



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 10:55 PM UTC

PDB ID : 9HAT / pdb_00009hat
EMDB ID : EMD-52006
Title : pT=3 virus-like particle of ssRNA phage Beihai26 coat protein
Authors : Kalnins, G.
Deposited on : 2024-11-05
Resolution : 3.60 Å (reported)
Based on initial model : .

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

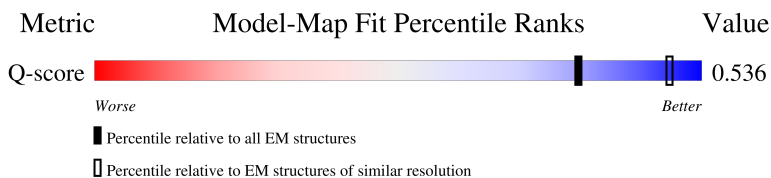
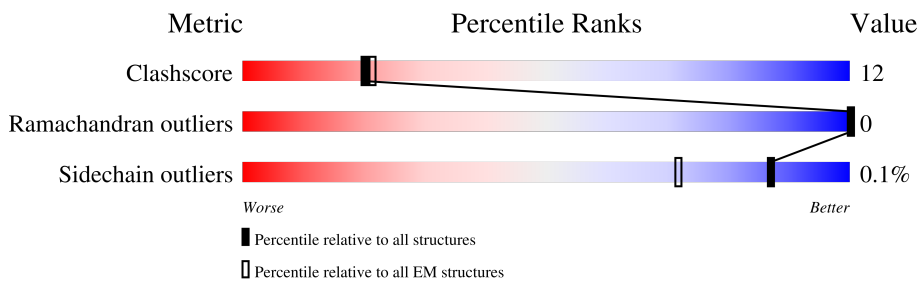
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.60 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	-
Q-score	-	25397	12797 (3.10 - 4.10)

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

Mol	Chain	Length	Quality of chain
1	AA	123	8% (red), 74% (green), 26% (yellow)
1	AC	123	69% (green), 31% (yellow)
1	AD	123	11% (red), 68% (green), 31% (yellow)
1	AE	123	7% (red), 75% (green), 25% (yellow)

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Mol	Chain	Length	Quality of chain
1	AG	123	76% 24%
1	AH	123	69% 30% 11%
1	AI	123	76% 24% 7%
1	AK	123	68% 32%
1	AL	123	67% 32% 12%
1	AM	123	73% 27% 8%
1	AO	123	68% 32%
1	AP	123	67% 32% 11%
1	AQ	123	72% 28% 7%
1	AS	123	72% 28%
1	AT	123	71% 29% 10%
1	AU	123	76% 24% 5%
1	AW	123	73% 27%
1	AX	123	67% 33% 12%
1	AY	123	75% 25% 7%
1	BA	123	70% 30%
1	BB	123	68% 31% 12%
1	BC	123	75% 25% 8%
1	BE	123	68% 32%
1	BF	123	67% 33% 11%
1	BG	123	74% 26% 7%
1	BI	123	72% 28%
1	BJ	123	70% 30% 10%
1	BK	123	75% 25% 7%
1	BM	123	70% 30%

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Mol	Chain	Length	Quality of chain
1	BN	123	
1	BO	123	
1	BQ	123	
1	BR	123	
1	BS	123	
1	BU	123	
1	BV	123	
1	BW	123	
1	BY	123	
1	BZ	123	
1	CA	123	
1	CC	123	
1	CD	123	
1	CE	123	
1	CG	123	
1	CH	123	
1	CI	123	
1	CK	123	
1	CL	123	
1	CM	123	
1	CO	123	
1	CP	123	
1	CQ	123	
1	CS	123	
1	CT	123	

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Mol	Chain	Length	Quality of chain	
1	CU	123	5%	76% 24%
1	CW	123	•	73% 27%
1	CX	123	12%	70% 30%
1	CY	123	7%	72% 28%
1	DA	123	•	73% 27%
1	DB	123	10%	69% 31%
1	DC	123	7%	76% 24%
1	DE	123	•	75% 25%
1	DF	123	11%	68% 31%
1	DG	123	5%	76% 24%
1	DI	123	•	72% 28%
1	DJ	123	12%	70% 30%
1	DK	123	8%	77% 23%
1	DM	123	•	70% 30%
1	DN	123	11%	67% 32%
1	DO	123	7%	74% 26%
1	DQ	123	•	69% 31%
1	DR	123	12%	68% 31%
1	DS	123	7%	79% 21%
1	DU	123	•	76% 24%
1	DV	123	11%	69% 30%
1	DW	123	5%	76% 24%
1	DY	123	•	72% 28%
1	DZ	123	12%	70% 30%
1	EA	123	8%	76% 24%

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Mol	Chain	Length	Quality of chain
1	EC	123	70% 30%
1	ED	123	67% 33% 11%
1	EE	123	77% 23% 7%
1	EG	123	76% 24%
1	EH	123	68% 31% 11%
1	EI	123	73% 27% 7%
1	EK	123	68% 32%
1	EL	123	68% 31% 12%
1	EM	123	72% 28% 7%
1	EO	123	72% 28%
1	EP	123	69% 31% 10%
1	EQ	123	74% 26% 8%
1	ES	123	69% 31%
1	ET	123	69% 30% 11%
1	EU	123	77% 23% 7%
1	EW	123	68% 32%
1	EX	123	67% 33% 12%
1	EY	123	76% 24% 7%
1	FA	123	76% 24%
1	FB	123	68% 31% 11%
1	FC	123	74% 26% 8%
1	FE	123	68% 32%
1	FF	123	67% 32% 11%
1	FG	123	76% 24% 5%
1	FI	123	72% 28%

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Mol	Chain	Length	Quality of chain	
1	FJ	123	12%	69% 31%
1	FK	123	7%	72% 28%
1	FM	123	•	72% 28%
1	FN	123	10%	71% 29%
1	FO	123	7%	75% 25%
1	FQ	123	•	76% 24%
1	FR	123	11%	69% 31%
1	FS	123	8%	73% 27%
1	FU	123	•	73% 27%
1	FV	123	11%	70% 30%
1	FW	123	5%	70% 30%
1	FY	123	•	76% 24%
1	FZ	123	11%	68% 32%
1	GA	123	8%	75% 24%
1	GC	123	•	80% 20%
1	GD	123	11%	70% 30%
1	GE	123	7%	68% 32%
1	GG	123	•	76% 24%
1	GH	123	11%	72% 27%
1	GI	123	7%	72% 28%
1	GK	123	•	75% 25%
1	GL	123	12%	70% 30%
1	GM	123	5%	73% 27%
1	GO	123	•	76% 24%
1	GP	123	11%	68% 32%













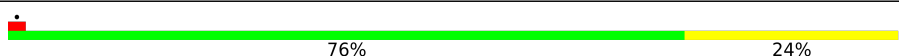
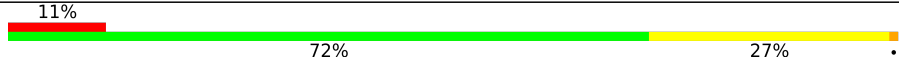
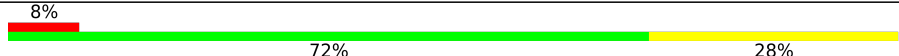

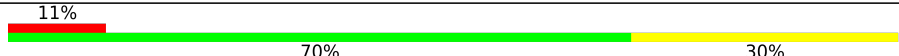
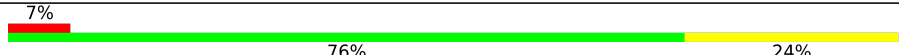
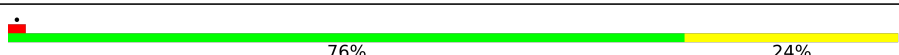
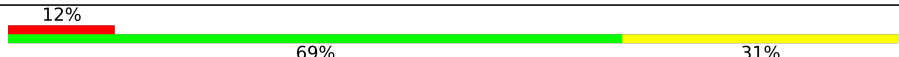
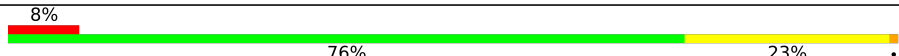



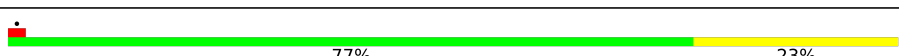
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Mol	Chain	Length	Quality of chain
1	GQ	123	8% 76% 23%
1	GS	123	1% 79% 21%
1	GT	123	11% 70% 30%
1	GU	123	7% 72% 28%
1	GW	123	1% 77% 23%
1	GX	123	11% 72% 28%
1	GY	123	5% 73% 27%
1	HA	123	1% 76% 24%
1	HB	123	11% 68% 32%
1	HC	123	7% 72% 28%
1	HE	123	1% 74% 26%
1	HF	123	12% 70% 30%
1	HG	123	8% 72% 28%
1	HI	123	1% 76% 24%
1	HJ	123	11% 68% 32%
1	HK	123	7% 72% 28%
1	HM	123	1% 76% 24%
1	HN	123	11% 71% 28%
1	HO	123	5% 73% 27%
1	HQ	123	1% 75% 25%
1	HR	123	11% 69% 31%
1	HS	123	7% 72% 28%
1	HU	123	1% 76% 24%
1	HV	123	12% 69% 31%
1	HW	123	7% 72% 28%

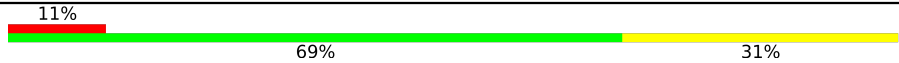
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Mol	Chain	Length	Quality of chain
1	HY	123	 76% 24%
1	HZ	123	 11% 72% 28%
1	IA	123	 8% 73% 27%
1	IC	123	 76% 24%
1	ID	123	 11% 68% 32%
1	IE	123	 8% 77% 22%
1	IG	123	 76% 24%
1	IH	123	 11% 67% 33%
1	II	123	 7% 75% 25%
1	IK	123	 76% 24%
1	IL	123	 12% 69% 31%
1	IM	123	 7% 72% 28%
1	IO	123	 76% 24%
1	IP	123	 11% 72% 27%
1	IQ	123	 8% 72% 28%
1	IS	123	 76% 24%
1	IT	123	 11% 70% 30%
1	IU	123	 7% 76% 24%
1	IW	123	 76% 24%
1	IX	123	 12% 69% 31%
1	IY	123	 8% 76% 23%
1	JA	123	 76% 24%
1	JB	123	 11% 67% 33%
1	JC	123	 5% 72% 28%
1	JE	123	 77% 23%

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Mol	Chain	Length	Quality of chain
1	JF	123	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '11%', a green segment in the middle labeled '69%', and a yellow segment on the right labeled '31%'. The segments are stacked horizontally to total 100%.</p>

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 163260 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AA	123	907	562	160	184	1	0	0
1	AC	123	907	562	160	184	1	0	0
1	AD	123	907	562	160	184	1	0	0
1	AE	123	907	562	160	184	1	0	0
1	AG	123	907	562	160	184	1	0	0
1	AH	123	907	562	160	184	1	0	0
1	AI	123	907	562	160	184	1	0	0
1	AK	123	907	562	160	184	1	0	0
1	AL	123	907	562	160	184	1	0	0
1	AM	123	907	562	160	184	1	0	0
1	AO	123	907	562	160	184	1	0	0
1	AP	123	907	562	160	184	1	0	0
1	AQ	123	907	562	160	184	1	0	0
1	AS	123	907	562	160	184	1	0	0
1	AT	123	907	562	160	184	1	0	0
1	AU	123	907	562	160	184	1	0	0
1	AW	123	907	562	160	184	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AX	123	907	562	160	184	1	0	0
1	AY	123	907	562	160	184	1	0	0
1	BA	123	907	562	160	184	1	0	0
1	BB	123	907	562	160	184	1	0	0
1	BC	123	907	562	160	184	1	0	0
1	BE	123	907	562	160	184	1	0	0
1	BF	123	907	562	160	184	1	0	0
1	BG	123	907	562	160	184	1	0	0
1	BI	123	907	562	160	184	1	0	0
1	BJ	123	907	562	160	184	1	0	0
1	BK	123	907	562	160	184	1	0	0
1	BM	123	907	562	160	184	1	0	0
1	BN	123	907	562	160	184	1	0	0
1	BO	123	907	562	160	184	1	0	0
1	BQ	123	907	562	160	184	1	0	0
1	BR	123	907	562	160	184	1	0	0
1	BS	123	907	562	160	184	1	0	0
1	BU	123	907	562	160	184	1	0	0
1	BV	123	907	562	160	184	1	0	0
1	BW	123	907	562	160	184	1	0	0
1	BY	123	907	562	160	184	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	BZ	123	907	562	160	184	1	0	0
1	CA	123	907	562	160	184	1	0	0
1	CC	123	907	562	160	184	1	0	0
1	CD	123	907	562	160	184	1	0	0
1	CE	123	907	562	160	184	1	0	0
1	CG	123	907	562	160	184	1	0	0
1	CH	123	907	562	160	184	1	0	0
1	CI	123	907	562	160	184	1	0	0
1	CK	123	907	562	160	184	1	0	0
1	CL	123	907	562	160	184	1	0	0
1	CM	123	907	562	160	184	1	0	0
1	CO	123	907	562	160	184	1	0	0
1	CP	123	907	562	160	184	1	0	0
1	CQ	123	907	562	160	184	1	0	0
1	CS	123	907	562	160	184	1	0	0
1	CT	123	907	562	160	184	1	0	0
1	CU	123	907	562	160	184	1	0	0
1	CW	123	907	562	160	184	1	0	0
1	CX	123	907	562	160	184	1	0	0
1	CY	123	907	562	160	184	1	0	0
1	DA	123	907	562	160	184	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	DB	123	907	562	160	184	1	0	0
1	DC	123	907	562	160	184	1	0	0
1	DE	123	907	562	160	184	1	0	0
1	DF	123	907	562	160	184	1	0	0
1	DG	123	907	562	160	184	1	0	0
1	DI	123	907	562	160	184	1	0	0
1	DJ	123	907	562	160	184	1	0	0
1	DK	123	907	562	160	184	1	0	0
1	DM	123	907	562	160	184	1	0	0
1	DN	123	907	562	160	184	1	0	0
1	DO	123	907	562	160	184	1	0	0
1	DQ	123	907	562	160	184	1	0	0
1	DR	123	907	562	160	184	1	0	0
1	DS	123	907	562	160	184	1	0	0
1	DU	123	907	562	160	184	1	0	0
1	DV	123	907	562	160	184	1	0	0
1	DW	123	907	562	160	184	1	0	0
1	DY	123	907	562	160	184	1	0	0
1	DZ	123	907	562	160	184	1	0	0
1	EA	123	907	562	160	184	1	0	0
1	EC	123	907	562	160	184	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	ED	123	907	562	160	184	1	0	0
1	EE	123	907	562	160	184	1	0	0
1	EG	123	907	562	160	184	1	0	0
1	EH	123	907	562	160	184	1	0	0
1	EI	123	907	562	160	184	1	0	0
1	EK	123	907	562	160	184	1	0	0
1	EL	123	907	562	160	184	1	0	0
1	EM	123	907	562	160	184	1	0	0
1	EO	123	907	562	160	184	1	0	0
1	EP	123	907	562	160	184	1	0	0
1	EQ	123	907	562	160	184	1	0	0
1	ES	123	907	562	160	184	1	0	0
1	ET	123	907	562	160	184	1	0	0
1	EU	123	907	562	160	184	1	0	0
1	EW	123	907	562	160	184	1	0	0
1	EX	123	907	562	160	184	1	0	0
1	EY	123	907	562	160	184	1	0	0
1	FA	123	907	562	160	184	1	0	0
1	FB	123	907	562	160	184	1	0	0
1	FC	123	907	562	160	184	1	0	0
1	FE	123	907	562	160	184	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	FF	123	907	562	160	184	1	0	0
1	FG	123	907	562	160	184	1	0	0
1	FI	123	907	562	160	184	1	0	0
1	FJ	123	907	562	160	184	1	0	0
1	FK	123	907	562	160	184	1	0	0
1	FM	123	907	562	160	184	1	0	0
1	FN	123	907	562	160	184	1	0	0
1	FO	123	907	562	160	184	1	0	0
1	FQ	123	907	562	160	184	1	0	0
1	FR	123	907	562	160	184	1	0	0
1	FS	123	907	562	160	184	1	0	0
1	FU	123	907	562	160	184	1	0	0
1	FV	123	907	562	160	184	1	0	0
1	FW	123	907	562	160	184	1	0	0
1	FY	123	907	562	160	184	1	0	0
1	FZ	123	907	562	160	184	1	0	0
1	GA	123	907	562	160	184	1	0	0
1	GC	123	907	562	160	184	1	0	0
1	GD	123	907	562	160	184	1	0	0
1	GE	123	907	562	160	184	1	0	0
1	GG	123	907	562	160	184	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	GH	123	907	562	160	184	1	0	0
1	GI	123	907	562	160	184	1	0	0
1	GK	123	907	562	160	184	1	0	0
1	GL	123	907	562	160	184	1	0	0
1	GM	123	907	562	160	184	1	0	0
1	GO	123	907	562	160	184	1	0	0
1	GP	123	907	562	160	184	1	0	0
1	GQ	123	907	562	160	184	1	0	0
1	GS	123	907	562	160	184	1	0	0
1	GT	123	907	562	160	184	1	0	0
1	GU	123	907	562	160	184	1	0	0
1	GW	123	907	562	160	184	1	0	0
1	GX	123	907	562	160	184	1	0	0
1	GY	123	907	562	160	184	1	0	0
1	HA	123	907	562	160	184	1	0	0
1	HB	123	907	562	160	184	1	0	0
1	HC	123	907	562	160	184	1	0	0
1	HE	123	907	562	160	184	1	0	0
1	HF	123	907	562	160	184	1	0	0
1	HG	123	907	562	160	184	1	0	0
1	HI	123	907	562	160	184	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	HJ	123	907	562	160	184	1	0	0
1	HK	123	907	562	160	184	1	0	0
1	HM	123	907	562	160	184	1	0	0
1	HN	123	907	562	160	184	1	0	0
1	HO	123	907	562	160	184	1	0	0
1	HQ	123	907	562	160	184	1	0	0
1	HR	123	907	562	160	184	1	0	0
1	HS	123	907	562	160	184	1	0	0
1	HU	123	907	562	160	184	1	0	0
1	HV	123	907	562	160	184	1	0	0
1	HW	123	907	562	160	184	1	0	0
1	HY	123	907	562	160	184	1	0	0
1	HZ	123	907	562	160	184	1	0	0
1	IA	123	907	562	160	184	1	0	0
1	IC	123	907	562	160	184	1	0	0
1	ID	123	907	562	160	184	1	0	0
1	IE	123	907	562	160	184	1	0	0
1	IG	123	907	562	160	184	1	0	0
1	IH	123	907	562	160	184	1	0	0
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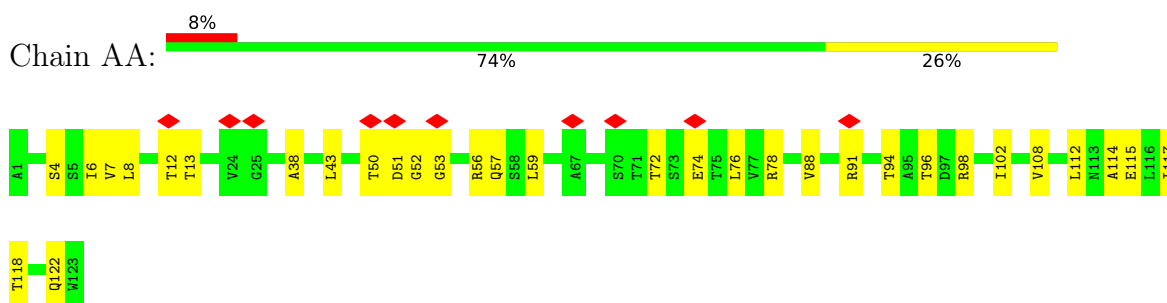
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	IL	123	Total	C	N	O	S	0	0
			907	562	160	184	1		
1	IM	123	Total	C	N	O	S	0	0
			907	562	160	184	1		
1	IO	123	Total	C	N	O	S	0	0
			907	562	160	184	1		
1	IP	123	Total	C	N	O	S	0	0
			907	562	160	184	1		
1	IQ	123	Total	C	N	O	S	0	0
			907	562	160	184	1		
1	IS	123	Total	C	N	O	S	0	0
			907	562	160	184	1		
1	IT	123	Total	C	N	O	S	0	0
			907	562	160	184	1		
1	IU	123	Total	C	N	O	S	0	0
			907	562	160	184	1		
1	IW	123	Total	C	N	O	S	0	0
			907	562	160	184	1		
1	IX	123	Total	C	N	O	S	0	0
			907	562	160	184	1		
1	IY	123	Total	C	N	O	S	0	0
			907	562	160	184	1		
1	JA	123	Total	C	N	O	S	0	0
			907	562	160	184	1		
1	JB	123	Total	C	N	O	S	0	0
			907	562	160	184	1		
1	JC	123	Total	C	N	O	S	0	0
			907	562	160	184	1		
1	JE	123	Total	C	N	O	S	0	0
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1	JF	123	Total	C	N	O	S	0	0
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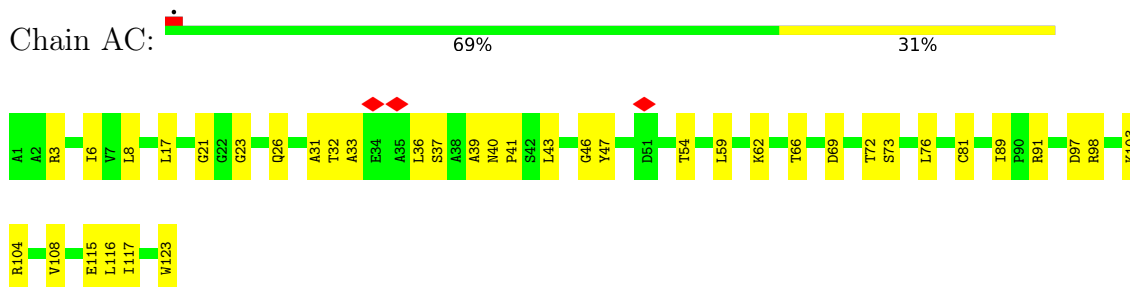
3 Residue-property plots [i](#)

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.

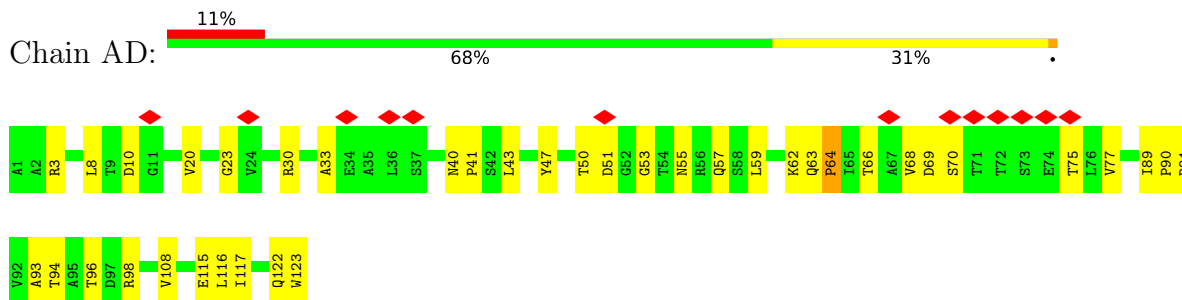
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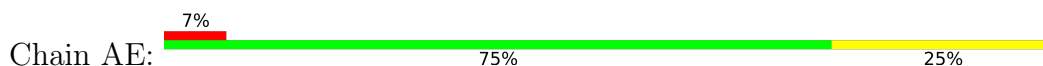
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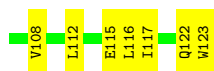


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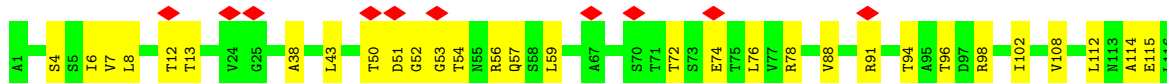
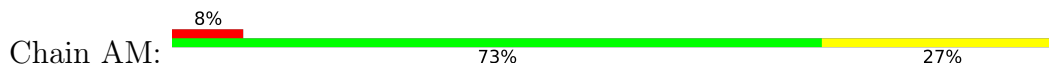


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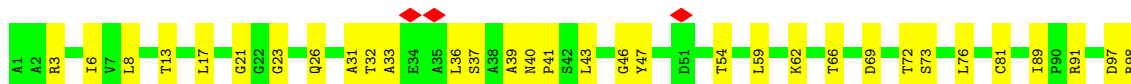




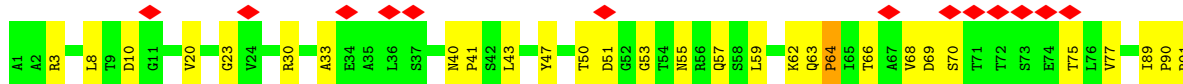
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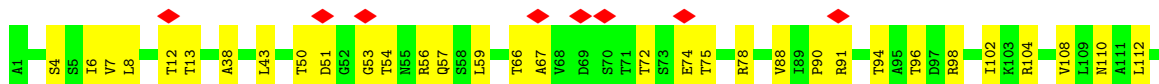
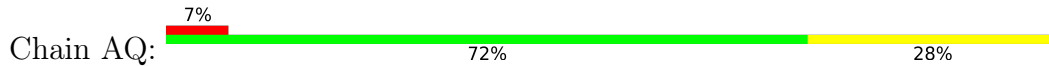
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• Molecule 1: Capsid protein

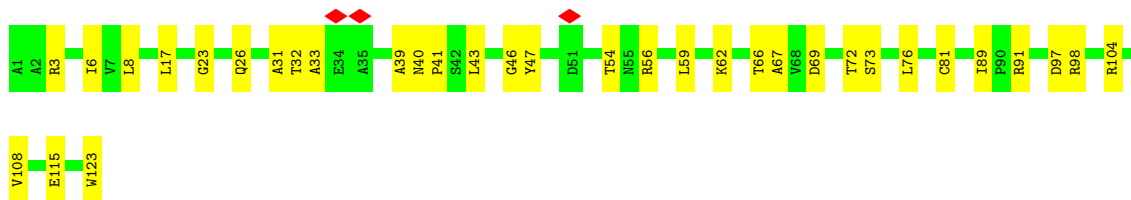


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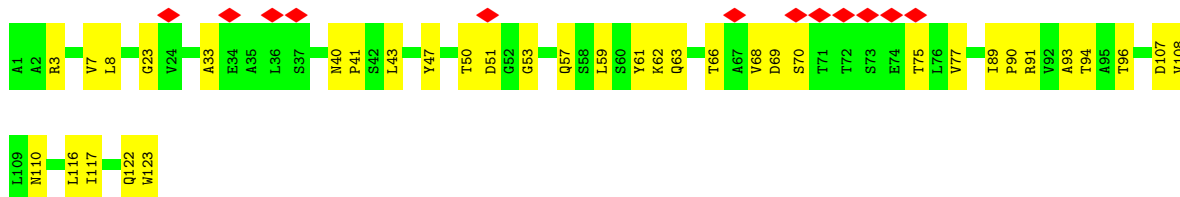


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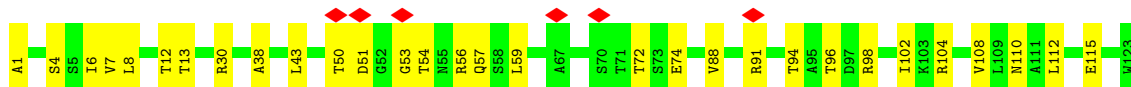
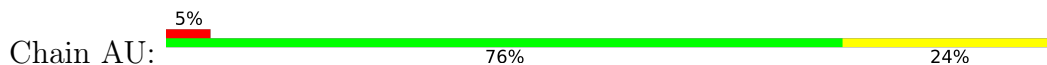




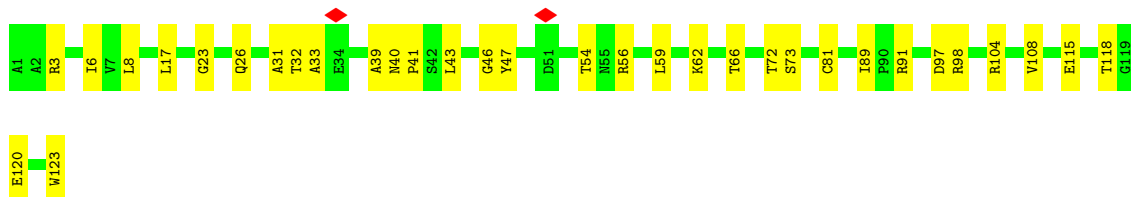
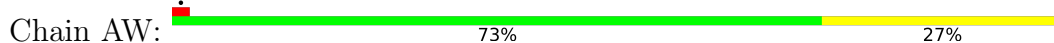
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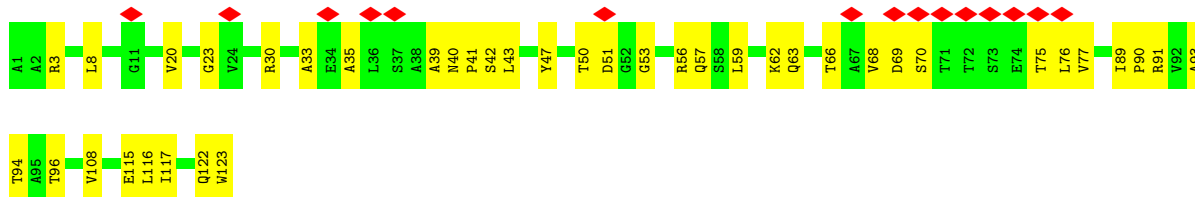
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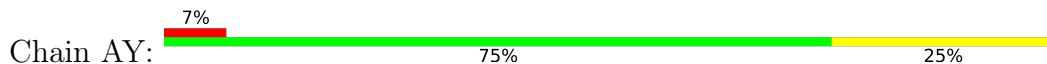
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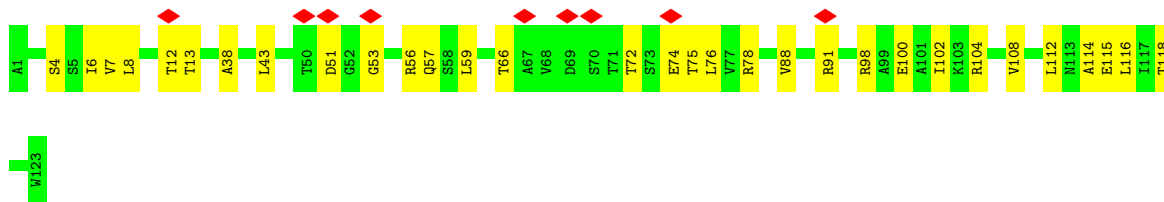


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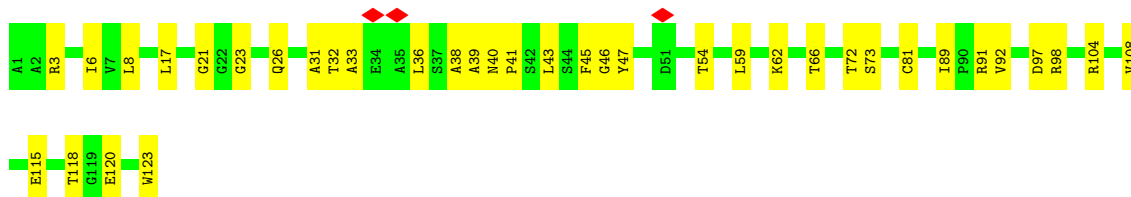


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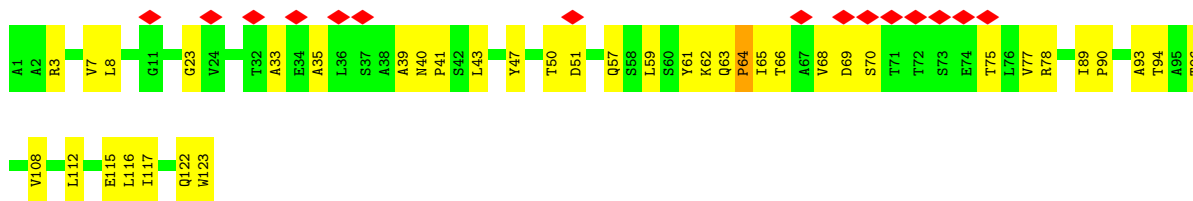




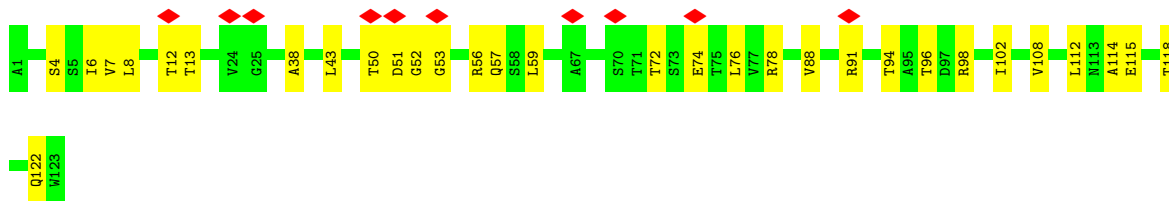
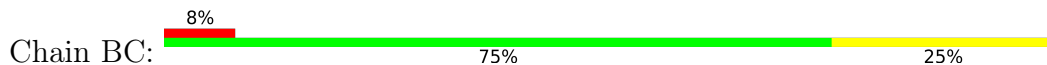
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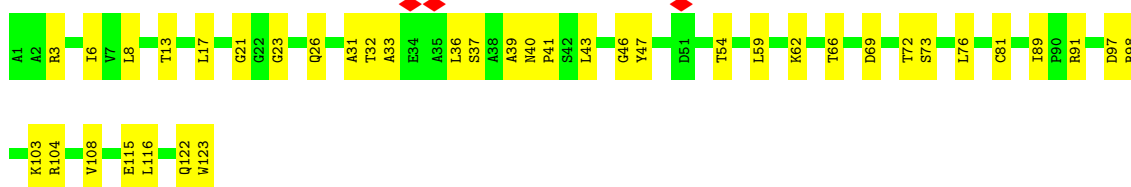
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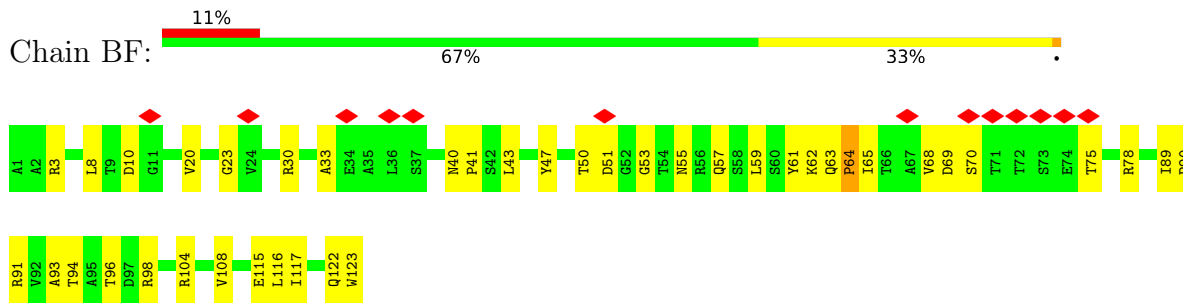
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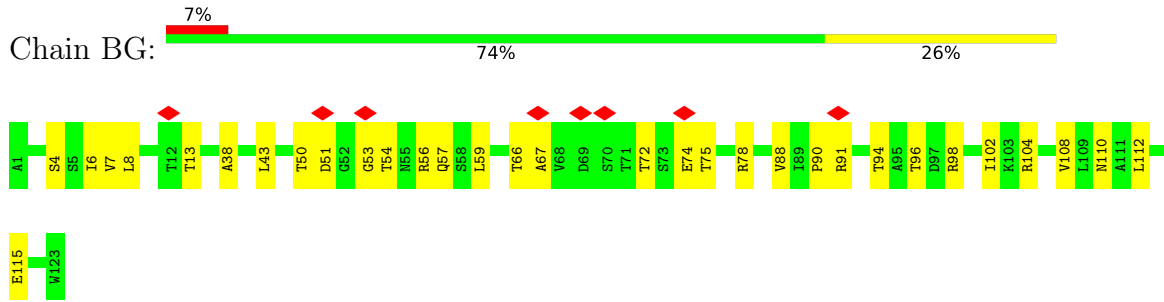
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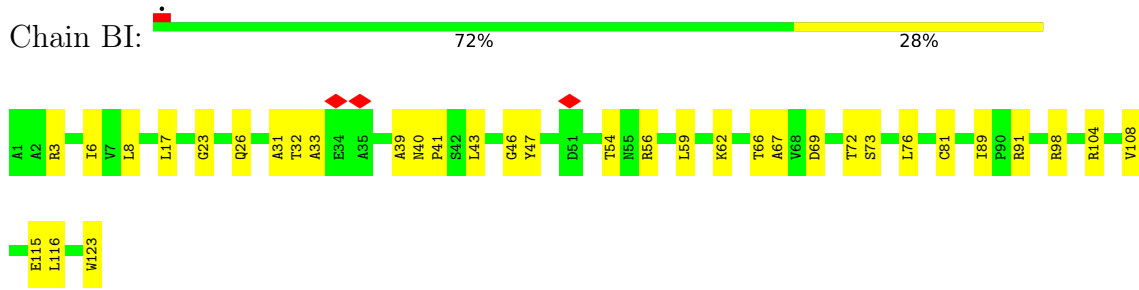
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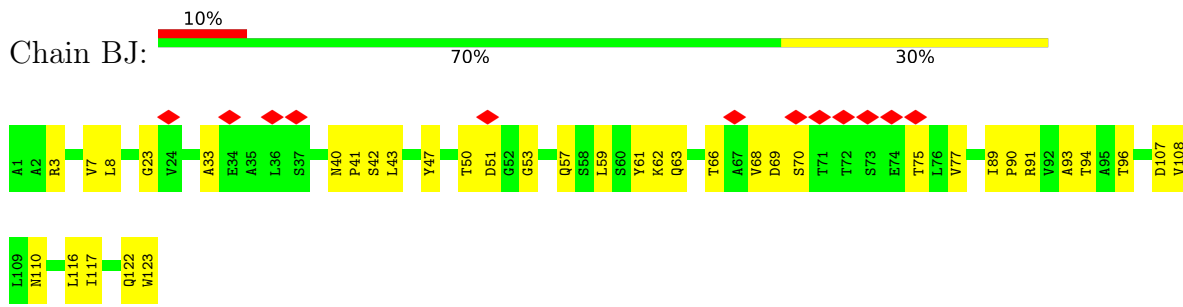
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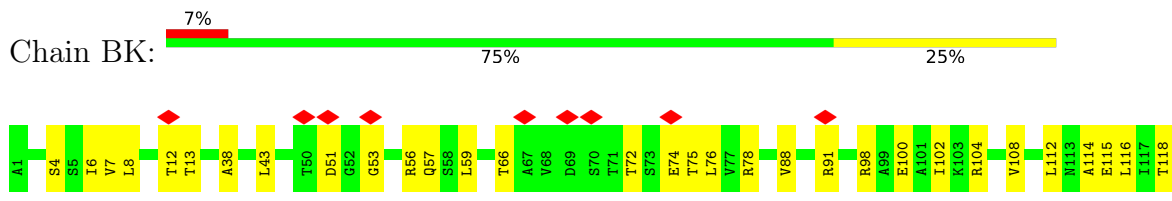
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• Molecule 1: Capsid protein

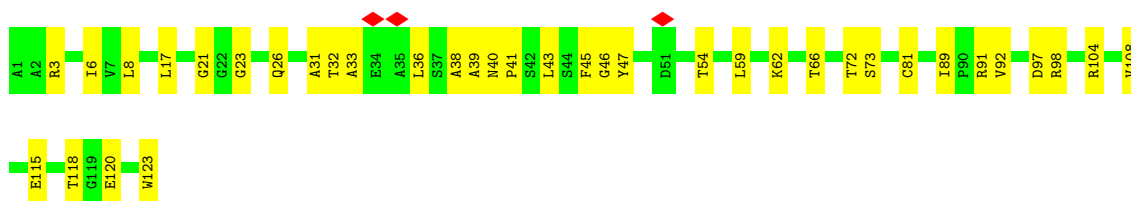


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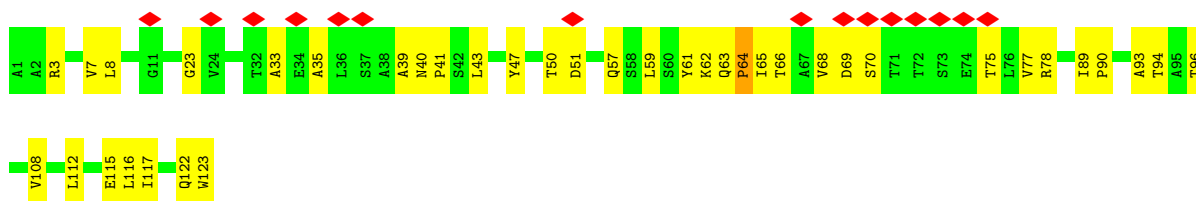




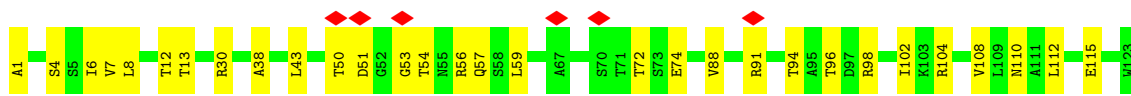
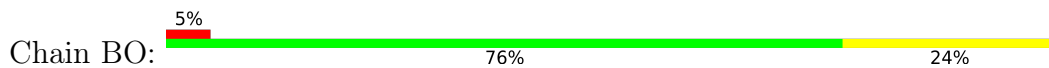
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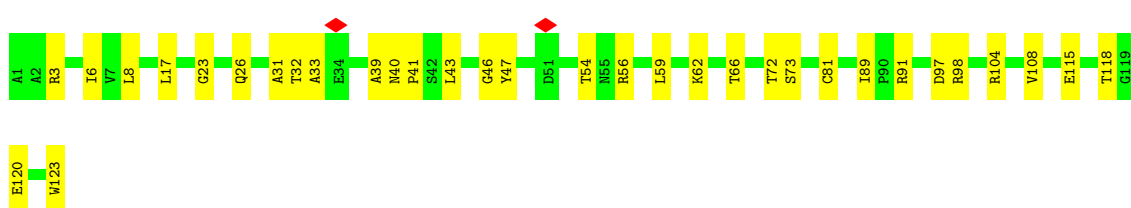
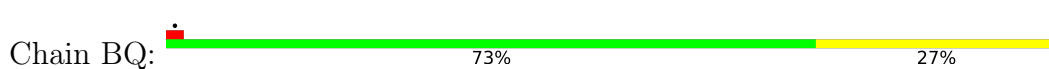
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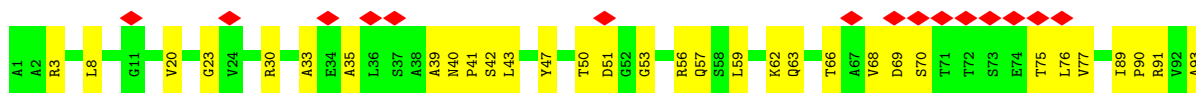
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• Molecule 1: Capsid protein

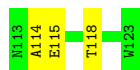
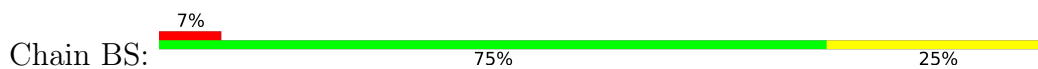


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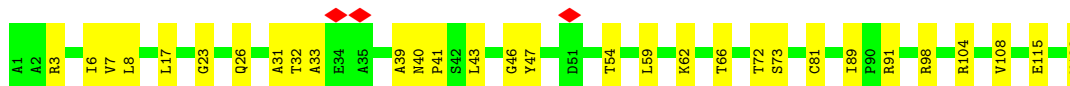
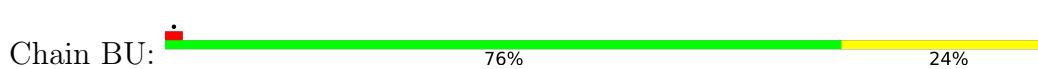




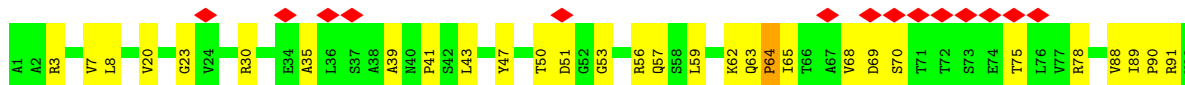
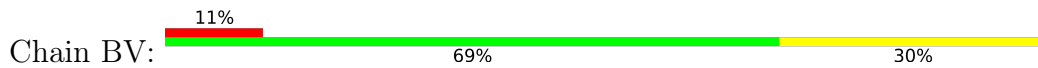
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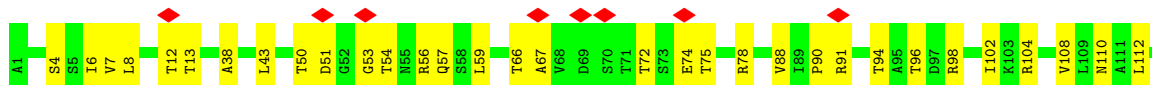
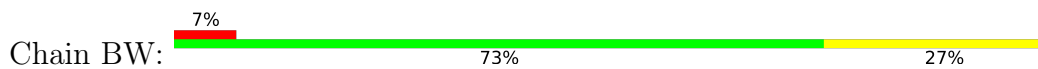
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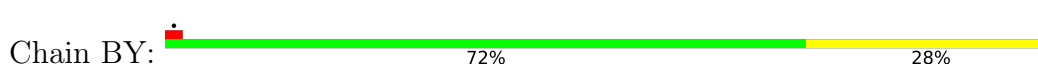
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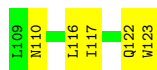
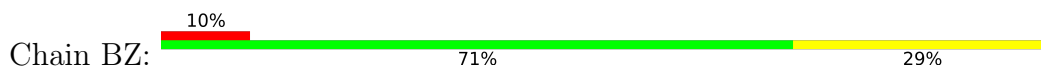


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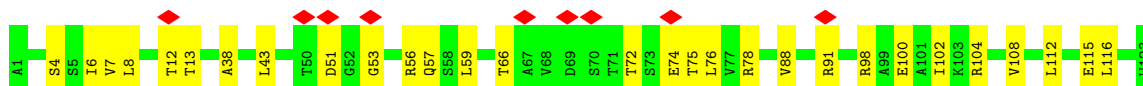
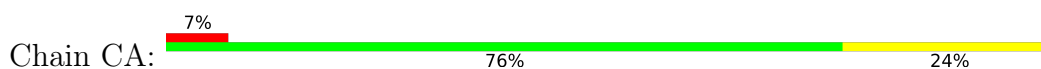




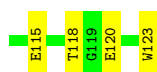
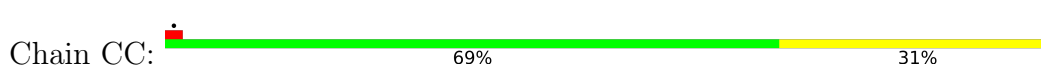
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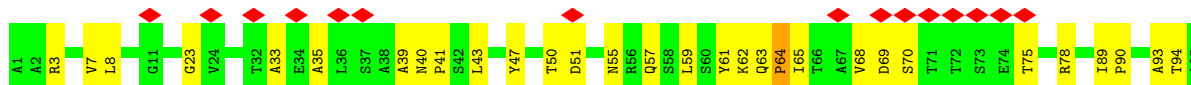
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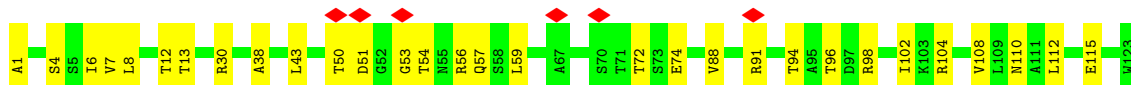
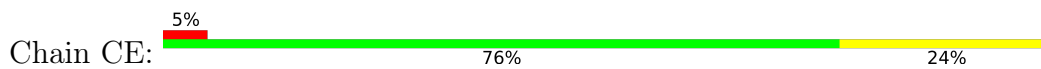
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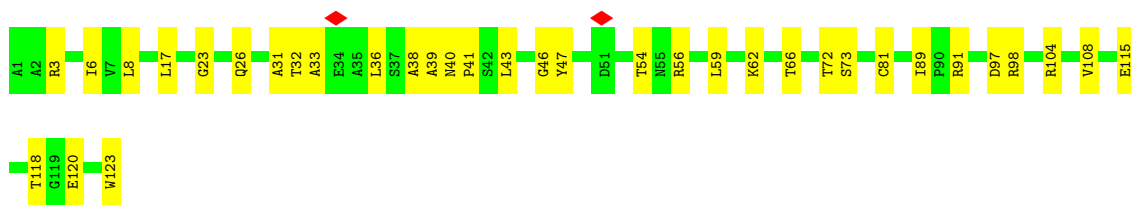
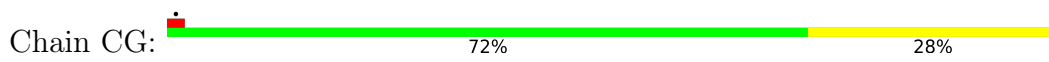
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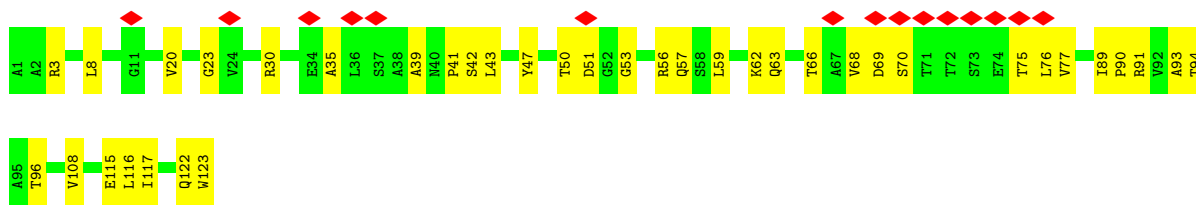
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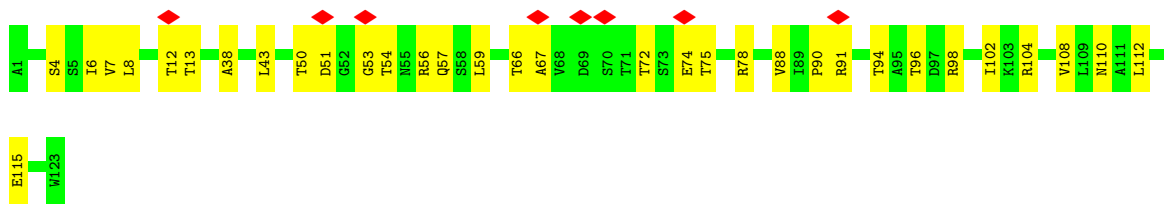
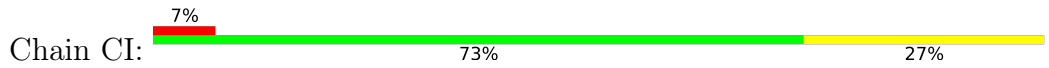
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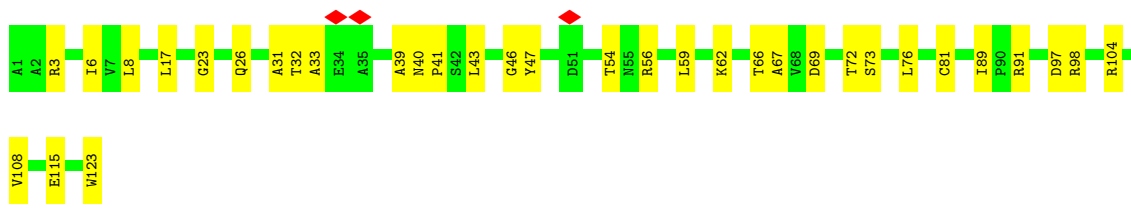
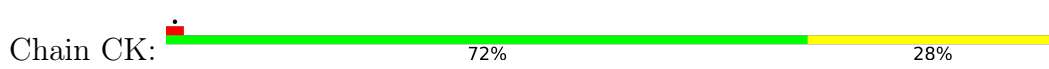
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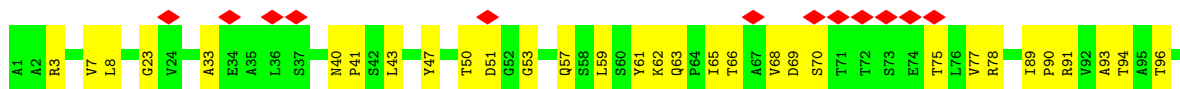
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• Molecule 1: Capsid protein

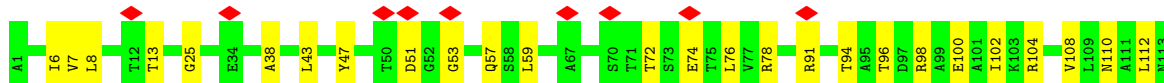
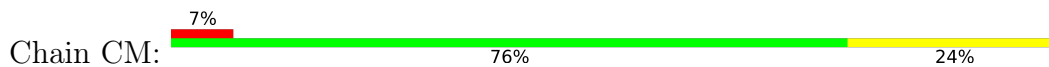


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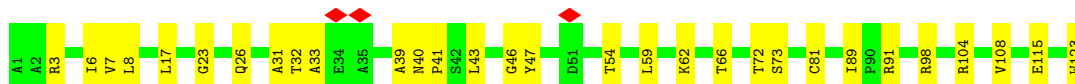
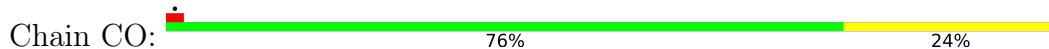




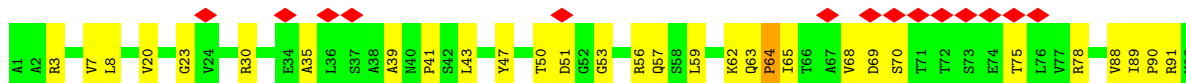
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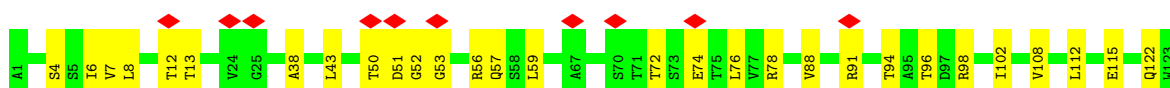
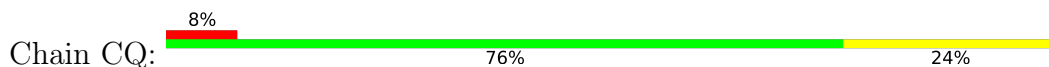
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• Molecule 1: Capsid protein



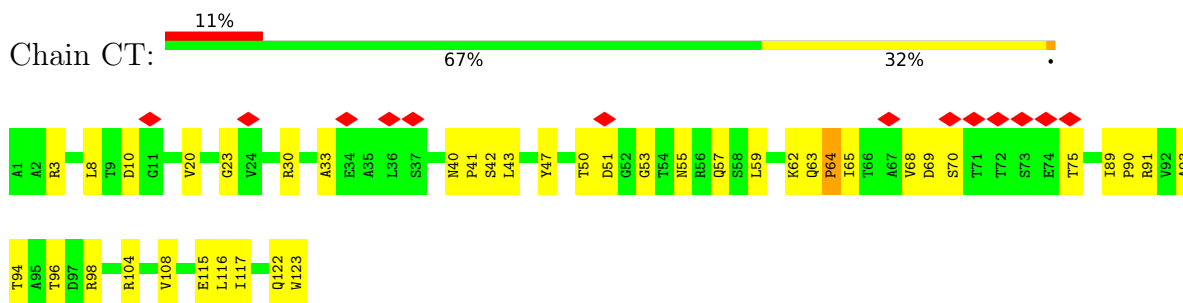
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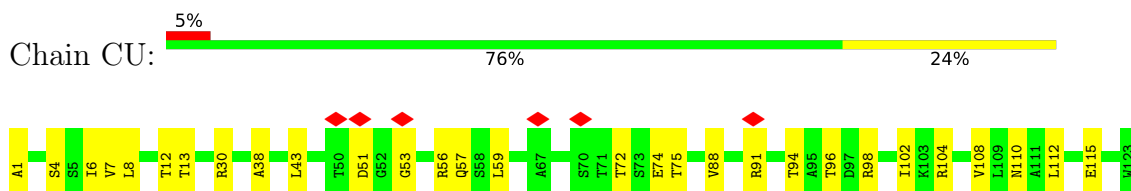
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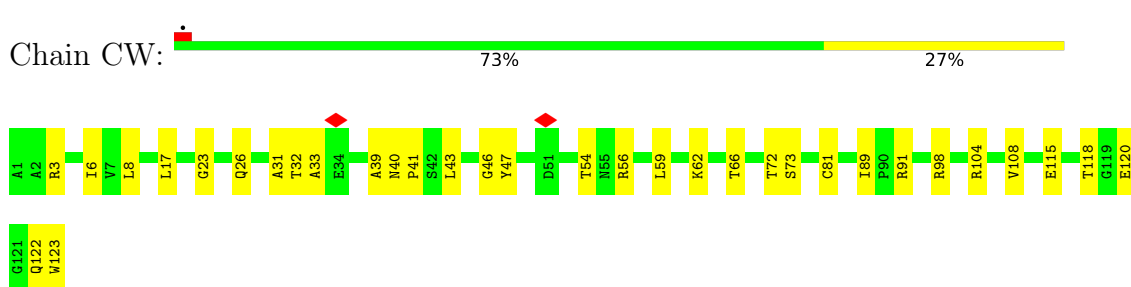
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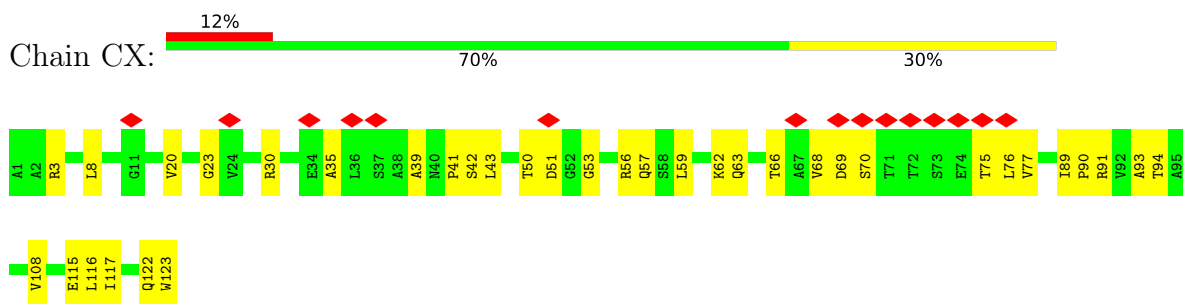
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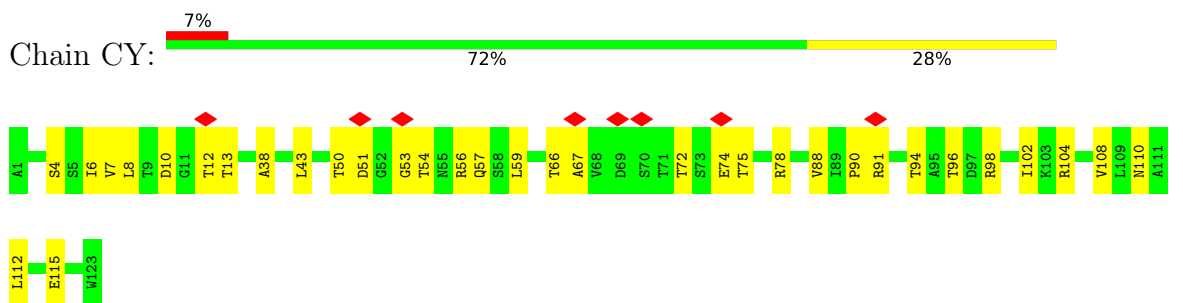
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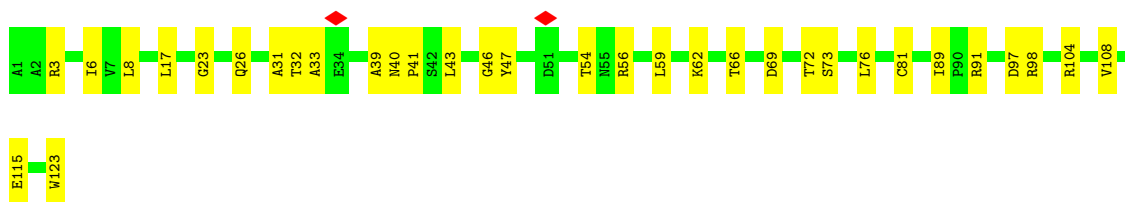
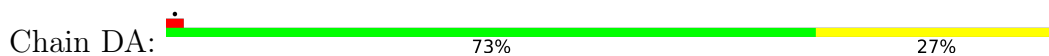
• Molecule 1: Capsid protein



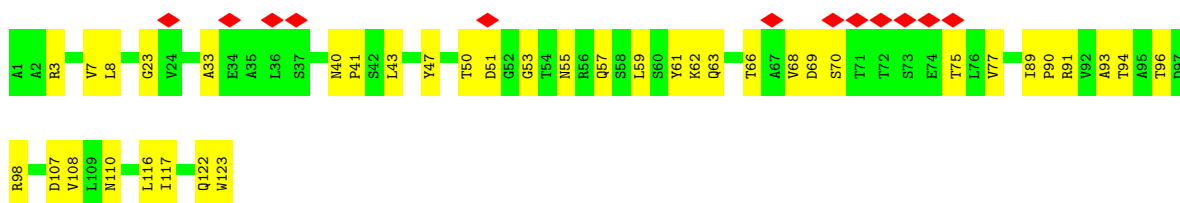
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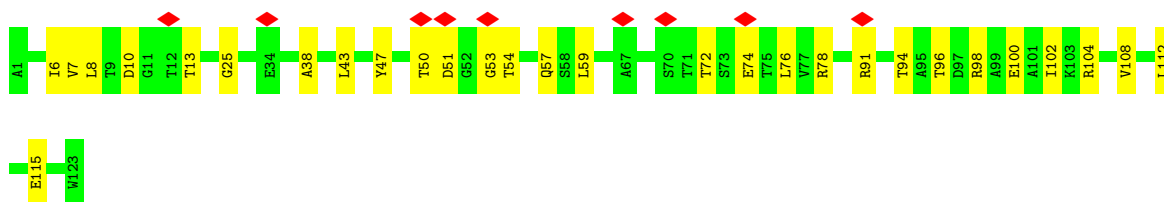
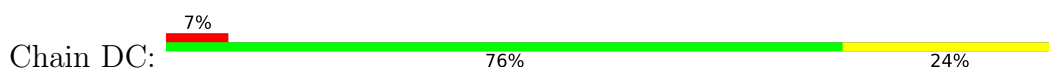
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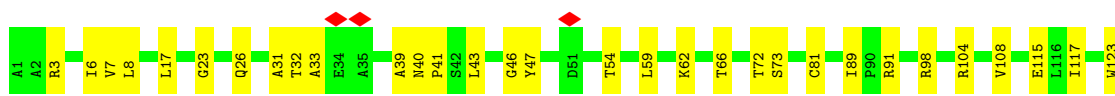
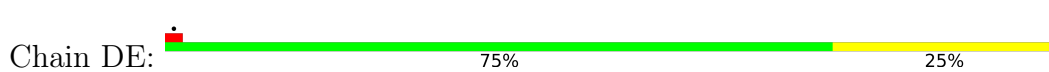
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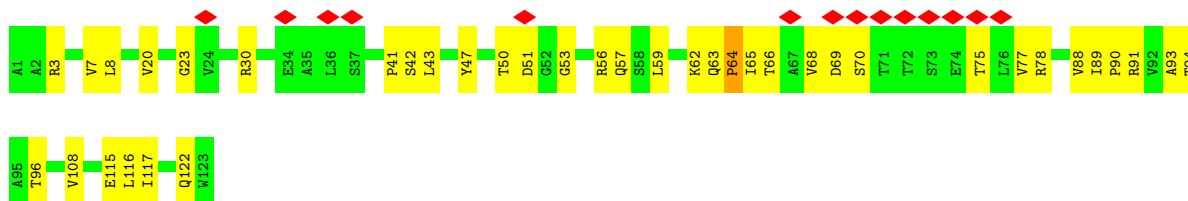
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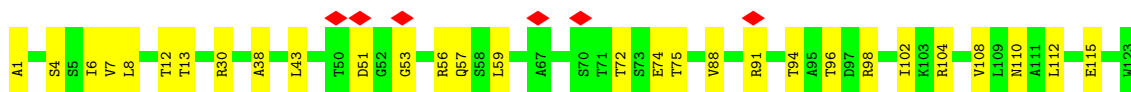
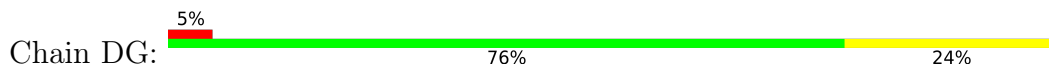
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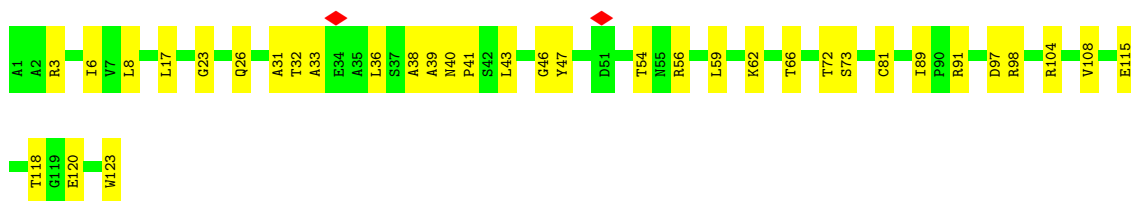
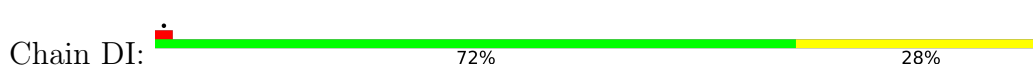
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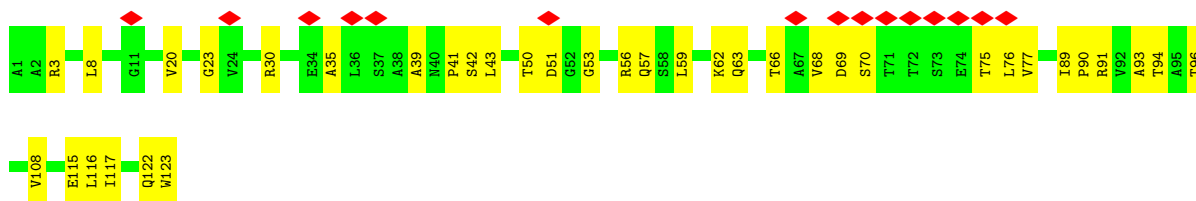
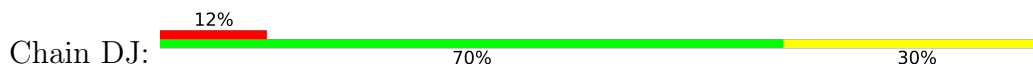
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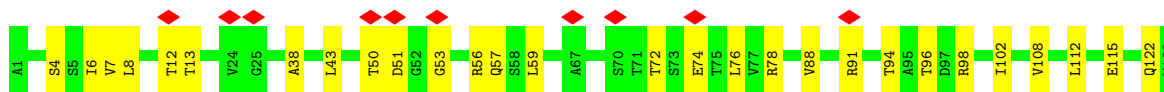
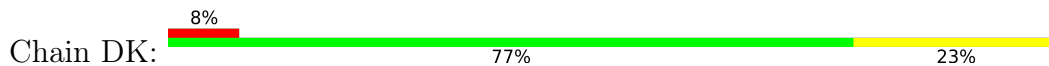
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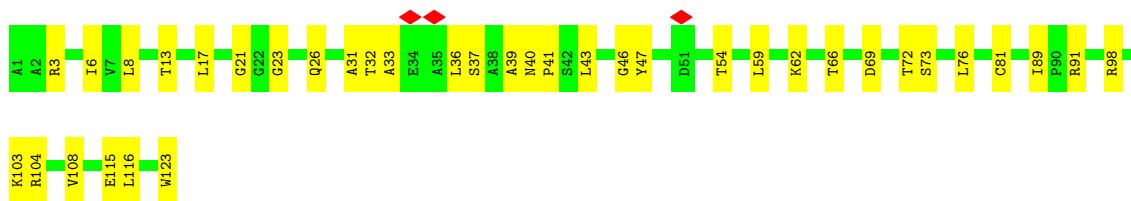
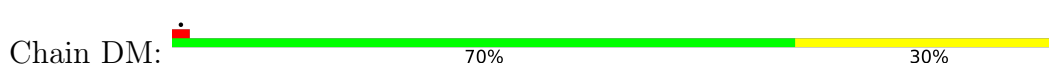
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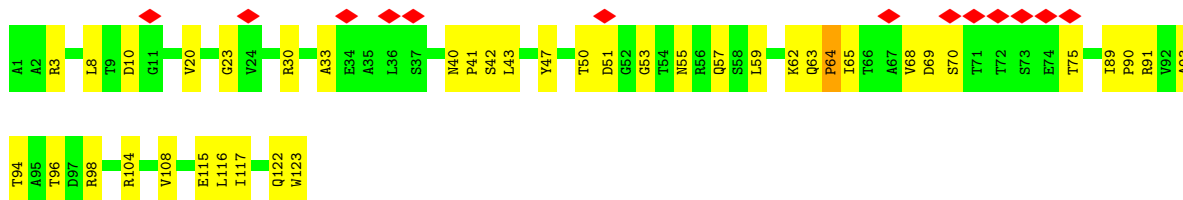


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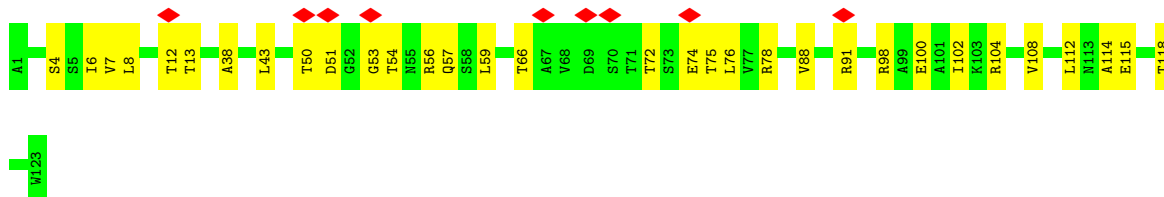
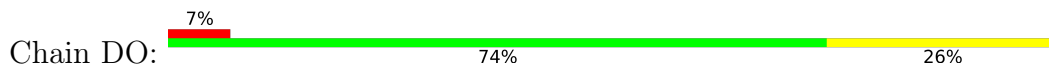


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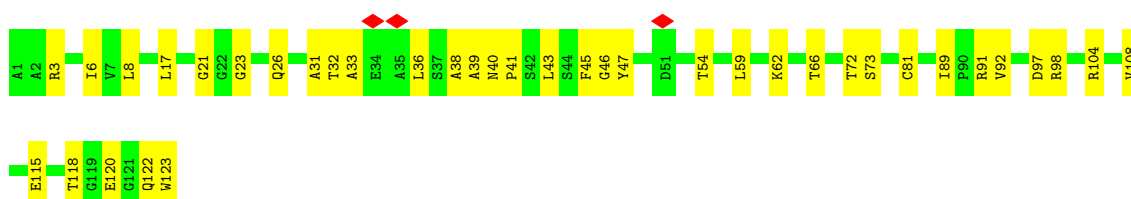




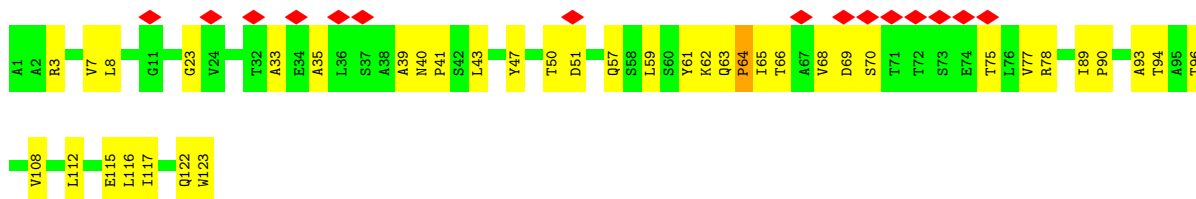
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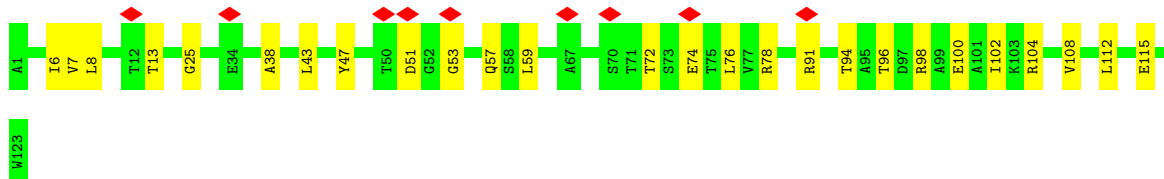
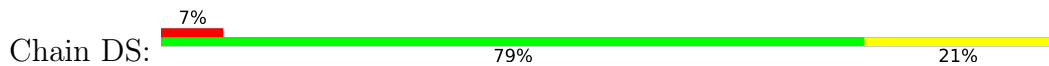
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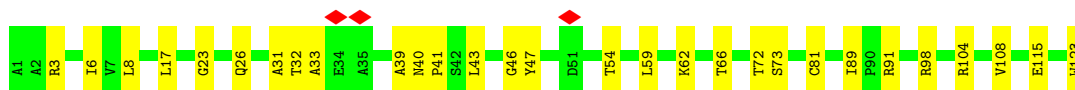
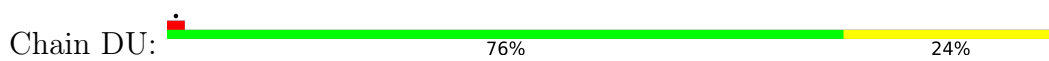
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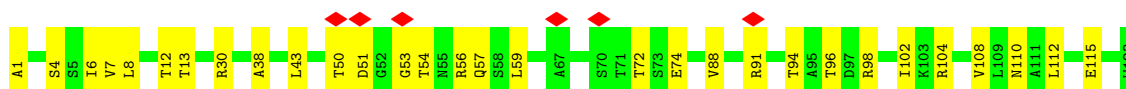
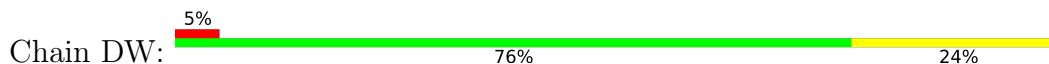
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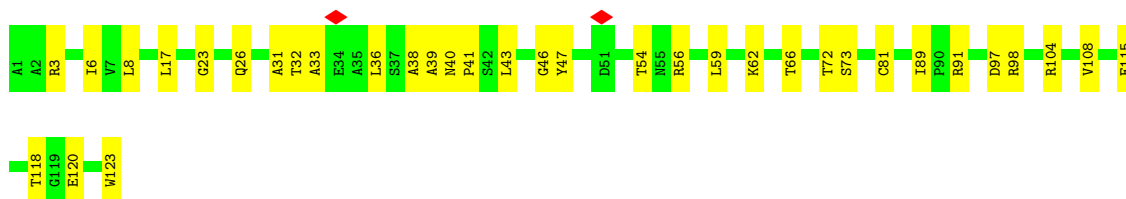
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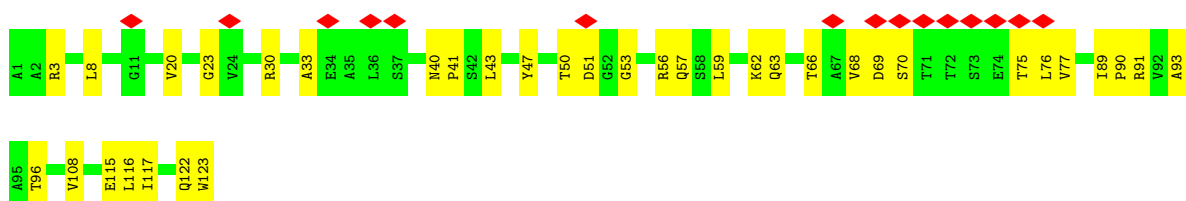
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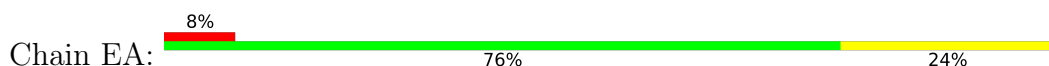
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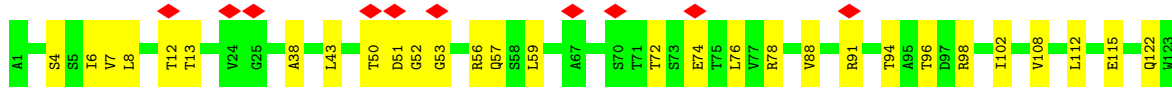


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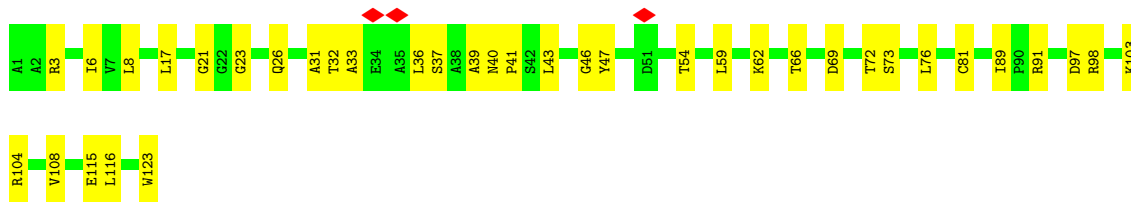


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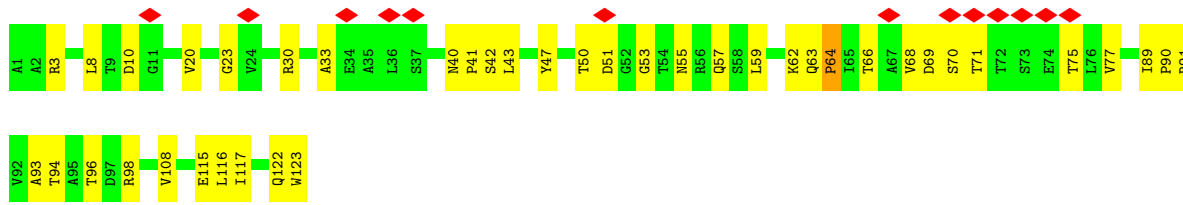




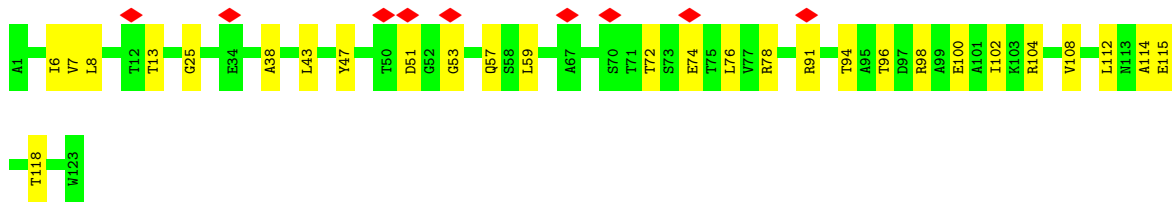
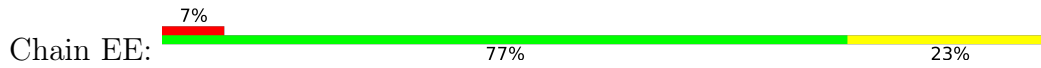
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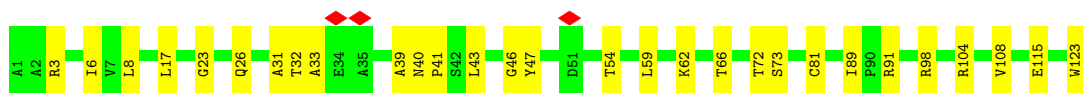
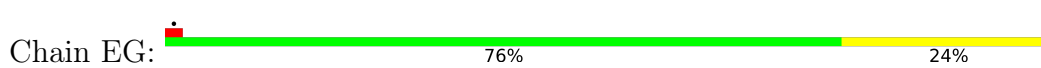
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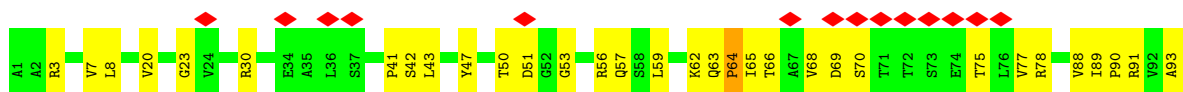
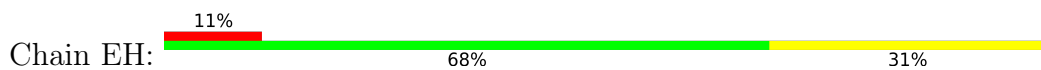
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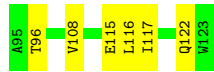


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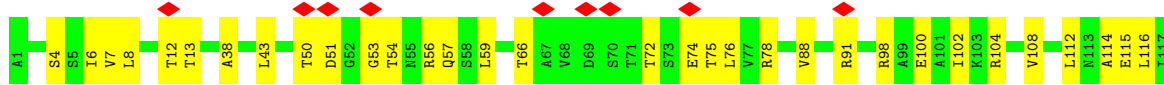
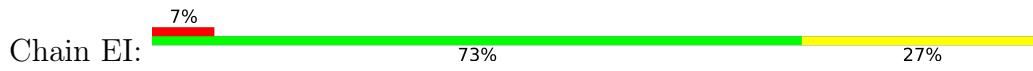


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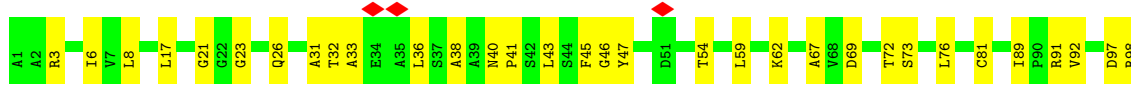




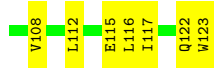
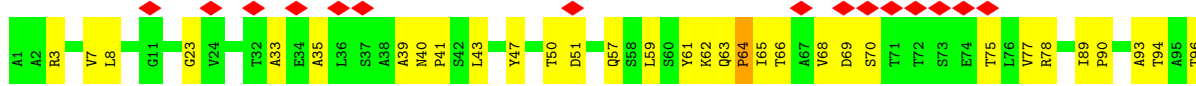
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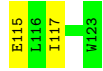
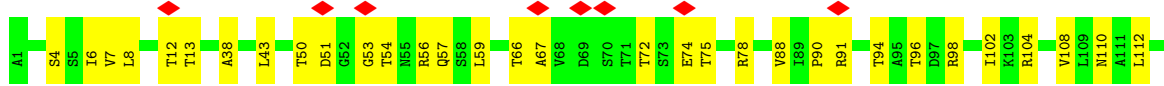
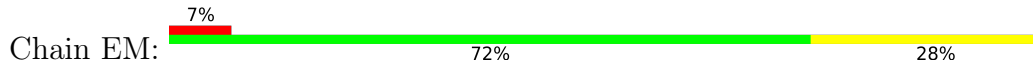
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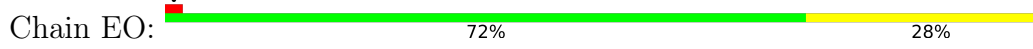
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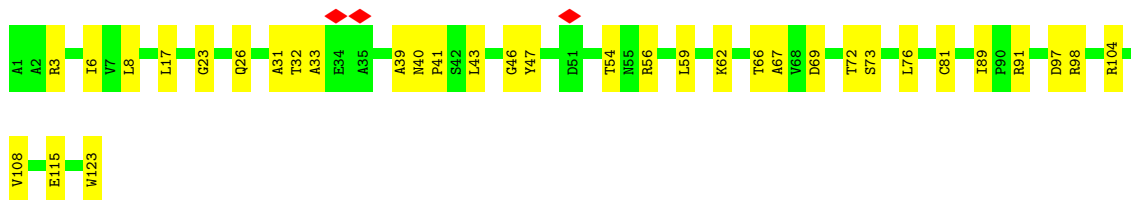


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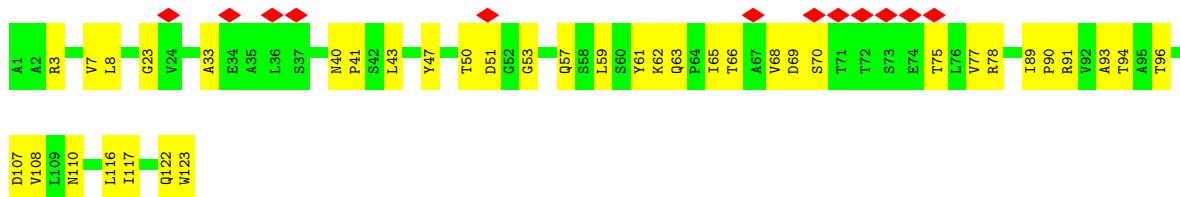


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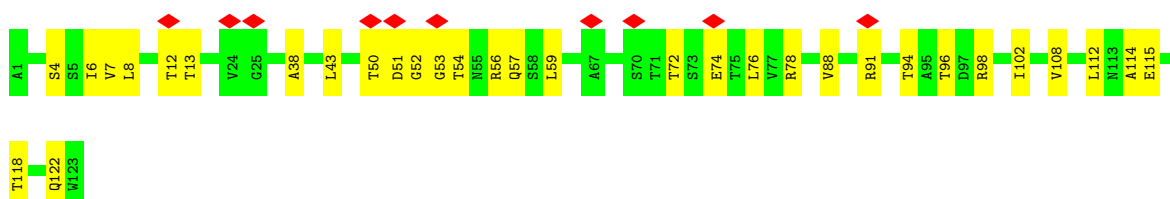
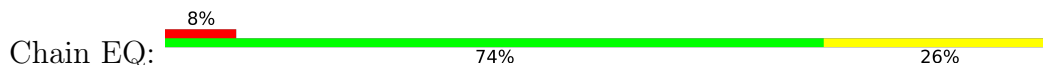




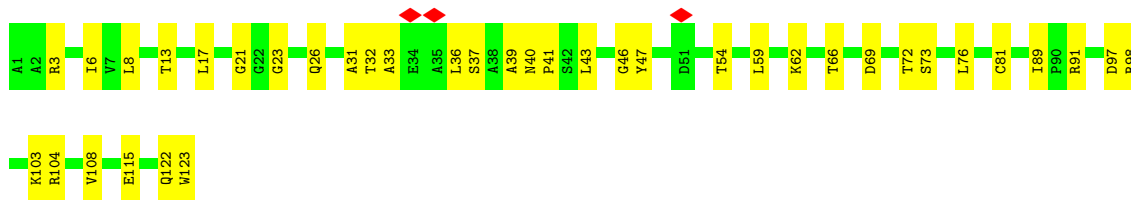
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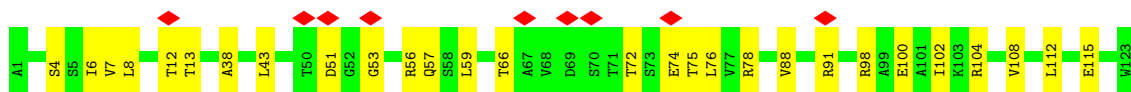
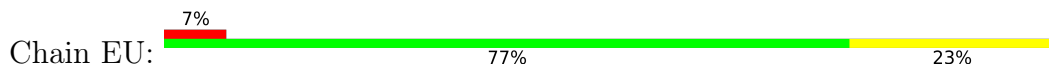
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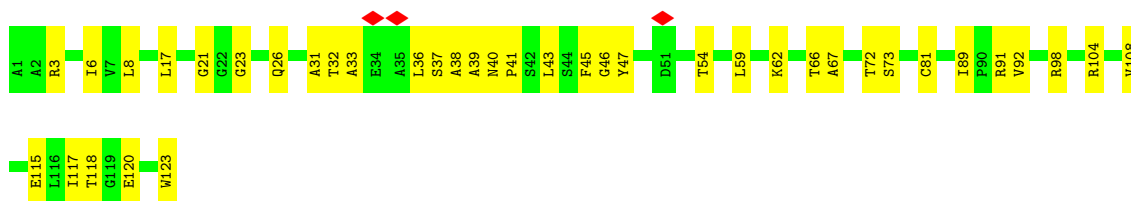
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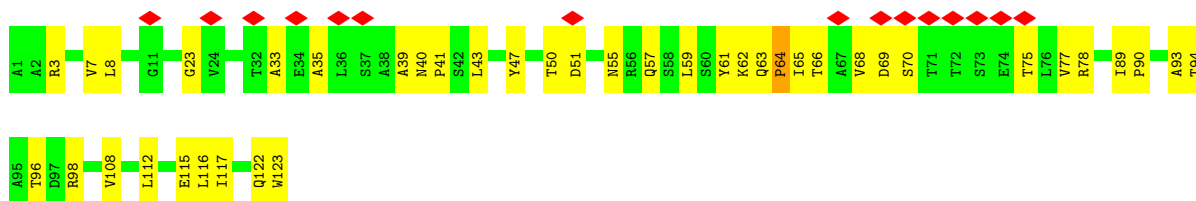
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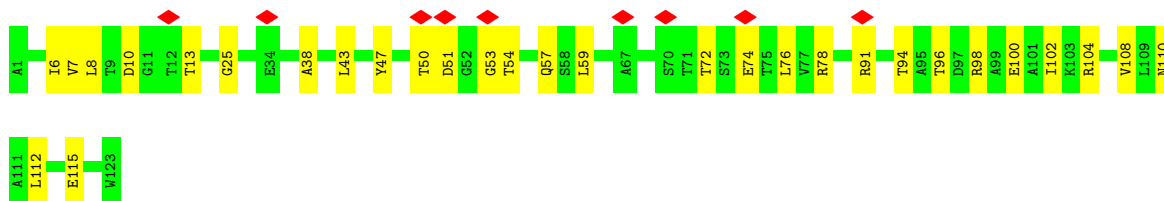
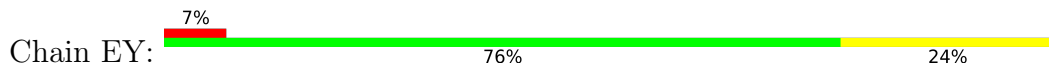
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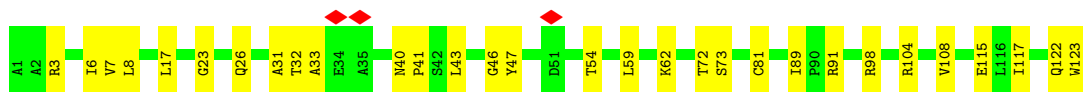
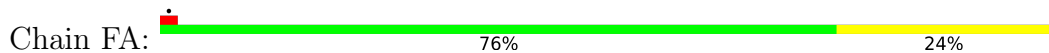
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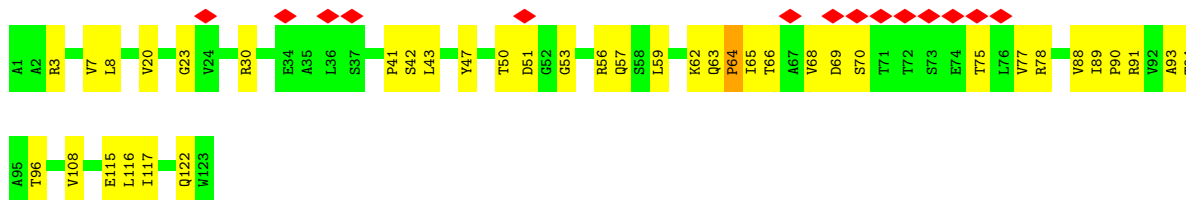


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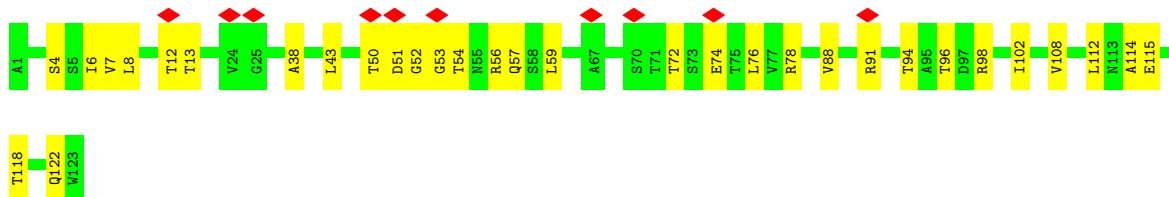
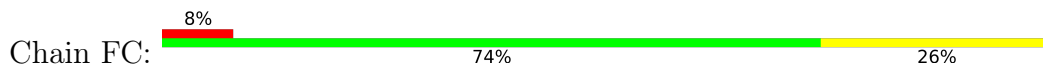


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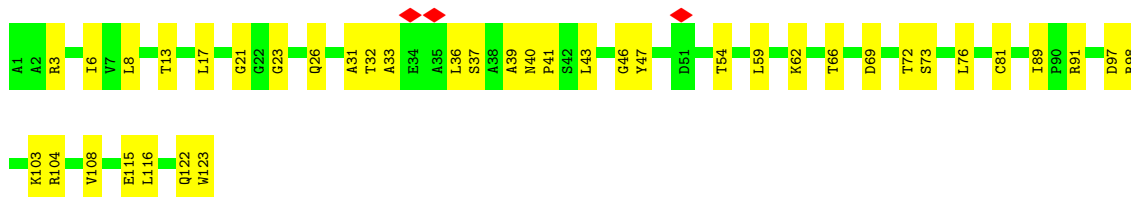




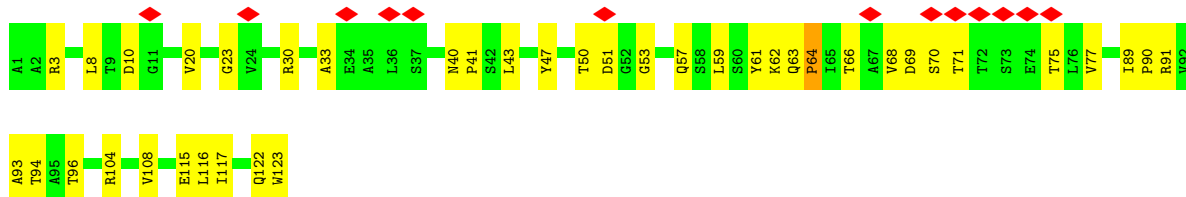
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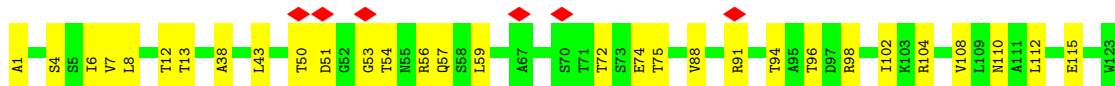
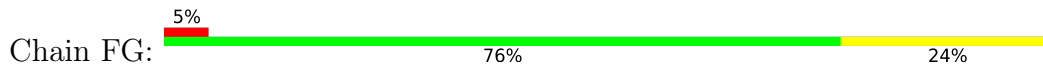
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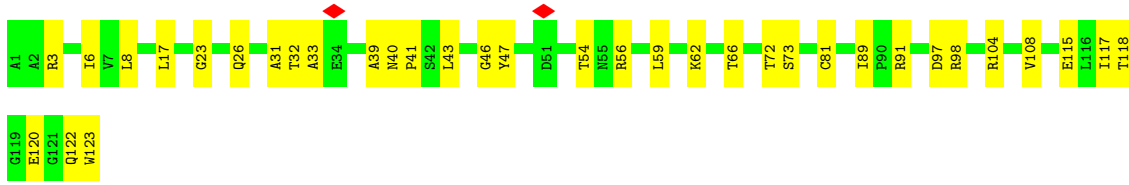


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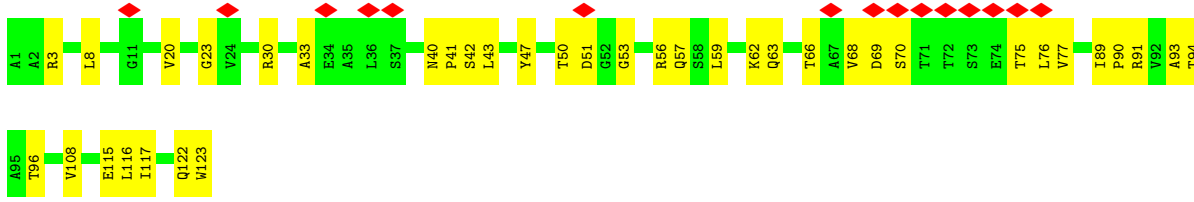


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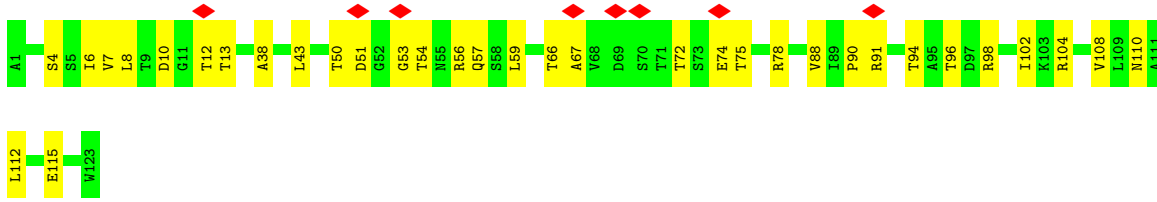
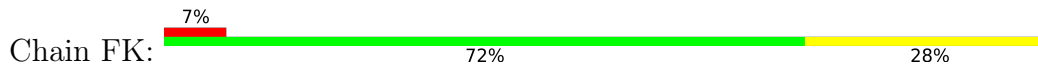




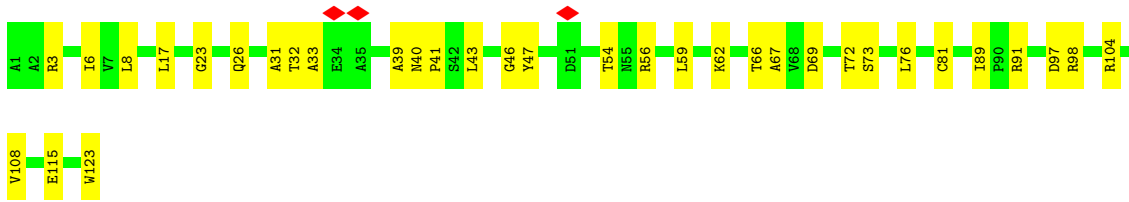
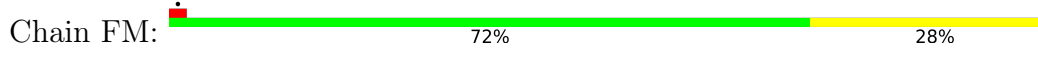
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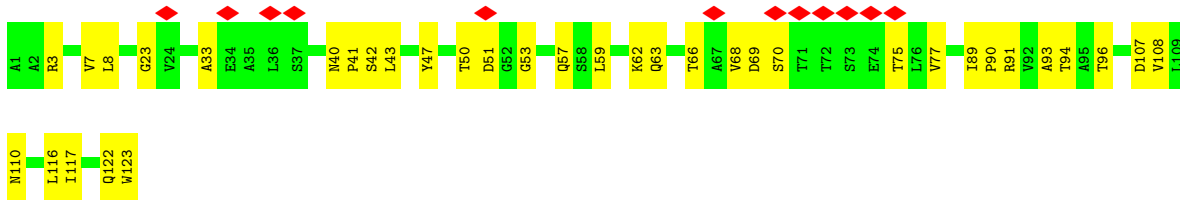
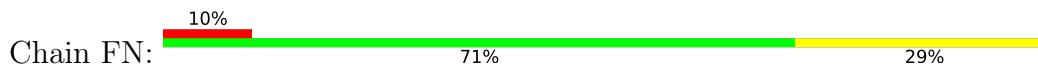
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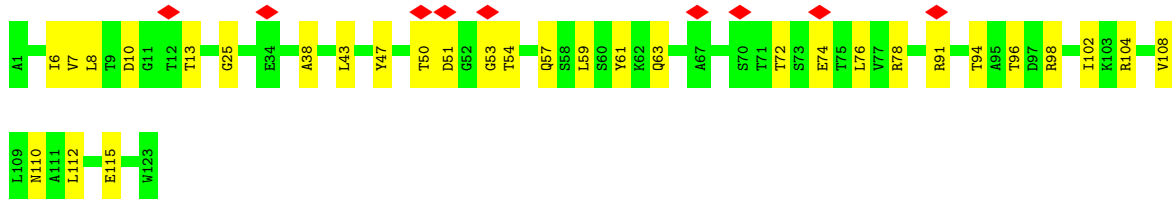
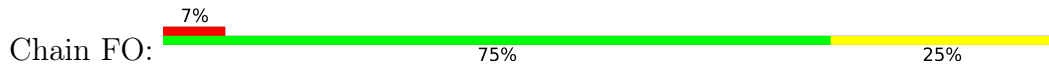
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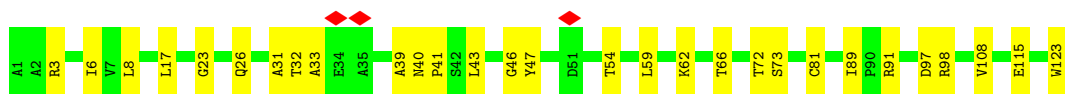
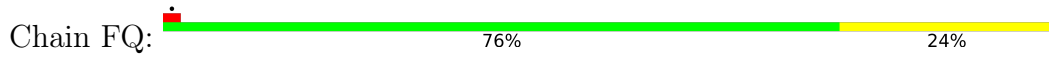
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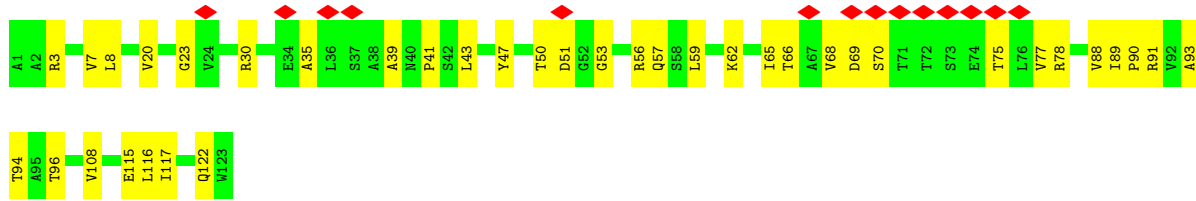
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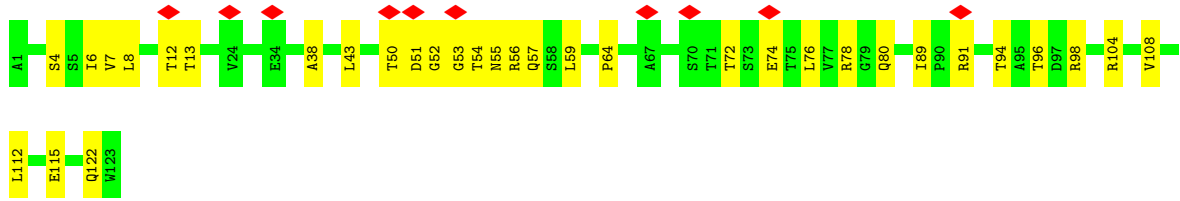
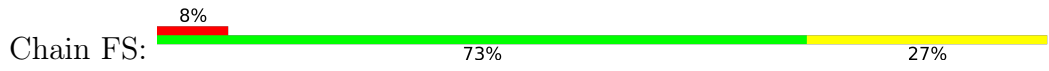
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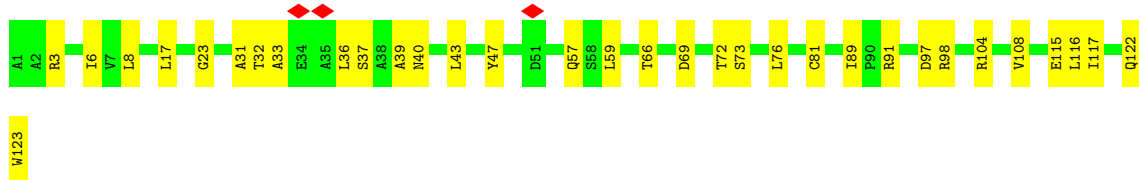
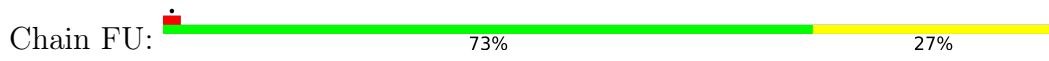
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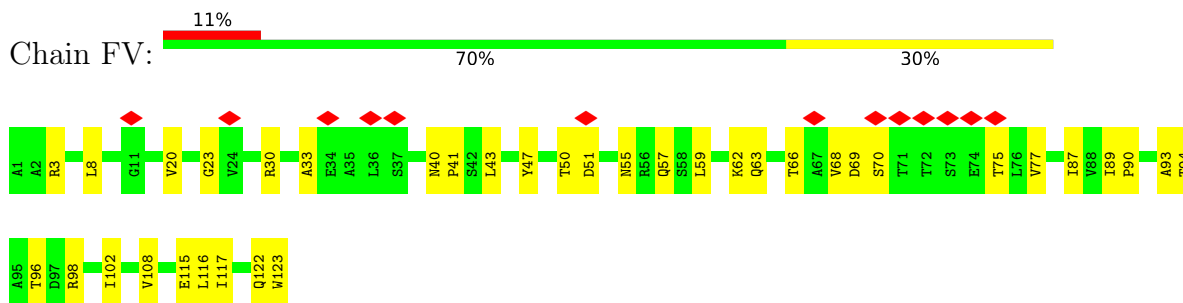
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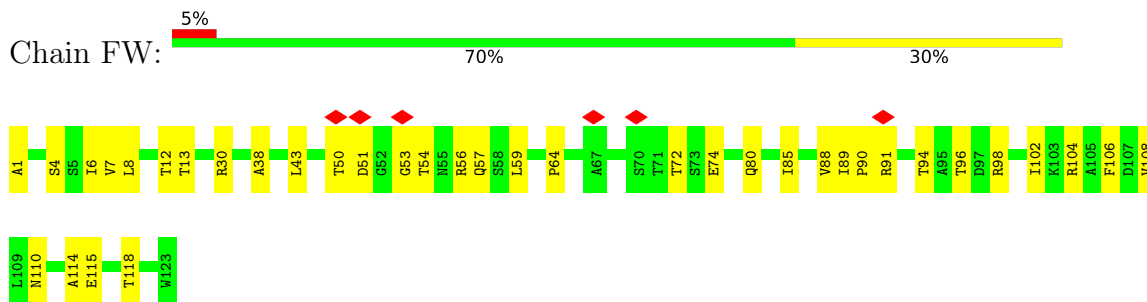
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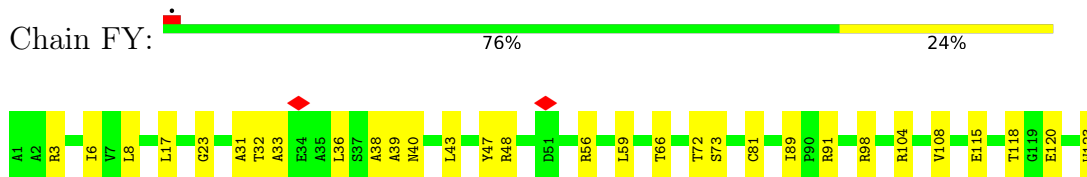
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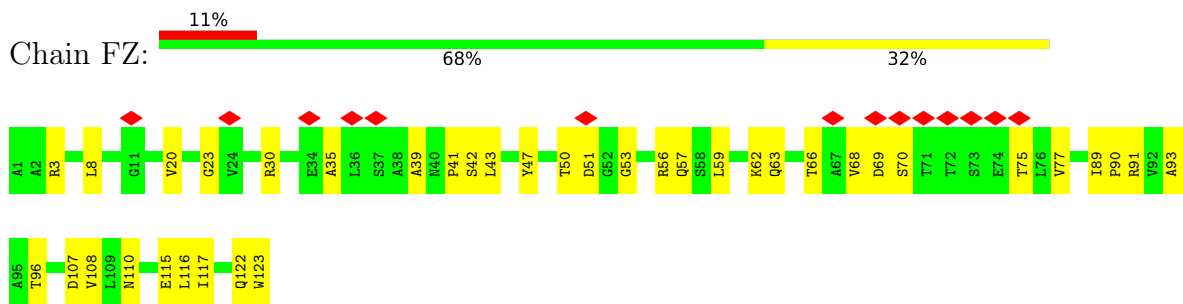
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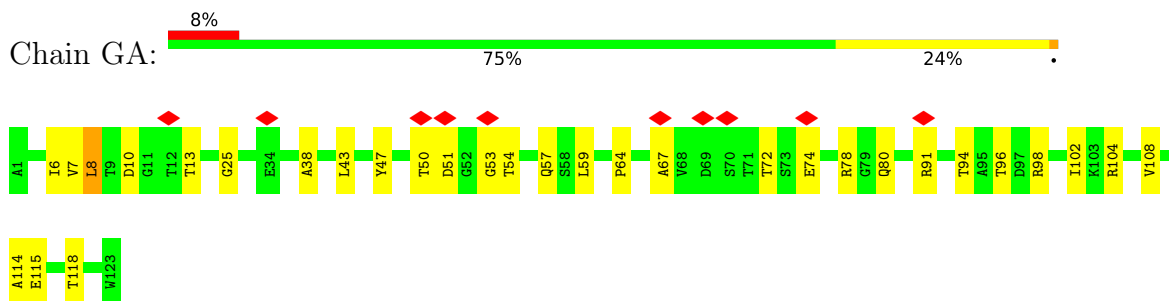
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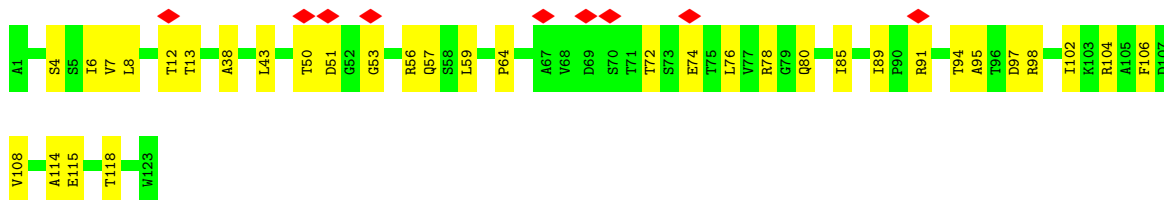
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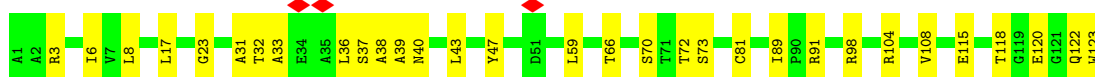
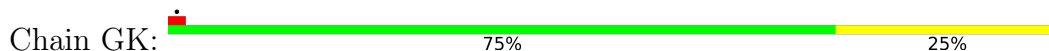
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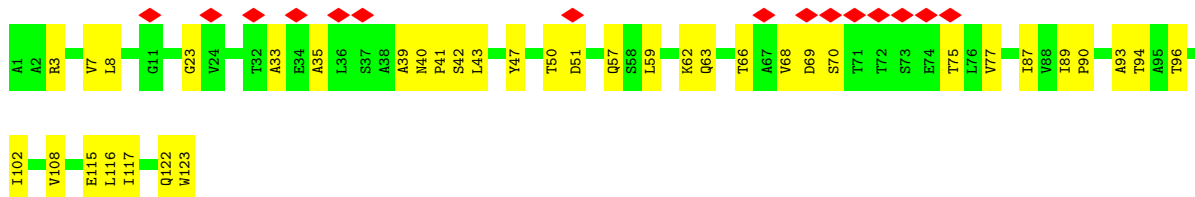
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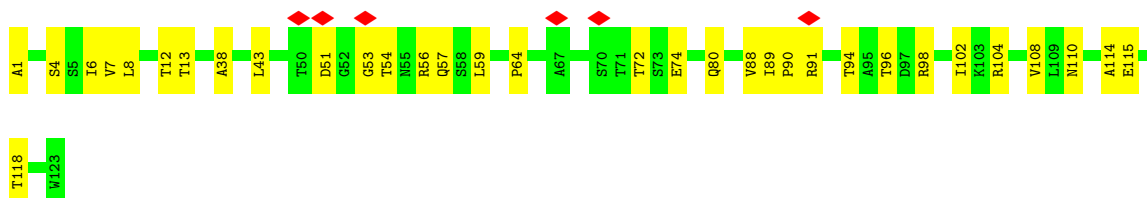
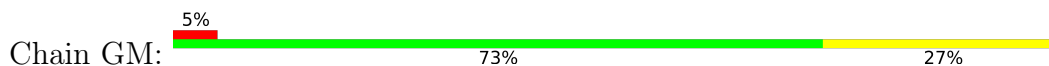
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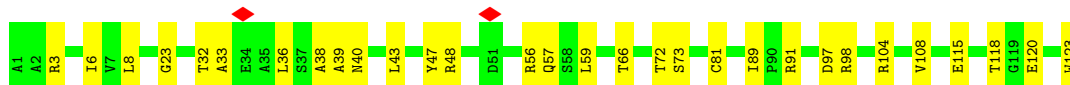
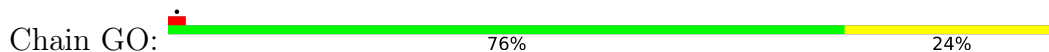
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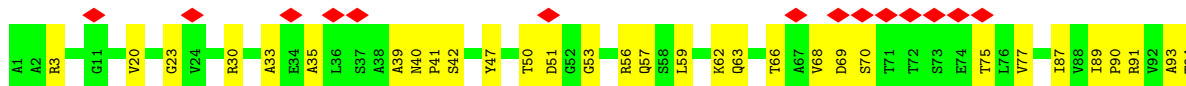
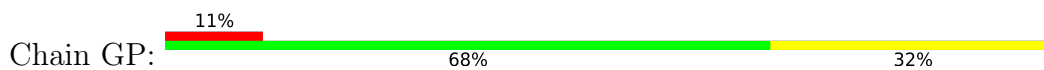
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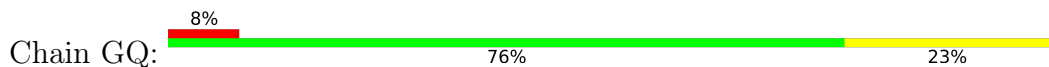


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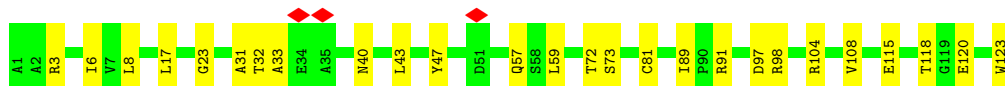
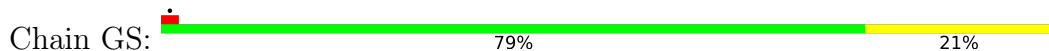




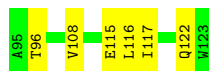
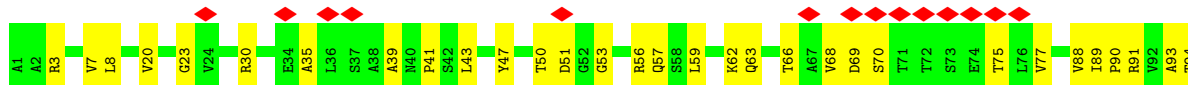
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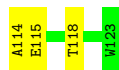
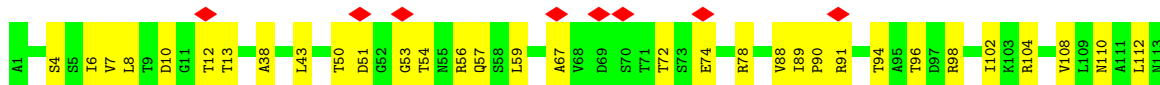
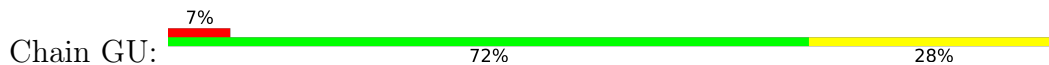
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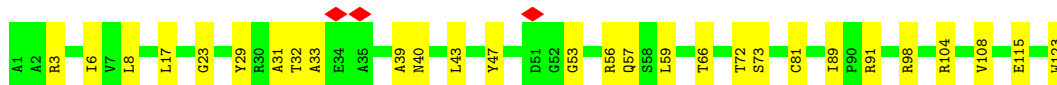
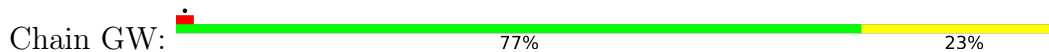
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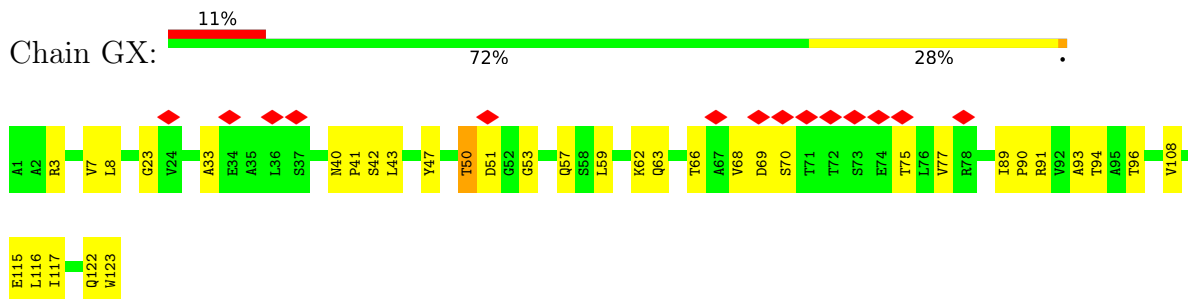
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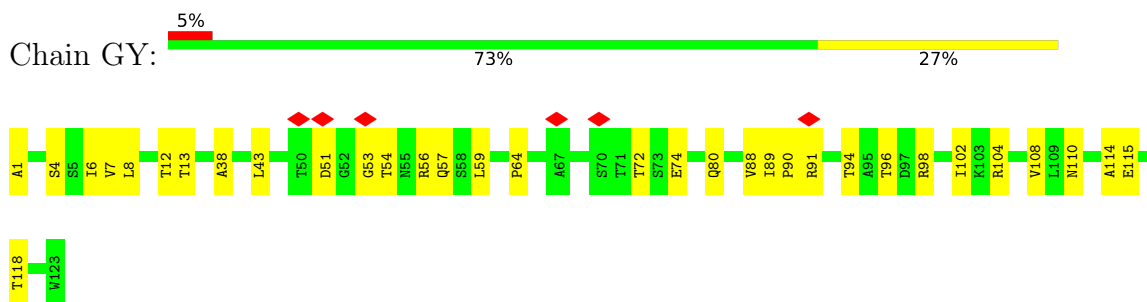
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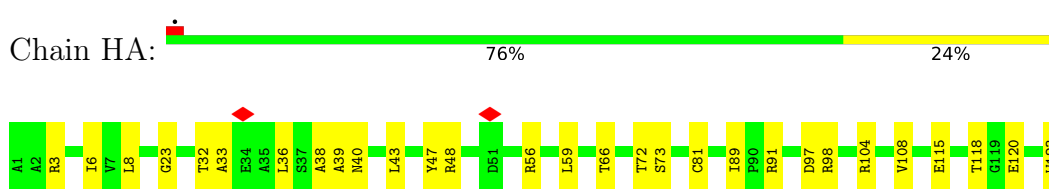
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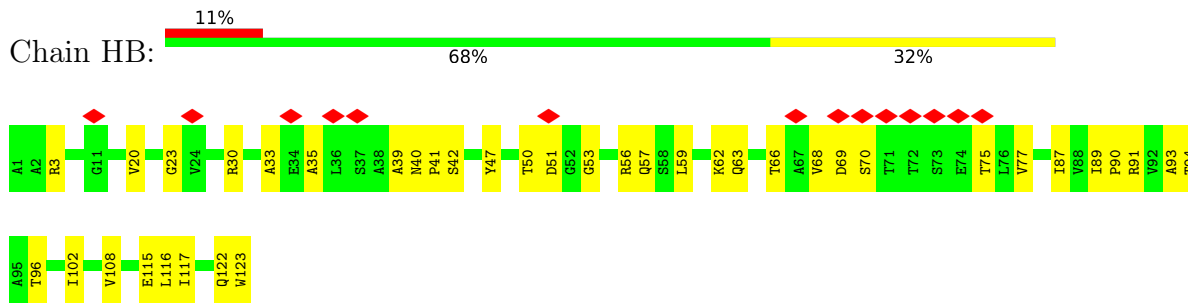
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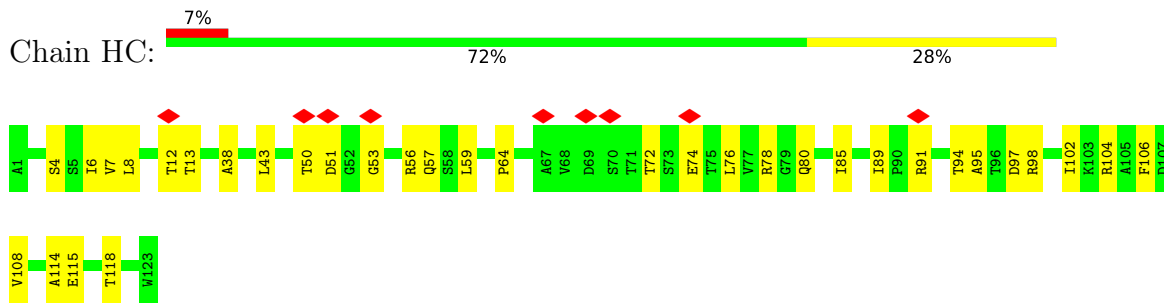
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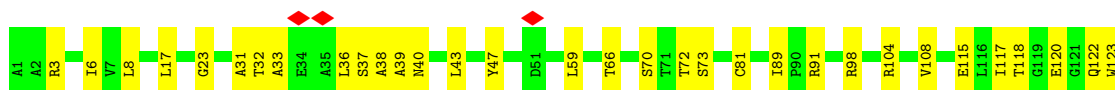
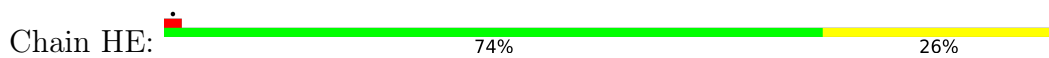
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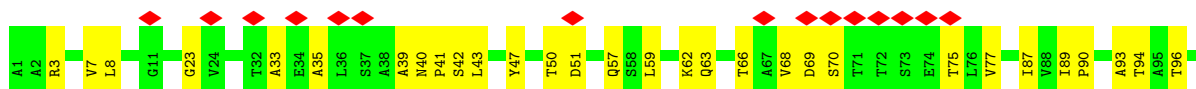
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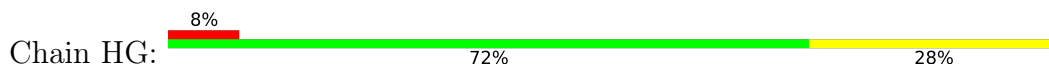
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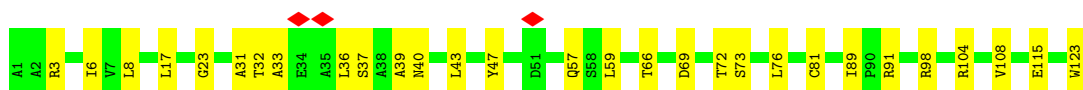
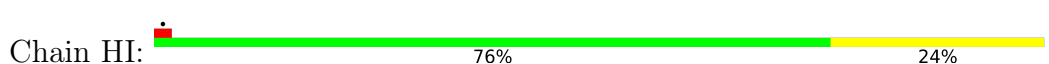
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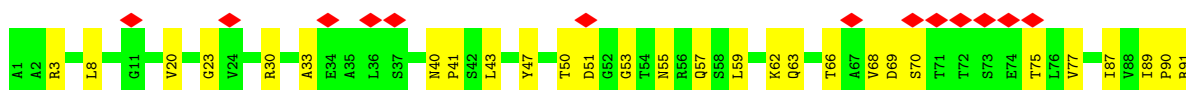
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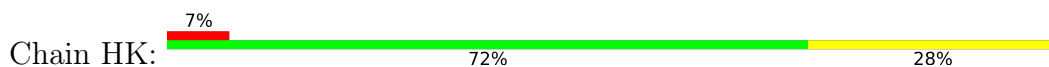
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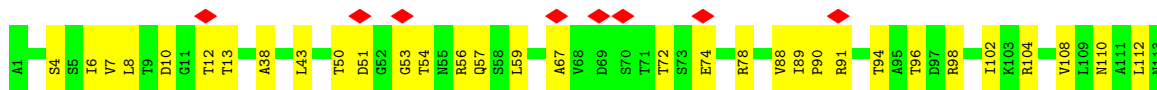


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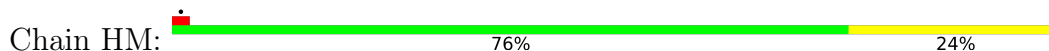


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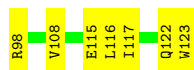
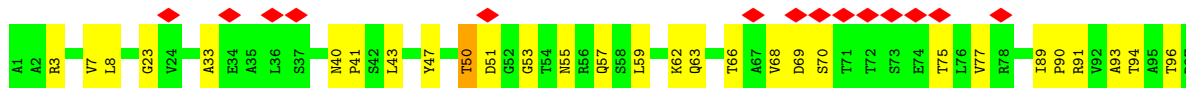




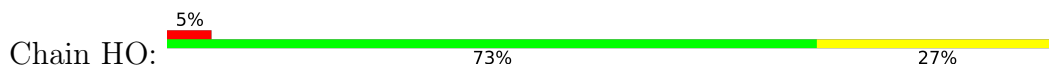
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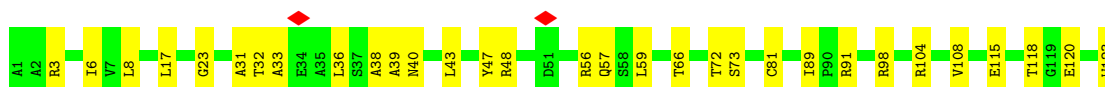
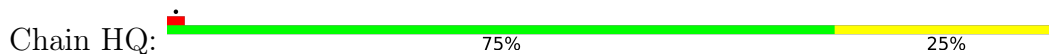
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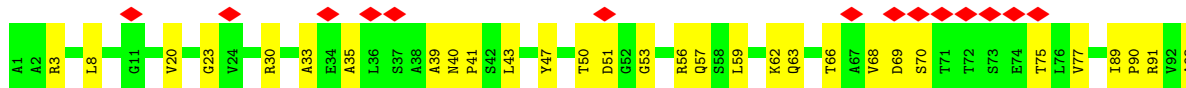
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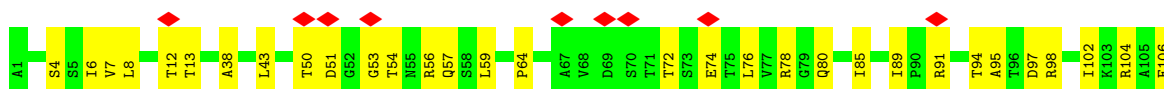
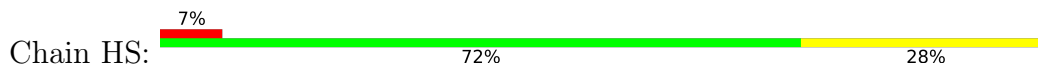


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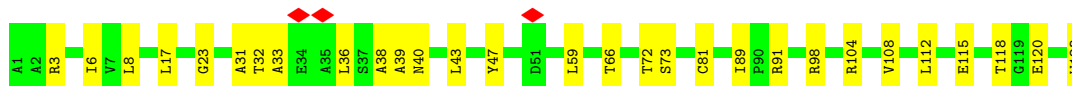
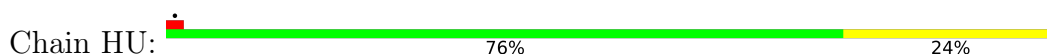




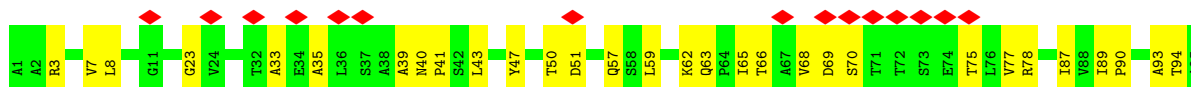
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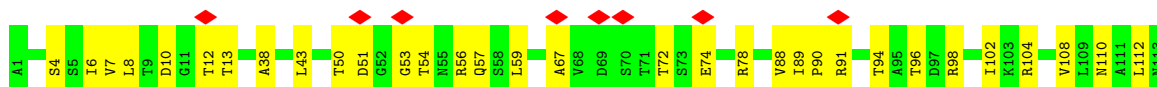
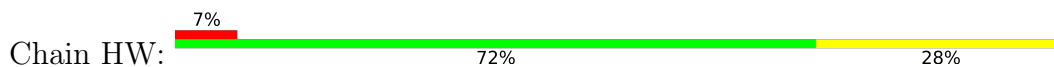
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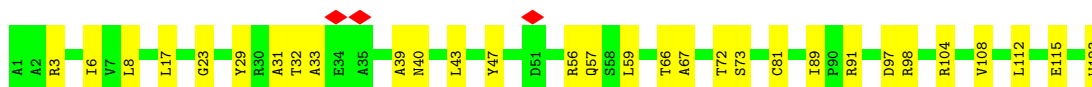
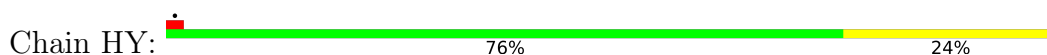
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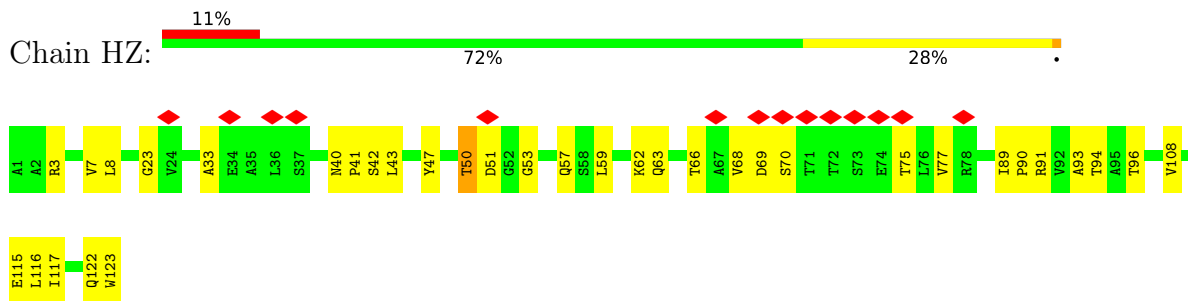
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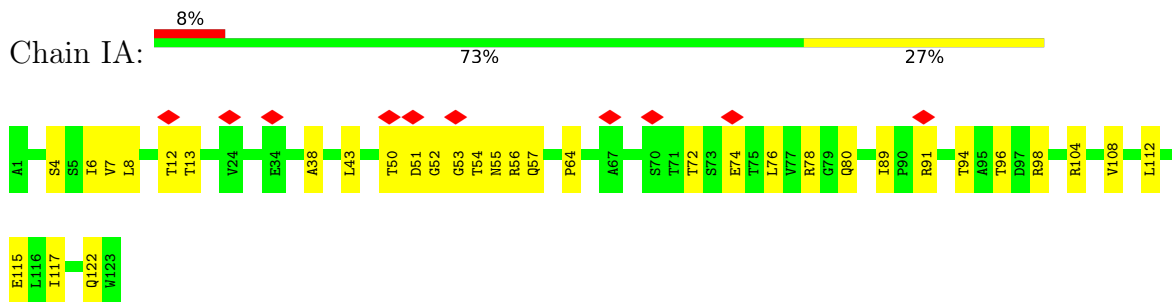
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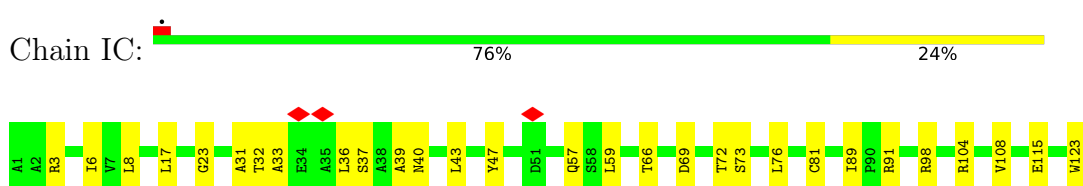
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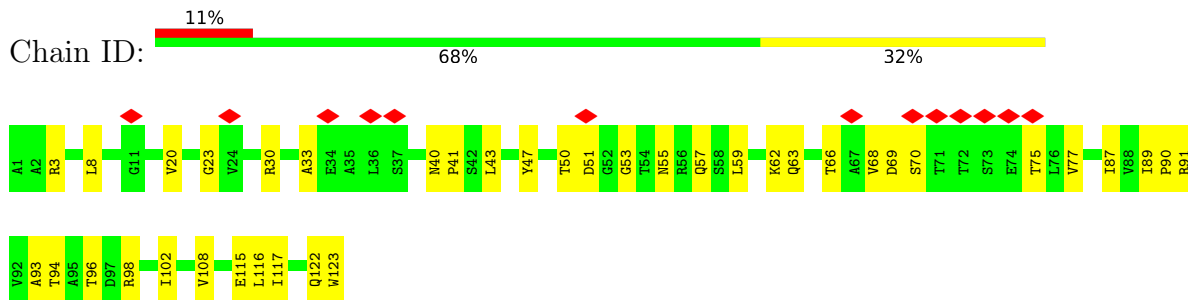
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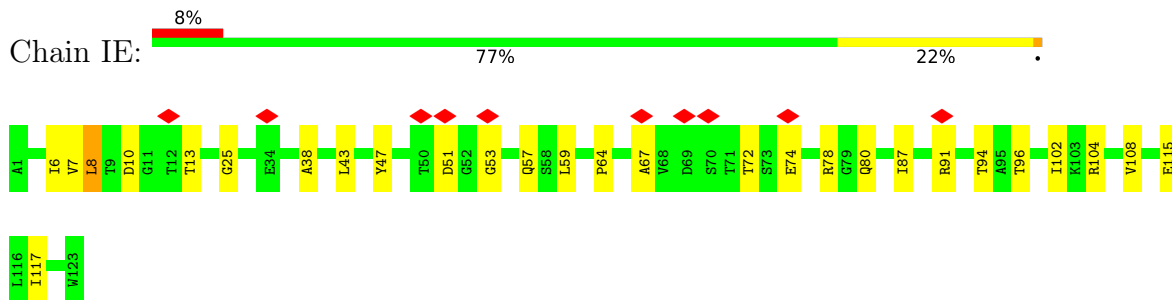
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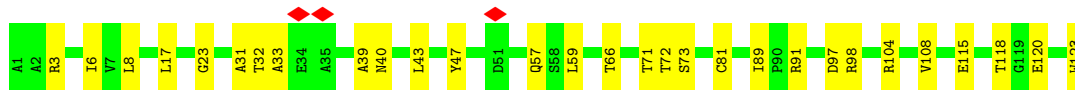
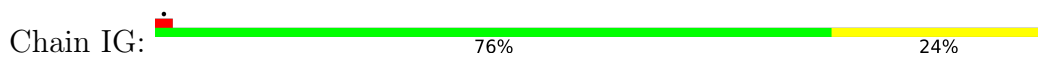
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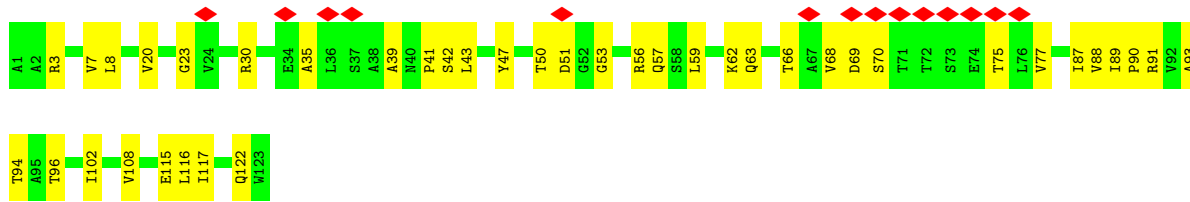
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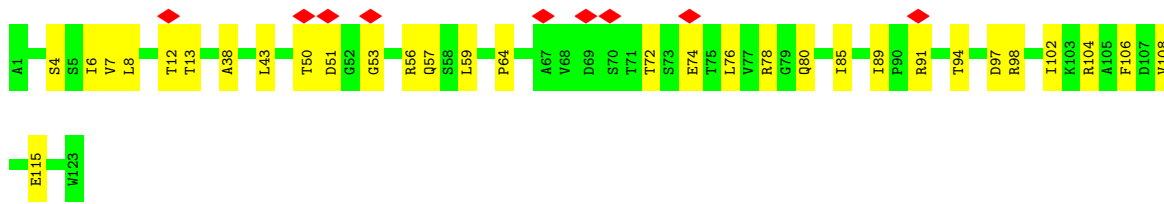
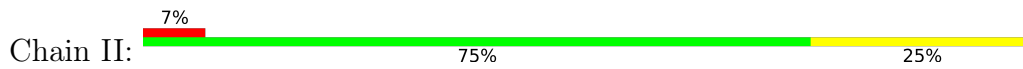
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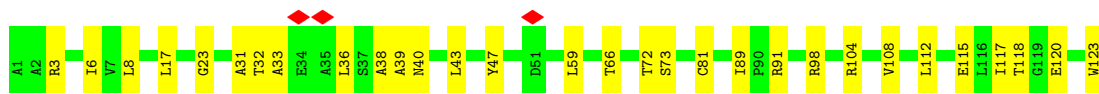
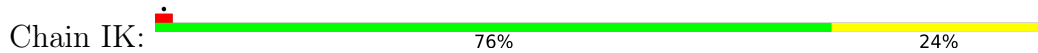
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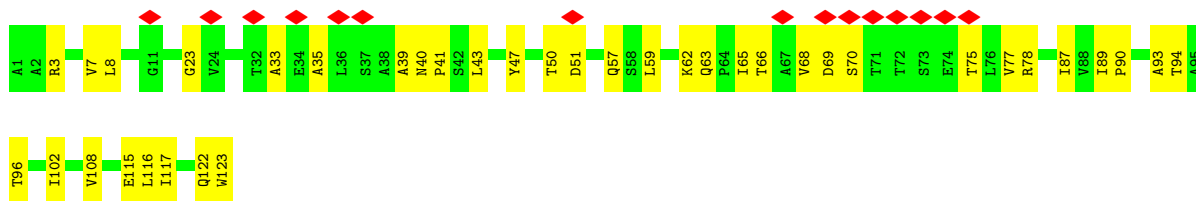
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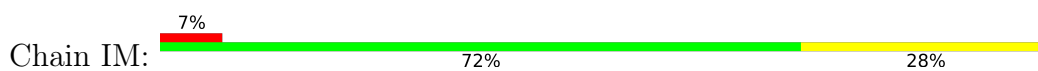
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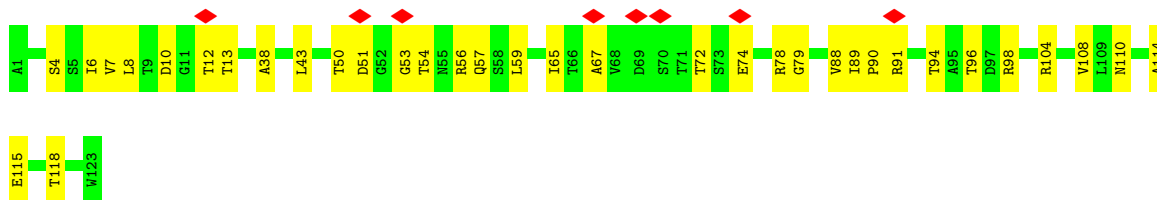


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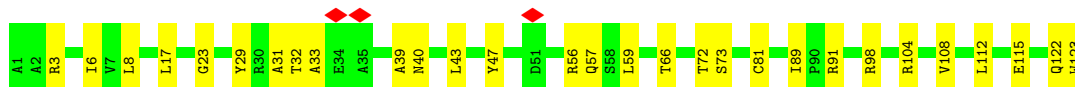
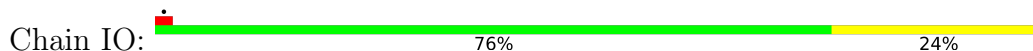


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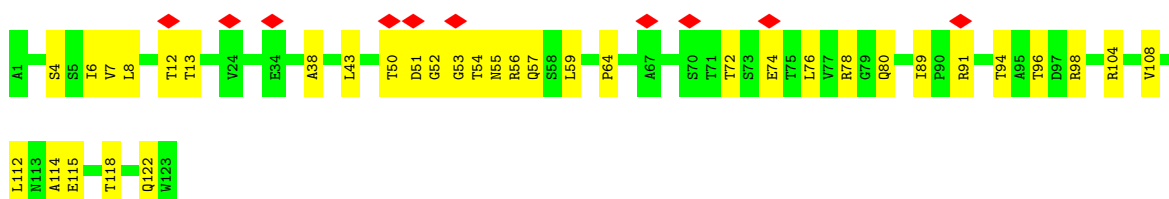
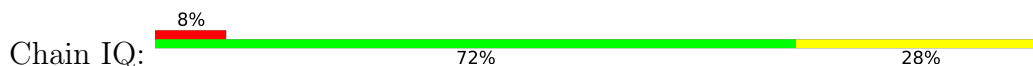
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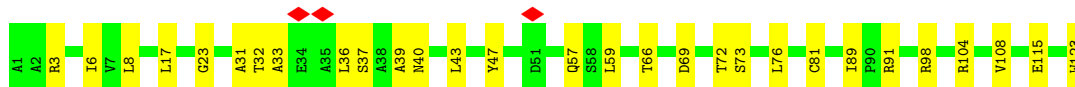
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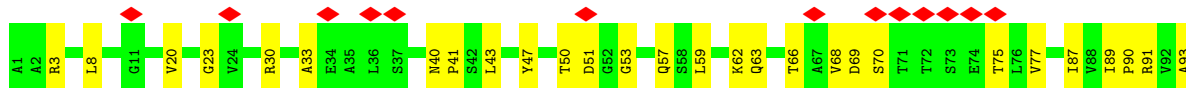
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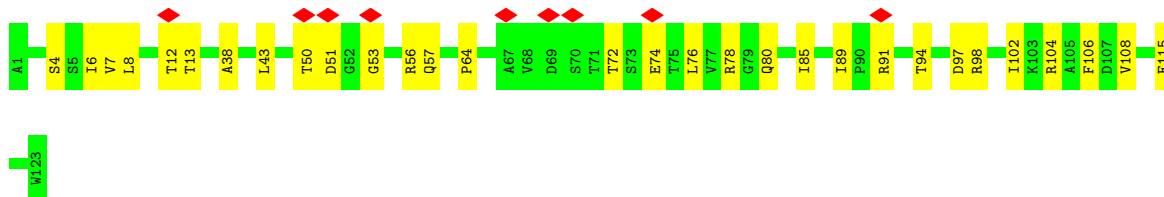
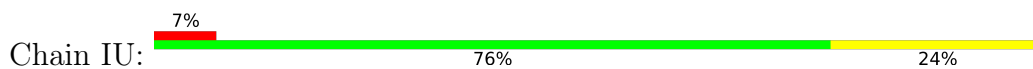


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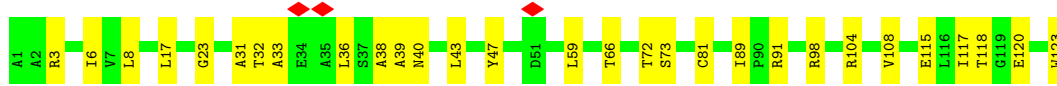
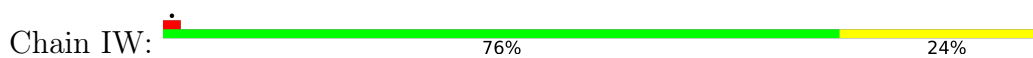




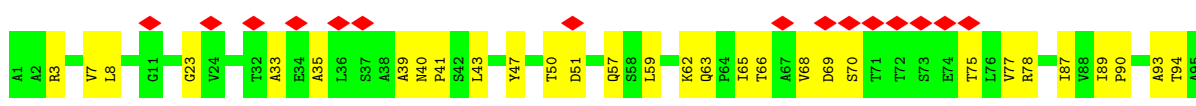
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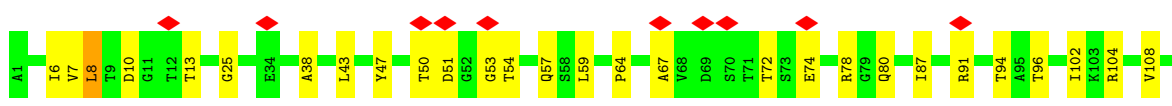
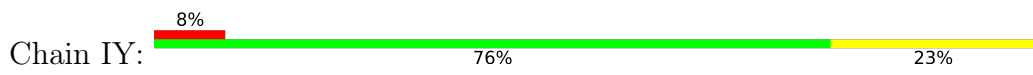
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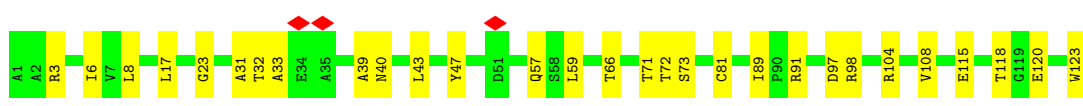
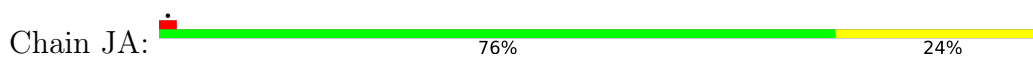
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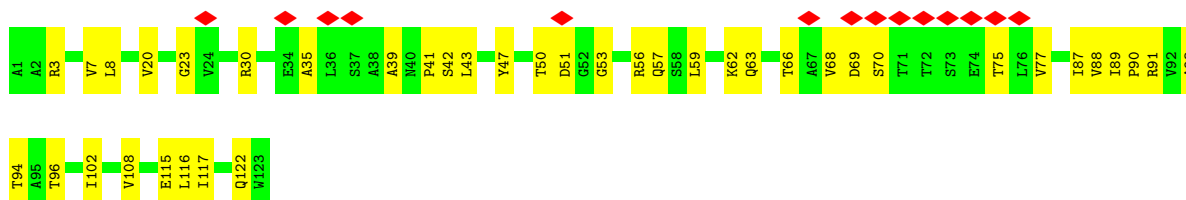
• Molecule 1: Capsid protein



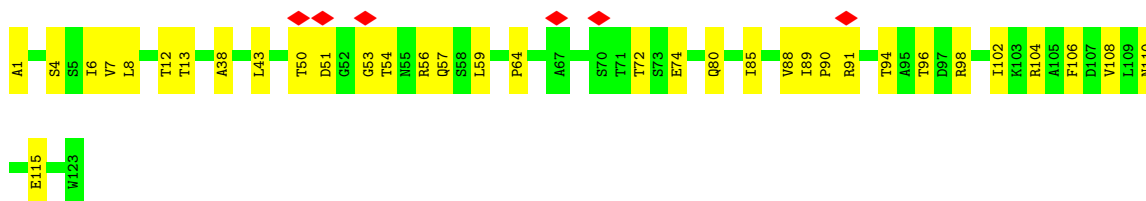
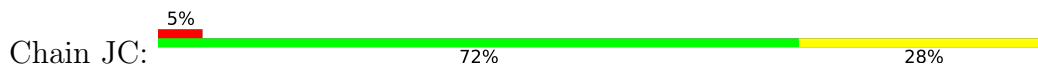
• Molecule 1: Capsid protein



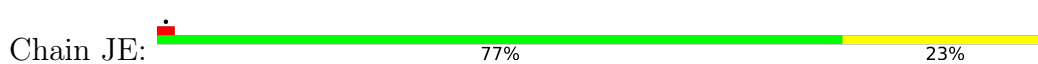
• Molecule 1: Capsid protein



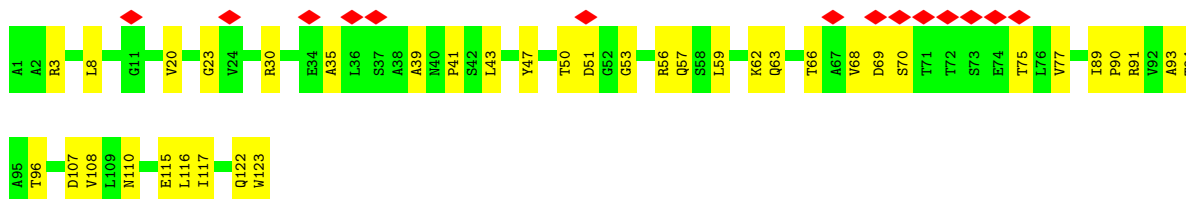
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28843	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.014	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.003	Depositor
Map size (\AA)	400.896, 400.896, 400.896	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.783, 0.783, 0.783	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.21	0/919	0.38	0/1254
1	AC	0.26	0/919	0.42	0/1254
1	AD	0.28	0/919	0.56	2/1254 (0.2%)
1	AE	0.22	0/919	0.38	0/1254
1	AG	0.26	0/919	0.41	0/1254
1	AH	0.28	0/919	0.60	2/1254 (0.2%)
1	AI	0.21	0/919	0.36	0/1254
1	AK	0.26	0/919	0.41	0/1254
1	AL	0.26	0/919	0.54	1/1254 (0.1%)
1	AM	0.21	0/919	0.38	0/1254
1	AO	0.26	0/919	0.42	0/1254
1	AP	0.28	0/919	0.56	2/1254 (0.2%)
1	AQ	0.22	0/919	0.38	0/1254
1	AS	0.26	0/919	0.42	0/1254
1	AT	0.22	0/919	0.38	0/1254
1	AU	0.21	0/919	0.36	0/1254
1	AW	0.26	0/919	0.41	0/1254
1	AX	0.22	0/919	0.39	0/1254
1	AY	0.21	0/919	0.36	0/1254
1	BA	0.26	0/919	0.41	0/1254
1	BB	0.26	0/919	0.54	1/1254 (0.1%)
1	BC	0.21	0/919	0.38	0/1254
1	BE	0.26	0/919	0.42	0/1254
1	BF	0.28	0/919	0.56	2/1254 (0.2%)
1	BG	0.22	0/919	0.38	0/1254
1	BI	0.26	0/919	0.42	0/1254
1	BJ	0.22	0/919	0.38	0/1254
1	BK	0.21	0/919	0.36	0/1254
1	BM	0.26	0/919	0.41	0/1254
1	BN	0.26	0/919	0.54	1/1254 (0.1%)
1	BO	0.21	0/919	0.36	0/1254
1	BQ	0.26	0/919	0.41	0/1254
1	BR	0.22	0/919	0.39	0/1254
1	BS	0.22	0/919	0.38	0/1254

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BU	0.26	0/919	0.41	0/1254
1	BV	0.28	0/919	0.60	2/1254 (0.2%)
1	BW	0.22	0/919	0.38	0/1254
1	BY	0.26	0/919	0.42	0/1254
1	BZ	0.22	0/919	0.38	0/1254
1	CA	0.21	0/919	0.36	0/1254
1	CC	0.26	0/919	0.41	0/1254
1	CD	0.26	0/919	0.54	1/1254 (0.1%)
1	CE	0.21	0/919	0.36	0/1254
1	CG	0.26	0/919	0.41	0/1254
1	CH	0.22	0/919	0.39	0/1254
1	CI	0.22	0/919	0.38	0/1254
1	CK	0.26	0/919	0.42	0/1254
1	CL	0.22	0/919	0.38	0/1254
1	CM	0.22	0/919	0.38	0/1254
1	CO	0.26	0/919	0.41	0/1254
1	CP	0.28	0/919	0.60	2/1254 (0.2%)
1	CQ	0.21	0/919	0.38	0/1254
1	CS	0.26	0/919	0.42	0/1254
1	CT	0.28	0/919	0.56	2/1254 (0.2%)
1	CU	0.21	0/919	0.37	0/1254
1	CW	0.26	0/919	0.41	0/1254
1	CX	0.22	0/919	0.39	0/1254
1	CY	0.22	0/919	0.39	0/1254
1	DA	0.26	0/919	0.42	0/1254
1	DB	0.22	0/919	0.38	0/1254
1	DC	0.22	0/919	0.38	0/1254
1	DE	0.26	0/919	0.41	0/1254
1	DF	0.28	0/919	0.60	2/1254 (0.2%)
1	DG	0.21	0/919	0.37	0/1254
1	DI	0.26	0/919	0.41	0/1254
1	DJ	0.22	0/919	0.39	0/1254
1	DK	0.21	0/919	0.38	0/1254
1	DM	0.26	0/919	0.42	0/1254
1	DN	0.28	0/919	0.56	2/1254 (0.2%)
1	DO	0.21	0/919	0.37	0/1254
1	DQ	0.26	0/919	0.41	0/1254
1	DR	0.26	0/919	0.54	1/1254 (0.1%)
1	DS	0.22	0/919	0.38	0/1254
1	DU	0.26	0/919	0.41	0/1254
1	DV	0.28	0/919	0.60	2/1254 (0.2%)
1	DW	0.21	0/919	0.36	0/1254
1	DY	0.26	0/919	0.41	0/1254

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	DZ	0.22	0/919	0.39	0/1254
1	EA	0.21	0/919	0.38	0/1254
1	EC	0.26	0/919	0.42	0/1254
1	ED	0.28	0/919	0.56	2/1254 (0.2%)
1	EE	0.22	0/919	0.38	0/1254
1	EG	0.26	0/919	0.41	0/1254
1	EH	0.28	0/919	0.60	2/1254 (0.2%)
1	EI	0.21	0/919	0.36	0/1254
1	EK	0.26	0/919	0.41	0/1254
1	EL	0.26	0/919	0.54	1/1254 (0.1%)
1	EM	0.22	0/919	0.38	0/1254
1	EO	0.26	0/919	0.42	0/1254
1	EP	0.22	0/919	0.38	0/1254
1	EQ	0.21	0/919	0.38	0/1254
1	ES	0.26	0/919	0.42	0/1254
1	ET	0.28	0/919	0.56	2/1254 (0.2%)
1	EU	0.21	0/919	0.37	0/1254
1	EW	0.26	0/919	0.41	0/1254
1	EX	0.26	0/919	0.54	1/1254 (0.1%)
1	EY	0.22	0/919	0.38	0/1254
1	FA	0.26	0/919	0.41	0/1254
1	FB	0.28	0/919	0.60	2/1254 (0.2%)
1	FC	0.21	0/919	0.38	0/1254
1	FE	0.26	0/919	0.42	0/1254
1	FF	0.28	0/919	0.56	2/1254 (0.2%)
1	FG	0.21	0/919	0.37	0/1254
1	FI	0.26	0/919	0.41	0/1254
1	FJ	0.22	0/919	0.39	0/1254
1	FK	0.22	0/919	0.40	0/1254
1	FM	0.26	0/919	0.42	0/1254
1	FN	0.22	0/919	0.38	0/1254
1	FO	0.22	0/919	0.38	0/1254
1	FQ	0.26	0/919	0.41	0/1254
1	FR	0.22	0/919	0.43	0/1254
1	FS	0.21	0/919	0.37	0/1254
1	FU	0.25	0/919	0.38	0/1254
1	FV	0.22	0/919	0.38	0/1254
1	FW	0.21	0/919	0.35	0/1254
1	FY	0.26	0/919	0.39	0/1254
1	FZ	0.22	0/919	0.38	0/1254
1	GA	0.22	0/919	0.38	0/1254
1	GC	0.25	0/919	0.38	0/1254
1	GD	0.22	0/919	0.42	0/1254

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	GE	0.22	0/919	0.39	0/1254
1	GG	0.25	0/919	0.39	0/1254
1	GH	0.22	0/919	0.37	0/1254
1	GI	0.21	0/919	0.35	0/1254
1	GK	0.25	0/919	0.38	0/1254
1	GL	0.22	0/919	0.38	0/1254
1	GM	0.21	0/919	0.35	0/1254
1	GO	0.26	0/919	0.39	0/1254
1	GP	0.22	0/919	0.38	0/1254
1	GQ	0.22	0/919	0.38	0/1254
1	GS	0.25	0/919	0.38	0/1254
1	GT	0.22	0/919	0.42	0/1254
1	GU	0.22	0/919	0.39	0/1254
1	GW	0.25	0/919	0.39	0/1254
1	GX	0.22	0/919	0.37	0/1254
1	GY	0.21	0/919	0.35	0/1254
1	HA	0.25	0/919	0.39	0/1254
1	HB	0.22	0/919	0.38	0/1254
1	HC	0.21	0/919	0.35	0/1254
1	HE	0.25	0/919	0.38	0/1254
1	HF	0.22	0/919	0.38	0/1254
1	HG	0.21	0/919	0.37	0/1254
1	HI	0.25	0/919	0.38	0/1254
1	HJ	0.22	0/919	0.39	0/1254
1	HK	0.21	0/919	0.39	0/1254
1	HM	0.25	0/919	0.40	0/1254
1	HN	0.22	0/919	0.37	0/1254
1	HO	0.21	0/919	0.35	0/1254
1	HQ	0.25	0/919	0.39	0/1254
1	HR	0.22	0/919	0.38	0/1254
1	HS	0.21	0/919	0.35	0/1254
1	HU	0.25	0/919	0.38	0/1254
1	HV	0.22	0/919	0.38	0/1254
1	HW	0.21	0/919	0.39	0/1254
1	HY	0.25	0/919	0.40	0/1254
1	HZ	0.22	0/919	0.37	0/1254
1	IA	0.21	0/919	0.37	0/1254
1	IC	0.25	0/919	0.38	0/1254
1	ID	0.22	0/919	0.39	0/1254
1	IE	0.22	0/919	0.38	0/1254
1	IG	0.25	0/919	0.38	0/1254
1	IH	0.22	0/919	0.42	0/1254
1	II	0.21	0/919	0.35	0/1254

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	IK	0.25	0/919	0.38	0/1254
1	IL	0.22	0/919	0.38	0/1254
1	IM	0.22	0/919	0.39	0/1254
1	IO	0.25	0/919	0.40	0/1254
1	IP	0.22	0/919	0.37	0/1254
1	IQ	0.21	0/919	0.37	0/1254
1	IS	0.25	0/919	0.38	0/1254
1	IT	0.22	0/919	0.39	0/1254
1	IU	0.21	0/919	0.35	0/1254
1	IW	0.25	0/919	0.38	0/1254
1	IX	0.22	0/919	0.38	0/1254
1	IY	0.22	0/919	0.38	0/1254
1	JA	0.25	0/919	0.38	0/1254
1	JB	0.22	0/919	0.42	0/1254
1	JC	0.21	0/919	0.35	0/1254
1	JE	0.26	0/919	0.39	0/1254
1	JF	0.22	0/919	0.38	0/1254
All	All	0.24	0/165420	0.41	37/225720 (0.0%)

There are no bond length outliers.

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BV	64	PRO	CA-N-CD	-10.74	96.97	112.00
1	CP	64	PRO	CA-N-CD	-10.74	96.97	112.00
1	DF	64	PRO	CA-N-CD	-10.74	96.97	112.00
1	EH	64	PRO	CA-N-CD	-10.74	96.97	112.00
1	AH	64	PRO	CA-N-CD	-10.71	97.00	112.00

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	AA	907	0	911	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AC	907	0	911	34	0
1	AD	907	0	911	29	0
1	AE	907	0	911	25	0
1	AG	907	0	911	27	0
1	AH	907	0	911	28	0
1	AI	907	0	911	24	0
1	AK	907	0	911	36	0
1	AL	907	0	911	32	0
1	AM	907	0	911	27	0
1	AO	907	0	911	35	0
1	AP	907	0	911	30	0
1	AQ	907	0	911	29	0
1	AS	907	0	911	33	0
1	AT	907	0	911	25	0
1	AU	907	0	911	24	0
1	AW	907	0	911	33	0
1	AX	907	0	911	29	0
1	AY	907	0	911	25	0
1	BA	907	0	911	36	0
1	BB	907	0	911	31	0
1	BC	907	0	911	26	0
1	BE	907	0	911	35	0
1	BF	907	0	911	32	0
1	BG	907	0	911	26	0
1	BI	907	0	911	31	0
1	BJ	907	0	911	27	0
1	BK	907	0	911	25	0
1	BM	907	0	911	35	0
1	BN	907	0	911	31	0
1	BO	907	0	911	22	0
1	BQ	907	0	911	32	0
1	BR	907	0	911	28	0
1	BS	907	0	911	27	0
1	BU	907	0	911	30	0
1	BV	907	0	911	27	0
1	BW	907	0	911	28	0
1	BY	907	0	911	32	0
1	BZ	907	0	911	26	0
1	CA	907	0	911	24	0
1	CC	907	0	911	36	0
1	CD	907	0	911	30	0
1	CE	907	0	911	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CG	907	0	911	33	0
1	CH	907	0	911	27	0
1	CI	907	0	911	27	0
1	CK	907	0	911	32	0
1	CL	907	0	911	27	0
1	CM	907	0	911	24	0
1	CO	907	0	911	29	0
1	CP	907	0	911	27	0
1	CQ	907	0	911	25	0
1	CS	907	0	911	33	0
1	CT	907	0	911	31	0
1	CU	907	0	911	21	0
1	CW	907	0	911	32	0
1	CX	907	0	911	26	0
1	CY	907	0	911	28	0
1	DA	907	0	911	32	0
1	DB	907	0	911	28	0
1	DC	907	0	911	23	0
1	DE	907	0	911	31	0
1	DF	907	0	911	29	0
1	DG	907	0	911	21	0
1	DI	907	0	911	34	0
1	DJ	907	0	911	26	0
1	DK	907	0	911	24	0
1	DM	907	0	911	32	0
1	DN	907	0	911	31	0
1	DO	907	0	911	25	0
1	DQ	907	0	911	36	0
1	DR	907	0	911	30	0
1	DS	907	0	911	20	0
1	DU	907	0	911	27	0
1	DV	907	0	911	27	0
1	DW	907	0	911	23	0
1	DY	907	0	911	34	0
1	DZ	907	0	911	26	0
1	EA	907	0	911	24	0
1	EC	907	0	911	33	0
1	ED	907	0	911	31	0
1	EE	907	0	911	22	0
1	EG	907	0	911	27	0
1	EH	907	0	911	28	0
1	EI	907	0	911	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	EK	907	0	911	36	0
1	EL	907	0	911	30	0
1	EM	907	0	911	29	0
1	EO	907	0	911	33	0
1	EP	907	0	911	26	0
1	EQ	907	0	911	26	0
1	ES	907	0	911	33	0
1	ET	907	0	911	28	0
1	EU	907	0	911	23	0
1	EW	907	0	911	37	0
1	EX	907	0	911	31	0
1	EY	907	0	911	24	0
1	FA	907	0	911	31	0
1	FB	907	0	911	29	0
1	FC	907	0	911	26	0
1	FE	907	0	911	34	0
1	FF	907	0	911	30	0
1	FG	907	0	911	21	0
1	FI	907	0	911	33	0
1	FJ	907	0	911	28	0
1	FK	907	0	911	28	0
1	FM	907	0	911	31	0
1	FN	907	0	911	26	0
1	FO	907	0	911	24	0
1	FQ	907	0	911	26	0
1	FR	907	0	911	26	0
1	FS	907	0	911	28	0
1	FU	907	0	911	31	0
1	FV	907	0	911	28	0
1	FW	907	0	911	26	0
1	FY	907	0	911	30	0
1	FZ	907	0	911	28	0
1	GA	907	0	911	23	0
1	GC	907	0	911	25	0
1	GD	907	0	911	27	0
1	GE	907	0	911	32	0
1	GG	907	0	911	30	0
1	GH	907	0	911	24	0
1	GI	907	0	911	26	0
1	GK	907	0	911	31	0
1	GL	907	0	911	27	0
1	GM	907	0	911	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	GO	907	0	911	30	0
1	GP	907	0	911	29	0
1	GQ	907	0	911	23	0
1	GS	907	0	911	26	0
1	GT	907	0	911	27	0
1	GU	907	0	911	31	0
1	GW	907	0	911	28	0
1	GX	907	0	911	25	0
1	GY	907	0	911	23	0
1	HA	907	0	911	29	0
1	HB	907	0	911	28	0
1	HC	907	0	911	26	0
1	HE	907	0	911	31	0
1	HF	907	0	911	27	0
1	HG	907	0	911	29	0
1	HI	907	0	911	26	0
1	HJ	907	0	911	27	0
1	HK	907	0	911	30	0
1	HM	907	0	911	32	0
1	HN	907	0	911	26	0
1	HO	907	0	911	24	0
1	HQ	907	0	911	32	0
1	HR	907	0	911	28	0
1	HS	907	0	911	27	0
1	HU	907	0	911	29	0
1	HV	907	0	911	27	0
1	HW	907	0	911	31	0
1	HY	907	0	911	31	0
1	HZ	907	0	911	25	0
1	IA	907	0	911	28	0
1	IC	907	0	911	26	0
1	ID	907	0	911	27	0
1	IE	907	0	911	21	0
1	IG	907	0	911	29	0
1	IH	907	0	911	29	0
1	II	907	0	911	24	0
1	IK	907	0	911	28	0
1	IL	907	0	911	27	0
1	IM	907	0	911	30	0
1	IO	907	0	911	31	0
1	IP	907	0	911	24	0
1	IQ	907	0	911	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	IS	907	0	911	27	0
1	IT	907	0	911	26	0
1	IU	907	0	911	23	0
1	IW	907	0	911	27	0
1	IX	907	0	911	27	0
1	IY	907	0	911	21	0
1	JA	907	0	911	29	0
1	JB	907	0	911	29	0
1	JC	907	0	911	24	0
1	JE	907	0	911	30	0
1	JF	907	0	911	27	0
All	All	163260	0	163980	4031	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 12.

The worst 5 of 4031 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CC:33:ALA:HB3	1:CC:40:ASN:HB3	1.65	0.78
1:EW:33:ALA:HB3	1:EW:40:ASN:HB3	1.65	0.78
1:HU:33:ALA:HB3	1:HU:40:ASN:HB3	1.65	0.78
1:DU:33:ALA:HB3	1:DU:40:ASN:HB3	1.66	0.78
1:EG:33:ALA:HB3	1:EG:40:ASN:HB3	1.66	0.78

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
1	AA	121/123 (98%)	102 (84%)	19 (16%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AC	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	AD	121/123 (98%)	105 (87%)	16 (13%)	0	100	100
1	AE	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	AG	121/123 (98%)	108 (89%)	13 (11%)	0	100	100
1	AH	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	AI	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	AK	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	AL	121/123 (98%)	109 (90%)	12 (10%)	0	100	100
1	AM	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	AO	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	AP	121/123 (98%)	105 (87%)	16 (13%)	0	100	100
1	AQ	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	AS	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	AT	121/123 (98%)	107 (88%)	14 (12%)	0	100	100
1	AU	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	AW	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	AX	121/123 (98%)	109 (90%)	12 (10%)	0	100	100
1	AY	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	BA	121/123 (98%)	107 (88%)	14 (12%)	0	100	100
1	BB	121/123 (98%)	109 (90%)	12 (10%)	0	100	100
1	BC	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	BE	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	BF	121/123 (98%)	105 (87%)	16 (13%)	0	100	100
1	BG	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	BI	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	BJ	121/123 (98%)	107 (88%)	14 (12%)	0	100	100
1	BK	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	BM	121/123 (98%)	107 (88%)	14 (12%)	0	100	100
1	BN	121/123 (98%)	109 (90%)	12 (10%)	0	100	100
1	BO	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	BQ	121/123 (98%)	106 (88%)	15 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BR	121/123 (98%)	109 (90%)	12 (10%)	0	100	100
1	BS	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	BU	121/123 (98%)	108 (89%)	13 (11%)	0	100	100
1	BV	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	BW	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	BY	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	BZ	121/123 (98%)	107 (88%)	14 (12%)	0	100	100
1	CA	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	CC	121/123 (98%)	107 (88%)	14 (12%)	0	100	100
1	CD	121/123 (98%)	109 (90%)	12 (10%)	0	100	100
1	CE	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	CG	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	CH	121/123 (98%)	109 (90%)	12 (10%)	0	100	100
1	CI	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	CK	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	CL	121/123 (98%)	107 (88%)	14 (12%)	0	100	100
1	CM	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	CO	121/123 (98%)	108 (89%)	13 (11%)	0	100	100
1	CP	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	CQ	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	CS	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	CT	121/123 (98%)	105 (87%)	16 (13%)	0	100	100
1	CU	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	CW	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	CX	121/123 (98%)	109 (90%)	12 (10%)	0	100	100
1	CY	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	DA	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	DB	121/123 (98%)	107 (88%)	14 (12%)	0	100	100
1	DC	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	DE	121/123 (98%)	108 (89%)	13 (11%)	0	100	100
1	DF	121/123 (98%)	106 (88%)	15 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DG	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	DI	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	DJ	121/123 (98%)	109 (90%)	12 (10%)	0	100	100
1	DK	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	DM	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	DN	121/123 (98%)	105 (87%)	16 (13%)	0	100	100
1	DO	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	DQ	121/123 (98%)	107 (88%)	14 (12%)	0	100	100
1	DR	121/123 (98%)	109 (90%)	12 (10%)	0	100	100
1	DS	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	DU	121/123 (98%)	108 (89%)	13 (11%)	0	100	100
1	DV	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	DW	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	DY	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	DZ	121/123 (98%)	109 (90%)	12 (10%)	0	100	100
1	EA	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	EC	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	ED	121/123 (98%)	105 (87%)	16 (13%)	0	100	100
1	EE	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	EG	121/123 (98%)	108 (89%)	13 (11%)	0	100	100
1	EH	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	EI	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	EK	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	EL	121/123 (98%)	109 (90%)	12 (10%)	0	100	100
1	EM	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	EO	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	EP	121/123 (98%)	107 (88%)	14 (12%)	0	100	100
1	EQ	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	ES	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	ET	121/123 (98%)	105 (87%)	16 (13%)	0	100	100
1	EU	121/123 (98%)	104 (86%)	17 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EW	121/123 (98%)	107 (88%)	14 (12%)	0	100	100
1	EX	121/123 (98%)	109 (90%)	12 (10%)	0	100	100
1	EY	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	FA	121/123 (98%)	108 (89%)	13 (11%)	0	100	100
1	FB	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	FC	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	FE	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	FF	121/123 (98%)	105 (87%)	16 (13%)	0	100	100
1	FG	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	FI	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	FJ	121/123 (98%)	109 (90%)	12 (10%)	0	100	100
1	FK	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	FM	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	FN	121/123 (98%)	107 (88%)	14 (12%)	0	100	100
1	FO	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	FQ	121/123 (98%)	108 (89%)	13 (11%)	0	100	100
1	FR	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	FS	121/123 (98%)	101 (84%)	20 (16%)	0	100	100
1	FU	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	FV	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	FW	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	FY	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	FZ	121/123 (98%)	107 (88%)	14 (12%)	0	100	100
1	GA	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	GC	121/123 (98%)	105 (87%)	16 (13%)	0	100	100
1	GD	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	GE	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	GG	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	GH	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	GI	121/123 (98%)	105 (87%)	16 (13%)	0	100	100
1	GK	121/123 (98%)	104 (86%)	17 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	GL	121/123 (98%)	107 (88%)	14 (12%)	0	100	100
1	GM	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	GO	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	GP	121/123 (98%)	107 (88%)	14 (12%)	0	100	100
1	GQ	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	GS	121/123 (98%)	105 (87%)	16 (13%)	0	100	100
1	GT	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	GU	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	GW	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	GX	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	GY	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	HA	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	HB	121/123 (98%)	107 (88%)	14 (12%)	0	100	100
1	HC	121/123 (98%)	105 (87%)	16 (13%)	0	100	100
1	HE	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	HF	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	HG	121/123 (98%)	101 (84%)	20 (16%)	0	100	100
1	HI	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	HJ	121/123 (98%)	105 (87%)	16 (13%)	0	100	100
1	HK	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	HM	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	HN	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	HO	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	HQ	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	HR	121/123 (98%)	107 (88%)	14 (12%)	0	100	100
1	HS	121/123 (98%)	105 (87%)	16 (13%)	0	100	100
1	HU	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	HV	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	HW	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	HY	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	HZ	121/123 (98%)	104 (86%)	17 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	IA	121/123 (98%)	101 (84%)	20 (16%)	0	100	100
1	IC	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	ID	121/123 (98%)	105 (87%)	16 (13%)	0	100	100
1	IE	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	IG	121/123 (98%)	105 (87%)	16 (13%)	0	100	100
1	IH	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	II	121/123 (98%)	105 (87%)	16 (13%)	0	100	100
1	IK	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	IL	121/123 (98%)	107 (88%)	14 (12%)	0	100	100
1	IM	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	IO	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	IP	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	IQ	121/123 (98%)	101 (84%)	20 (16%)	0	100	100
1	IS	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	IT	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	IU	121/123 (98%)	105 (87%)	16 (13%)	0	100	100
1	IW	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	IX	121/123 (98%)	106 (88%)	15 (12%)	0	100	100
1	IY	121/123 (98%)	103 (85%)	18 (15%)	0	100	100
1	JA	121/123 (98%)	105 (87%)	16 (13%)	0	100	100
1	JB	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	JC	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
1	JE	121/123 (98%)	102 (84%)	19 (16%)	0	100	100
1	JF	121/123 (98%)	107 (88%)	14 (12%)	0	100	100
All	All	21780/22140 (98%)	18872 (87%)	2908 (13%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	97/97 (100%)	97 (100%)	0	100	100
1	AC	97/97 (100%)	97 (100%)	0	100	100
1	AD	97/97 (100%)	97 (100%)	0	100	100
1	AE	97/97 (100%)	97 (100%)	0	100	100
1	AG	97/97 (100%)	97 (100%)	0	100	100
1	AH	97/97 (100%)	97 (100%)	0	100	100
1	AI	97/97 (100%)	97 (100%)	0	100	100
1	AK	97/97 (100%)	97 (100%)	0	100	100
1	AL	97/97 (100%)	97 (100%)	0	100	100
1	AM	97/97 (100%)	97 (100%)	0	100	100
1	AO	97/97 (100%)	97 (100%)	0	100	100
1	AP	97/97 (100%)	97 (100%)	0	100	100
1	AQ	97/97 (100%)	97 (100%)	0	100	100
1	AS	97/97 (100%)	97 (100%)	0	100	100
1	AT	97/97 (100%)	97 (100%)	0	100	100
1	AU	97/97 (100%)	97 (100%)	0	100	100
1	AW	97/97 (100%)	97 (100%)	0	100	100
1	AX	97/97 (100%)	96 (99%)	1 (1%)	68	75
1	AY	97/97 (100%)	97 (100%)	0	100	100
1	BA	97/97 (100%)	97 (100%)	0	100	100
1	BB	97/97 (100%)	97 (100%)	0	100	100
1	BC	97/97 (100%)	97 (100%)	0	100	100
1	BE	97/97 (100%)	97 (100%)	0	100	100
1	BF	97/97 (100%)	97 (100%)	0	100	100
1	BG	97/97 (100%)	97 (100%)	0	100	100
1	BI	97/97 (100%)	97 (100%)	0	100	100
1	BJ	97/97 (100%)	97 (100%)	0	100	100
1	BK	97/97 (100%)	97 (100%)	0	100	100
1	BM	97/97 (100%)	97 (100%)	0	100	100
1	BN	97/97 (100%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BO	97/97 (100%)	97 (100%)	0	100	100
1	BQ	97/97 (100%)	97 (100%)	0	100	100
1	BR	97/97 (100%)	96 (99%)	1 (1%)	68	75
1	BS	97/97 (100%)	97 (100%)	0	100	100
1	BU	97/97 (100%)	97 (100%)	0	100	100
1	BV	97/97 (100%)	97 (100%)	0	100	100
1	BW	97/97 (100%)	97 (100%)	0	100	100
1	BY	97/97 (100%)	97 (100%)	0	100	100
1	BZ	97/97 (100%)	97 (100%)	0	100	100
1	CA	97/97 (100%)	97 (100%)	0	100	100
1	CC	97/97 (100%)	97 (100%)	0	100	100
1	CD	97/97 (100%)	97 (100%)	0	100	100
1	CE	97/97 (100%)	97 (100%)	0	100	100
1	CG	97/97 (100%)	97 (100%)	0	100	100
1	CH	97/97 (100%)	96 (99%)	1 (1%)	68	75
1	CI	97/97 (100%)	97 (100%)	0	100	100
1	CK	97/97 (100%)	97 (100%)	0	100	100
1	CL	97/97 (100%)	97 (100%)	0	100	100
1	CM	97/97 (100%)	97 (100%)	0	100	100
1	CO	97/97 (100%)	97 (100%)	0	100	100
1	CP	97/97 (100%)	97 (100%)	0	100	100
1	CQ	97/97 (100%)	97 (100%)	0	100	100
1	CS	97/97 (100%)	97 (100%)	0	100	100
1	CT	97/97 (100%)	97 (100%)	0	100	100
1	CU	97/97 (100%)	96 (99%)	1 (1%)	68	75
1	CW	97/97 (100%)	97 (100%)	0	100	100
1	CX	97/97 (100%)	96 (99%)	1 (1%)	68	75
1	CY	97/97 (100%)	97 (100%)	0	100	100
1	DA	97/97 (100%)	97 (100%)	0	100	100
1	DB	97/97 (100%)	97 (100%)	0	100	100
1	DC	97/97 (100%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DE	97/97 (100%)	97 (100%)	0	100	100
1	DF	97/97 (100%)	97 (100%)	0	100	100
1	DG	97/97 (100%)	96 (99%)	1 (1%)	68	75
1	DI	97/97 (100%)	97 (100%)	0	100	100
1	DJ	97/97 (100%)	96 (99%)	1 (1%)	68	75
1	DK	97/97 (100%)	97 (100%)	0	100	100
1	DM	97/97 (100%)	97 (100%)	0	100	100
1	DN	97/97 (100%)	97 (100%)	0	100	100
1	DO	97/97 (100%)	97 (100%)	0	100	100
1	DQ	97/97 (100%)	97 (100%)	0	100	100
1	DR	97/97 (100%)	97 (100%)	0	100	100
1	DS	97/97 (100%)	97 (100%)	0	100	100
1	DU	97/97 (100%)	97 (100%)	0	100	100
1	DV	97/97 (100%)	97 (100%)	0	100	100
1	DW	97/97 (100%)	97 (100%)	0	100	100
1	DY	97/97 (100%)	97 (100%)	0	100	100
1	DZ	97/97 (100%)	96 (99%)	1 (1%)	68	75
1	EA	97/97 (100%)	97 (100%)	0	100	100
1	EC	97/97 (100%)	97 (100%)	0	100	100
1	ED	97/97 (100%)	97 (100%)	0	100	100
1	EE	97/97 (100%)	97 (100%)	0	100	100
1	EG	97/97 (100%)	97 (100%)	0	100	100
1	EH	97/97 (100%)	97 (100%)	0	100	100
1	EI	97/97 (100%)	97 (100%)	0	100	100
1	EK	97/97 (100%)	97 (100%)	0	100	100
1	EL	97/97 (100%)	97 (100%)	0	100	100
1	EM	97/97 (100%)	97 (100%)	0	100	100
1	EO	97/97 (100%)	97 (100%)	0	100	100
1	EP	97/97 (100%)	97 (100%)	0	100	100
1	EQ	97/97 (100%)	97 (100%)	0	100	100
1	ES	97/97 (100%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	ET	97/97 (100%)	97 (100%)	0	100	100
1	EU	97/97 (100%)	97 (100%)	0	100	100
1	EW	97/97 (100%)	97 (100%)	0	100	100
1	EX	97/97 (100%)	97 (100%)	0	100	100
1	EY	97/97 (100%)	97 (100%)	0	100	100
1	FA	97/97 (100%)	97 (100%)	0	100	100
1	FB	97/97 (100%)	97 (100%)	0	100	100
1	FC	97/97 (100%)	97 (100%)	0	100	100
1	FE	97/97 (100%)	97 (100%)	0	100	100
1	FF	97/97 (100%)	97 (100%)	0	100	100
1	FG	97/97 (100%)	96 (99%)	1 (1%)	68	75
1	FI	97/97 (100%)	97 (100%)	0	100	100
1	FJ	97/97 (100%)	96 (99%)	1 (1%)	68	75
1	FK	97/97 (100%)	97 (100%)	0	100	100
1	FM	97/97 (100%)	97 (100%)	0	100	100
1	FN	97/97 (100%)	97 (100%)	0	100	100
1	FO	97/97 (100%)	97 (100%)	0	100	100
1	FQ	97/97 (100%)	97 (100%)	0	100	100
1	FR	97/97 (100%)	97 (100%)	0	100	100
1	FS	97/97 (100%)	97 (100%)	0	100	100
1	FU	97/97 (100%)	97 (100%)	0	100	100
1	FV	97/97 (100%)	97 (100%)	0	100	100
1	FW	97/97 (100%)	97 (100%)	0	100	100
1	FY	97/97 (100%)	97 (100%)	0	100	100
1	FZ	97/97 (100%)	97 (100%)	0	100	100
1	GA	97/97 (100%)	96 (99%)	1 (1%)	68	75
1	GC	97/97 (100%)	97 (100%)	0	100	100
1	GD	97/97 (100%)	97 (100%)	0	100	100
1	GE	97/97 (100%)	97 (100%)	0	100	100
1	GG	97/97 (100%)	97 (100%)	0	100	100
1	GH	97/97 (100%)	96 (99%)	1 (1%)	68	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GI	97/97 (100%)	97 (100%)	0	100	100
1	GK	97/97 (100%)	97 (100%)	0	100	100
1	GL	97/97 (100%)	97 (100%)	0	100	100
1	GM	97/97 (100%)	97 (100%)	0	100	100
1	GO	97/97 (100%)	97 (100%)	0	100	100
1	GP	97/97 (100%)	97 (100%)	0	100	100
1	GQ	97/97 (100%)	96 (99%)	1 (1%)	68	75
1	GS	97/97 (100%)	97 (100%)	0	100	100
1	GT	97/97 (100%)	97 (100%)	0	100	100
1	GU	97/97 (100%)	97 (100%)	0	100	100
1	GW	97/97 (100%)	97 (100%)	0	100	100
1	GX	97/97 (100%)	96 (99%)	1 (1%)	68	75
1	GY	97/97 (100%)	97 (100%)	0	100	100
1	HA	97/97 (100%)	97 (100%)	0	100	100
1	HB	97/97 (100%)	97 (100%)	0	100	100
1	HC	97/97 (100%)	97 (100%)	0	100	100
1	HE	97/97 (100%)	97 (100%)	0	100	100
1	HF	97/97 (100%)	97 (100%)	0	100	100
1	HG	97/97 (100%)	97 (100%)	0	100	100
1	HI	97/97 (100%)	97 (100%)	0	100	100
1	HJ	97/97 (100%)	97 (100%)	0	100	100
1	HK	97/97 (100%)	97 (100%)	0	100	100
1	HM	97/97 (100%)	97 (100%)	0	100	100
1	HN	97/97 (100%)	96 (99%)	1 (1%)	68	75
1	HO	97/97 (100%)	97 (100%)	0	100	100
1	HQ	97/97 (100%)	97 (100%)	0	100	100
1	HR	97/97 (100%)	97 (100%)	0	100	100
1	HS	97/97 (100%)	97 (100%)	0	100	100
1	HU	97/97 (100%)	97 (100%)	0	100	100
1	HV	97/97 (100%)	97 (100%)	0	100	100
1	HW	97/97 (100%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	HY	97/97 (100%)	97 (100%)	0	100	100
1	HZ	97/97 (100%)	96 (99%)	1 (1%)	68	75
1	IA	97/97 (100%)	97 (100%)	0	100	100
1	IC	97/97 (100%)	97 (100%)	0	100	100
1	ID	97/97 (100%)	97 (100%)	0	100	100
1	IE	97/97 (100%)	96 (99%)	1 (1%)	68	75
1	IG	97/97 (100%)	97 (100%)	0	100	100
1	IH	97/97 (100%)	97 (100%)	0	100	100
1	II	97/97 (100%)	97 (100%)	0	100	100
1	IK	97/97 (100%)	97 (100%)	0	100	100
1	IL	97/97 (100%)	97 (100%)	0	100	100
1	IM	97/97 (100%)	97 (100%)	0	100	100
1	IO	97/97 (100%)	97 (100%)	0	100	100
1	IP	97/97 (100%)	96 (99%)	1 (1%)	68	75
1	IQ	97/97 (100%)	97 (100%)	0	100	100
1	IS	97/97 (100%)	97 (100%)	0	100	100
1	IT	97/97 (100%)	97 (100%)	0	100	100
1	IU	97/97 (100%)	97 (100%)	0	100	100
1	IW	97/97 (100%)	97 (100%)	0	100	100
1	IX	97/97 (100%)	97 (100%)	0	100	100
1	IY	97/97 (100%)	96 (99%)	1 (1%)	68	75
1	JA	97/97 (100%)	97 (100%)	0	100	100
1	JB	97/97 (100%)	97 (100%)	0	100	100
1	JC	97/97 (100%)	97 (100%)	0	100	100
1	JE	97/97 (100%)	97 (100%)	0	100	100
1	JF	97/97 (100%)	97 (100%)	0	100	100
All	All	17460/17460 (100%)	17441 (100%)	19 (0%)	87	87

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

Mol	Chain	Res	Type
1	HN	50	THR
1	IP	50	THR

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Mol	Chain	Res	Type
1	IY	8	LEU
1	IE	8	LEU
1	FG	75	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	EY	55	ASN
1	GQ	122	GLN
1	FV	55	ASN
1	GY	122	GLN
1	CT	55	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

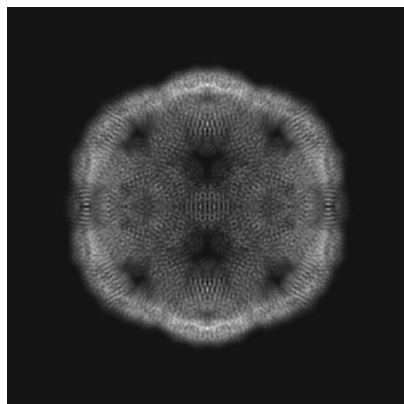
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52006. These allow visual inspection of the internal detail of the map and identification of artifacts.

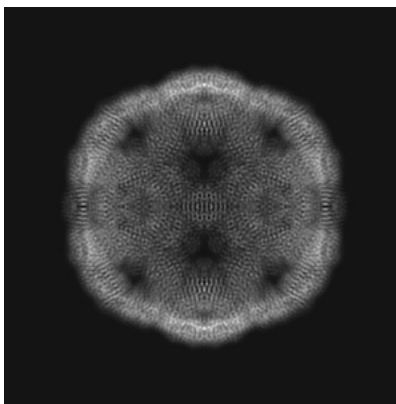
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

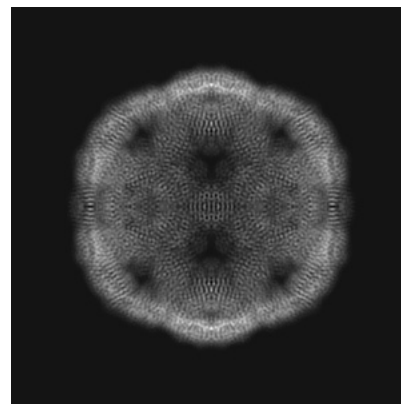
6.1.1 Primary map



X

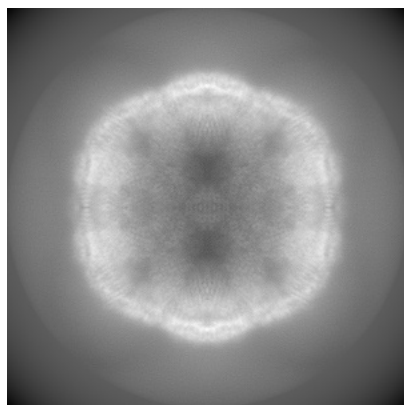


Y

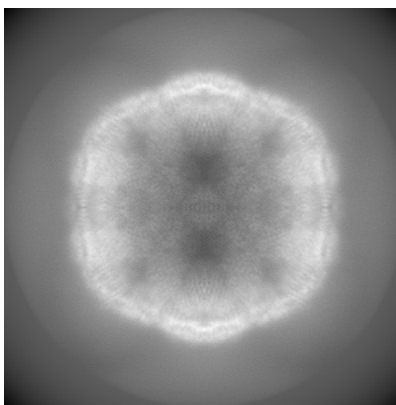


Z

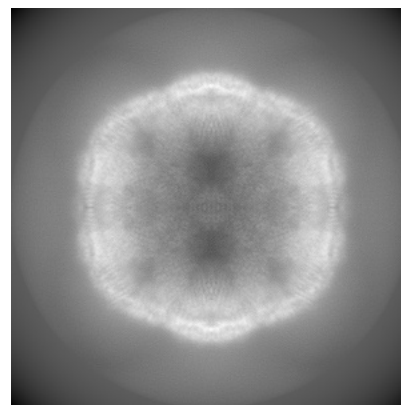
6.1.2 Raw map



X



Y

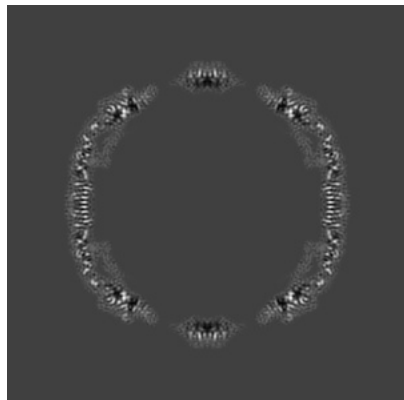


Z

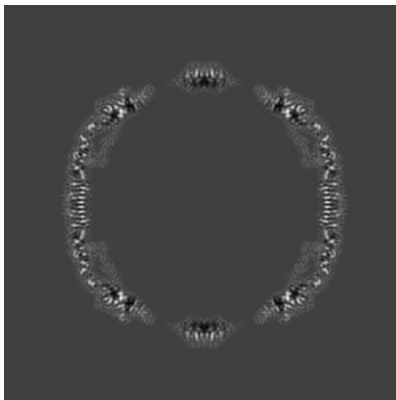
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

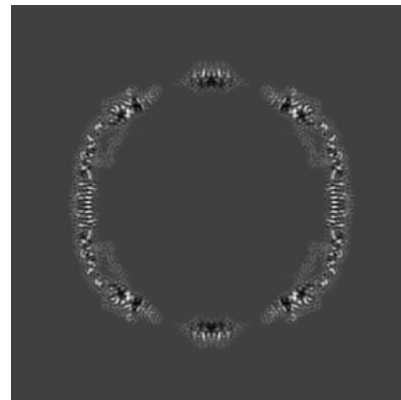
6.2.1 Primary map



X Index: 256

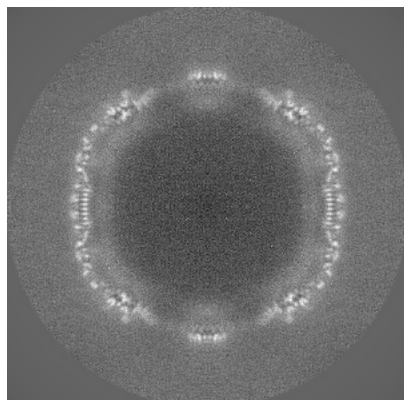


Y Index: 256

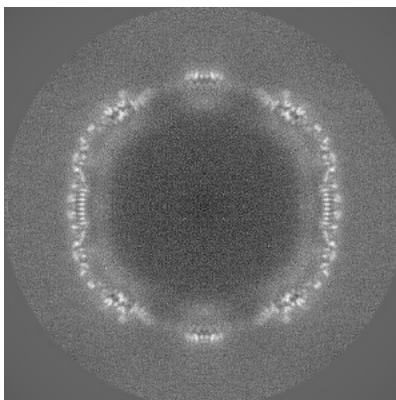


Z Index: 256

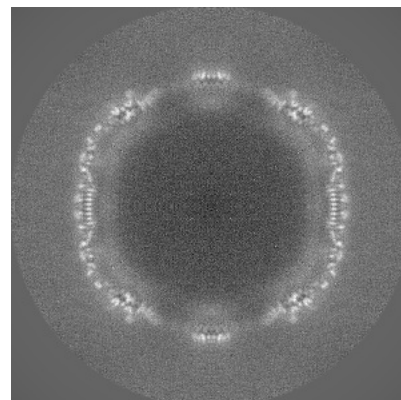
6.2.2 Raw map



X Index: 256



Y Index: 256

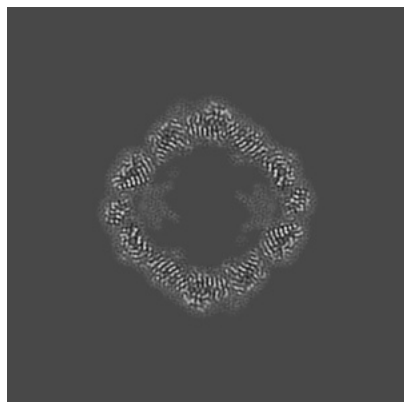


Z Index: 256

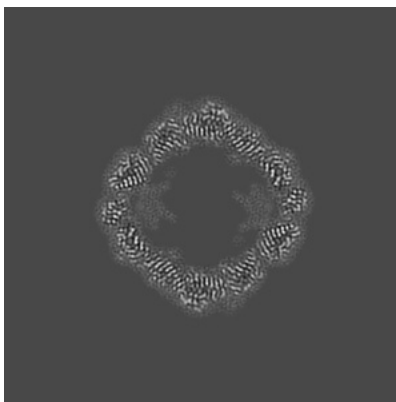
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

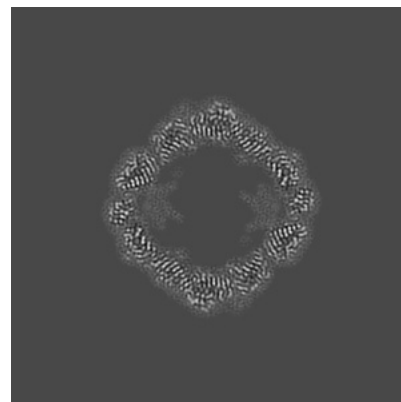
6.3.1 Primary map



X Index: 130

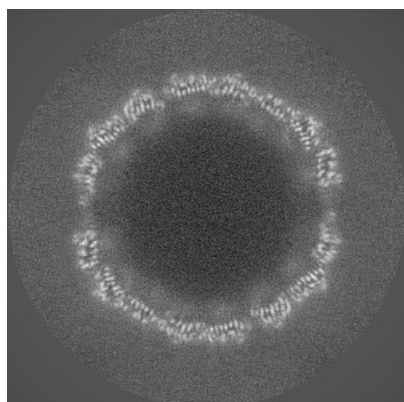


Y Index: 130

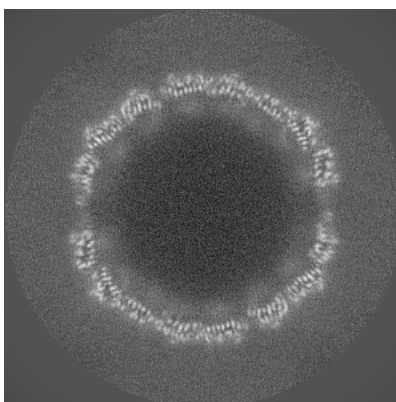


Z Index: 130

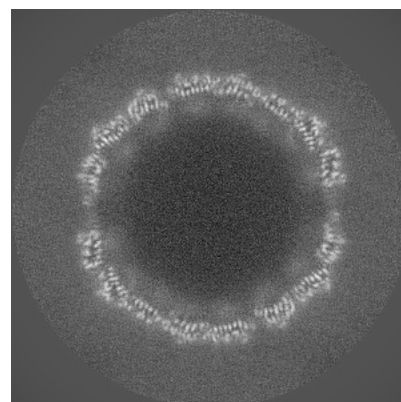
6.3.2 Raw map



X Index: 218



Y Index: 218

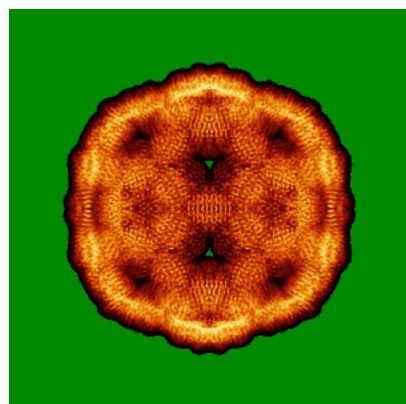


Z Index: 218

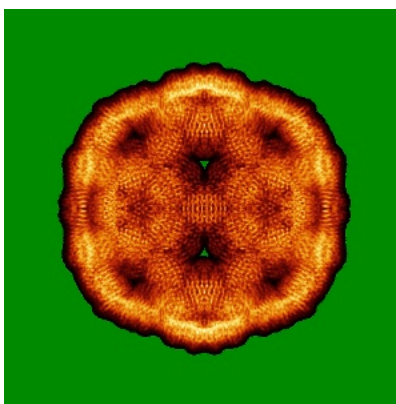
The images above show the largest variance slices of the map in three orthogonal directions.

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

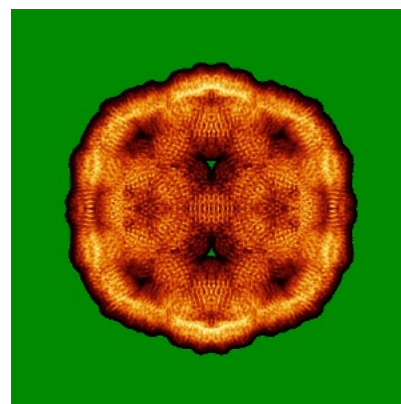
6.4.1 Primary map



X

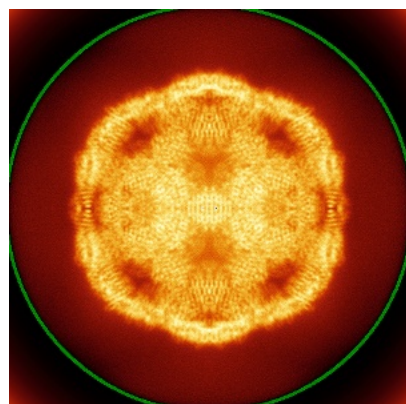


Y

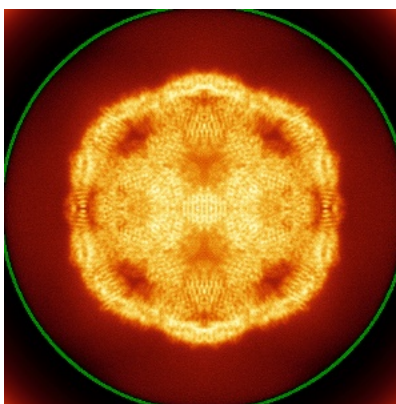


Z

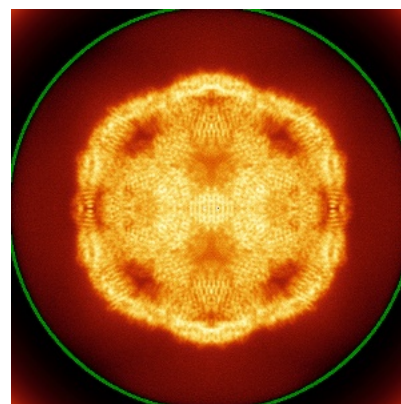
6.4.2 Raw map



X



Y

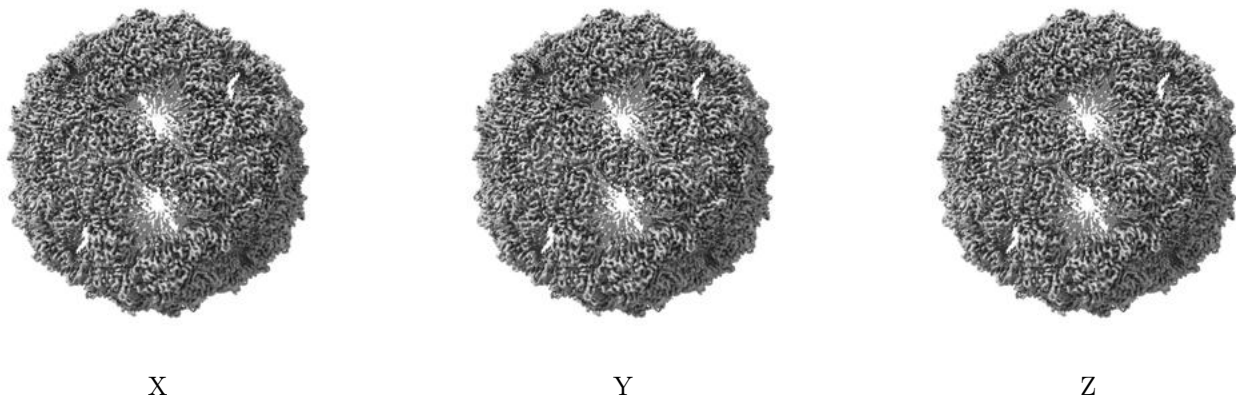


Z

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.

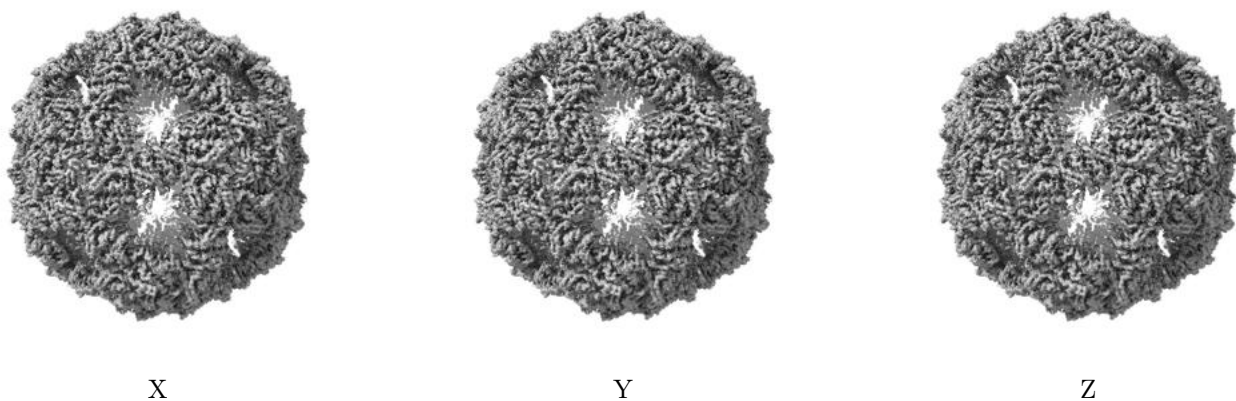
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.003. 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.

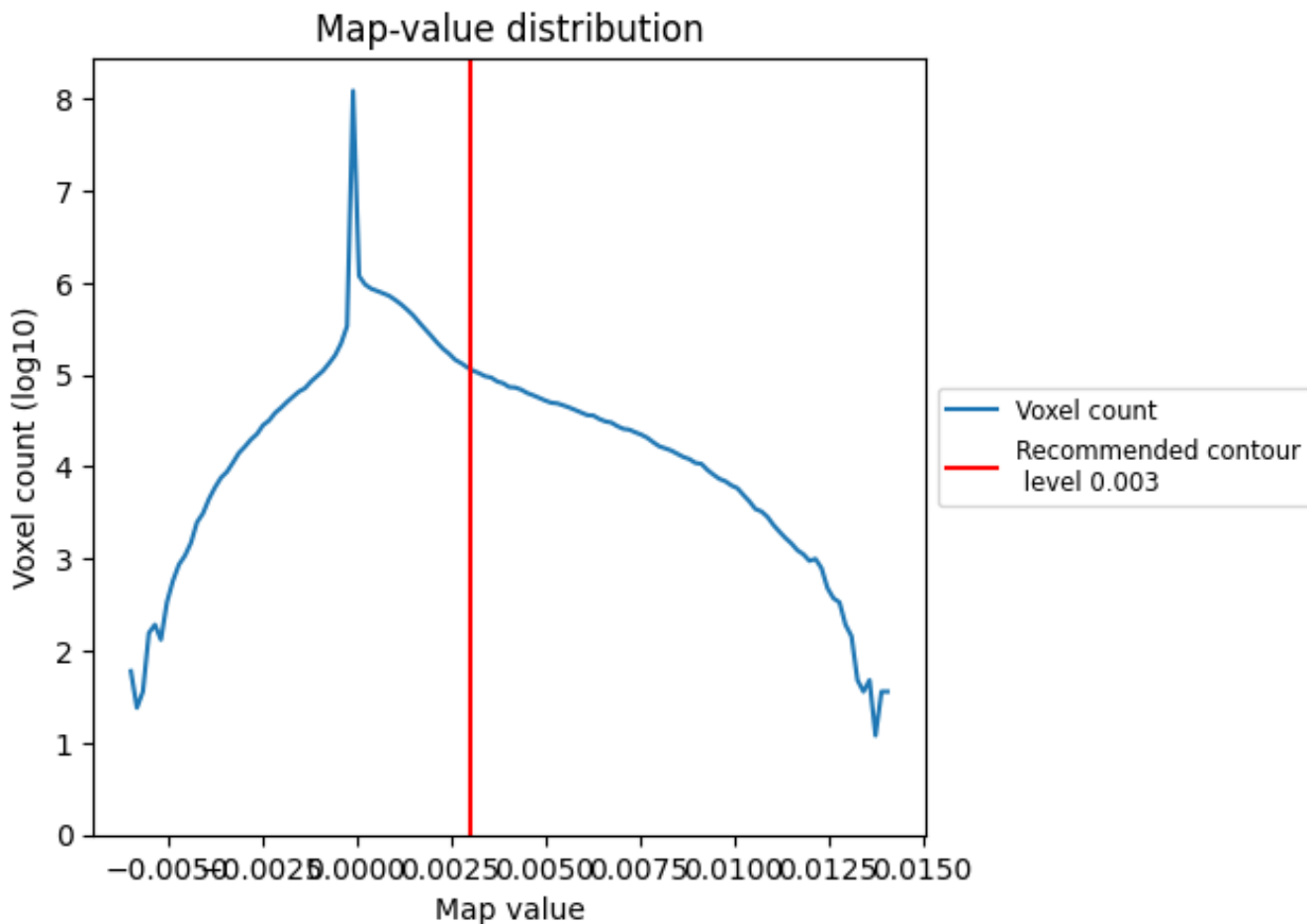
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

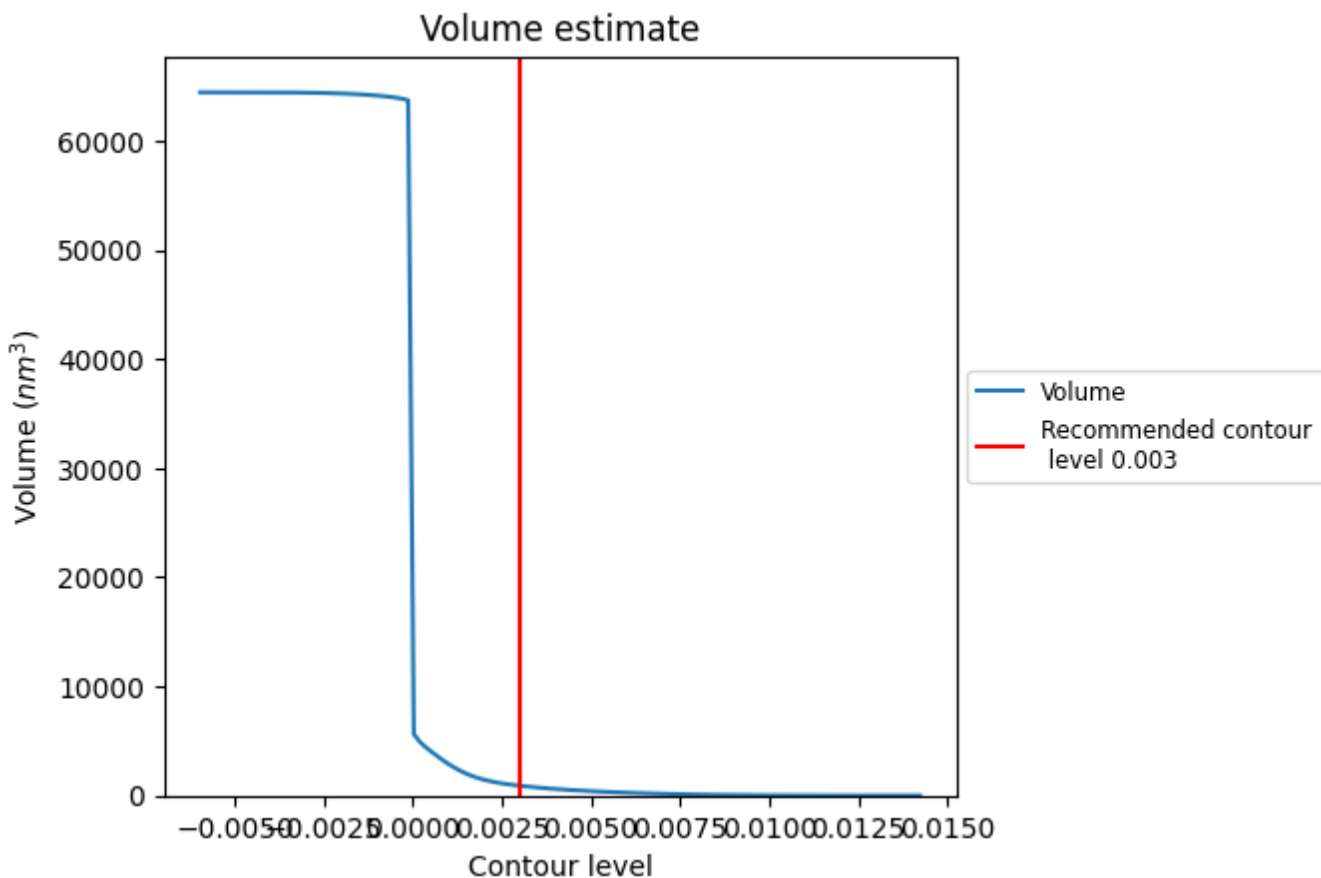
This section contains the results of statistical analysis of the map.

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.

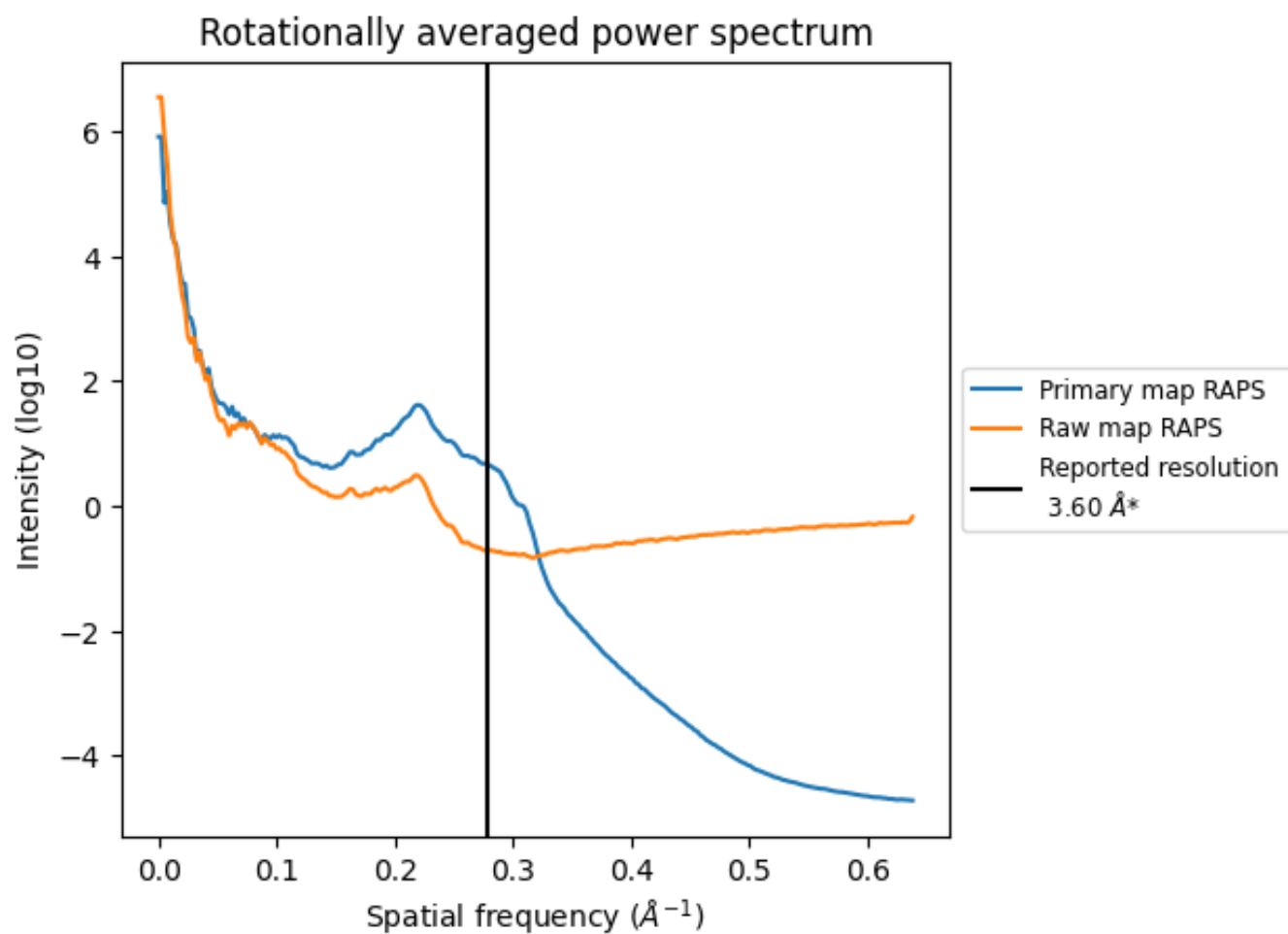
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 898 nm³; this corresponds to an approximate mass of 811 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

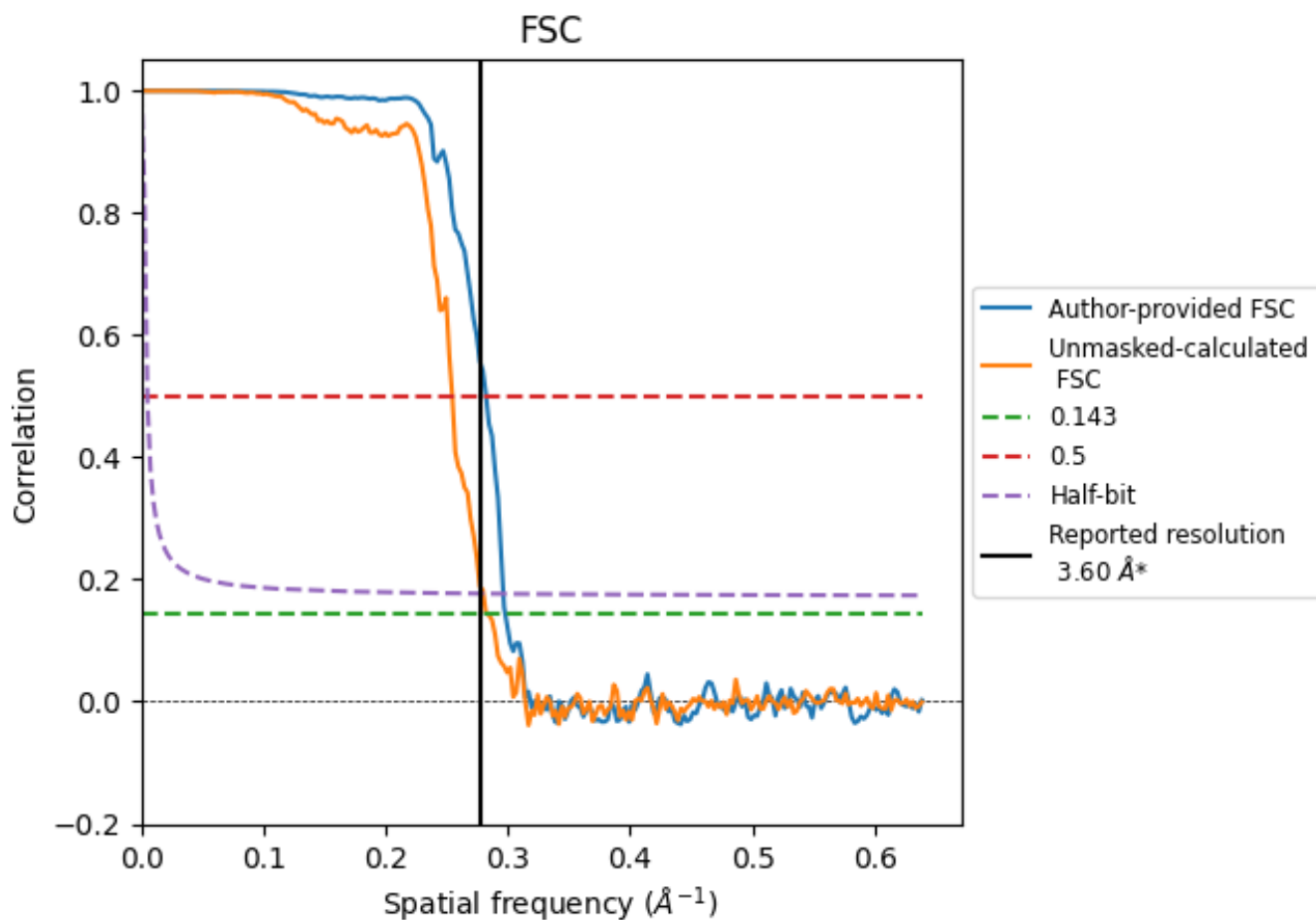


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

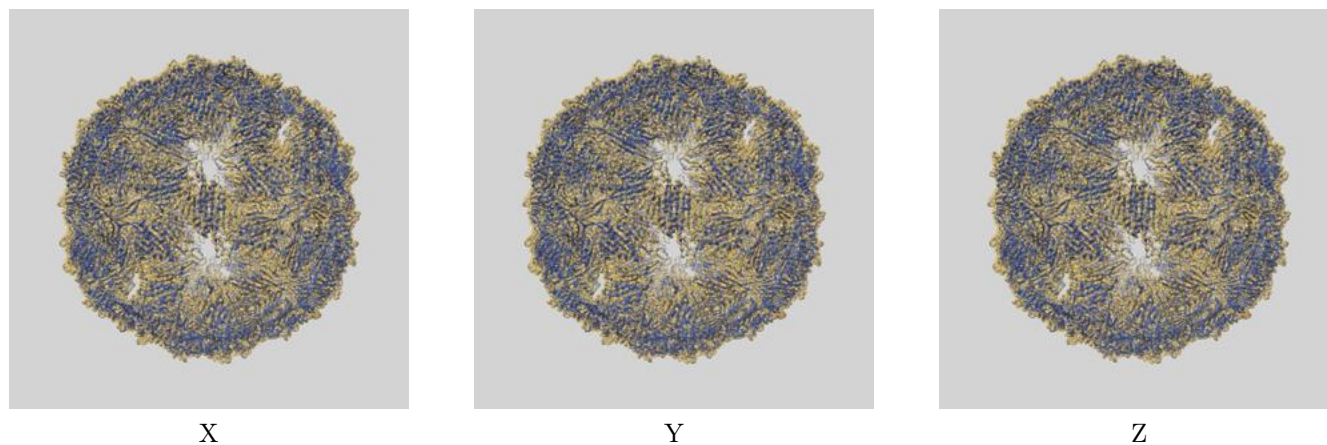
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.36	3.55	3.38
Unmasked-calculated*	3.53	3.93	3.57

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

9 Map-model fit [i](#)

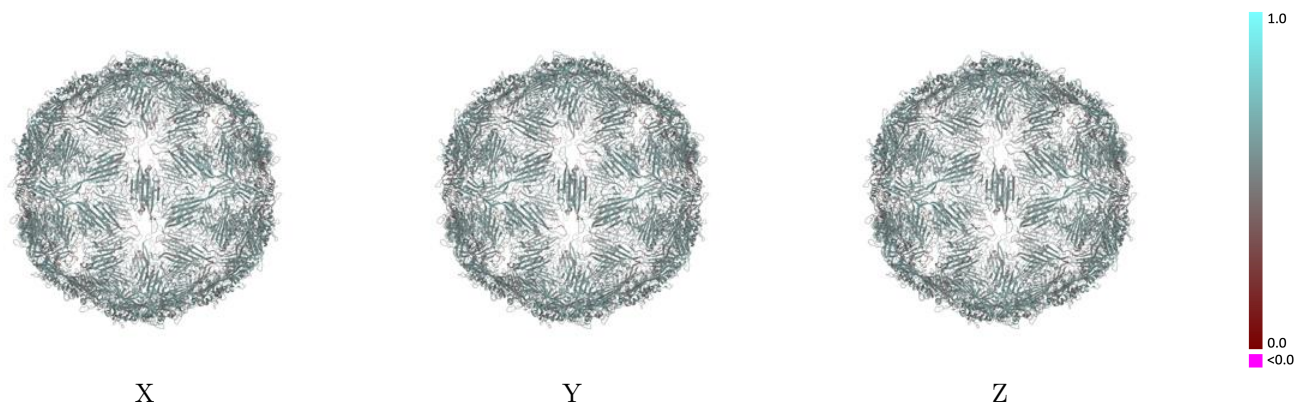
This section contains information regarding the fit between EMDB map EMD-52006 and PDB model 9HAT. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



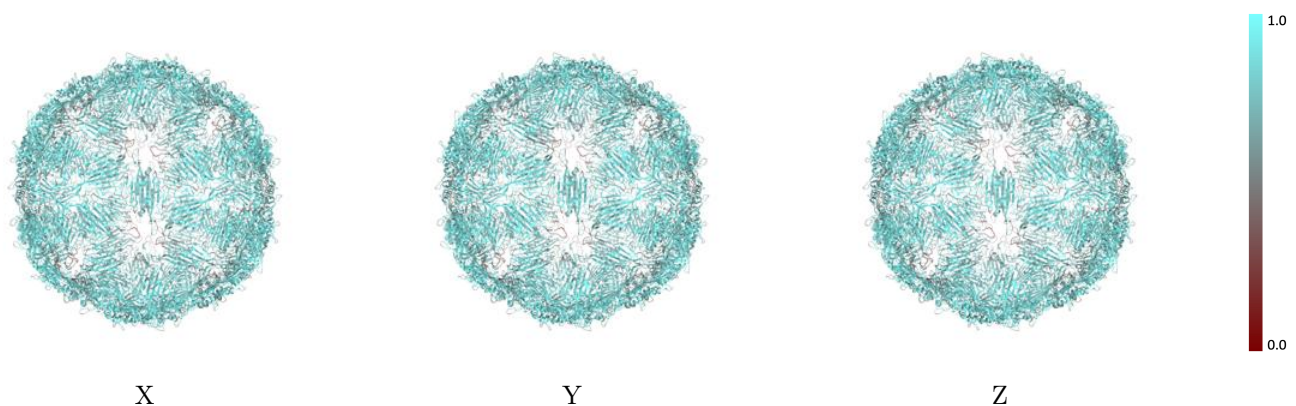
The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



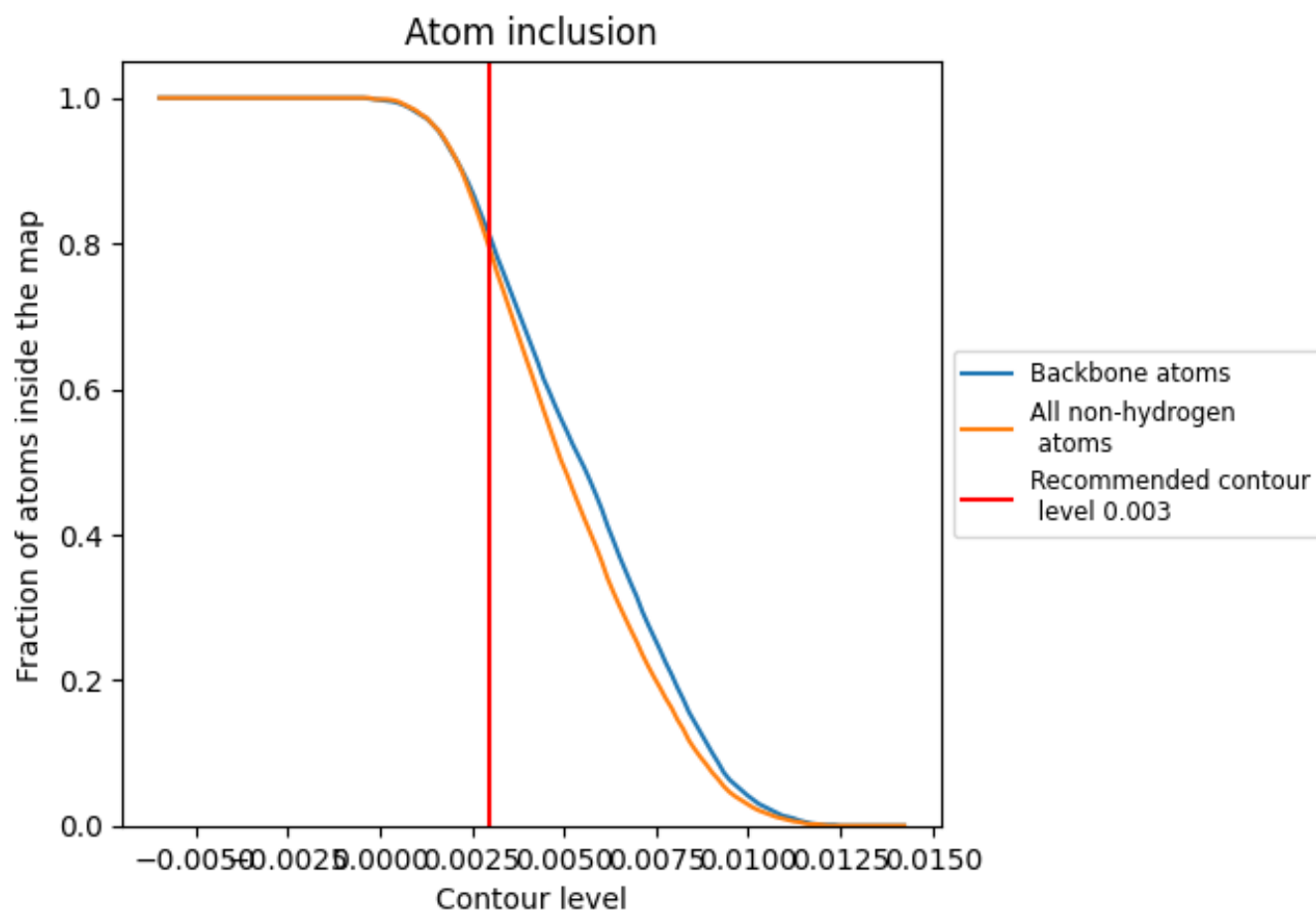
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.003).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 79% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7900	 0.5360
AA	 0.7680	 0.5300
AC	 0.8440	 0.5520
AD	 0.7580	 0.5220
AE	 0.7670	 0.5250
AG	 0.8460	 0.5560
AH	 0.7420	 0.5240
AI	 0.7710	 0.5290
AK	 0.8440	 0.5550
AL	 0.7460	 0.5220
AM	 0.7680	 0.5350
AO	 0.8440	 0.5550
AP	 0.7580	 0.5220
AQ	 0.7700	 0.5240
AS	 0.8510	 0.5530
AT	 0.7500	 0.5230
AU	 0.7730	 0.5280
AW	 0.8550	 0.5560
AX	 0.7540	 0.5250
AY	 0.7710	 0.5270
BA	 0.8440	 0.5560
BB	 0.7460	 0.5250
BC	 0.7680	 0.5270
BE	 0.8440	 0.5550
BF	 0.7580	 0.5200
BG	 0.7700	 0.5310
BI	 0.8510	 0.5570
BJ	 0.7500	 0.5220
BK	 0.7710	 0.5310
BM	 0.8440	 0.5550
BN	 0.7460	 0.5230
BO	 0.7730	 0.5300
BQ	 0.8550	 0.5550
BR	 0.7540	 0.5260
BS	 0.7670	 0.5230























































































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Chain	Atom inclusion	Q-score
BU	 0.8460	 0.5510
BV	 0.7420	 0.5200
BW	 0.7700	 0.5270
BY	 0.8510	 0.5560
BZ	 0.7500	 0.5220
CA	 0.7710	 0.5330
CC	 0.8440	 0.5590
CD	 0.7460	 0.5250
CE	 0.7730	 0.5270
CG	 0.8550	 0.5510
CH	 0.7540	 0.5220
CI	 0.7700	 0.5280
CK	 0.8510	 0.5550
CL	 0.7500	 0.5210
CM	 0.7670	 0.5200
CO	 0.8470	 0.5520
CP	 0.7420	 0.5180
CQ	 0.7680	 0.5310
CS	 0.8440	 0.5590
CT	 0.7580	 0.5270
CU	 0.7730	 0.5310
CW	 0.8550	 0.5530
CX	 0.7540	 0.5220
CY	 0.7710	 0.5290
DA	 0.8520	 0.5520
DB	 0.7500	 0.5170
DC	 0.7620	 0.5260
DE	 0.8470	 0.5590
DF	 0.7420	 0.5270
DG	 0.7730	 0.5330
DI	 0.8550	 0.5550
DJ	 0.7540	 0.5230
DK	 0.7650	 0.5280
DM	 0.8440	 0.5580
DN	 0.7580	 0.5260
DO	 0.7710	 0.5260
DQ	 0.8440	 0.5520
DR	 0.7460	 0.5160
DS	 0.7620	 0.5290
DU	 0.8470	 0.5550
DV	 0.7420	 0.5240
DW	 0.7730	 0.5270





















































































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Chain	Atom inclusion	Q-score
DY	 0.8550	 0.5560
DZ	 0.7540	 0.5270
EA	 0.7680	 0.5290
EC	 0.8440	 0.5530
ED	 0.7580	 0.5230
EE	 0.7670	 0.5290
EG	 0.8470	 0.5530
EH	 0.7420	 0.5220
EI	 0.7710	 0.5280
EK	 0.8440	 0.5520
EL	 0.7460	 0.5200
EM	 0.7700	 0.5250
EO	 0.8510	 0.5560
EP	 0.7500	 0.5250
EQ	 0.7650	 0.5290
ES	 0.8440	 0.5520
ET	 0.7590	 0.5210
EU	 0.7710	 0.5300
EW	 0.8440	 0.5570
EX	 0.7460	 0.5240
EY	 0.7620	 0.5260
FA	 0.8470	 0.5570
FB	 0.7420	 0.5250
FC	 0.7650	 0.5340
FE	 0.8440	 0.5540
FF	 0.7580	 0.5220
FG	 0.7730	 0.5270
FI	 0.8550	 0.5530
FJ	 0.7540	 0.5230
FK	 0.7710	 0.5280
FM	 0.8510	 0.5550
FN	 0.7500	 0.5230
FO	 0.7620	 0.5310
FQ	 0.8500	 0.5560
FR	 0.7430	 0.5230
FS	 0.7690	 0.5300
FU	 0.8430	 0.5560
FV	 0.7620	 0.5200
FW	 0.7730	 0.5290
FY	 0.8570	 0.5560
FZ	 0.7560	 0.5250
GA	 0.7680	 0.5340









































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Chain	Atom inclusion	Q-score
GC	 0.8510	 0.5550
GD	 0.7430	 0.5210
GE	 0.7760	 0.5310
GG	 0.8530	 0.5550
GH	 0.7520	 0.5270
GI	 0.7770	 0.5290
GK	 0.8490	 0.5550
GL	 0.7520	 0.5200
GM	 0.7730	 0.5300
GO	 0.8570	 0.5530
GP	 0.7560	 0.5250
GQ	 0.7680	 0.5290
GS	 0.8510	 0.5580
GT	 0.7430	 0.5280
GU	 0.7760	 0.5290
GW	 0.8530	 0.5510
GX	 0.7520	 0.5190
GY	 0.7730	 0.5350
HA	 0.8570	 0.5530
HB	 0.7560	 0.5240
HC	 0.7770	 0.5260
HE	 0.8490	 0.5510
HF	 0.7520	 0.5170
HG	 0.7690	 0.5290
HI	 0.8430	 0.5580
HJ	 0.7610	 0.5280
HK	 0.7760	 0.5300
HM	 0.8530	 0.5550
HN	 0.7520	 0.5230
HO	 0.7730	 0.5300
HQ	 0.8570	 0.5530
HR	 0.7560	 0.5250
HS	 0.7770	 0.5330
HU	 0.8490	 0.5560
HV	 0.7520	 0.5250
HW	 0.7760	 0.5340
HY	 0.8530	 0.5530
HZ	 0.7520	 0.5220
IA	 0.7690	 0.5310
IC	 0.8430	 0.5580
ID	 0.7610	 0.5280
IE	 0.7680	 0.5220

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Chain	Atom inclusion	Q-score
IG	 0.8510	 0.5530
IH	 0.7430	 0.5200
II	 0.7770	 0.5290
IK	 0.8490	 0.5570
IL	 0.7520	 0.5250
IM	 0.7760	 0.5340
IO	 0.8530	 0.5540
IP	 0.7520	 0.5240
IQ	 0.7690	 0.5280
IS	 0.8430	 0.5550
IT	 0.7610	 0.5230
IU	 0.7770	 0.5330
IW	 0.8490	 0.5550
IX	 0.7520	 0.5210
IY	 0.7680	 0.5220
JA	 0.8510	 0.5520
JB	 0.7430	 0.5220
JC	 0.7730	 0.5310
JE	 0.8570	 0.5550
JF	 0.7560	 0.5250