



wwPDB EM Validation Summary Report ⓘ

Nov 11, 2023 – 11:27 pm GMT

PDB ID : 8PKH
EMDB ID : EMD-17739
Title : Borrelia bacteriophage BB1 procapsid, fivefold-symmetrized outer shell
Authors : Rumnieks, J.; Fuzik, T.; Tars, K.
Deposited on : 2023-06-26
Resolution : 3.35 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.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

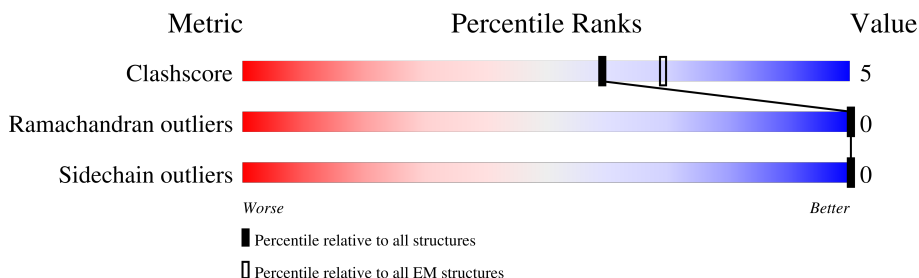
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.35 Å.

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




























Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	AA	319	
1	AB	319	
1	AC	319	
1	AD	319	
1	AE	319	
1	AF	319	
1	AG	319	
1	AH	319	


























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Mol	Chain	Length	Quality of chain
1	AI	319	 87% 12%
1	AJ	319	 82% 15%
1	AK	319	 83% 15%
1	AL	319	 84% 14%
1	AM	319	 83% 13%
1	AN	319	 83% 15%
1	AO	319	 83% 15%
1	AP	319	 81% 16%
1	AQ	319	 86% 12%
1	AR	319	 84% 14%
1	AS	319	 78% 20%
1	AT	319	 81% 17%
1	AU	319	 81% 18%
1	AV	319	 79% 19%
1	AW	319	 85% 13%
1	AX	319	 81% 18%
1	AY	319	 81% 17%
1	AZ	319	 82% 16%
1	BA	319	 79% 19%
1	BB	319	 85% 13%
1	BC	319	 83% 11% 6%
1	BD	319	 85% 12%
1	BE	319	 87% 11%
1	BF	319	 87% 12%
1	BG	319	 84% 13%







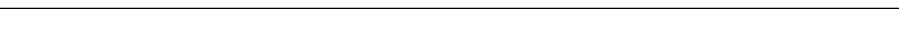
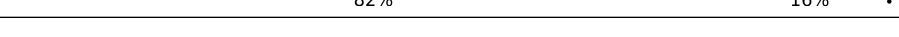
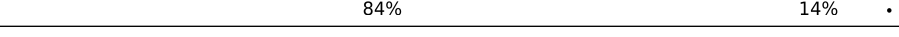












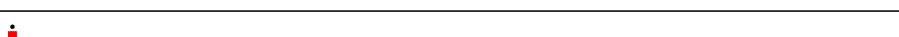

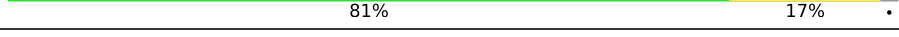

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Mol	Chain	Length	Quality of chain
1	BH	319	 85% 13%
1	BI	319	 86% 12%
1	BJ	319	 83% 14%
1	BK	319	 83% 15%
1	BL	319	 87% 11%
1	BM	319	 85% 13%
1	BN	319	 88% 10%
1	BO	319	 85% 13%
1	BP	319	 82% 15%
1	BQ	319	 86% 12%
1	BR	319	 84% 14%
1	BS	319	 82% 16%
1	BT	319	 81% 13% 7%
1	BU	319	 82% 17%
1	BV	319	 83% 15%
1	BW	319	 87% 11%
1	BX	319	 82% 11% 7%
1	BY	319	 78% 20%
1	BZ	319	 83% 15%
1	CA	319	 81% 18%
1	CB	319	 82% 16%
1	CC	319	 85% 13%
1	CD	319	 84% 14%
1	CE	319	 84% 14%
1	CF	319	 80% 18%


























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Mol	Chain	Length	Quality of chain
1	CG	319	 82% 16%
1	CH	319	 82% 17%
1	CI	319	 87% 11%
1	CJ	319	 86% 12%
1	CK	319	 80% 18%
1	CL	319	 80% 18%
1	CM	319	 82% 16%
1	CN	319	 84% 14%
1	CO	319	 79% 19%
1	CP	319	 81% 17%
1	CQ	319	 84% 14%
1	CR	319	 85% 13%
1	CS	319	 83% 15%
1	CT	319	 83% 15%
1	CU	319	 78% 20%
1	CV	319	 81% 18%
1	CW	319	 82% 17%
1	CX	319	 86% 12%
1	CY	319	 86% 12%
1	CZ	319	 82% 16%
1	DA	319	 81% 17%
1	DB	319	 84% 14%
1	DC	319	 83% 15%
1	DD	319	 80% 18%
1	DE	319	 82% 16%


























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Mol	Chain	Length	Quality of chain
2	DF	185	 78% 6% 16%
2	DG	185	 75% 8% 18%
2	DH	185	 75% 8% 17%
2	DI	185	 77% 5% 17%
2	DJ	185	 72% 11% 17%
2	DK	185	 72% 11% 17%
2	DL	185	 74% 9% 17%
2	DM	185	 73% 10% 17%
2	DN	185	 72% 11% 17%
2	DO	185	 74% 9% 17%
2	DP	185	 69% 14% 17%
2	DQ	185	 73% 9% 18%
2	DR	185	 75% 9% 17%
2	DS	185	 81% 10% 9%
2	DT	185	 65% 18% 17%
2	DU	185	 71% 11% 17%
2	DV	185	 70% 12% 17%
2	DW	185	 71% 11% 17%
2	DX	185	 75% 10% 15%
2	DY	185	 69% 13% 18%
2	DZ	185	 73% 10% 17%
2	EA	185	 57% 8% 35%
2	EB	185	 72% 13% 15%
2	EC	185	 73% 10% 17%
2	ED	185	 79% 7% 14%

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Mol	Chain	Length	Quality of chain
2	EE	185	 75% 10% 15%
2	EF	185	 72% 11% 17%
2	EG	185	 82% 13% 5%
2	EH	185	 72% 10% 17%
2	EI	185	 75% 10% 15%
2	EJ	185	 83% 7% 10%
2	EK	185	 78% 13% 9%
2	EL	185	 73% 9% 18%
2	EM	185	 68% 16% 17%
2	EN	185	 70% 13% 17%
2	EO	185	 82% 10% 8%
2	EP	185	 68% 15% 17%
2	EQ	185	 77% 8% 15%
2	ER	185	 68% 14% 18%
2	ES	185	 74% 10% 17%
2	ET	185	 69% 14% 17%
2	EU	185	 74% 12% 15%
2	EV	185	 69% 12% 18%
2	EW	185	 73% 10% 17%
2	EX	185	 72% 11% 17%
2	EY	185	 76% 10% 15%
2	EZ	185	 71% 10% 18%
2	FA	185	 74% 10% 17%
2	FB	185	 70% 12% 17%
2	FC	185	 76% 10% 15%

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Mol	Chain	Length	Quality of chain
2	FD	185	68% 14% 18%
2	FE	185	72% 11% 17%
2	FF	185	72% 11% 17%
2	FG	185	73% 12% 15%
2	FH	185	69% 12% 18%
2	FI	185	74% 9% 17%
3	FJ	254	55% 9% 37%
4	FK	190	71% 9% 20%
4	FL	190	70% 10% 20%
4	FM	190	72% 9% 19%
4	FN	190	68% 12% 20%
4	FO	190	71% 12% 18%
4	FP	190	68% 12% 20%
4	FQ	190	75% 15% 10%
4	FR	190	5% 77% 13% 10%
4	FS	190	74% 16% 10%
4	FT	190	67% 8% 24%
4	FU	190	69% 11% 21%
4	FV	190	71% 10% 19%
4	FW	190	66% 15% 19%
4	FX	190	71% 9% 21%
4	FY	190	68% 11% 21%
4	FZ	190	66% 14% 20%
4	GA	190	77% 13% 10%
4	GB	190	77% 13% 10%








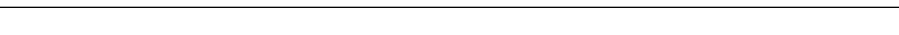
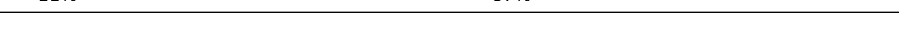
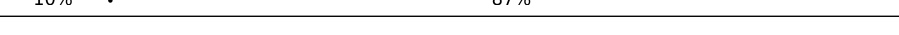
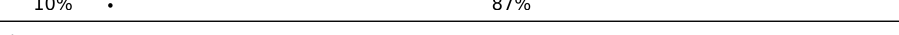
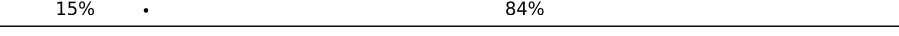













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Mol	Chain	Length	Quality of chain
4	GC	190	75% 15% 10%
4	GD	190	74% 16% 10%
4	GE	190	76% 14% 10%
4	GF	190	77% 13% 10%
4	GG	190	74% 16% 10%
4	GH	190	74% 16% 10%
4	GI	190	75% 15% 10%
4	GJ	190	77% 13% 10%
5	GK	230	12% 87%
5	GL	230	13% 84%
5	GM	230	14% 84%
5	GN	230	15% 84%
5	GO	230	15% 84%
5	GP	230	16% 84%
5	GQ	230	13% 84%
5	GR	230	16% 84%
5	GS	230	14% 84%
5	GT	230	16% 84%
5	GU	230	14% 84%
5	GV	230	15% 84%
5	GW	230	12% 87%
5	GX	230	13% 84%
5	GY	230	13% 84%
5	GZ	230	14% 84%
5	HA	230	15% 84%


























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Mol	Chain	Length	Quality of chain	
5	HB	230		84%
5	HC	230		84%
5	HD	230		87%
5	HE	230		84%
5	HF	230		84%
5	HG	230		84%
5	HH	230		87%
5	HI	230		87%
5	HJ	230		87%
5	HK	230		87%
5	HL	230		84%
5	HM	230		87%
5	HN	230		84%
5	HO	230		84%
5	HP	230		84%
5	HQ	230		84%
5	HR	230		84%
5	HS	230		84%
5	HT	230		84%
5	HU	230		84%
5	HV	230		84%
5	HW	230		88%
5	HX	230		84%
5	HY	230		84%
5	HZ	230		84%














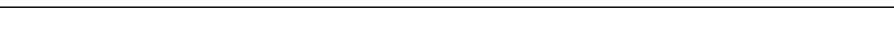
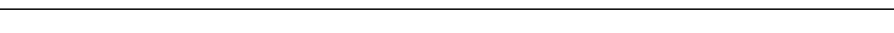
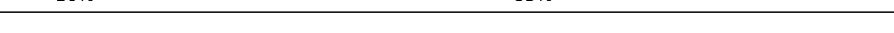
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Mol	Chain	Length	Quality of chain	
5	IA	230		84%
5	IB	230		87%
5	IC	230		84%
5	ID	230		87%
5	IE	230		84%
5	IF	230		84%
5	IG	230		84%
5	IH	230		87%
5	II	230		87%
5	IJ	230		87%
5	IK	230		87%
5	IL	230		83%
5	IM	230		84%
5	IN	230		84%
5	IO	230		83%
5	IP	230		84%
5	IQ	230		84%
5	IR	230		83%
5	IS	230		84%
5	IT	230		84%
5	IU	230		83%
5	IV	230		84%
5	IW	230		84%
5	IX	230		84%
5	IY	230		83%

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Mol	Chain	Length	Quality of chain	
5	IZ	230		84%
5	JA	230		83%
5	JB	230		84%
5	JC	230		84%
5	JD	230		83%
5	JE	230		84%
5	JF	230		84%
5	JG	230		83%
5	JH	230		84%
5	JI	230		84%
5	JJ	230		83%
5	JK	230		84%
5	JL	230		84%
5	JM	230		84%
5	JN	230		83%
5	JO	230		84%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 333778 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AA	309	2488	1604	400	475	9	0	0
1	AB	313	2510	1616	404	481	9	0	0
1	AC	313	2510	1616	404	481	9	0	0
1	AD	309	2488	1604	400	475	9	0	0
1	AE	313	2510	1616	404	481	9	0	0
1	AF	313	2510	1616	404	481	9	0	0
1	AG	309	2488	1604	400	475	9	0	0
1	AH	313	2510	1616	404	481	9	0	0
1	AI	313	2510	1616	404	481	9	0	0
1	AJ	309	2488	1604	400	475	9	0	0
1	AK	313	2510	1616	404	481	9	0	0
1	AL	313	2510	1616	404	481	9	0	0
1	AM	309	2488	1604	400	475	9	0	0
1	AN	313	2510	1616	404	481	9	0	0
1	AO	313	2510	1616	404	481	9	0	0
1	AP	309	2488	1604	400	475	9	0	0
1	AQ	313	2510	1616	404	481	9	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AR	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	AS	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	AT	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	AU	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	AV	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	AW	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	AX	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	AY	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	AZ	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	BA	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	BB	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	BC	300	Total	C	N	O	S	0	0
			2405	1549	390	457	9		
1	BD	309	Total	C	N	O	S	0	0
			2488	1604	400	475	9		
1	BE	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	BF	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	BG	309	Total	C	N	O	S	0	0
			2488	1604	400	475	9		
1	BH	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	BI	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	BJ	309	Total	C	N	O	S	0	0
			2488	1604	400	475	9		
1	BK	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	BL	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	BM	311	Total	C	N	O	S	0	0
			2505	1614	402	479	10		
1	BN	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	BO	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	BP	309	Total	C	N	O	S	0	0
			2488	1604	400	475	9		
1	BQ	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	BR	311	Total	C	N	O	S	0	0
			2505	1614	402	479	10		
1	BS	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	BT	297	Total	C	N	O	S	0	0
			2383	1532	385	457	9		
1	BU	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	BV	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	BW	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	BX	297	Total	C	N	O	S	0	0
			2383	1532	385	457	9		
1	BY	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	BZ	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CA	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CB	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CC	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CD	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CE	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CF	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CG	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	CH	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CI	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CJ	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CK	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CL	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CM	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CN	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CO	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CP	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CQ	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CR	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CS	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CT	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CU	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CV	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CW	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CX	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CY	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	CZ	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	DA	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	DB	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	DC	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	DD	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		
1	DE	313	Total	C	N	O	S	0	0
			2510	1616	404	481	9		

- Molecule 2 is a protein called Decorator protein P03.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	DF	155	Total	C	N	O	S	0	0
			1178	742	197	235	4		
2	DG	152	Total	C	N	O	S	0	0
			1160	730	194	232	4		
2	DH	154	Total	C	N	O	S	0	0
			1173	739	196	234	4		
2	DI	153	Total	C	N	O	S	0	0
			1165	733	195	233	4		
2	DJ	154	Total	C	N	O	S	0	0
			1173	739	196	234	4		
2	DK	153	Total	C	N	O	S	0	0
			1165	733	195	233	4		
2	DL	154	Total	C	N	O	S	0	0
			1173	739	196	234	4		
2	DM	154	Total	C	N	O	S	0	0
			1170	736	196	234	4		
2	DN	154	Total	C	N	O	S	0	0
			1173	739	196	234	4		
2	DO	153	Total	C	N	O	S	0	0
			1165	733	195	233	4		
2	DP	153	Total	C	N	O	S	0	0
			1165	733	195	233	4		
2	DQ	152	Total	C	N	O	S	0	0
			1160	730	194	232	4		
2	DR	154	Total	C	N	O	S	0	0
			1173	739	196	234	4		
2	DS	168	Total	C	N	O	S	0	0
			1288	813	215	256	4		
2	DT	154	Total	C	N	O	S	0	0
			1173	739	196	234	4		
2	DU	153	Total	C	N	O	S	0	0
			1161	730	194	233	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	DV	153	Total	C	N	O	S	0	0
			1165	733	195	233	4		
2	DW	153	Total	C	N	O	S	0	0
			1161	730	194	233	4		
2	DX	158	Total	C	N	O	S	0	0
			1198	750	202	242	4		
2	DY	151	Total	C	N	O	S	0	0
			1148	721	192	231	4		
2	DZ	154	Total	C	N	O	S	0	0
			1173	739	196	234	4		
2	EA	120	Total	C	N	O	S	0	0
			917	584	151	180	2		
2	EB	158	Total	C	N	O	S	0	0
			1198	750	202	242	4		
2	EC	153	Total	C	N	O	S	0	0
			1164	733	194	233	4		
2	ED	160	Total	C	N	O	S	0	0
			1211	759	204	244	4		
2	EE	158	Total	C	N	O	S	0	0
			1194	747	201	242	4		
2	EF	154	Total	C	N	O	S	0	0
			1173	739	196	234	4		
2	EG	175	Total	C	N	O	S	0	0
			1337	840	225	268	4		
2	EH	153	Total	C	N	O	S	0	0
			1165	733	195	233	4		
2	EI	157	Total	C	N	O	S	0	0
			1189	744	200	241	4		
2	EJ	166	Total	C	N	O	S	0	0
			1275	804	213	254	4		
2	EK	168	Total	C	N	O	S	0	0
			1288	813	215	256	4		
2	EL	152	Total	C	N	O	S	0	0
			1160	730	194	232	4		
2	EM	154	Total	C	N	O	S	0	0
			1173	739	196	234	4		
2	EN	153	Total	C	N	O	S	0	0
			1165	733	195	233	4		
2	EO	170	Total	C	N	O	S	0	0
			1304	823	218	259	4		
2	EP	153	Total	C	N	O	S	0	0
			1161	730	194	233	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	EQ	158	1198	750	202	242	4	0	0
2	ER	151	1148	721	192	231	4	0	0
2	ES	154	1173	739	196	234	4	0	0
2	ET	153	1161	730	194	233	4	0	0
2	EU	158	1198	750	202	242	4	0	0
2	EV	151	1148	721	192	231	4	0	0
2	EW	154	1173	739	196	234	4	0	0
2	EX	153	1161	730	194	233	4	0	0
2	EY	158	1198	750	202	242	4	0	0
2	EZ	151	1148	721	192	231	4	0	0
2	FA	154	1173	739	196	234	4	0	0
2	FB	153	1161	730	194	233	4	0	0
2	FC	158	1198	750	202	242	4	0	0
2	FD	151	1148	721	192	231	4	0	0
2	FE	154	1173	739	196	234	4	0	0
2	FF	153	1161	730	194	233	4	0	0
2	FG	158	1198	750	202	242	4	0	0
2	FH	151	1148	721	192	231	4	0	0
2	FI	154	1173	739	196	234	4	0	0

- Molecule 3 is a protein called Decorator protein P04.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	FJ	161	1252	801	199	245	7	0	0

- Molecule 4 is a protein called Decorator protein P05.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	FK	152	1195	761	203	229	2	0	0
4	FL	152	1195	761	203	229	2	0	0
4	FM	153	1203	767	203	231	2	0	0
4	FN	152	1197	764	202	229	2	0	0
4	FO	156	1222	776	208	235	3	0	0
4	FP	152	1191	758	202	229	2	0	0
4	FQ	171	1358	865	231	260	2	0	0
4	FR	171	1358	865	231	260	2	0	0
4	FS	171	1358	865	231	260	2	0	0
4	FT	144	1137	726	191	218	2	0	0
4	FU	151	1187	755	201	229	2	0	0
4	FV	154	1208	769	205	231	3	0	0
4	FW	154	1208	769	205	231	3	0	0
4	FX	151	1186	755	201	228	2	0	0
4	FY	151	1186	755	201	228	2	0	0
4	FZ	152	1195	761	203	229	2	0	0
4	GA	171	1358	865	231	260	2	0	0
4	GB	171	1358	865	231	260	2	0	0
4	GC	171	1358	865	231	260	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	GD	171	Total	C	N	O	S	0	0
			1358	865	231	260	2		
4	GE	171	Total	C	N	O	S	0	0
			1358	865	231	260	2		
4	GF	171	Total	C	N	O	S	0	0
			1358	865	231	260	2		
4	GG	171	Total	C	N	O	S	0	0
			1358	865	231	260	2		
4	GH	171	Total	C	N	O	S	0	0
			1358	865	231	260	2		
4	GI	171	Total	C	N	O	S	0	0
			1358	865	231	260	2		
4	GJ	171	Total	C	N	O	S	0	0
			1358	865	231	260	2		

- Molecule 5 is a protein called Scaffold protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	GK	30	Total	C	N	O	0	0
			266	174	47	45		
5	GL	37	Total	C	N	O	0	0
			315	203	55	57		
5	GM	37	Total	C	N	O	0	0
			315	203	55	57		
5	GN	37	Total	C	N	O	0	0
			315	203	55	57		
5	GO	37	Total	C	N	O	0	0
			315	203	55	57		
5	GP	37	Total	C	N	O	0	0
			315	203	55	57		
5	GQ	37	Total	C	N	O	0	0
			315	203	55	57		
5	GR	37	Total	C	N	O	0	0
			315	203	55	57		
5	GS	37	Total	C	N	O	0	0
			315	203	55	57		
5	GT	37	Total	C	N	O	0	0
			315	203	55	57		
5	GU	37	Total	C	N	O	0	0
			315	203	55	57		
5	GV	37	Total	C	N	O	0	0
			315	203	55	57		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	GW	30	Total 266	C 174	N 47	O 45	0	0
5	GX	37	Total 315	C 203	N 55	O 57	0	0
5	GY	37	Total 315	C 203	N 55	O 57	0	0
5	GZ	37	Total 315	C 203	N 55	O 57	0	0
5	HA	37	Total 315	C 203	N 55	O 57	0	0
5	HB	37	Total 315	C 203	N 55	O 57	0	0
5	HC	37	Total 315	C 203	N 55	O 57	0	0
5	HD	30	Total 266	C 174	N 47	O 45	0	0
5	HE	37	Total 315	C 203	N 55	O 57	0	0
5	HF	37	Total 315	C 203	N 55	O 57	0	0
5	HG	37	Total 315	C 203	N 55	O 57	0	0
5	HH	30	Total 266	C 174	N 47	O 45	0	0
5	HI	30	Total 266	C 174	N 47	O 45	0	0
5	HJ	30	Total 266	C 174	N 47	O 45	0	0
5	HK	30	Total 266	C 174	N 47	O 45	0	0
5	HL	37	Total 315	C 203	N 55	O 57	0	0
5	HM	29	Total 255	C 165	N 46	O 44	0	0
5	HN	37	Total 315	C 203	N 55	O 57	0	0
5	HO	37	Total 315	C 203	N 55	O 57	0	0
5	HP	37	Total 315	C 203	N 55	O 57	0	0
5	HQ	37	Total 315	C 203	N 55	O 57	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	HR	37	Total 315	C 203	N 55	O 57	0	0
5	HS	37	Total 315	C 203	N 55	O 57	0	0
5	HT	37	Total 315	C 203	N 55	O 57	0	0
5	HU	37	Total 315	C 203	N 55	O 57	0	0
5	HV	37	Total 315	C 203	N 55	O 57	0	0
5	HW	28	Total 248	C 160	N 45	O 43	0	0
5	HX	37	Total 315	C 203	N 55	O 57	0	0
5	HY	37	Total 315	C 203	N 55	O 57	0	0
5	HZ	37	Total 315	C 203	N 55	O 57	0	0
5	IA	37	Total 315	C 203	N 55	O 57	0	0
5	IB	29	Total 255	C 165	N 46	O 44	0	0
5	IC	37	Total 315	C 203	N 55	O 57	0	0
5	ID	29	Total 255	C 165	N 46	O 44	0	0
5	IE	37	Total 315	C 203	N 55	O 57	0	0
5	IF	37	Total 315	C 203	N 55	O 57	0	0
5	IG	37	Total 315	C 203	N 55	O 57	0	0
5	IH	29	Total 255	C 165	N 46	O 44	0	0
5	II	30	Total 266	C 174	N 47	O 45	0	0
5	IJ	30	Total 266	C 174	N 47	O 45	0	0
5	IK	30	Total 266	C 174	N 47	O 45	0	0
5	IL	40	Total 345	C 221	N 64	O 60	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	IM	37	Total 315	C 203	N 55	O 57	0	0
5	IN	37	Total 315	C 203	N 55	O 57	0	0
5	IO	40	Total 345	C 221	N 64	O 60	0	0
5	IP	37	Total 315	C 203	N 55	O 57	0	0
5	IQ	37	Total 315	C 203	N 55	O 57	0	0
5	IR	40	Total 345	C 221	N 64	O 60	0	0
5	IS	37	Total 315	C 203	N 55	O 57	0	0
5	IT	37	Total 315	C 203	N 55	O 57	0	0
5	IU	40	Total 345	C 221	N 64	O 60	0	0
5	IV	37	Total 315	C 203	N 55	O 57	0	0
5	IW	37	Total 315	C 203	N 55	O 57	0	0
5	IX	37	Total 315	C 203	N 55	O 57	0	0
5	IY	40	Total 345	C 221	N 64	O 60	0	0
5	IZ	37	Total 315	C 203	N 55	O 57	0	0
5	JA	40	Total 345	C 221	N 64	O 60	0	0
5	JB	37	Total 315	C 203	N 55	O 57	0	0
5	JC	37	Total 315	C 203	N 55	O 57	0	0
5	JD	40	Total 345	C 221	N 64	O 60	0	0
5	JE	37	Total 315	C 203	N 55	O 57	0	0
5	JF	37	Total 315	C 203	N 55	O 57	0	0
5	JG	40	Total 345	C 221	N 64	O 60	0	0

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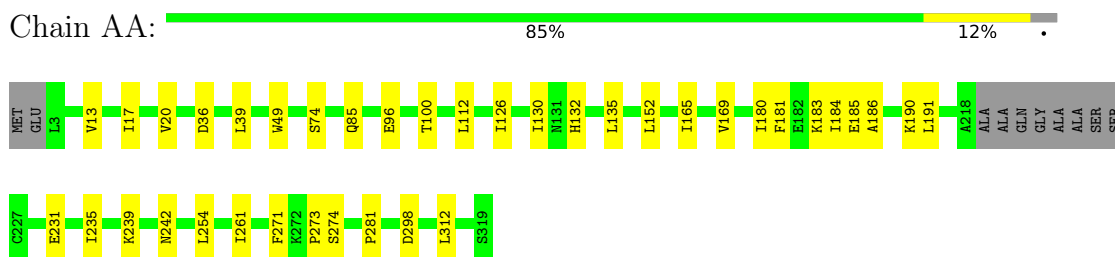
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Mol	Chain	Residues	Atoms				AltConf	Trace
5	JH	37	Total	C	N	O	0	0
			315	203	55	57		
5	JI	37	Total	C	N	O	0	0
			315	203	55	57		
5	JJ	40	Total	C	N	O	0	0
			345	221	64	60		
5	JK	37	Total	C	N	O	0	0
			315	203	55	57		
5	JL	37	Total	C	N	O	0	0
			315	203	55	57		
5	JM	37	Total	C	N	O	0	0
			315	203	55	57		
5	JN	40	Total	C	N	O	0	0
			345	221	64	60		
5	JO	37	Total	C	N	O	0	0
			315	203	55	57		

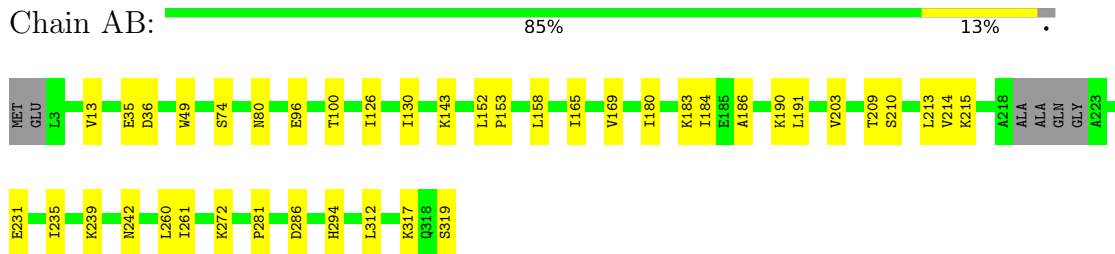
3 Residue-property plots

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

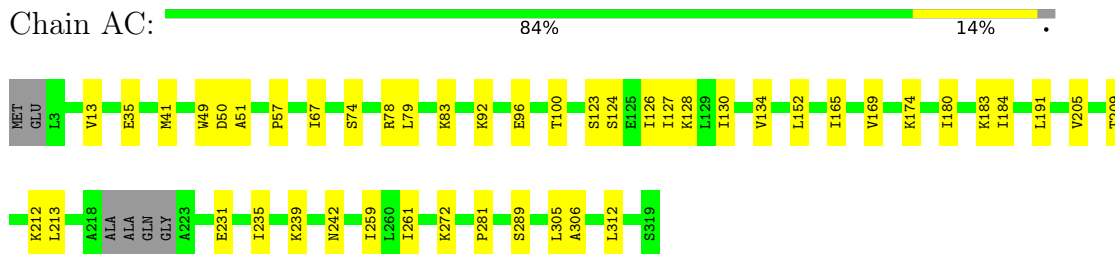
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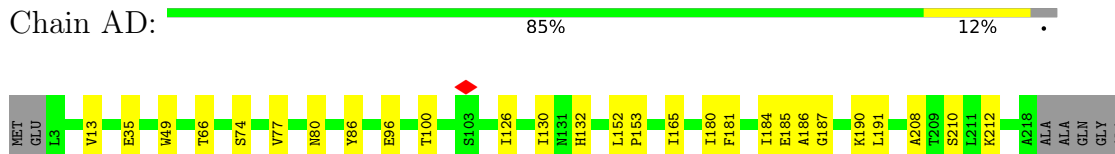
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein

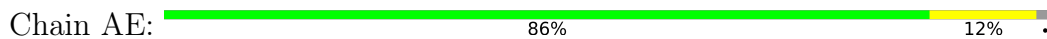


- Molecule 1: Major capsid protein

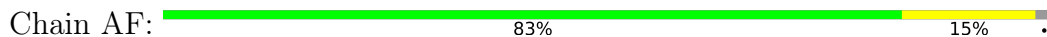




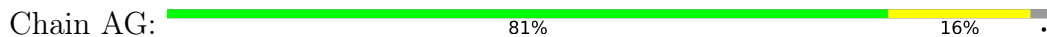
• Molecule 1: Major capsid protein



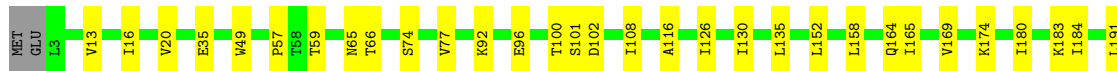
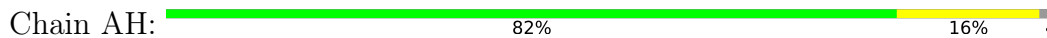
• Molecule 1: Major capsid protein



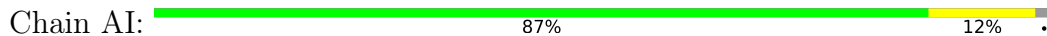
• Molecule 1: Major capsid protein

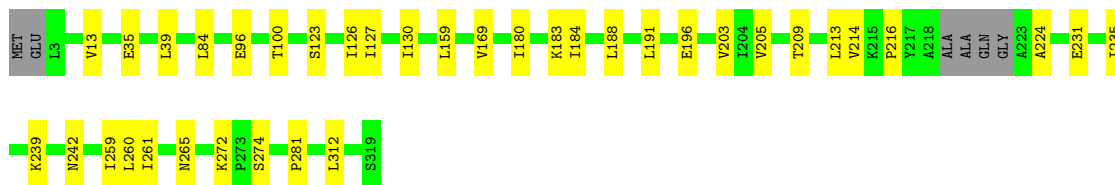


• Molecule 1: Major capsid protein

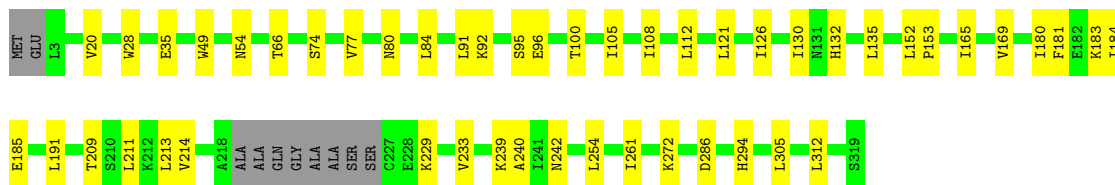
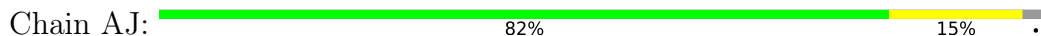


• Molecule 1: Major capsid protein

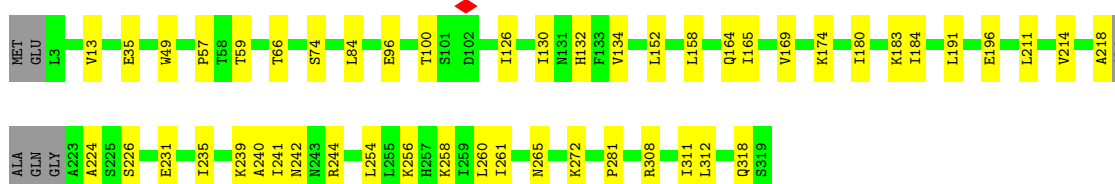
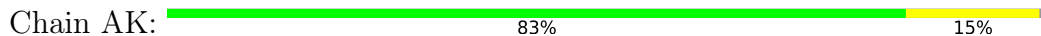




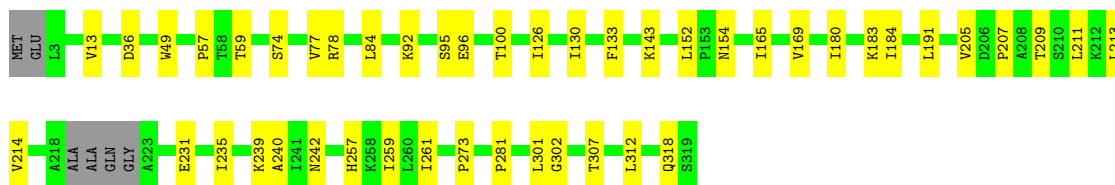
• Molecule 1: Major capsid protein



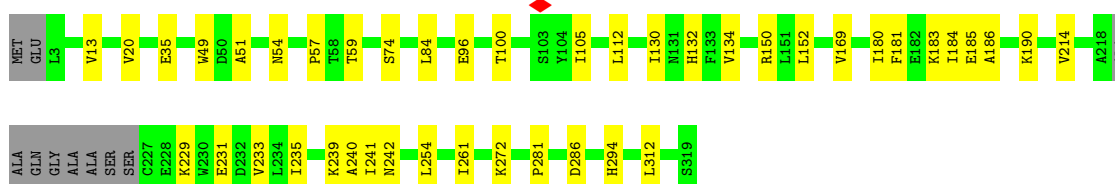
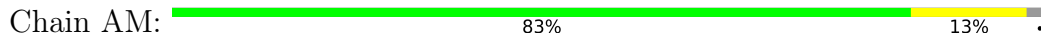
• Molecule 1: Major capsid protein




• Molecule 1: Major capsid protein

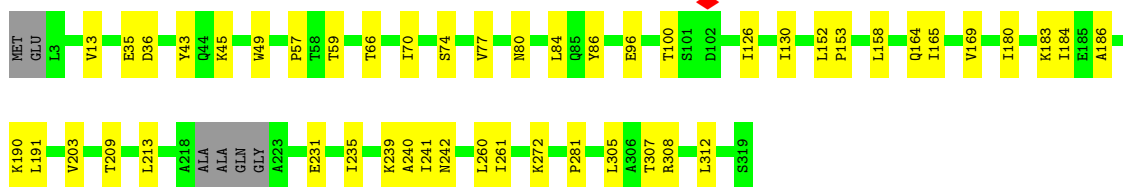


• Molecule 1: Major capsid protein




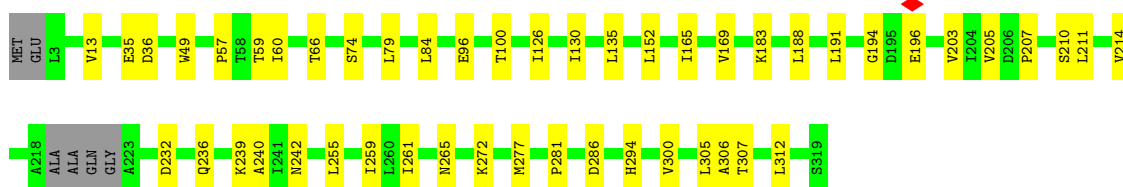
• Molecule 1: Major capsid protein

Chain AN:  83% 15%




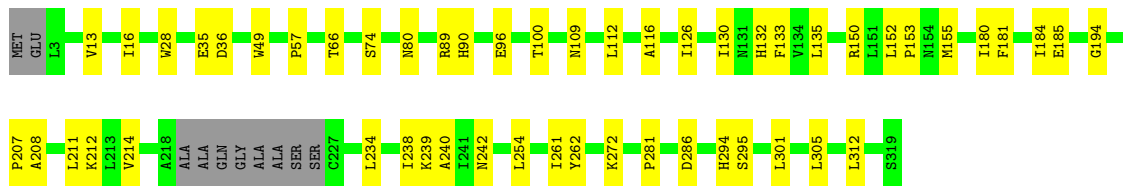
• Molecule 1: Major capsid protein

Chain AO:  83% 15%




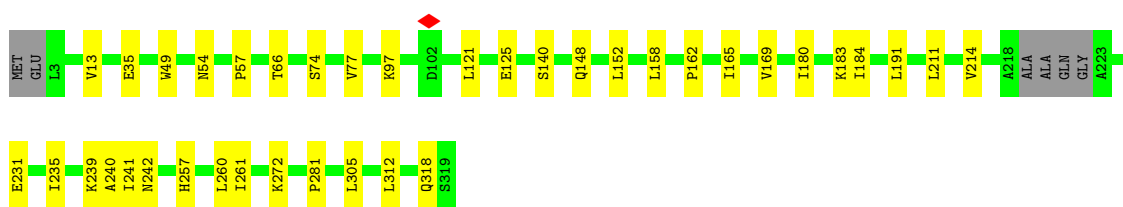
• Molecule 1: Major capsid protein

Chain AP:  81% 16%




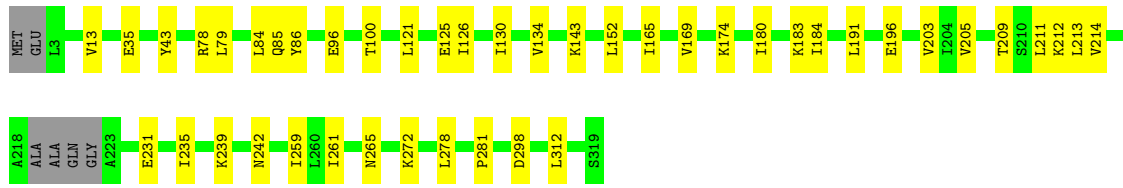
• Molecule 1: Major capsid protein

Chain AQ:  86% 12%




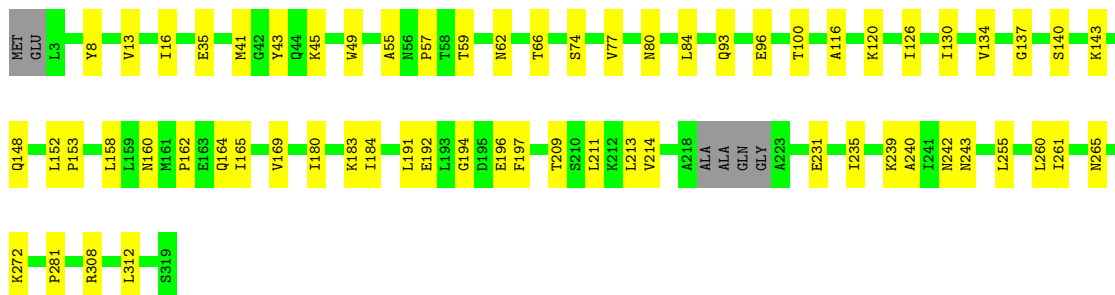
• Molecule 1: Major capsid protein

Chain AR:  84% 14%




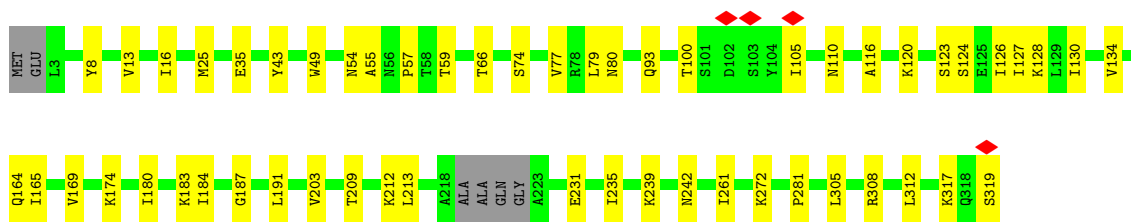
• Molecule 1: Major capsid protein

Chain AS:  78% 20%




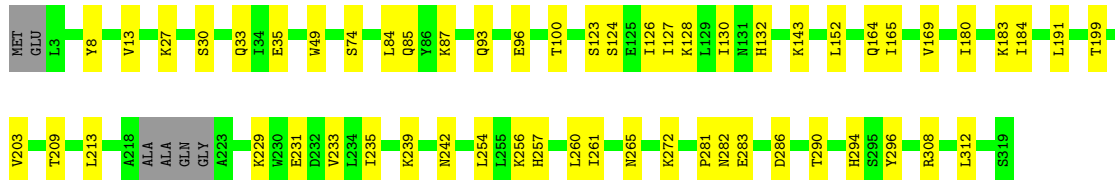
• Molecule 1: Major capsid protein

Chain AT:  81% 17%




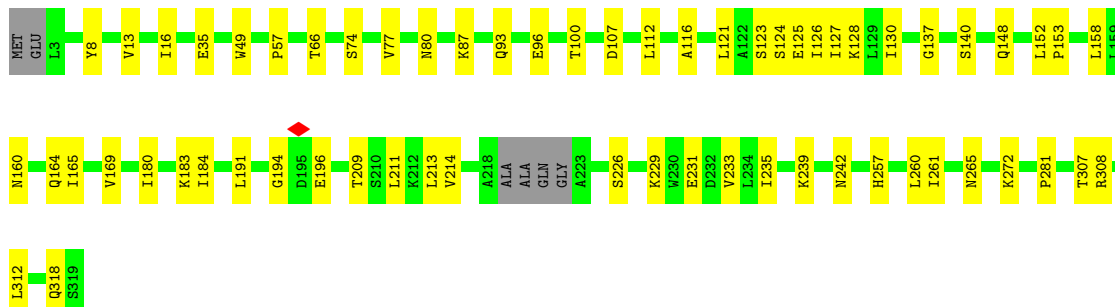
• Molecule 1: Major capsid protein

Chain AU:  81% 18%




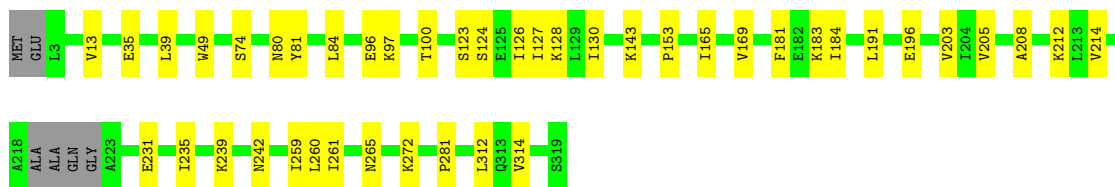
• Molecule 1: Major capsid protein

Chain AV:  79% 19%




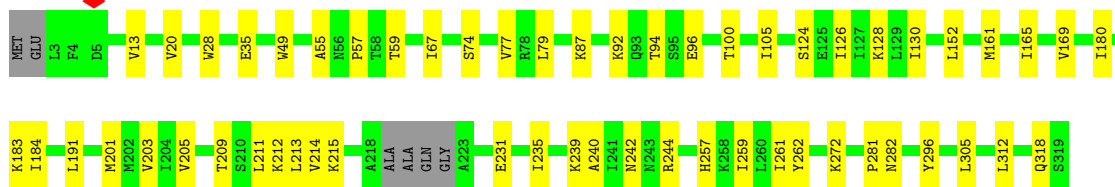
• Molecule 1: Major capsid protein

Chain AW:  85% 13%




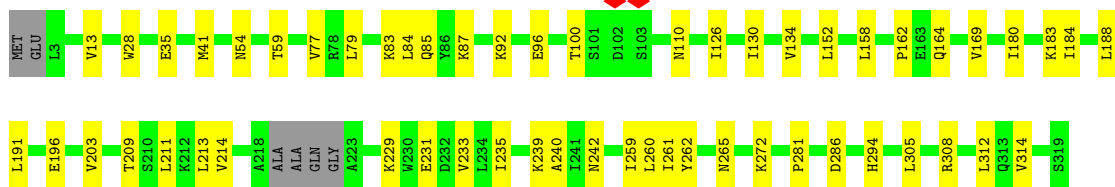
• Molecule 1: Major capsid protein

Chain AX:  81% 18%




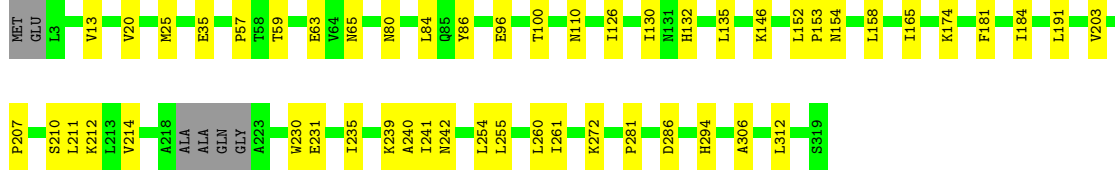
• Molecule 1: Major capsid protein

Chain AY:  81% 17%




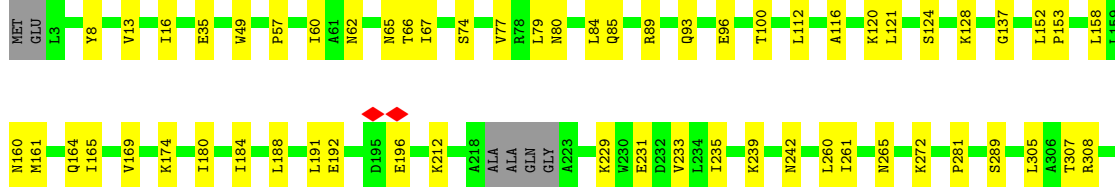
• Molecule 1: Major capsid protein

Chain AZ:  82% 16%



• Molecule 1: Major capsid protein

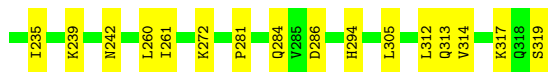
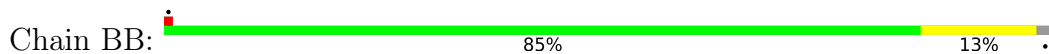
Chain BA:  79% 19%



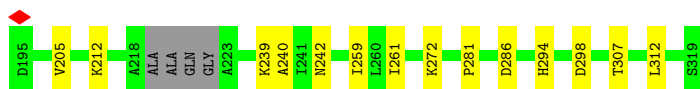
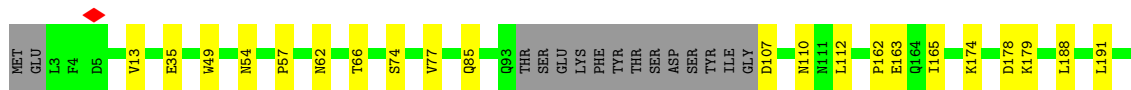
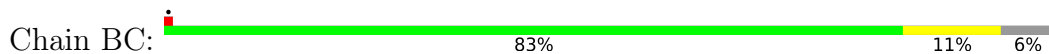
• Molecule 1: Major capsid protein



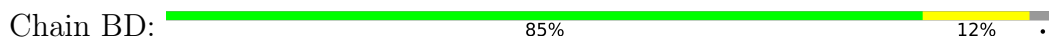
• Molecule 1: Major capsid protein



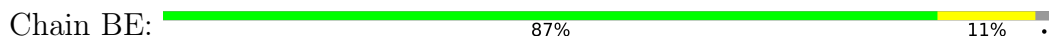
• Molecule 1: Major capsid protein



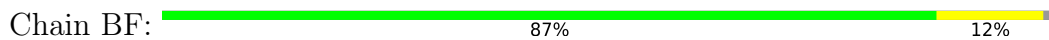
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein

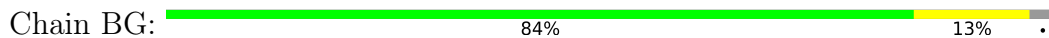


• Molecule 1: Major capsid protein

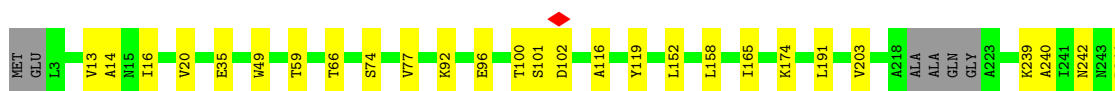
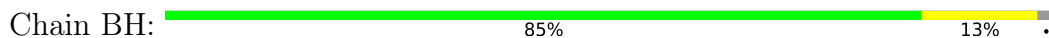




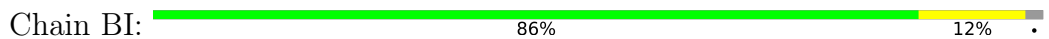
• Molecule 1: Major capsid protein



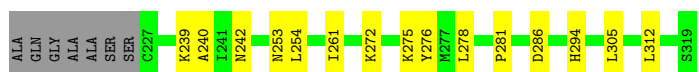
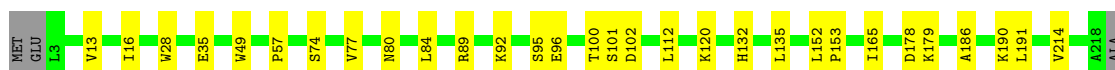
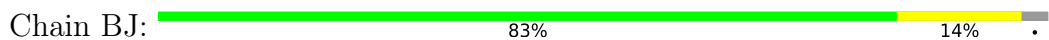
• Molecule 1: Major capsid protein



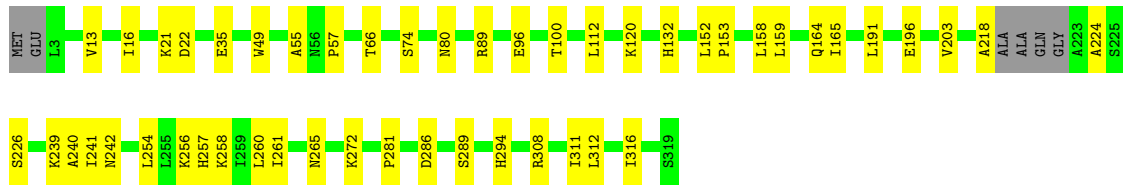
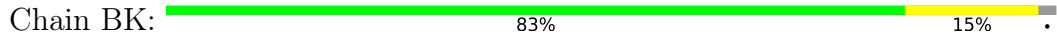
• Molecule 1: Major capsid protein



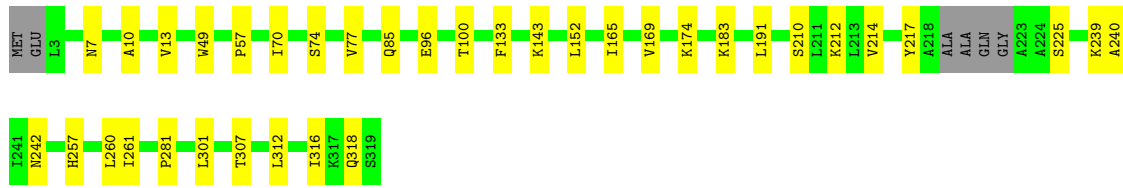
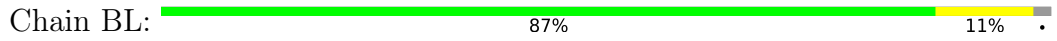
• Molecule 1: Major capsid protein



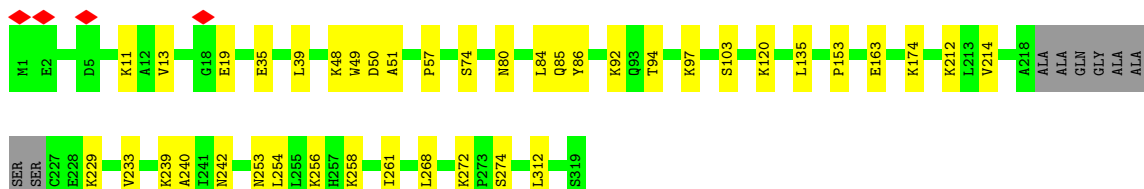
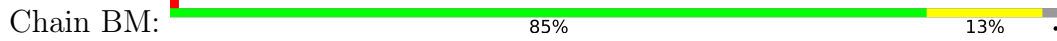
• Molecule 1: Major capsid protein



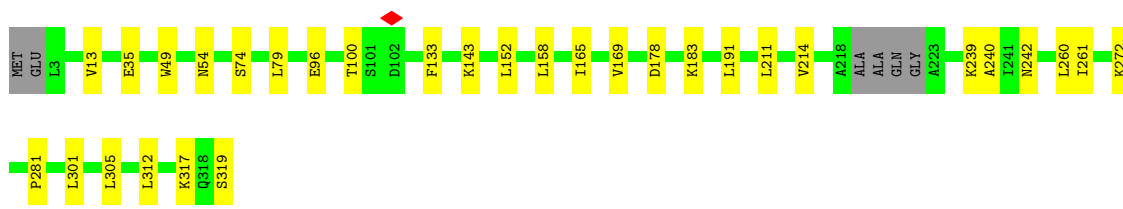
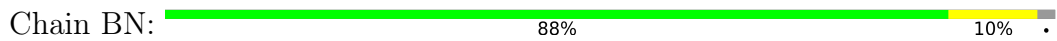
• Molecule 1: Major capsid protein



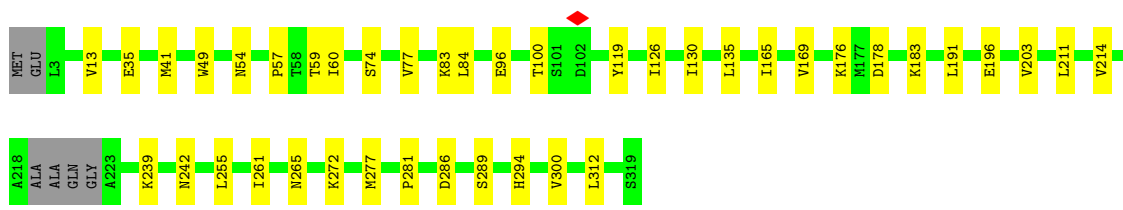
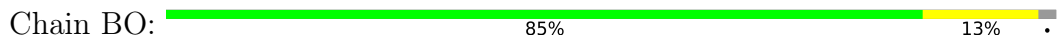
• Molecule 1: Major capsid protein



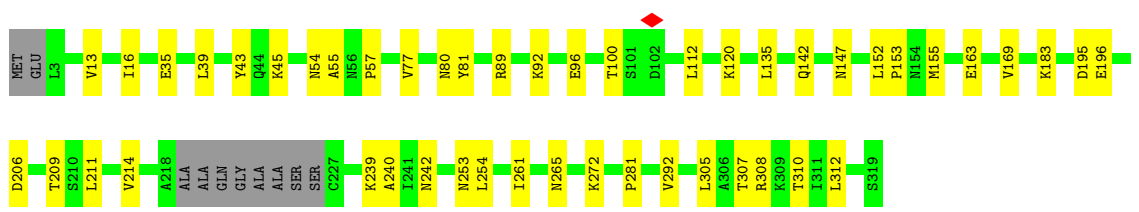
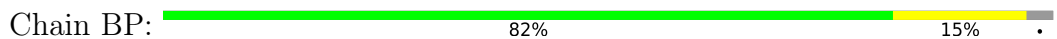
• Molecule 1: Major capsid protein



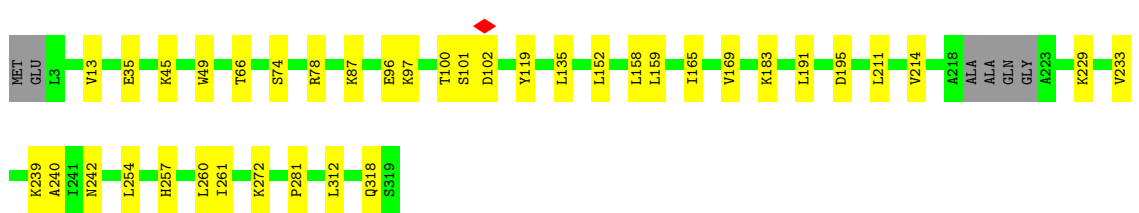
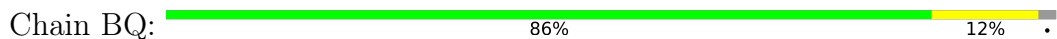
• Molecule 1: Major capsid protein



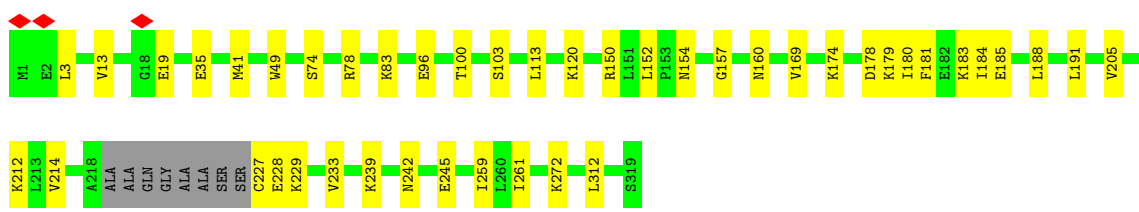
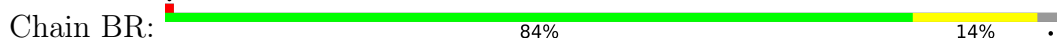
• Molecule 1: Major capsid protein



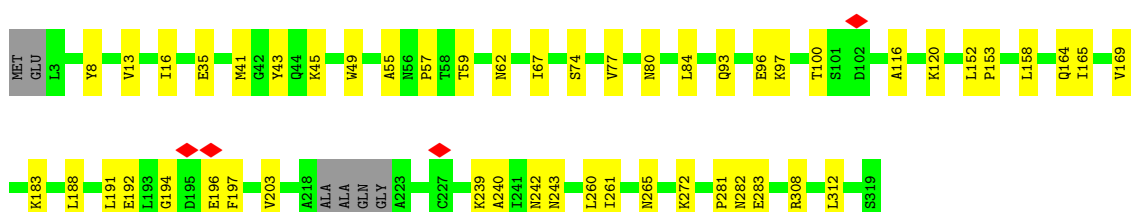
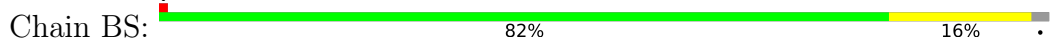
• Molecule 1: Major capsid protein



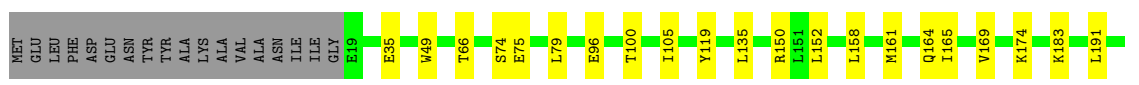
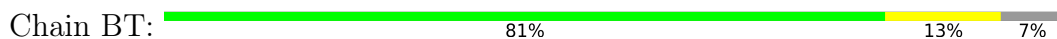
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein

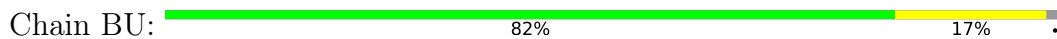


• Molecule 1: Major capsid protein

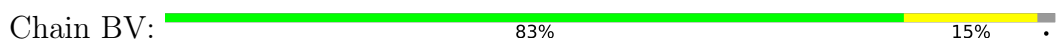




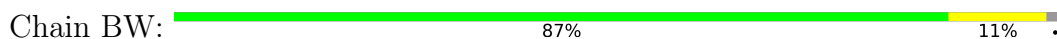
• Molecule 1: Major capsid protein



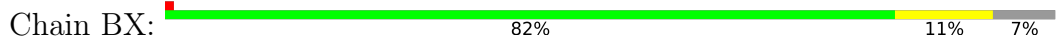
• Molecule 1: Major capsid protein



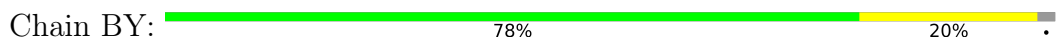
• Molecule 1: Major capsid protein

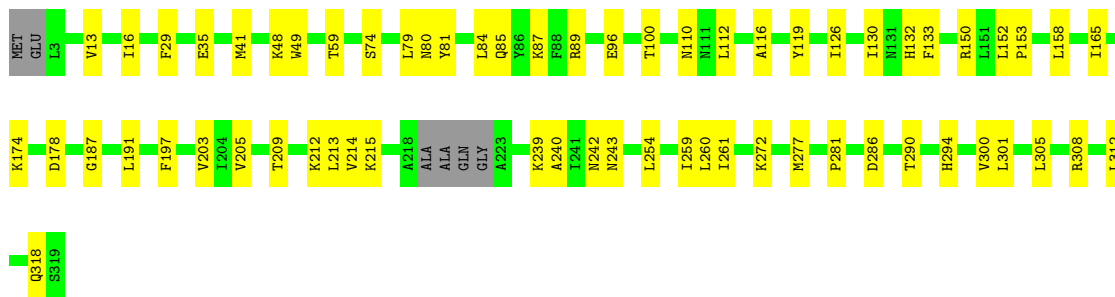


• Molecule 1: Major capsid protein

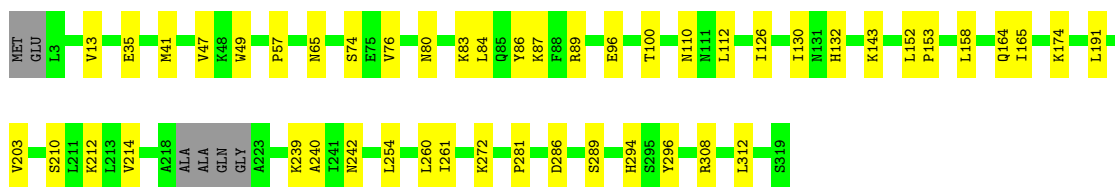
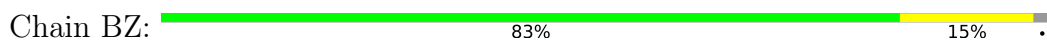


• Molecule 1: Major capsid protein

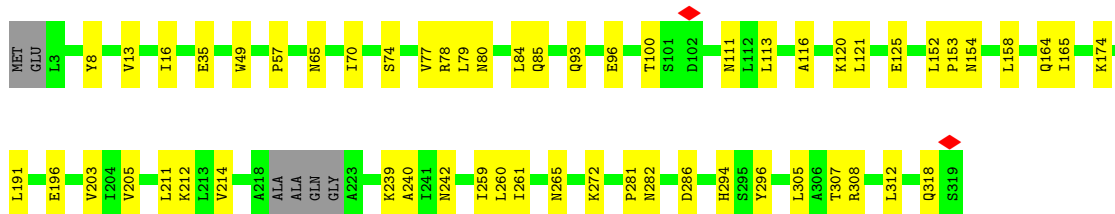
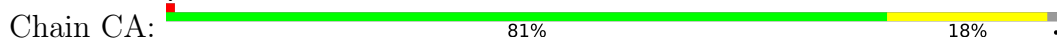




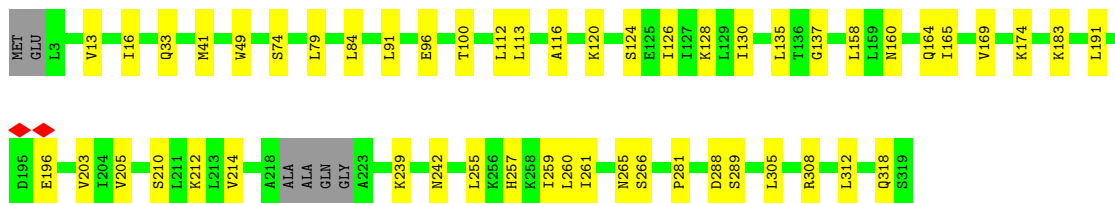
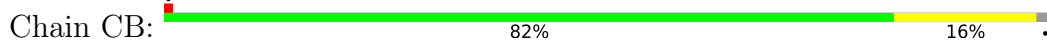
• Molecule 1: Major capsid protein



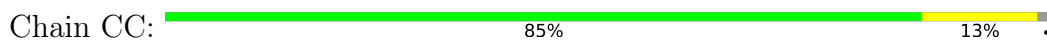
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein

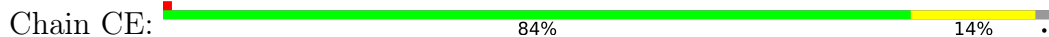




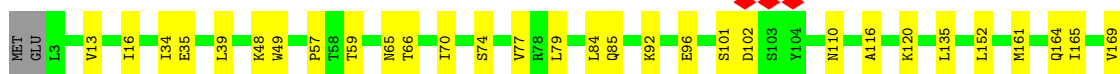
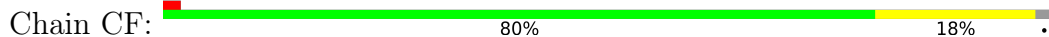
• Molecule 1: Major capsid protein



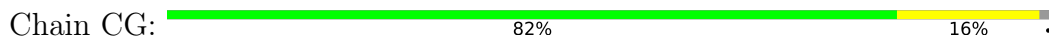
• Molecule 1: Major capsid protein



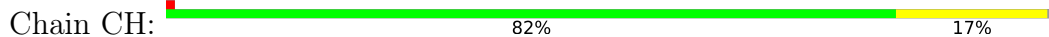
• Molecule 1: Major capsid protein

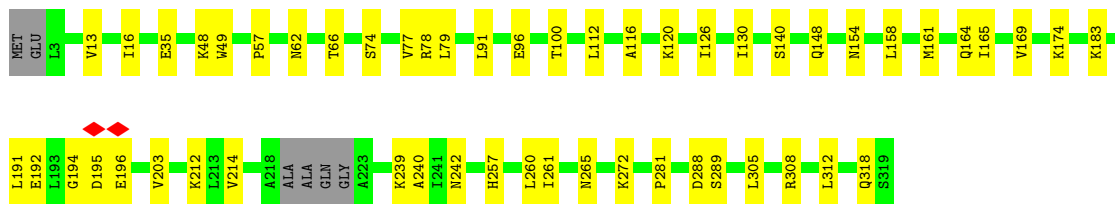


• Molecule 1: Major capsid protein

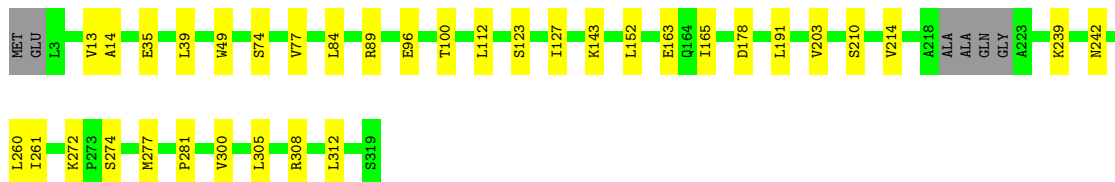
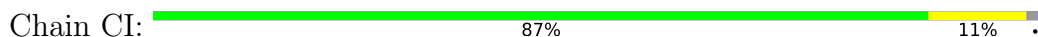


• Molecule 1: Major capsid protein

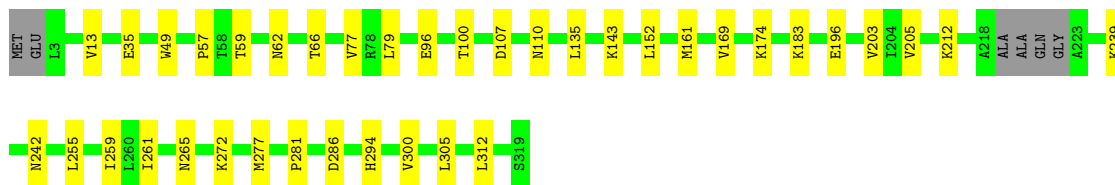
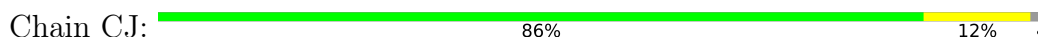




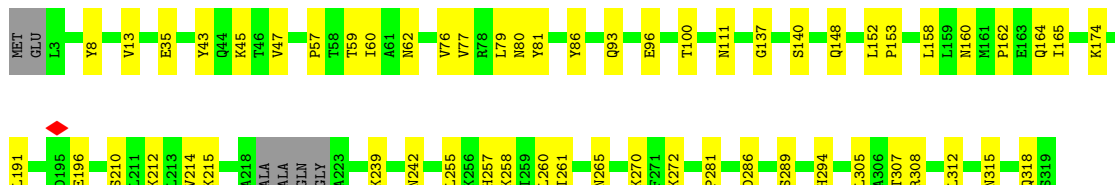
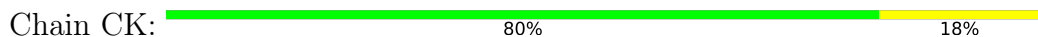
• Molecule 1: Major capsid protein



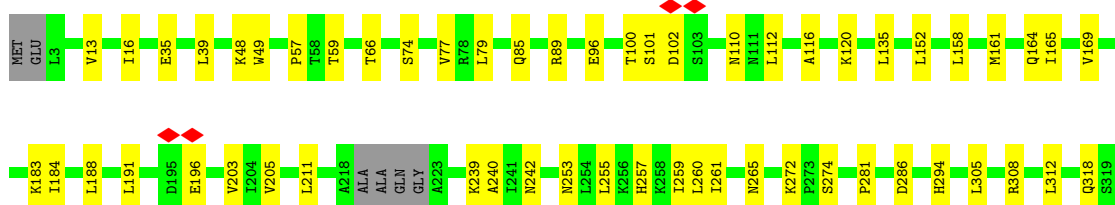
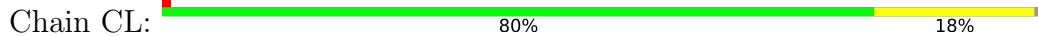
• Molecule 1: Major capsid protein




• Molecule 1: Major capsid protein

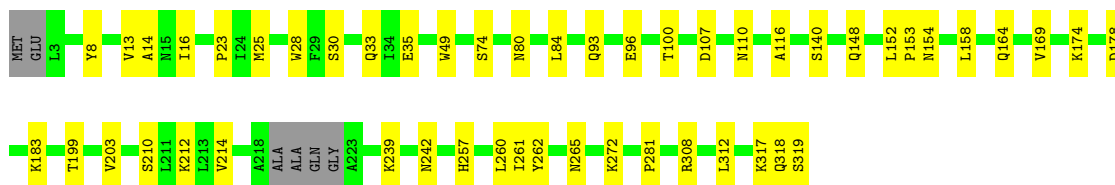


• Molecule 1: Major capsid protein




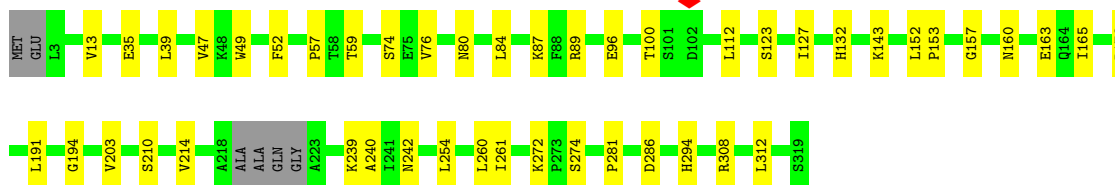
• Molecule 1: Major capsid protein

Chain CM:  82% 16%




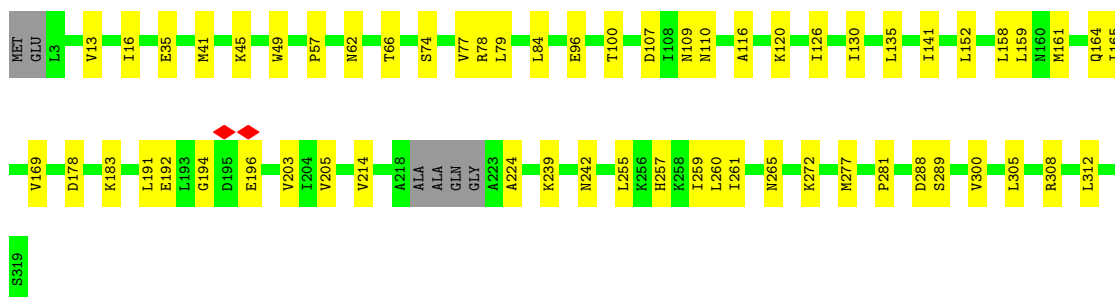
• Molecule 1: Major capsid protein

Chain CN:  84% 14%




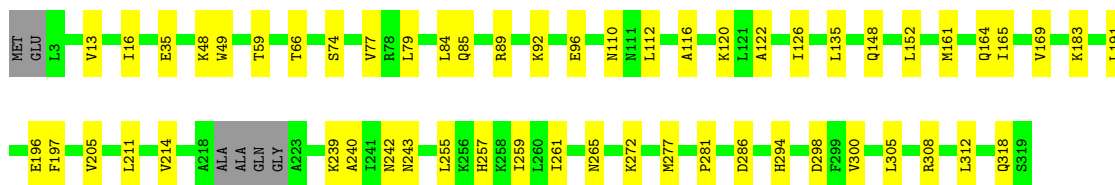
• Molecule 1: Major capsid protein

Chain CO:  79% 19%




• Molecule 1: Major capsid protein

Chain CP:  81% 17%



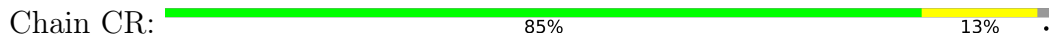
• Molecule 1: Major capsid protein

Chain CQ:  84% 14%

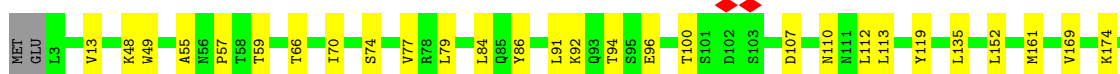
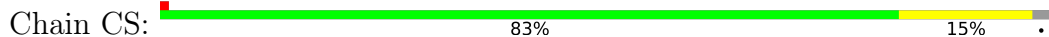




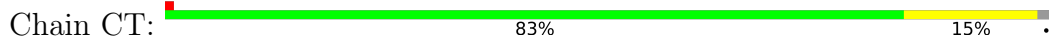
• Molecule 1: Major capsid protein



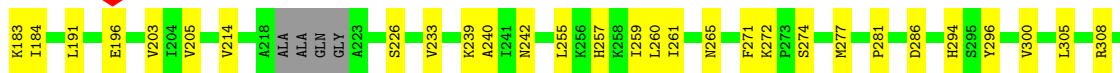
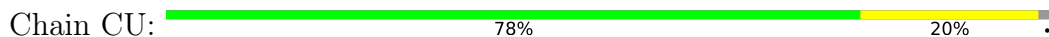
• Molecule 1: Major capsid protein




• Molecule 1: Major capsid protein

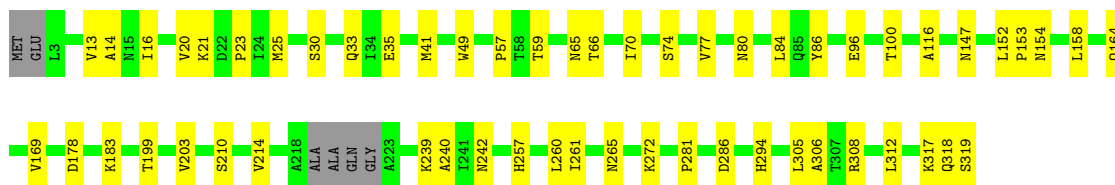


• Molecule 1: Major capsid protein




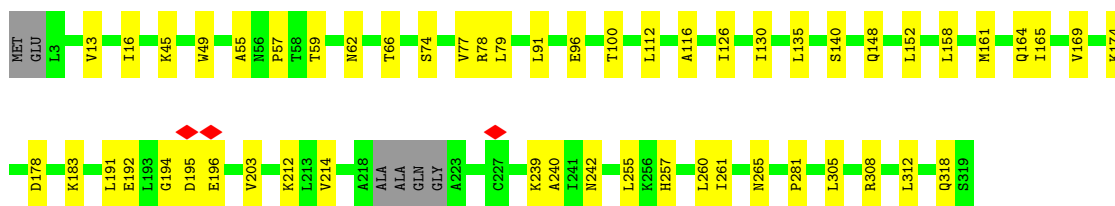
• Molecule 1: Major capsid protein

Chain CV:  81% 18%




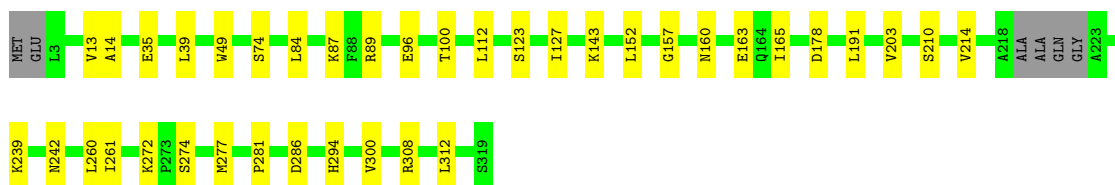
• Molecule 1: Major capsid protein

Chain CW:  82% 17%




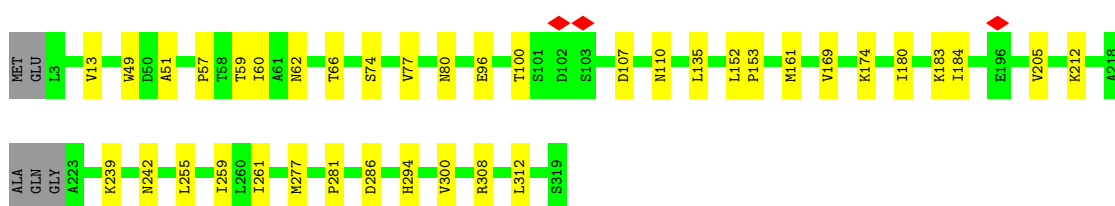
• Molecule 1: Major capsid protein

Chain CX:  86% 12%



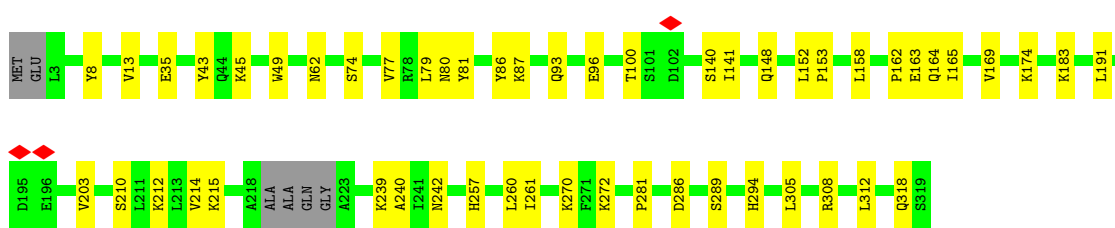
• Molecule 1: Major capsid protein

Chain CY:  86% 12%

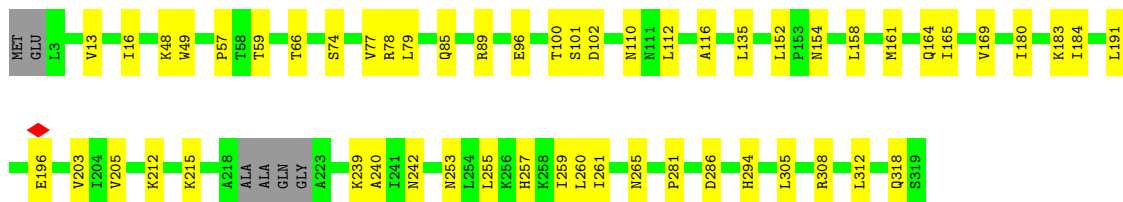
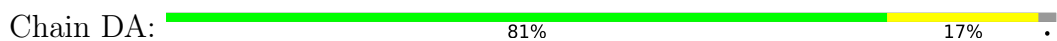


• Molecule 1: Major capsid protein

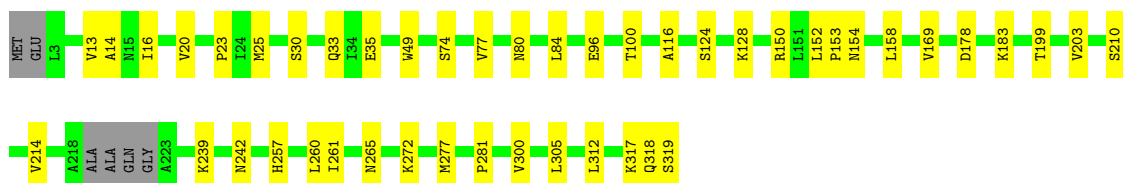
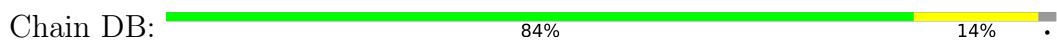
Chain CZ:  82% 16%



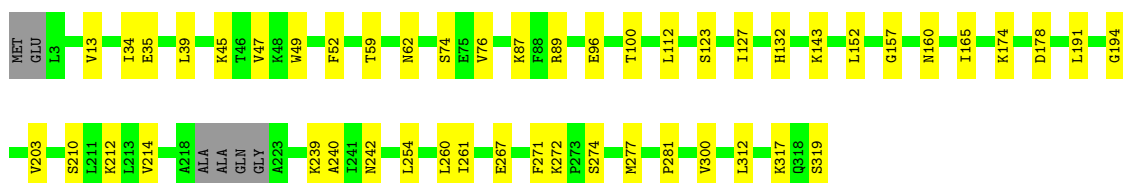
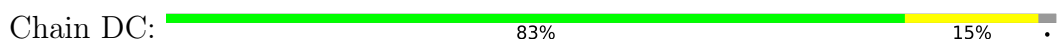
• Molecule 1: Major capsid protein



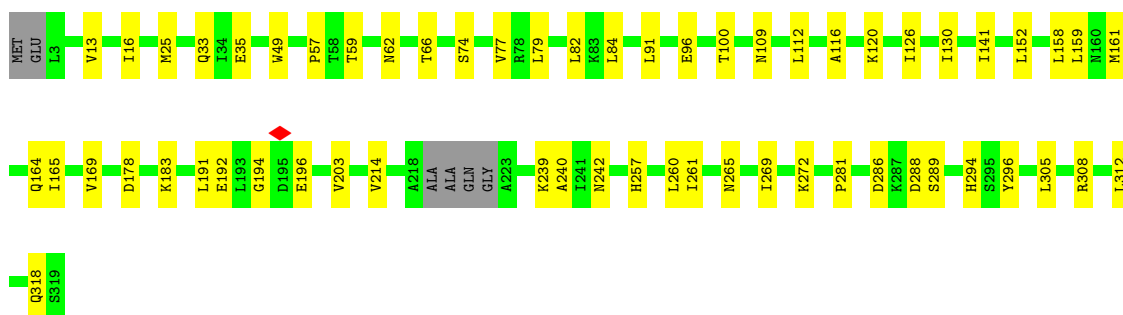
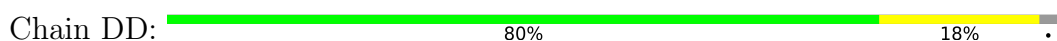
• Molecule 1: Major capsid protein



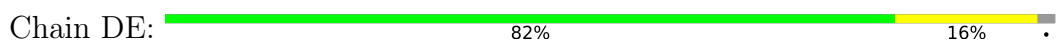
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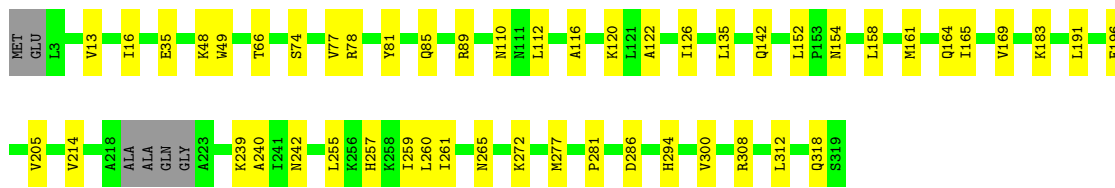


• Molecule 1: Major capsid protein

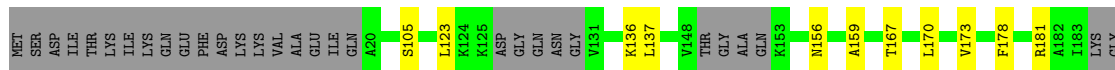
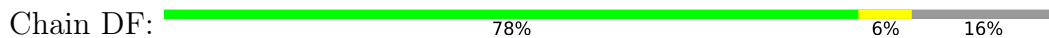


• Molecule 1: Major capsid protein

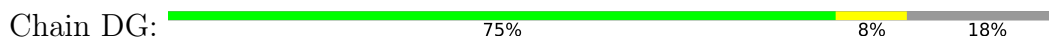




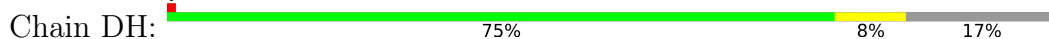
• Molecule 2: Decorator protein P03



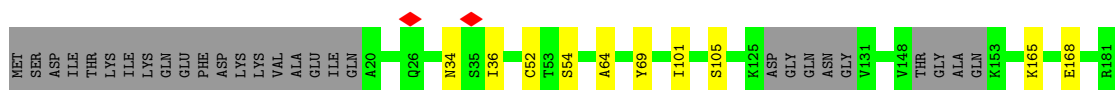
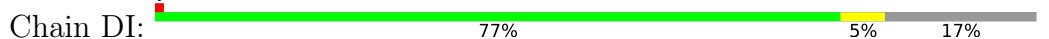
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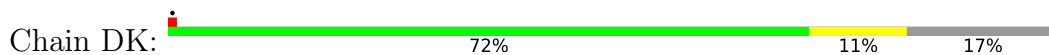


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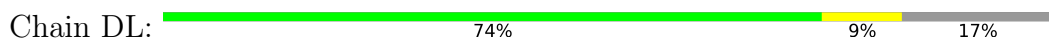




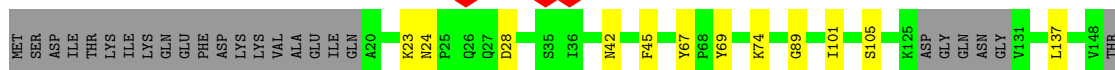
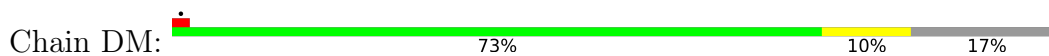
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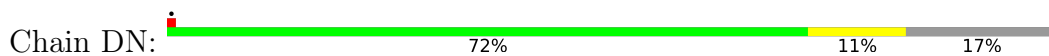
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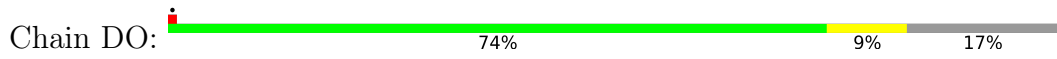
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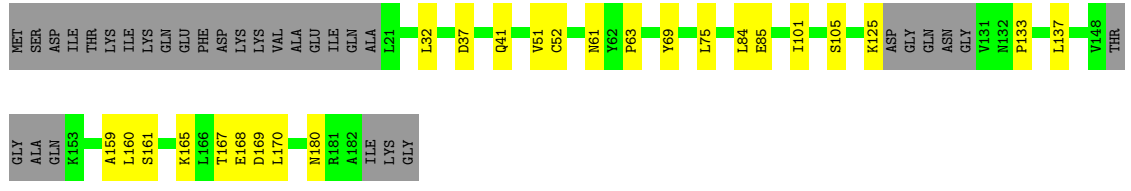
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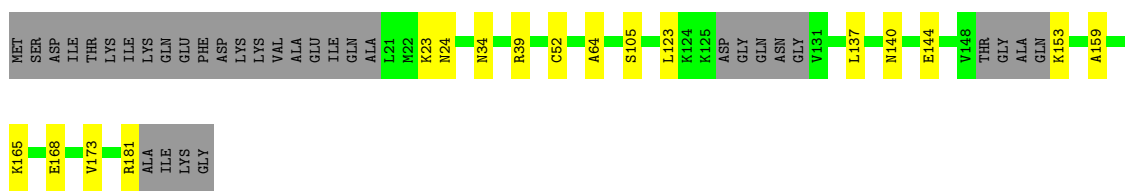
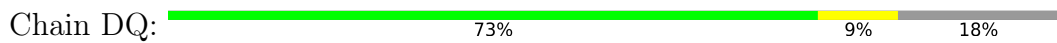
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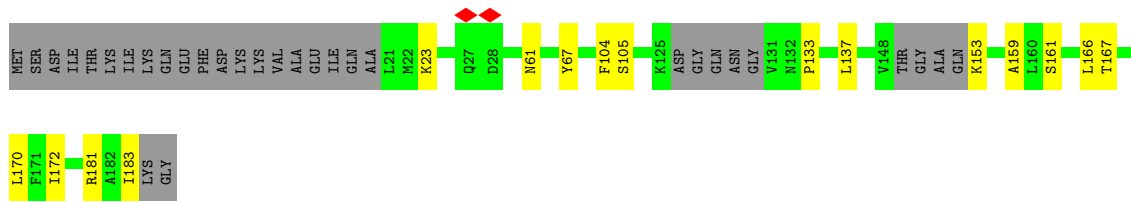
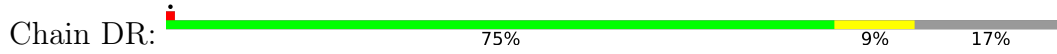
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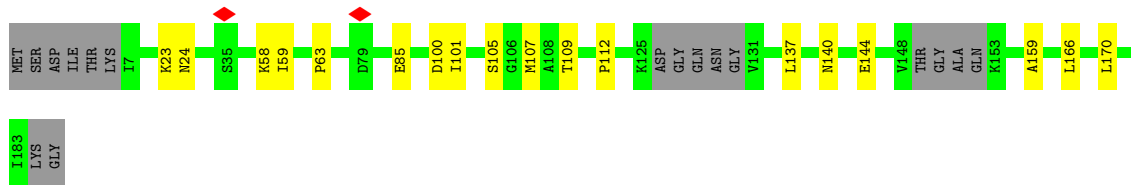
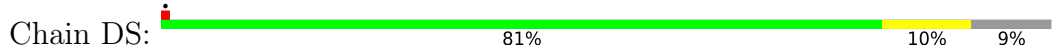
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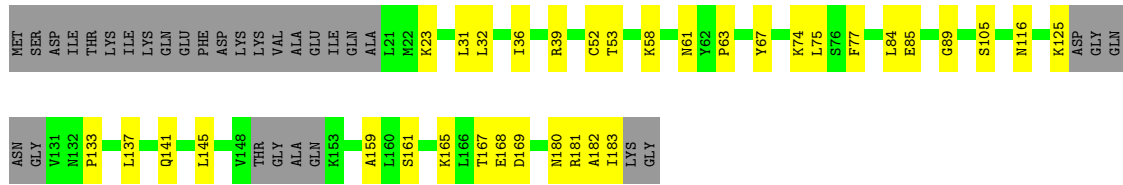
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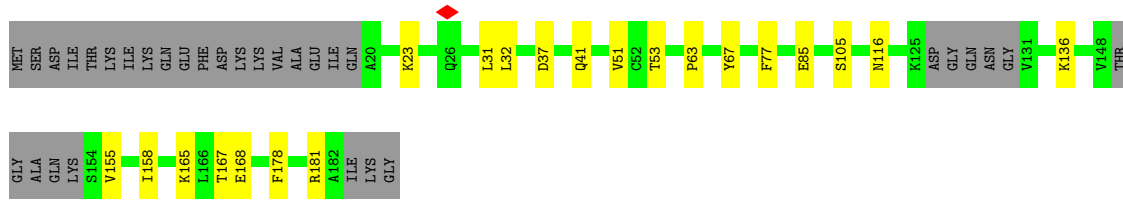
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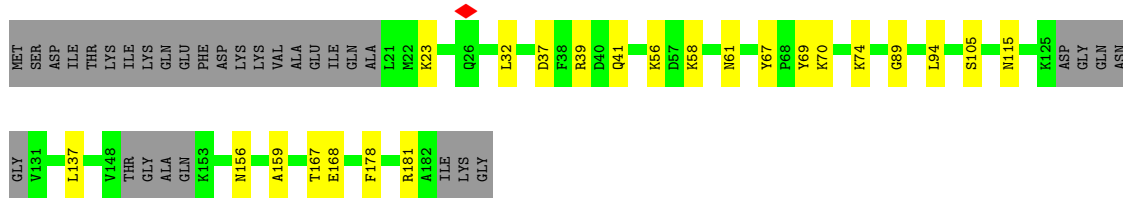
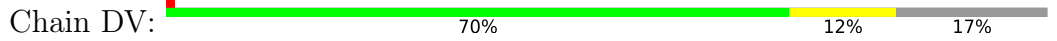
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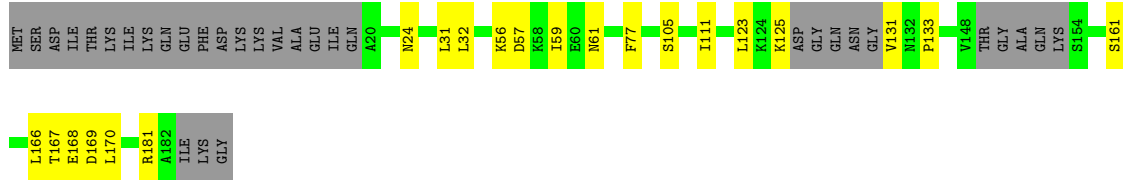
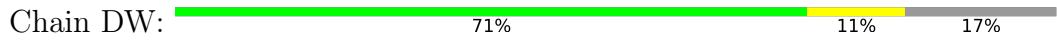
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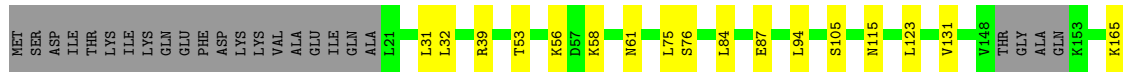
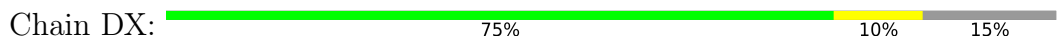
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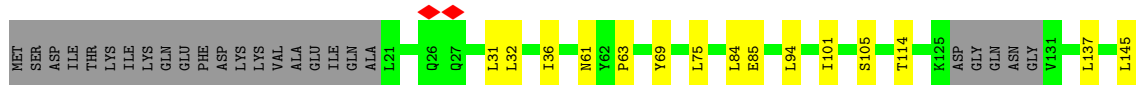




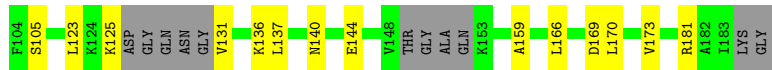
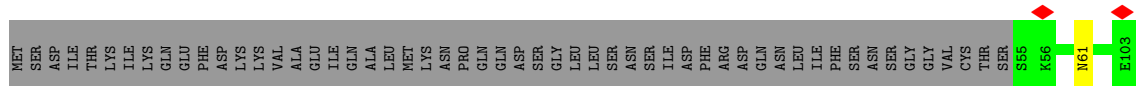
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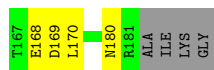
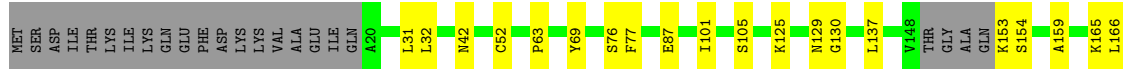
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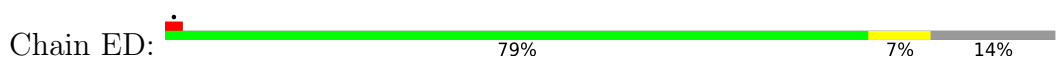


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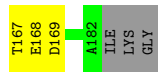
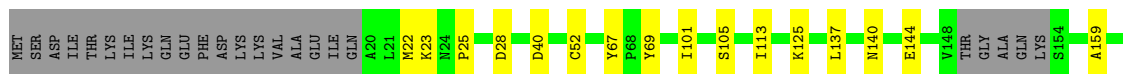
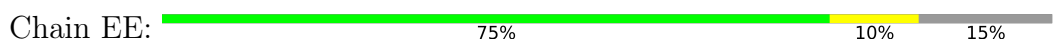




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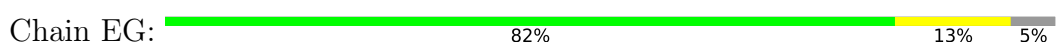
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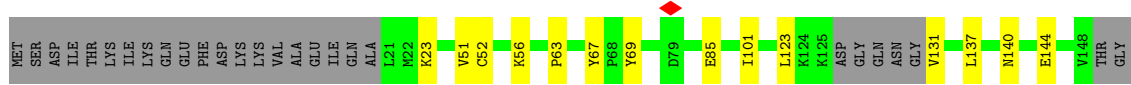
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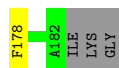
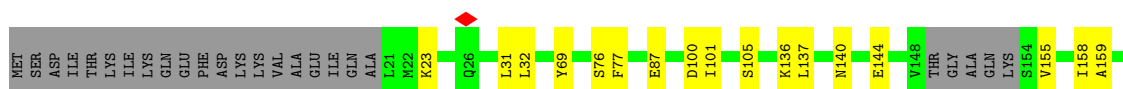
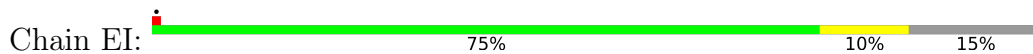


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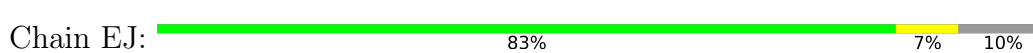




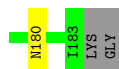
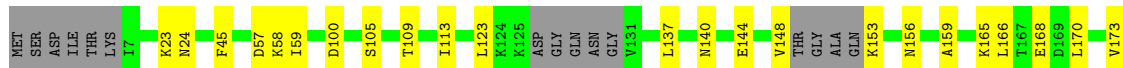
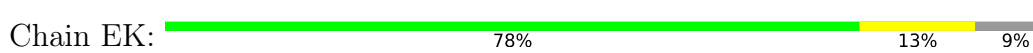
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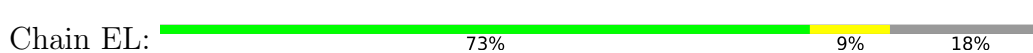
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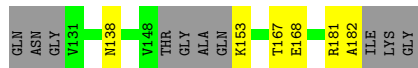
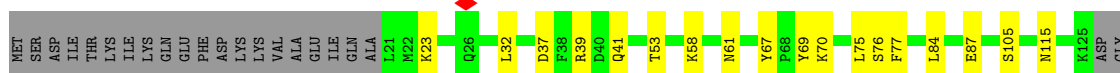


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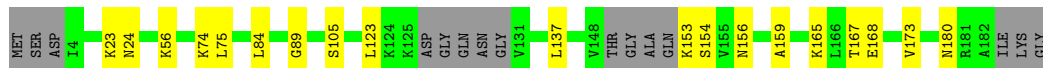




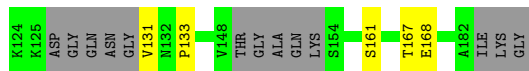
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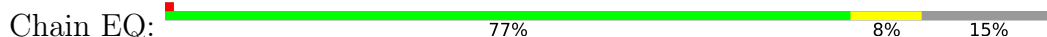
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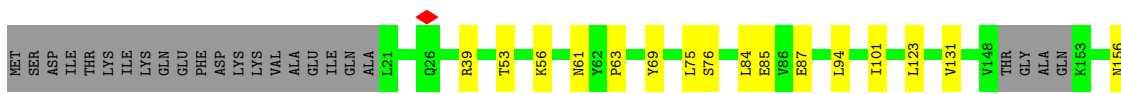
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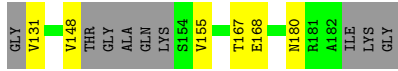
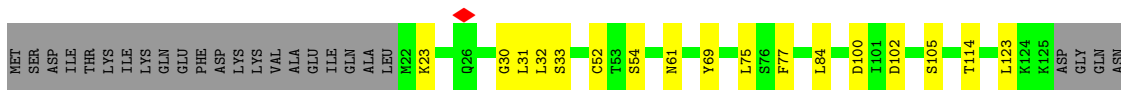
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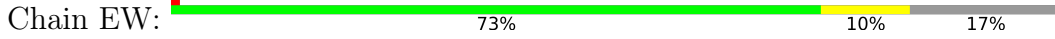
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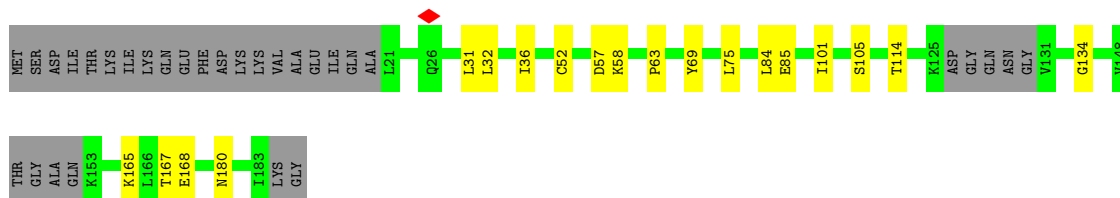


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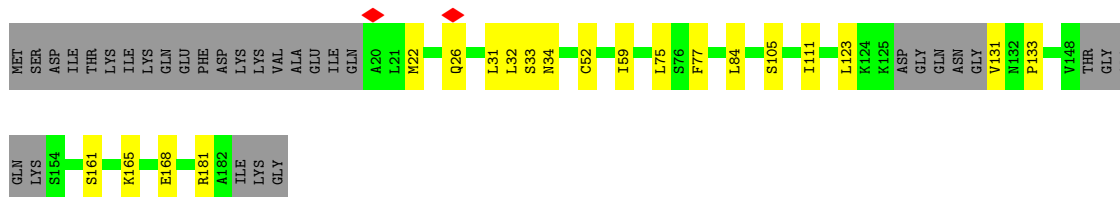


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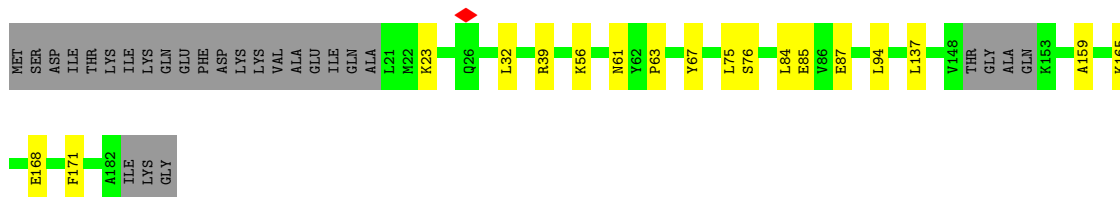
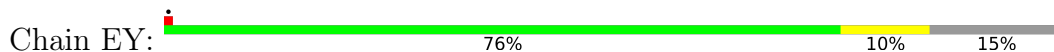




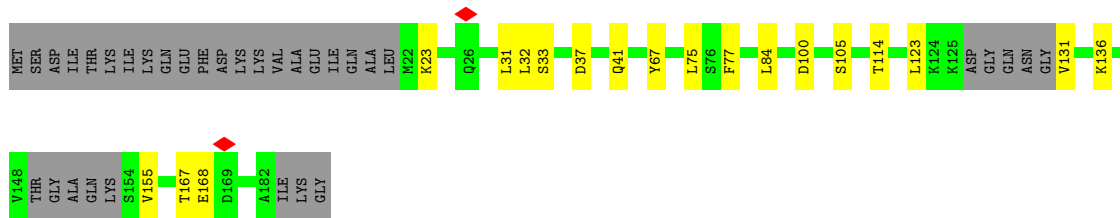
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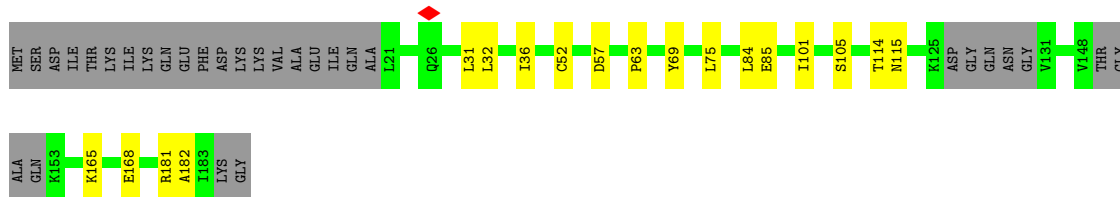
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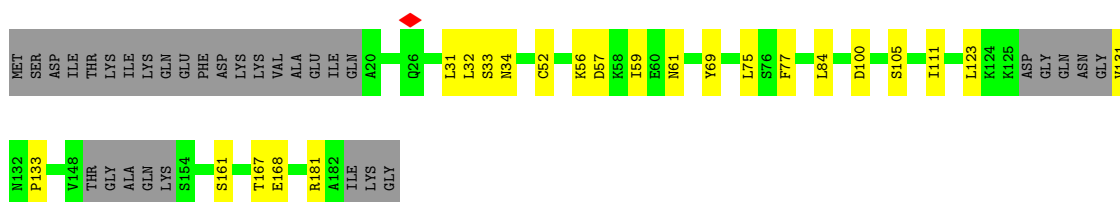
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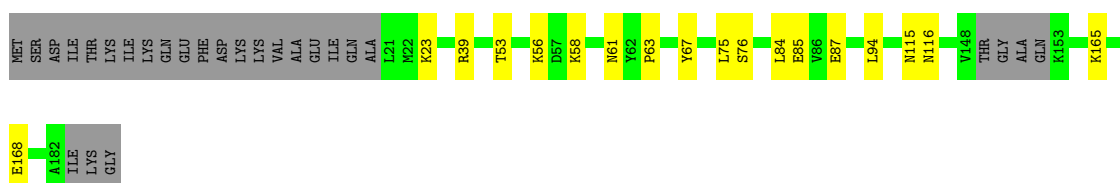
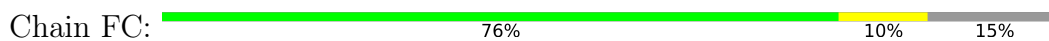
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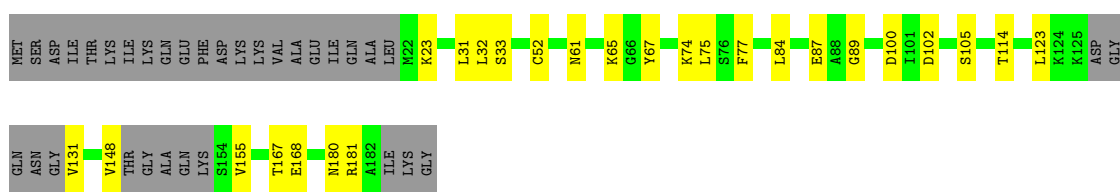
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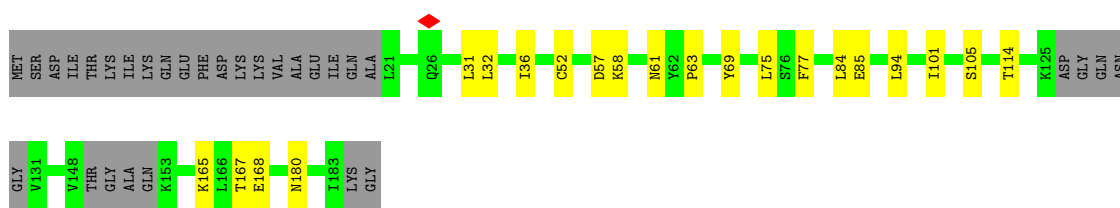
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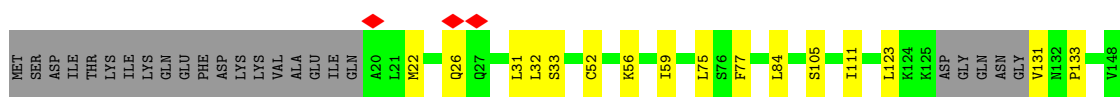
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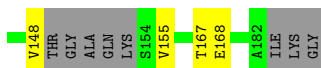
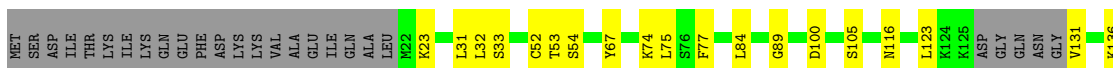




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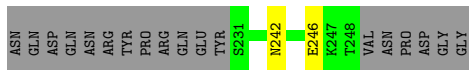
• Molecule 2: Decorator protein P03



• Molecule 2: Decorator protein P03



• Molecule 3: Decorator protein P04



• Molecule 4: Decorator protein P05





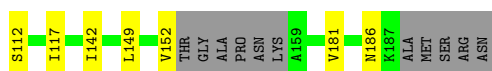
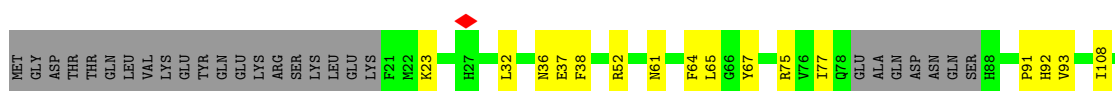
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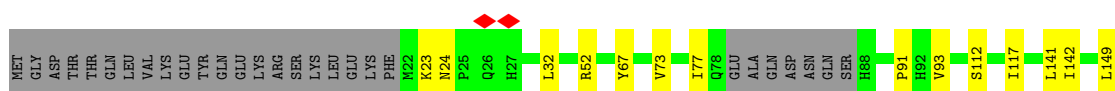
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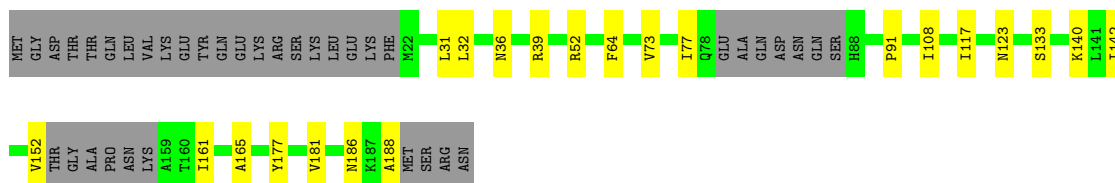
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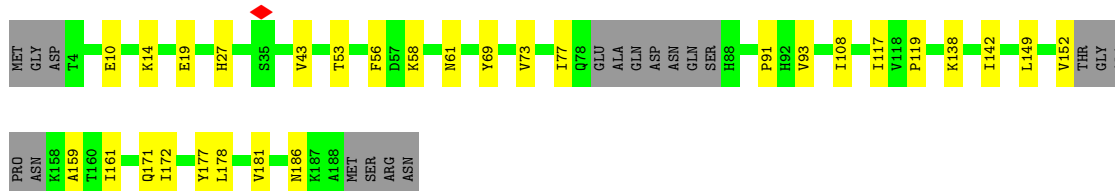
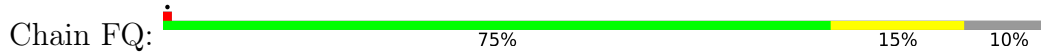
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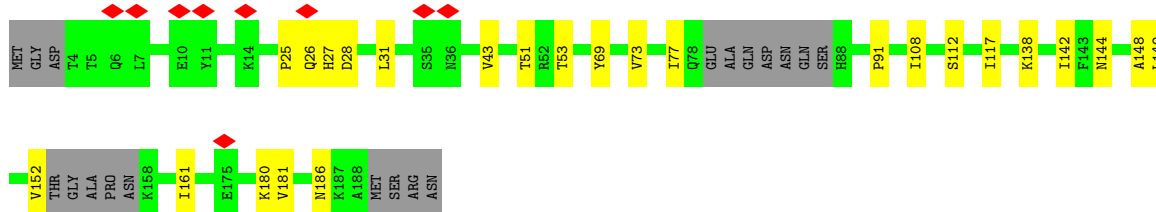
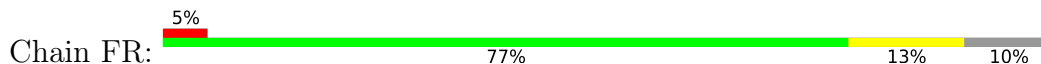
• Molecule 4: Decorator protein P05



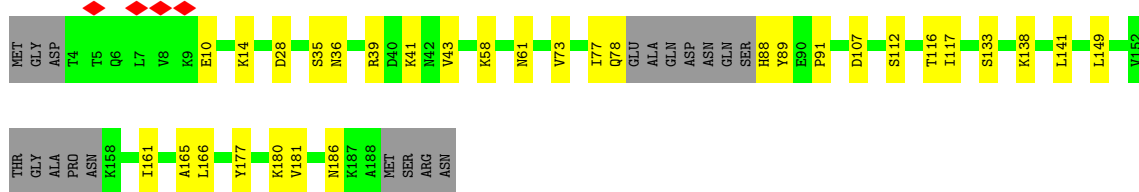
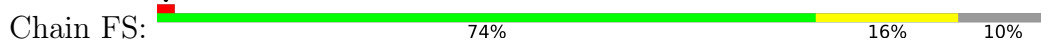
• Molecule 4: Decorator protein P05



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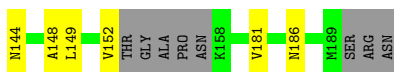
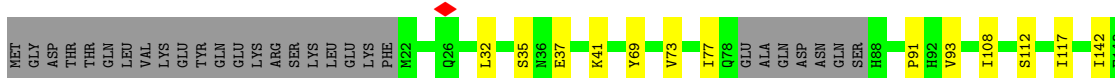




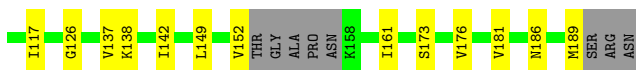
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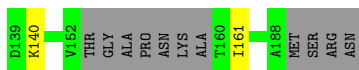
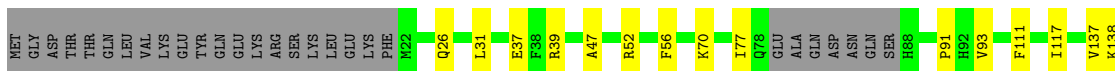
• Molecule 4: Decorator protein P05



• Molecule 4: Decorator protein P05

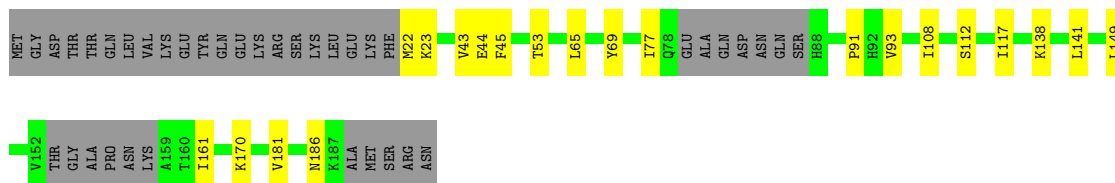


• Molecule 4: Decorator protein P05

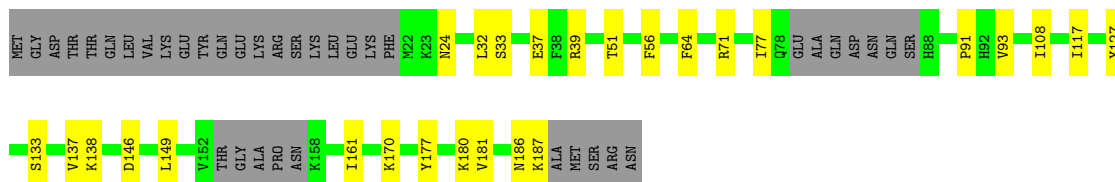


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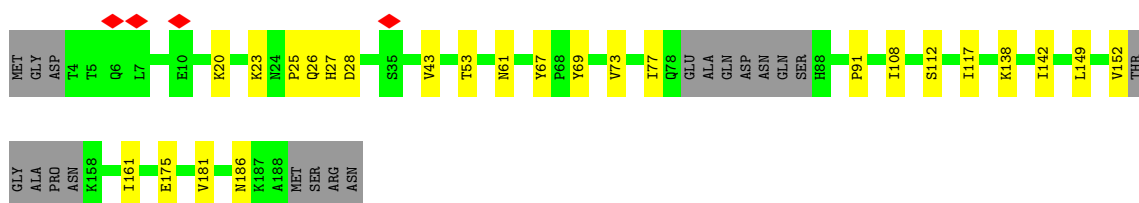
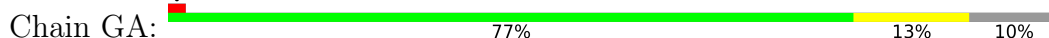




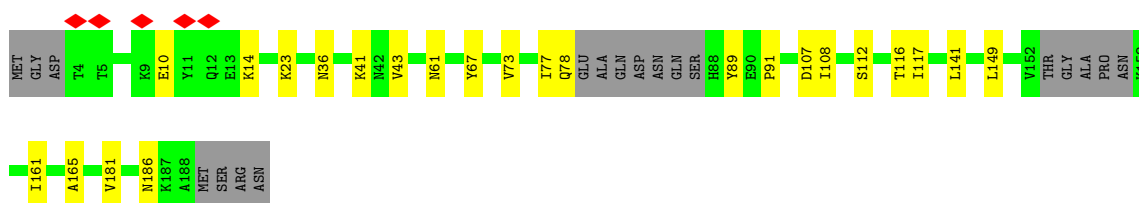
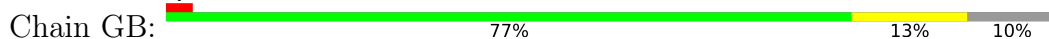
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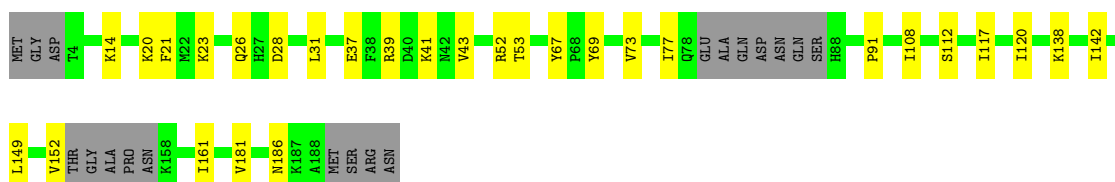
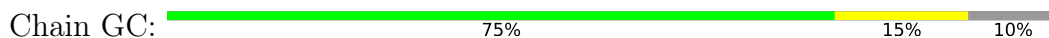
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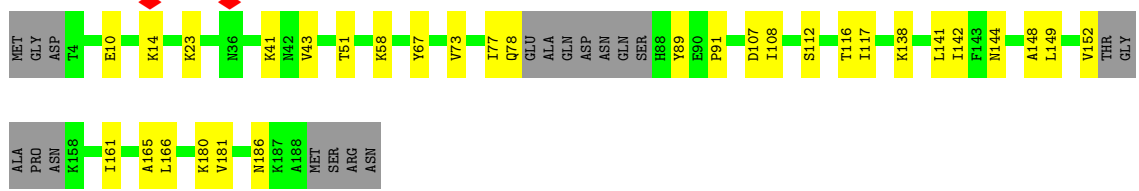
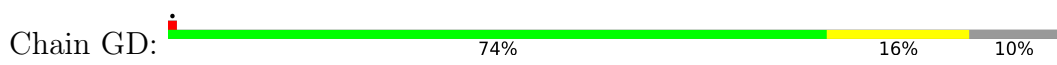
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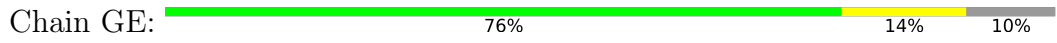
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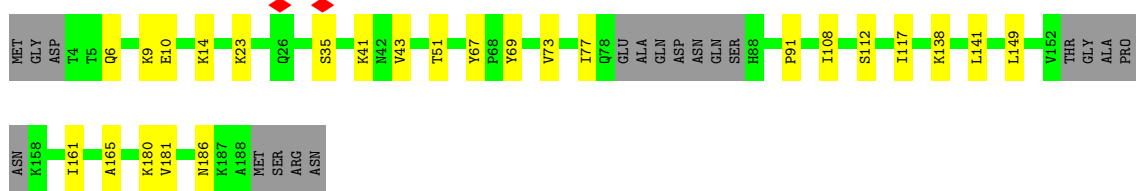
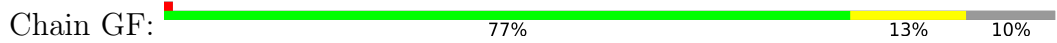
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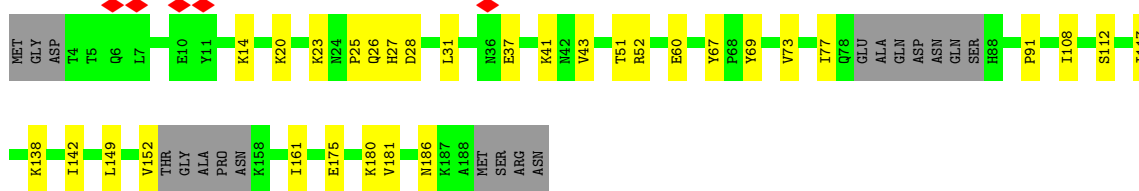
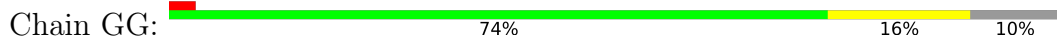
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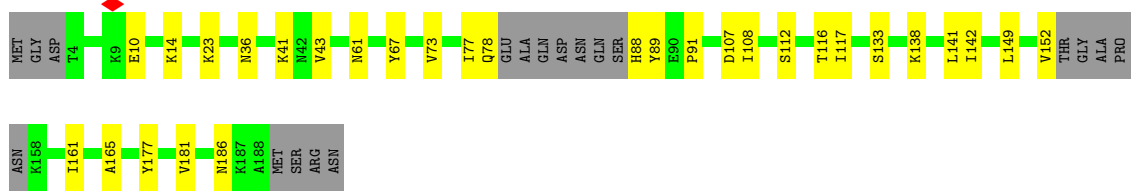
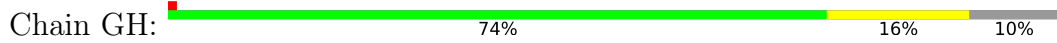
• Molecule 4: Decorator protein P05



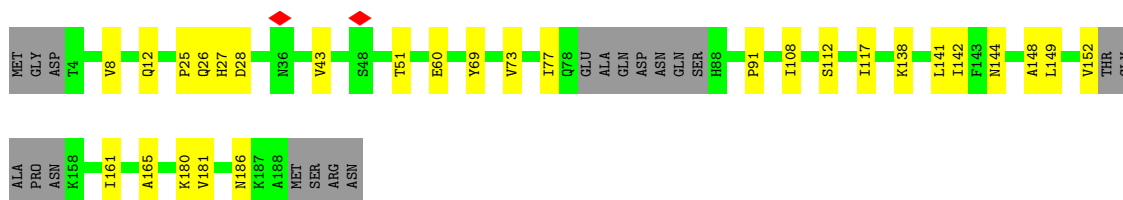
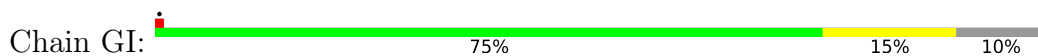
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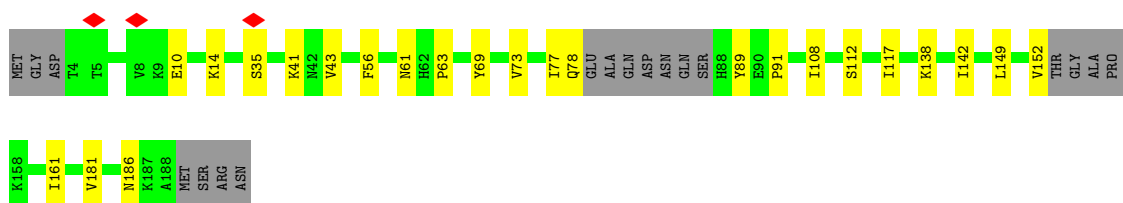
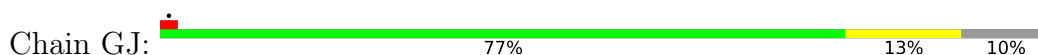
• Molecule 4: Decorator protein P05



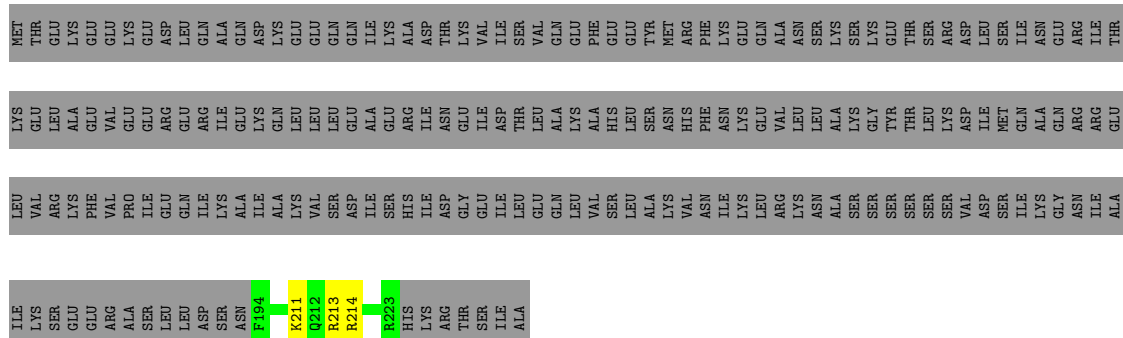
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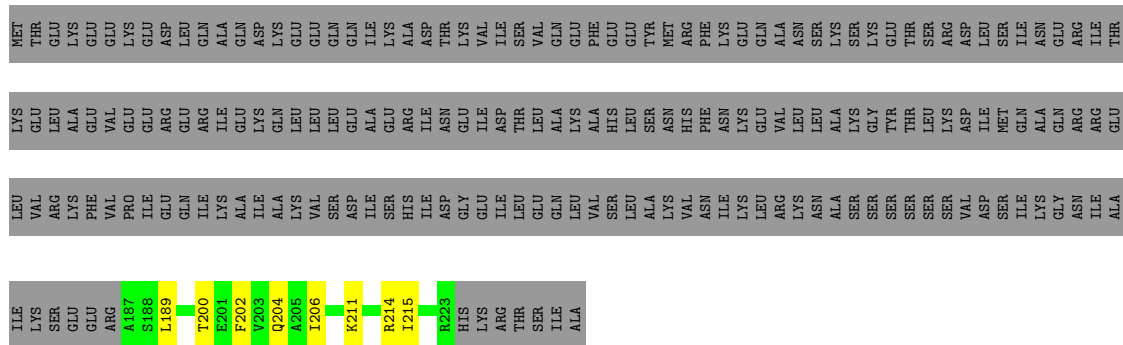
• Molecule 4: Decorator protein P05



• Molecule 5: Scaffold protein



• Molecule 5: Scaffold protein



- Molecule 5: Scaffold protein

Chain GM:  14% 84%

MET	THR	GLU	LEU	LYS	GLU	GLY	LYS	ASP	GLN	GLN	ALA	GLN	ASP	LYS	GLU	GLU	GLN	GLN	ILE	LYS	ALA	ALA	ASP	THR	LYS	VAL	ILE	SER	THR	GLN	GLN	ALA	GLN	PHE	GLU	GLU	TYR	MET	ARG	MET	ARG	PHE	LYS	GLU	GLN	ALA	ALA	ASN	SER	LYS	SER	LYS	GLY	TYR	THR	THR	SER	SER	ARG	ASP	ILE	LEU	SER	MET	ILE	GLN	ILE	ASN	GLU	ARG	ILE	THR	
LYS	GLU	LYS	ALA	GLU	VAL	VAL	GLU	GLU	ARG	GLN	ARG	ILE	GLY	LYS	GLN	LEU	LEU	GLY	ALA	ILE	GLU	ARG	ALA	ILE	THR	GLY	ILE	ILE	THR	THR	VAL	GLN	ALA	LYS	ALA	PHE	HIS	GLU	ASN	THR	ASN	PHE	ASN	LYS	GLU	VAL	VAL	ASN	LYS	LEU	ALA	LYS	SER	LYS	GLY	TYR	THR	THR	LEU	LYS	ASP	ILE	LEU	SER	MET	ILE	GLN	ILE	ASN	GLU	ARG	ILE	THR
LEU	VAL	ARG	LYS	GLU	PHE	GLU	PRO	ILE	GLU	GLN	ILE	ILE	ALA	ILE	ALA	VAL	SER	ASP	ILE	ILE	SER	HIS	ALA	THR	THR	GLY	ILE	ILE	THR	THR	GLN	ALA	GLN	LYS	VAL	GLU	GLU	VAL	ASN	VAL	ILE	ILE	LYS	LEU	ALA	ALA	LYS	SER	GLY	SER	GLY	TYR	THR	THR	SER	SER	VAL	VAL	ASP	ILE	LEU	SER	MET	ILE	GLN	ILE	ASN	GLY	ASN	ALA	ARG	ILE	THR
ILE	LYS	SER	GLU	GLU	ARG	A197	M193	T200	Q204	K211	I215	F223	HIS	LYS	THR	SER	GLY	ILE	ILE	ASP	THR	ALA	ASP	THR	LYS	VAL	ILE	ILE	SER	THR	GLN	ALA	GLN	LYS	VAL	PHE	GLU	GLU	TYR	MET	ARG	ARG	PHE	LYS	GLU	GLN	ALA	ASN	SER	LYS	SER	LYS	GLY	TYR	THR	THR	LEU	SER	ARG	ASP	ILE	LEU	SER	MET	ILE	GLN	ILE	ASN	GLU	ARG	ILE	THR	

- Molecule 5: Scaffold protein

Chain GN:  15% 84%

MET	THR	GLU	LEU	LYS	GLU	GLY	LYS	ASP	GLN	GLN	ALA	GLN	ASP	LYS	GLU	GLU	GLN	GLN	ILE	LYS	ALA	ALA	ASP	THR	LYS	VAL	ILE	SER	THR	GLN	GLN	ALA	GLN	PHE	GLU	GLU	TYR	MET	ARG	MET	ARG	PHE	LYS	GLU	GLN	ALA	ASN	SER	LYS	SER	LYS	GLY	TYR	THR	THR	SER	SER	ARG	ASP	ILE	LEU	SER	MET	ILE	GLN	ILE	ASN	GLU	ARG	ILE	THR									
LYS	GLU	LYS	ALA	GLU	VAL	VAL	GLU	GLU	ARG	GLN	ARG	ILE	GLY	LYS	GLN	LEU	LEU	GLY	ALA	ILE	GLU	ARG	ALA	ASP	THR	GLY	ILE	ILE	THR	THR	VAL	GLN	ALA	LYS	VAL	ALA	GLU	GLU	TYR	MET	LYS	ASN	HIS	ASN	PHE	ASN	LYS	VAL	VAL	ASN	ILE	LYS	GLU	VAL	ASN	LYS	ALA	LYS	SER	GLY	TYR	THR	THR	LEU	LYS	ASP	ILE	LEU	SER	MET	ILE	GLN	ILE	ASN	GLY	ASN	ALA	ARG	ILE	THR
LEU	VAL	ARG	LYS	GLU	PHE	GLU	PRO	ILE	GLU	GLN	ILE	ILE	ALA	ILE	ALA	VAL	SER	ASP	ILE	ILE	SER	HIS	ALA	THR	THR	GLY	ILE	ILE	THR	THR	GLN	ALA	GLN	LYS	VAL	GLU	GLU	VAL	ASN	VAL	ILE	ILE	LYS	LEU	ALA	ALA	LYS	SER	GLY	SER	GLY	TYR	THR	THR	SER	SER	VAL	VAL	ASP	ILE	LEU	SER	MET	ILE	GLN	ILE	ASN	GLY	ASN	ALA	ARG	ILE	THR							
ILE	LYS	SER	GLU	GLU	ARG	A197	M193	F202	I206	F223	HIS	LYS	THR	SER	ILE	GLY	ARG	THR	SER	ILE	ASP	THR	ALA	ASP	THR	LYS	VAL	ILE	ILE	THR	GLN	ALA	GLN	LYS	VAL	ALA	GLU	GLU	TYR	MET	ARG	ARG	PHE	LYS	GLU	GLN	ALA	ASN	SER	LYS	SER	LYS	GLY	TYR	THR	THR	LEU	LYS	ASP	ILE	LEU	SER	MET	ILE	GLN	ILE	ASN	GLY	ASN	ALA	ARG	ILE	THR							

- Molecule 5: Scaffold protein

Chain GO:  15% 84%

MET	THR	GLU	LEU	LYS	GLU	GLY	LYS	ASP	GLN	GLN	ALA	GLN	ASP	LYS	GLU	GLU	GLN	GLN	ILE	LYS	ALA	ALA	ASP	THR	LYS	VAL	ILE	SER	THR	GLN	GLN	ALA	GLN	PHE	GLU	GLU	TYR	MET	ARG	MET	ARG	PHE	LYS	GLU	GLN	ALA	ASN	SER	LYS	SER	LYS	GLY	TYR	THR	THR	SER	SER	ARG	ASP	ILE	LEU	SER	MET	ILE	GLN	ILE	ASN	GLU	ARG	ILE	THR									
LYS	GLU	LEU	ALA	GLU	VAL	VAL	GLU	GLU	ARG	GLN	ARG	ILE	GLY	LYS	GLN	LEU	LEU	GLY	ALA	ILE	GLU	ARG	ALA	ASP	THR	GLY	ILE	ILE	THR	THR	VAL	GLN	ALA	LYS	VAL	ALA	GLU	GLU	TYR	MET	LYS	ASN	HIS	ASN	PHE	ASN	LYS	VAL	VAL	ASN	ILE	LYS	GLU	VAL	ASN	LYS	ALA	LYS	SER	GLY	TYR	THR	THR	LEU	LYS	ASP	ILE	LEU	SER	MET	ILE	GLN	ILE	ASN	GLY	ASN	ALA	ARG	ILE	THR
LEU	VAL	ARG	LYS	GLU	PHE	GLU	PRO	ILE	GLU	GLN	ILE	ILE	ALA	ILE	ALA	VAL	SER	ASP	ILE	ILE	SER	HIS	ALA	THR	THR	GLY	ILE	ILE	THR	THR	GLN	ALA	GLN	LYS	VAL	GLU	GLU	VAL	ASN	VAL	ILE	ILE	LYS	LEU	ALA	ALA	LYS	SER	GLY	SER	GLY	TYR	THR	THR	SER	SER	VAL	VAL	ASP	ILE	LEU	SER	MET	ILE	GLN	ILE	ASN	GLY	ASN	ALA	ARG	ILE	THR							
ILE	LYS	SER	GLU	GLU	ARG	A197	F202	I206	F223	HIS	LYS	THR	SER	ILE	GLY	ARG	THR	SER	ILE	ASP	THR	ALA	ASP	THR	LYS	VAL	ILE	ILE	THR	GLN	ALA	GLN	LYS	VAL	ALA	GLU	GLU	TYR	MET	ARG	ARG	PHE	LYS	GLU	GLN	ALA	ASN	SER	LYS	SER	LYS	GLY	TYR	THR	THR	LEU	LYS	ASP	ILE	LEU	SER	MET	ILE	GLN	ILE	ASN	GLY	ASN	ALA	ARG	ILE	THR								

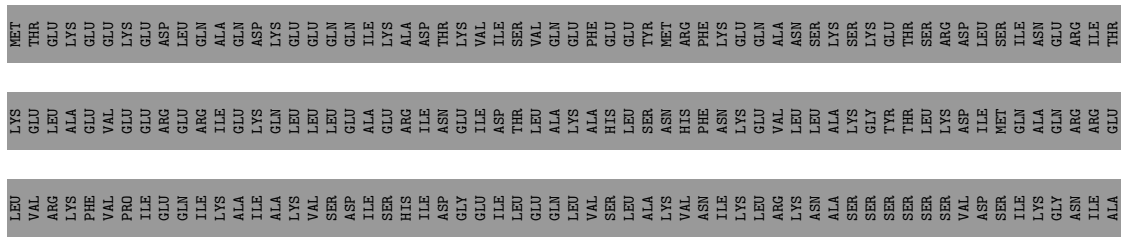
- Molecule 5: Scaffold protein

Chain GP:  16% 84%

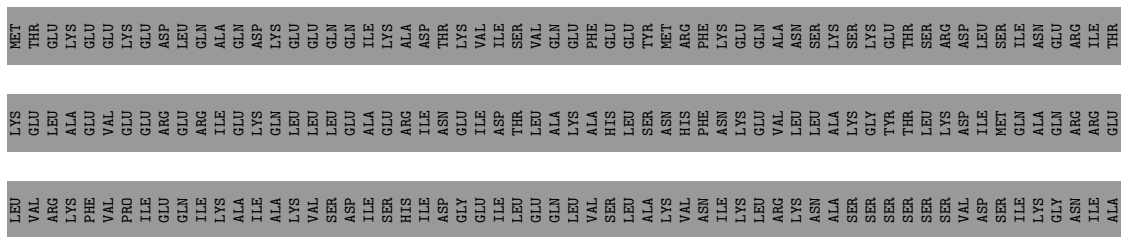
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-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



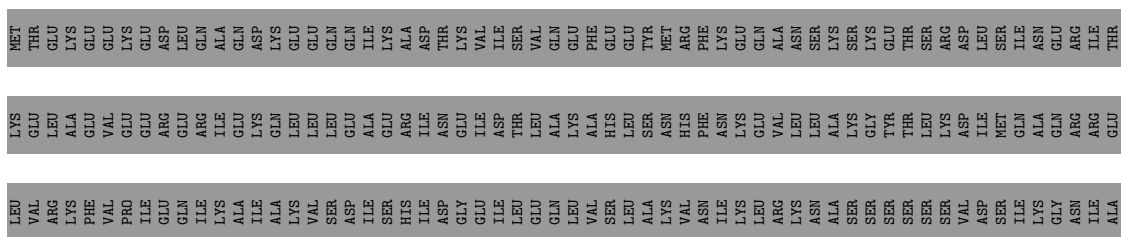
• Molecule 5: Scaffold protein



• Molecule 5: Scaffold protein



• Molecule 5: Scaffold protein

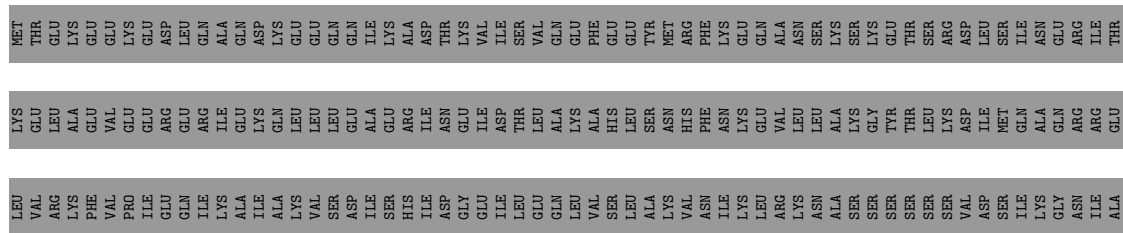


• Molecule 5: Scaffold protein

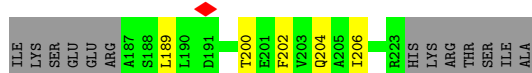
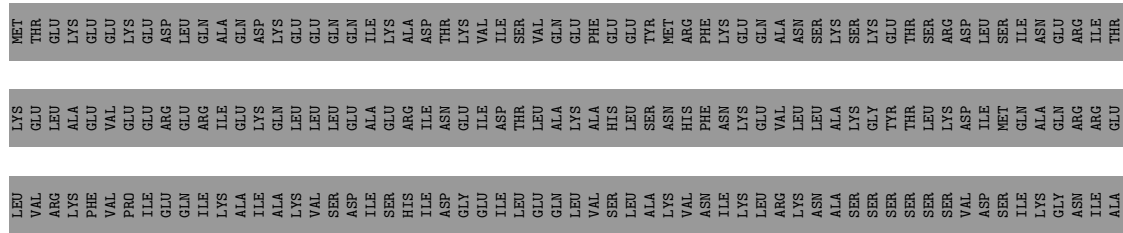




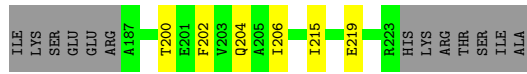
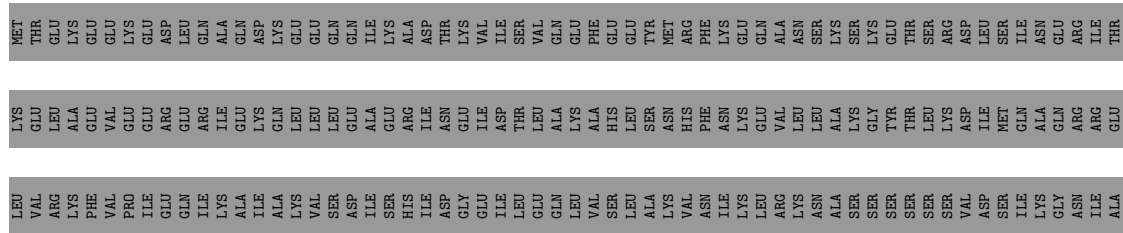
● Molecule 5: Scaffold protein



● Molecule 5: Scaffold protein



● Molecule 5: Scaffold protein

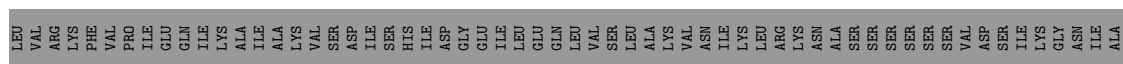
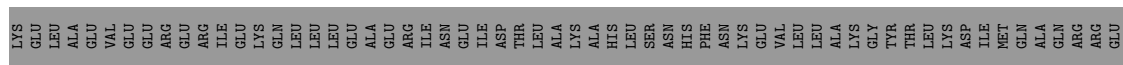
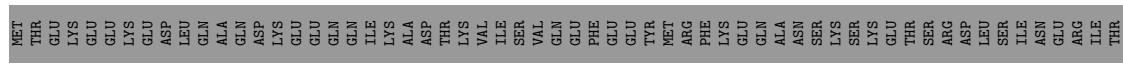


● Molecule 5: Scaffold protein

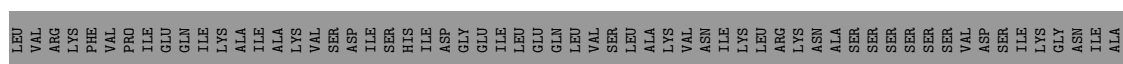
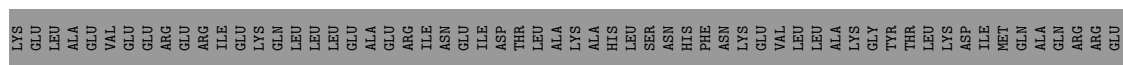
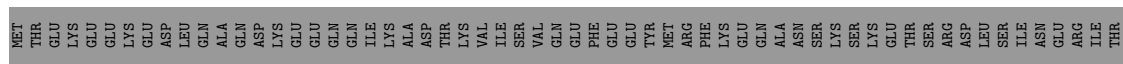




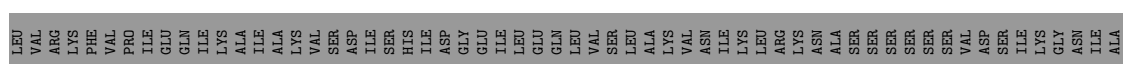
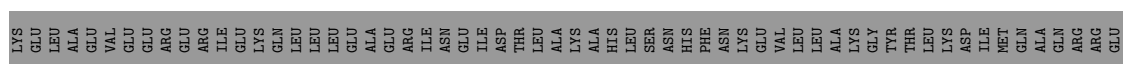
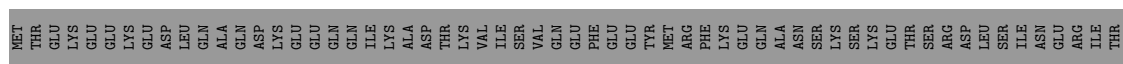
• Molecule 5: Scaffold protein



• Molecule 5: Scaffold protein



• Molecule 5: Scaffold protein



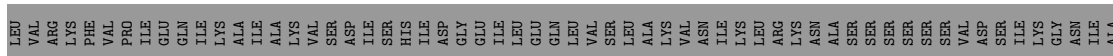
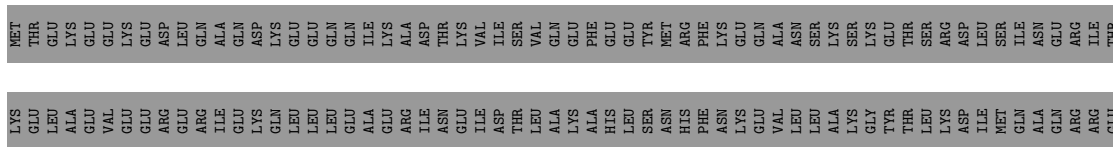
• Molecule 5: Scaffold protein





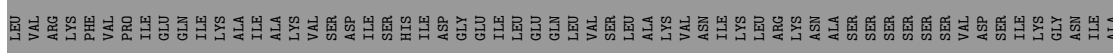
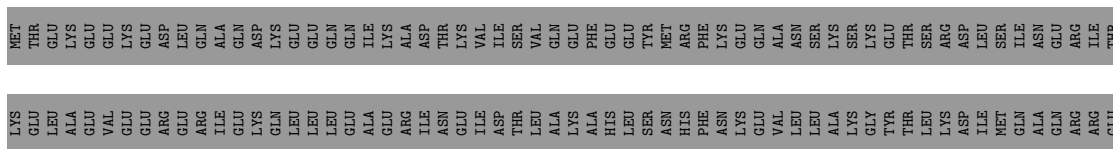
- Molecule 5: Scaffold protein

Chain HO: 16% 84%



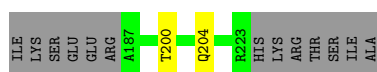
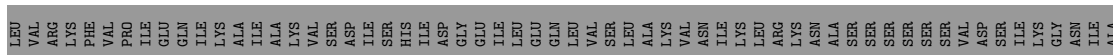
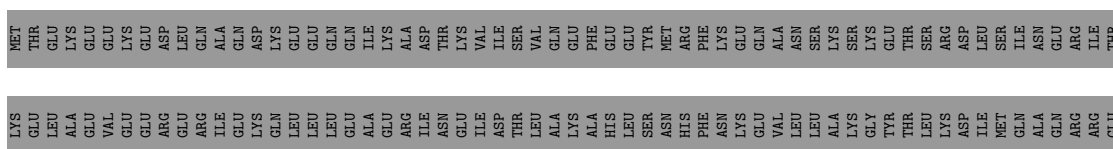
- Molecule 5: Scaffold protein

Chain HP: 16% 84%



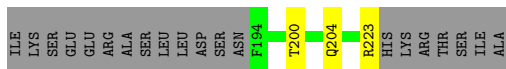
- Molecule 5: Scaffold protein

Chain HQ: 15% 84%



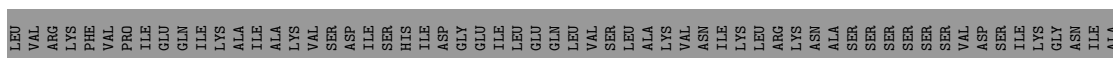
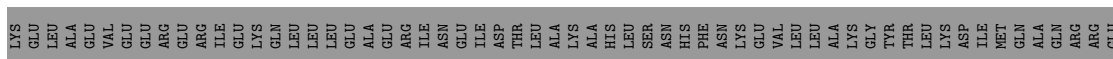
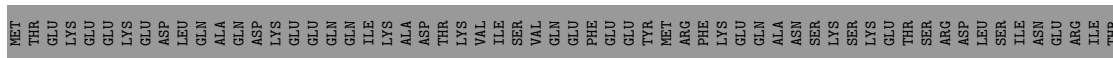
- Molecule 5: Scaffold protein

Chain HR: 15% 84%



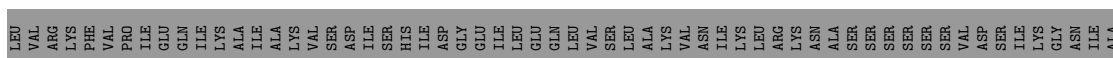
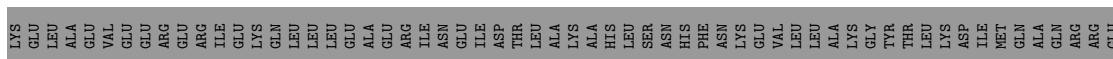
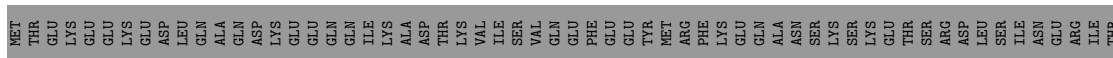
• Molecule 5: Scaffold protein

Chain IJ: 12% . 87%



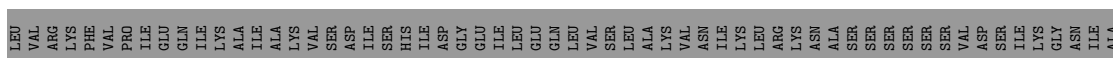
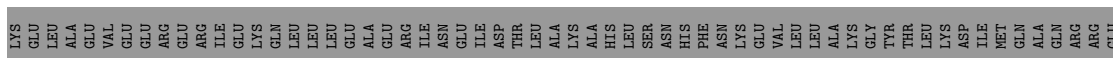
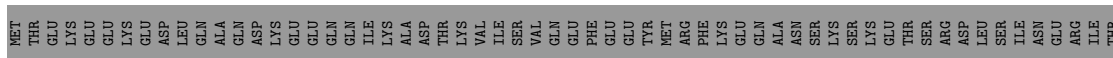
• Molecule 5: Scaffold protein

Chain IK: 12% . 87%



• Molecule 5: Scaffold protein

Chain IL: 16% . 83%



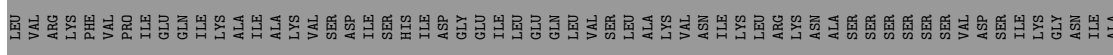
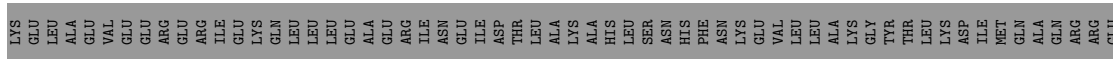
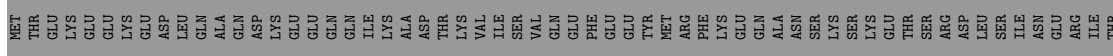
• Molecule 5: Scaffold protein

Chain IM: 16% . 84%



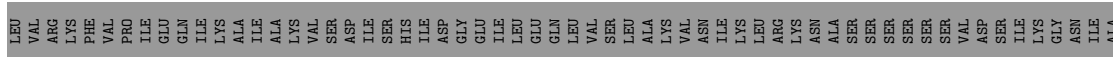
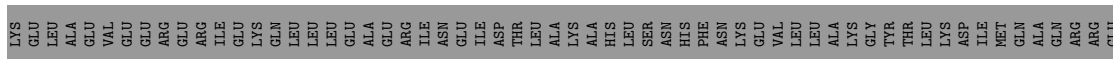
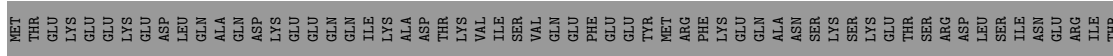
- Molecule 5: Scaffold protein

Chain IX:  16% 84%



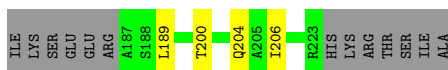
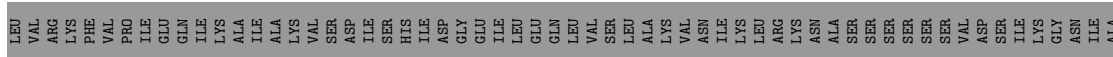
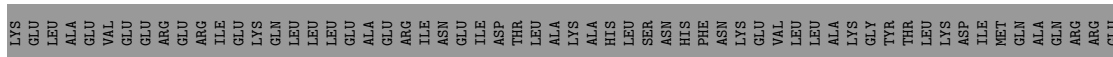
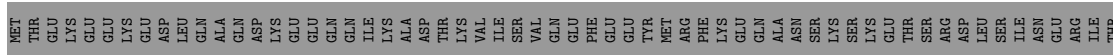
- Molecule 5: Scaffold protein

Chain IV:  17% 83%



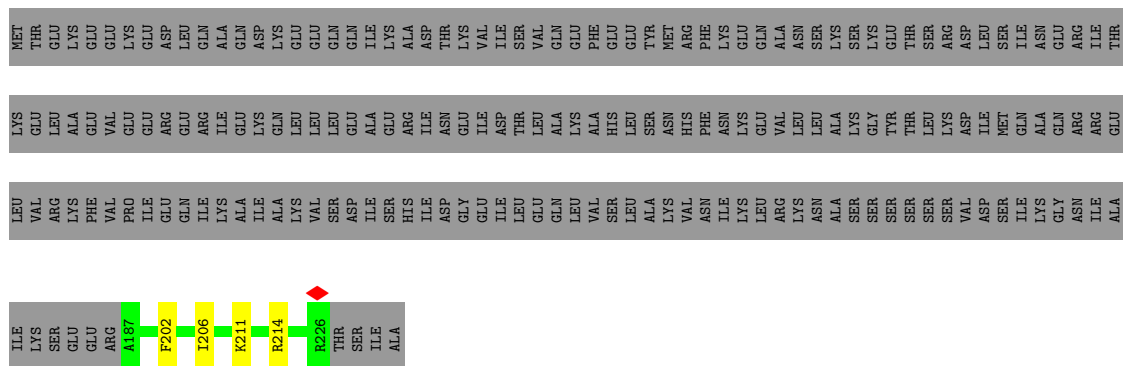
- Molecule 5: Scaffold protein

Chain IZ:  14% 84%



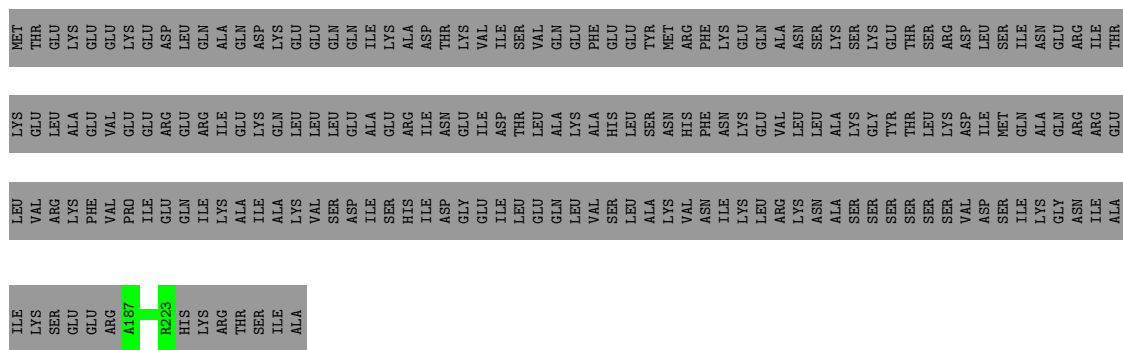
- Molecule 5: Scaffold protein

Chain JA:  16% 83%



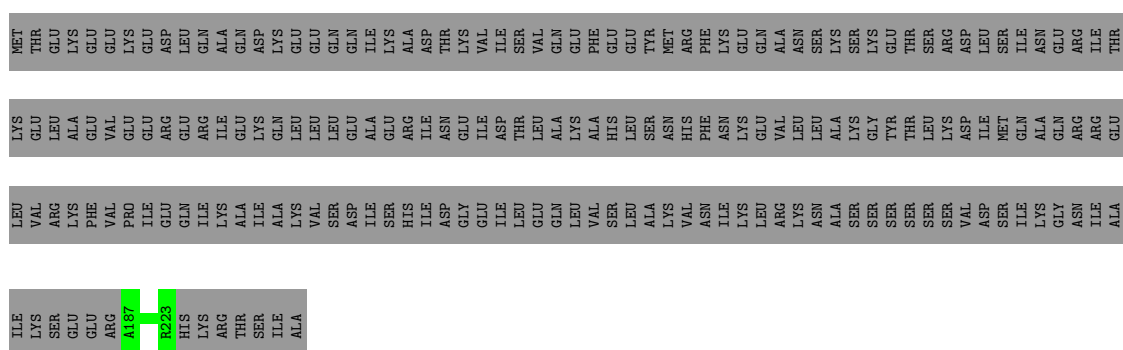
• Molecule 5: Scaffold protein

Chain JB: 16% 84%



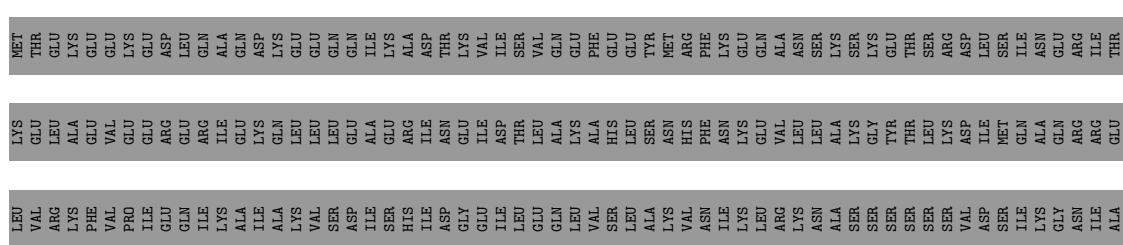
• Molecule 5: Scaffold protein

Chain JC: 16% 84%



• Molecule 5: Scaffold protein

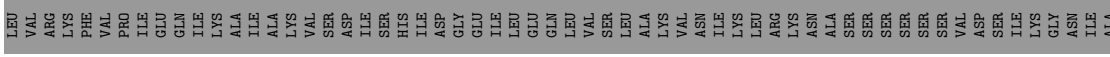
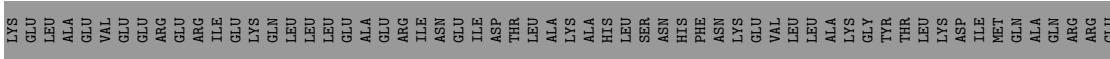
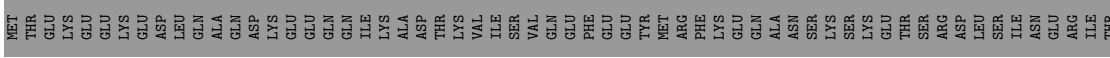
Chain JD: 17% 83%





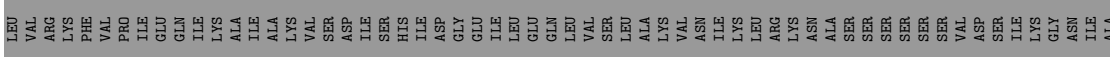
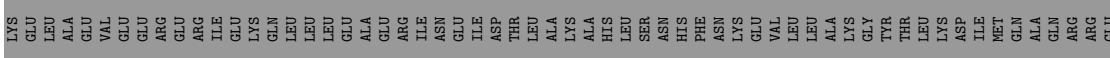
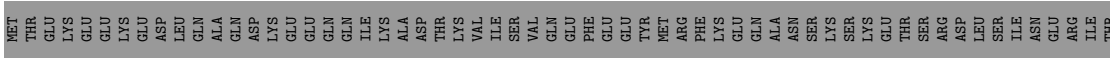
• Molecule 5: Scaffold protein

Chain JE: 15% 84%



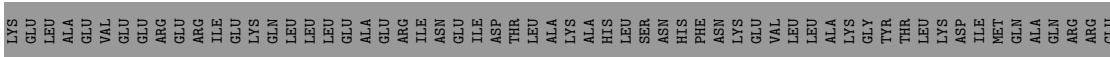
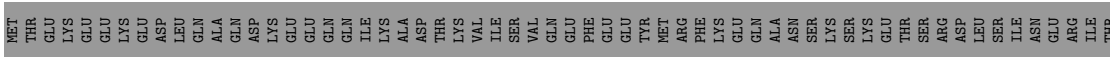
• Molecule 5: Scaffold protein

Chain JF: 15% 84%



• Molecule 5: Scaffold protein

Chain JG: 15% 83%



• Molecule 5: Scaffold protein

Chain JH: 15% 84%

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

ILE	ILE
LYS	LYS
SER	SER
GLU	GLU
GLU	GLU
ARG	ARG
A187	A187
S186	S186
L189	L189
T200	T200
Q204	Q204
A205	A205
I206	I206
R223	R223
HIS	HIS
LYS	LYS
ARG	ARG
THR	THR
SER	SER
ILE	ILE
ALA	ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	25958	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	16500	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.098	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	1200.384, 1200.384, 1200.384	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.6672001, 1.6672001, 1.6672001	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	0.25	0/2536	0.43	0/3428
1	AB	0.24	0/2558	0.43	0/3458
1	AC	0.25	0/2558	0.43	0/3458
1	AD	0.24	0/2536	0.43	0/3428
1	AE	0.24	0/2558	0.43	0/3458
1	AF	0.25	0/2558	0.43	0/3458
1	AG	0.25	0/2536	0.43	0/3428
1	AH	0.24	0/2558	0.43	0/3458
1	AI	0.25	0/2558	0.43	0/3458
1	AJ	0.24	0/2536	0.43	0/3428
1	AK	0.24	0/2558	0.43	0/3458
1	AL	0.24	0/2558	0.43	0/3458
1	AM	0.24	0/2536	0.43	0/3428
1	AN	0.24	0/2558	0.44	0/3458
1	AO	0.24	0/2558	0.43	0/3458
1	AP	0.25	0/2536	0.43	0/3428
1	AQ	0.24	0/2558	0.44	0/3458
1	AR	0.25	0/2558	0.43	0/3458
1	AS	0.24	0/2558	0.43	0/3458
1	AT	0.25	0/2558	0.44	0/3458
1	AU	0.24	0/2558	0.44	0/3458
1	AV	0.24	0/2558	0.44	0/3458
1	AW	0.24	0/2558	0.44	0/3458
1	AX	0.24	0/2558	0.43	0/3458
1	AY	0.24	0/2558	0.43	0/3458
1	AZ	0.24	0/2558	0.44	0/3458
1	BA	0.24	0/2558	0.43	0/3458
1	BB	0.24	0/2558	0.42	0/3458
1	BC	0.24	0/2449	0.42	0/3309
1	BD	0.24	0/2536	0.42	0/3428
1	BE	0.24	0/2558	0.42	0/3458
1	BF	0.24	0/2558	0.42	0/3458
1	BG	0.24	0/2536	0.42	0/3428
1	BH	0.24	0/2558	0.43	0/3458

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BI	0.24	0/2558	0.43	0/3458
1	BJ	0.24	0/2536	0.43	0/3428
1	BK	0.24	0/2558	0.43	0/3458
1	BL	0.24	0/2558	0.42	0/3458
1	BM	0.24	0/2553	0.43	0/3450
1	BN	0.24	0/2558	0.43	0/3458
1	BO	0.24	0/2558	0.43	0/3458
1	BP	0.24	0/2536	0.42	0/3428
1	BQ	0.24	0/2558	0.43	0/3458
1	BR	0.25	0/2553	0.44	0/3450
1	BS	0.24	0/2558	0.42	0/3458
1	BT	0.24	0/2428	0.43	0/3281
1	BU	0.24	0/2558	0.43	0/3458
1	BV	0.24	0/2558	0.43	0/3458
1	BW	0.24	0/2558	0.43	0/3458
1	BX	0.24	0/2428	0.43	0/3281
1	BY	0.24	0/2558	0.43	0/3458
1	BZ	0.24	0/2558	0.42	0/3458
1	CA	0.24	0/2558	0.42	0/3458
1	CB	0.24	0/2558	0.43	0/3458
1	CC	0.24	0/2558	0.43	0/3458
1	CD	0.24	0/2558	0.42	0/3458
1	CE	0.24	0/2558	0.42	0/3458
1	CF	0.24	0/2558	0.42	0/3458
1	CG	0.24	0/2558	0.43	0/3458
1	CH	0.24	0/2558	0.43	0/3458
1	CI	0.24	0/2558	0.43	0/3458
1	CJ	0.24	0/2558	0.43	0/3458
1	CK	0.24	0/2558	0.43	0/3458
1	CL	0.24	0/2558	0.42	0/3458
1	CM	0.24	0/2558	0.43	0/3458
1	CN	0.24	0/2558	0.43	0/3458
1	CO	0.24	0/2558	0.42	0/3458
1	CP	0.24	0/2558	0.42	0/3458
1	CQ	0.24	0/2558	0.42	0/3458
1	CR	0.24	0/2558	0.43	0/3458
1	CS	0.24	0/2558	0.43	0/3458
1	CT	0.24	0/2558	0.42	0/3458
1	CU	0.24	0/2558	0.42	0/3458
1	CV	0.24	0/2558	0.42	0/3458
1	CW	0.24	0/2558	0.43	0/3458
1	CX	0.24	0/2558	0.43	0/3458
1	CY	0.24	0/2558	0.42	0/3458

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	CZ	0.24	0/2558	0.42	0/3458
1	DA	0.24	0/2558	0.42	0/3458
1	DB	0.24	0/2558	0.42	0/3458
1	DC	0.24	0/2558	0.43	0/3458
1	DD	0.24	0/2558	0.42	0/3458
1	DE	0.24	0/2558	0.42	0/3458
2	DF	0.25	0/1195	0.46	0/1608
2	DG	0.25	0/1177	0.44	0/1583
2	DH	0.24	0/1190	0.44	0/1601
2	DI	0.25	0/1182	0.46	0/1590
2	DJ	0.25	0/1190	0.45	0/1601
2	DK	0.24	0/1182	0.45	0/1590
2	DL	0.25	0/1190	0.46	0/1601
2	DM	0.25	0/1187	0.45	0/1597
2	DN	0.25	0/1190	0.45	0/1601
2	DO	0.25	0/1182	0.46	0/1590
2	DP	0.24	0/1182	0.44	0/1590
2	DQ	0.25	0/1177	0.45	0/1583
2	DR	0.24	0/1190	0.45	0/1601
2	DS	0.26	0/1306	0.46	0/1755
2	DT	0.25	0/1190	0.45	0/1601
2	DU	0.25	0/1178	0.44	0/1586
2	DV	0.24	0/1182	0.43	0/1590
2	DW	0.24	0/1178	0.44	0/1586
2	DX	0.25	0/1216	0.44	0/1637
2	DY	0.24	0/1165	0.43	0/1568
2	DZ	0.25	0/1190	0.45	0/1601
2	EA	0.24	0/931	0.44	0/1252
2	EB	0.25	0/1216	0.45	0/1637
2	EC	0.25	0/1181	0.44	0/1590
2	ED	0.25	0/1229	0.46	0/1655
2	EE	0.25	0/1212	0.45	0/1633
2	EF	0.24	0/1190	0.44	0/1601
2	EG	0.25	0/1356	0.44	0/1823
2	EH	0.25	0/1182	0.45	0/1590
2	EI	0.24	0/1207	0.44	0/1626
2	EJ	0.24	0/1293	0.44	0/1737
2	EK	0.24	0/1306	0.44	0/1755
2	EL	0.25	0/1177	0.44	0/1583
2	EM	0.24	0/1190	0.45	0/1601
2	EN	0.25	0/1182	0.44	0/1590
2	EO	0.24	0/1322	0.44	0/1776
2	EP	0.24	0/1178	0.44	0/1586

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	EQ	0.24	0/1216	0.44	0/1637
2	ER	0.25	0/1165	0.43	0/1568
2	ES	0.25	0/1190	0.44	0/1601
2	ET	0.24	0/1178	0.44	0/1586
2	EU	0.24	0/1216	0.44	0/1637
2	EV	0.25	0/1165	0.43	0/1568
2	EW	0.24	0/1190	0.45	0/1601
2	EX	0.24	0/1178	0.45	0/1586
2	EY	0.24	0/1216	0.44	0/1637
2	EZ	0.25	0/1165	0.44	0/1568
2	FA	0.24	0/1190	0.44	0/1601
2	FB	0.25	0/1178	0.45	0/1586
2	FC	0.25	0/1216	0.44	0/1637
2	FD	0.24	0/1165	0.43	0/1568
2	FE	0.24	0/1190	0.45	0/1601
2	FF	0.25	0/1178	0.45	0/1586
2	FG	0.24	0/1216	0.44	0/1637
2	FH	0.25	0/1165	0.44	0/1568
2	FI	0.25	0/1190	0.45	0/1601
3	FJ	0.26	0/1274	0.46	0/1721
4	FK	0.25	0/1216	0.46	0/1636
4	FL	0.25	0/1216	0.46	0/1636
4	FM	0.25	0/1225	0.46	0/1649
4	FN	0.25	0/1219	0.46	0/1641
4	FO	0.25	0/1243	0.47	0/1672
4	FP	0.24	0/1212	0.46	0/1632
4	FQ	0.24	0/1381	0.45	0/1855
4	FR	0.24	0/1381	0.45	0/1855
4	FS	0.24	0/1381	0.45	0/1855
4	FT	0.24	0/1158	0.44	0/1559
4	FU	0.25	0/1208	0.45	0/1626
4	FV	0.24	0/1229	0.45	0/1653
4	FW	0.25	0/1229	0.46	0/1653
4	FX	0.25	0/1207	0.45	0/1625
4	FY	0.24	0/1207	0.45	0/1625
4	FZ	0.24	0/1216	0.45	0/1636
4	GA	0.24	0/1381	0.45	0/1855
4	GB	0.24	0/1381	0.44	0/1855
4	GC	0.24	0/1381	0.44	0/1855
4	GD	0.24	0/1381	0.44	0/1855
4	GE	0.24	0/1381	0.44	0/1855
4	GF	0.24	0/1381	0.44	0/1855
4	GG	0.24	0/1381	0.44	0/1855

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	GH	0.24	0/1381	0.45	0/1855
4	GI	0.24	0/1381	0.45	0/1855
4	GJ	0.24	0/1381	0.45	0/1855
5	GK	0.26	0/272	0.46	0/365
5	GL	0.26	0/321	0.45	0/432
5	GM	0.26	0/321	0.45	0/432
5	GN	0.26	0/321	0.44	0/432
5	GO	0.26	0/321	0.44	0/432
5	GP	0.26	0/321	0.44	0/432
5	GQ	0.25	0/321	0.44	0/432
5	GR	0.26	0/321	0.45	0/432
5	GS	0.26	0/321	0.44	0/432
5	GT	0.26	0/321	0.45	0/432
5	GU	0.26	0/321	0.45	0/432
5	GV	0.26	0/321	0.44	0/432
5	GW	0.26	0/272	0.46	0/365
5	GX	0.26	0/321	0.46	0/432
5	GY	0.26	0/321	0.46	0/432
5	GZ	0.26	0/321	0.45	0/432
5	HA	0.26	0/321	0.45	0/432
5	HB	0.25	0/321	0.45	0/432
5	HC	0.26	0/321	0.44	0/432
5	HD	0.27	0/272	0.47	0/365
5	HE	0.25	0/321	0.44	0/432
5	HF	0.25	0/321	0.45	0/432
5	HG	0.26	0/321	0.45	0/432
5	HH	0.26	0/272	0.47	0/365
5	HI	0.26	0/272	0.47	0/365
5	HJ	0.26	0/272	0.49	0/365
5	HK	0.26	0/272	0.46	0/365
5	HL	0.25	0/321	0.43	0/432
5	HM	0.25	0/260	0.45	0/349
5	HN	0.25	0/321	0.43	0/432
5	HO	0.25	0/321	0.43	0/432
5	HP	0.25	0/321	0.43	0/432
5	HQ	0.25	0/321	0.43	0/432
5	HR	0.25	0/321	0.43	0/432
5	HS	0.25	0/321	0.43	0/432
5	HT	0.25	0/321	0.44	0/432
5	HU	0.26	0/321	0.44	0/432
5	HV	0.25	0/321	0.43	0/432
5	HW	0.25	0/253	0.45	0/338
5	HX	0.25	0/321	0.44	0/432

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	HY	0.25	0/321	0.44	0/432
5	HZ	0.25	0/321	0.43	0/432
5	IA	0.25	0/321	0.43	0/432
5	IB	0.25	0/260	0.45	0/349
5	IC	0.26	0/321	0.43	0/432
5	ID	0.25	0/260	0.45	0/349
5	IE	0.25	0/321	0.43	0/432
5	IF	0.25	0/321	0.44	0/432
5	IG	0.25	0/321	0.43	0/432
5	IH	0.26	0/260	0.46	0/349
5	II	0.26	0/272	0.45	0/365
5	IJ	0.26	0/272	0.47	0/365
5	IK	0.25	0/272	0.45	0/365
5	IL	0.25	0/352	0.46	0/472
5	IM	0.26	0/321	0.43	0/432
5	IN	0.25	0/321	0.43	0/432
5	IO	0.25	0/352	0.45	0/472
5	IP	0.25	0/321	0.43	0/432
5	IQ	0.26	0/321	0.44	0/432
5	IR	0.25	0/352	0.46	0/472
5	IS	0.26	0/321	0.43	0/432
5	IT	0.25	0/321	0.43	0/432
5	IU	0.25	0/352	0.46	0/472
5	IV	0.25	0/321	0.43	0/432
5	IW	0.25	0/321	0.43	0/432
5	IX	0.25	0/321	0.43	0/432
5	IY	0.25	0/352	0.47	0/472
5	IZ	0.25	0/321	0.43	0/432
5	JA	0.25	0/352	0.46	0/472
5	JB	0.25	0/321	0.43	0/432
5	JC	0.25	0/321	0.42	0/432
5	JD	0.25	0/352	0.45	0/472
5	JE	0.25	0/321	0.43	0/432
5	JF	0.25	0/321	0.43	0/432
5	JG	0.25	0/352	0.47	0/472
5	JH	0.26	0/321	0.43	0/432
5	JI	0.25	0/321	0.43	0/432
5	JJ	0.25	0/352	0.46	0/472
5	JK	0.25	0/321	0.43	0/432
5	JL	0.25	0/321	0.44	0/432
5	JM	0.26	0/321	0.43	0/432
5	JN	0.25	0/352	0.46	0/472
5	JO	0.25	0/321	0.43	0/432

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.24	0/339816	0.43	0/458503

There are no bond length outliers.

There are no bond angle outliers.

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	2488	0	2527	23	0
1	AB	2510	0	2547	23	0
1	AC	2510	0	2547	27	0
1	AD	2488	0	2527	24	0
1	AE	2510	0	2547	25	0
1	AF	2510	0	2547	31	0
1	AG	2488	0	2527	32	0
1	AH	2510	0	2547	30	0
1	AI	2510	0	2547	20	0
1	AJ	2488	0	2527	30	0
1	AK	2510	0	2547	31	0
1	AL	2510	0	2547	29	0
1	AM	2488	0	2527	29	0
1	AN	2510	0	2547	32	0
1	AO	2510	0	2547	37	0
1	AP	2488	0	2527	33	0
1	AQ	2510	0	2547	24	0
1	AR	2510	0	2547	30	0
1	AS	2510	0	2547	43	0
1	AT	2510	0	2547	33	0
1	AU	2510	0	2547	35	0
1	AV	2510	0	2547	37	0
1	AW	2510	0	2547	26	0
1	AX	2510	0	2547	37	0
1	AY	2510	0	2547	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AZ	2510	0	2547	38	0
1	BA	2510	0	2547	39	0
1	BB	2510	0	2547	25	0
1	BC	2405	0	2453	23	0
1	BD	2488	0	2527	26	0
1	BE	2510	0	2547	22	0
1	BF	2510	0	2547	25	0
1	BG	2488	0	2527	27	0
1	BH	2510	0	2547	26	0
1	BI	2510	0	2547	23	0
1	BJ	2488	0	2527	31	0
1	BK	2510	0	2547	35	0
1	BL	2510	0	2547	25	0
1	BM	2505	0	2545	27	0
1	BN	2510	0	2547	22	0
1	BO	2510	0	2547	32	0
1	BP	2488	0	2527	33	0
1	BQ	2510	0	2547	24	0
1	BR	2505	0	2545	26	0
1	BS	2510	0	2547	34	0
1	BT	2383	0	2425	24	0
1	BU	2510	0	2547	34	0
1	BV	2510	0	2547	32	0
1	BW	2510	0	2547	24	0
1	BX	2383	0	2425	26	0
1	BY	2510	0	2547	42	0
1	BZ	2510	0	2547	32	0
1	CA	2510	0	2547	38	0
1	CB	2510	0	2547	29	0
1	CC	2510	0	2547	28	0
1	CD	2510	0	2547	29	0
1	CE	2510	0	2547	30	0
1	CF	2510	0	2547	39	0
1	CG	2510	0	2547	33	0
1	CH	2510	0	2547	35	0
1	CI	2510	0	2547	22	0
1	CJ	2510	0	2547	25	0
1	CK	2510	0	2547	38	0
1	CL	2510	0	2547	39	0
1	CM	2510	0	2547	29	0
1	CN	2510	0	2547	28	0
1	CO	2510	0	2547	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CP	2510	0	2547	35	0
1	CQ	2510	0	2547	25	0
1	CR	2510	0	2547	29	0
1	CS	2510	0	2547	35	0
1	CT	2510	0	2547	35	0
1	CU	2510	0	2547	41	0
1	CV	2510	0	2547	40	0
1	CW	2510	0	2547	37	0
1	CX	2510	0	2547	24	0
1	CY	2510	0	2547	24	0
1	CZ	2510	0	2547	36	0
1	DA	2510	0	2547	36	0
1	DB	2510	0	2547	28	0
1	DC	2510	0	2547	34	0
1	DD	2510	0	2547	43	0
1	DE	2510	0	2547	31	0
2	DF	1178	0	1163	6	0
2	DG	1160	0	1142	9	0
2	DH	1173	0	1158	10	0
2	DI	1165	0	1147	9	0
2	DJ	1173	0	1158	13	0
2	DK	1165	0	1147	12	0
2	DL	1173	0	1158	10	0
2	DM	1170	0	1152	12	0
2	DN	1173	0	1158	16	0
2	DO	1165	0	1147	12	0
2	DP	1165	0	1147	17	0
2	DQ	1160	0	1142	12	0
2	DR	1173	0	1158	10	0
2	DS	1288	0	1279	13	0
2	DT	1173	0	1158	31	0
2	DU	1161	0	1139	15	0
2	DV	1165	0	1147	17	0
2	DW	1161	0	1139	17	0
2	DX	1198	0	1172	17	0
2	DY	1148	0	1123	19	0
2	DZ	1173	0	1158	15	0
2	EA	917	0	912	9	0
2	EB	1198	0	1172	18	0
2	EC	1164	0	1145	10	0
2	ED	1211	0	1188	9	0
2	EE	1194	0	1164	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	EF	1173	0	1158	15	0
2	EG	1337	0	1324	15	0
2	EH	1165	0	1147	11	0
2	EI	1189	0	1159	11	0
2	EJ	1275	0	1263	9	0
2	EK	1288	0	1279	17	0
2	EL	1160	0	1142	14	0
2	EM	1173	0	1158	22	0
2	EN	1165	0	1147	17	0
2	EO	1304	0	1299	12	0
2	EP	1161	0	1139	21	0
2	EQ	1198	0	1172	13	0
2	ER	1148	0	1123	18	0
2	ES	1173	0	1158	16	0
2	ET	1161	0	1139	18	0
2	EU	1198	0	1172	14	0
2	EV	1148	0	1123	18	0
2	EW	1173	0	1158	18	0
2	EX	1161	0	1139	15	0
2	EY	1198	0	1172	14	0
2	EZ	1148	0	1123	13	0
2	FA	1173	0	1158	13	0
2	FB	1161	0	1139	19	0
2	FC	1198	0	1172	12	0
2	FD	1148	0	1123	19	0
2	FE	1173	0	1158	19	0
2	FF	1161	0	1139	15	0
2	FG	1198	0	1172	18	0
2	FH	1148	0	1123	17	0
2	FI	1173	0	1158	15	0
3	FJ	1252	0	1235	17	0
4	FK	1195	0	1189	12	0
4	FL	1195	0	1189	12	0
4	FM	1203	0	1190	11	0
4	FN	1197	0	1185	15	0
4	FO	1222	0	1214	14	0
4	FP	1191	0	1181	17	0
4	FQ	1358	0	1361	19	0
4	FR	1358	0	1361	16	0
4	FS	1358	0	1361	21	0
4	FT	1137	0	1125	10	0
4	FU	1187	0	1176	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	FV	1208	0	1203	12	0
4	FW	1208	0	1203	20	0
4	FX	1186	0	1176	12	0
4	FY	1186	0	1176	15	0
4	FZ	1195	0	1189	18	0
4	GA	1358	0	1361	15	0
4	GB	1358	0	1361	15	0
4	GC	1358	0	1361	19	0
4	GD	1358	0	1361	23	0
4	GE	1358	0	1361	18	0
4	GF	1358	0	1361	14	0
4	GG	1358	0	1361	20	0
4	GH	1358	0	1361	20	0
4	GI	1358	0	1361	18	0
4	GJ	1358	0	1361	15	0
5	GK	266	0	265	3	0
5	GL	315	0	312	5	0
5	GM	315	0	312	2	0
5	GN	315	0	312	1	0
5	GO	315	0	312	1	0
5	GP	315	0	312	0	0
5	GQ	315	0	312	5	0
5	GR	315	0	312	1	0
5	GS	315	0	312	2	0
5	GT	315	0	312	1	0
5	GU	315	0	312	3	0
5	GV	315	0	312	2	0
5	GW	266	0	265	2	0
5	GX	315	0	312	4	0
5	GY	315	0	312	4	0
5	GZ	315	0	312	4	0
5	HA	315	0	312	1	0
5	HB	315	0	312	4	0
5	HC	315	0	312	5	0
5	HD	266	0	265	2	0
5	HE	315	0	312	2	0
5	HF	315	0	312	3	0
5	HG	315	0	312	0	0
5	HH	266	0	265	3	0
5	HI	266	0	265	2	0
5	HJ	266	0	265	4	0
5	HK	266	0	265	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	HL	315	0	312	2	0
5	HM	255	0	256	1	0
5	HN	315	0	312	2	0
5	HO	315	0	312	1	0
5	HP	315	0	312	1	0
5	HQ	315	0	312	1	0
5	HR	315	0	312	2	0
5	HS	315	0	312	0	0
5	HT	315	0	312	0	0
5	HU	315	0	312	1	0
5	HV	315	0	312	2	0
5	HW	248	0	248	0	0
5	HX	315	0	312	0	0
5	HY	315	0	312	1	0
5	HZ	315	0	312	1	0
5	IA	315	0	312	1	0
5	IB	255	0	256	2	0
5	IC	315	0	312	2	0
5	ID	255	0	256	0	0
5	IE	315	0	312	2	0
5	IF	315	0	312	2	0
5	IG	315	0	312	0	0
5	IH	255	0	256	3	0
5	II	266	0	265	2	0
5	IJ	266	0	265	1	0
5	IK	266	0	265	1	0
5	IL	345	0	345	2	0
5	IM	315	0	312	0	0
5	IN	315	0	312	1	0
5	IO	345	0	345	1	0
5	IP	315	0	312	1	0
5	IQ	315	0	312	2	0
5	IR	345	0	345	2	0
5	IS	315	0	312	2	0
5	IT	315	0	312	0	0
5	IU	345	0	345	1	0
5	IV	315	0	312	1	0
5	IW	315	0	312	1	0
5	IX	315	0	312	0	0
5	IY	345	0	345	1	0
5	IZ	315	0	312	2	0
5	JA	345	0	345	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	JB	315	0	312	0	0
5	JC	315	0	312	0	0
5	JD	345	0	345	1	0
5	JE	315	0	312	1	0
5	JF	315	0	312	2	0
5	JG	345	0	345	3	0
5	JH	315	0	312	2	0
5	JI	315	0	312	1	0
5	JJ	345	0	345	1	0
5	JK	315	0	312	2	0
5	JL	315	0	312	2	0
5	JM	315	0	312	1	0
5	JN	345	0	345	2	0
5	JO	315	0	312	2	0
All	All	333778	0	335560	3234	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 5.

The worst 5 of 3234 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:BY:165:ILE:HD13	1:BY:191:LEU:HD23	1.62	0.79
1:CF:165:ILE:HD13	1:CF:191:LEU:HD23	1.64	0.79
4:FX:77:ILE:HG13	4:FX:91:PRO:HB3	1.66	0.77
1:CU:165:ILE:HD13	1:CU:191:LEU:HD23	1.64	0.77
1:CP:165:ILE:HD13	1:CP:191:LEU:HD23	1.67	0.76

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	305/319 (96%)	302 (99%)	3 (1%)	0	100	100
1	AB	309/319 (97%)	302 (98%)	7 (2%)	0	100	100
1	AC	309/319 (97%)	303 (98%)	6 (2%)	0	100	100
1	AD	305/319 (96%)	302 (99%)	3 (1%)	0	100	100
1	AE	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	AF	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	AG	305/319 (96%)	301 (99%)	4 (1%)	0	100	100
1	AH	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	AI	309/319 (97%)	307 (99%)	2 (1%)	0	100	100
1	AJ	305/319 (96%)	300 (98%)	5 (2%)	0	100	100
1	AK	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	AL	309/319 (97%)	304 (98%)	5 (2%)	0	100	100
1	AM	305/319 (96%)	301 (99%)	4 (1%)	0	100	100
1	AN	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	AO	309/319 (97%)	304 (98%)	5 (2%)	0	100	100
1	AP	305/319 (96%)	301 (99%)	4 (1%)	0	100	100
1	AQ	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	AR	309/319 (97%)	304 (98%)	5 (2%)	0	100	100
1	AS	309/319 (97%)	303 (98%)	6 (2%)	0	100	100
1	AT	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	AU	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	AV	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	AW	309/319 (97%)	307 (99%)	2 (1%)	0	100	100
1	AX	309/319 (97%)	307 (99%)	2 (1%)	0	100	100
1	AY	309/319 (97%)	302 (98%)	7 (2%)	0	100	100
1	AZ	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	BA	309/319 (97%)	307 (99%)	2 (1%)	0	100	100
1	BB	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	BC	294/319 (92%)	286 (97%)	8 (3%)	0	100	100
1	BD	305/319 (96%)	301 (99%)	4 (1%)	0	100	100
1	BE	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	BF	309/319 (97%)	304 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BG	305/319 (96%)	300 (98%)	5 (2%)	0	100	100
1	BH	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	BI	309/319 (97%)	304 (98%)	5 (2%)	0	100	100
1	BJ	305/319 (96%)	299 (98%)	6 (2%)	0	100	100
1	BK	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	BL	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	BM	307/319 (96%)	304 (99%)	3 (1%)	0	100	100
1	BN	309/319 (97%)	304 (98%)	5 (2%)	0	100	100
1	BO	309/319 (97%)	304 (98%)	5 (2%)	0	100	100
1	BP	305/319 (96%)	302 (99%)	3 (1%)	0	100	100
1	BQ	309/319 (97%)	307 (99%)	2 (1%)	0	100	100
1	BR	307/319 (96%)	302 (98%)	5 (2%)	0	100	100
1	BS	309/319 (97%)	303 (98%)	6 (2%)	0	100	100
1	BT	293/319 (92%)	290 (99%)	3 (1%)	0	100	100
1	BU	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	BV	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	BW	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	BX	293/319 (92%)	289 (99%)	4 (1%)	0	100	100
1	BY	309/319 (97%)	304 (98%)	5 (2%)	0	100	100
1	BZ	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	CA	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	CB	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	CC	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	CD	309/319 (97%)	304 (98%)	5 (2%)	0	100	100
1	CE	309/319 (97%)	302 (98%)	7 (2%)	0	100	100
1	CF	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	CG	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	CH	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	CI	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	CJ	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	CK	309/319 (97%)	302 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CL	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	CM	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	CN	309/319 (97%)	307 (99%)	2 (1%)	0	100	100
1	CO	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	CP	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	CQ	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	CR	309/319 (97%)	307 (99%)	2 (1%)	0	100	100
1	CS	309/319 (97%)	304 (98%)	5 (2%)	0	100	100
1	CT	309/319 (97%)	303 (98%)	6 (2%)	0	100	100
1	CU	309/319 (97%)	307 (99%)	2 (1%)	0	100	100
1	CV	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	CW	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	CX	309/319 (97%)	307 (99%)	2 (1%)	0	100	100
1	CY	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	CZ	309/319 (97%)	302 (98%)	7 (2%)	0	100	100
1	DA	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	DB	309/319 (97%)	305 (99%)	4 (1%)	0	100	100
1	DC	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	DD	309/319 (97%)	306 (99%)	3 (1%)	0	100	100
1	DE	309/319 (97%)	304 (98%)	5 (2%)	0	100	100
2	DF	149/185 (80%)	148 (99%)	1 (1%)	0	100	100
2	DG	146/185 (79%)	145 (99%)	1 (1%)	0	100	100
2	DH	148/185 (80%)	147 (99%)	1 (1%)	0	100	100
2	DI	147/185 (80%)	143 (97%)	4 (3%)	0	100	100
2	DJ	148/185 (80%)	146 (99%)	2 (1%)	0	100	100
2	DK	147/185 (80%)	145 (99%)	2 (1%)	0	100	100
2	DL	148/185 (80%)	148 (100%)	0	0	100	100
2	DM	148/185 (80%)	146 (99%)	2 (1%)	0	100	100
2	DN	148/185 (80%)	146 (99%)	2 (1%)	0	100	100
2	DO	147/185 (80%)	144 (98%)	3 (2%)	0	100	100
2	DP	147/185 (80%)	145 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	DQ	146/185 (79%)	145 (99%)	1 (1%)	0	100	100
2	DR	148/185 (80%)	147 (99%)	1 (1%)	0	100	100
2	DS	162/185 (88%)	160 (99%)	2 (1%)	0	100	100
2	DT	148/185 (80%)	145 (98%)	3 (2%)	0	100	100
2	DU	147/185 (80%)	145 (99%)	2 (1%)	0	100	100
2	DV	147/185 (80%)	146 (99%)	1 (1%)	0	100	100
2	DW	147/185 (80%)	145 (99%)	2 (1%)	0	100	100
2	DX	154/185 (83%)	153 (99%)	1 (1%)	0	100	100
2	DY	145/185 (78%)	142 (98%)	3 (2%)	0	100	100
2	DZ	148/185 (80%)	147 (99%)	1 (1%)	0	100	100
2	EA	114/185 (62%)	113 (99%)	1 (1%)	0	100	100
2	EB	154/185 (83%)	152 (99%)	2 (1%)	0	100	100
2	EC	147/185 (80%)	146 (99%)	1 (1%)	0	100	100
2	ED	156/185 (84%)	153 (98%)	3 (2%)	0	100	100
2	EE	154/185 (83%)	153 (99%)	1 (1%)	0	100	100
2	EF	148/185 (80%)	146 (99%)	2 (1%)	0	100	100
2	EG	171/185 (92%)	168 (98%)	3 (2%)	0	100	100
2	EH	147/185 (80%)	146 (99%)	1 (1%)	0	100	100
2	EI	153/185 (83%)	152 (99%)	1 (1%)	0	100	100
2	EJ	160/185 (86%)	159 (99%)	1 (1%)	0	100	100
2	EK	162/185 (88%)	161 (99%)	1 (1%)	0	100	100
2	EL	146/185 (79%)	144 (99%)	2 (1%)	0	100	100
2	EM	148/185 (80%)	146 (99%)	2 (1%)	0	100	100
2	EN	147/185 (80%)	145 (99%)	2 (1%)	0	100	100
2	EO	164/185 (89%)	163 (99%)	1 (1%)	0	100	100
2	EP	147/185 (80%)	145 (99%)	2 (1%)	0	100	100
2	EQ	154/185 (83%)	153 (99%)	1 (1%)	0	100	100
2	ER	145/185 (78%)	142 (98%)	3 (2%)	0	100	100
2	ES	148/185 (80%)	146 (99%)	2 (1%)	0	100	100
2	ET	147/185 (80%)	145 (99%)	2 (1%)	0	100	100
2	EU	154/185 (83%)	153 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	EV	145/185 (78%)	143 (99%)	2 (1%)	0	100	100
2	EW	148/185 (80%)	145 (98%)	3 (2%)	0	100	100
2	EX	147/185 (80%)	146 (99%)	1 (1%)	0	100	100
2	EY	154/185 (83%)	152 (99%)	2 (1%)	0	100	100
2	EZ	145/185 (78%)	144 (99%)	1 (1%)	0	100	100
2	FA	148/185 (80%)	147 (99%)	1 (1%)	0	100	100
2	FB	147/185 (80%)	146 (99%)	1 (1%)	0	100	100
2	FC	154/185 (83%)	152 (99%)	2 (1%)	0	100	100
2	FD	145/185 (78%)	142 (98%)	3 (2%)	0	100	100
2	FE	148/185 (80%)	147 (99%)	1 (1%)	0	100	100
2	FF	147/185 (80%)	146 (99%)	1 (1%)	0	100	100
2	FG	154/185 (83%)	152 (99%)	2 (1%)	0	100	100
2	FH	145/185 (78%)	142 (98%)	3 (2%)	0	100	100
2	FI	148/185 (80%)	147 (99%)	1 (1%)	0	100	100
3	FJ	153/254 (60%)	152 (99%)	1 (1%)	0	100	100
4	FK	146/190 (77%)	144 (99%)	2 (1%)	0	100	100
4	FL	146/190 (77%)	145 (99%)	1 (1%)	0	100	100
4	FM	147/190 (77%)	144 (98%)	3 (2%)	0	100	100
4	FN	146/190 (77%)	145 (99%)	1 (1%)	0	100	100
4	FO	150/190 (79%)	146 (97%)	4 (3%)	0	100	100
4	FP	146/190 (77%)	145 (99%)	1 (1%)	0	100	100
4	FQ	165/190 (87%)	160 (97%)	5 (3%)	0	100	100
4	FR	165/190 (87%)	162 (98%)	3 (2%)	0	100	100
4	FS	165/190 (87%)	162 (98%)	3 (2%)	0	100	100
4	FT	138/190 (73%)	136 (99%)	2 (1%)	0	100	100
4	FU	145/190 (76%)	141 (97%)	4 (3%)	0	100	100
4	FV	148/190 (78%)	145 (98%)	3 (2%)	0	100	100
4	FW	148/190 (78%)	145 (98%)	3 (2%)	0	100	100
4	FX	145/190 (76%)	141 (97%)	4 (3%)	0	100	100
4	FY	145/190 (76%)	142 (98%)	3 (2%)	0	100	100
4	FZ	146/190 (77%)	145 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	GA	165/190 (87%)	164 (99%)	1 (1%)	0	100	100
4	GB	165/190 (87%)	161 (98%)	4 (2%)	0	100	100
4	GC	165/190 (87%)	164 (99%)	1 (1%)	0	100	100
4	GD	165/190 (87%)	163 (99%)	2 (1%)	0	100	100
4	GE	165/190 (87%)	163 (99%)	2 (1%)	0	100	100
4	GF	165/190 (87%)	163 (99%)	2 (1%)	0	100	100
4	GG	165/190 (87%)	163 (99%)	2 (1%)	0	100	100
4	GH	165/190 (87%)	163 (99%)	2 (1%)	0	100	100
4	GI	165/190 (87%)	164 (99%)	1 (1%)	0	100	100
4	GJ	165/190 (87%)	162 (98%)	3 (2%)	0	100	100
5	GK	28/230 (12%)	28 (100%)	0	0	100	100
5	GL	35/230 (15%)	35 (100%)	0	0	100	100
5	GM	35/230 (15%)	35 (100%)	0	0	100	100
5	GN	35/230 (15%)	35 (100%)	0	0	100	100
5	GO	35/230 (15%)	35 (100%)	0	0	100	100
5	GP	35/230 (15%)	35 (100%)	0	0	100	100
5	GQ	35/230 (15%)	35 (100%)	0	0	100	100
5	GR	35/230 (15%)	35 (100%)	0	0	100	100
5	GS	35/230 (15%)	35 (100%)	0	0	100	100
5	GT	35/230 (15%)	35 (100%)	0	0	100	100
5	GU	35/230 (15%)	35 (100%)	0	0	100	100
5	GV	35/230 (15%)	35 (100%)	0	0	100	100
5	GW	28/230 (12%)	28 (100%)	0	0	100	100
5	GX	35/230 (15%)	35 (100%)	0	0	100	100
5	GY	35/230 (15%)	35 (100%)	0	0	100	100
5	GZ	35/230 (15%)	35 (100%)	0	0	100	100
5	HA	35/230 (15%)	35 (100%)	0	0	100	100
5	HB	35/230 (15%)	35 (100%)	0	0	100	100
5	HC	35/230 (15%)	35 (100%)	0	0	100	100
5	HD	28/230 (12%)	28 (100%)	0	0	100	100
5	HE	35/230 (15%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	HF	35/230 (15%)	35 (100%)	0	0	100	100
5	HG	35/230 (15%)	35 (100%)	0	0	100	100
5	HH	28/230 (12%)	28 (100%)	0	0	100	100
5	HI	28/230 (12%)	28 (100%)	0	0	100	100
5	HJ	28/230 (12%)	28 (100%)	0	0	100	100
5	HK	28/230 (12%)	28 (100%)	0	0	100	100
5	HL	35/230 (15%)	35 (100%)	0	0	100	100
5	HM	27/230 (12%)	27 (100%)	0	0	100	100
5	HN	35/230 (15%)	35 (100%)	0	0	100	100
5	HO	35/230 (15%)	35 (100%)	0	0	100	100
5	HP	35/230 (15%)	35 (100%)	0	0	100	100
5	HQ	35/230 (15%)	35 (100%)	0	0	100	100
5	HR	35/230 (15%)	35 (100%)	0	0	100	100
5	HS	35/230 (15%)	35 (100%)	0	0	100	100
5	HT	35/230 (15%)	35 (100%)	0	0	100	100
5	HU	35/230 (15%)	35 (100%)	0	0	100	100
5	HV	35/230 (15%)	35 (100%)	0	0	100	100
5	HW	26/230 (11%)	26 (100%)	0	0	100	100
5	HX	35/230 (15%)	35 (100%)	0	0	100	100
5	HY	35/230 (15%)	35 (100%)	0	0	100	100
5	HZ	35/230 (15%)	35 (100%)	0	0	100	100
5	IA	35/230 (15%)	35 (100%)	0	0	100	100
5	IB	27/230 (12%)	27 (100%)	0	0	100	100
5	IC	35/230 (15%)	35 (100%)	0	0	100	100
5	ID	27/230 (12%)	27 (100%)	0	0	100	100
5	IE	35/230 (15%)	35 (100%)	0	0	100	100
5	IF	35/230 (15%)	35 (100%)	0	0	100	100
5	IG	35/230 (15%)	35 (100%)	0	0	100	100
5	IH	27/230 (12%)	27 (100%)	0	0	100	100
5	II	28/230 (12%)	28 (100%)	0	0	100	100
5	IJ	28/230 (12%)	28 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	IK	28/230 (12%)	28 (100%)	0	0	100	100
5	IL	38/230 (16%)	38 (100%)	0	0	100	100
5	IM	35/230 (15%)	35 (100%)	0	0	100	100
5	IN	35/230 (15%)	35 (100%)	0	0	100	100
5	IO	38/230 (16%)	38 (100%)	0	0	100	100
5	IP	35/230 (15%)	35 (100%)	0	0	100	100
5	IQ	35/230 (15%)	35 (100%)	0	0	100	100
5	IR	38/230 (16%)	38 (100%)	0	0	100	100
5	IS	35/230 (15%)	35 (100%)	0	0	100	100
5	IT	35/230 (15%)	35 (100%)	0	0	100	100
5	IU	38/230 (16%)	38 (100%)	0	0	100	100
5	IV	35/230 (15%)	35 (100%)	0	0	100	100
5	IW	35/230 (15%)	35 (100%)	0	0	100	100
5	IX	35/230 (15%)	35 (100%)	0	0	100	100
5	IY	38/230 (16%)	38 (100%)	0	0	100	100
5	IZ	35/230 (15%)	35 (100%)	0	0	100	100
5	JA	38/230 (16%)	38 (100%)	0	0	100	100
5	JB	35/230 (15%)	35 (100%)	0	0	100	100
5	JC	35/230 (15%)	35 (100%)	0	0	100	100
5	JD	38/230 (16%)	38 (100%)	0	0	100	100
5	JE	35/230 (15%)	35 (100%)	0	0	100	100
5	JF	35/230 (15%)	35 (100%)	0	0	100	100
5	JG	38/230 (16%)	38 (100%)	0	0	100	100
5	JH	35/230 (15%)	35 (100%)	0	0	100	100
5	JI	35/230 (15%)	35 (100%)	0	0	100	100
5	JJ	38/230 (16%)	38 (100%)	0	0	100	100
5	JK	35/230 (15%)	35 (100%)	0	0	100	100
5	JL	35/230 (15%)	35 (100%)	0	0	100	100
5	JM	35/230 (15%)	35 (100%)	0	0	100	100
5	JN	38/230 (16%)	38 (100%)	0	0	100	100
5	JO	35/230 (15%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	40930/61121 (67%)	40441 (99%)	489 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	281/286 (98%)	281 (100%)	0	100	100
1	AB	283/286 (99%)	283 (100%)	0	100	100
1	AC	283/286 (99%)	283 (100%)	0	100	100
1	AD	281/286 (98%)	281 (100%)	0	100	100
1	AE	283/286 (99%)	283 (100%)	0	100	100
1	AF	283/286 (99%)	283 (100%)	0	100	100
1	AG	281/286 (98%)	281 (100%)	0	100	100
1	AH	283/286 (99%)	283 (100%)	0	100	100
1	AI	283/286 (99%)	283 (100%)	0	100	100
1	AJ	281/286 (98%)	281 (100%)	0	100	100
1	AK	283/286 (99%)	283 (100%)	0	100	100
1	AL	283/286 (99%)	283 (100%)	0	100	100
1	AM	281/286 (98%)	281 (100%)	0	100	100
1	AN	283/286 (99%)	283 (100%)	0	100	100
1	AO	283/286 (99%)	283 (100%)	0	100	100
1	AP	281/286 (98%)	281 (100%)	0	100	100
1	AQ	283/286 (99%)	283 (100%)	0	100	100
1	AR	283/286 (99%)	283 (100%)	0	100	100
1	AS	283/286 (99%)	283 (100%)	0	100	100
1	AT	283/286 (99%)	283 (100%)	0	100	100
1	AU	283/286 (99%)	283 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AV	283/286 (99%)	283 (100%)	0	100	100
1	AW	283/286 (99%)	283 (100%)	0	100	100
1	AX	283/286 (99%)	283 (100%)	0	100	100
1	AY	283/286 (99%)	283 (100%)	0	100	100
1	AZ	283/286 (99%)	283 (100%)	0	100	100
1	BA	283/286 (99%)	283 (100%)	0	100	100
1	BB	283/286 (99%)	283 (100%)	0	100	100
1	BC	271/286 (95%)	271 (100%)	0	100	100
1	BD	281/286 (98%)	281 (100%)	0	100	100
1	BE	283/286 (99%)	283 (100%)	0	100	100
1	BF	283/286 (99%)	283 (100%)	0	100	100
1	BG	281/286 (98%)	281 (100%)	0	100	100
1	BH	283/286 (99%)	283 (100%)	0	100	100
1	BI	283/286 (99%)	283 (100%)	0	100	100
1	BJ	281/286 (98%)	281 (100%)	0	100	100
1	BK	283/286 (99%)	283 (100%)	0	100	100
1	BL	283/286 (99%)	283 (100%)	0	100	100
1	BM	283/286 (99%)	283 (100%)	0	100	100
1	BN	283/286 (99%)	283 (100%)	0	100	100
1	BO	283/286 (99%)	283 (100%)	0	100	100
1	BP	281/286 (98%)	281 (100%)	0	100	100
1	BQ	283/286 (99%)	283 (100%)	0	100	100
1	BR	283/286 (99%)	283 (100%)	0	100	100
1	BS	283/286 (99%)	283 (100%)	0	100	100
1	BT	271/286 (95%)	271 (100%)	0	100	100
1	BU	283/286 (99%)	283 (100%)	0	100	100
1	BV	283/286 (99%)	283 (100%)	0	100	100
1	BW	283/286 (99%)	283 (100%)	0	100	100
1	BX	271/286 (95%)	271 (100%)	0	100	100
1	BY	283/286 (99%)	283 (100%)	0	100	100
1	BZ	283/286 (99%)	283 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CA	283/286 (99%)	283 (100%)	0	100	100
1	CB	283/286 (99%)	283 (100%)	0	100	100
1	CC	283/286 (99%)	283 (100%)	0	100	100
1	CD	283/286 (99%)	283 (100%)	0	100	100
1	CE	283/286 (99%)	283 (100%)	0	100	100
1	CF	283/286 (99%)	283 (100%)	0	100	100
1	CG	283/286 (99%)	283 (100%)	0	100	100
1	CH	283/286 (99%)	283 (100%)	0	100	100
1	CI	283/286 (99%)	283 (100%)	0	100	100
1	CJ	283/286 (99%)	283 (100%)	0	100	100
1	CK	283/286 (99%)	283 (100%)	0	100	100
1	CL	283/286 (99%)	283 (100%)	0	100	100
1	CM	283/286 (99%)	283 (100%)	0	100	100
1	CN	283/286 (99%)	283 (100%)	0	100	100
1	CO	283/286 (99%)	283 (100%)	0	100	100
1	CP	283/286 (99%)	283 (100%)	0	100	100
1	CQ	283/286 (99%)	283 (100%)	0	100	100
1	CR	283/286 (99%)	283 (100%)	0	100	100
1	CS	283/286 (99%)	283 (100%)	0	100	100
1	CT	283/286 (99%)	283 (100%)	0	100	100
1	CU	283/286 (99%)	283 (100%)	0	100	100
1	CV	283/286 (99%)	283 (100%)	0	100	100
1	CW	283/286 (99%)	283 (100%)	0	100	100
1	CX	283/286 (99%)	283 (100%)	0	100	100
1	CY	283/286 (99%)	283 (100%)	0	100	100
1	CZ	283/286 (99%)	283 (100%)	0	100	100
1	DA	283/286 (99%)	283 (100%)	0	100	100
1	DB	283/286 (99%)	283 (100%)	0	100	100
1	DC	283/286 (99%)	283 (100%)	0	100	100
1	DD	283/286 (99%)	283 (100%)	0	100	100
1	DE	283/286 (99%)	283 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	DF	130/154 (84%)	130 (100%)	0	100	100
2	DG	129/154 (84%)	129 (100%)	0	100	100
2	DH	130/154 (84%)	130 (100%)	0	100	100
2	DI	129/154 (84%)	129 (100%)	0	100	100
2	DJ	130/154 (84%)	130 (100%)	0	100	100
2	DK	129/154 (84%)	129 (100%)	0	100	100
2	DL	130/154 (84%)	130 (100%)	0	100	100
2	DM	129/154 (84%)	129 (100%)	0	100	100
2	DN	130/154 (84%)	130 (100%)	0	100	100
2	DO	129/154 (84%)	129 (100%)	0	100	100
2	DP	129/154 (84%)	129 (100%)	0	100	100
2	DQ	129/154 (84%)	129 (100%)	0	100	100
2	DR	130/154 (84%)	130 (100%)	0	100	100
2	DS	142/154 (92%)	142 (100%)	0	100	100
2	DT	130/154 (84%)	130 (100%)	0	100	100
2	DU	128/154 (83%)	128 (100%)	0	100	100
2	DV	129/154 (84%)	129 (100%)	0	100	100
2	DW	128/154 (83%)	128 (100%)	0	100	100
2	DX	132/154 (86%)	132 (100%)	0	100	100
2	DY	127/154 (82%)	127 (100%)	0	100	100
2	DZ	130/154 (84%)	130 (100%)	0	100	100
2	EA	99/154 (64%)	99 (100%)	0	100	100
2	EB	132/154 (86%)	132 (100%)	0	100	100
2	EC	129/154 (84%)	129 (100%)	0	100	100
2	ED	133/154 (86%)	133 (100%)	0	100	100
2	EE	131/154 (85%)	131 (100%)	0	100	100
2	EF	130/154 (84%)	130 (100%)	0	100	100
2	EG	147/154 (96%)	147 (100%)	0	100	100
2	EH	129/154 (84%)	129 (100%)	0	100	100
2	EI	131/154 (85%)	131 (100%)	0	100	100
2	EJ	141/154 (92%)	141 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	EK	142/154 (92%)	142 (100%)	0	100	100
2	EL	129/154 (84%)	129 (100%)	0	100	100
2	EM	130/154 (84%)	130 (100%)	0	100	100
2	EN	129/154 (84%)	129 (100%)	0	100	100
2	EO	144/154 (94%)	144 (100%)	0	100	100
2	EP	128/154 (83%)	128 (100%)	0	100	100
2	EQ	132/154 (86%)	132 (100%)	0	100	100
2	ER	127/154 (82%)	127 (100%)	0	100	100
2	ES	130/154 (84%)	130 (100%)	0	100	100
2	ET	128/154 (83%)	128 (100%)	0	100	100
2	EU	132/154 (86%)	132 (100%)	0	100	100
2	EV	127/154 (82%)	127 (100%)	0	100	100
2	EW	130/154 (84%)	130 (100%)	0	100	100
2	EX	128/154 (83%)	128 (100%)	0	100	100
2	EY	132/154 (86%)	132 (100%)	0	100	100
2	EZ	127/154 (82%)	127 (100%)	0	100	100
2	FA	130/154 (84%)	130 (100%)	0	100	100
2	FB	128/154 (83%)	128 (100%)	0	100	100
2	FC	132/154 (86%)	132 (100%)	0	100	100
2	FD	127/154 (82%)	127 (100%)	0	100	100
2	FE	130/154 (84%)	130 (100%)	0	100	100
2	FF	128/154 (83%)	128 (100%)	0	100	100
2	FG	132/154 (86%)	132 (100%)	0	100	100
2	FH	127/154 (82%)	127 (100%)	0	100	100
2	FI	130/154 (84%)	130 (100%)	0	100	100
3	FJ	141/218 (65%)	141 (100%)	0	100	100
4	FK	130/163 (80%)	130 (100%)	0	100	100
4	FL	130/163 (80%)	130 (100%)	0	100	100
4	FM	131/163 (80%)	131 (100%)	0	100	100
4	FN	130/163 (80%)	130 (100%)	0	100	100
4	FO	133/163 (82%)	133 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	FP	129/163 (79%)	129 (100%)	0	100	100
4	FQ	148/163 (91%)	148 (100%)	0	100	100
4	FR	148/163 (91%)	148 (100%)	0	100	100
4	FS	148/163 (91%)	148 (100%)	0	100	100
4	FT	124/163 (76%)	124 (100%)	0	100	100
4	FU	130/163 (80%)	130 (100%)	0	100	100
4	FV	131/163 (80%)	131 (100%)	0	100	100
4	FW	131/163 (80%)	131 (100%)	0	100	100
4	FX	129/163 (79%)	129 (100%)	0	100	100
4	FY	129/163 (79%)	129 (100%)	0	100	100
4	FZ	130/163 (80%)	130 (100%)	0	100	100
4	GA	148/163 (91%)	148 (100%)	0	100	100
4	GB	148/163 (91%)	148 (100%)	0	100	100
4	GC	148/163 (91%)	148 (100%)	0	100	100
4	GD	148/163 (91%)	148 (100%)	0	100	100
4	GE	148/163 (91%)	148 (100%)	0	100	100
4	GF	148/163 (91%)	148 (100%)	0	100	100
4	GG	148/163 (91%)	148 (100%)	0	100	100
4	GH	148/163 (91%)	148 (100%)	0	100	100
4	GI	148/163 (91%)	148 (100%)	0	100	100
4	GJ	148/163 (91%)	148 (100%)	0	100	100
5	GK	29/210 (14%)	29 (100%)	0	100	100
5	GL	35/210 (17%)	35 (100%)	0	100	100
5	GM	35/210 (17%)	35 (100%)	0	100	100
5	GN	35/210 (17%)	35 (100%)	0	100	100
5	GO	35/210 (17%)	35 (100%)	0	100	100
5	GP	35/210 (17%)	35 (100%)	0	100	100
5	GQ	35/210 (17%)	35 (100%)	0	100	100
5	GR	35/210 (17%)	35 (100%)	0	100	100
5	GS	35/210 (17%)	35 (100%)	0	100	100
5	GT	35/210 (17%)	35 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	GU	35/210 (17%)	35 (100%)	0	100	100
5	GV	35/210 (17%)	35 (100%)	0	100	100
5	GW	29/210 (14%)	29 (100%)	0	100	100
5	GX	35/210 (17%)	35 (100%)	0	100	100
5	GY	35/210 (17%)	35 (100%)	0	100	100
5	GZ	35/210 (17%)	35 (100%)	0	100	100
5	HA	35/210 (17%)	35 (100%)	0	100	100
5	HB	35/210 (17%)	35 (100%)	0	100	100
5	HC	35/210 (17%)	35 (100%)	0	100	100
5	HD	29/210 (14%)	29 (100%)	0	100	100
5	HE	35/210 (17%)	35 (100%)	0	100	100
5	HF	35/210 (17%)	35 (100%)	0	100	100
5	HG	35/210 (17%)	35 (100%)	0	100	100
5	HH	29/210 (14%)	29 (100%)	0	100	100
5	HI	29/210 (14%)	29 (100%)	0	100	100
5	HJ	29/210 (14%)	29 (100%)	0	100	100
5	HK	29/210 (14%)	29 (100%)	0	100	100
5	HL	35/210 (17%)	35 (100%)	0	100	100
5	HM	28/210 (13%)	28 (100%)	0	100	100
5	HN	35/210 (17%)	35 (100%)	0	100	100
5	HO	35/210 (17%)	35 (100%)	0	100	100
5	HP	35/210 (17%)	35 (100%)	0	100	100
5	HQ	35/210 (17%)	35 (100%)	0	100	100
5	HR	35/210 (17%)	35 (100%)	0	100	100
5	HS	35/210 (17%)	35 (100%)	0	100	100
5	HT	35/210 (17%)	35 (100%)	0	100	100
5	HU	35/210 (17%)	35 (100%)	0	100	100
5	HV	35/210 (17%)	35 (100%)	0	100	100
5	HW	27/210 (13%)	27 (100%)	0	100	100
5	HX	35/210 (17%)	35 (100%)	0	100	100
5	HY	35/210 (17%)	35 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	HZ	35/210 (17%)	35 (100%)	0	100	100
5	IA	35/210 (17%)	35 (100%)	0	100	100
5	IB	28/210 (13%)	28 (100%)	0	100	100
5	IC	35/210 (17%)	35 (100%)	0	100	100
5	ID	28/210 (13%)	28 (100%)	0	100	100
5	IE	35/210 (17%)	35 (100%)	0	100	100
5	IF	35/210 (17%)	35 (100%)	0	100	100
5	IG	35/210 (17%)	35 (100%)	0	100	100
5	IH	28/210 (13%)	28 (100%)	0	100	100
5	II	29/210 (14%)	29 (100%)	0	100	100
5	IJ	29/210 (14%)	29 (100%)	0	100	100
5	IK	29/210 (14%)	29 (100%)	0	100	100
5	IL	38/210 (18%)	38 (100%)	0	100	100
5	IM	35/210 (17%)	35 (100%)	0	100	100
5	IN	35/210 (17%)	35 (100%)	0	100	100
5	IO	38/210 (18%)	38 (100%)	0	100	100
5	IP	35/210 (17%)	35 (100%)	0	100	100
5	IQ	35/210 (17%)	35 (100%)	0	100	100
5	IR	38/210 (18%)	38 (100%)	0	100	100
5	IS	35/210 (17%)	35 (100%)	0	100	100
5	IT	35/210 (17%)	35 (100%)	0	100	100
5	IU	38/210 (18%)	38 (100%)	0	100	100
5	IV	35/210 (17%)	35 (100%)	0	100	100
5	IW	35/210 (17%)	35 (100%)	0	100	100
5	IX	35/210 (17%)	35 (100%)	0	100	100
5	IY	38/210 (18%)	38 (100%)	0	100	100
5	IZ	35/210 (17%)	35 (100%)	0	100	100
5	JA	38/210 (18%)	38 (100%)	0	100	100
5	JB	35/210 (17%)	35 (100%)	0	100	100
5	JC	35/210 (17%)	35 (100%)	0	100	100
5	JD	38/210 (18%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	JE	35/210 (17%)	35 (100%)	0	100	100
5	JF	35/210 (17%)	35 (100%)	0	100	100
5	JG	38/210 (18%)	38 (100%)	0	100	100
5	JH	35/210 (17%)	35 (100%)	0	100	100
5	JI	35/210 (17%)	35 (100%)	0	100	100
5	JJ	38/210 (18%)	38 (100%)	0	100	100
5	JK	35/210 (17%)	35 (100%)	0	100	100
5	JL	35/210 (17%)	35 (100%)	0	100	100
5	JM	35/210 (17%)	35 (100%)	0	100	100
5	JN	38/210 (18%)	38 (100%)	0	100	100
5	JO	35/210 (17%)	35 (100%)	0	100	100
All	All	37314/54248 (69%)	37314 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	CH	62	ASN
4	GJ	88	HIS
2	DV	115	ASN
4	GH	88	HIS
4	FO	162	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

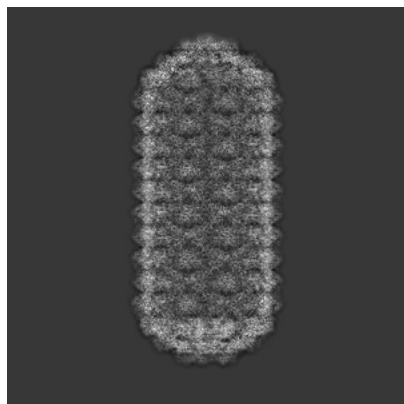
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17739. These allow visual inspection of the internal detail of the map and identification of artifacts.

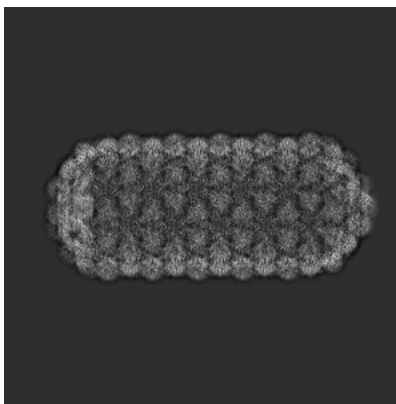
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

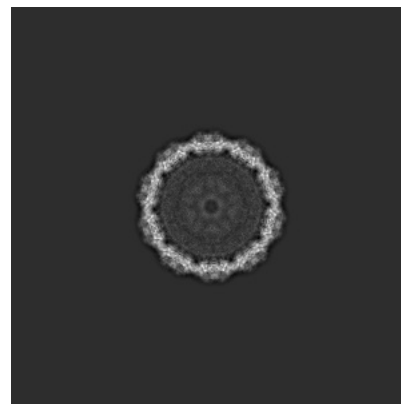
6.1.1 Primary map



X

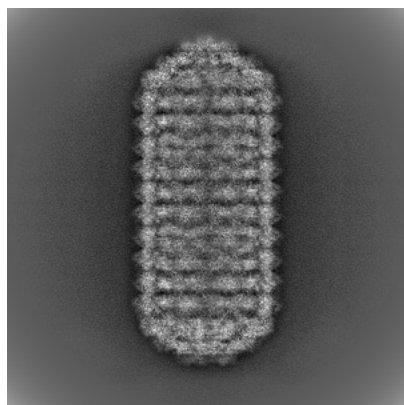


Y

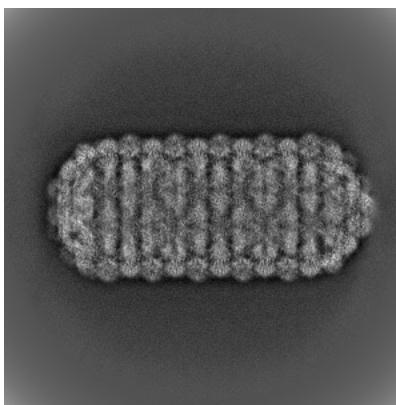


Z

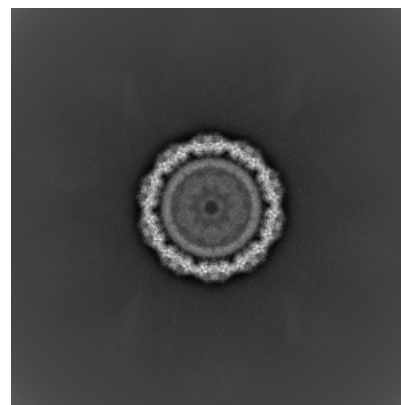
6.1.2 Raw map



X



Y



Z

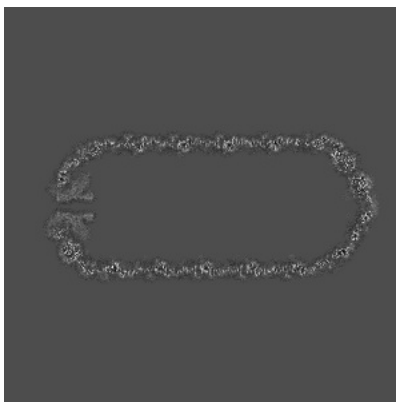
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 360

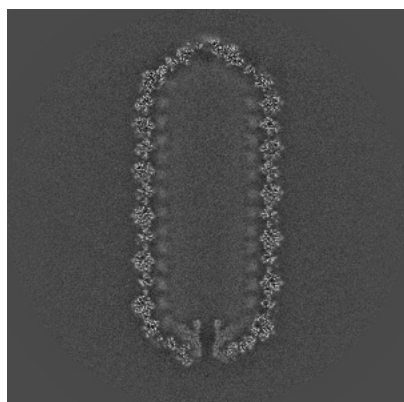


Y Index: 360

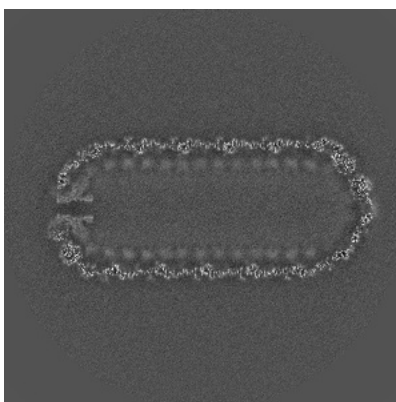


Z Index: 360

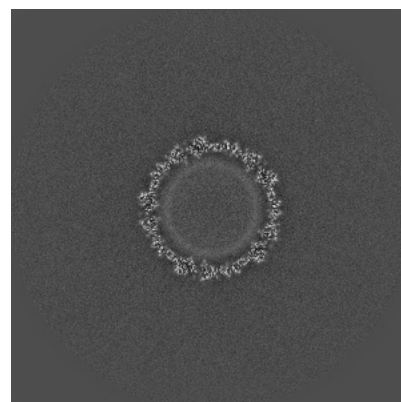
6.2.2 Raw map



X Index: 360



Y Index: 360

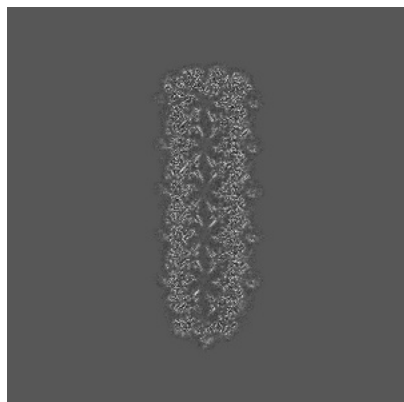


Z Index: 360

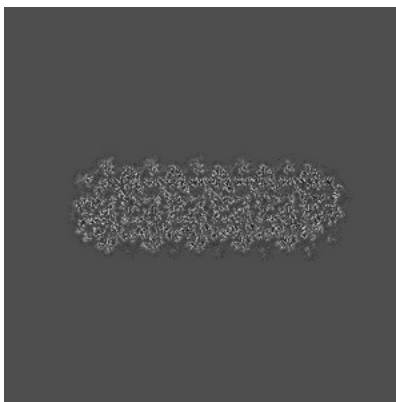
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

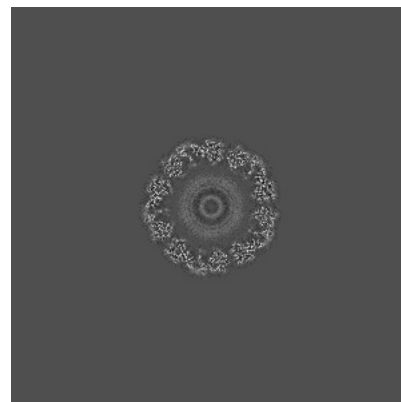
6.3.1 Primary map



X Index: 260

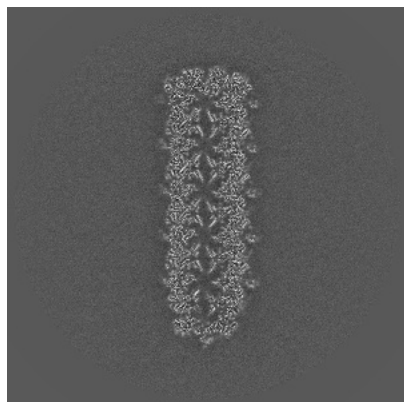


Y Index: 465

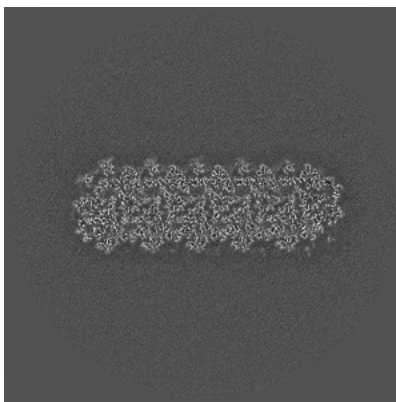


Z Index: 145

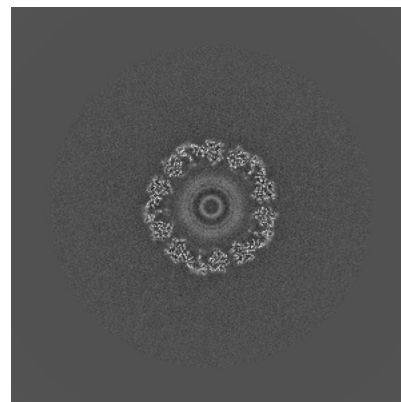
6.3.2 Raw map



X Index: 260



Y Index: 465

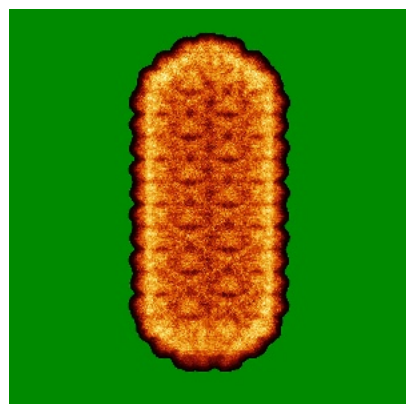


Z Index: 145

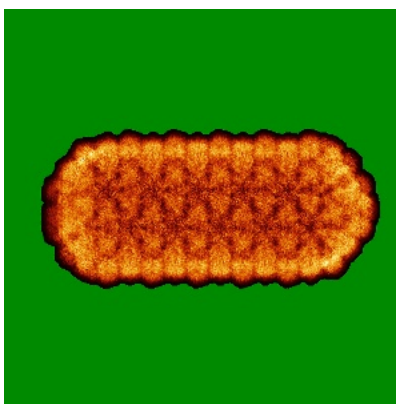
The images above show the largest variance slices of the map in three orthogonal directions.

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

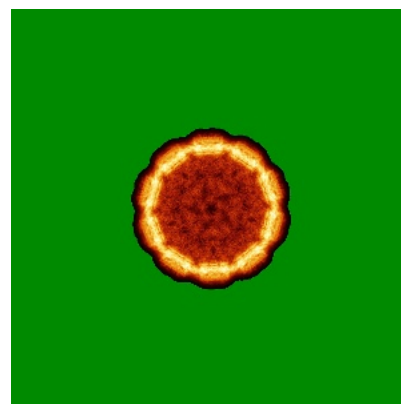
6.4.1 Primary map



X

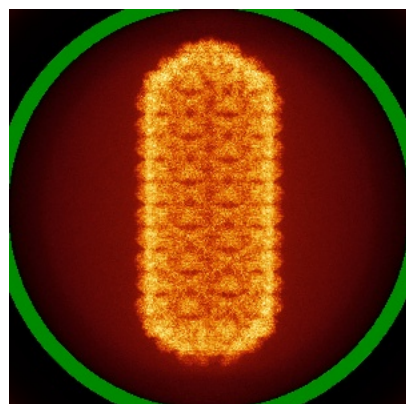


Y

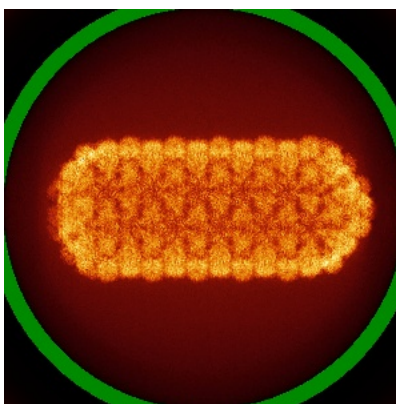


Z

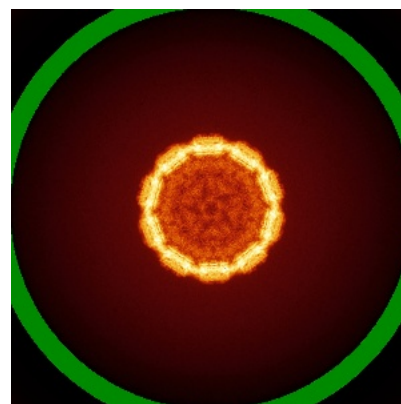
6.4.2 Raw map



X



Y

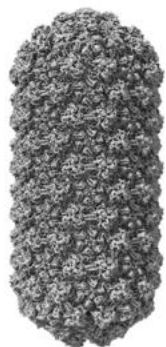


Z

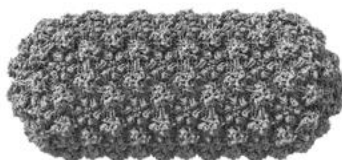
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

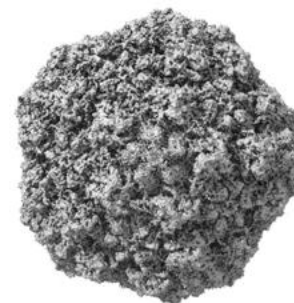
6.5.1 Primary map



X



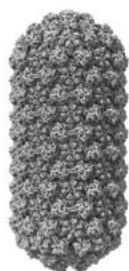
Y



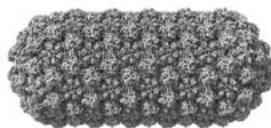
Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

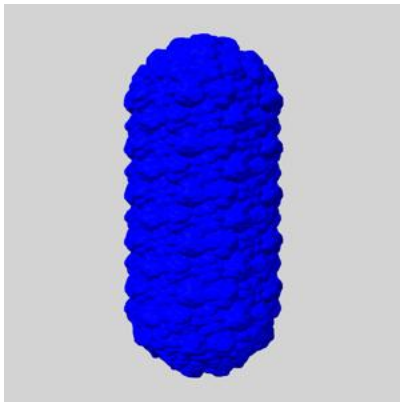
6.6 Mask visualisation [i](#)

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

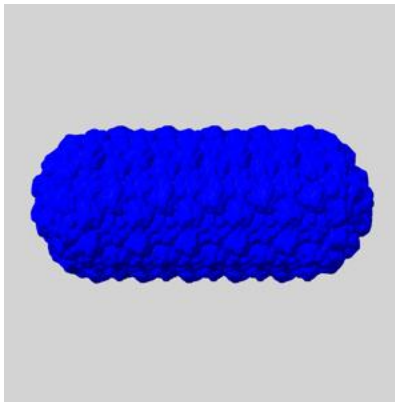
A mask typically either:

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

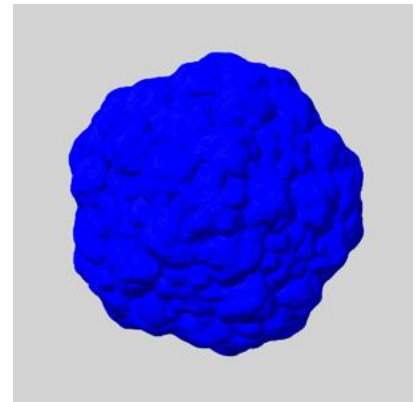
6.6.1 emd_17739_msk_1.map [i](#)



X



Y

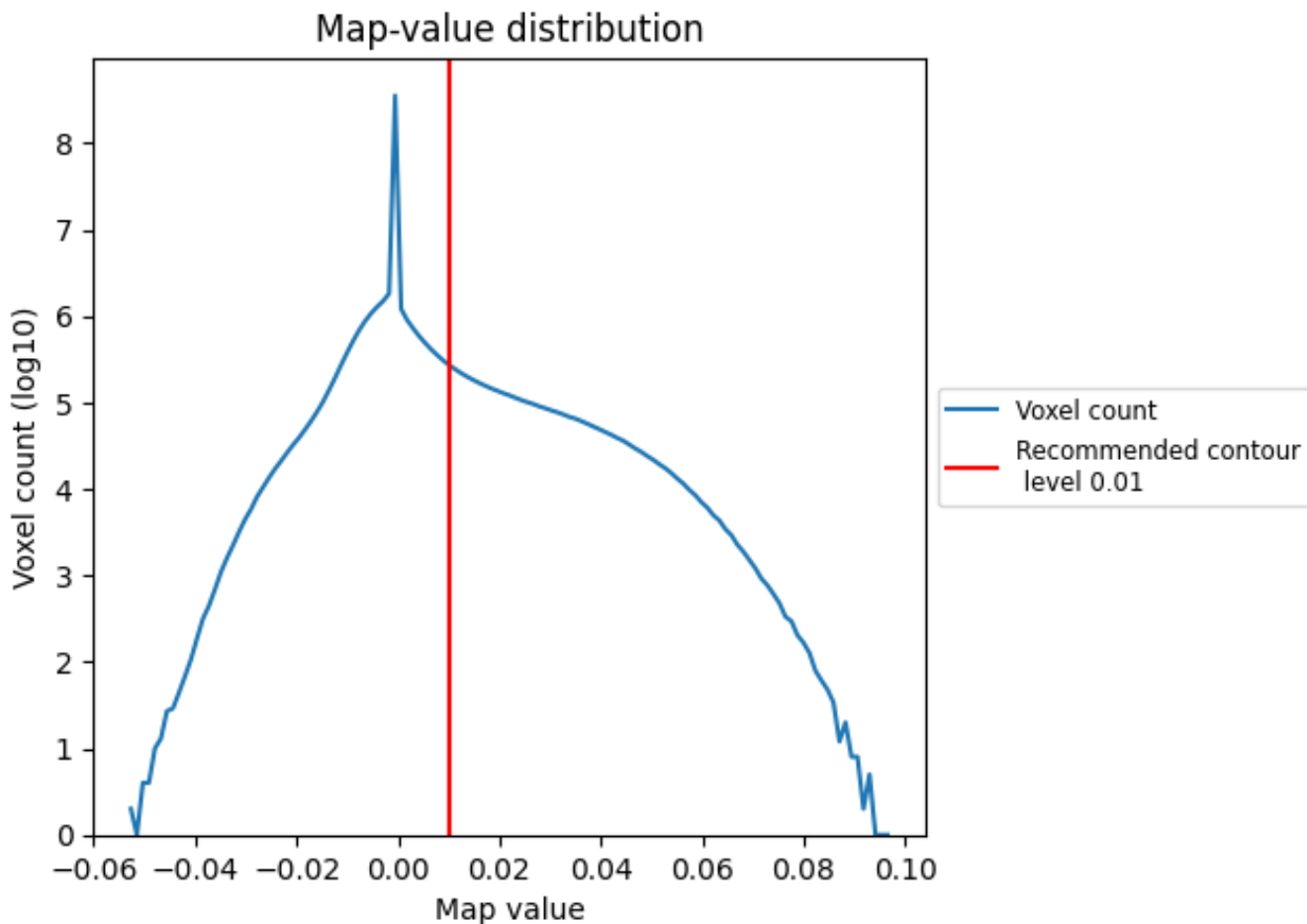


Z

7 Map analysis [i](#)

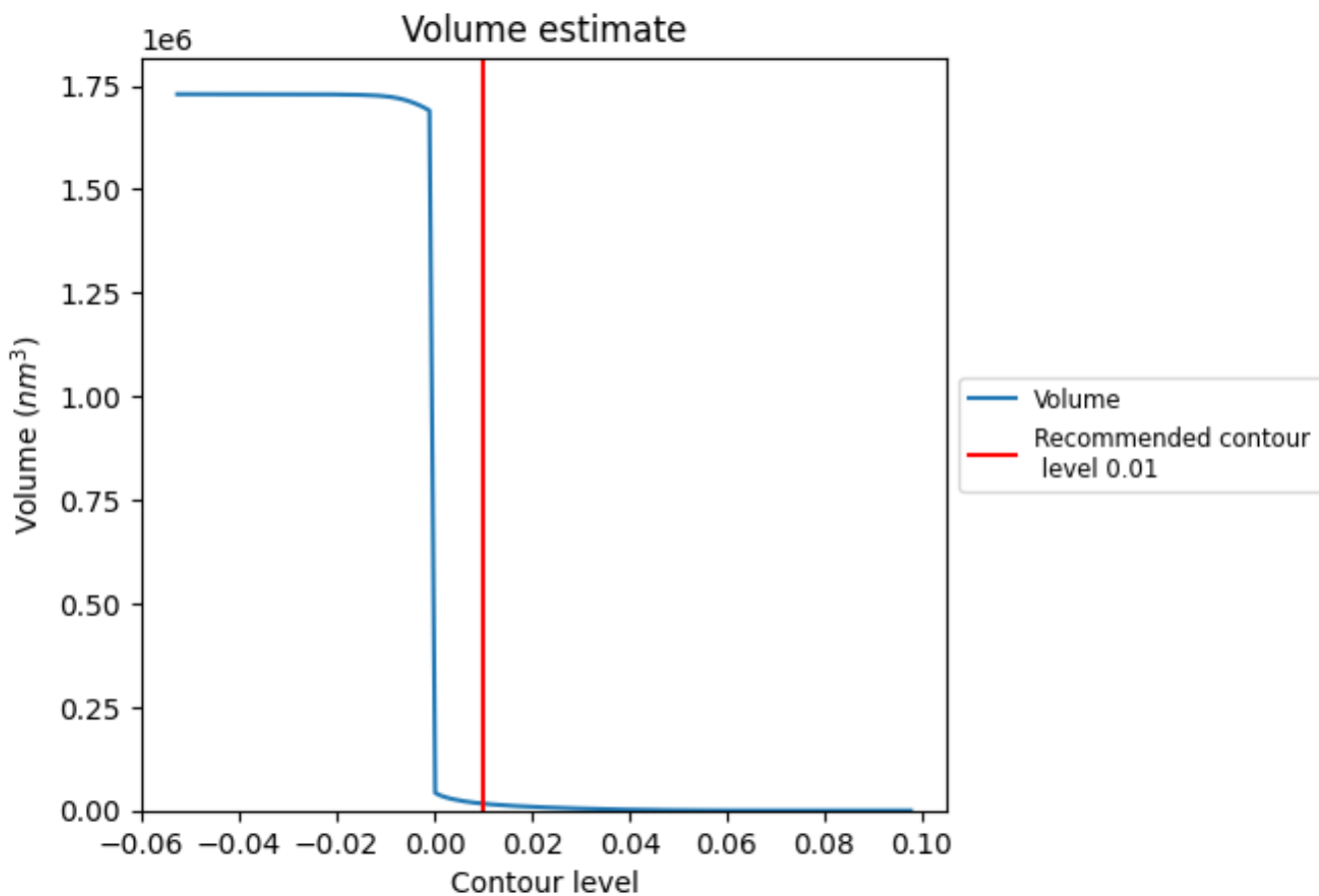
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

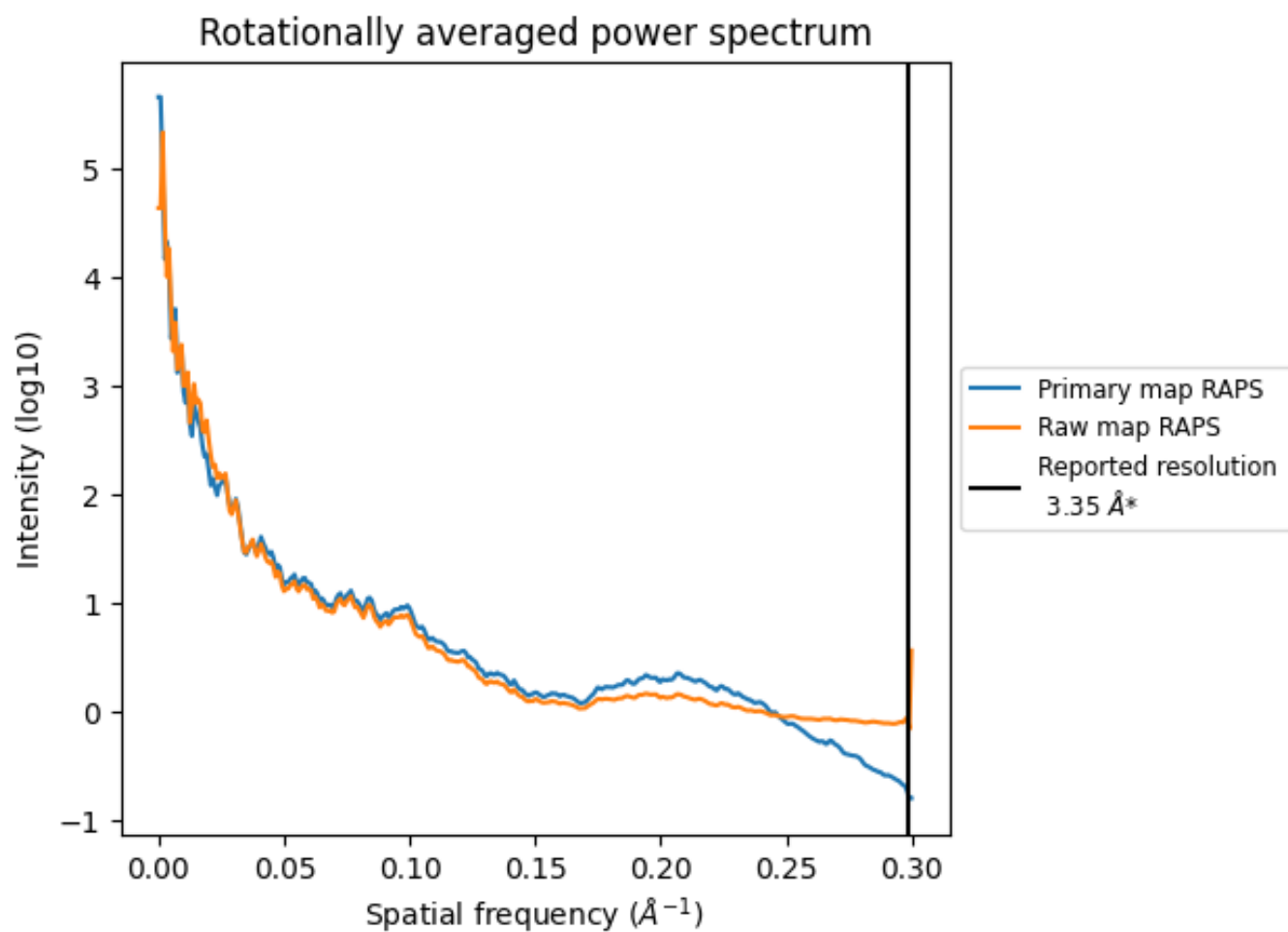
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 16709 nm^3 ; this corresponds to an approximate mass of 15093 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

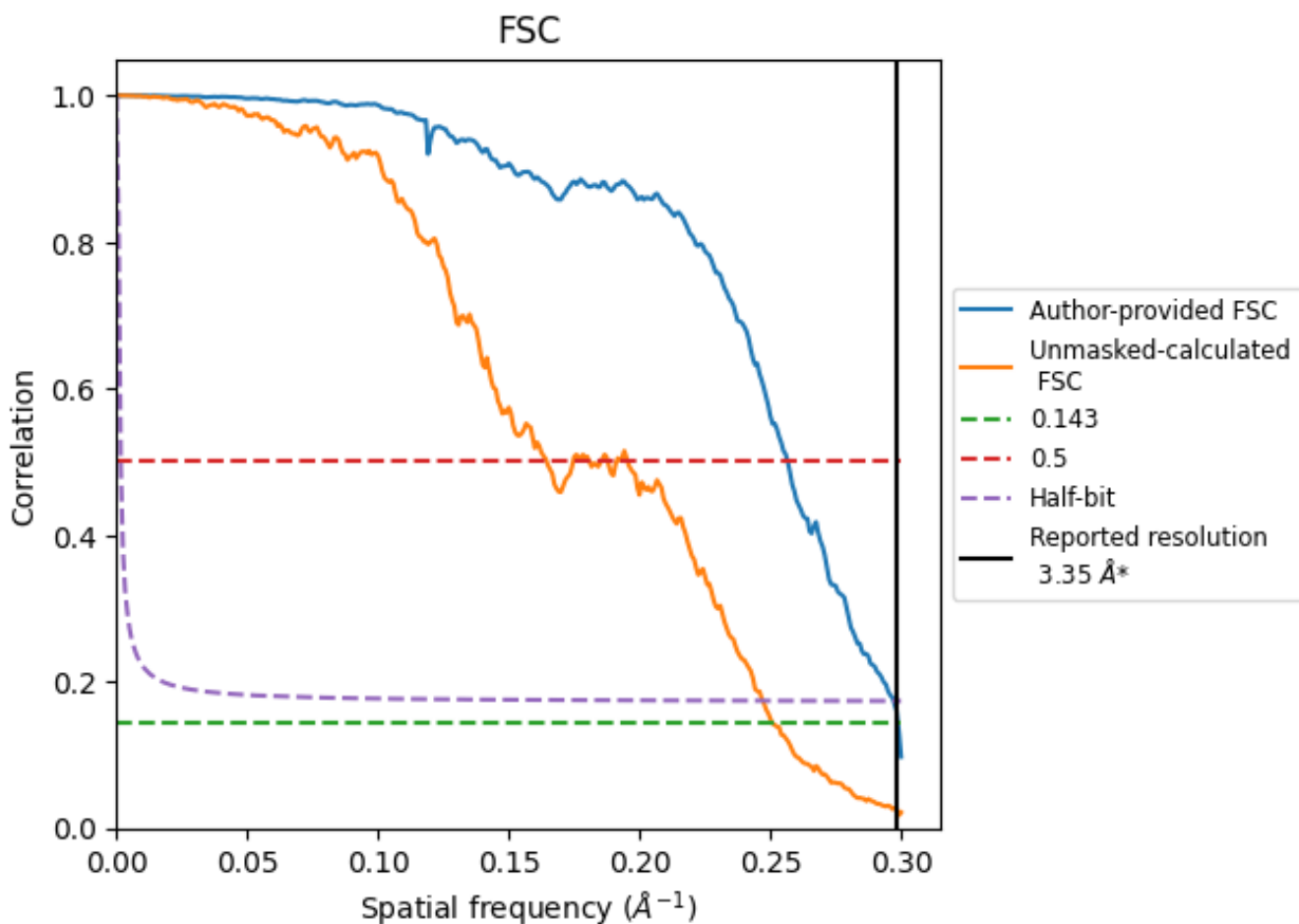


*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

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 0.299 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	3.35	3.90	3.37
Unmasked-calculated*	3.99	6.08	4.05

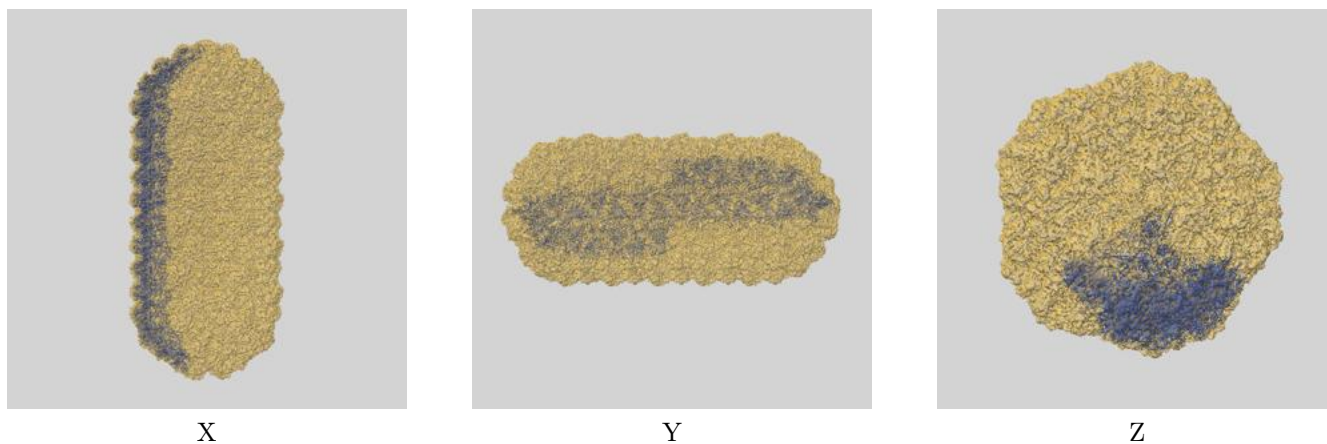
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.99 differs from the reported value 3.35 by more than 10 %

9 Map-model fit [i](#)

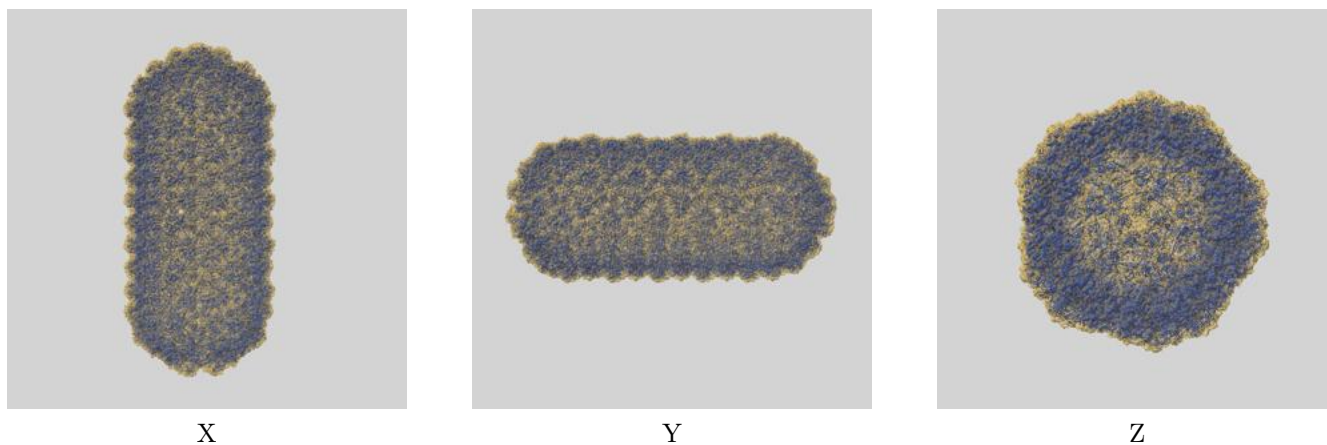
This section contains information regarding the fit between EMDB map EMD-17739 and PDB model 8PKH. Per-residue inclusion information can be found in section 3 on page 26.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

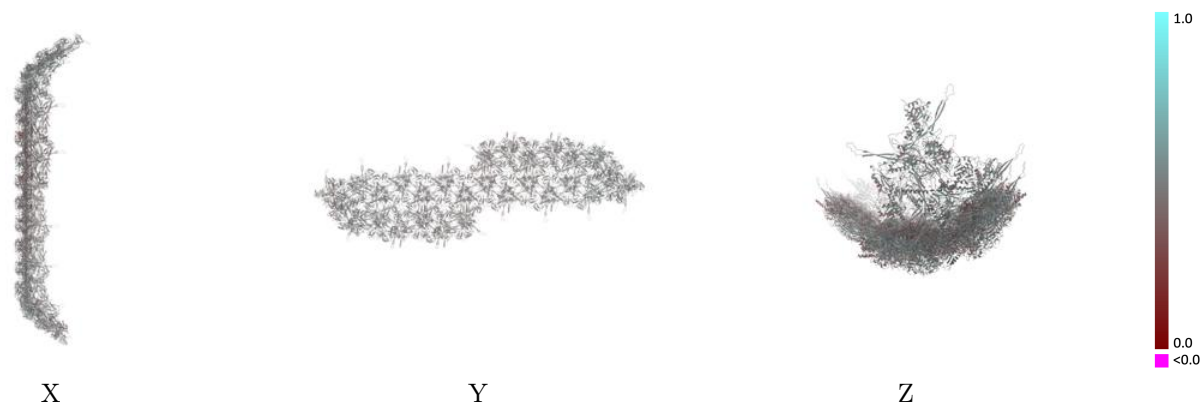


9.1.2 Map-model assembly overlay [i](#)



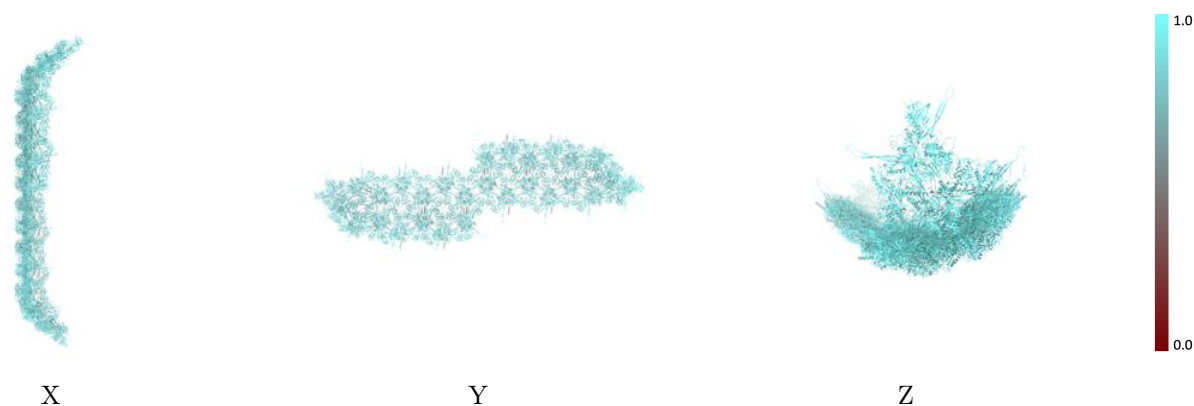
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



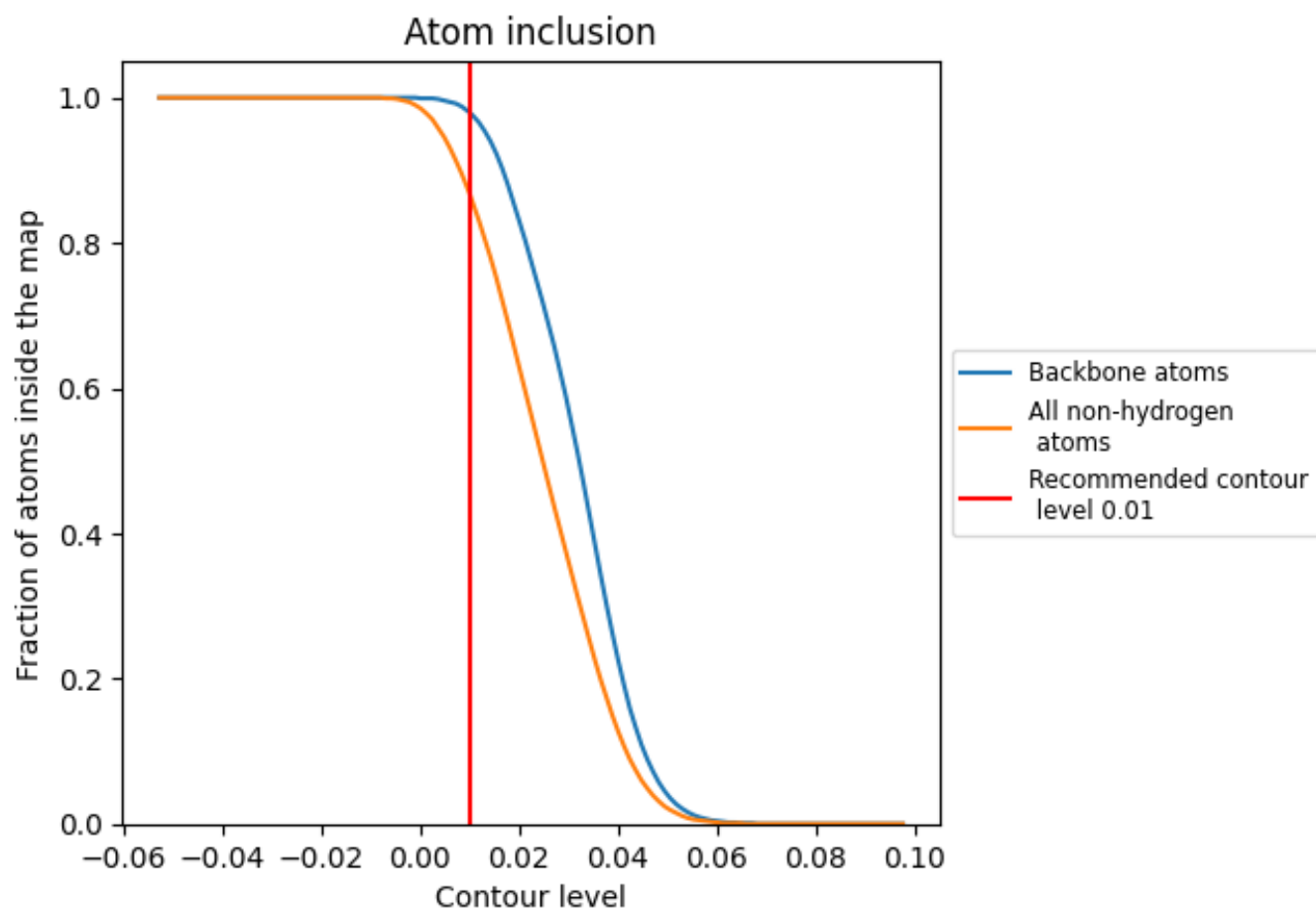
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 87% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8690	 0.4550
AA	 0.8950	 0.4860
AB	 0.8860	 0.4790
AC	 0.8930	 0.4840
AD	 0.8850	 0.4920
AE	 0.8880	 0.4860
AF	 0.8930	 0.4880
AG	 0.8900	 0.4880
AH	 0.8820	 0.4790
AI	 0.8860	 0.4850
AJ	 0.8840	 0.4840
AK	 0.8740	 0.4650
AL	 0.8800	 0.4740
AM	 0.8830	 0.4910
AN	 0.8850	 0.4820
AO	 0.8710	 0.4740
AP	 0.8950	 0.4920
AQ	 0.8850	 0.4810
AR	 0.8890	 0.4880
AS	 0.8660	 0.4530
AT	 0.8610	 0.4650
AU	 0.8600	 0.4460
AV	 0.8710	 0.4600
AW	 0.8650	 0.4660
AX	 0.8650	 0.4590
AY	 0.8590	 0.4530
AZ	 0.8540	 0.4440
BA	 0.8600	 0.4510
BB	 0.8580	 0.4510
BC	 0.8660	 0.4510
BD	 0.8770	 0.4820
BE	 0.8730	 0.4720
BF	 0.8850	 0.4770
BG	 0.8940	 0.4880
BH	 0.8810	 0.4800























































































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Chain	Atom inclusion	Q-score
BI	 0.8920	 0.4770
BJ	 0.8950	 0.4900
BK	 0.8790	 0.4760
BL	 0.8900	 0.4790
BM	 0.8890	 0.4860
BN	 0.8900	 0.4820
BO	 0.8870	 0.4750
BP	 0.8930	 0.4850
BQ	 0.8790	 0.4760
BR	 0.8630	 0.4690
BS	 0.8760	 0.4590
BT	 0.8780	 0.4720
BU	 0.8780	 0.4590
BV	 0.8890	 0.4690
BW	 0.8790	 0.4660
BX	 0.8620	 0.4540
BY	 0.8890	 0.4740
BZ	 0.8810	 0.4520
CA	 0.8730	 0.4530
CB	 0.8670	 0.4440
CC	 0.8590	 0.4430
CD	 0.8670	 0.4510
CE	 0.8720	 0.4490
CF	 0.8530	 0.4400
CG	 0.8590	 0.4370
CH	 0.8650	 0.4470
CI	 0.8610	 0.4470
CJ	 0.8730	 0.4480
CK	 0.8680	 0.4430
CL	 0.8560	 0.4450
CM	 0.8660	 0.4460
CN	 0.8670	 0.4470
CO	 0.8660	 0.4510
CP	 0.8690	 0.4470
CQ	 0.8660	 0.4390
CR	 0.8580	 0.4410
CS	 0.8520	 0.4400
CT	 0.8610	 0.4380
CU	 0.8680	 0.4440
CV	 0.8540	 0.4380
CW	 0.8590	 0.4470
CX	 0.8650	 0.4410





















































































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Chain	Atom inclusion	Q-score
CY	 0.8530	 0.4430
CZ	 0.8580	 0.4390
DA	 0.8650	 0.4500
DB	 0.8530	 0.4430
DC	 0.8670	 0.4430
DD	 0.8700	 0.4520
DE	 0.8700	 0.4480
DF	 0.9060	 0.4760
DG	 0.8910	 0.4710
DH	 0.8650	 0.4710
DI	 0.8760	 0.4800
DJ	 0.8850	 0.4710
DK	 0.8880	 0.4830
DL	 0.8820	 0.4770
DM	 0.8340	 0.4460
DN	 0.8600	 0.4720
DO	 0.8640	 0.4720
DP	 0.8760	 0.4790
DQ	 0.9020	 0.4870
DR	 0.8810	 0.4830
DS	 0.8390	 0.4190
DT	 0.8700	 0.4600
DU	 0.8700	 0.4640
DV	 0.8570	 0.4650
DW	 0.8500	 0.4140
DX	 0.8640	 0.4470
DY	 0.8790	 0.4490
DZ	 0.8570	 0.4410
EA	 0.8070	 0.3940
EB	 0.8660	 0.4690
EC	 0.9020	 0.4880
ED	 0.8730	 0.4660
EE	 0.8990	 0.4780
EF	 0.8710	 0.4690
EG	 0.8680	 0.4740
EH	 0.8440	 0.4430
EI	 0.8870	 0.4760
EJ	 0.8760	 0.4760
EK	 0.8790	 0.4450
EL	 0.8830	 0.4650
EM	 0.8820	 0.4530
EN	 0.8640	 0.4610





















































































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Chain	Atom inclusion	Q-score
EO	 0.8650	 0.4430
EP	 0.8760	 0.4580
EQ	 0.8720	 0.4560
ER	 0.8460	 0.4240
ES	 0.8670	 0.4490
ET	 0.8890	 0.4530
EU	 0.8710	 0.4540
EV	 0.8440	 0.4130
EW	 0.8810	 0.4480
EX	 0.8650	 0.4510
EY	 0.8790	 0.4550
EZ	 0.8450	 0.4190
FA	 0.8740	 0.4580
FB	 0.8390	 0.4060
FC	 0.8690	 0.4540
FD	 0.8760	 0.4470
FE	 0.8690	 0.4490
FF	 0.8380	 0.4210
FG	 0.8700	 0.4500
FH	 0.8660	 0.4530
FI	 0.8630	 0.4500
FJ	 0.8660	 0.4640
FK	 0.8880	 0.4770
FL	 0.8830	 0.4810
FM	 0.8690	 0.4690
FN	 0.8580	 0.4730
FO	 0.8820	 0.4810
FP	 0.8730	 0.4610
FQ	 0.8430	 0.4410
FR	 0.7830	 0.3770
FS	 0.8260	 0.4130
FT	 0.8570	 0.4530
FU	 0.8690	 0.4690
FV	 0.8750	 0.4670
FW	 0.8690	 0.4680
FX	 0.8770	 0.4740
FY	 0.8710	 0.4580
FZ	 0.8700	 0.4380
GA	 0.8230	 0.4120
GB	 0.8030	 0.3970
GC	 0.8360	 0.4250
GD	 0.7890	 0.3740





















































































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Chain	Atom inclusion	Q-score
GE	 0.8460	 0.4230
GF	 0.8050	 0.3810
GG	 0.7830	 0.3850
GH	 0.8230	 0.4150
GI	 0.8060	 0.3890
GJ	 0.8260	 0.4160
GK	 0.8450	 0.4430
GL	 0.8630	 0.4520
GM	 0.8340	 0.4420
GN	 0.8370	 0.4490
GO	 0.8860	 0.4550
GP	 0.8760	 0.4290
GQ	 0.7950	 0.4300
GR	 0.8700	 0.4480
GS	 0.8700	 0.4290
GT	 0.8760	 0.4550
GU	 0.8730	 0.4430
GV	 0.8890	 0.4410
GW	 0.8570	 0.4560
GX	 0.8760	 0.4350
GY	 0.8630	 0.4380
GZ	 0.8890	 0.4490
HA	 0.8600	 0.4450
HB	 0.8370	 0.4480
HC	 0.8990	 0.4180
HD	 0.8640	 0.4230
HE	 0.8730	 0.4200
HF	 0.8760	 0.4120
HG	 0.8660	 0.4260
HH	 0.8490	 0.4240
HI	 0.8610	 0.3990
HJ	 0.8800	 0.3940
HK	 0.8950	 0.3990
HL	 0.7590	 0.3960
HM	 0.8300	 0.3880
HN	 0.8790	 0.4560
HO	 0.8760	 0.4460
HP	 0.8600	 0.4340
HQ	 0.8400	 0.4290
HR	 0.9120	 0.4650
HS	 0.8140	 0.4200
HT	 0.8830	 0.4590











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Chain	Atom inclusion	Q-score
HU	 0.8730	 0.4420
HV	 0.9020	 0.4500
HW	 0.7830	 0.4290
HX	 0.8860	 0.4450
HY	 0.8920	 0.4530
HZ	 0.8760	 0.4370
IA	 0.8440	 0.4320
IB	 0.7730	 0.4380
IC	 0.8920	 0.4360
ID	 0.8580	 0.4180
IE	 0.8960	 0.4490
IF	 0.8990	 0.4330
IG	 0.8760	 0.4440
IH	 0.8620	 0.3980
II	 0.8840	 0.4400
IJ	 0.9030	 0.4140
IK	 0.9190	 0.4140
IL	 0.8780	 0.4070
IM	 0.8890	 0.4240
IN	 0.8630	 0.4090
IO	 0.8660	 0.3970
IP	 0.8730	 0.4010
IQ	 0.8790	 0.4020
IR	 0.8570	 0.4000
IS	 0.8700	 0.4130
IT	 0.8830	 0.4230
IU	 0.8540	 0.4070
IV	 0.8370	 0.4000
IW	 0.8860	 0.4240
IX	 0.8790	 0.4120
IY	 0.8780	 0.4060
IZ	 0.8660	 0.4200
JA	 0.8720	 0.4130
JB	 0.8760	 0.4020
JC	 0.8600	 0.4000
JD	 0.8870	 0.4080
JE	 0.8530	 0.4110
JF	 0.8730	 0.3960
JG	 0.8570	 0.3960
JH	 0.8790	 0.4010
JI	 0.8470	 0.4310
JJ	 0.8720	 0.4050

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Chain	Atom inclusion	Q-score
JK	 0.8700	 0.4090
JL	 0.8790	 0.4350
JM	 0.8660	 0.4050
JN	 0.8780	 0.4070
JO	 0.8600	 0.4140