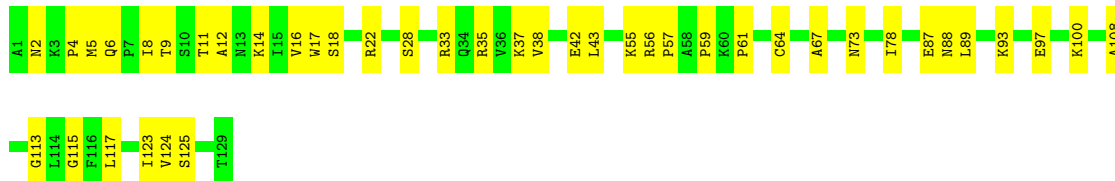
• Molecule 3: Coat protein



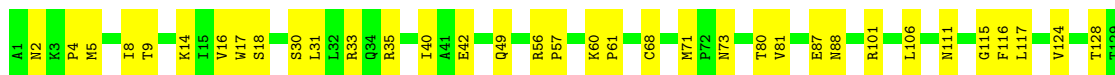
• Molecule 3: Coat protein



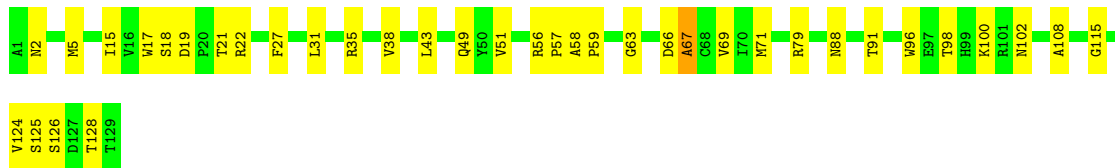
• Molecule 3: Coat protein



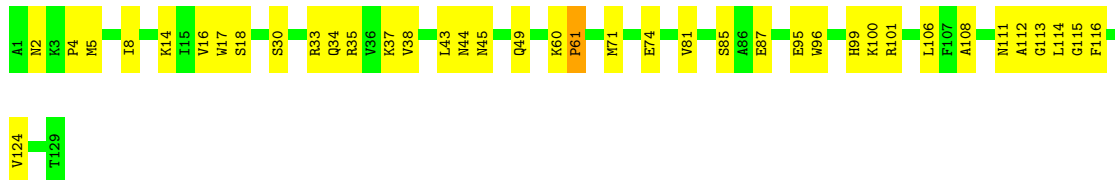
• Molecule 3: Coat protein



• Molecule 3: Coat protein



• Molecule 3: Coat protein

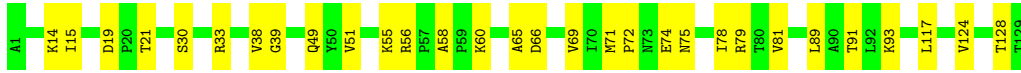
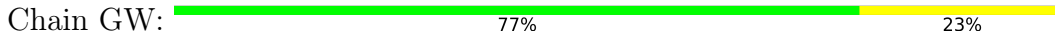


• Molecule 3: Coat protein

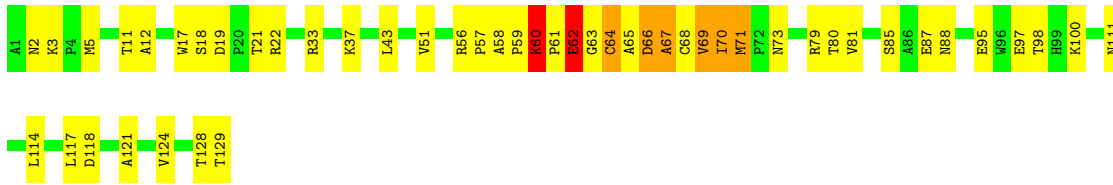




• Molecule 3: Coat protein



• Molecule 3: Coat protein



• Molecule 3: Coat protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	150000	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	1.710	Depositor
Minimum map value	-0.308	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.121	Depositor
Recommended contour level	0.128	Depositor
Map size ( $\text{\AA}$ )	487.59998, 487.59998, 487.59998	wwPDB
Map dimensions	460, 460, 460	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

### 5.1 Standard geometry

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	R	0.09	0/101047	0.20	0/157333
2	a	0.15	0/4409	0.38	0/5964
2	b	0.13	0/4409	0.37	0/5964
3	AB	0.18	0/985	0.41	1/1342 (0.1%)
3	AC	0.17	0/985	0.41	1/1342 (0.1%)
3	AE	0.21	0/985	0.47	1/1342 (0.1%)
3	AF	0.20	0/985	0.44	0/1342
3	AG	0.20	0/985	0.40	0/1342
3	AH	0.19	0/985	0.35	0/1342
3	AI	0.21	0/985	0.40	0/1342
3	AJ	0.20	0/985	0.35	0/1342
3	AK	0.21	0/985	0.38	0/1342
3	AL	0.19	0/985	0.35	0/1342
3	AM	0.19	0/985	0.36	0/1342
3	AN	0.20	0/985	0.38	0/1342
3	AO	0.19	0/985	0.36	0/1342
3	AP	0.26	0/985	0.45	0/1342
3	AQ	0.22	0/985	0.41	0/1342
3	AS	0.21	0/985	0.39	0/1342
3	AT	0.19	0/985	0.42	0/1342
3	AU	0.21	0/985	0.41	0/1342
3	AV	0.21	0/985	0.43	0/1342
3	AW	0.21	0/985	0.39	0/1342
3	AX	0.20	0/985	0.41	0/1342
3	AY	0.19	0/985	0.41	0/1342
3	AZ	0.31	0/985	0.49	1/1342 (0.1%)
3	Ac	0.20	0/985	0.37	0/1342
3	BA	0.20	0/985	0.41	0/1342
3	BB	0.20	0/985	0.43	0/1342
3	BC	0.22	0/985	0.46	0/1342
3	BD	0.19	0/985	0.36	0/1342
3	BE	0.20	0/985	0.38	0/1342
3	BF	0.20	0/985	0.39	0/1342
3	BG	0.22	0/985	0.41	1/1342 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	BH	0.20	0/985	0.37	0/1342
3	BI	0.20	0/985	0.41	0/1342
3	BJ	0.19	0/985	0.38	0/1342
3	BK	0.19	0/985	0.41	0/1342
3	BL	0.20	0/985	0.40	0/1342
3	BM	0.21	0/985	0.40	0/1342
3	BN	0.41	0/985	0.52	0/1342
3	BO	0.20	0/985	0.42	0/1342
3	BP	0.20	0/985	0.38	0/1342
3	BQ	0.19	0/985	0.40	0/1342
3	BS	0.20	0/985	0.39	0/1342
3	BT	0.21	0/985	0.41	0/1342
3	BU	0.21	0/985	0.42	0/1342
3	BV	0.33	1/985 (0.1%)	0.50	1/1342 (0.1%)
3	BW	0.20	0/985	0.41	0/1342
3	BX	0.20	0/985	0.40	0/1342
3	BY	0.20	0/985	0.34	0/1342
3	BZ	0.21	0/985	0.44	0/1342
3	Bc	0.20	0/985	0.43	0/1342
3	CA	0.22	0/985	0.47	0/1342
3	CB	0.20	0/985	0.38	0/1342
3	CC	0.21	0/985	0.39	0/1342
3	CD	0.20	0/985	0.43	0/1342
3	CE	0.21	0/985	0.44	0/1342
3	CF	0.19	0/985	0.40	0/1342
3	CG	0.19	0/985	0.35	0/1342
3	CH	0.19	0/985	0.35	0/1342
3	CI	0.21	0/985	0.42	0/1342
3	CJ	0.21	0/985	0.42	0/1342
3	CK	0.19	0/985	0.41	0/1342
3	CL	0.19	0/985	0.38	0/1342
3	CM	0.18	0/985	0.43	0/1342
3	CN	0.21	0/985	0.45	0/1342
3	CO	0.19	0/985	0.42	0/1342
3	CP	0.21	0/985	0.44	0/1342
3	CQ	0.19	0/985	0.36	0/1342
3	CS	0.20	0/985	0.40	0/1342
3	CT	0.19	0/985	0.38	0/1342
3	CU	0.21	0/985	0.39	0/1342
3	CV	0.20	0/985	0.41	0/1342
3	CW	0.19	0/985	0.35	0/1342
3	CX	0.19	0/985	0.34	0/1342
3	CY	0.19	0/985	0.42	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	CZ	0.19	0/985	0.37	0/1342
3	Cc	0.21	0/985	0.36	0/1342
3	DA	0.20	0/985	0.39	0/1342
3	DB	0.20	0/985	0.38	0/1342
3	DC	0.19	0/985	0.46	0/1342
3	DD	0.21	0/985	0.39	0/1342
3	DE	0.20	0/985	0.40	0/1342
3	DF	0.21	0/985	0.41	0/1342
3	DG	0.21	0/985	0.39	0/1342
3	DH	0.19	0/985	0.38	0/1342
3	DI	0.17	0/985	0.36	0/1342
3	DJ	0.18	0/985	0.39	0/1342
3	DK	0.20	0/985	0.39	0/1342
3	DL	0.21	0/985	0.42	0/1342
3	DM	0.20	0/985	0.38	0/1342
3	DN	0.21	0/985	0.45	0/1342
3	DO	0.19	0/985	0.45	0/1342
3	DQ	0.20	0/985	0.41	0/1342
3	DS	0.20	0/985	0.43	0/1342
3	DT	0.22	0/985	0.45	1/1342 (0.1%)
3	DU	0.19	0/985	0.36	0/1342
3	DV	0.23	0/985	0.41	0/1342
3	DW	0.19	0/985	0.41	0/1342
3	DX	0.20	0/985	0.39	0/1342
3	DY	0.21	0/985	0.41	0/1342
3	DZ	0.20	0/985	0.40	0/1342
3	Dc	0.19	0/985	0.35	0/1342
3	EA	0.20	0/985	0.37	0/1342
3	EB	0.20	0/985	0.38	0/1342
3	EC	0.20	0/985	0.40	0/1342
3	ED	0.20	0/985	0.40	0/1342
3	EE	0.29	0/985	0.43	0/1342
3	EF	0.21	0/985	0.41	0/1342
3	EG	0.35	0/985	0.44	1/1342 (0.1%)
3	EH	0.22	0/985	0.41	0/1342
3	EI	0.20	0/985	0.40	0/1342
3	EJ	0.20	0/985	0.39	0/1342
3	EK	0.19	0/985	0.39	0/1342
3	EL	0.21	0/985	0.41	0/1342
3	EM	0.19	0/985	0.40	0/1342
3	EN	0.20	0/985	0.42	2/1342 (0.1%)
3	EO	0.21	0/985	0.43	0/1342
3	EP	0.20	0/985	0.39	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	EQ	0.21	0/985	0.40	0/1342
3	ES	0.19	0/985	0.38	0/1342
3	ET	0.21	0/985	0.42	2/1342 (0.1%)
3	EU	0.19	0/985	0.43	0/1342
3	EV	0.19	0/985	0.42	0/1342
3	EW	0.20	0/985	0.37	0/1342
3	EX	0.27	0/985	0.41	0/1342
3	EY	0.20	0/985	0.40	0/1342
3	EZ	0.22	0/985	0.44	0/1342
3	Ec	0.21	0/985	0.42	0/1342
3	FA	0.18	0/985	0.40	0/1342
3	FB	0.21	0/985	0.47	1/1342 (0.1%)
3	FC	0.18	0/985	0.38	0/1342
3	FD	0.20	0/985	0.40	0/1342
3	FE	0.20	0/985	0.42	0/1342
3	FF	0.20	0/985	0.49	1/1342 (0.1%)
3	FG	0.18	0/985	0.39	0/1342
3	FH	0.21	0/985	0.42	0/1342
3	FI	0.20	0/985	0.37	0/1342
3	FJ	0.20	0/985	0.40	1/1342 (0.1%)
3	FK	0.21	0/985	0.39	0/1342
3	FL	0.20	0/985	0.39	0/1342
3	FM	0.19	0/985	0.40	0/1342
3	FN	0.21	0/985	0.43	1/1342 (0.1%)
3	FO	0.22	0/985	0.44	0/1342
3	FP	0.20	0/985	0.38	0/1342
3	FQ	0.19	0/985	0.37	0/1342
3	FS	0.20	0/985	0.38	0/1342
3	FT	0.20	0/985	0.41	0/1342
3	FU	0.20	0/985	0.36	0/1342
3	FV	0.19	0/985	0.39	0/1342
3	FW	0.25	0/985	0.47	1/1342 (0.1%)
3	FX	0.22	0/985	0.43	0/1342
3	FY	0.19	0/985	0.37	0/1342
3	FZ	0.22	0/985	0.44	0/1342
3	Fc	0.21	0/985	0.41	0/1342
3	GA	0.21	0/985	0.43	0/1342
3	GB	0.21	0/985	0.41	0/1342
3	GC	0.56	1/985 (0.1%)	0.58	1/1342 (0.1%)
3	GD	0.20	0/985	0.35	0/1342
3	GE	0.20	0/985	0.41	0/1342
3	GF	0.19	0/985	0.43	0/1342
3	GG	0.20	0/985	0.37	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	GH	0.21	0/985	0.43	0/1342
3	GI	0.19	0/985	0.38	0/1342
3	GJ	0.20	0/985	0.38	0/1342
3	GK	0.21	0/985	0.39	0/1342
3	GL	0.19	0/985	0.38	0/1342
3	GM	0.19	0/985	0.40	0/1342
3	GN	0.21	0/985	0.39	0/1342
3	GO	0.19	0/985	0.36	0/1342
3	GP	0.19	0/985	0.35	0/1342
3	GQ	0.19	0/985	0.41	0/1342
3	GS	0.20	0/985	0.40	0/1342
3	GT	0.19	0/985	0.35	0/1342
3	GU	0.20	0/985	0.39	0/1342
3	GV	0.21	0/985	0.43	0/1342
3	GW	0.20	0/985	0.40	0/1342
3	GX	0.49	0/985	0.54	1/1342 (0.1%)
3	GY	0.20	0/985	0.43	0/1342
3	Gc	0.20	0/985	0.40	0/1342
All	All	0.18	2/285195 (0.0%)	0.34	19/408137 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	GC	66	ASP	CA-C	-8.71	1.48	1.53
3	BV	67	ALA	CA-C	-5.00	1.47	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	GC	66	ASP	N-CA-C	-11.12	99.66	108.78
3	BV	67	ALA	N-CA-C	-9.49	100.05	112.68
3	FF	66	ASP	CB-CA-C	-7.57	107.83	116.54
3	AZ	63	GLY	N-CA-C	-6.99	103.61	115.08
3	DT	66	ASP	CB-CA-C	-6.78	108.77	116.63

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	R	90441	0	45709	2519	0
2	a	4304	0	4314	175	0
2	b	4304	0	4315	148	0
3	AB	968	0	974	55	0
3	AC	968	0	973	46	0
3	AE	968	0	973	35	0
3	AF	968	0	973	31	0
3	AG	968	0	973	37	0
3	AH	968	0	973	33	0
3	AI	968	0	973	39	0
3	AJ	968	0	973	30	0
3	AK	968	0	973	22	0
3	AL	968	0	973	44	0
3	AM	968	0	973	31	0
3	AN	968	0	973	43	0
3	AO	968	0	973	39	0
3	AP	968	0	973	40	0
3	AQ	968	0	973	28	0
3	AS	968	0	973	37	0
3	AT	968	0	973	40	0
3	AU	968	0	973	43	0
3	AV	968	0	973	43	0
3	AW	968	0	973	36	0
3	AX	968	0	973	40	0
3	AY	968	0	973	30	0
3	AZ	968	0	973	34	0
3	Ac	968	0	973	40	0
3	BA	968	0	973	36	0
3	BB	968	0	973	28	0
3	BC	968	0	973	27	0
3	BD	968	0	973	41	0
3	BE	968	0	973	37	0
3	BF	968	0	973	31	0
3	BG	968	0	973	43	0
3	BH	968	0	973	38	0
3	BI	968	0	973	36	0
3	BJ	968	0	974	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BK	968	0	973	41	0
3	BL	968	0	973	30	0
3	BM	968	0	973	32	0
3	BN	968	0	973	48	0
3	BO	968	0	973	40	0
3	BP	968	0	974	34	0
3	BQ	968	0	973	35	0
3	BS	968	0	973	46	0
3	BT	968	0	973	37	0
3	BU	968	0	973	47	0
3	BV	968	0	974	38	0
3	BW	968	0	973	51	0
3	BX	968	0	973	34	0
3	BY	968	0	973	33	0
3	BZ	968	0	973	34	0
3	Bc	968	0	973	36	0
3	CA	968	0	973	31	0
3	CB	968	0	973	34	0
3	CC	968	0	973	40	0
3	CD	968	0	973	18	0
3	CE	968	0	973	40	0
3	CF	968	0	973	33	0
3	CG	968	0	973	35	0
3	CH	968	0	973	35	0
3	CI	968	0	973	40	0
3	CJ	968	0	973	29	0
3	CK	968	0	973	43	0
3	CL	968	0	973	32	0
3	CM	968	0	974	53	0
3	CN	968	0	973	58	0
3	CO	968	0	973	65	0
3	CP	968	0	973	32	0
3	CQ	968	0	973	34	0
3	CS	968	0	974	36	0
3	CT	968	0	973	27	0
3	CU	968	0	973	34	0
3	CV	968	0	973	37	0
3	CW	968	0	973	33	0
3	CX	968	0	973	44	0
3	CY	968	0	973	28	0
3	CZ	968	0	973	33	0
3	Cc	968	0	973	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	DA	968	0	973	31	0
3	DB	968	0	973	43	0
3	DC	968	0	973	34	0
3	DD	968	0	973	35	0
3	DE	968	0	973	30	0
3	DF	968	0	973	39	0
3	DG	968	0	973	29	0
3	DH	968	0	973	46	0
3	DI	968	0	973	40	0
3	DJ	968	0	973	49	0
3	DK	968	0	973	38	0
3	DL	968	0	973	37	0
3	DM	968	0	973	34	0
3	DN	968	0	973	48	0
3	DO	968	0	973	58	0
3	DQ	968	0	973	27	0
3	DS	968	0	973	38	0
3	DT	968	0	973	31	0
3	DU	968	0	973	36	0
3	DV	968	0	974	37	0
3	DW	968	0	973	26	0
3	DX	968	0	973	24	0
3	DY	968	0	973	31	0
3	DZ	968	0	973	37	0
3	Dc	968	0	973	40	0
3	EA	968	0	973	40	0
3	EB	968	0	973	18	0
3	EC	968	0	973	27	0
3	ED	968	0	973	38	0
3	EE	968	0	973	56	0
3	EF	968	0	973	40	0
3	EG	968	0	974	46	0
3	EH	968	0	973	44	0
3	EI	968	0	973	38	0
3	EJ	968	0	973	42	0
3	EK	968	0	973	38	0
3	EL	968	0	973	36	0
3	EM	968	0	973	39	0
3	EN	968	0	973	31	0
3	EO	968	0	973	38	0
3	EP	968	0	973	35	0
3	EQ	968	0	973	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	ES	968	0	973	31	0
3	ET	968	0	973	40	0
3	EU	968	0	973	40	0
3	EV	968	0	973	45	0
3	EW	968	0	973	42	0
3	EX	968	0	973	32	0
3	EY	968	0	973	37	0
3	EZ	968	0	973	30	0
3	Ec	968	0	973	50	0
3	FA	968	0	973	42	0
3	FB	968	0	973	49	0
3	FC	968	0	973	27	0
3	FD	968	0	973	46	0
3	FE	968	0	973	34	0
3	FF	968	0	973	35	0
3	FG	968	0	974	46	0
3	FH	968	0	973	29	0
3	FI	968	0	973	56	0
3	FJ	968	0	973	29	0
3	FK	968	0	973	36	0
3	FL	968	0	973	35	0
3	FM	968	0	973	36	0
3	FN	968	0	973	41	0
3	FO	968	0	973	38	0
3	FP	968	0	973	36	0
3	FQ	968	0	973	41	0
3	FS	968	0	973	30	0
3	FT	968	0	973	32	0
3	FU	968	0	973	41	0
3	FV	968	0	973	23	0
3	FW	968	0	974	45	0
3	FX	968	0	973	44	0
3	FY	968	0	973	32	0
3	FZ	968	0	973	44	0
3	Fc	968	0	973	31	0
3	GA	968	0	973	68	0
3	GB	968	0	973	30	0
3	GC	968	0	974	42	0
3	GD	968	0	973	36	0
3	GE	968	0	973	49	0
3	GF	968	0	973	42	0
3	GG	968	0	973	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	GH	968	0	973	37	0
3	GI	968	0	973	34	0
3	GJ	968	0	973	33	0
3	GK	968	0	973	23	0
3	GL	968	0	974	37	0
3	GM	968	0	973	36	0
3	GN	968	0	973	35	0
3	GO	968	0	973	19	0
3	GP	968	0	973	41	0
3	GQ	968	0	973	28	0
3	GS	968	0	973	38	0
3	GT	968	0	973	36	0
3	GU	968	0	973	35	0
3	GV	968	0	973	49	0
3	GW	968	0	973	25	0
3	GX	968	0	974	44	0
3	GY	968	0	973	33	0
3	Gc	968	0	973	46	0
All	All	271353	0	227545	7666	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 16.

The worst 5 of 7666 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)
3:BP:68:CYS:SG	3:EG:64:CYS:SG	1.31	1.31
3:CS:64:CYS:SG	3:DV:68:CYS:SG	1.30	1.29
3:BP:68:CYS:CB	3:EG:64:CYS:SG	2.27	1.22
1:R:3429:G:H1	1:R:3449:A:N6	1.48	1.10
1:R:2499:A:N6	1:R:2542:G:H1	1.50	1.09

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	a	532/534 (100%)	492 (92%)	38 (7%)	2 (0%)	30	60
2	b	532/534 (100%)	488 (92%)	41 (8%)	3 (1%)	21	50
3	AB	127/129 (98%)	114 (90%)	13 (10%)	0	100	100
3	AC	127/129 (98%)	119 (94%)	6 (5%)	2 (2%)	7	29
3	AE	127/129 (98%)	114 (90%)	12 (9%)	1 (1%)	16	45
3	AF	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	7	29
3	AG	127/129 (98%)	112 (88%)	15 (12%)	0	100	100
3	AH	127/129 (98%)	120 (94%)	5 (4%)	2 (2%)	7	29
3	AI	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	AJ	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	16	45
3	AK	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	16	45
3	AL	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
3	AM	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	16	45
3	AN	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	16	45
3	AO	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	16	45
3	AP	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	AQ	127/129 (98%)	113 (89%)	11 (9%)	3 (2%)	4	21
3	AS	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	45
3	AT	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	16	45
3	AU	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
3	AV	127/129 (98%)	114 (90%)	11 (9%)	2 (2%)	7	29
3	AW	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	45
3	AX	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	16	45
3	AY	127/129 (98%)	120 (94%)	5 (4%)	2 (2%)	7	29
3	AZ	127/129 (98%)	115 (91%)	7 (6%)	5 (4%)	2	13
3	Ac	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
3	BA	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	16	45
3	BB	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
3	BC	127/129 (98%)	112 (88%)	13 (10%)	2 (2%)	7	29
3	BD	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	16	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	BE	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	16	45
3	BF	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	16	45
3	BG	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	BH	127/129 (98%)	120 (94%)	5 (4%)	2 (2%)	7	29
3	BI	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	BJ	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
3	BK	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	16	45
3	BL	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
3	BM	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	16	45
3	BN	127/129 (98%)	113 (89%)	12 (9%)	2 (2%)	7	29
3	BO	127/129 (98%)	114 (90%)	11 (9%)	2 (2%)	7	29
3	BP	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	16	45
3	BQ	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	16	45
3	BS	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
3	BT	127/129 (98%)	114 (90%)	11 (9%)	2 (2%)	7	29
3	BU	127/129 (98%)	121 (95%)	4 (3%)	2 (2%)	7	29
3	BV	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	16	45
3	BW	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
3	BX	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	7	29
3	BY	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
3	BZ	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	16	45
3	Bc	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	45
3	CA	127/129 (98%)	115 (91%)	10 (8%)	2 (2%)	7	29
3	CB	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
3	CC	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	16	45
3	CD	127/129 (98%)	116 (91%)	9 (7%)	2 (2%)	7	29
3	CE	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	16	45
3	CF	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	45
3	CG	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	45
3	CH	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
3	CI	127/129 (98%)	120 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	CJ	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	CK	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	CL	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	16	45
3	CM	127/129 (98%)	116 (91%)	9 (7%)	2 (2%)	7	29
3	CN	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	7	29
3	CO	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
3	CP	127/129 (98%)	115 (91%)	10 (8%)	2 (2%)	7	29
3	CQ	127/129 (98%)	122 (96%)	3 (2%)	2 (2%)	7	29
3	CS	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	16	45
3	CT	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
3	CU	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
3	CV	127/129 (98%)	117 (92%)	7 (6%)	3 (2%)	4	21
3	CW	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	16	45
3	CX	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	16	45
3	CY	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	45
3	CZ	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	16	45
3	Cc	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	16	45
3	DA	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	16	45
3	DB	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
3	DC	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	16	45
3	DD	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	7	29
3	DE	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
3	DF	127/129 (98%)	121 (95%)	4 (3%)	2 (2%)	7	29
3	DG	127/129 (98%)	116 (91%)	10 (8%)	1 (1%)	16	45
3	DH	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	DI	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
3	DJ	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
3	DK	127/129 (98%)	119 (94%)	6 (5%)	2 (2%)	7	29
3	DL	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
3	DM	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	16	45
3	DN	127/129 (98%)	116 (91%)	11 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	DO	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
3	DQ	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	16	45
3	DS	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	7	29
3	DT	127/129 (98%)	116 (91%)	10 (8%)	1 (1%)	16	45
3	DU	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
3	DV	127/129 (98%)	117 (92%)	7 (6%)	3 (2%)	4	21
3	DW	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	16	45
3	DX	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
3	DY	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
3	DZ	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
3	Dc	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
3	EA	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
3	EB	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
3	EC	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
3	ED	127/129 (98%)	120 (94%)	5 (4%)	2 (2%)	7	29
3	EE	127/129 (98%)	115 (91%)	8 (6%)	4 (3%)	3	17
3	EF	127/129 (98%)	115 (91%)	12 (9%)	0	100	100
3	EG	127/129 (98%)	120 (94%)	3 (2%)	4 (3%)	3	17
3	EH	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	16	45
3	EI	127/129 (98%)	115 (91%)	10 (8%)	2 (2%)	7	29
3	EJ	127/129 (98%)	119 (94%)	5 (4%)	3 (2%)	4	21
3	EK	127/129 (98%)	123 (97%)	2 (2%)	2 (2%)	7	29
3	EL	127/129 (98%)	119 (94%)	6 (5%)	2 (2%)	7	29
3	EM	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
3	EN	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	16	45
3	EO	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	16	45
3	EP	127/129 (98%)	119 (94%)	6 (5%)	2 (2%)	7	29
3	EQ	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	7	29
3	ES	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	ET	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	45
3	EU	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	16	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	EV	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	16	45
3	EW	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	45
3	EX	127/129 (98%)	110 (87%)	13 (10%)	4 (3%)	3	17
3	EY	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
3	EZ	127/129 (98%)	119 (94%)	6 (5%)	2 (2%)	7	29
3	Ec	127/129 (98%)	116 (91%)	10 (8%)	1 (1%)	16	45
3	FA	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
3	FB	127/129 (98%)	115 (91%)	9 (7%)	3 (2%)	4	21
3	FC	127/129 (98%)	118 (93%)	6 (5%)	3 (2%)	4	21
3	FD	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
3	FE	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
3	FF	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	16	45
3	FG	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
3	FH	127/129 (98%)	115 (91%)	12 (9%)	0	100	100
3	FI	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
3	FJ	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	16	45
3	FK	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
3	FL	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	16	45
3	FM	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	7	29
3	FN	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	16	45
3	FO	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	45
3	FP	127/129 (98%)	120 (94%)	5 (4%)	2 (2%)	7	29
3	FQ	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	FS	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	16	45
3	FT	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	16	45
3	FU	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
3	FV	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	45
3	FW	127/129 (98%)	112 (88%)	11 (9%)	4 (3%)	3	17
3	FX	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	7	29
3	FY	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
3	FZ	127/129 (98%)	113 (89%)	11 (9%)	3 (2%)	4	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Fc	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	7	29
3	GA	127/129 (98%)	116 (91%)	10 (8%)	1 (1%)	16	45
3	GB	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	GC	127/129 (98%)	117 (92%)	7 (6%)	3 (2%)	4	21
3	GD	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
3	GE	127/129 (98%)	119 (94%)	5 (4%)	3 (2%)	4	21
3	GF	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	16	45
3	GG	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	45
3	GH	127/129 (98%)	122 (96%)	3 (2%)	2 (2%)	7	29
3	GI	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	16	45
3	GJ	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	16	45
3	GK	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	16	45
3	GL	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
3	GM	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
3	GN	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	7	29
3	GO	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	16	45
3	GP	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	16	45
3	GQ	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	45
3	GS	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
3	GT	127/129 (98%)	119 (94%)	6 (5%)	2 (2%)	7	29
3	GU	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	16	45
3	GV	127/129 (98%)	116 (91%)	9 (7%)	2 (2%)	7	29
3	GW	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
3	GX	127/129 (98%)	114 (90%)	9 (7%)	4 (3%)	3	17
3	GY	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	16	45
3	Gc	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
All	All	23670/24030 (98%)	22117 (93%)	1356 (6%)	197 (1%)	18	45

5 of 197 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	a	148	ILE
2	b	148	ILE

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Mol	Chain	Res	Type
3	AV	66	ASP
3	AX	70	ILE
3	AY	67	ALA

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	a	466/466 (100%)	466 (100%)	0	100	100
2	b	466/466 (100%)	466 (100%)	0	100	100
3	AB	108/108 (100%)	108 (100%)	0	100	100
3	AC	108/108 (100%)	108 (100%)	0	100	100
3	AE	108/108 (100%)	108 (100%)	0	100	100
3	AF	108/108 (100%)	108 (100%)	0	100	100
3	AG	108/108 (100%)	108 (100%)	0	100	100
3	AH	108/108 (100%)	108 (100%)	0	100	100
3	AI	108/108 (100%)	108 (100%)	0	100	100
3	AJ	108/108 (100%)	108 (100%)	0	100	100
3	AK	108/108 (100%)	108 (100%)	0	100	100
3	AL	108/108 (100%)	108 (100%)	0	100	100
3	AM	108/108 (100%)	108 (100%)	0	100	100
3	AN	108/108 (100%)	108 (100%)	0	100	100
3	AO	108/108 (100%)	108 (100%)	0	100	100
3	AP	108/108 (100%)	107 (99%)	1 (1%)	70	78
3	AQ	108/108 (100%)	108 (100%)	0	100	100
3	AS	108/108 (100%)	108 (100%)	0	100	100
3	AT	108/108 (100%)	108 (100%)	0	100	100
3	AU	108/108 (100%)	108 (100%)	0	100	100
3	AV	108/108 (100%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AW	108/108 (100%)	108 (100%)	0	100	100
3	AX	108/108 (100%)	108 (100%)	0	100	100
3	AY	108/108 (100%)	108 (100%)	0	100	100
3	AZ	108/108 (100%)	106 (98%)	2 (2%)	50	71
3	Ac	108/108 (100%)	108 (100%)	0	100	100
3	BA	108/108 (100%)	108 (100%)	0	100	100
3	BB	108/108 (100%)	108 (100%)	0	100	100
3	BC	108/108 (100%)	108 (100%)	0	100	100
3	BD	108/108 (100%)	108 (100%)	0	100	100
3	BE	108/108 (100%)	108 (100%)	0	100	100
3	BF	108/108 (100%)	108 (100%)	0	100	100
3	BG	108/108 (100%)	108 (100%)	0	100	100
3	BH	108/108 (100%)	108 (100%)	0	100	100
3	BI	108/108 (100%)	108 (100%)	0	100	100
3	BJ	108/108 (100%)	108 (100%)	0	100	100
3	BK	108/108 (100%)	108 (100%)	0	100	100
3	BL	108/108 (100%)	108 (100%)	0	100	100
3	BM	108/108 (100%)	108 (100%)	0	100	100
3	BN	108/108 (100%)	106 (98%)	2 (2%)	50	71
3	BO	108/108 (100%)	108 (100%)	0	100	100
3	BP	108/108 (100%)	108 (100%)	0	100	100
3	BQ	108/108 (100%)	108 (100%)	0	100	100
3	BS	108/108 (100%)	108 (100%)	0	100	100
3	BT	108/108 (100%)	108 (100%)	0	100	100
3	BU	108/108 (100%)	108 (100%)	0	100	100
3	BV	108/108 (100%)	108 (100%)	0	100	100
3	BW	108/108 (100%)	108 (100%)	0	100	100
3	BX	108/108 (100%)	108 (100%)	0	100	100
3	BY	108/108 (100%)	108 (100%)	0	100	100
3	BZ	108/108 (100%)	108 (100%)	0	100	100
3	Bc	108/108 (100%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	CA	108/108 (100%)	108 (100%)	0	100	100
3	CB	108/108 (100%)	108 (100%)	0	100	100
3	CC	108/108 (100%)	108 (100%)	0	100	100
3	CD	108/108 (100%)	108 (100%)	0	100	100
3	CE	108/108 (100%)	108 (100%)	0	100	100
3	CF	108/108 (100%)	108 (100%)	0	100	100
3	CG	108/108 (100%)	108 (100%)	0	100	100
3	CH	108/108 (100%)	108 (100%)	0	100	100
3	CI	108/108 (100%)	108 (100%)	0	100	100
3	CJ	108/108 (100%)	108 (100%)	0	100	100
3	CK	108/108 (100%)	108 (100%)	0	100	100
3	CL	108/108 (100%)	108 (100%)	0	100	100
3	CM	108/108 (100%)	108 (100%)	0	100	100
3	CN	108/108 (100%)	108 (100%)	0	100	100
3	CO	108/108 (100%)	108 (100%)	0	100	100
3	CP	108/108 (100%)	108 (100%)	0	100	100
3	CQ	108/108 (100%)	108 (100%)	0	100	100
3	CS	108/108 (100%)	108 (100%)	0	100	100
3	CT	108/108 (100%)	108 (100%)	0	100	100
3	CU	108/108 (100%)	108 (100%)	0	100	100
3	CV	108/108 (100%)	108 (100%)	0	100	100
3	CW	108/108 (100%)	108 (100%)	0	100	100
3	CX	108/108 (100%)	108 (100%)	0	100	100
3	CY	108/108 (100%)	108 (100%)	0	100	100
3	CZ	108/108 (100%)	108 (100%)	0	100	100
3	Cc	108/108 (100%)	108 (100%)	0	100	100
3	DA	108/108 (100%)	108 (100%)	0	100	100
3	DB	108/108 (100%)	108 (100%)	0	100	100
3	DC	108/108 (100%)	108 (100%)	0	100	100
3	DD	108/108 (100%)	108 (100%)	0	100	100
3	DE	108/108 (100%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	DF	108/108 (100%)	108 (100%)	0	100	100
3	DG	108/108 (100%)	108 (100%)	0	100	100
3	DH	108/108 (100%)	108 (100%)	0	100	100
3	DI	108/108 (100%)	108 (100%)	0	100	100
3	DJ	108/108 (100%)	108 (100%)	0	100	100
3	DK	108/108 (100%)	108 (100%)	0	100	100
3	DL	108/108 (100%)	108 (100%)	0	100	100
3	DM	108/108 (100%)	108 (100%)	0	100	100
3	DN	108/108 (100%)	108 (100%)	0	100	100
3	DO	108/108 (100%)	108 (100%)	0	100	100
3	DQ	108/108 (100%)	108 (100%)	0	100	100
3	DS	108/108 (100%)	108 (100%)	0	100	100
3	DT	108/108 (100%)	108 (100%)	0	100	100
3	DU	108/108 (100%)	108 (100%)	0	100	100
3	DV	108/108 (100%)	107 (99%)	1 (1%)	70	78
3	DW	108/108 (100%)	108 (100%)	0	100	100
3	DX	108/108 (100%)	108 (100%)	0	100	100
3	DY	108/108 (100%)	108 (100%)	0	100	100
3	DZ	108/108 (100%)	108 (100%)	0	100	100
3	Dc	108/108 (100%)	108 (100%)	0	100	100
3	EA	108/108 (100%)	108 (100%)	0	100	100
3	EB	108/108 (100%)	108 (100%)	0	100	100
3	EC	108/108 (100%)	108 (100%)	0	100	100
3	ED	108/108 (100%)	108 (100%)	0	100	100
3	EE	108/108 (100%)	107 (99%)	1 (1%)	70	78
3	EF	108/108 (100%)	108 (100%)	0	100	100
3	EG	108/108 (100%)	108 (100%)	0	100	100
3	EH	108/108 (100%)	108 (100%)	0	100	100
3	EI	108/108 (100%)	108 (100%)	0	100	100
3	EJ	108/108 (100%)	108 (100%)	0	100	100
3	EK	108/108 (100%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	EL	108/108 (100%)	108 (100%)	0	100	100
3	EM	108/108 (100%)	108 (100%)	0	100	100
3	EN	108/108 (100%)	108 (100%)	0	100	100
3	EO	108/108 (100%)	108 (100%)	0	100	100
3	EP	108/108 (100%)	108 (100%)	0	100	100
3	EQ	108/108 (100%)	108 (100%)	0	100	100
3	ES	108/108 (100%)	108 (100%)	0	100	100
3	ET	108/108 (100%)	108 (100%)	0	100	100
3	EU	108/108 (100%)	108 (100%)	0	100	100
3	EV	108/108 (100%)	108 (100%)	0	100	100
3	EW	108/108 (100%)	108 (100%)	0	100	100
3	EX	108/108 (100%)	108 (100%)	0	100	100
3	EY	108/108 (100%)	108 (100%)	0	100	100
3	EZ	108/108 (100%)	108 (100%)	0	100	100
3	Ec	108/108 (100%)	108 (100%)	0	100	100
3	FA	108/108 (100%)	108 (100%)	0	100	100
3	FB	108/108 (100%)	108 (100%)	0	100	100
3	FC	108/108 (100%)	108 (100%)	0	100	100
3	FD	108/108 (100%)	108 (100%)	0	100	100
3	FE	108/108 (100%)	108 (100%)	0	100	100
3	FF	108/108 (100%)	108 (100%)	0	100	100
3	FG	108/108 (100%)	108 (100%)	0	100	100
3	FH	108/108 (100%)	108 (100%)	0	100	100
3	FI	108/108 (100%)	108 (100%)	0	100	100
3	FJ	108/108 (100%)	108 (100%)	0	100	100
3	FK	108/108 (100%)	108 (100%)	0	100	100
3	FL	108/108 (100%)	108 (100%)	0	100	100
3	FM	108/108 (100%)	108 (100%)	0	100	100
3	FN	108/108 (100%)	108 (100%)	0	100	100
3	FO	108/108 (100%)	108 (100%)	0	100	100
3	FP	108/108 (100%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	FQ	108/108 (100%)	108 (100%)	0	100	100
3	FS	108/108 (100%)	108 (100%)	0	100	100
3	FT	108/108 (100%)	108 (100%)	0	100	100
3	FU	108/108 (100%)	108 (100%)	0	100	100
3	FV	108/108 (100%)	108 (100%)	0	100	100
3	FW	108/108 (100%)	107 (99%)	1 (1%)	70	78
3	FX	108/108 (100%)	108 (100%)	0	100	100
3	FY	108/108 (100%)	108 (100%)	0	100	100
3	FZ	108/108 (100%)	108 (100%)	0	100	100
3	Fc	108/108 (100%)	108 (100%)	0	100	100
3	GA	108/108 (100%)	108 (100%)	0	100	100
3	GB	108/108 (100%)	108 (100%)	0	100	100
3	GC	108/108 (100%)	104 (96%)	4 (4%)	30	59
3	GD	108/108 (100%)	108 (100%)	0	100	100
3	GE	108/108 (100%)	108 (100%)	0	100	100
3	GF	108/108 (100%)	108 (100%)	0	100	100
3	GG	108/108 (100%)	108 (100%)	0	100	100
3	GH	108/108 (100%)	108 (100%)	0	100	100
3	GI	108/108 (100%)	108 (100%)	0	100	100
3	GJ	108/108 (100%)	108 (100%)	0	100	100
3	GK	108/108 (100%)	108 (100%)	0	100	100
3	GL	108/108 (100%)	108 (100%)	0	100	100
3	GM	108/108 (100%)	108 (100%)	0	100	100
3	GN	108/108 (100%)	108 (100%)	0	100	100
3	GO	108/108 (100%)	108 (100%)	0	100	100
3	GP	108/108 (100%)	108 (100%)	0	100	100
3	GQ	108/108 (100%)	108 (100%)	0	100	100
3	GS	108/108 (100%)	108 (100%)	0	100	100
3	GT	108/108 (100%)	108 (100%)	0	100	100
3	GU	108/108 (100%)	108 (100%)	0	100	100
3	GV	108/108 (100%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	GW	108/108 (100%)	108 (100%)	0	100	100
3	GX	108/108 (100%)	101 (94%)	7 (6%)	15	42
3	GY	108/108 (100%)	108 (100%)	0	100	100
3	Gc	108/108 (100%)	108 (100%)	0	100	100
All	All	20156/20156 (100%)	20137 (100%)	19 (0%)	87	90

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	GX	64	CYS
3	GX	71	MET
3	GX	73	ASN
3	GX	70	ILE
3	GC	60	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 133 such sidechains are listed below:

Mol	Chain	Res	Type
3	FO	49	GLN
3	FY	2	ASN
3	GX	73	ASN
3	BU	44	ASN
3	BU	34	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	4269/4269 (100%)	689 (16%)	7 (0%)

5 of 689 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	G
1	R	4	G
1	R	17	G
1	R	29	A
1	R	37	U

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	317	C
1	R	993	C
1	R	3833	A
1	R	2865	A
1	R	60	A

#### 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.

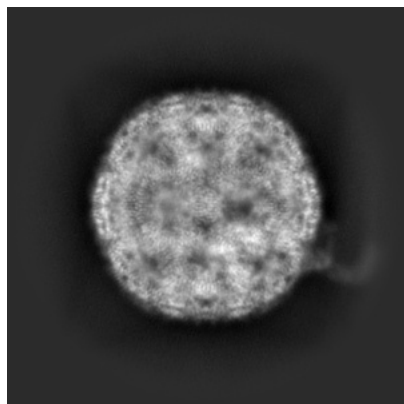
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41443. These allow visual inspection of the internal detail of the map and identification of artifacts.

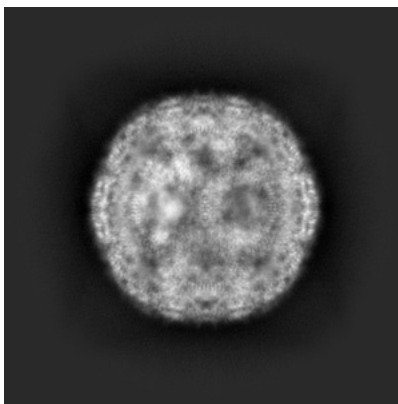
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

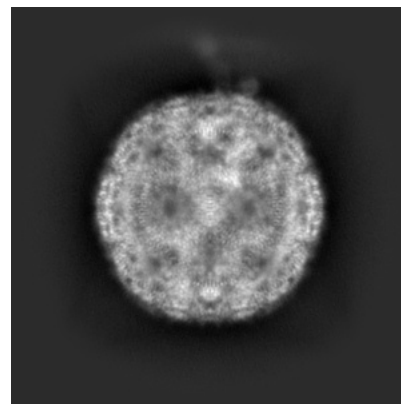
#### 6.1.1 Primary map



X

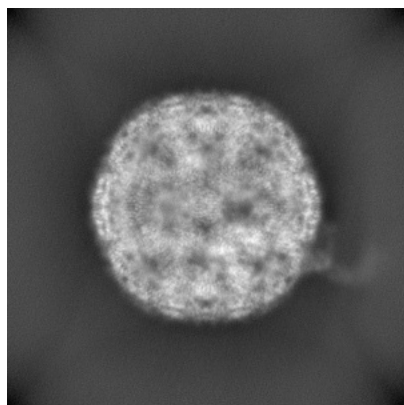


Y

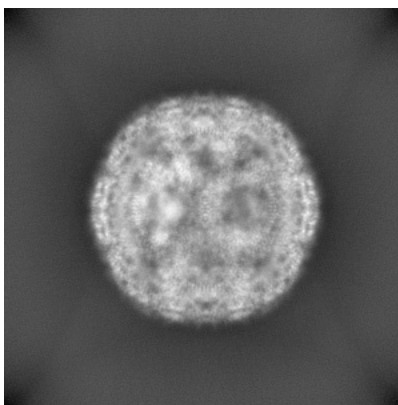


Z

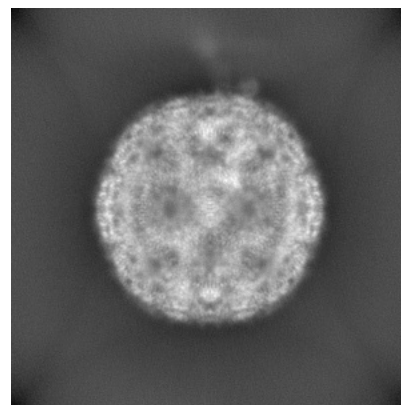
#### 6.1.2 Raw map



X



Y

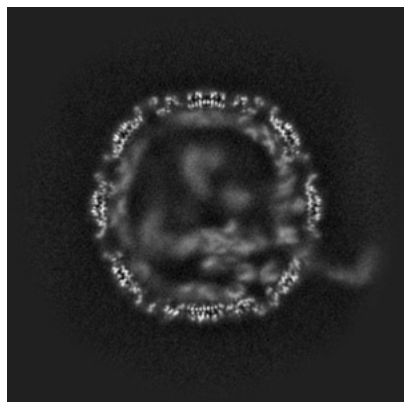


Z

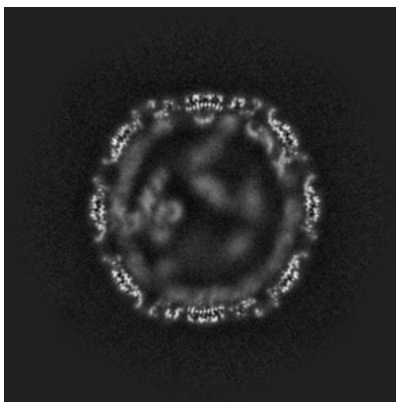
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

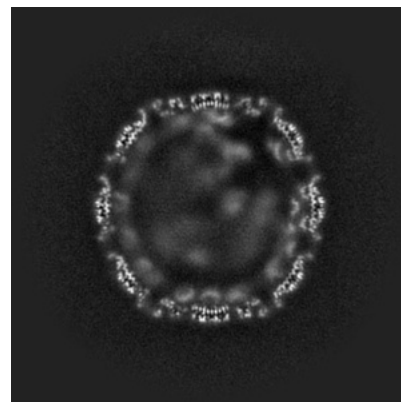
### 6.2.1 Primary map



X Index: 230

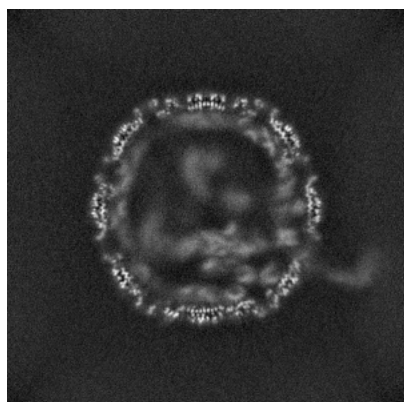


Y Index: 230

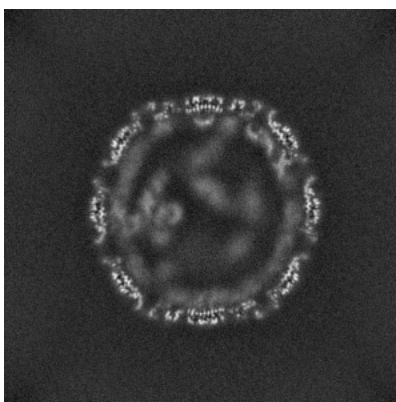


Z Index: 230

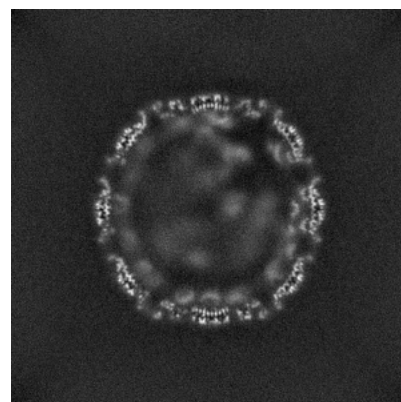
### 6.2.2 Raw map



X Index: 230



Y Index: 230

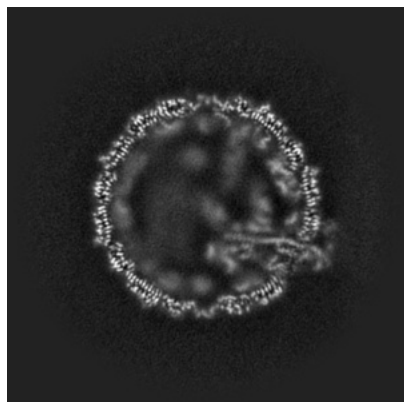


Z Index: 230

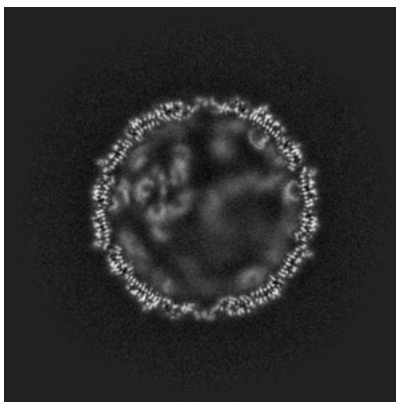
The images above show central slices of the map in three orthogonal directions.

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

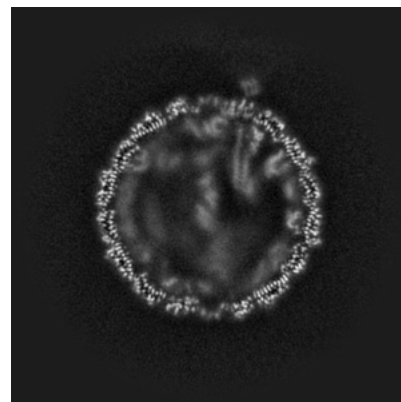
### 6.3.1 Primary map



X Index: 262

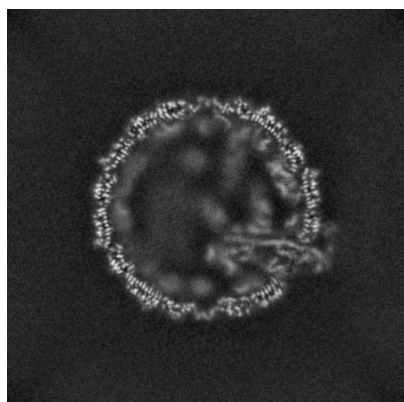


Y Index: 262

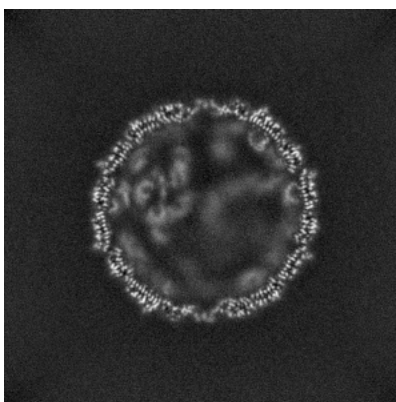


Z Index: 194

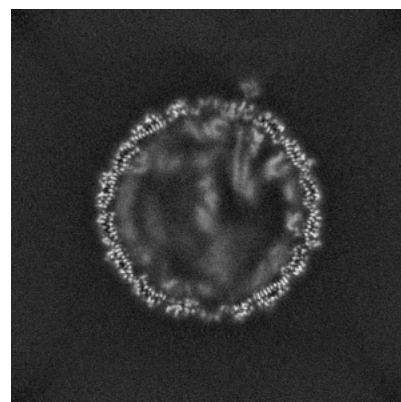
### 6.3.2 Raw map



X Index: 262



Y Index: 262

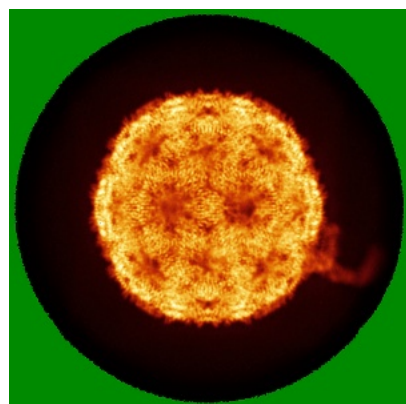


Z Index: 194

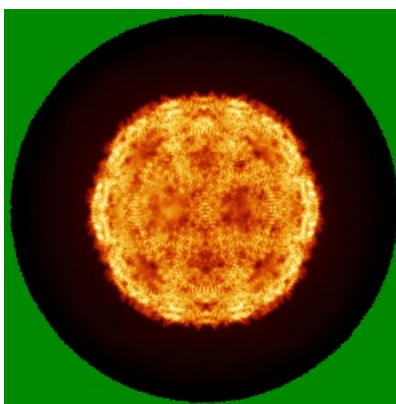
The images above show the largest variance slices of the map in three orthogonal directions.

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

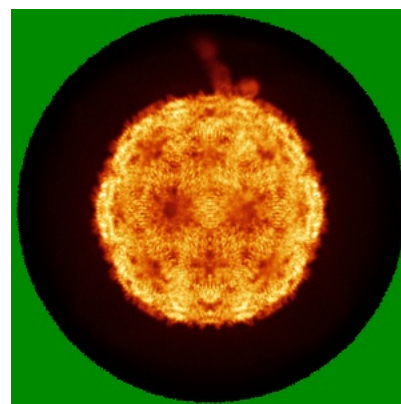
### 6.4.1 Primary map



X

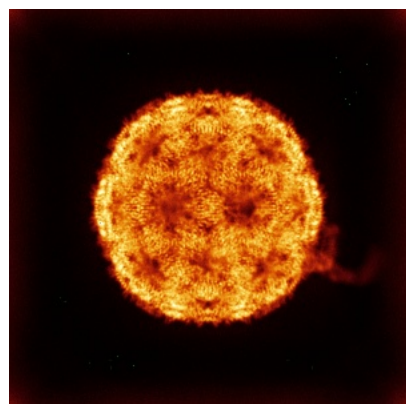


Y

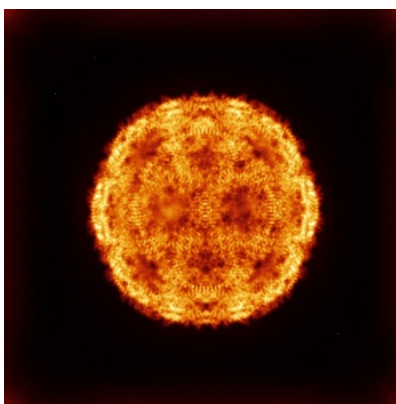


Z

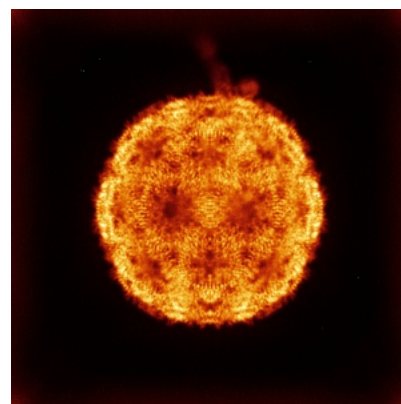
### 6.4.2 Raw map



X



Y

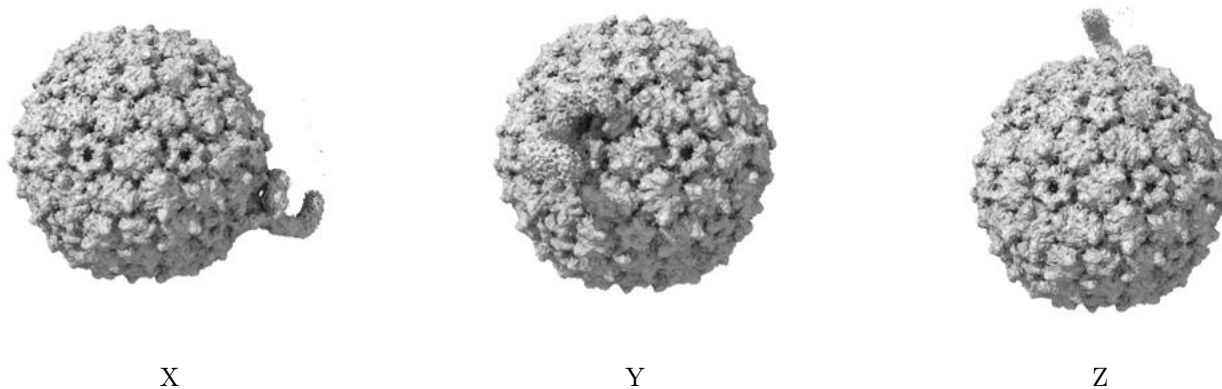


Z

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

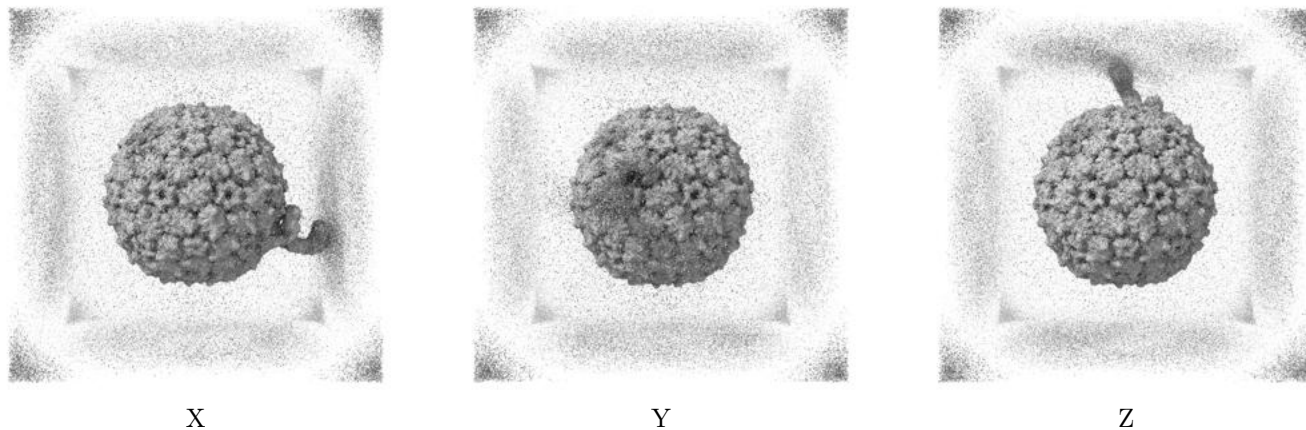
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.128. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

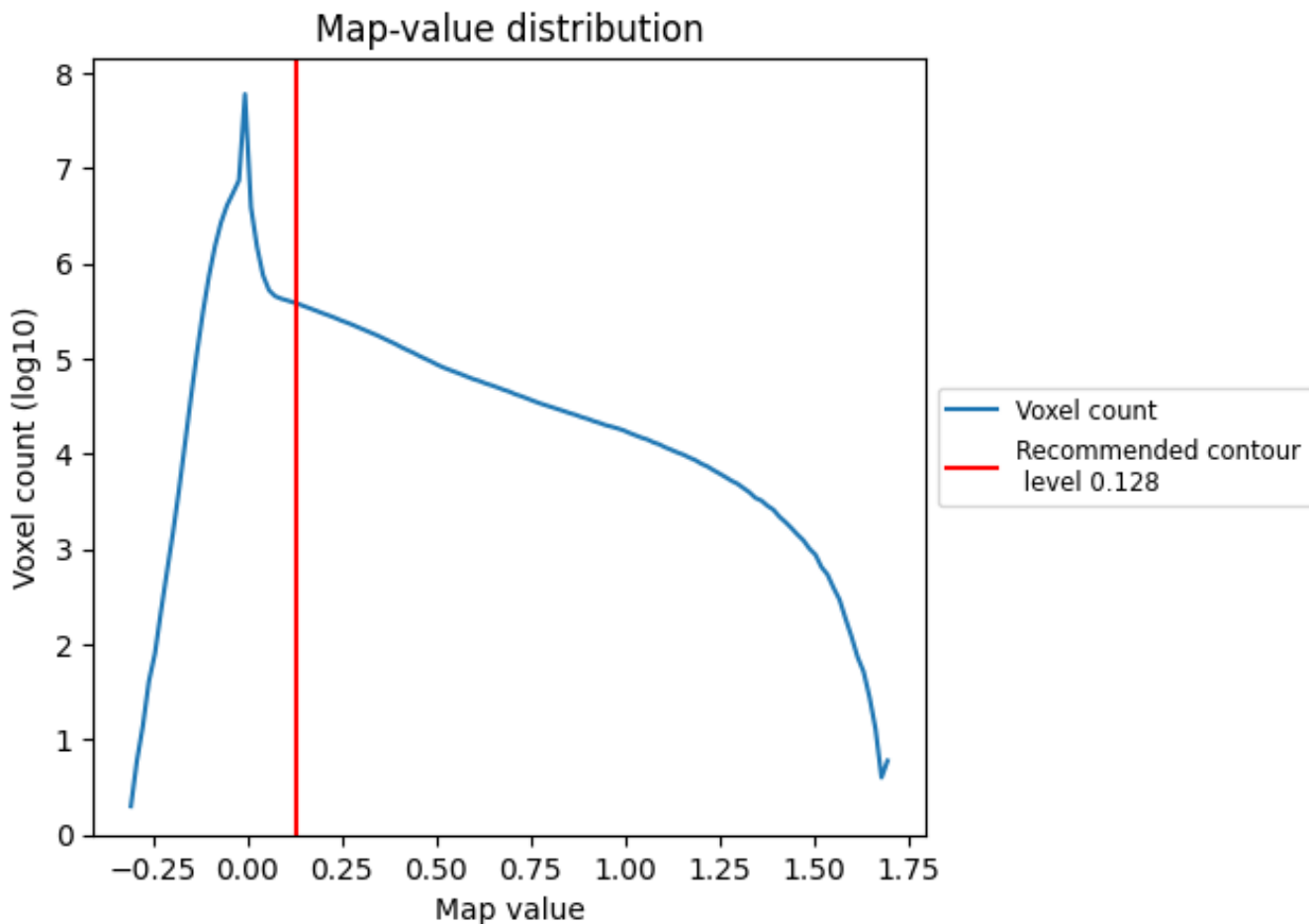
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

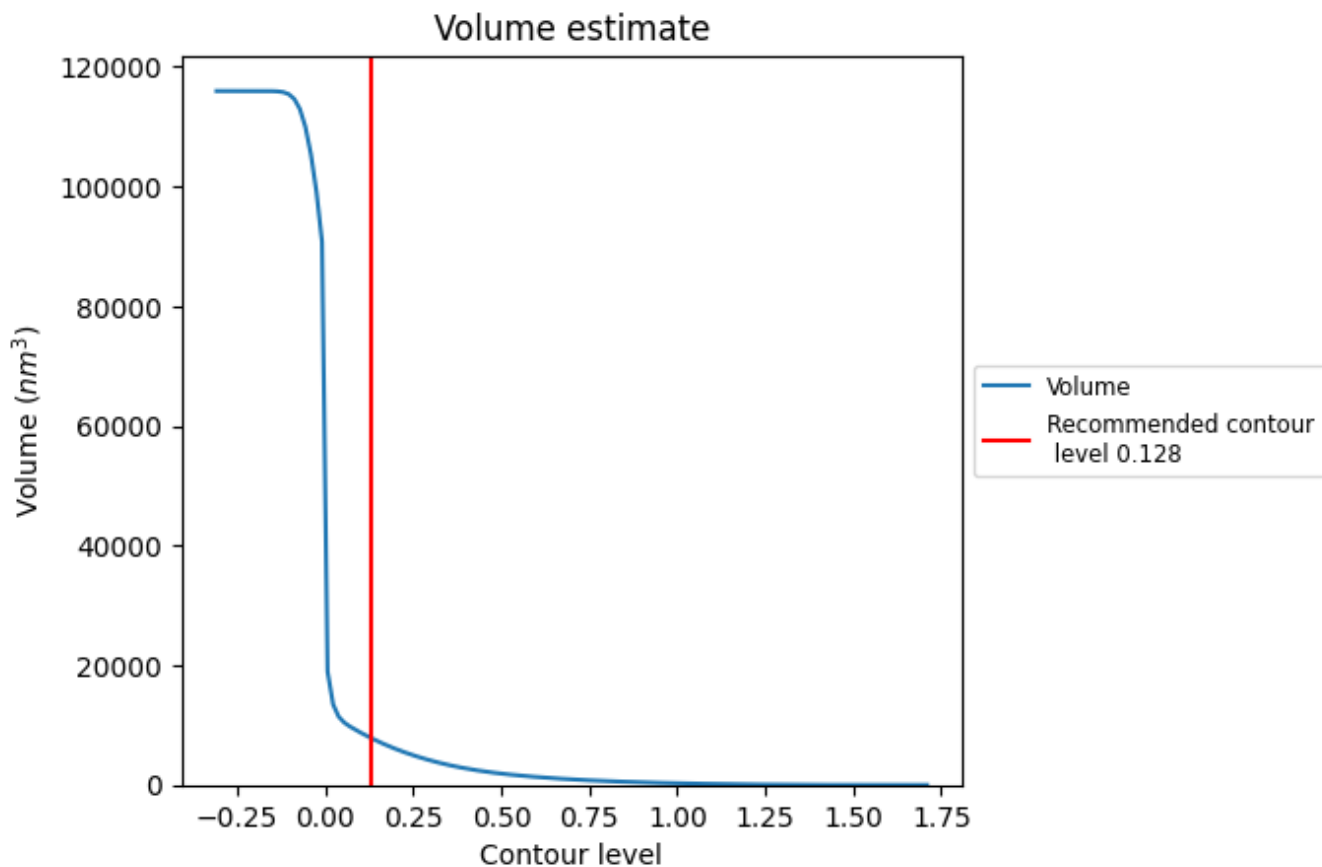
This section contains the results of statistical analysis of the map.

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



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

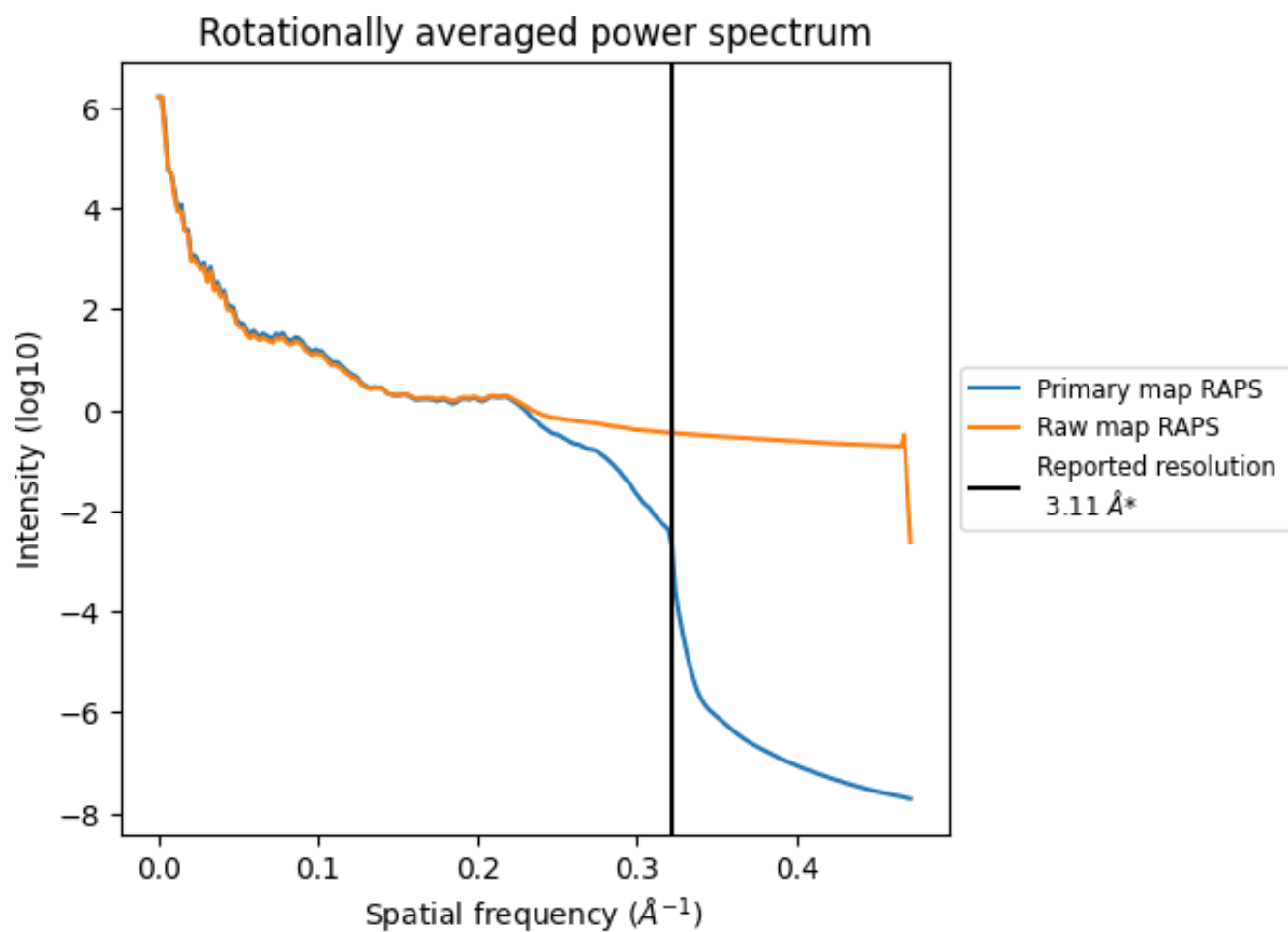
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 7917  $\text{nm}^3$ ; this corresponds to an approximate mass of 7152 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)

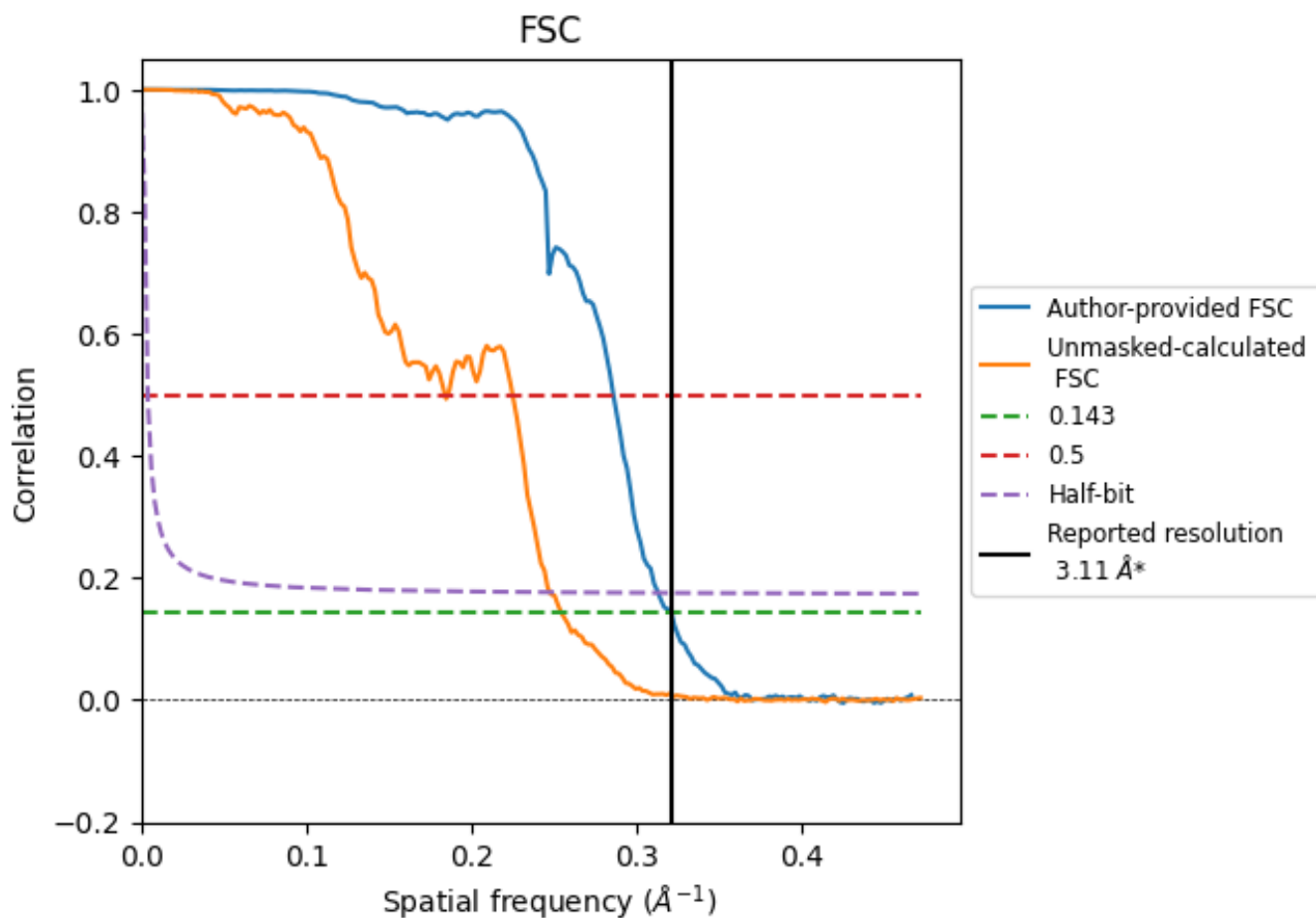


\*Reported resolution corresponds to spatial frequency of 0.322 Å<sup>-1</sup>

## 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 0.322 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

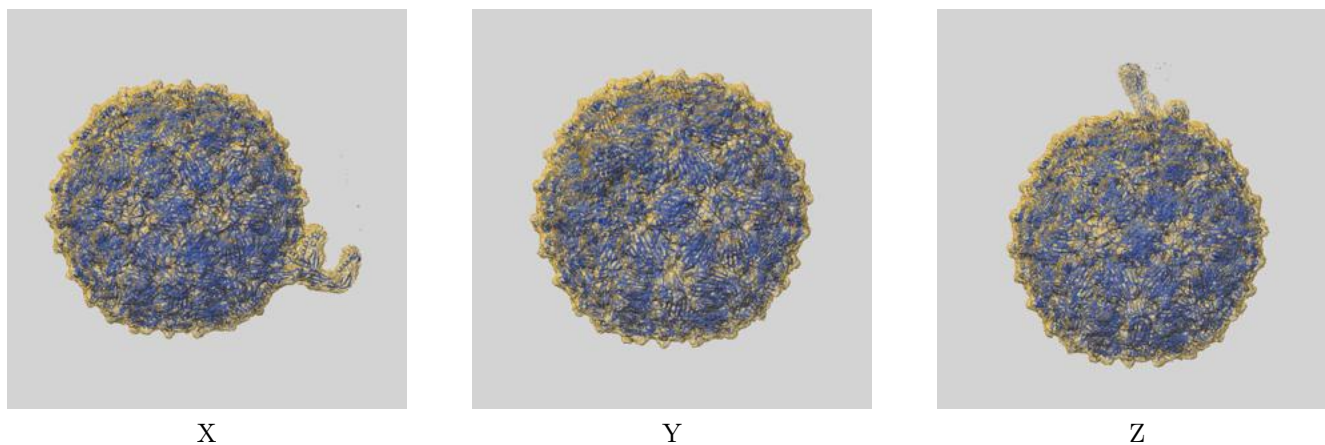
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	3.12	3.50	3.19
Unmasked-calculated*	3.93	5.44	4.04

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.93 differs from the reported value 3.11 by more than 10 %

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

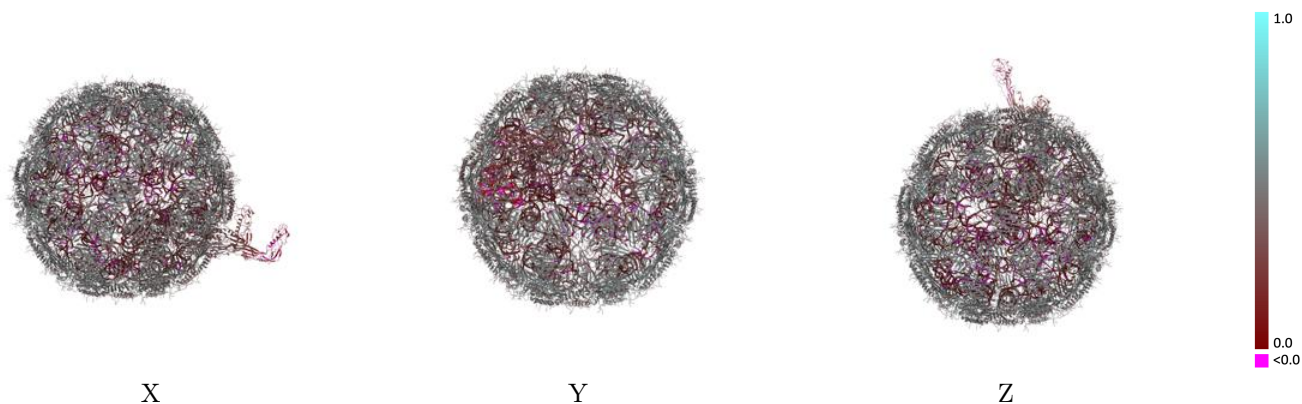
This section contains information regarding the fit between EMDB map EMD-41443 and PDB model 8TOC. Per-residue inclusion information can be found in section [3](#) on page [20](#).

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



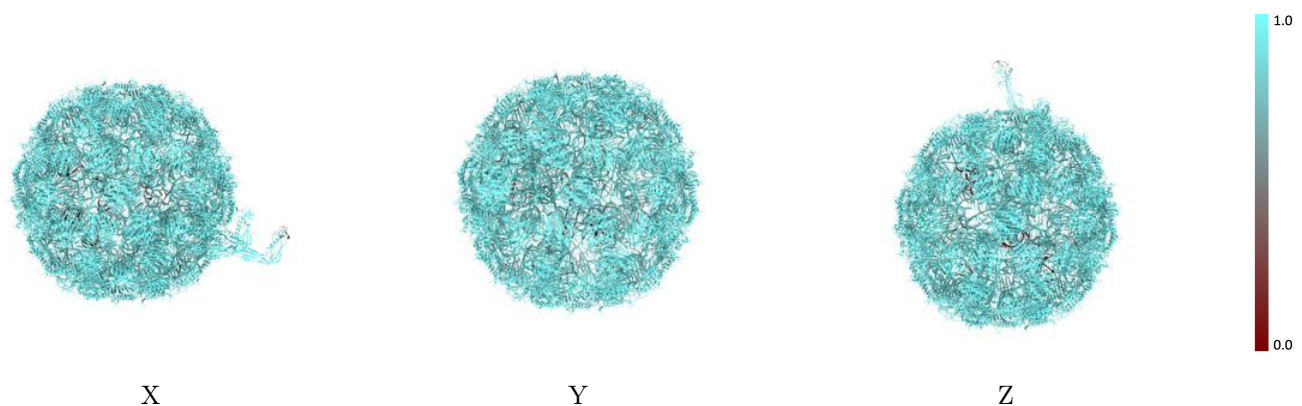
The images above show the 3D surface view of the map at the recommended contour level 0.128 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



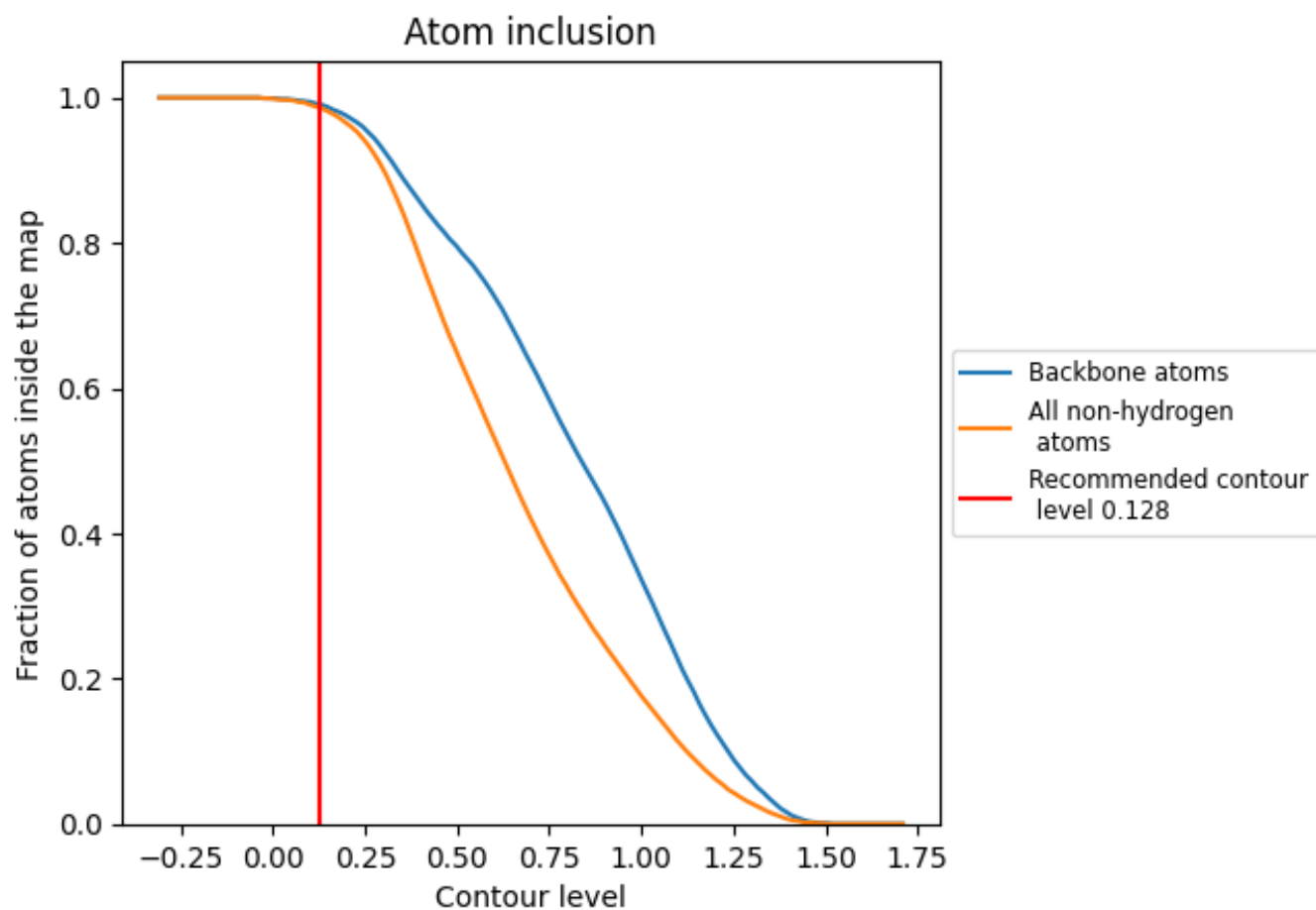
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.128).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.128) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9860	0.3540
AB	1.0000	0.4070
AC	1.0000	0.4160
AE	1.0000	0.4640
AF	0.9990	0.4650
AG	1.0000	0.4690
AH	1.0000	0.4680
AI	1.0000	0.4600
AJ	0.9980	0.4630
AK	1.0000	0.4690
AL	1.0000	0.4660
AM	1.0000	0.4790
AN	1.0000	0.4450
AO	1.0000	0.4540
AP	1.0000	0.4620
AQ	1.0000	0.4640
AS	1.0000	0.4600
AT	1.0000	0.4570
AU	1.0000	0.4650
AV	1.0000	0.4560
AW	1.0000	0.4680
AX	0.9980	0.4650
AY	1.0000	0.4670
AZ	1.0000	0.4650
Ac	1.0000	0.4610
BA	1.0000	0.4630
BB	1.0000	0.4670
BC	1.0000	0.4620
BD	0.9990	0.4660
BE	1.0000	0.4690
BF	1.0000	0.4680
BG	0.9990	0.4710
BH	0.9990	0.4650
BI	1.0000	0.4480
BJ	1.0000	0.4610



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Chain	Atom inclusion	Q-score
BK	1.0000	0.4460
BL	1.0000	0.4610
BM	1.0000	0.4700
BN	1.0000	0.4700
BO	1.0000	0.4610
BP	1.0000	0.4600
BQ	1.0000	0.4550
BS	1.0000	0.4530
BT	1.0000	0.4610
BU	1.0000	0.4580
BV	0.9970	0.4490
BW	1.0000	0.4440
BX	1.0000	0.4680
BY	0.9990	0.4680
BZ	1.0000	0.4670
Bc	1.0000	0.4680
CA	1.0000	0.4620
CB	1.0000	0.4660
CC	0.9970	0.4600
CD	1.0000	0.4690
CE	1.0000	0.4690
CF	1.0000	0.4690
CG	1.0000	0.4650
CH	1.0000	0.4720
CI	1.0000	0.4620
CJ	1.0000	0.4570
CK	1.0000	0.4520
CL	1.0000	0.4640
CM	1.0000	0.4070
CN	0.9960	0.4330
CO	1.0000	0.4300
CP	1.0000	0.4680
CQ	0.9990	0.4660
CS	1.0000	0.4740
CT	1.0000	0.4700
CU	1.0000	0.4740
CV	1.0000	0.4650
CW	1.0000	0.4630
CX	0.9990	0.4650
CY	1.0000	0.4700
CZ	1.0000	0.4740
Cc	1.0000	0.4630





















































































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Chain	Atom inclusion	Q-score
DA	1.0000	0.4670
DB	0.9990	0.4620
DC	0.9990	0.4680
DD	1.0000	0.4670
DE	1.0000	0.4670
DF	0.9990	0.4680
DG	1.0000	0.4710
DH	1.0000	0.4530
DI	1.0000	0.4240
DJ	1.0000	0.4480
DK	0.9990	0.4760
DL	1.0000	0.4660
DM	0.9990	0.4720
DN	0.9990	0.4270
DO	0.9990	0.3930
DQ	1.0000	0.4760
DS	1.0000	0.4650
DT	1.0000	0.4580
DU	1.0000	0.4660
DV	1.0000	0.4640
DW	1.0000	0.4670
DX	1.0000	0.4730
DY	1.0000	0.4660
DZ	1.0000	0.4670
Dc	0.9990	0.4670
EA	1.0000	0.4680
EB	1.0000	0.4600
EC	1.0000	0.4540
ED	1.0000	0.4560
EE	1.0000	0.4620
EF	1.0000	0.4570
EG	0.9990	0.4640
EH	1.0000	0.4620
EI	0.9990	0.4590
EJ	1.0000	0.4630
EK	1.0000	0.4680
EL	1.0000	0.4660
EM	1.0000	0.4660
EN	1.0000	0.4640
EO	1.0000	0.4700
EP	1.0000	0.4640
EQ	1.0000	0.4670











































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Chain	Atom inclusion	Q-score
ES	 1.0000	 0.4650
ET	 0.9990	 0.4640
EU	 1.0000	 0.4410
EV	 0.9990	 0.4380
EW	 1.0000	 0.4500
EX	 1.0000	 0.4690
EY	 0.9980	 0.4630
EZ	 1.0000	 0.4680
Ec	 1.0000	 0.4640
FA	 1.0000	 0.4520
FB	 1.0000	 0.4330
FC	 1.0000	 0.4500
FD	 1.0000	 0.4660
FE	 0.9990	 0.4620
FF	 1.0000	 0.4650
FG	 1.0000	 0.4200
FH	 1.0000	 0.4470
FI	 1.0000	 0.4500
FJ	 1.0000	 0.4710
FK	 1.0000	 0.4630
FL	 1.0000	 0.4660
FM	 1.0000	 0.4660
FN	 0.9990	 0.4660
FO	 1.0000	 0.4620
FP	 1.0000	 0.4730
FQ	 1.0000	 0.4710
FS	 1.0000	 0.4660
FT	 1.0000	 0.4570
FU	 0.9990	 0.4660
FV	 1.0000	 0.4660
FW	 0.9990	 0.4650
FX	 0.9990	 0.4590
FY	 1.0000	 0.4630
FZ	 1.0000	 0.4500
Fc	 1.0000	 0.4710
GA	 1.0000	 0.4320
GB	 0.9990	 0.4630
GC	 1.0000	 0.4690
GD	 1.0000	 0.4700
GE	 1.0000	 0.4710
GF	 1.0000	 0.4640
GG	 1.0000	 0.4720

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Chain	Atom inclusion	Q-score
GH	 1.0000	 0.4570
GI	 1.0000	 0.4630
GJ	 1.0000	 0.4670
GK	 1.0000	 0.4710
GL	 1.0000	 0.4690
GM	 0.9990	 0.4710
GN	 1.0000	 0.4730
GO	 1.0000	 0.4650
GP	 1.0000	 0.4710
GQ	 0.9990	 0.4690
GS	 1.0000	 0.4660
GT	 1.0000	 0.4570
GU	 1.0000	 0.4480
GV	 0.9990	 0.4480
GW	 1.0000	 0.4680
GX	 0.9990	 0.4720
GY	 1.0000	 0.4730
Gc	 1.0000	 0.4660
R	 0.9600	 0.1610
a	 0.9970	 0.2750
b	 0.9600	 0.2190