



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 01:35 AM UTC

PDB ID : 6TBA / pdb_00006tba
EMDB ID : EMD-10443
Title : Virion of native gene transfer agent (GTA) particle
Authors : Bardy, P.; Fuzik, T.; Hrebik, D.; Pantucek, R.; Beatty, J.T.; Plevka, P.
Deposited on : 2019-11-01
Resolution : 4.54 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

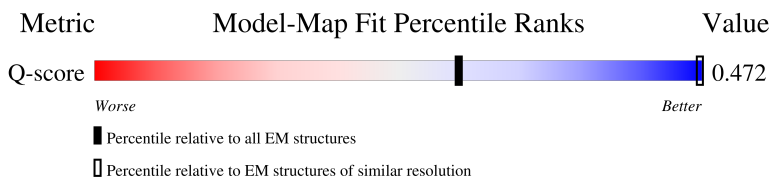
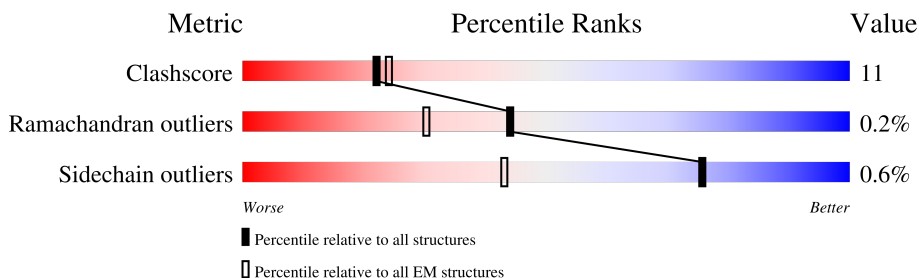
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.54 Å.

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



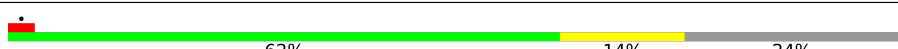
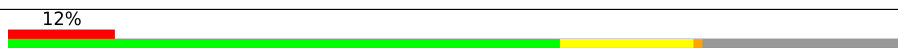
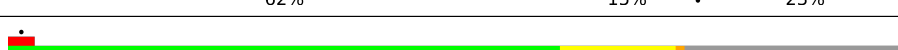
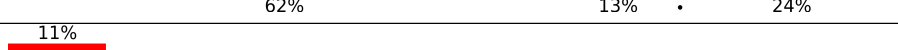
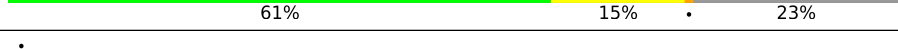
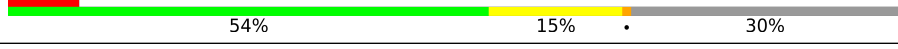
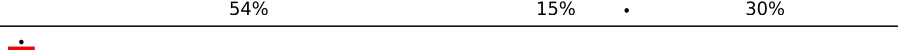
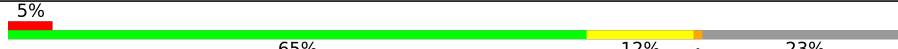
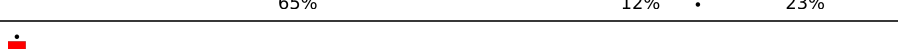
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2475 (4.04 - 5.04)

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	A4	385	
1	A5	385	
1	A9	385	
1	AA	385	

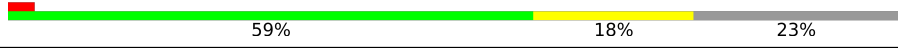
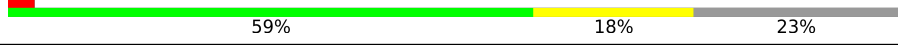
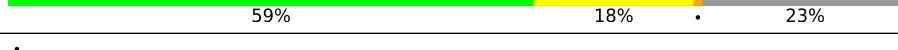
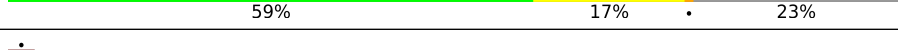
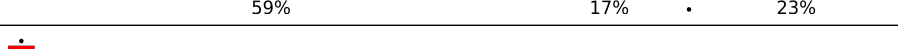
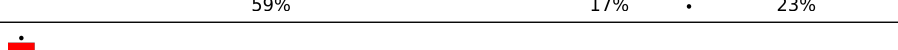
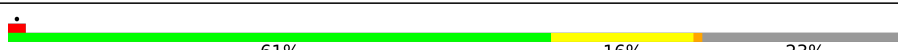
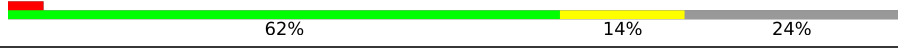
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Mol	Chain	Length	Quality of chain
1	AE	385	
1	AF	385	
1	AJ	385	
1	AK	385	
1	AO	385	
1	AP	385	
1	B4	385	
1	B5	385	
1	B9	385	
1	BA	385	
1	BE	385	
1	BF	385	
1	BJ	385	
1	BK	385	
1	BO	385	
1	BP	385	
1	C4	385	
1	C5	385	
1	C9	385	
1	CA	385	
1	CE	385	
1	CF	385	
1	CJ	385	
1	CK	385	
1	CO	385	

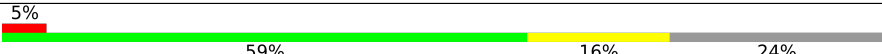
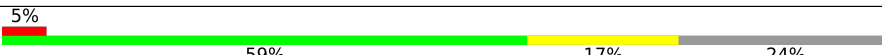
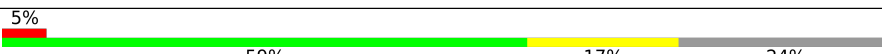
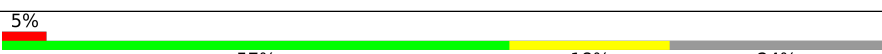
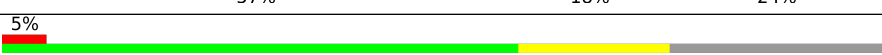
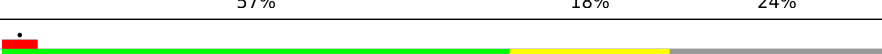
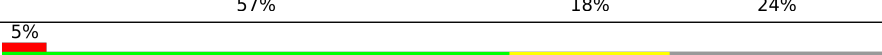
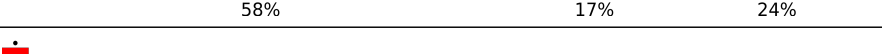
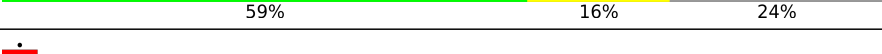
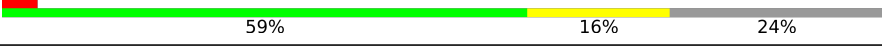
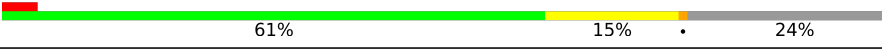
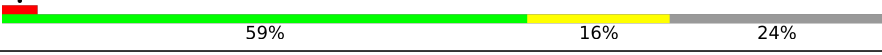
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Mol	Chain	Length	Quality of chain
1	CP	385	
1	D4	385	
1	D9	385	
1	DE	385	
1	DJ	385	
1	DO	385	
1	E4	385	
1	E9	385	
1	EE	385	
1	EJ	385	
1	EO	385	
1	F4	385	
1	F9	385	
1	FE	385	
1	FJ	385	
1	FO	385	
1	G4	385	
1	G9	385	
1	GE	385	
1	GJ	385	
1	GO	385	
1	H4	385	
1	H9	385	
1	HE	385	
1	HJ	385	

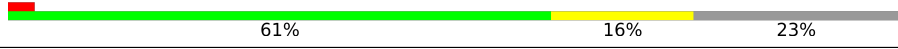
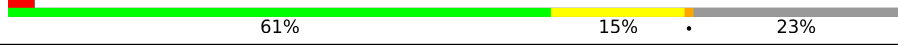
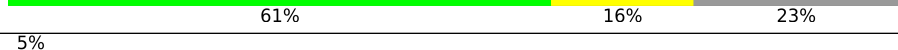
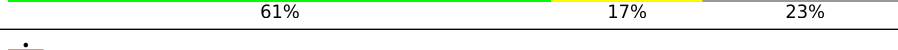
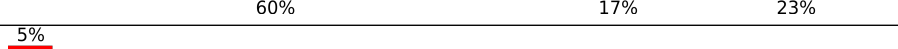
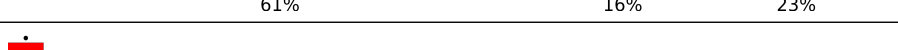
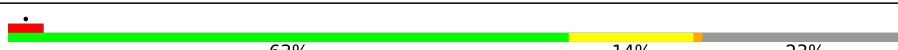
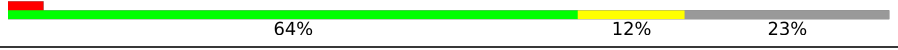
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Mol	Chain	Length	Quality of chain
1	HO	385	
1	I4	385	
1	I9	385	
1	IE	385	
1	IJ	385	
1	IO	385	
1	J4	385	
1	J9	385	
1	JE	385	
1	JJ	385	
1	JO	385	
1	K4	385	
1	K9	385	
1	KE	385	
1	KJ	385	
1	KO	385	
1	L4	385	
1	L9	385	
1	LE	385	
1	LJ	385	
1	LO	385	
1	M4	385	
1	M9	385	
1	ME	385	
1	MJ	385	

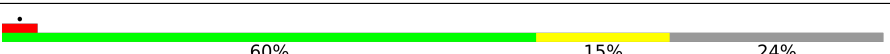
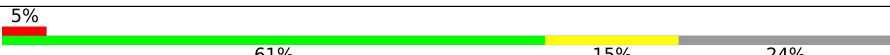
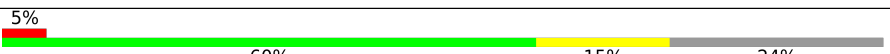
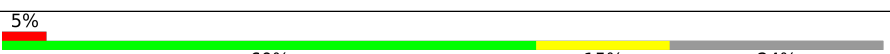
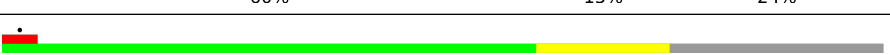
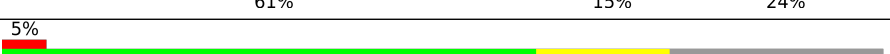
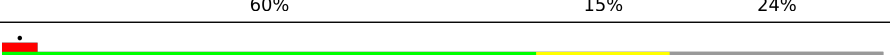
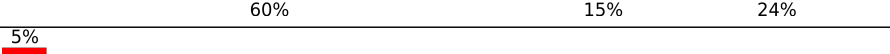
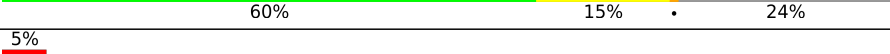
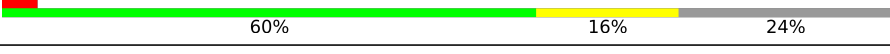
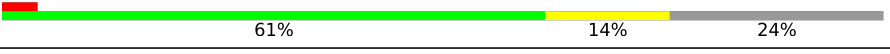
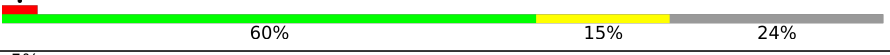
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Mol	Chain	Length	Quality of chain
1	MO	385	
1	N4	385	
1	N9	385	
1	NE	385	
1	NJ	385	
1	NO	385	
1	O4	385	
1	O9	385	
1	OE	385	
1	OJ	385	
1	OO	385	
1	P4	385	
1	P9	385	
1	PE	385	
1	PJ	385	
1	PO	385	
1	Q4	385	
1	Q9	385	
1	QE	385	
1	QJ	385	
1	QO	385	
1	R4	385	
1	R9	385	
1	RE	385	
1	RJ	385	

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Mol	Chain	Length	Quality of chain
1	RO	385	
1	S4	385	
1	S9	385	
1	SE	385	
1	SJ	385	
1	SO	385	
1	T4	385	
1	T9	385	
1	TE	385	
1	TJ	385	
1	TO	385	
1	U4	385	
1	U9	385	
1	UE	385	
1	UJ	385	
1	UO	385	
1	V4	385	
1	V9	385	
1	VE	385	
1	VJ	385	
1	VO	385	
1	W4	385	
1	W9	385	
1	WE	385	
1	WJ	385	

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Mol	Chain	Length	Quality of chain
1	WO	385	
1	X4	385	
1	X9	385	
1	XE	385	
1	XJ	385	
1	XO	385	
1	Y4	385	
1	Y9	385	
1	YE	385	
1	YJ	385	
1	YO	385	
1	Z4	385	
1	Z9	385	
1	ZE	385	
1	ZJ	385	
1	ZO	385	
2	A1	84	
2	A2	84	
2	A3	84	
2	A6	84	
2	A7	84	
2	A8	84	
2	AB	84	
2	AC	84	
2	AD	84	

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Mol	Chain	Length	Quality of chain
2	AG	84	7% 65% 35%
2	AH	84	17% 64% 36%
2	AI	84	29% 69% 31%
2	AL	84	7% 67% 33%
2	AM	84	18% 65% 35%
2	AN	84	23% 69% 31%
2	B2	84	17% 65% 35%
2	B3	84	19% 65% 35%
2	B7	84	19% 68% 32%
2	B8	84	21% 65% 35%
2	BC	84	18% 67% 33%
2	BD	84	20% 65% 35%
2	BH	84	17% 67% 33%
2	BI	84	21% 65% 35%
2	BM	84	19% 67% 33%
2	BN	84	21% 65% 35%
2	C2	84	24% 68% 32%
2	C3	84	21% 68% 32%
2	C7	84	21% 69% 31%
2	C8	84	26% 68% 32%
2	CC	84	20% 67% 33%
2	CD	84	24% 68% 32%
2	CH	84	20% 67% 33%
2	CI	84	21% 68% 32%
2	CM	84	21% 68% 32%

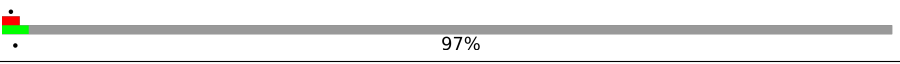
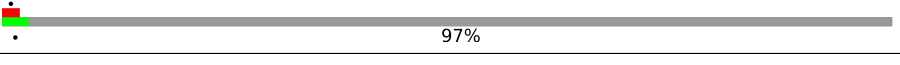
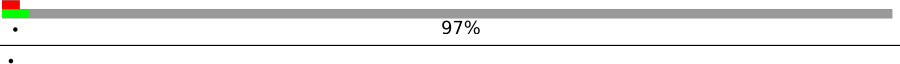
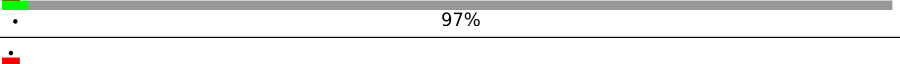
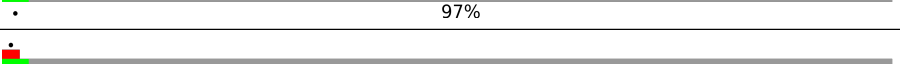
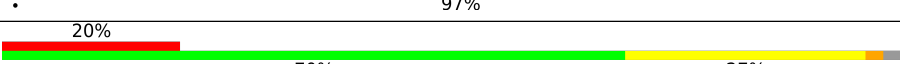
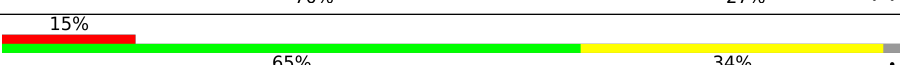
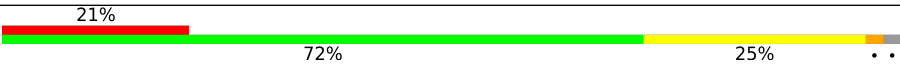
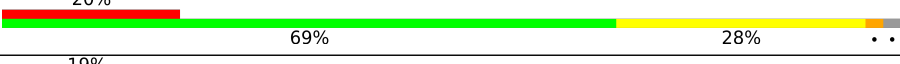
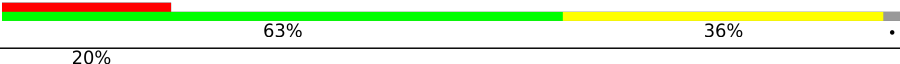
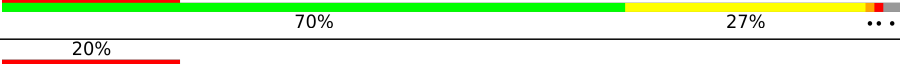
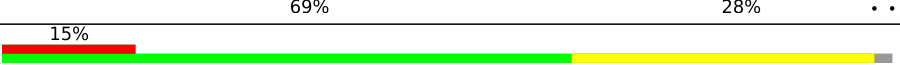
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Mol	Chain	Length	Quality of chain
2	CN	84	
2	D2	84	
2	D3	84	
2	D7	84	
2	D8	84	
2	DC	84	
2	DD	84	
2	DH	84	
2	DI	84	
2	DM	84	
2	DN	84	
2	E2	84	
2	E3	84	
2	E7	84	
2	E8	84	
2	EC	84	
2	ED	84	
2	EH	84	
2	EI	84	
2	EM	84	
2	EN	84	
3	F2	325	
3	F3	325	
3	F7	325	
3	F8	325	

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Mol	Chain	Length	Quality of chain
3	FC	325	 97%
3	FD	325	 97%
3	FH	325	 97%
3	FI	325	 97%
3	FM	325	 97%
3	FN	325	 97%
4	2A	197	 20% 70% 27% ..
4	2B	197	 15% 65% 34% .
4	2C	197	 21% 72% 25% ..
4	2D	197	 17% 65% 34% .
4	2E	197	 20% 69% 28% ..
4	2F	197	 19% 63% 36% .
4	2G	197	 20% 70% 27% ...
4	2H	197	 20% 64% 35% .
4	2I	197	 20% 69% 28% ..
4	2J	197	 15% 64% 34% .
4	2K	197	 18% 71% 26% ..
4	2L	197	 16% 65% 34% .
5	1A	396	 15% 73% 17% . 9%
5	1B	396	 17% 73% 18% 9%
5	1C	396	 18% 73% 17% . 9%
5	1D	396	 18% 72% 18% 9%
5	1E	396	 20% 72% 18% . 9%
5	1F	396	 20% 71% 19% 9%
5	1G	396	 19% 72% 18% . 9%

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Mol	Chain	Length	Quality of chain
5	1H	396	
5	1I	396	
5	1J	396	
5	1K	396	
5	1L	396	
6	4A	135	
6	4B	135	
6	4C	135	
6	4D	135	
6	4E	135	
6	4F	135	
7	3A	112	
7	3B	112	
7	3C	112	
7	3D	112	
7	3E	112	
7	3F	112	
8	50	137	
8	51	137	
8	52	137	
8	53	137	
8	5A	137	
8	5B	137	
8	5C	137	
8	5D	137	

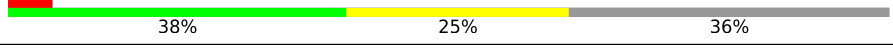
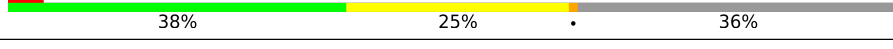
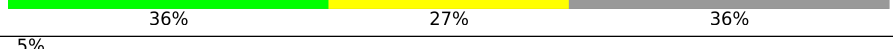
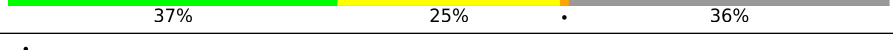
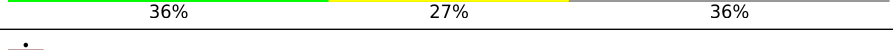
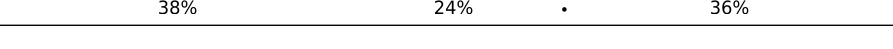
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Mol	Chain	Length	Quality of chain
8	5E	137	
8	5F	137	
8	5G	137	
8	5H	137	
8	5I	137	
8	5J	137	
8	5K	137	
8	5L	137	
8	5M	137	
8	5N	137	
8	5O	137	
8	5P	137	
8	5Q	137	
8	5R	137	
8	5S	137	
8	5T	137	
8	5U	137	
8	5V	137	
8	5W	137	
8	5X	137	
8	5Y	137	
8	5Z	137	
9	7A	296	
9	7B	296	
9	7C	296	

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Mol	Chain	Length	Quality of chain
10	8A	1304	
10	8B	1304	
10	8C	1304	
11	6A	210	
11	6B	210	
11	6C	210	
11	6D	210	
11	6E	210	
11	6F	210	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 465916 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 Phage major capsid protein, HK97 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C5	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	X4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	Y4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	Z4	297	Total	C	N	O	S	0	0
			2207	1399	377	425	6		
1	A5	297	Total	C	N	O	S	0	0
			2199	1394	377	422	6		
1	B5	271	Total	C	N	O	S	0	0
			2009	1278	342	383	6		
1	N4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	R4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	M4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	Q4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	O4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	P4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	W4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	U4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	T4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	S4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	K4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	J4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	V4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	L4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	H4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	I4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	A4	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	D4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	E4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	F4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	G4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	B4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	C4	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	CP	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	XO	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	YO	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	ZO	297	Total	C	N	O	S	0	0
			2207	1399	377	425	6		
1	AP	297	Total	C	N	O	S	0	0
			2201	1396	377	422	6		
1	BP	271	Total	C	N	O	S	0	0
			2009	1280	342	381	6		
1	NO	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	RO	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	MO	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	QO	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	OO	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	PO	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	WO	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	UO	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	TO	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	SO	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	KO	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	JO	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	VO	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	LO	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	HO	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	IO	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	AO	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	DO	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	EO	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	FO	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	GO	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	BO	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	CO	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	CK	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	XJ	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	YJ	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	ZJ	297	Total	C	N	O	S	0	0
			2207	1399	377	425	6		
1	AK	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	BK	271	Total	C	N	O	S	0	0
			2009	1278	342	383	6		
1	NJ	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	RJ	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	MJ	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	QJ	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	OJ	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	PJ	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	WJ	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	UJ	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	TJ	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	SJ	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	KJ	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	JJ	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	VJ	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	LJ	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	HJ	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	IJ	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AJ	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	DJ	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	EJ	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	FJ	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	GJ	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	BJ	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	CJ	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	CF	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	XE	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	YE	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	ZE	297	Total	C	N	O	S	0	0
			2207	1399	377	425	6		
1	AF	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	BF	271	Total	C	N	O	S	0	0
			2015	1283	344	382	6		
1	NE	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	RE	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	ME	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	QE	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	OE	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	PE	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	WE	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	UE	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	TE	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	SE	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	KE	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	JE	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	VE	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	LE	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	HE	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	IE	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	AE	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	DE	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	EE	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	FE	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	GE	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	BE	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	CE	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	CA	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	X9	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	Y9	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	Z9	297	Total	C	N	O	S	0	0
			2207	1399	377	425	6		
1	AA	297	Total	C	N	O	S	0	0
			2205	1398	377	424	6		
1	BA	271	Total	C	N	O	S	0	0
			2014	1281	344	383	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	N9	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	R9	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	M9	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	Q9	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	O9	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	P9	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	W9	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	U9	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	T9	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	S9	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	K9	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	J9	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	V9	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	L9	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	H9	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	I9	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	A9	291	Total	C	N	O	S	0	0
			2173	1379	371	417	6		
1	D9	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	E9	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	F9	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	G9	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	B9	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		
1	C9	297	Total	C	N	O	S	0	0
			2209	1400	377	426	6		

- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E3	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	D3	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	A3	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	C3	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	B3	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	A1	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	E2	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	D2	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	A2	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	C2	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	B2	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	EN	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	DN	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	AN	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	CN	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	BN	84	Total	C	N	O	S	0	0
			640	403	115	121	1		
2	AL	84	Total	C	N	O	S	0	0
			640	403	115	121	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	EM	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	DM	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	AM	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	CM	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	BM	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	EI	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	DI	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	AI	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	CI	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	BI	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	AG	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	EH	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	DH	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	AH	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	CH	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	BH	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	ED	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	DD	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	AD	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	CD	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	BD	84	Total 640	C 403	N 115	O 121	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	EC	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	DC	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	AC	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	CC	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	BC	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	E8	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	D8	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	A8	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	C8	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	B8	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	A6	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	E7	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	D7	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	A7	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	C7	84	Total 640	C 403	N 115	O 121	S 1	0	0
2	B7	84	Total 640	C 403	N 115	O 121	S 1	0	0

- Molecule 3 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	F3	10	Total 62	C 42	N 10	O 10	0	0
3	F2	10	Total 62	C 42	N 10	O 10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	FN	10	Total	C	N	O	0	0
			62	42	10	10		
3	FM	10	Total	C	N	O	0	0
			62	42	10	10		
3	FI	10	Total	C	N	O	0	0
			62	42	10	10		
3	FH	10	Total	C	N	O	0	0
			62	42	10	10		
3	FD	10	Total	C	N	O	0	0
			62	42	10	10		
3	FC	10	Total	C	N	O	0	0
			62	42	10	10		
3	F8	10	Total	C	N	O	0	0
			62	42	10	10		
3	F7	10	Total	C	N	O	0	0
			62	42	10	10		

- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2A	194	Total	C	N	O	S	0	0
			1450	931	259	253	7		
4	2B	194	Total	C	N	O	S	0	0
			1453	933	259	253	8		
4	2K	194	Total	C	N	O	S	0	0
			1448	929	259	253	7		
4	2L	194	Total	C	N	O	S	0	0
			1456	936	259	253	8		
4	2I	194	Total	C	N	O	S	0	0
			1450	931	259	253	7		
4	2J	194	Total	C	N	O	S	0	0
			1456	936	259	253	8		
4	2G	194	Total	C	N	O	S	0	0
			1447	929	259	253	6		
4	2H	194	Total	C	N	O	S	0	0
			1453	934	259	253	7		
4	2E	194	Total	C	N	O	S	0	0
			1450	931	259	253	7		
4	2F	194	Total	C	N	O	S	0	0
			1456	936	259	253	8		
4	2C	194	Total	C	N	O	S	0	0
			1450	931	259	253	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	2D	194	Total	C	N	O	S	0	0
			1456	936	259	253	8		

- Molecule 5 is a protein called Portal protein Rcc01684.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1A	360	Total	C	N	O	S	0	0
			2714	1729	483	490	12		
5	1B	360	Total	C	N	O	S	0	0
			2723	1734	486	490	13		
5	1K	360	Total	C	N	O	S	0	0
			2717	1731	483	490	13		
5	1L	360	Total	C	N	O	S	0	0
			2717	1731	483	490	13		
5	1I	360	Total	C	N	O	S	0	0
			2717	1731	483	490	13		
5	1J	360	Total	C	N	O	S	0	0
			2717	1731	483	490	13		
5	1G	360	Total	C	N	O	S	0	0
			2723	1734	486	490	13		
5	1H	360	Total	C	N	O	S	0	0
			2717	1731	483	490	13		
5	1E	360	Total	C	N	O	S	0	0
			2717	1731	483	490	13		
5	1F	360	Total	C	N	O	S	0	0
			2717	1731	483	490	13		
5	1C	360	Total	C	N	O	S	0	0
			2711	1728	480	490	13		
5	1D	360	Total	C	N	O	S	0	0
			2720	1732	486	490	12		

- Molecule 6 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4A	134	Total	C	N	O	S	0	0
			968	613	174	180	1		
6	4F	134	Total	C	N	O	S	0	0
			968	613	174	180	1		
6	4E	134	Total	C	N	O	S	0	0
			968	613	174	180	1		
6	4D	134	Total	C	N	O	S	0	0
			968	613	174	180	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	4C	134	Total	C	N	O	S	0	0
			968	613	174	180	1		
6	4B	134	Total	C	N	O	S	0	0
			968	613	174	180	1		

- Molecule 7 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	3A	110	Total	C	N	O	S	0	0
			859	536	171	151	1		
7	3F	110	Total	C	N	O	S	0	0
			859	536	171	151	1		
7	3E	110	Total	C	N	O	S	0	0
			859	536	171	151	1		
7	3D	110	Total	C	N	O	S	0	0
			859	536	171	151	1		
7	3C	110	Total	C	N	O	S	0	0
			859	536	171	151	1		
7	3B	110	Total	C	N	O	S	0	0
			859	536	171	151	1		

- Molecule 8 is a protein called Phage major tail protein, TP901-1 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	5A	130	Total	C	N	O	S	0	0
			972	612	163	195	2		
8	5S	130	Total	C	N	O	S	0	0
			972	612	163	195	2		
8	5G	130	Total	C	N	O	S	0	0
			972	612	163	195	2		
8	5M	130	Total	C	N	O	S	0	0
			972	612	163	195	2		
8	5F	130	Total	C	N	O	S	0	0
			972	612	163	195	2		
8	5X	130	Total	C	N	O	S	0	0
			972	612	163	195	2		
8	5L	130	Total	C	N	O	S	0	0
			972	612	163	195	2		
8	5R	130	Total	C	N	O	S	0	0
			972	612	163	195	2		
8	5E	130	Total	C	N	O	S	0	0
			972	612	163	195	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	5W	130	Total 972	C 612	N 163	O 195	S 2	0	0
8	5K	130	Total 972	C 612	N 163	O 195	S 2	0	0
8	5Q	130	Total 972	C 612	N 163	O 195	S 2	0	0
8	5D	130	Total 972	C 612	N 163	O 195	S 2	0	0
8	5V	130	Total 972	C 612	N 163	O 195	S 2	0	0
8	5J	130	Total 972	C 612	N 163	O 195	S 2	0	0
8	5P	130	Total 972	C 612	N 163	O 195	S 2	0	0
8	5C	130	Total 972	C 612	N 163	O 195	S 2	0	0
8	5U	130	Total 972	C 612	N 163	O 195	S 2	0	0
8	5I	130	Total 972	C 612	N 163	O 195	S 2	0	0
8	5O	130	Total 972	C 612	N 163	O 195	S 2	0	0
8	5B	130	Total 972	C 612	N 163	O 195	S 2	0	0
8	5T	130	Total 972	C 612	N 163	O 195	S 2	0	0
8	5H	130	Total 972	C 612	N 163	O 195	S 2	0	0
8	5N	130	Total 972	C 612	N 163	O 195	S 2	0	0
8	5Y	130	Total 972	C 612	N 163	O 195	S 2	0	0
8	5Z	130	Total 972	C 612	N 163	O 195	S 2	0	0
8	52	130	Total 972	C 612	N 163	O 195	S 2	0	0
8	53	130	Total 972	C 612	N 163	O 195	S 2	0	0
8	50	130	Total 972	C 612	N 163	O 195	S 2	0	0
8	51	130	Total 972	C 612	N 163	O 195	S 2	0	0

- Molecule 9 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	7A	292	Total	C	N	O	S	0	0
			2179	1369	395	408	7		
9	7C	292	Total	C	N	O	S	0	0
			2179	1369	395	408	7		
9	7B	292	Total	C	N	O	S	0	0
			2179	1369	395	408	7		

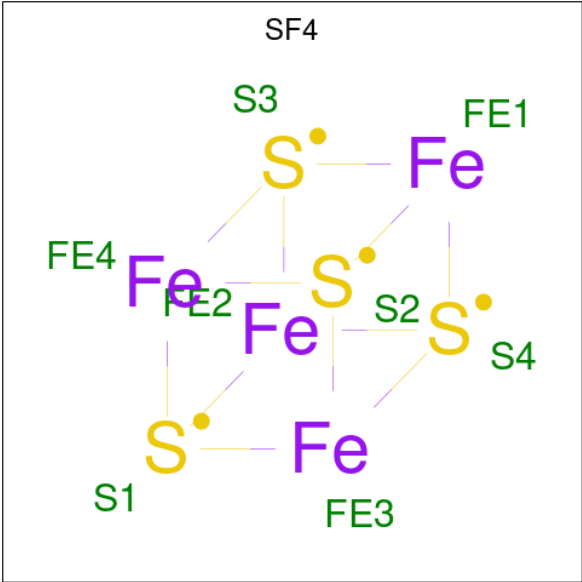
- Molecule 10 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	8A	439	Total	C	N	O	S	0	0
			3246	2028	590	621	7		
10	8C	439	Total	C	N	O	S	0	0
			3246	2028	590	621	7		
10	8B	439	Total	C	N	O	S	0	0
			3246	2028	590	621	7		

- Molecule 11 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	6B	134	Total	C	N	O	0	0
			1056	665	198	193		
11	6A	134	Total	C	N	O	0	0
			1056	665	198	193		
11	6F	134	Total	C	N	O	0	0
			1056	665	198	193		
11	6E	134	Total	C	N	O	0	0
			1056	665	198	193		
11	6D	134	Total	C	N	O	0	0
			1056	665	198	193		
11	6C	134	Total	C	N	O	0	0
			1056	665	198	193		

- Molecule 12 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

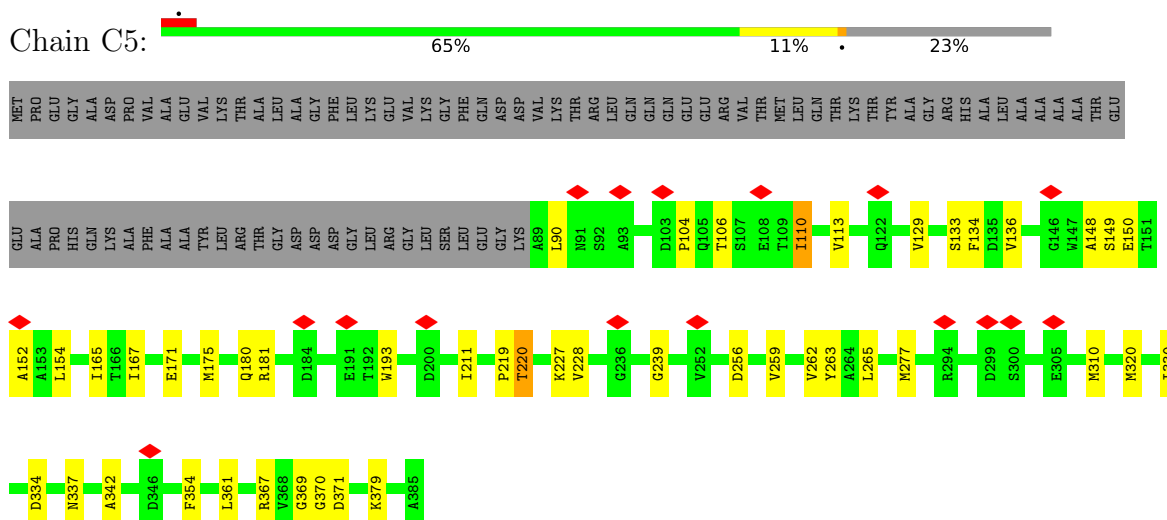


Mol	Chain	Residues	Atoms			AltConf
12	7A	1	Total	Fe	S	0
			8	4	4	
12	7C	1	Total	Fe	S	0
			8	4	4	
12	7B	1	Total	Fe	S	0
			8	4	4	

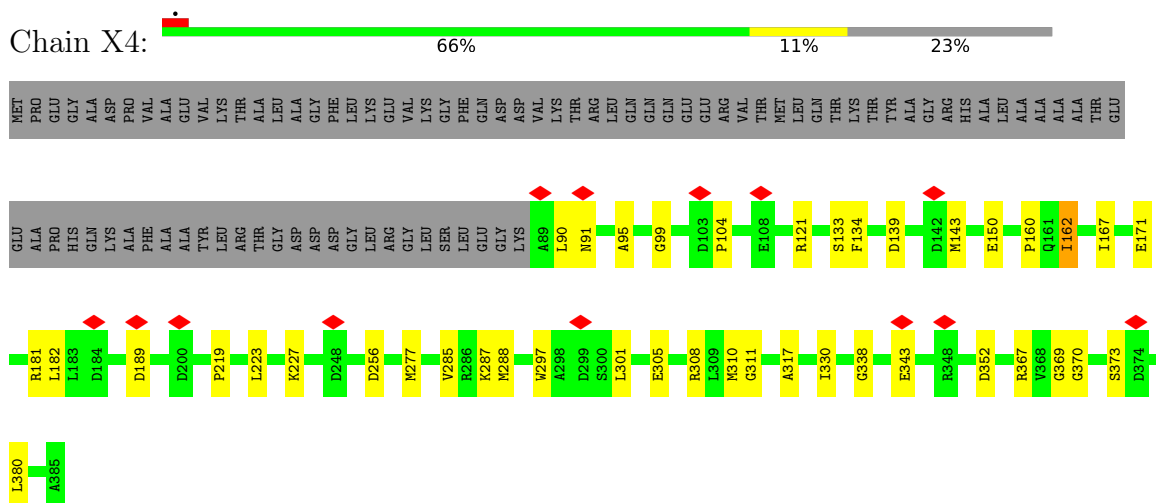
3 Residue-property plots

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

- Molecule 1: Phage major capsid protein, HK97 family

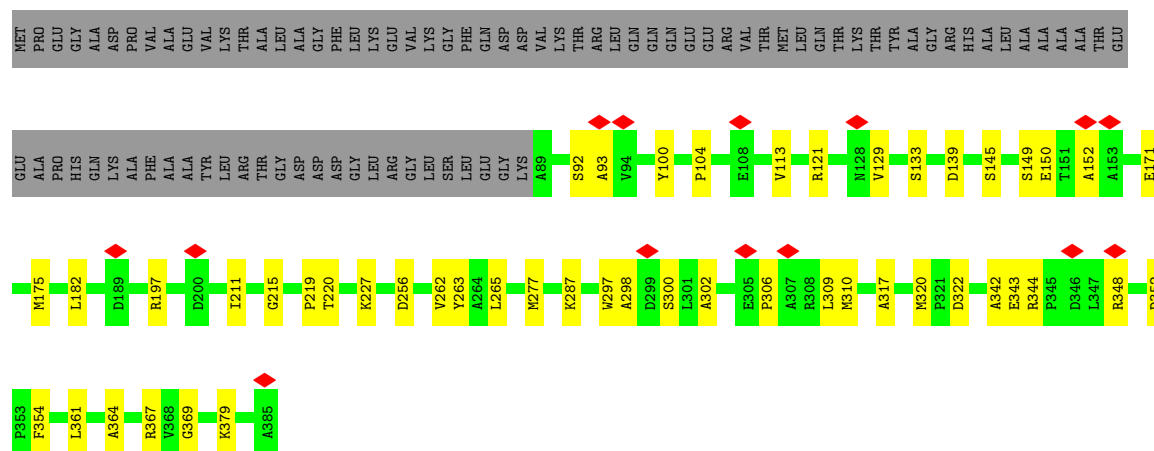


- Molecule 1: Phage major capsid protein, HK97 family



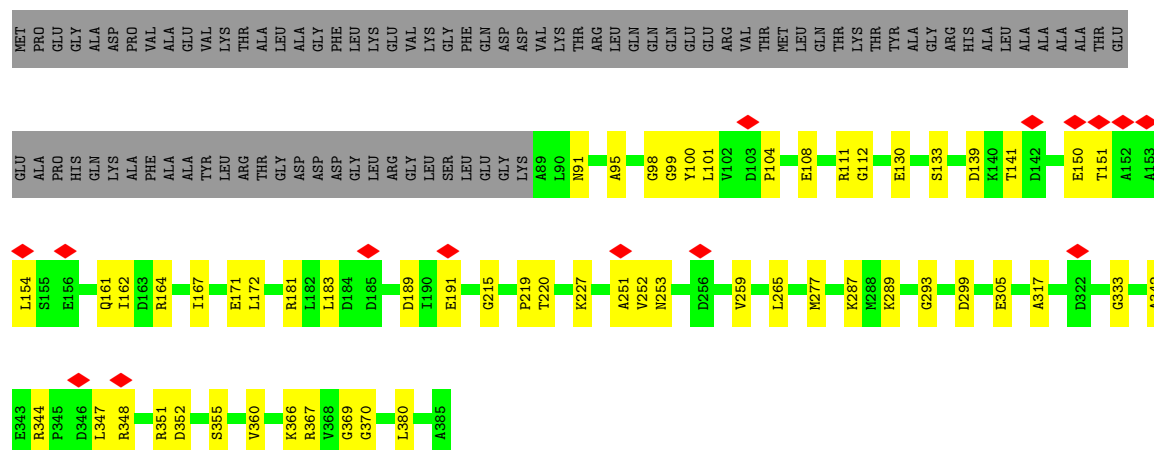
- Molecule 1: Phage major capsid protein, HK97 family





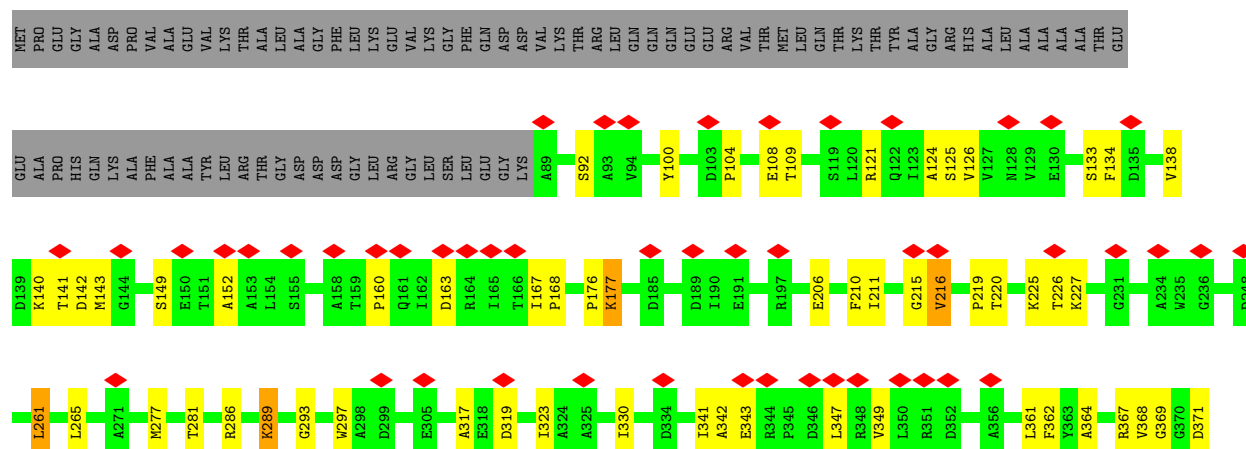
- Molecule 1: Phage major capsid protein, HK97 family

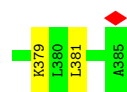
Chain Z4: 62% 15% 23%



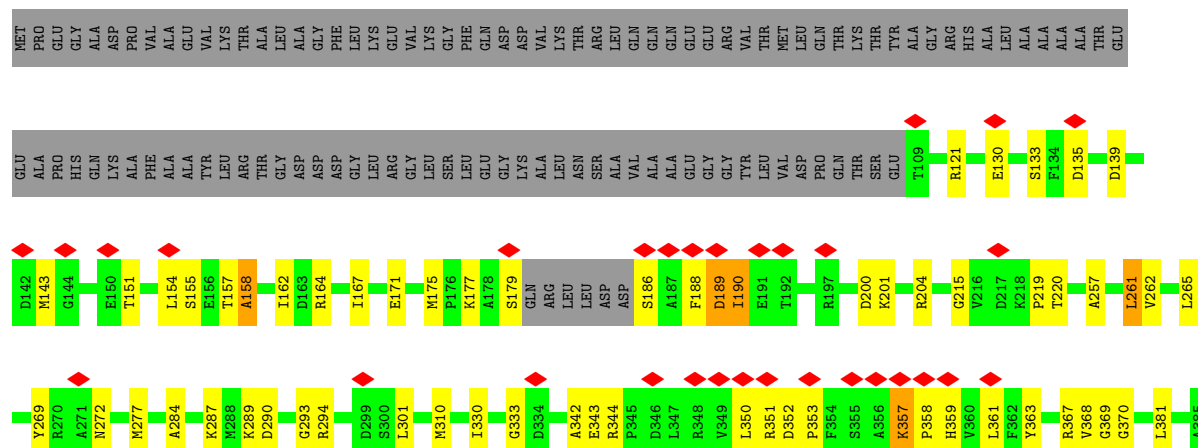
- Molecule 1: Phage major capsid protein, HK97 family

Chain A5: 13% 62% 15% 23%

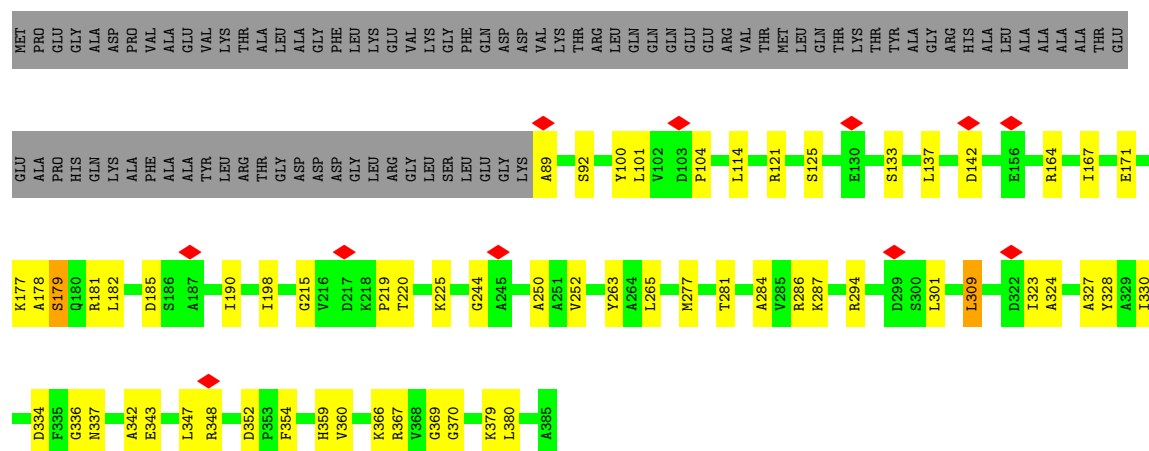




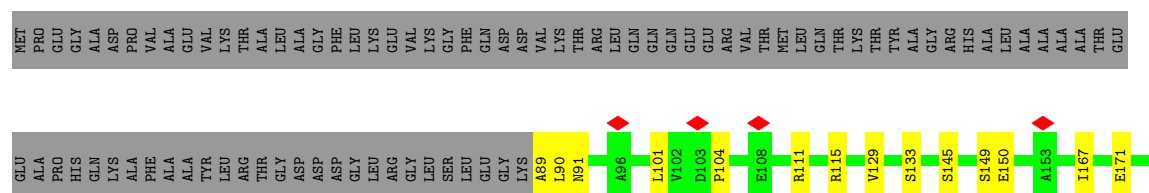
- Molecule 1: Phage major capsid protein, HK97 family

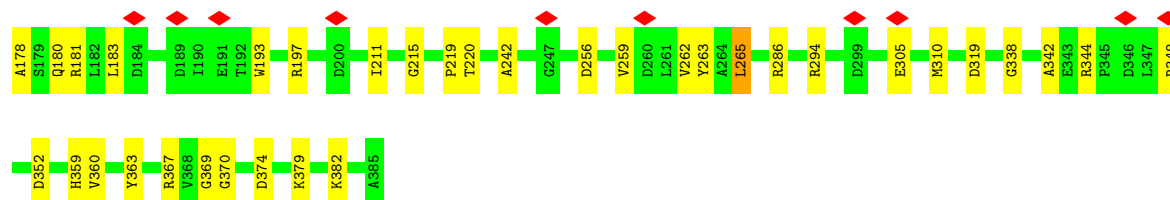


- Molecule 1: Phage major capsid protein, HK97 family

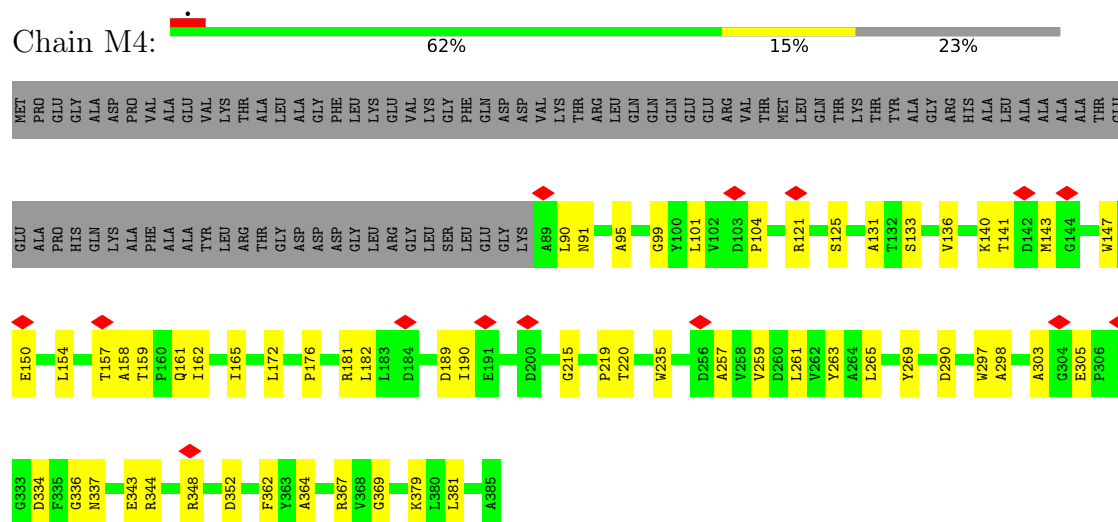


- Molecule 1: Phage major capsid protein, HK97 family

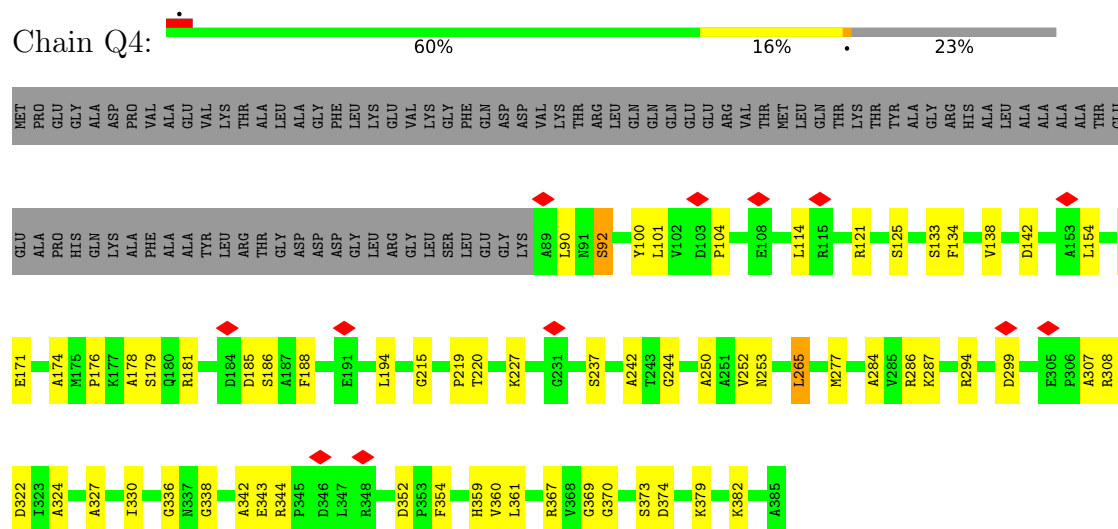




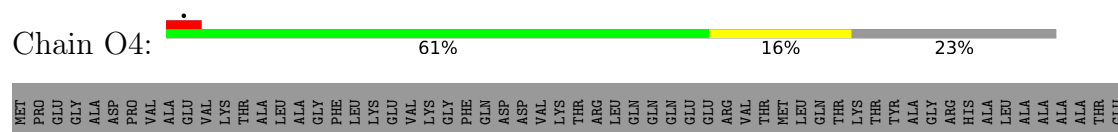
- Molecule 1: Phage major capsid protein, HK97 family

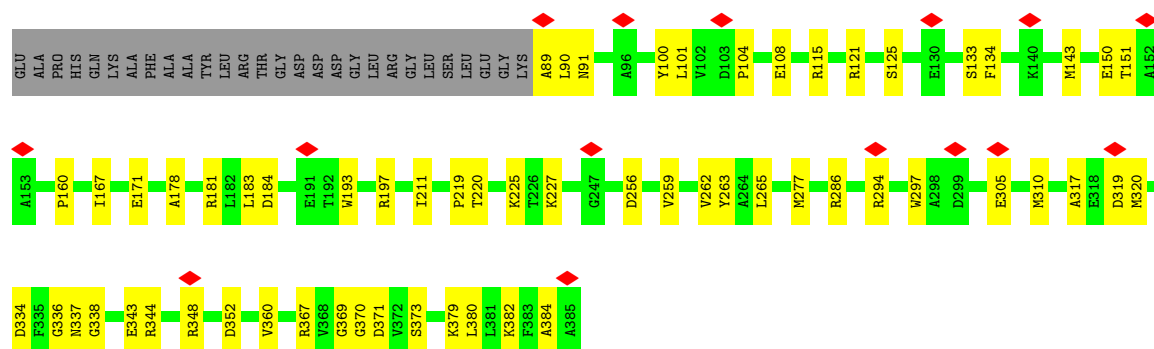


- Molecule 1: Phage major capsid protein, HK97 family



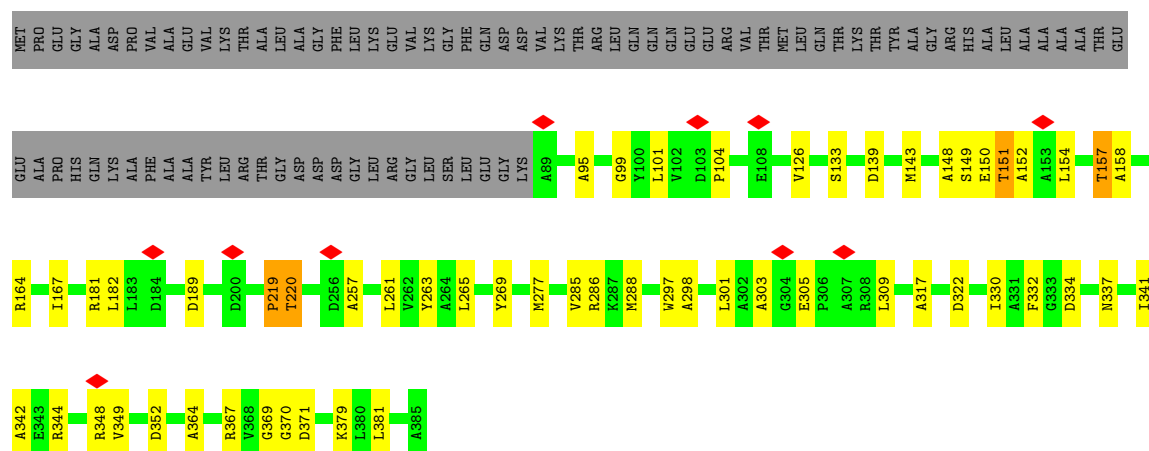
- Molecule 1: Phage major capsid protein, HK97 family





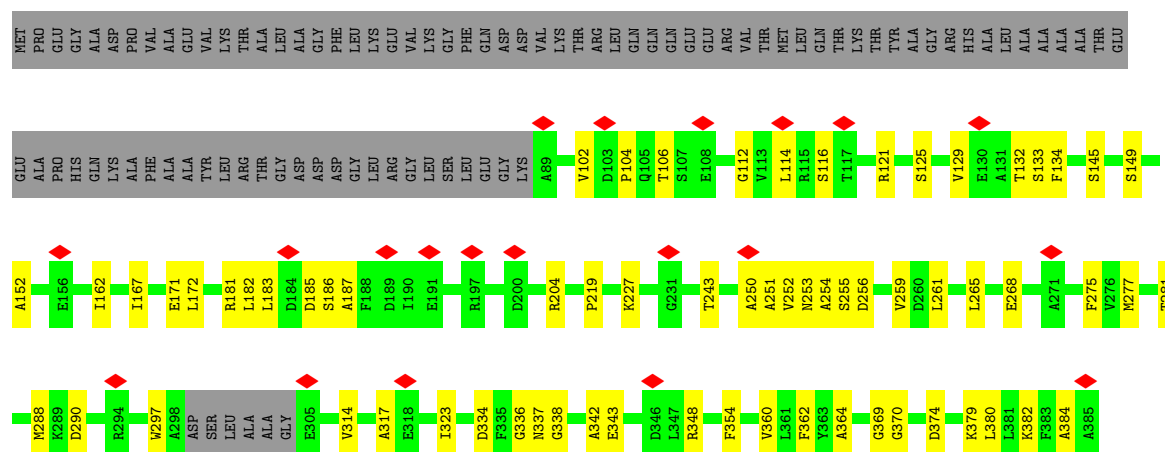
- Molecule 1: Phage major capsid protein, HK97 family

Chain P4: 62% 14% 23%



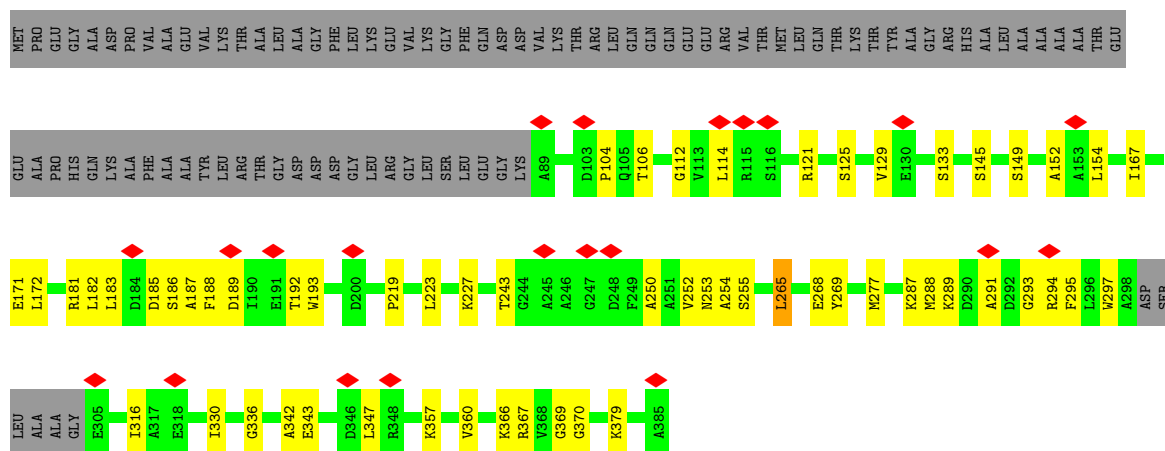
- Molecule 1: Phage major capsid protein, HK97 family

Chain W4: 5% 58% 17% 24%

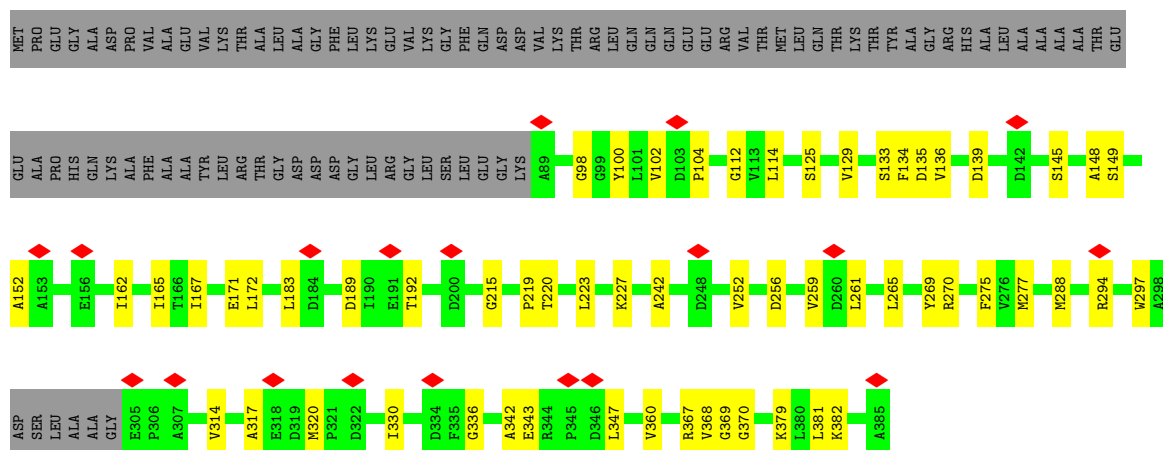


- Molecule 1: Phage major capsid protein, HK97 family

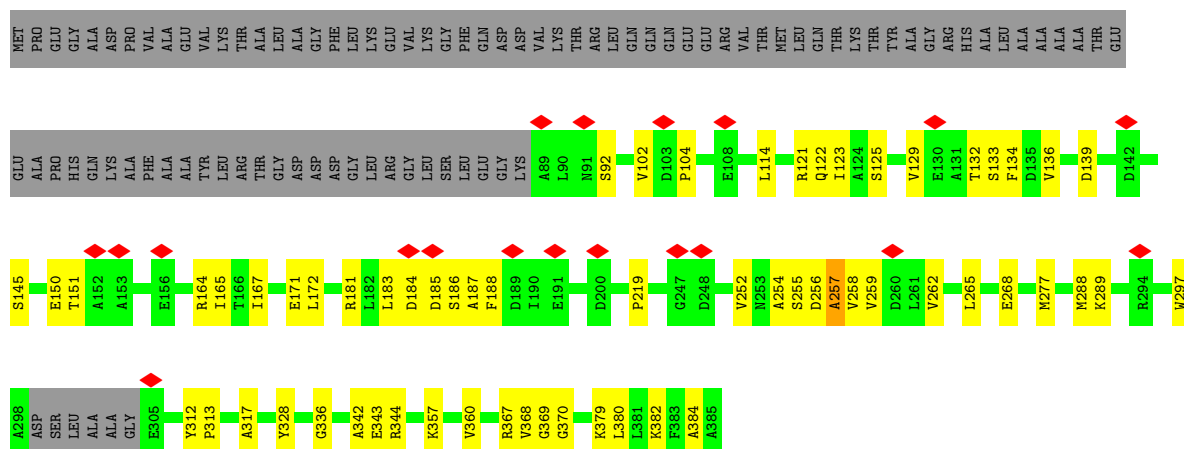
Chain U4: 5% 60% 15% 24%



- Molecule 1: Phage major capsid protein, HK97 family

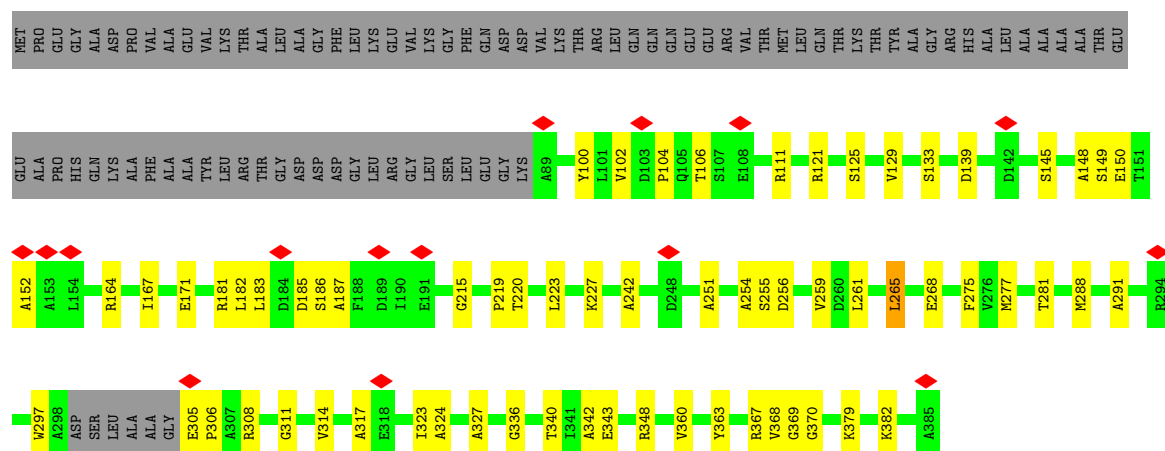


- Molecule 1: Phage major capsid protein, HK97 family



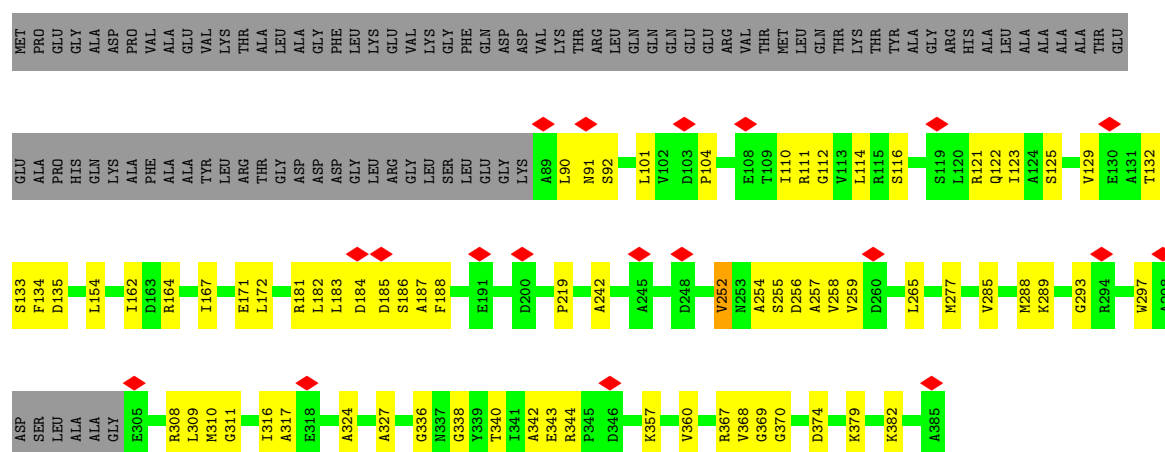
- Molecule 1: Phage major capsid protein, HK97 family

Chain K4:  58% 17% 24%



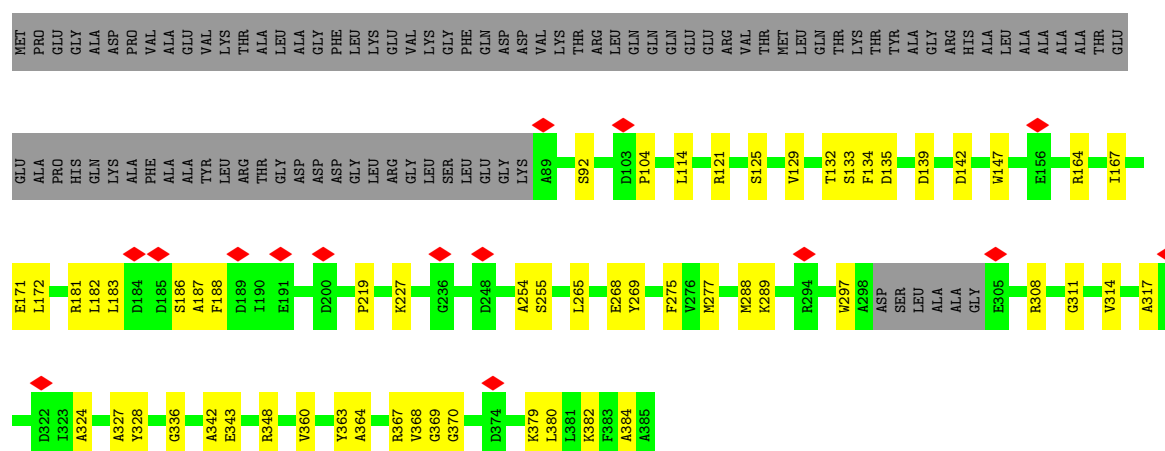
- Molecule 1: Phage major capsid protein, HK97 family

Chain J4:  5% 57% 18% 24%



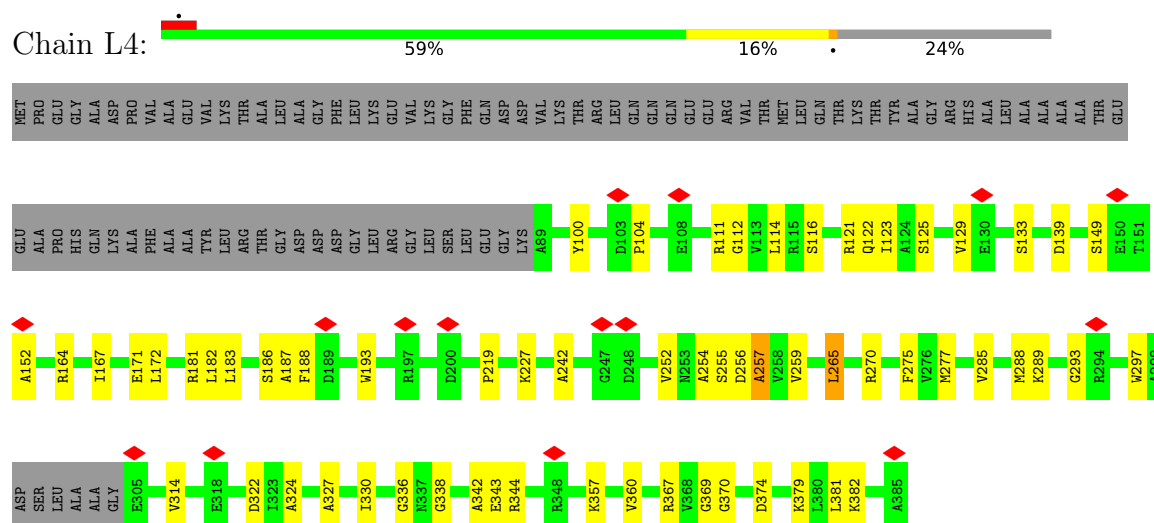
- Molecule 1: Phage major capsid protein, HK97 family

Chain V4:  61% 15% 24%



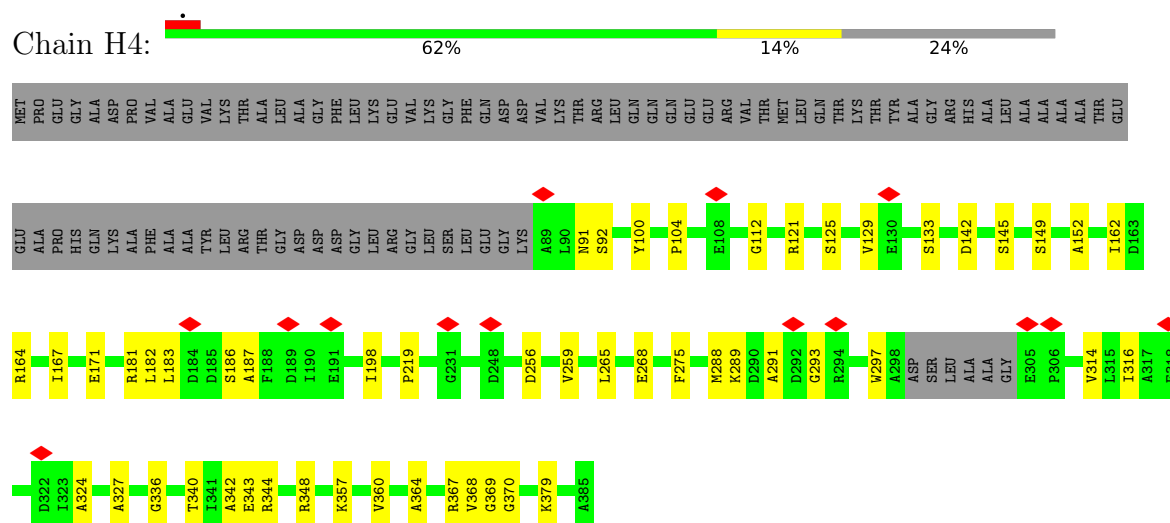
- Molecule 1: Phage major capsid protein, HK97 family

Chain L4:



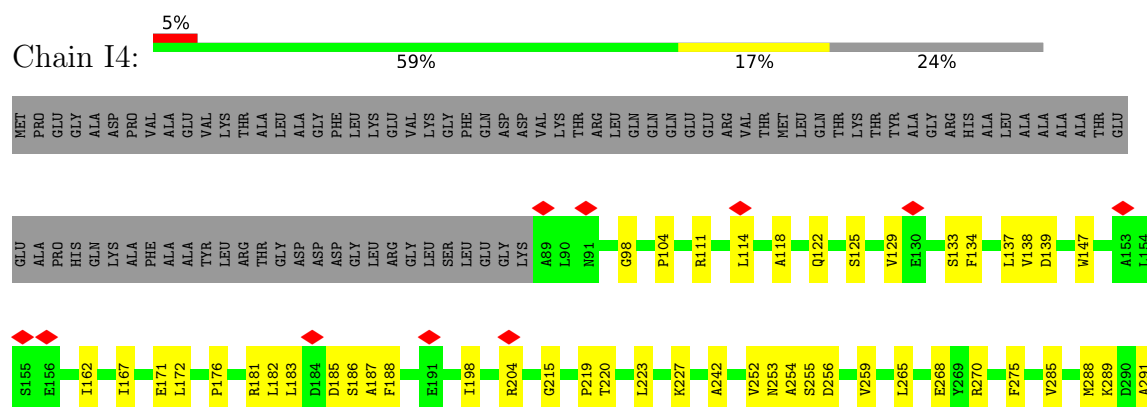
- Molecule 1: Phage major capsid protein, HK97 family

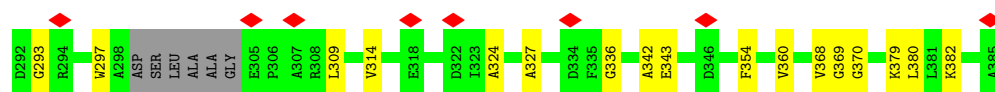
Chain H4:



- Molecule 1: Phage major capsid protein, HK97 family

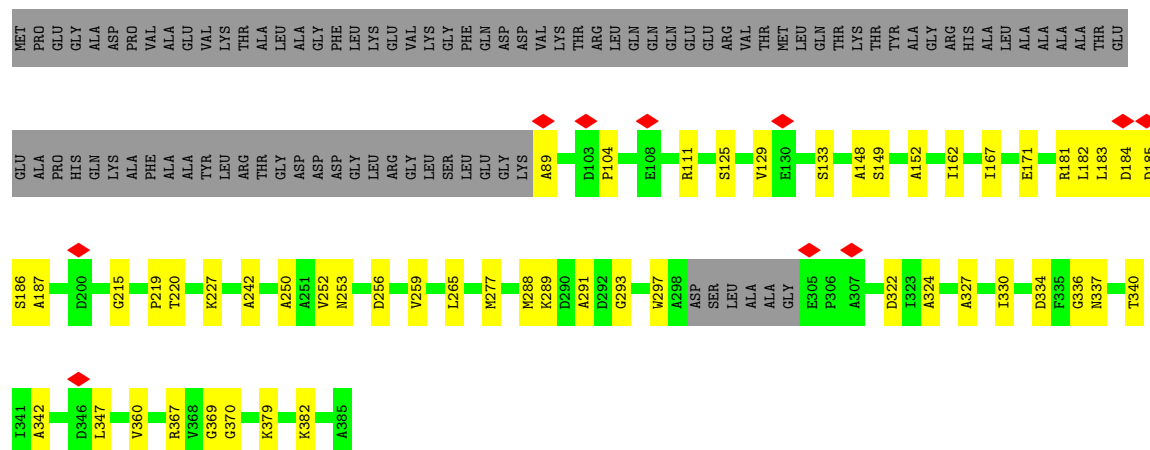
Chain I4:





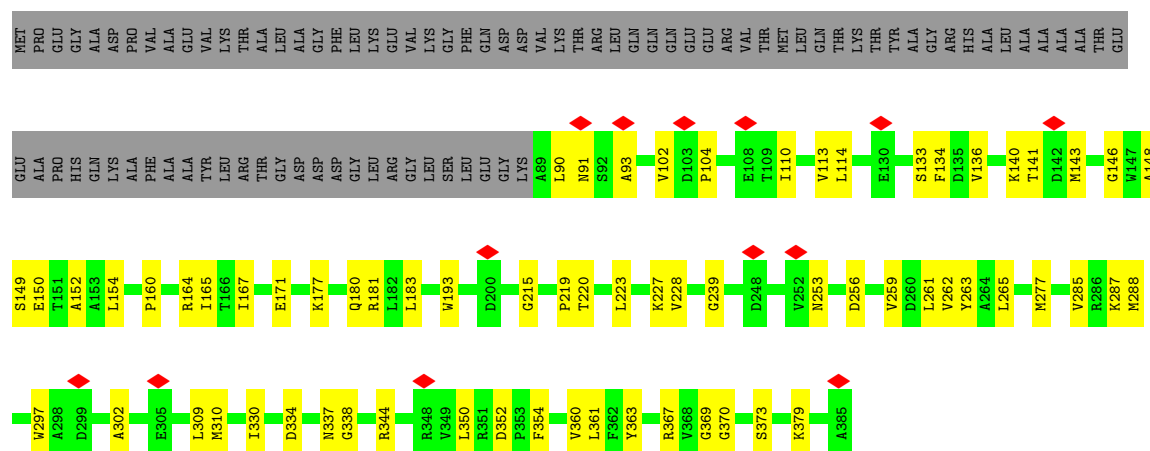
- Molecule 1: Phage major capsid protein, HK97 family

Chain A4: 62% 14% 24%



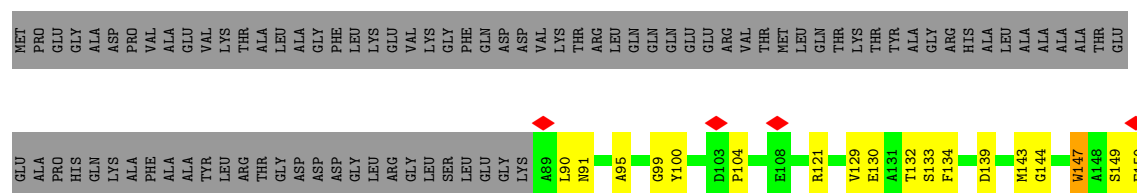
- Molecule 1: Phage major capsid protein, HK97 family

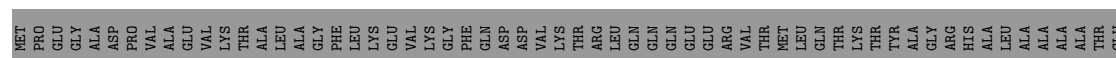
Chain D4: 59% 18% 23%

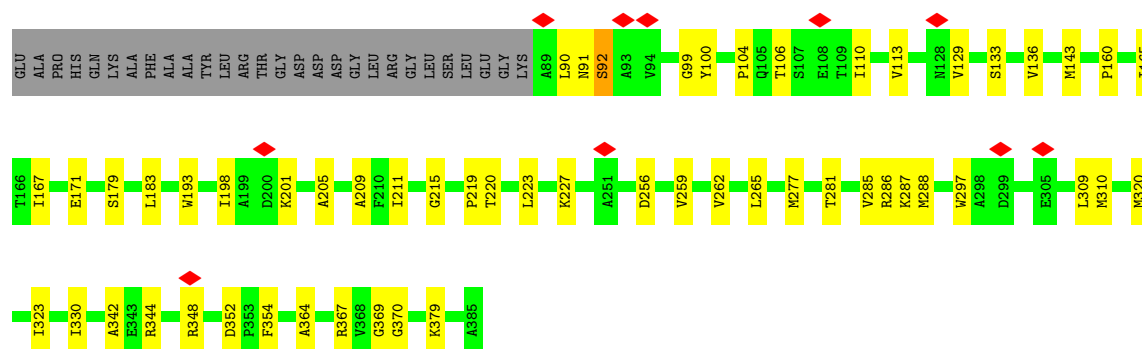


- Molecule 1: Phage major capsid protein, HK97 family

Chain E4: 59% 18% 23%

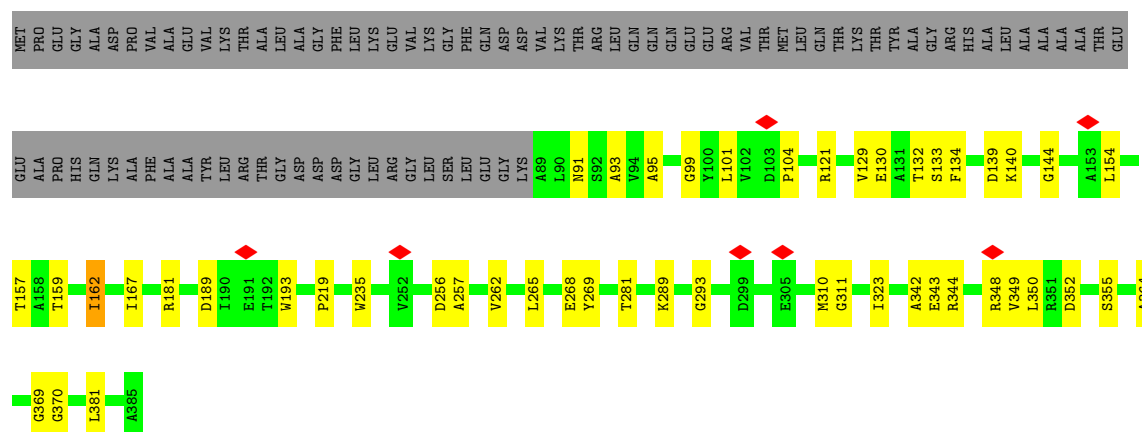






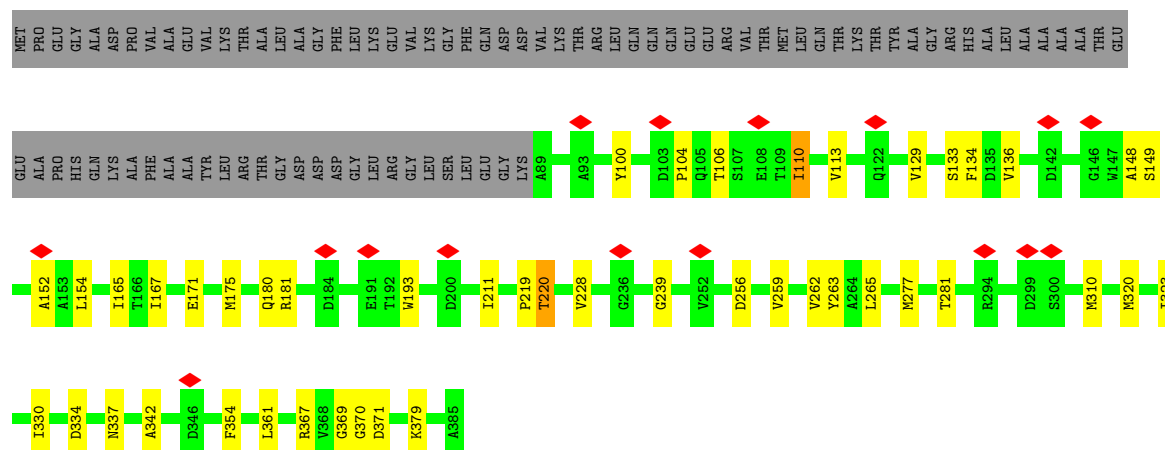
- Molecule 1: Phage major capsid protein, HK97 family

Chain C4: 64% 12% 23%



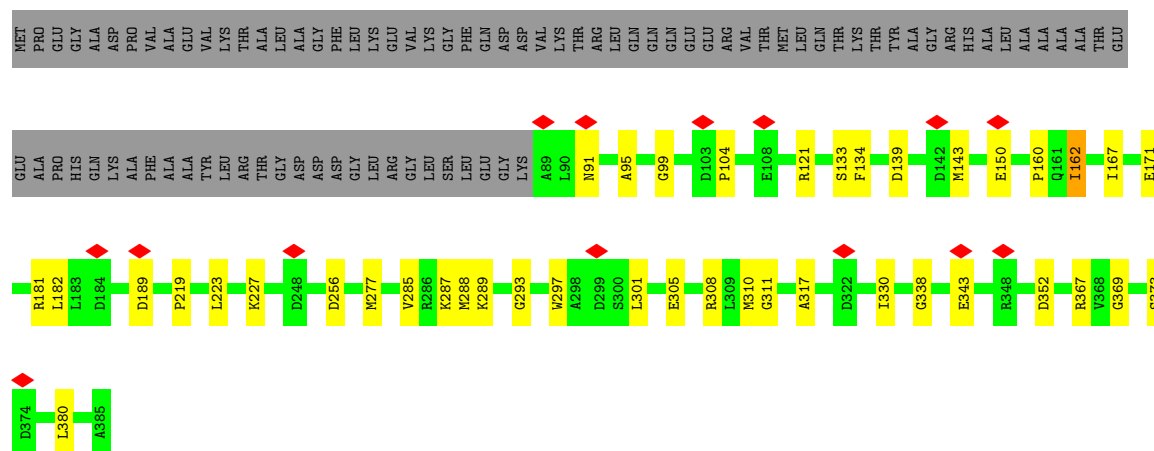
- Molecule 1: Phage major capsid protein, HK97 family

Chain CP: 65% 11% 23%



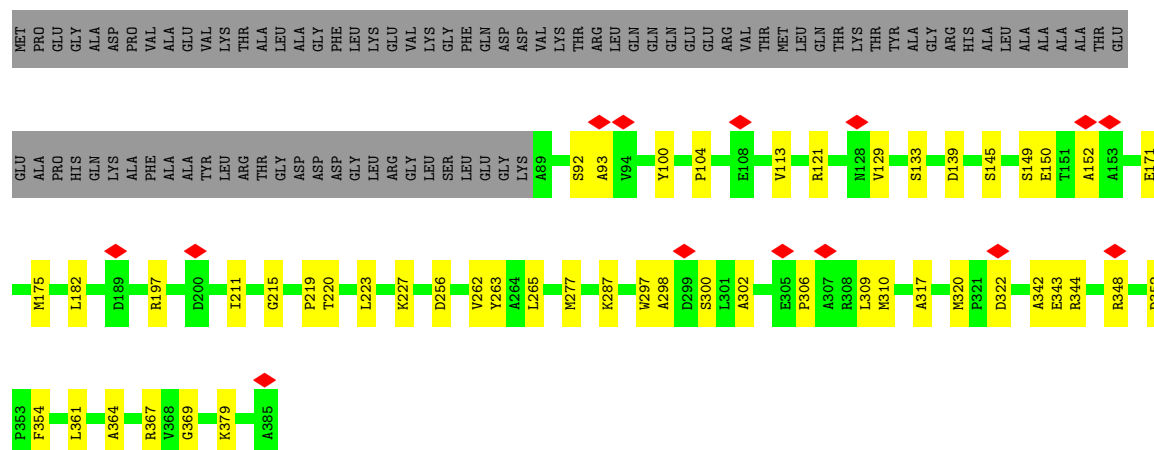
- Molecule 1: Phage major capsid protein, HK97 family

Chain XO: 66% 11% 23%



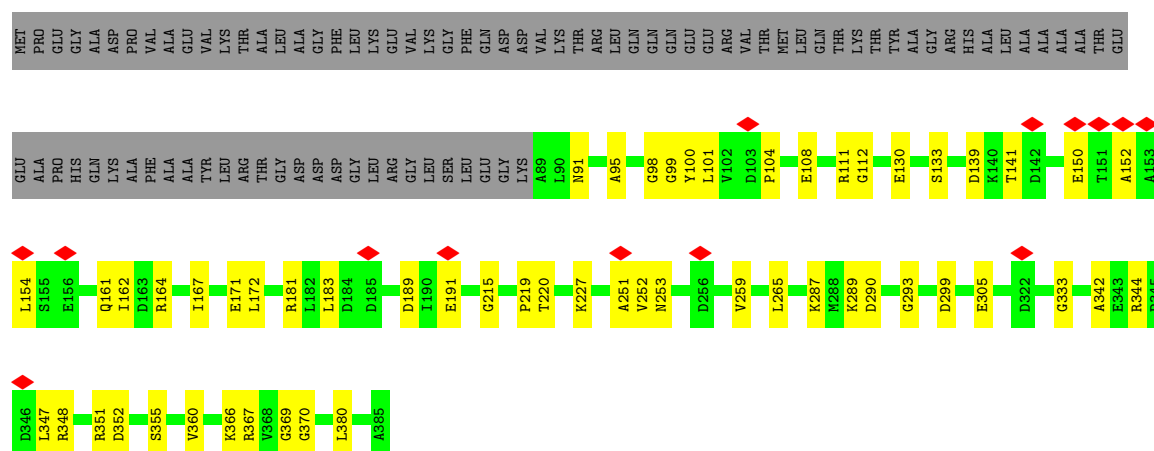
- Molecule 1: Phage major capsid protein, HK97 family

Chain YO: 64% 13% 23%

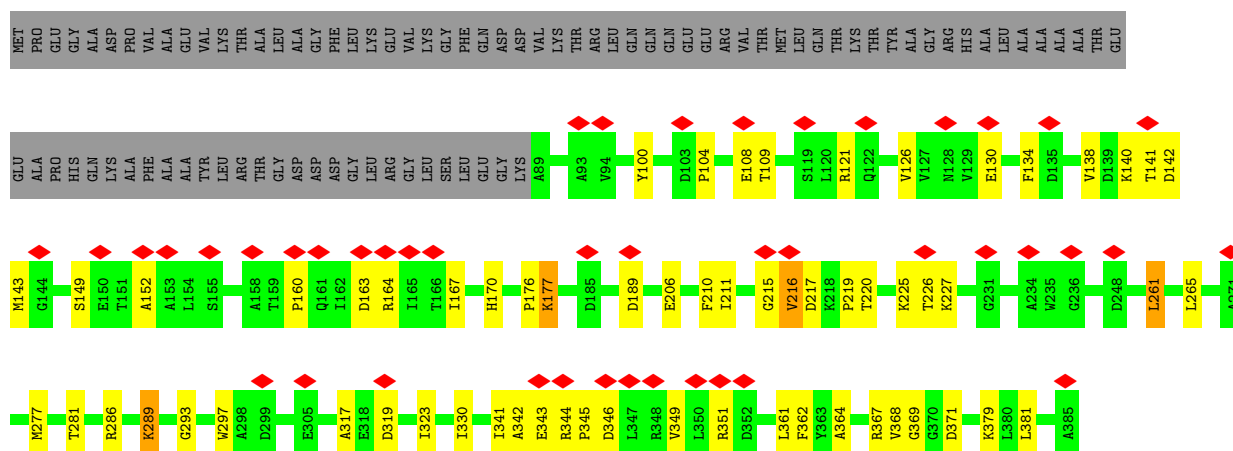


- Molecule 1: Phage major capsid protein, HK97 family

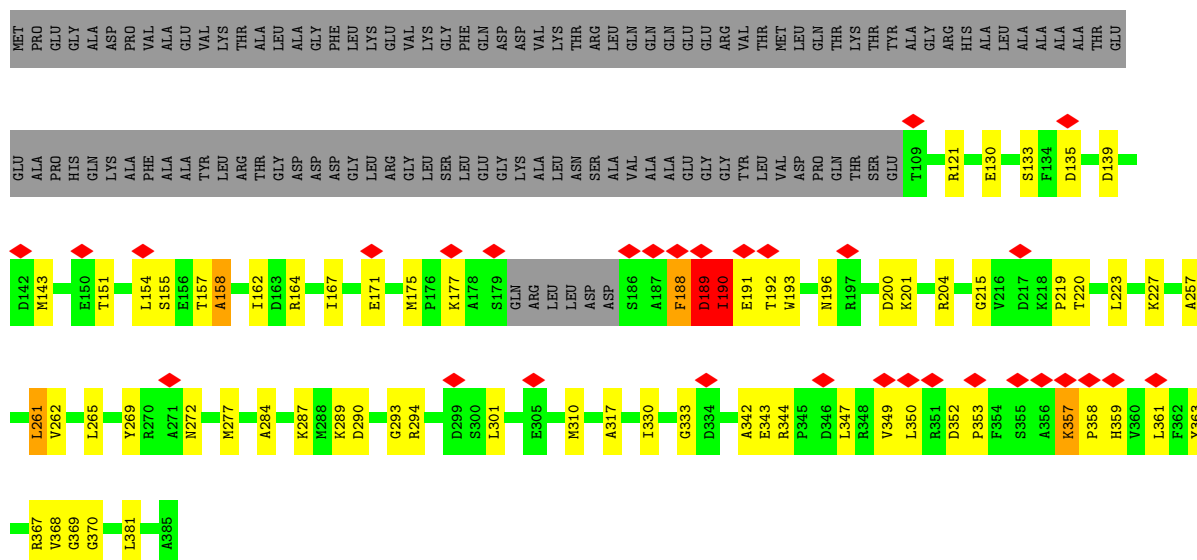
Chain ZO: 63% 15% 23%



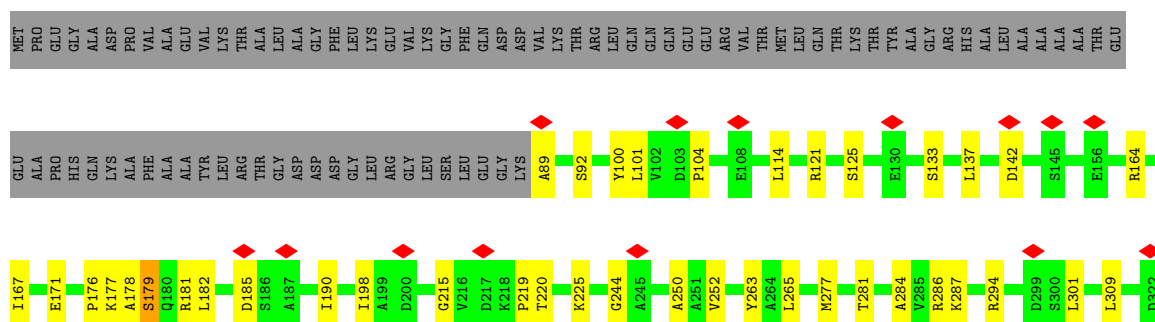
- Molecule 1: Phage major capsid protein, HK97 family

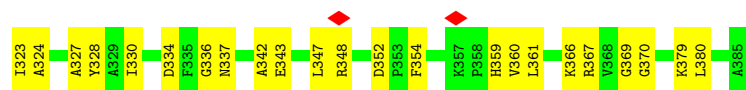


- Molecule 1: Phage major capsid protein, HK97 family



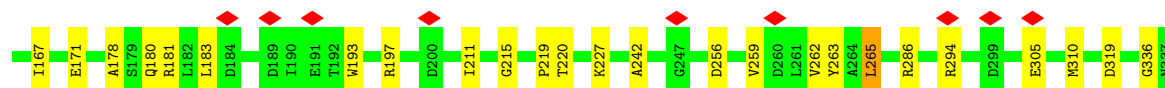
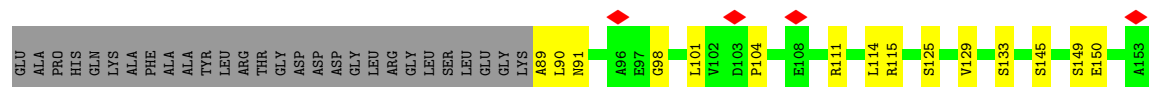
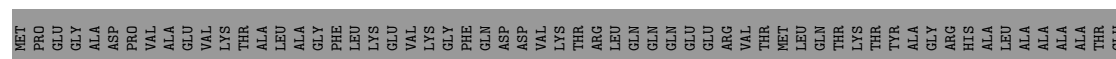
- Molecule 1: Phage major capsid protein, HK97 family





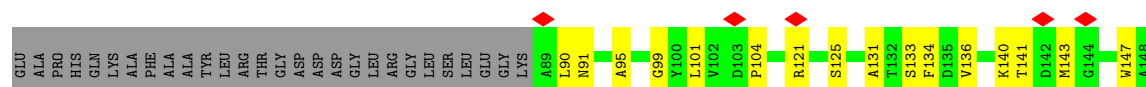
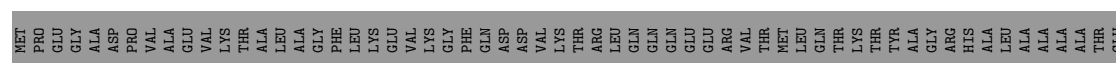
- Molecule 1: Phage major capsid protein, HK97 family

Chain RO: 63% 14% 23%



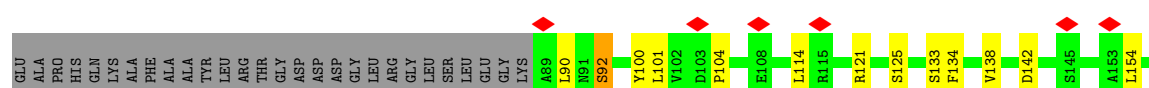
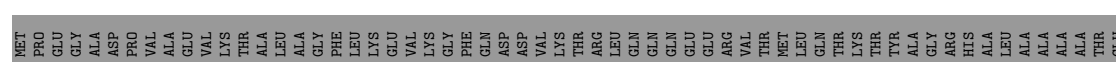
- Molecule 1: Phage major capsid protein, HK97 family

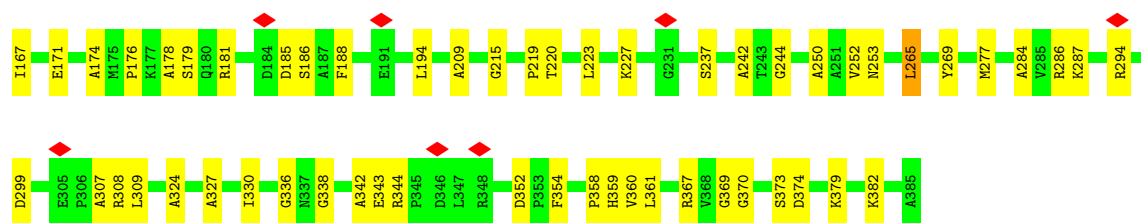
Chain MO: 60% 17% 23%



- Molecule 1: Phage major capsid protein, HK97 family

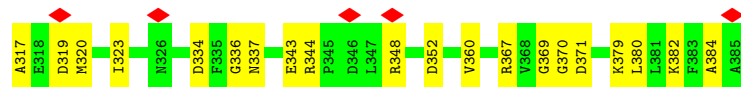
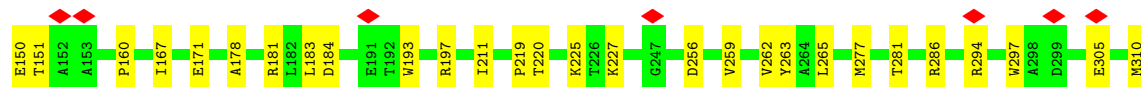
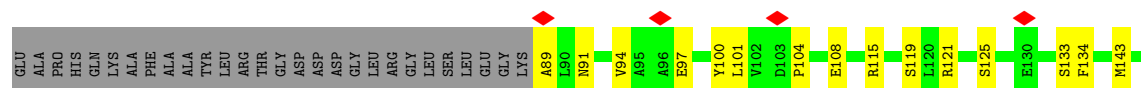
Chain QO: 59% 17% 23%





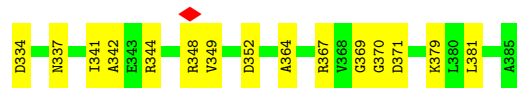
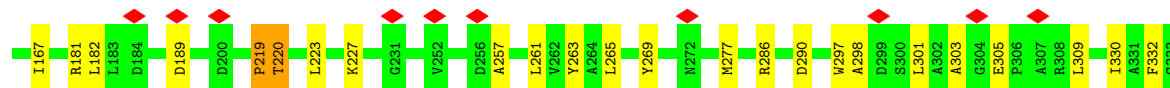
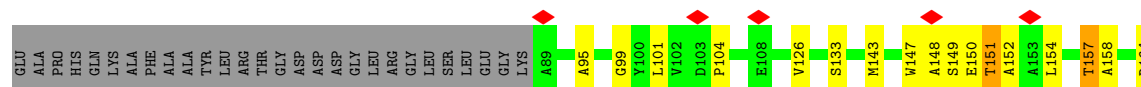
- Molecule 1: Phage major capsid protein, HK97 family

Chain OO: 61% 16% 23%



- Molecule 1: Phage major capsid protein, HK97 family

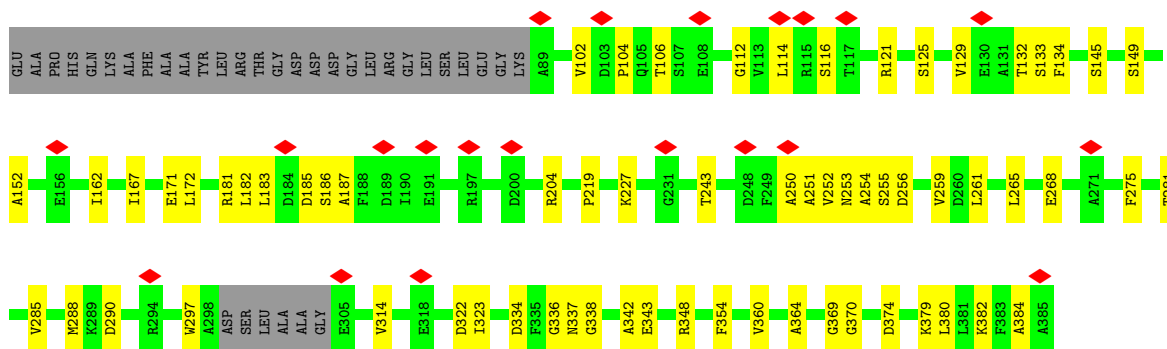
Chain PO: 63% 14% 23%



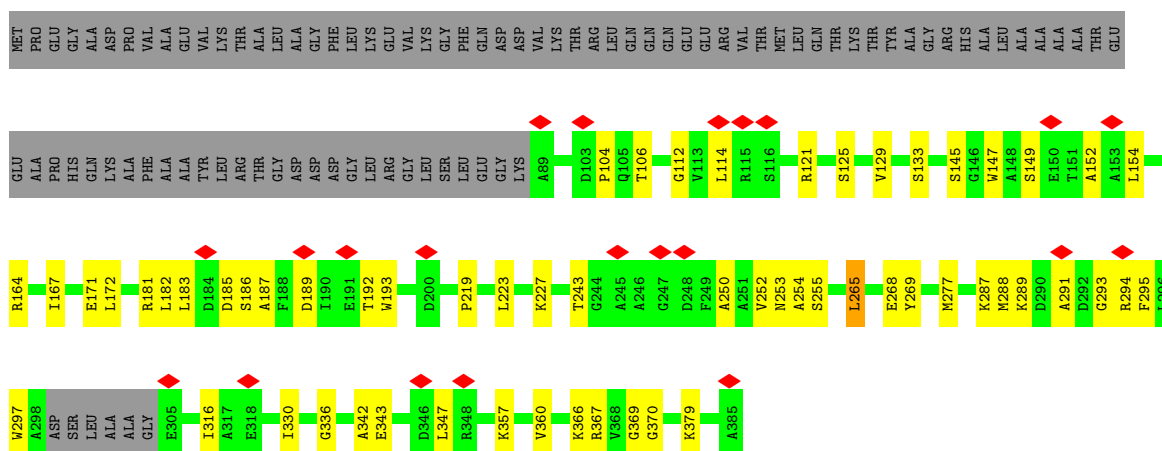
- Molecule 1: Phage major capsid protein, HK97 family

Chain WO: 5% 58% 24%

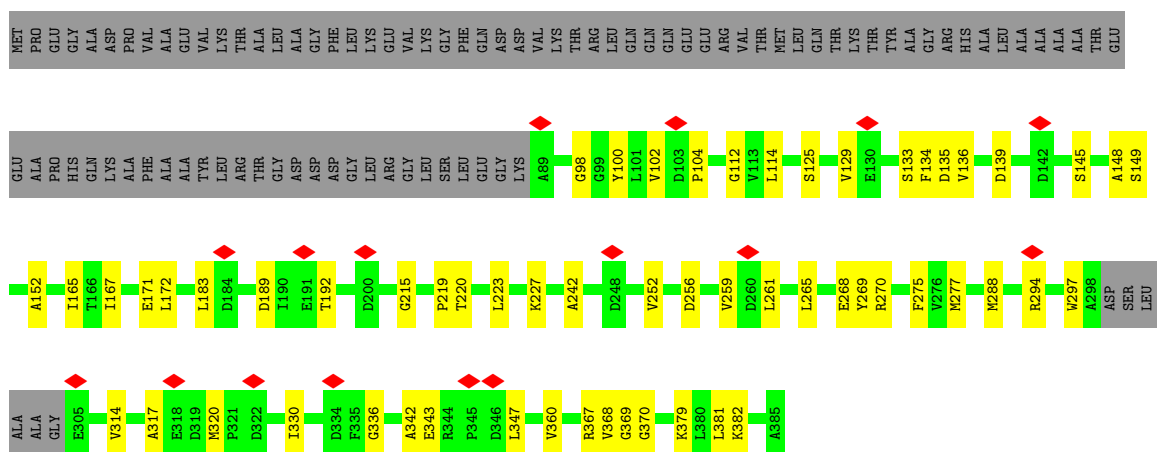




- Molecule 1: Phage major capsid protein, HK97 family



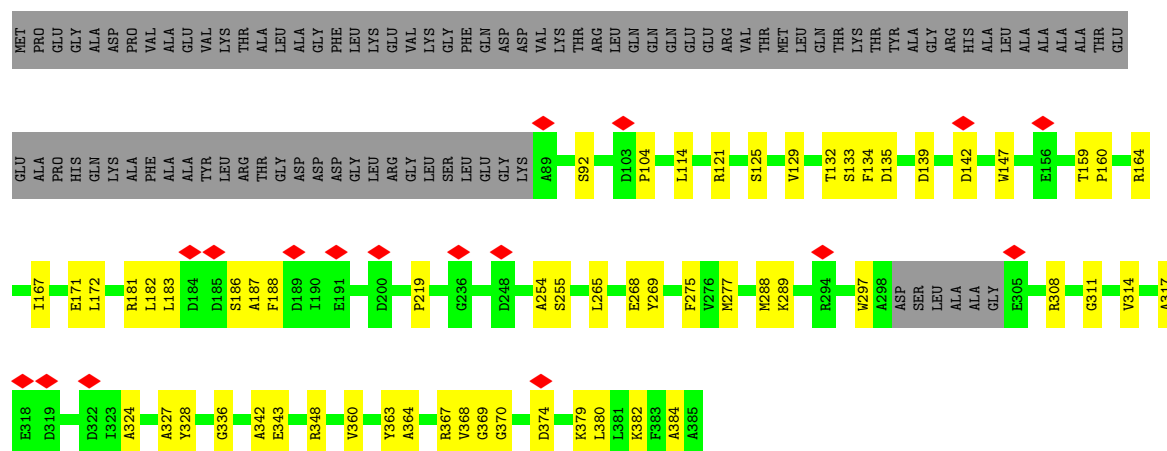
- Molecule 1: Phage major capsid protein, HK97 family



- Molecule 1: Phage major capsid protein, HK97 family

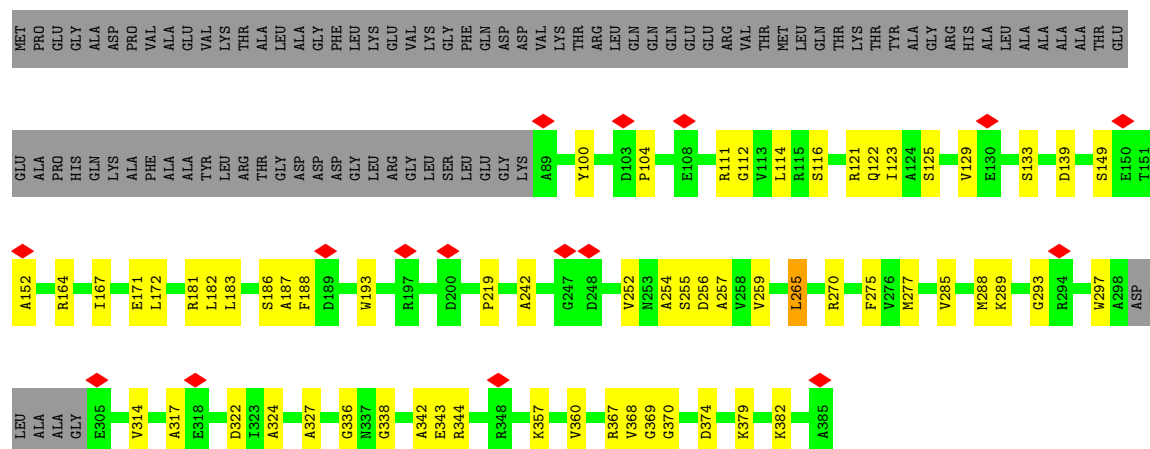


Chain VO: 



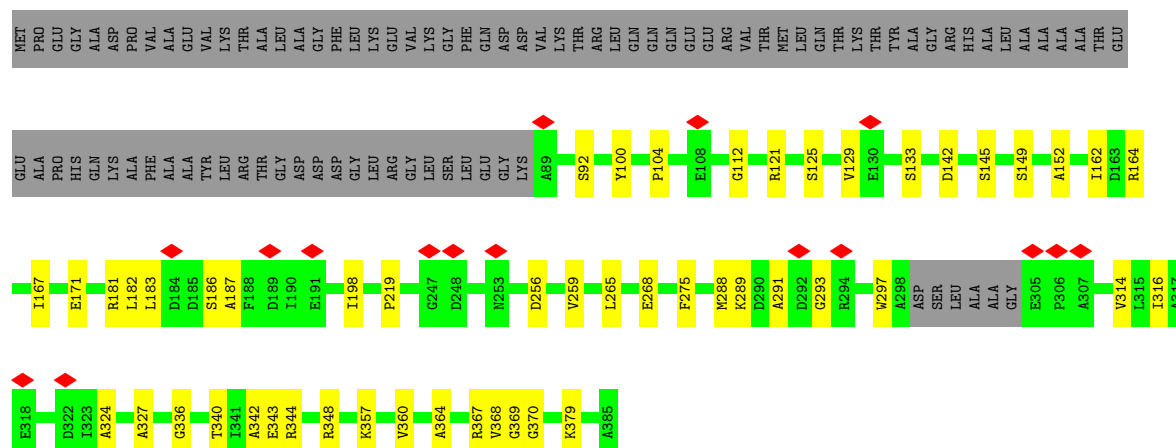
- Molecule 1: Phage major capsid protein, HK97 family

Chain LO: 

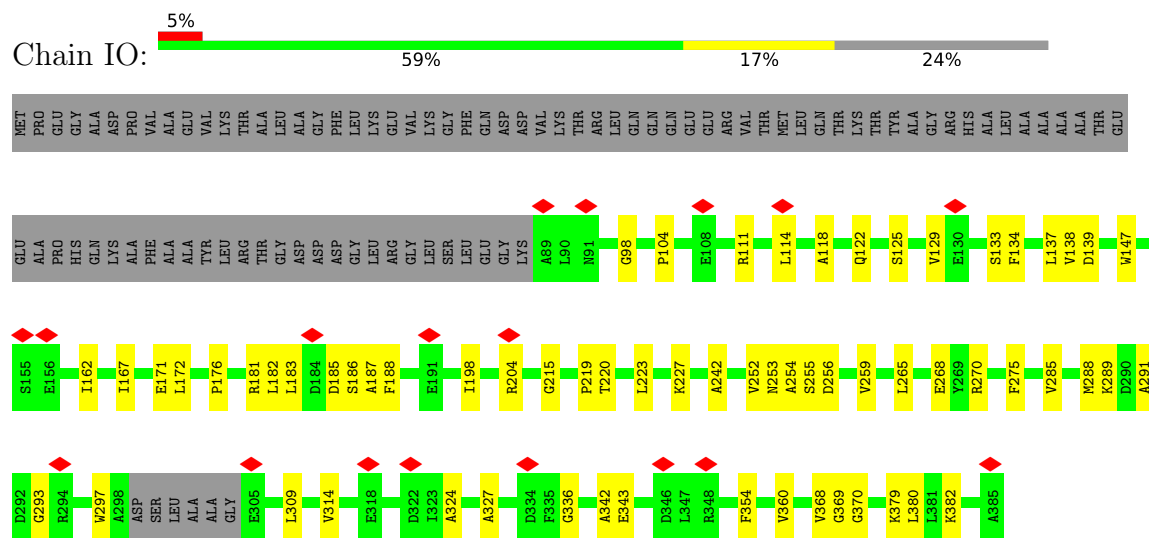


- Molecule 1: Phage major capsid protein, HK97 family

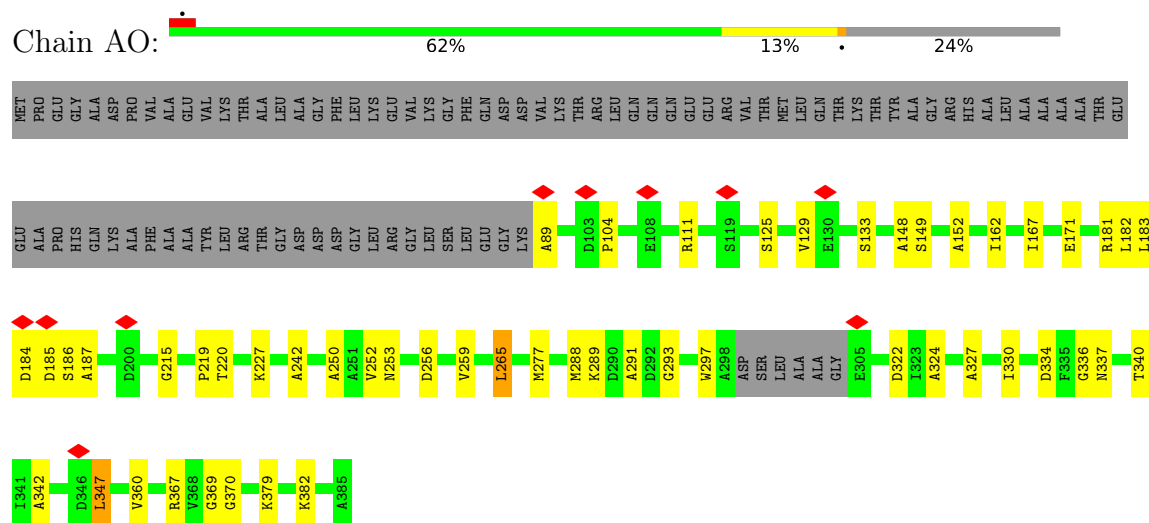
Chain HO: 



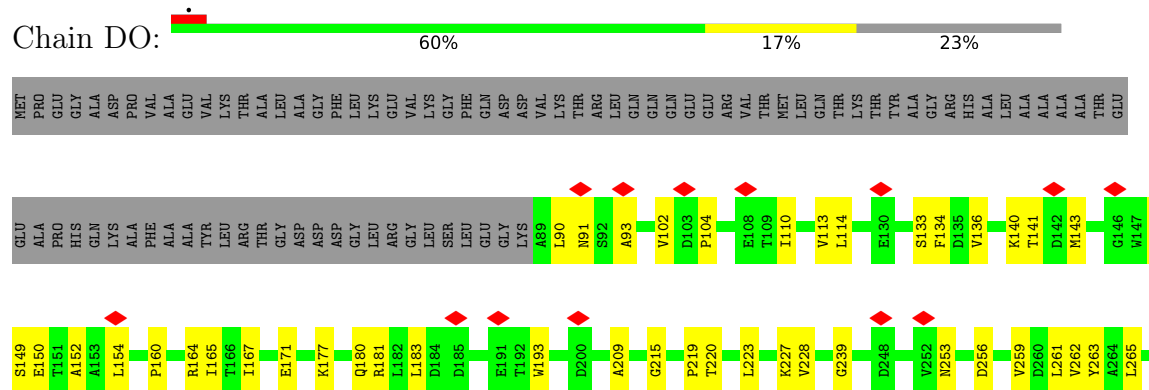
- Molecule 1: Phage major capsid protein, HK97 family

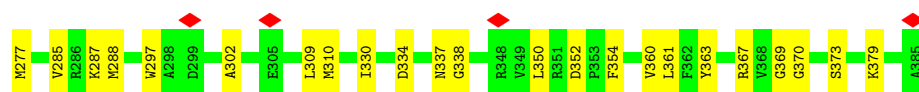


- Molecule 1: Phage major capsid protein, HK97 family



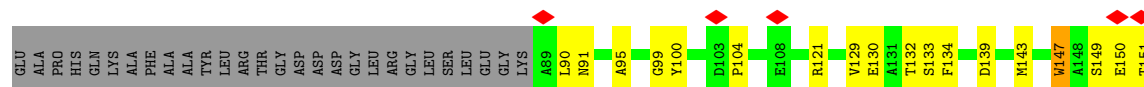
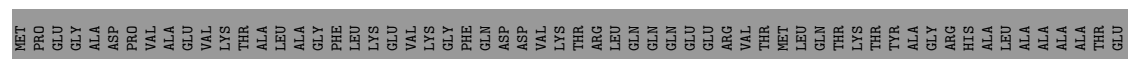
- Molecule 1: Phage major capsid protein, HK97 family





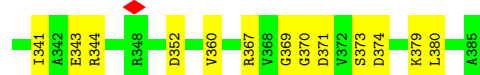
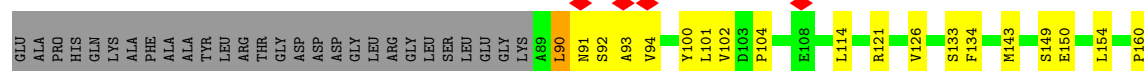
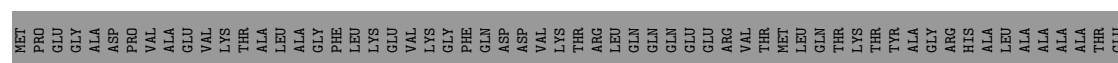
- Molecule 1: Phage major capsid protein, HK97 family

Chain EO: 59% 17% 23%



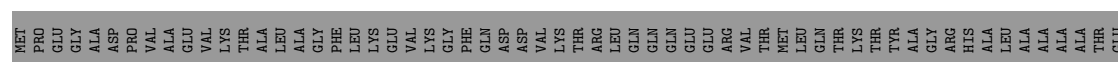
- Molecule 1: Phage major capsid protein, HK97 family

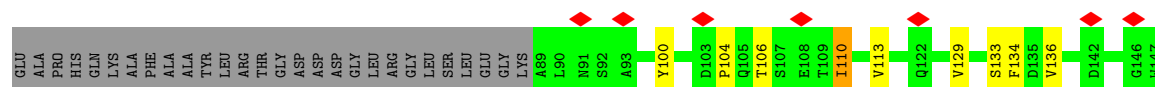
Chain FO: 61% 16% 23%

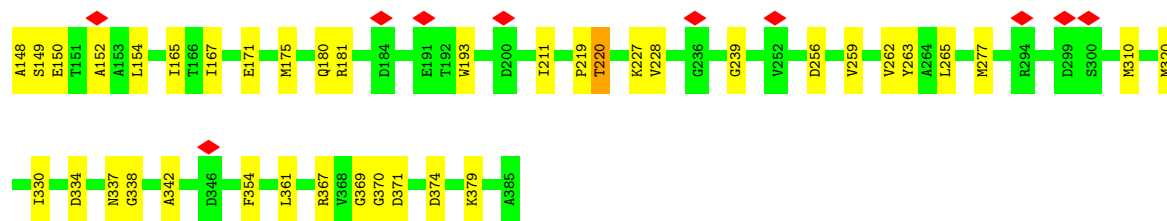


- Molecule 1: Phage major capsid protein, HK97 family

Chain GO: 63% 14% 23%

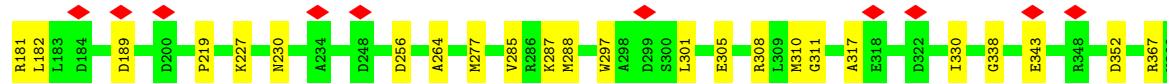
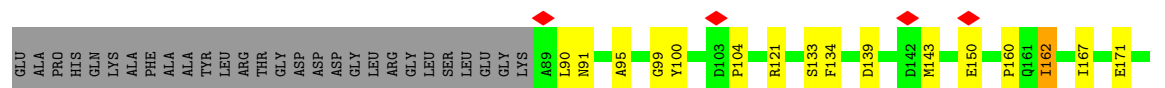
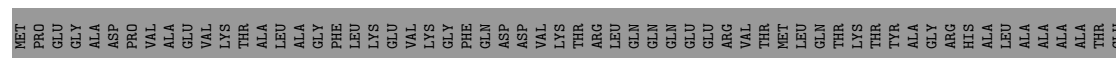






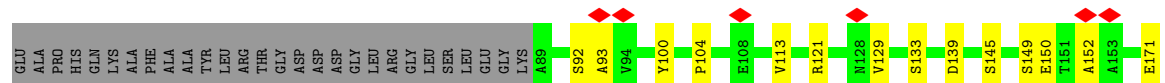
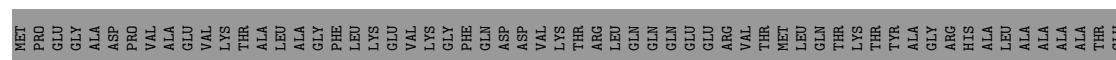
- Molecule 1: Phage major capsid protein, HK97 family

Chain XJ: 66% 11% 23%



- Molecule 1: Phage major capsid protein, HK97 family

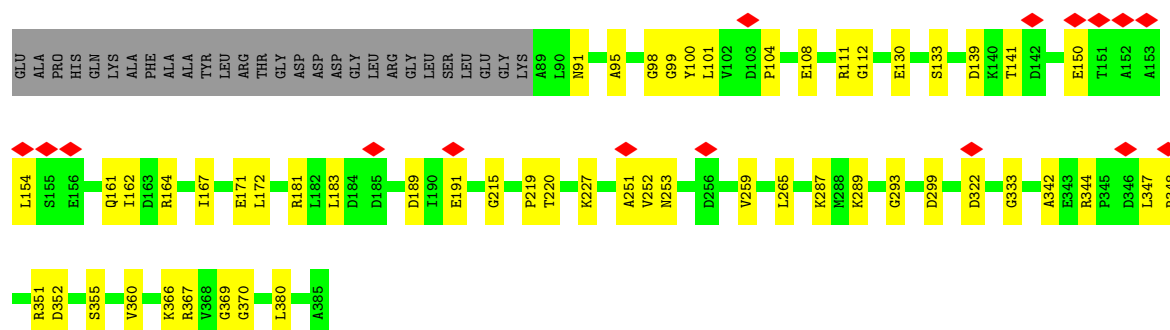
Chain YJ: 64% 13% 23%



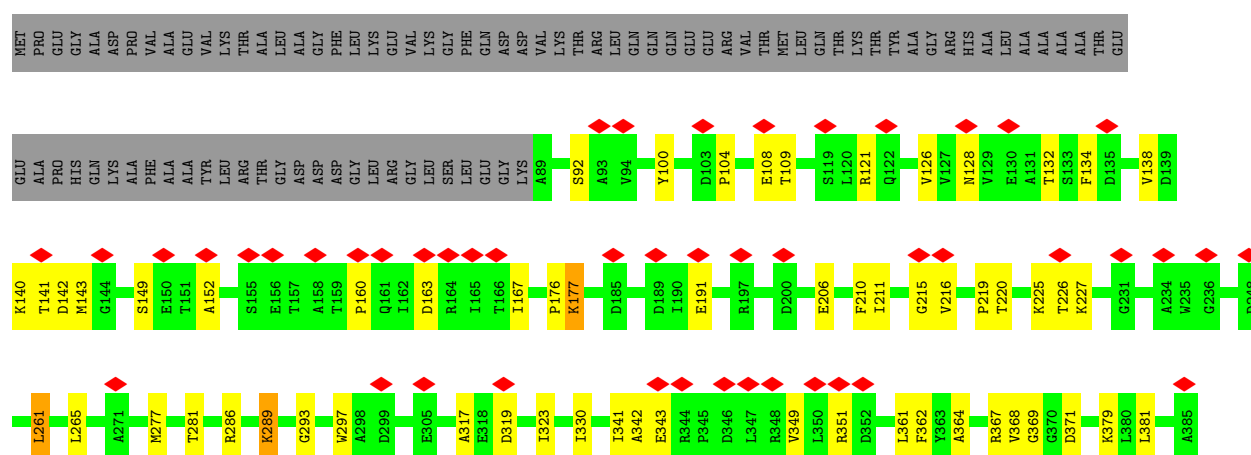
- Molecule 1: Phage major capsid protein, HK97 family

Chain ZJ: 63% 14% 23%

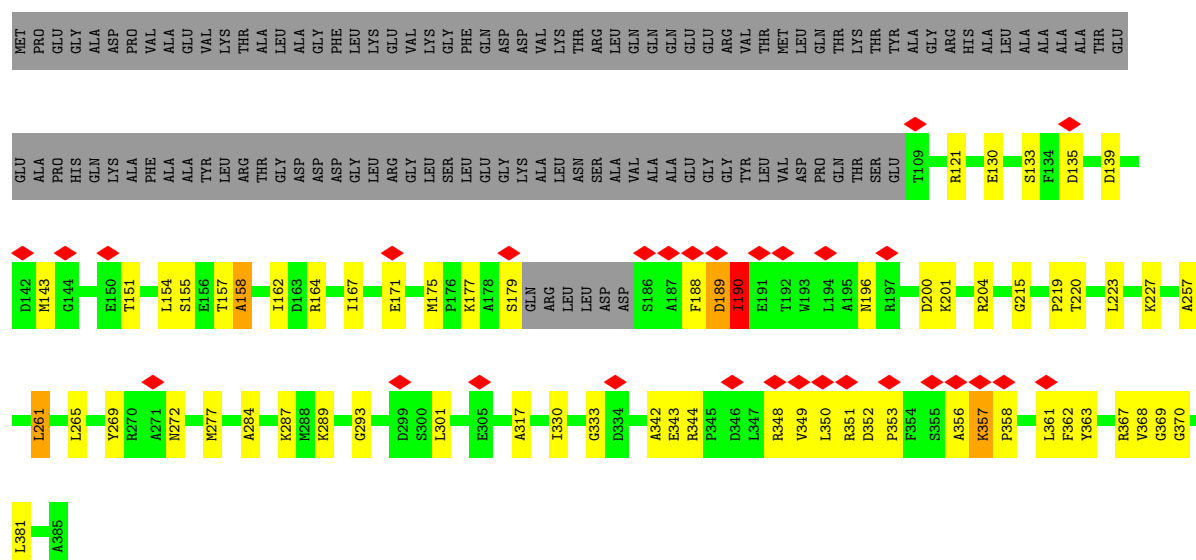




- Molecule 1: Phage major capsid protein, HK97 family

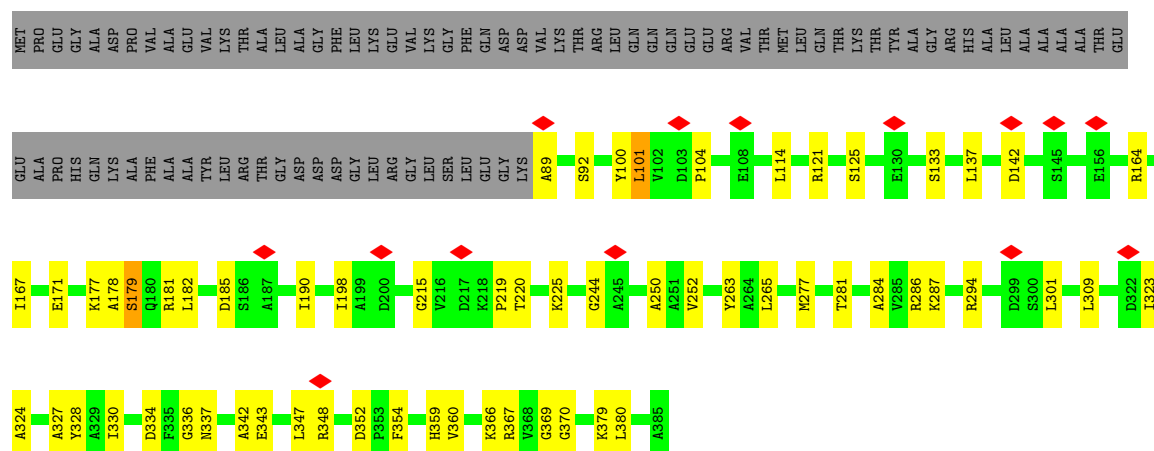


- Molecule 1: Phage major capsid protein, HK97 family



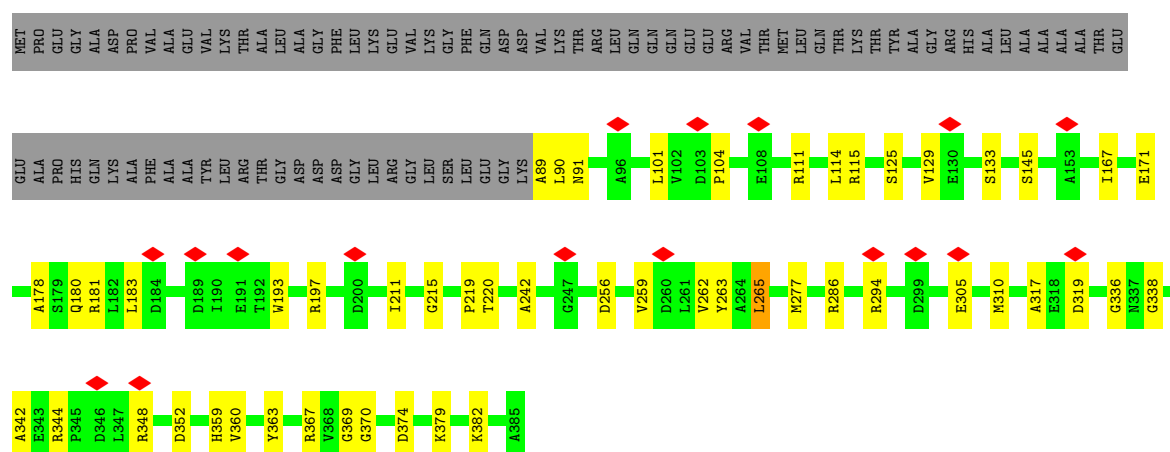
- Molecule 1: Phage major capsid protein, HK97 family

Chain NJ:  61% 15% 23%



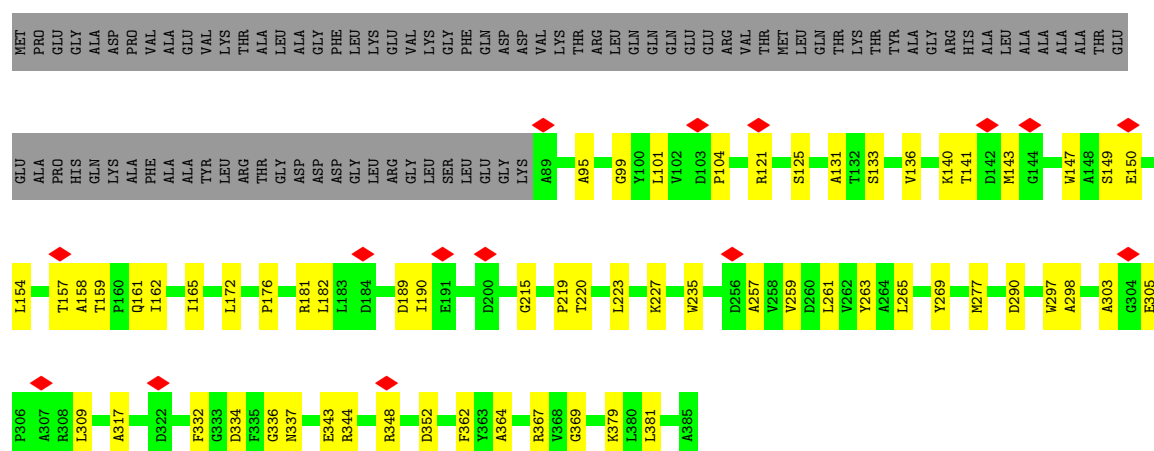
• Molecule 1: Phage major capsid protein, HK97 family

Chain RJ:  64% 13% 23%

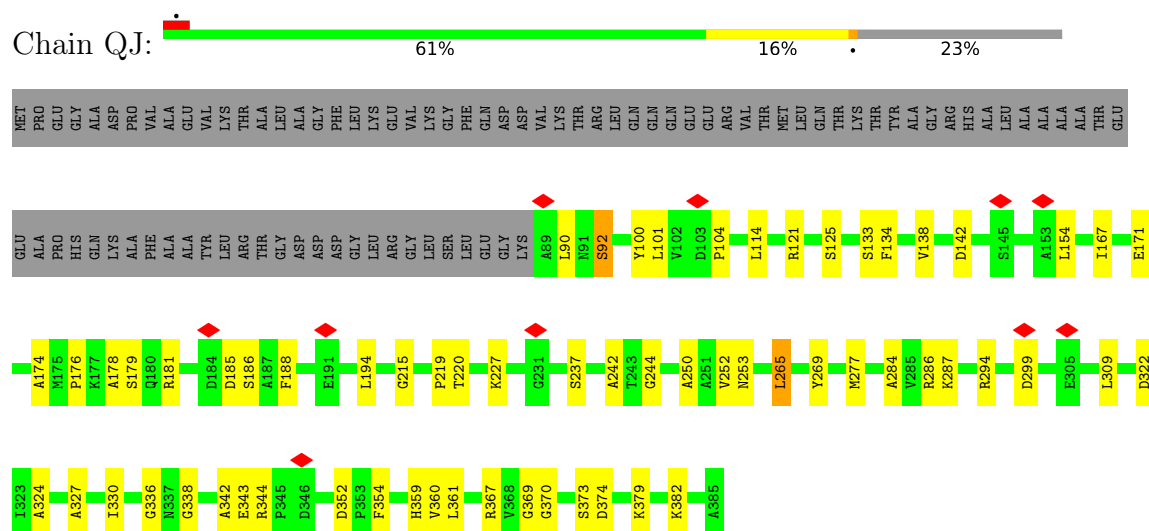


• Molecule 1: Phage major capsid protein, HK97 family

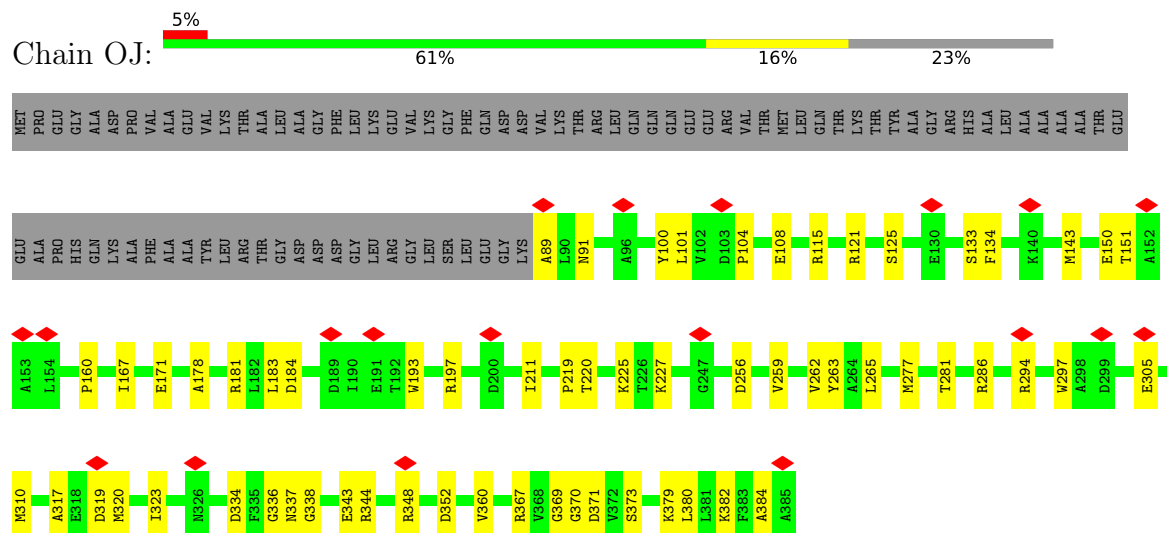
Chain MJ:  61% 16% 23%



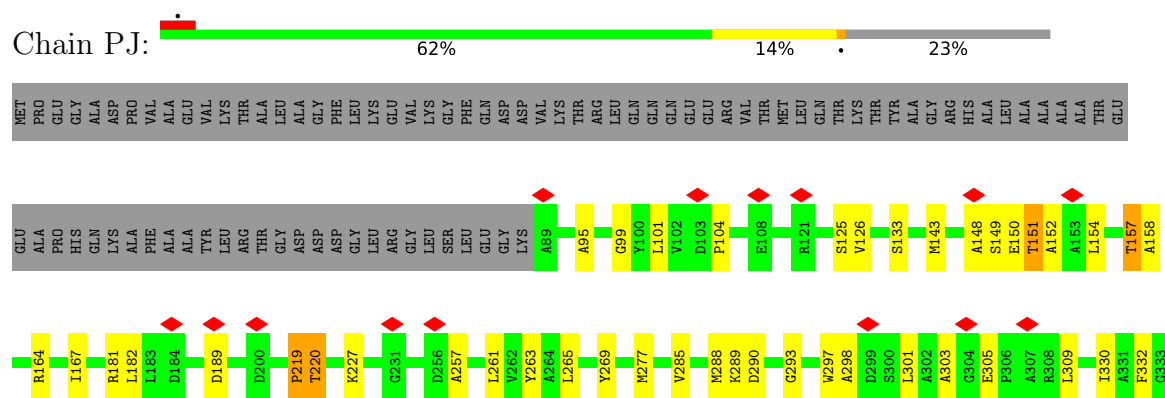
- Molecule 1: Phage major capsid protein, HK97 family

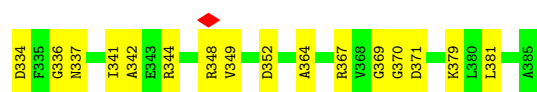


- Molecule 1: Phage major capsid protein, HK97 family

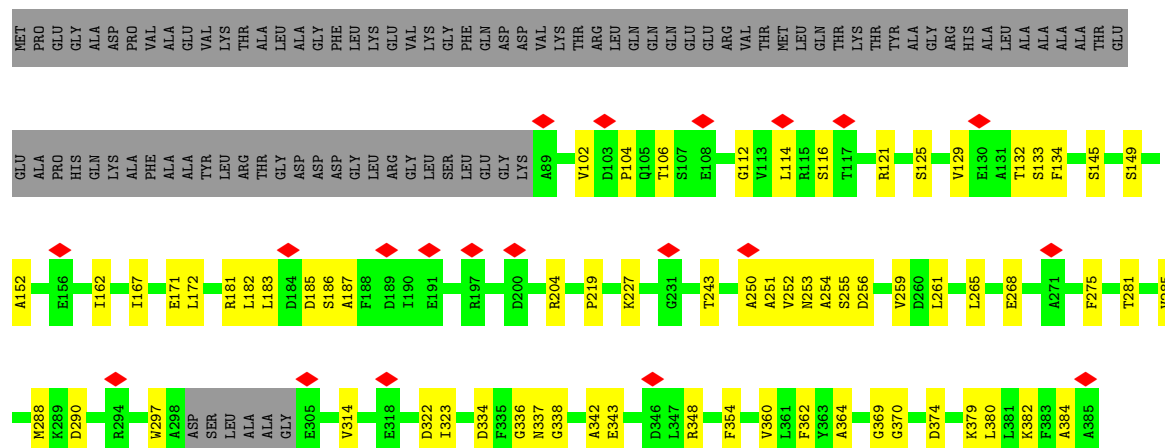


- Molecule 1: Phage major capsid protein, HK97 family

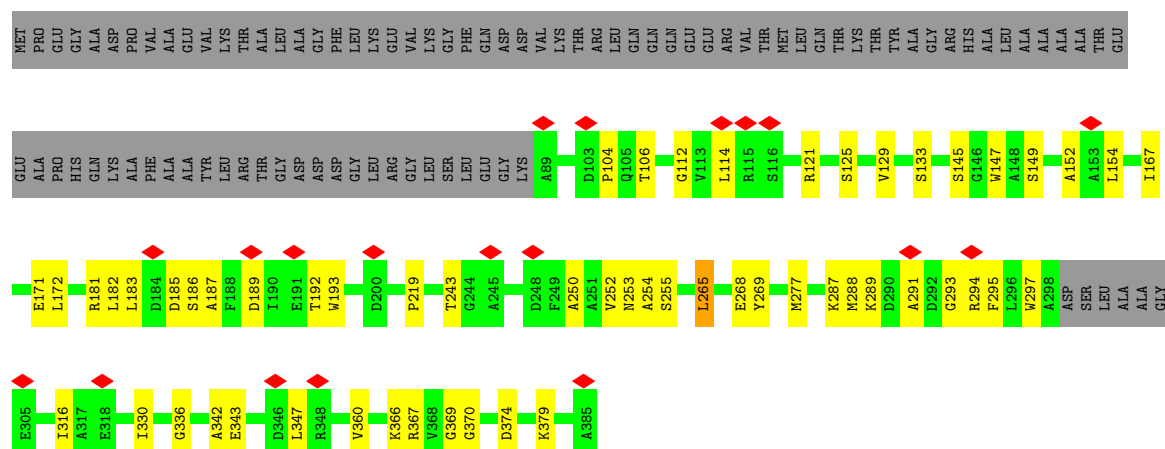




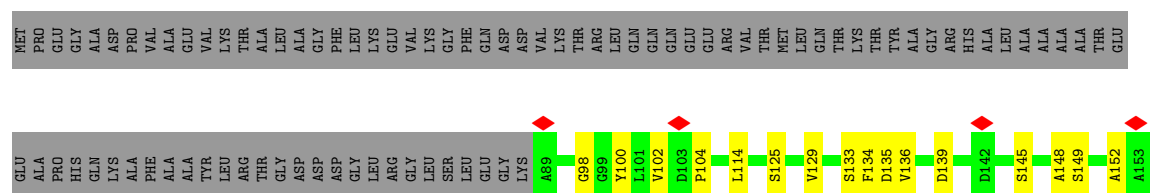
- Molecule 1: Phage major capsid protein, HK97 family

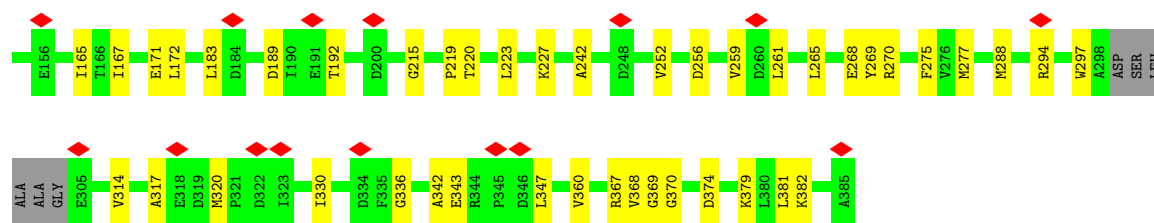


- Molecule 1: Phage major capsid protein, HK97 family

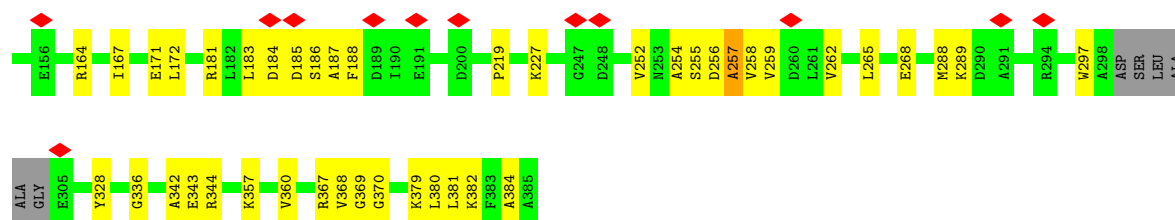
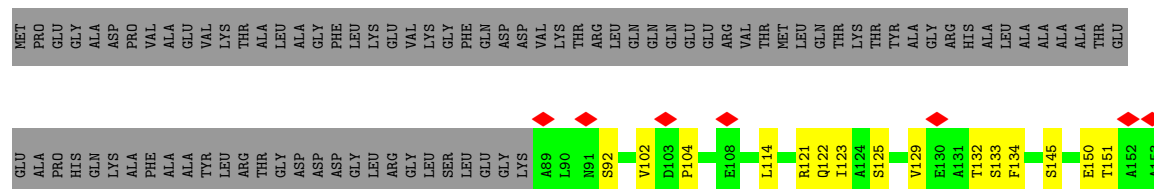


- Molecule 1: Phage major capsid protein, HK97 family

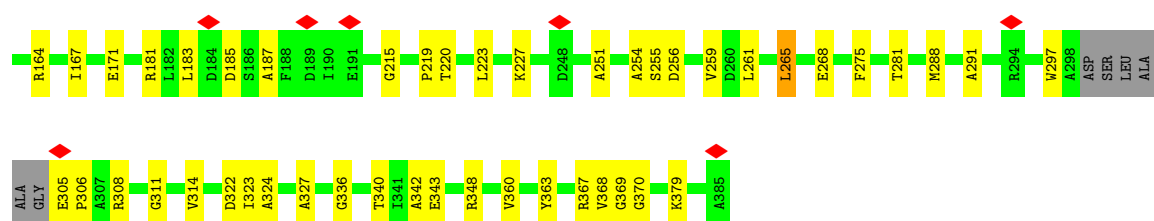
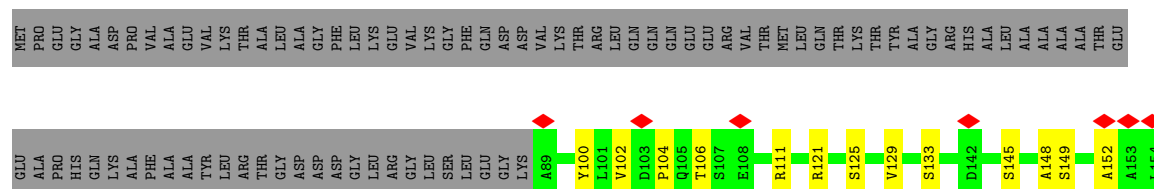




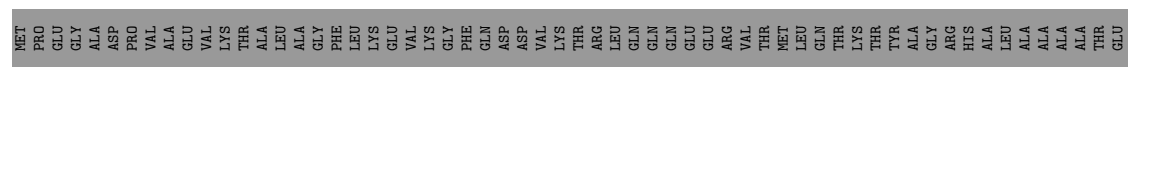
- Molecule 1: Phage major capsid protein, HK97 family

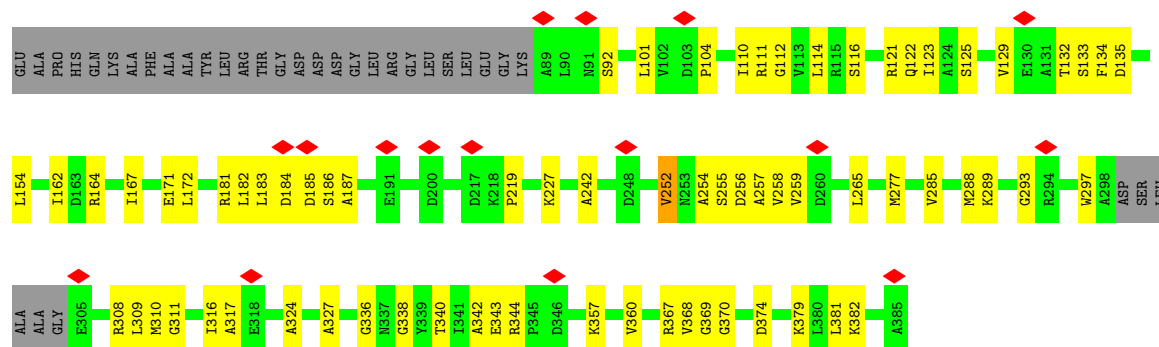


- Molecule 1: Phage major capsid protein, HK97 family



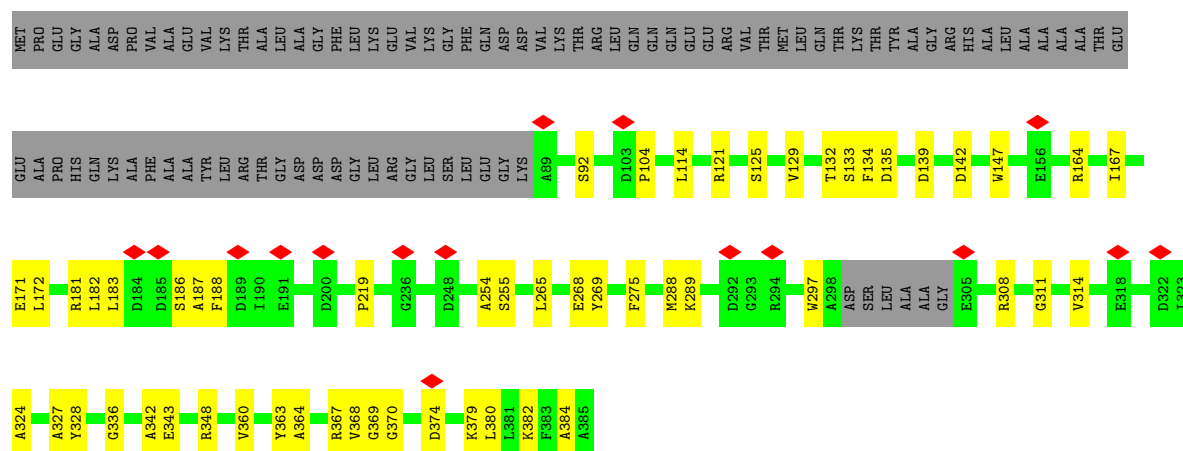
- Molecule 1: Phage major capsid protein, HK97 family





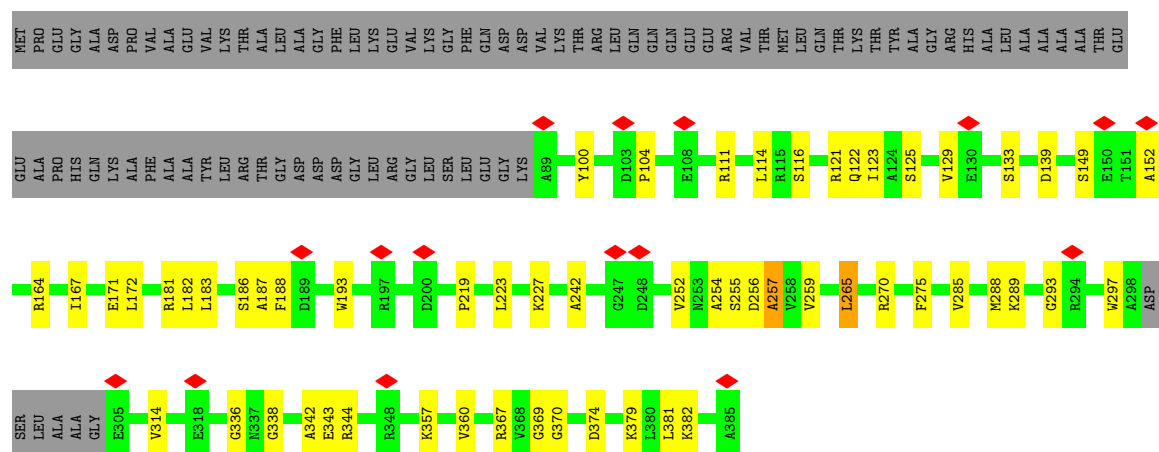
- Molecule 1: Phage major capsid protein, HK97 family

Chain VJ: 61% 14% 24%



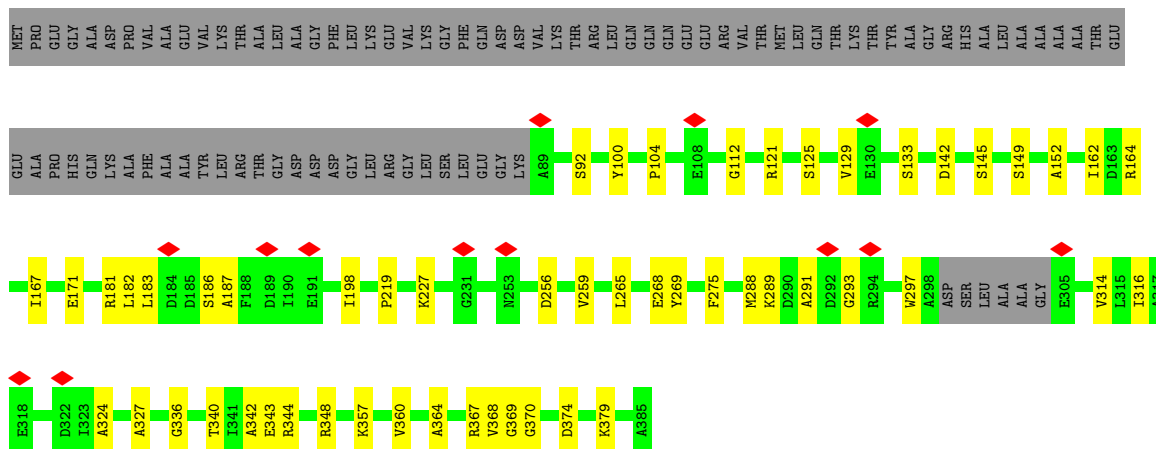
- Molecule 1: Phage major capsid protein, HK97 family

Chain LJ: 61% 15% 24%

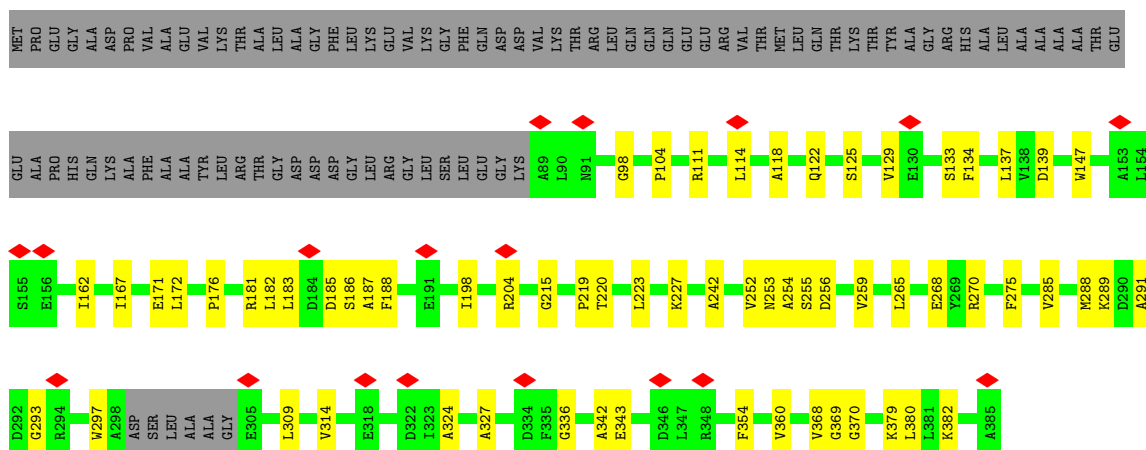


- Molecule 1: Phage major capsid protein, HK97 family

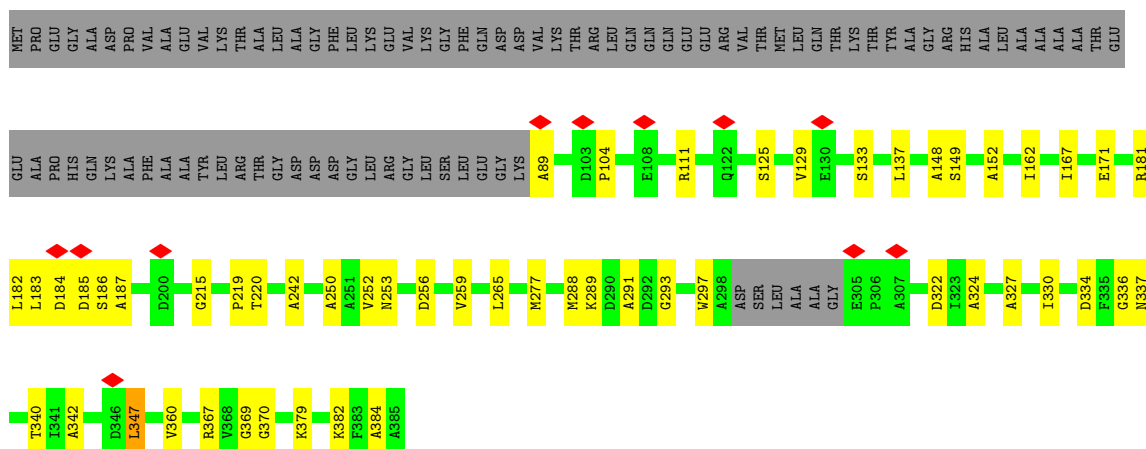
Chain HJ: 62% 14% 24%



- Molecule 1: Phage major capsid protein, HK97 family

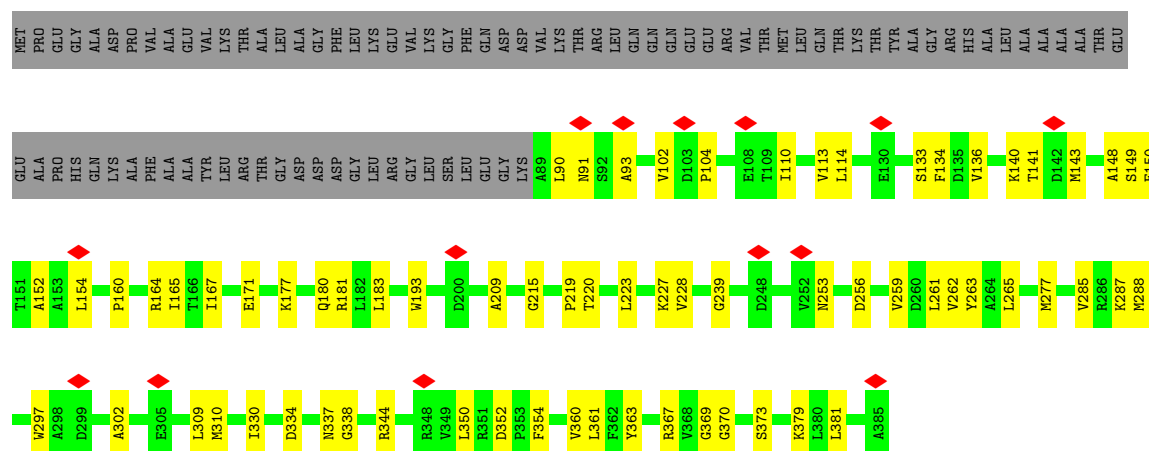


- Molecule 1: Phage major capsid protein, HK97 family



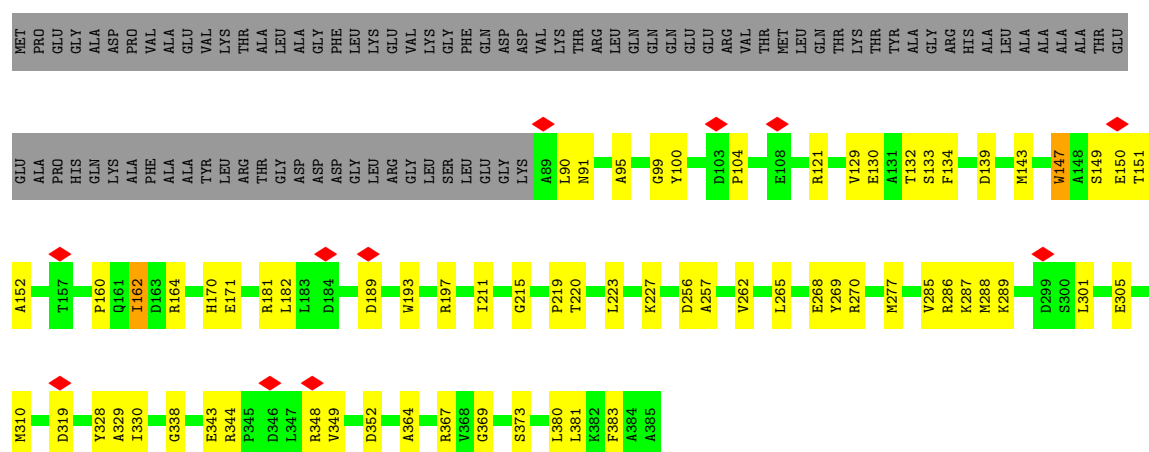
- Molecule 1: Phage major capsid protein, HK97 family

Chain DJ:  59% 18% 23%



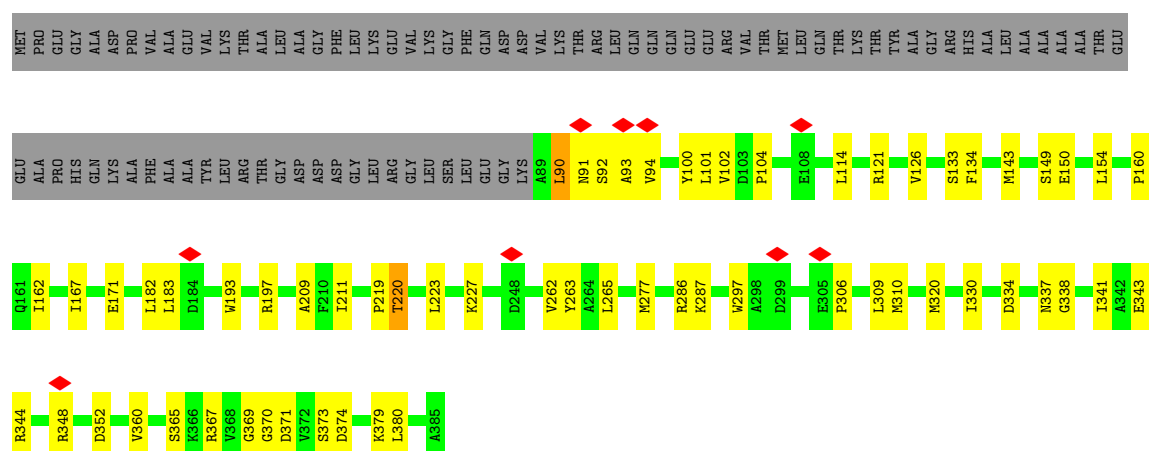
- Molecule 1: Phage major capsid protein, HK97 family

Chain EJ:  59% 17% 23%



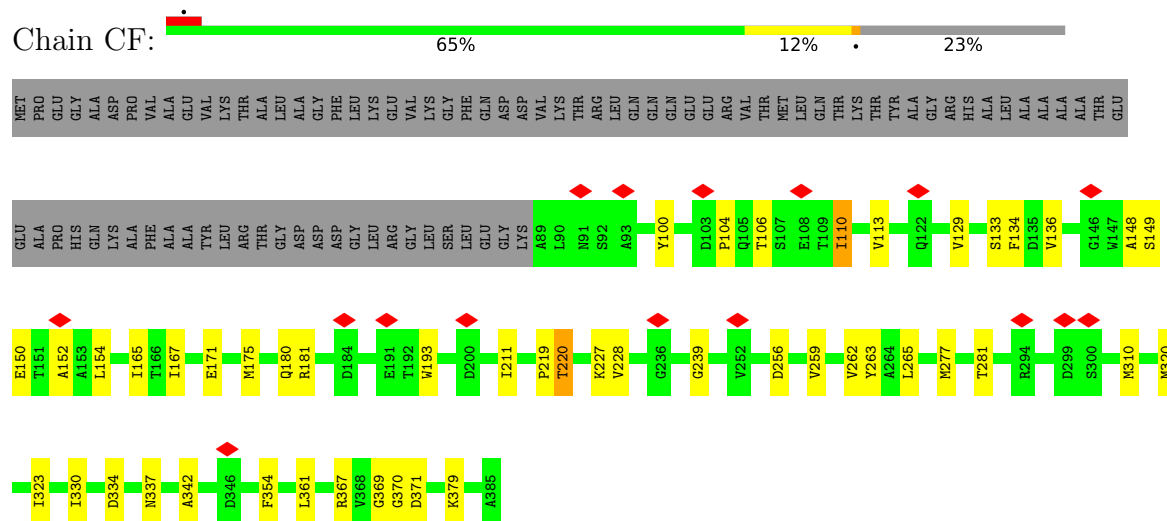
- Molecule 1: Phage major capsid protein, HK97 family

Chain FJ:  61% 16% 23%



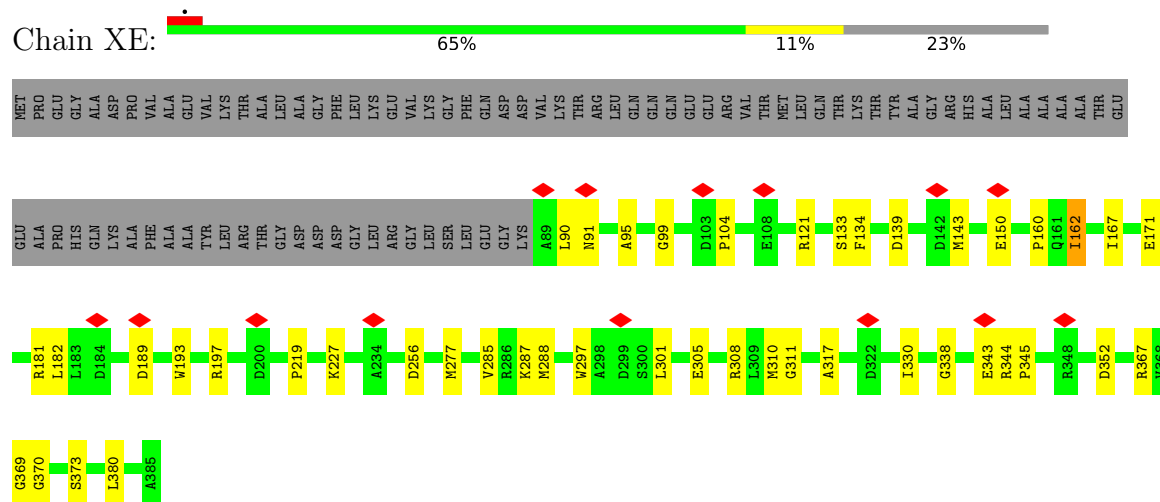
- Molecule 1: Phage major capsid protein, HK97 family

Chain CF:



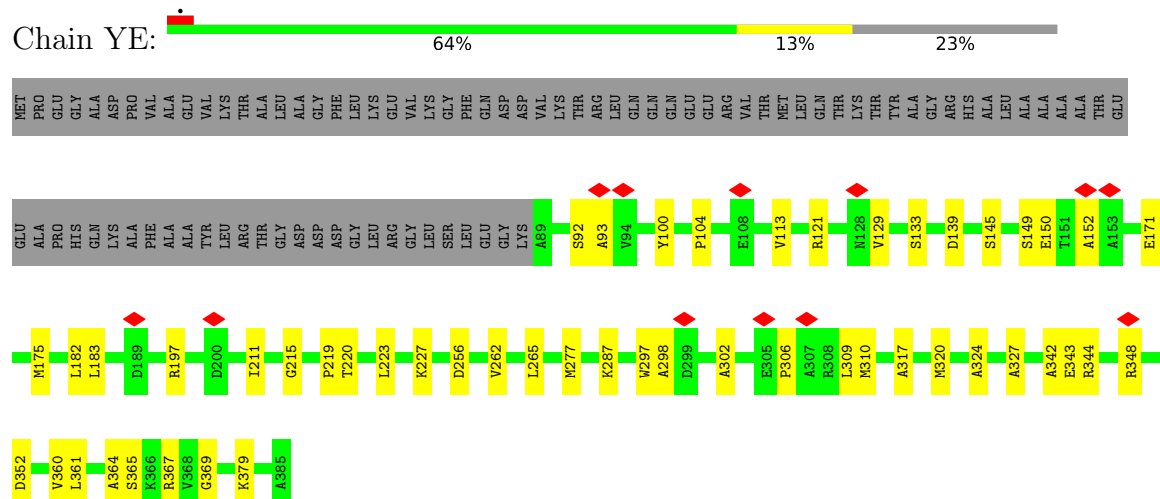
- Molecule 1: Phage major capsid protein, HK97 family

Chain XE:

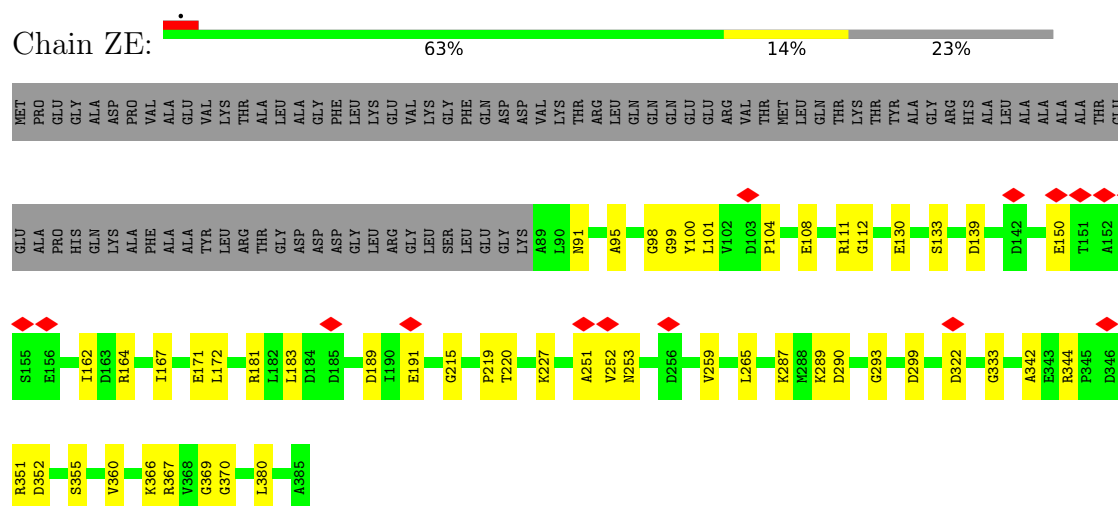


- Molecule 1: Phage major capsid protein, HK97 family

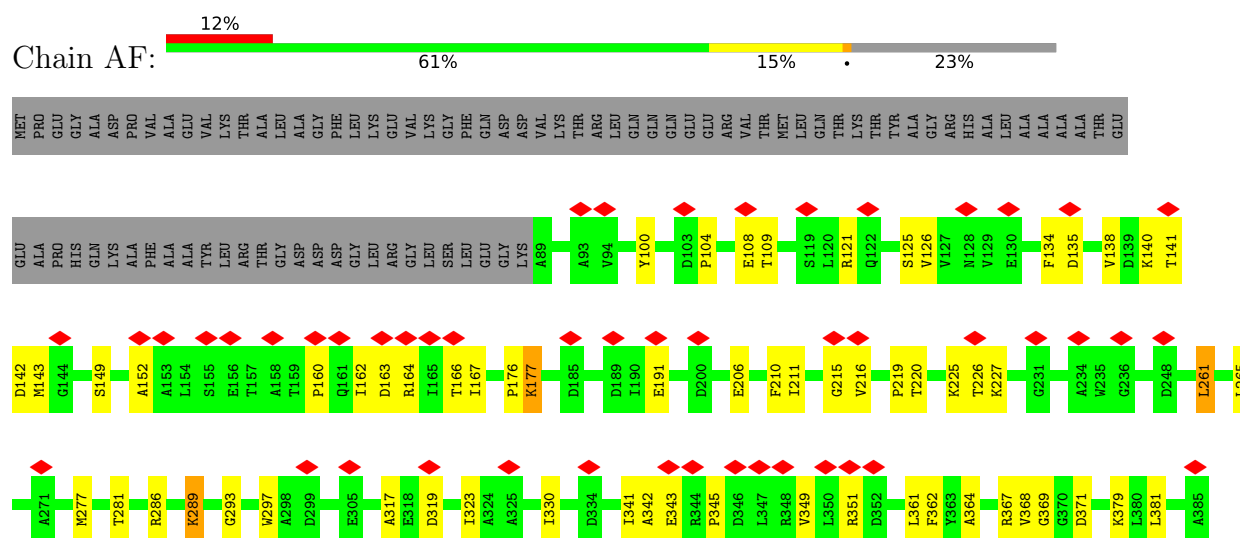
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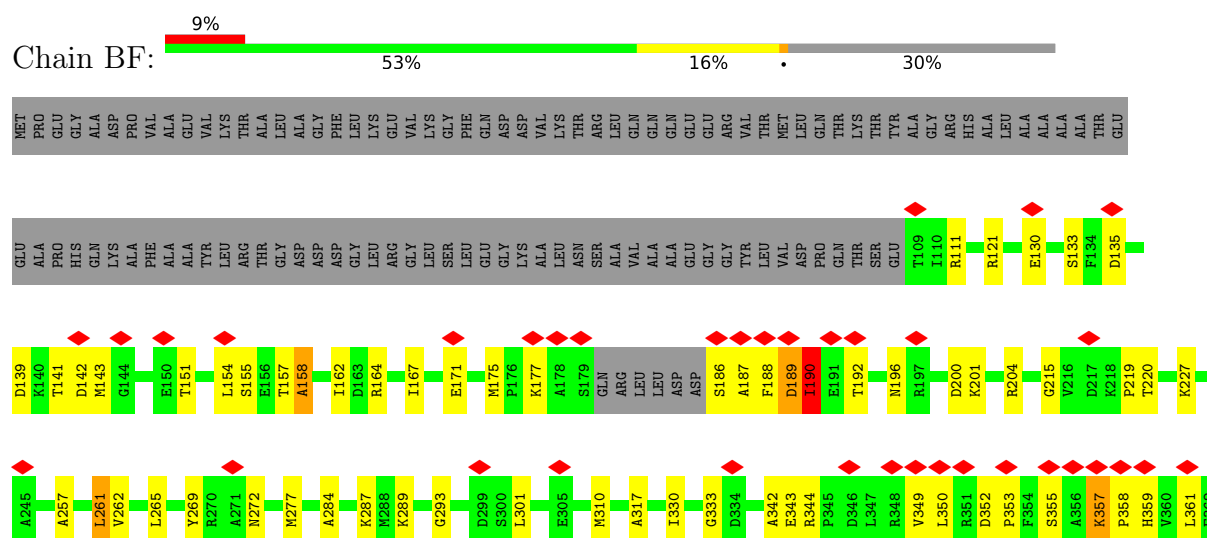
- Molecule 1: Phage major capsid protein, HK97 family

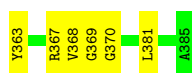


- Molecule 1: Phage major capsid protein, HK97 family



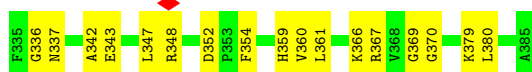
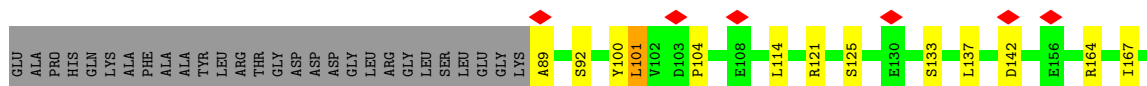
- Molecule 1: Phage major capsid protein, HK97 family





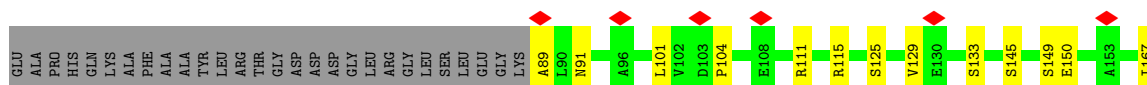
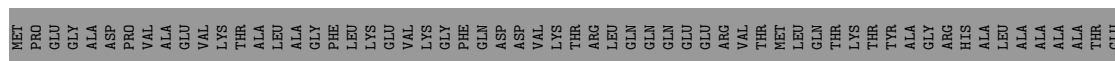
- Molecule 1: Phage major capsid protein, HK97 family

Chain NE: 61% 15% 23%



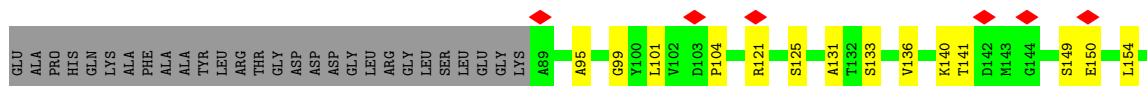
- Molecule 1: Phage major capsid protein, HK97 family

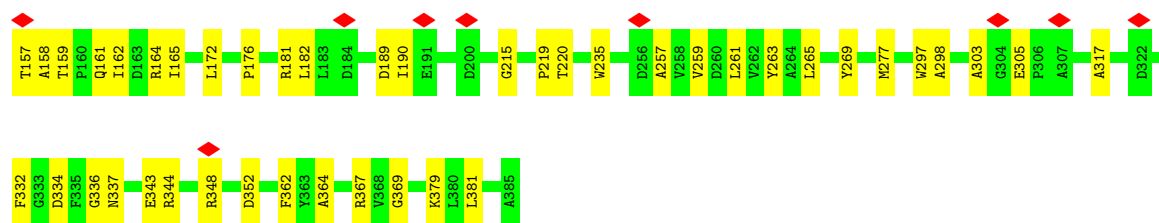
Chain RE: 63% 14% 23%



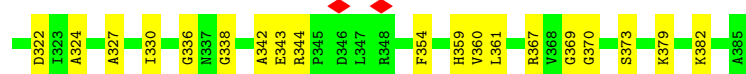
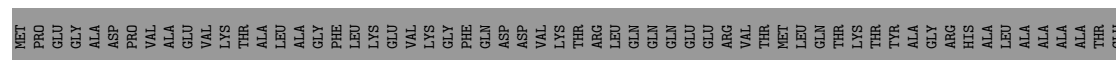
- Molecule 1: Phage major capsid protein, HK97 family

Chain ME: 62% 15% 23%

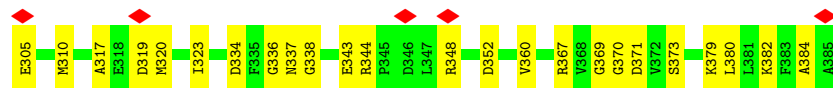
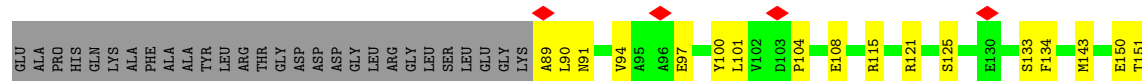
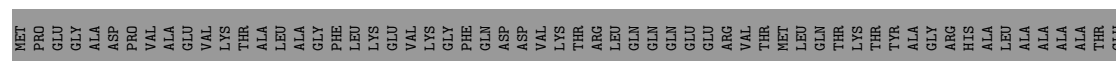




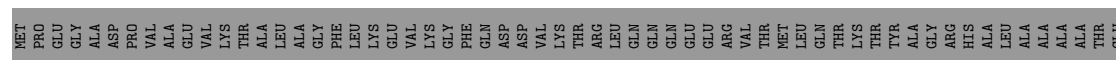
- Molecule 1: Phage major capsid protein, HK97 family

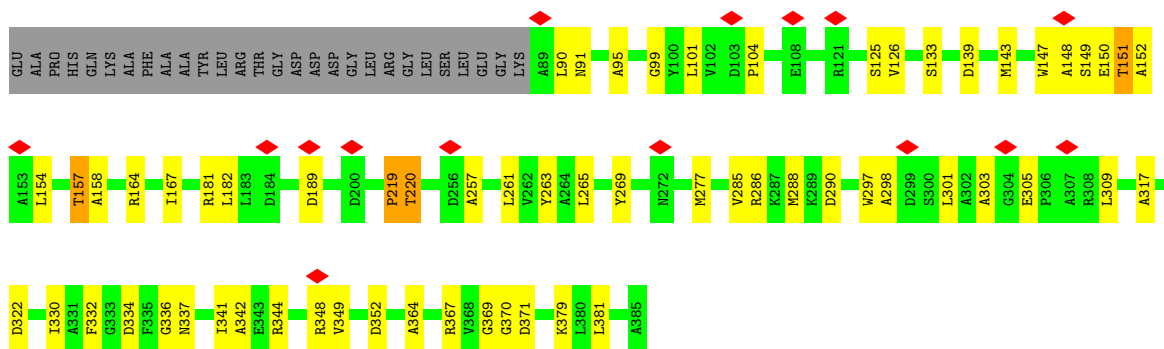


- Molecule 1: Phage major capsid protein, HK97 family

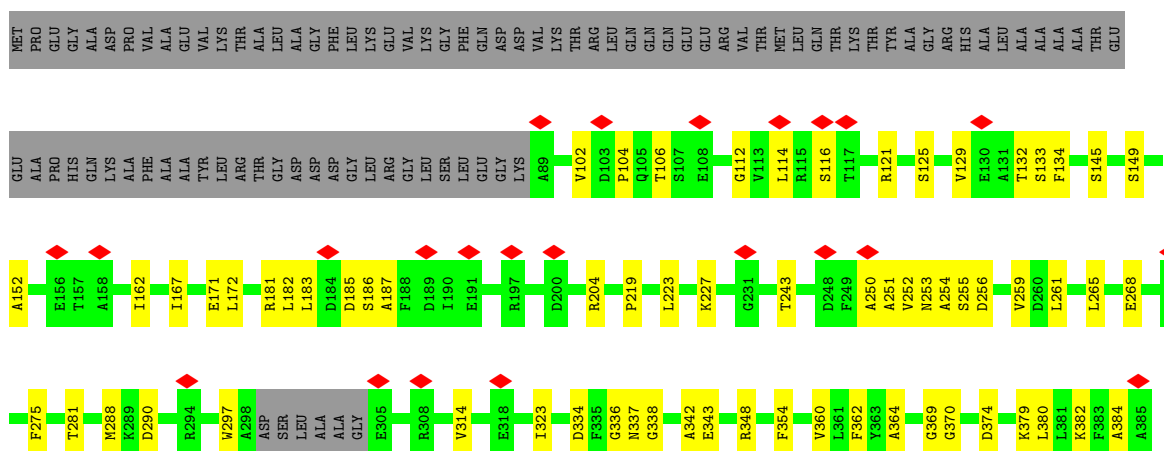


- Molecule 1: Phage major capsid protein, HK97 family

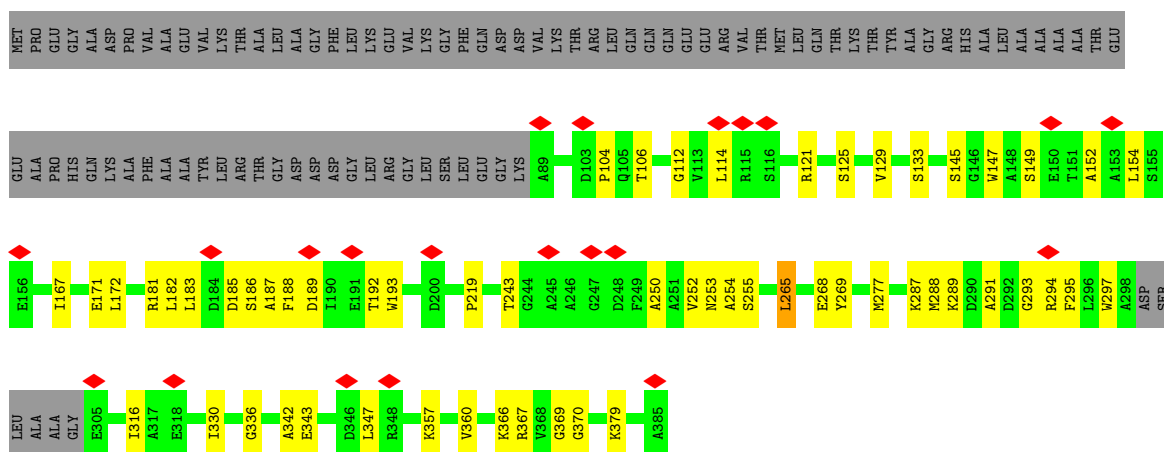




- Molecule 1: Phage major capsid protein, HK97 family

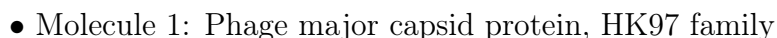


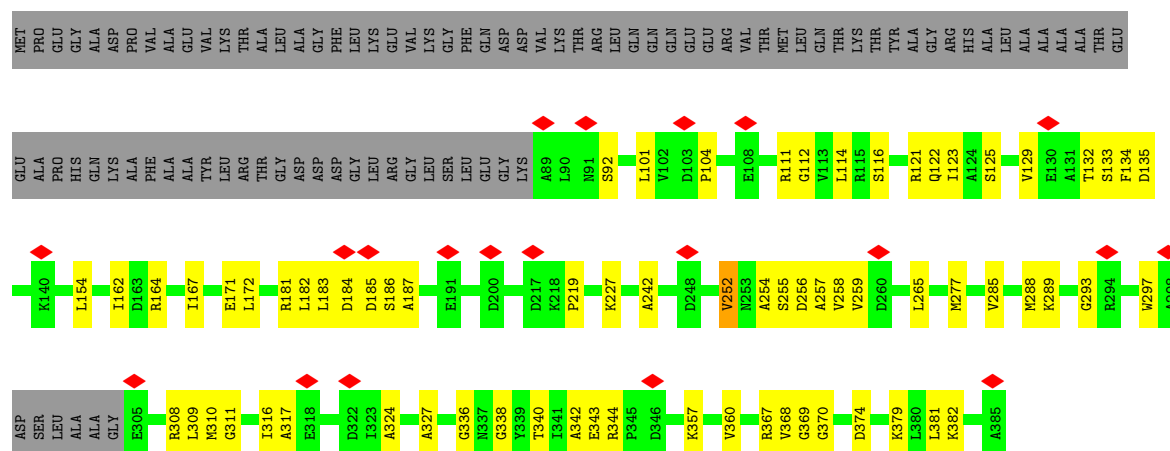
- Molecule 1: Phage major capsid protein, HK97 family



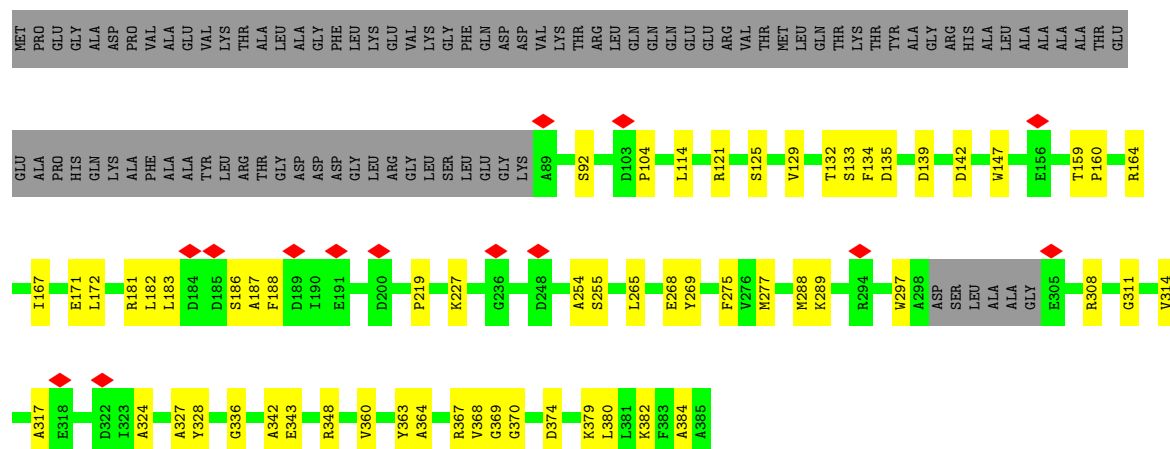
- Molecule 1: Phage major capsid protein, HK97 family



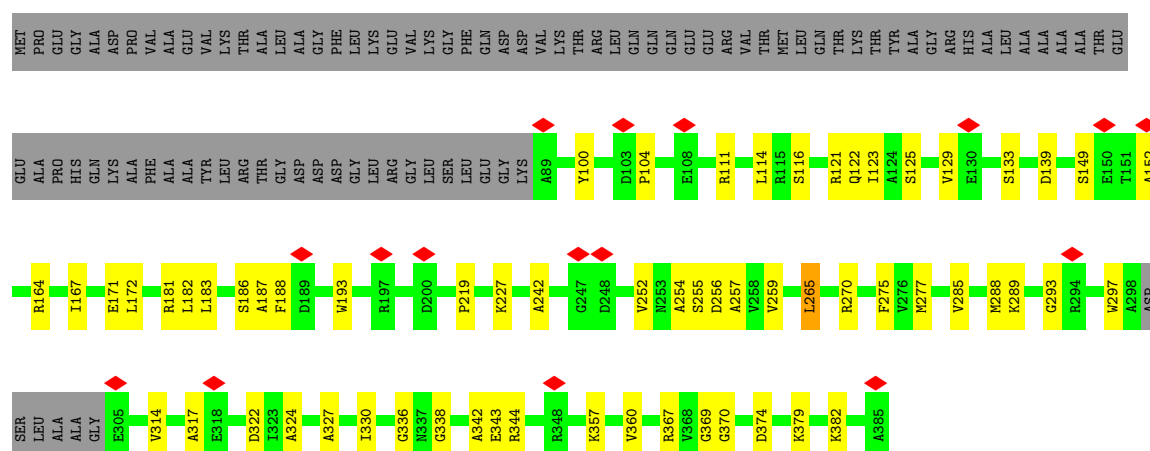




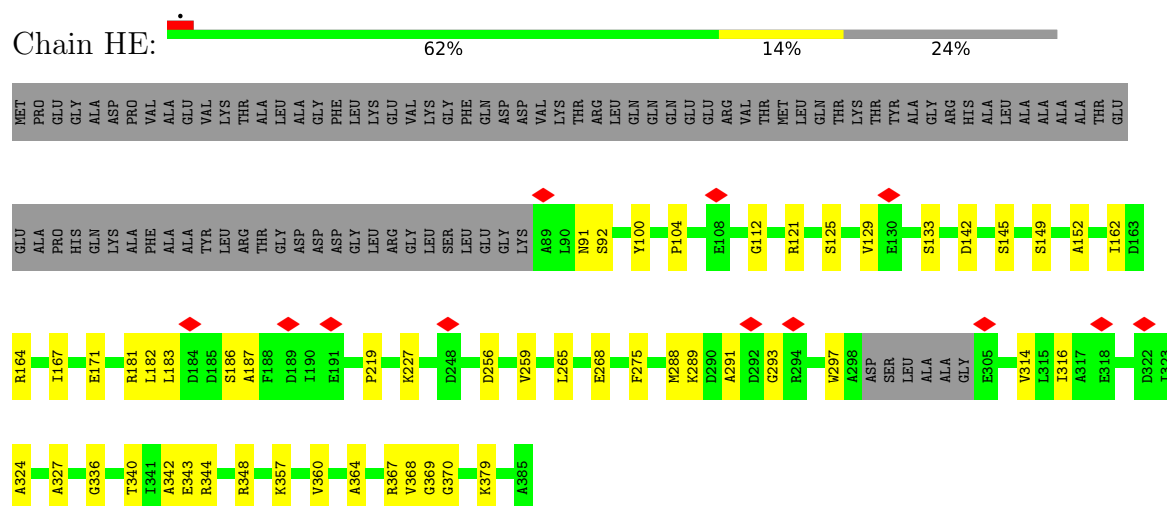
- Molecule 1: Phage major capsid protein, HK97 family



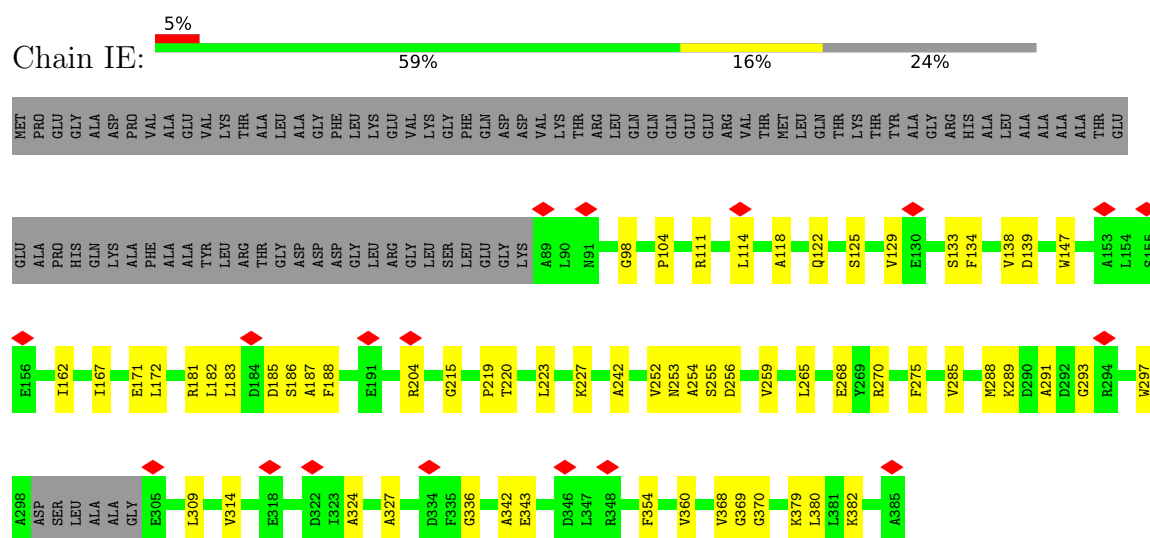
- Molecule 1: Phage major capsid protein, HK97 family



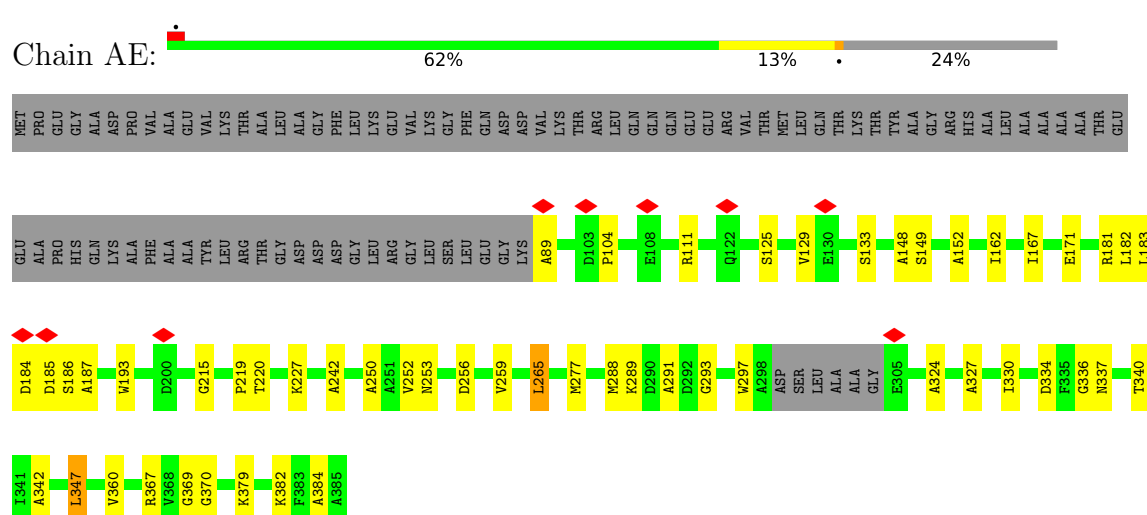
- Molecule 1: Phage major capsid protein, HK97 family



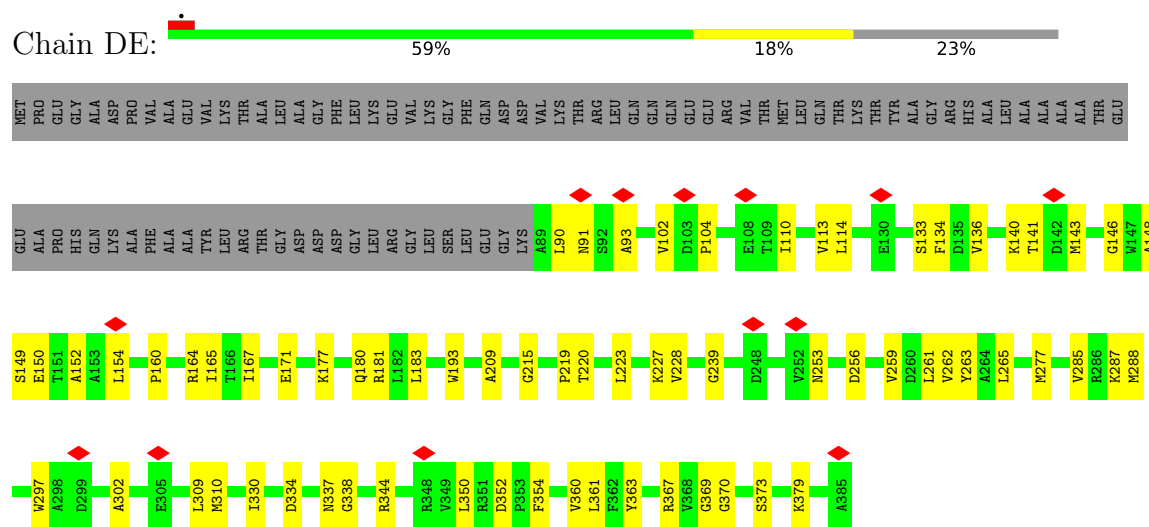
- Molecule 1: Phage major capsid protein, HK97 family



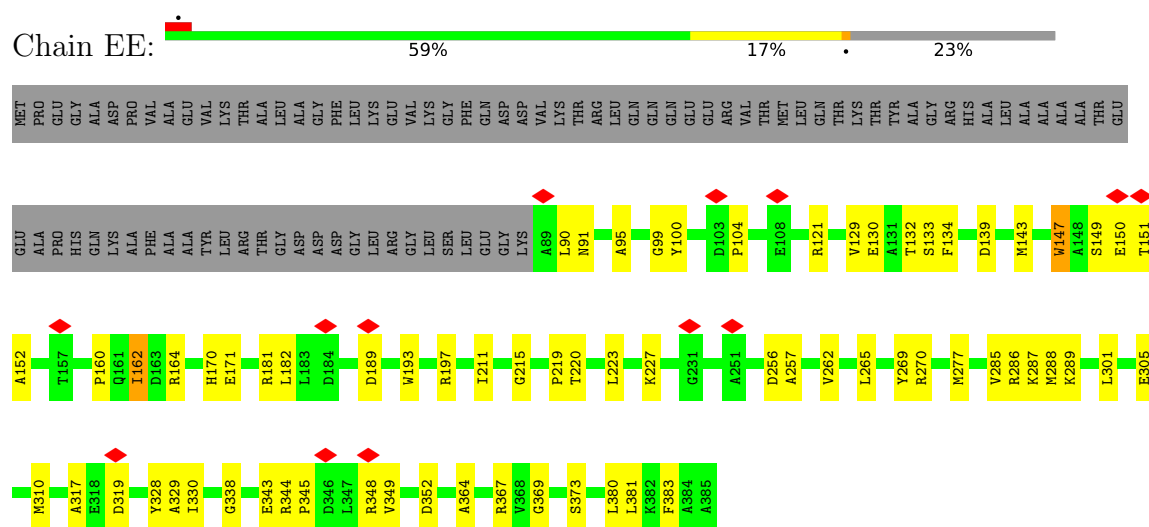
- Molecule 1: Phage major capsid protein, HK97 family



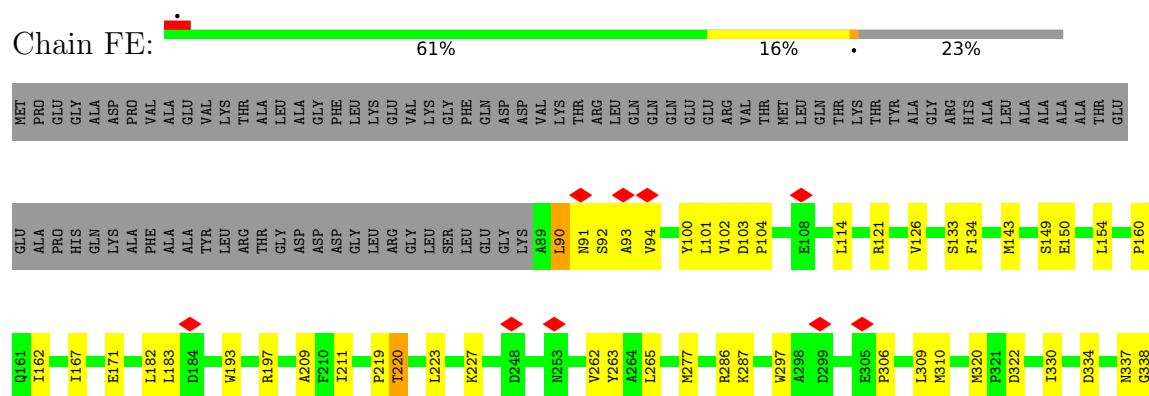
- Molecule 1: Phage major capsid protein, HK97 family

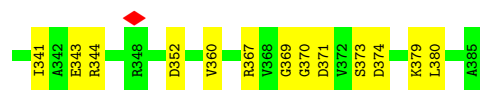


- Molecule 1: Phage major capsid protein, HK97 family

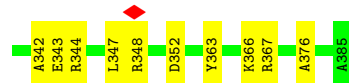
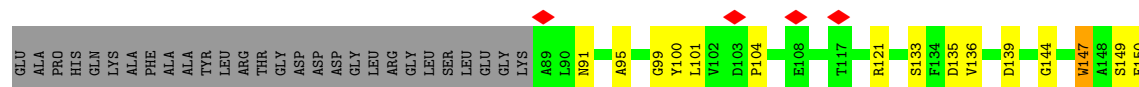


- Molecule 1: Phage major capsid protein, HK97 family

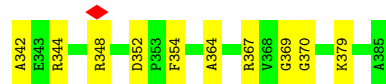
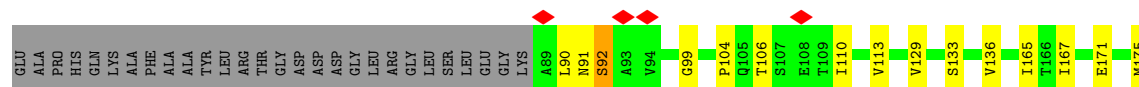
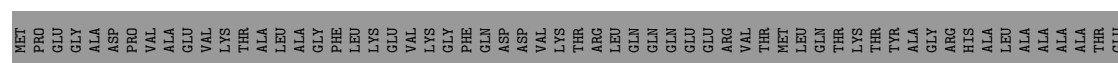




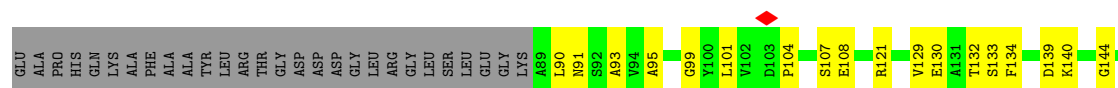
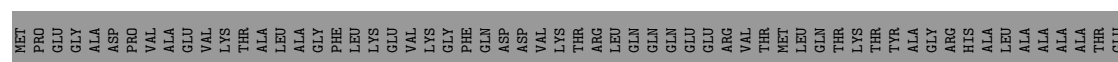
- Molecule 1: Phage major capsid protein, HK97 family

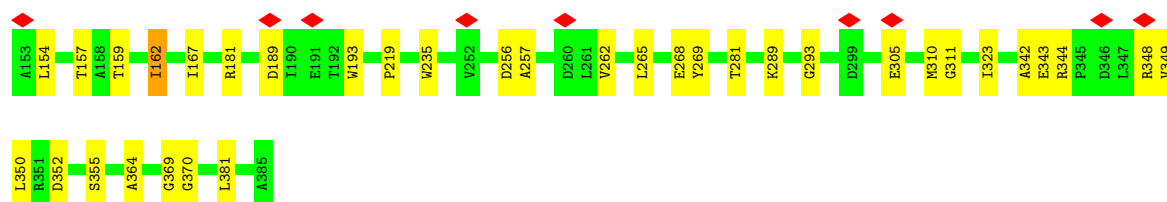


- Molecule 1: Phage major capsid protein, HK97 family

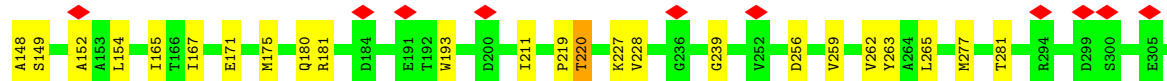
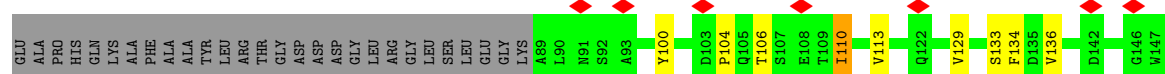
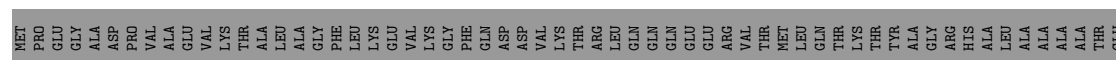


- Molecule 1: Phage major capsid protein, HK97 family

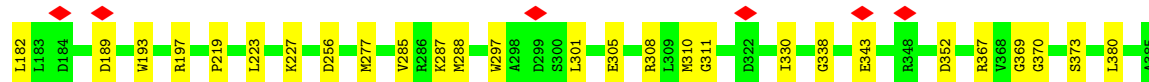
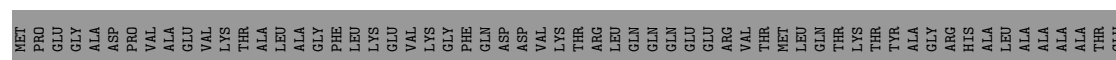




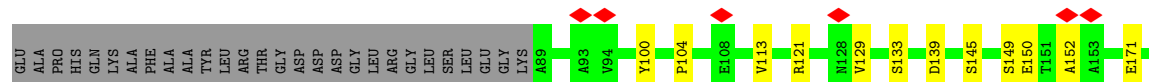
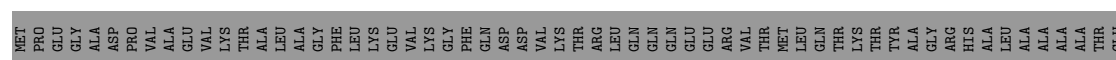
- Molecule 1: Phage major capsid protein, HK97 family

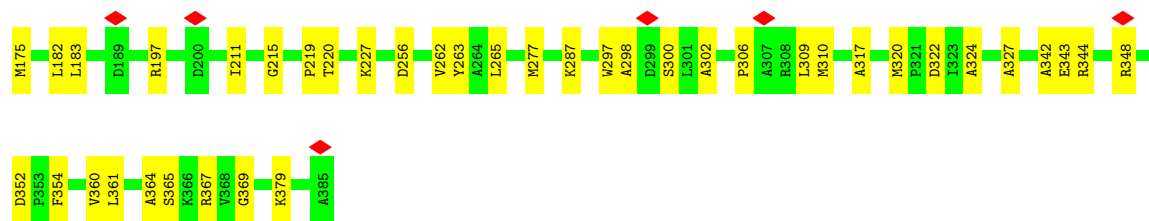


- Molecule 1: Phage major capsid protein, HK97 family



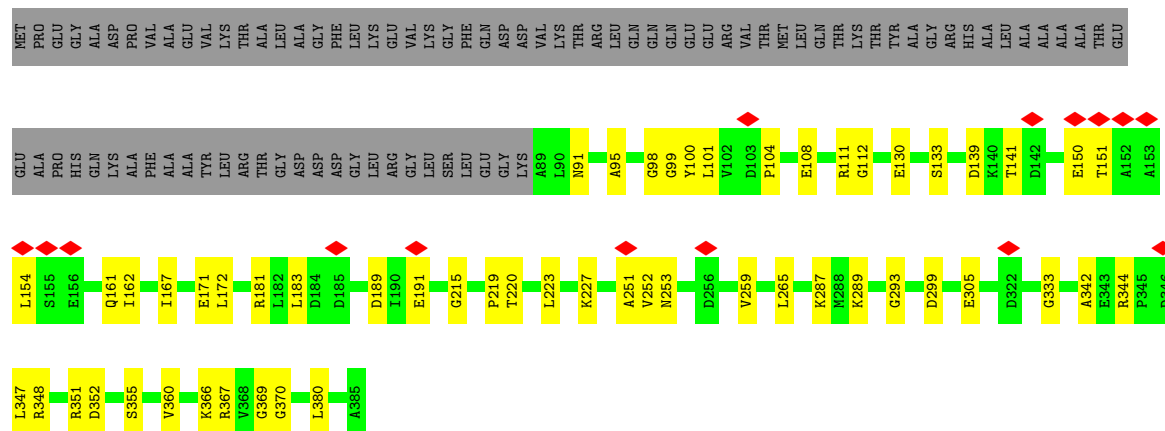
- Molecule 1: Phage major capsid protein, HK97 family





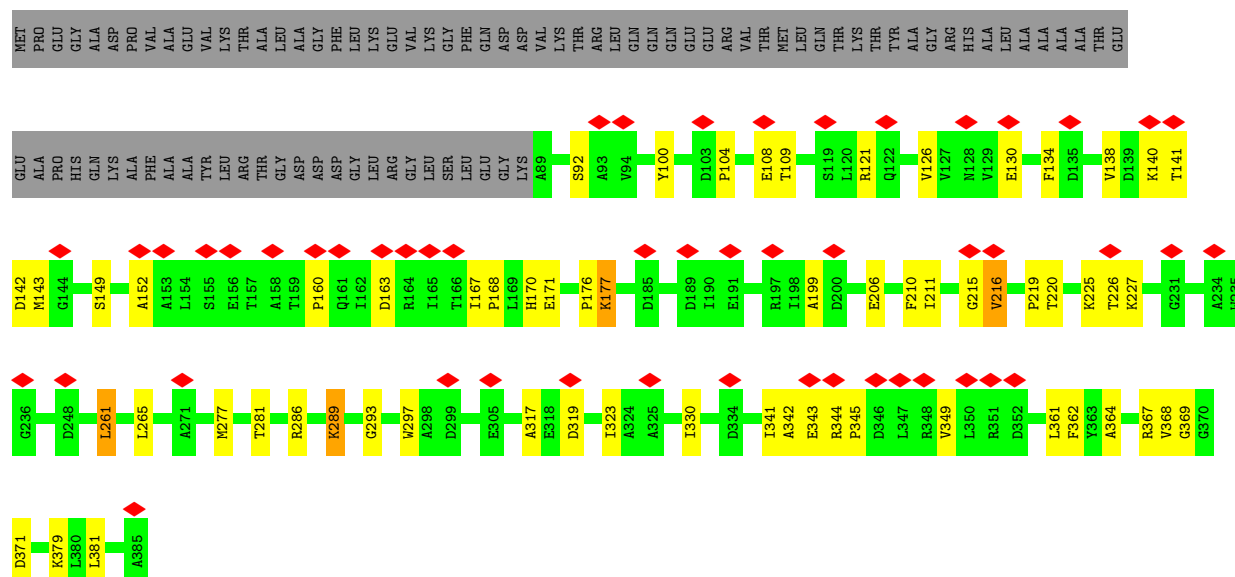
- Molecule 1: Phage major capsid protein, HK97 family

Chain Z9: 63% 14% 23%



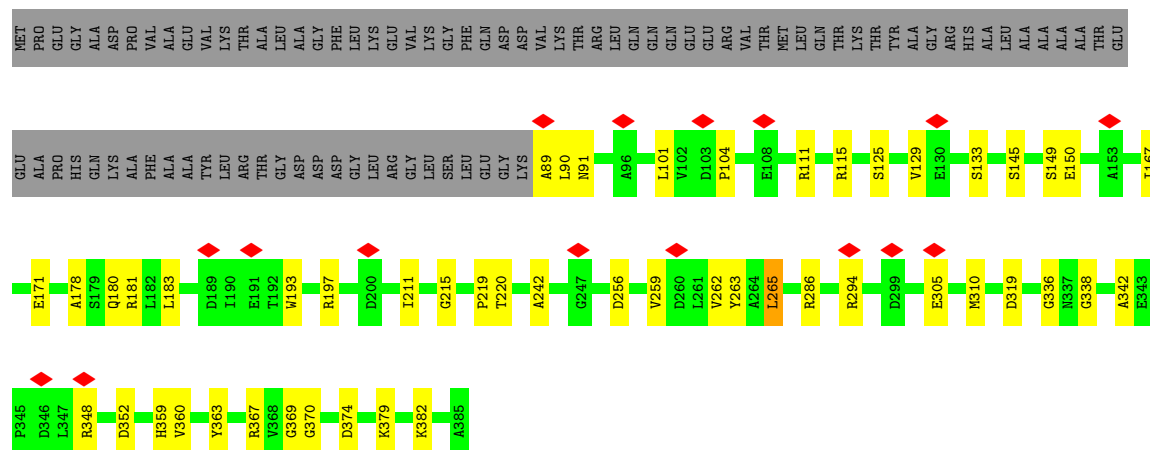
- Molecule 1: Phage major capsid protein, HK97 family

Chain AA: 13% 61% 15% 23%



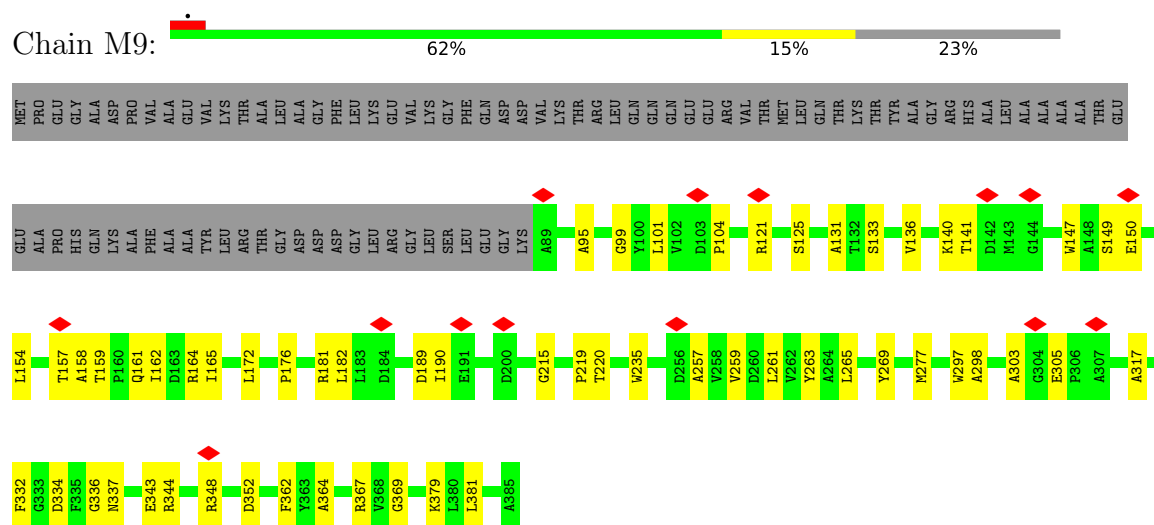
- Molecule 1: Phage major capsid protein, HK97 family

Chain BA: 9% 54% 15% 30%



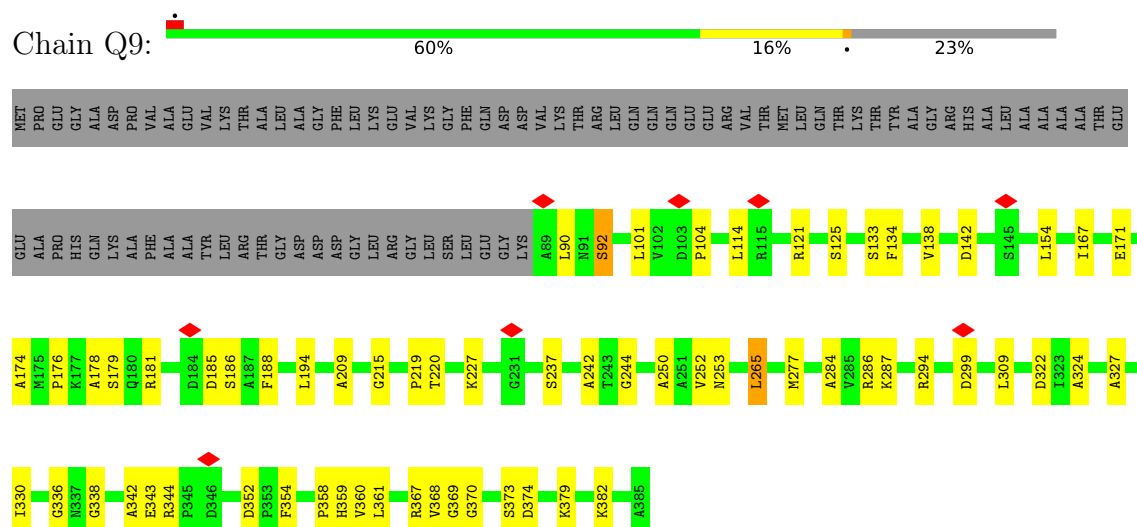
- Molecule 1: Phage major capsid protein, HK97 family

Chain M9:



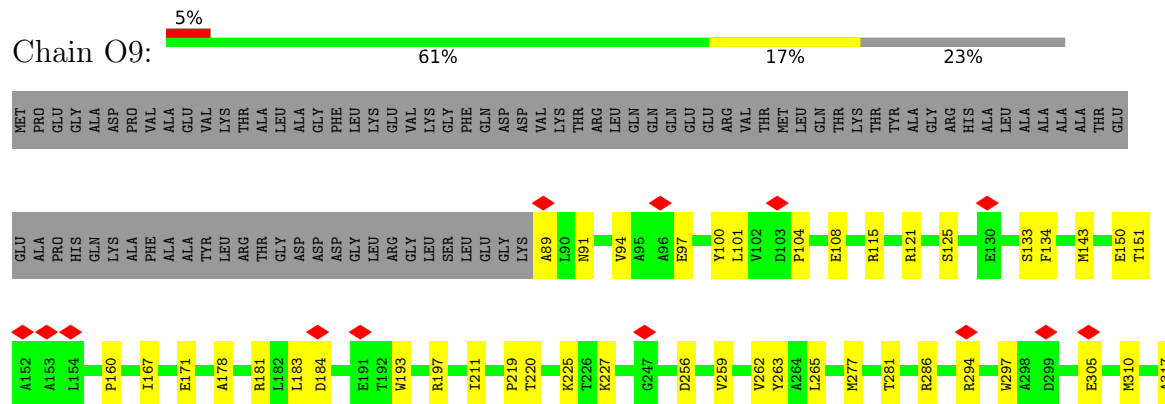
- Molecule 1: Phage major capsid protein, HK97 family

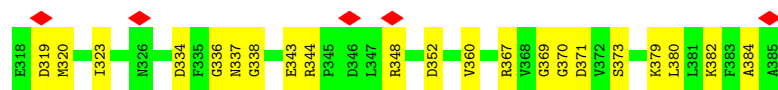
Chain Q9:



- Molecule 1: Phage major capsid protein, HK97 family

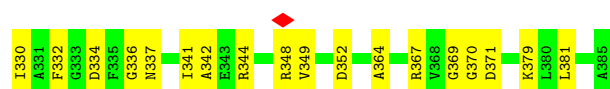
Chain O9:





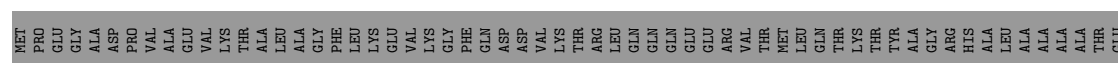
- Molecule 1: Phage major capsid protein, HK97 family

Chain P9: 61% 15% 23%



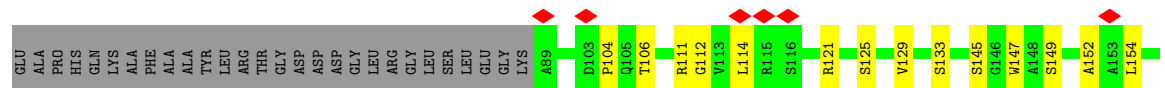
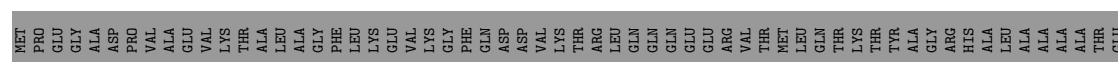
- Molecule 1: Phage major capsid protein, HK97 family

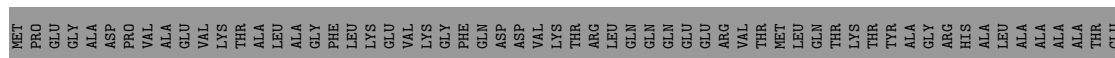
Chain W9: 5% 58% 17% 24%

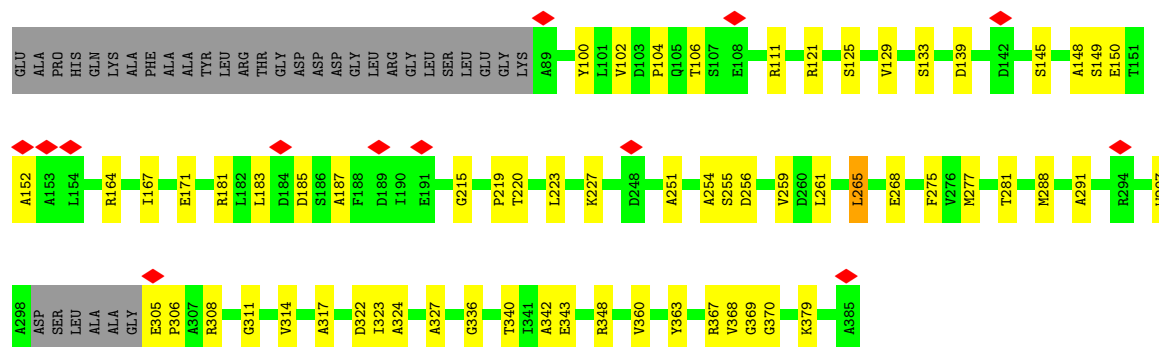


- Molecule 1: Phage major capsid protein, HK97 family

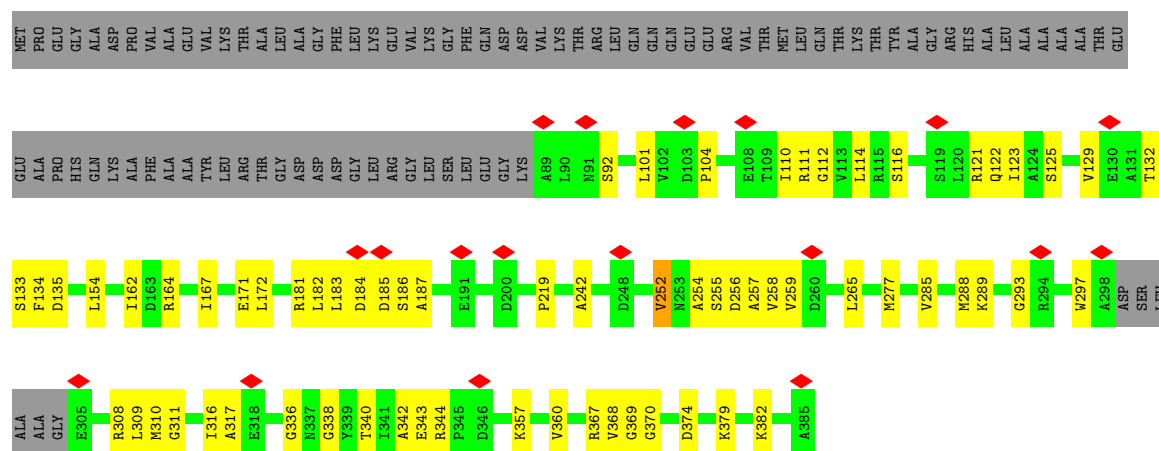
Chain U9: 5% 60% 15% 24%



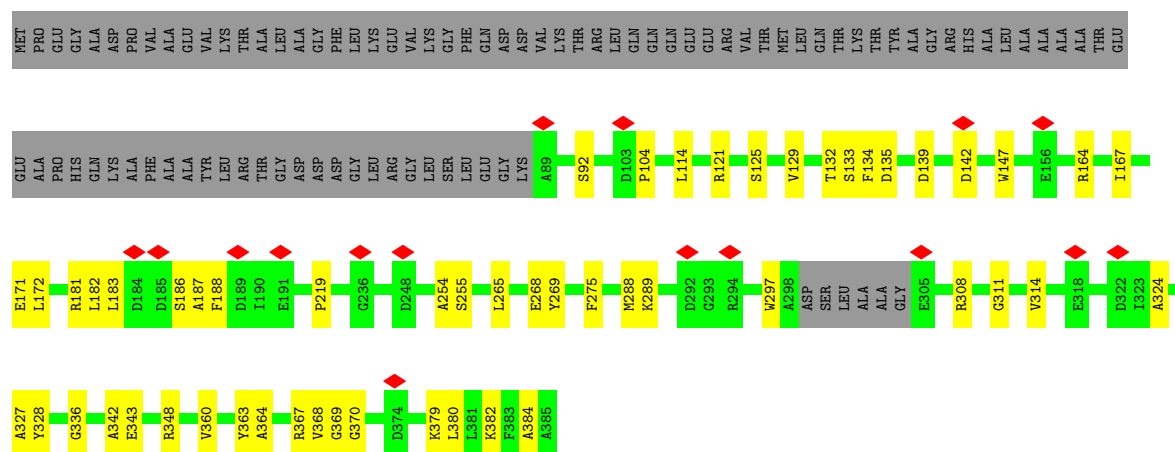




- Molecule 1: Phage major capsid protein, HK97 family

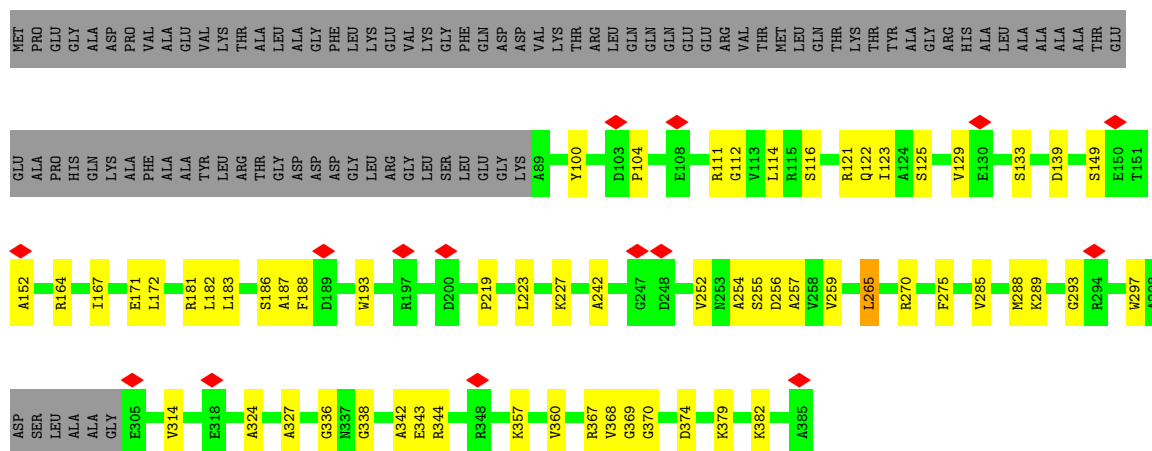


- Molecule 1: Phage major capsid protein, HK97 family

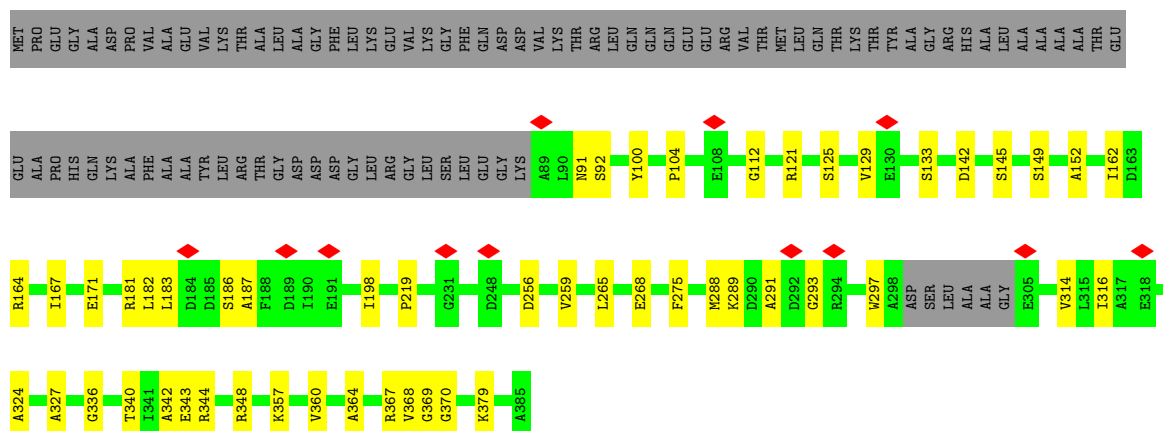


- Molecule 1: Phage major capsid protein, HK97 family

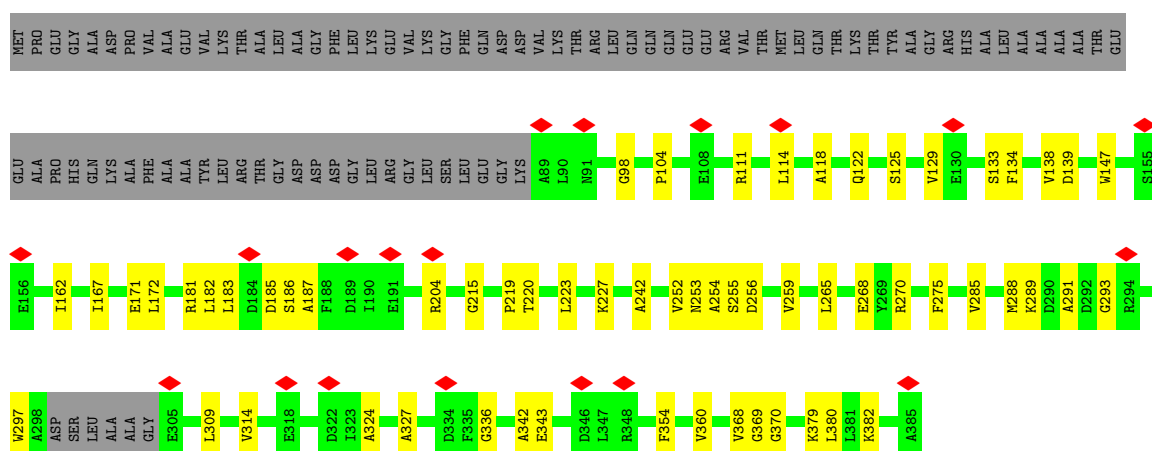




- Molecule 1: Phage major capsid protein, HK97 family

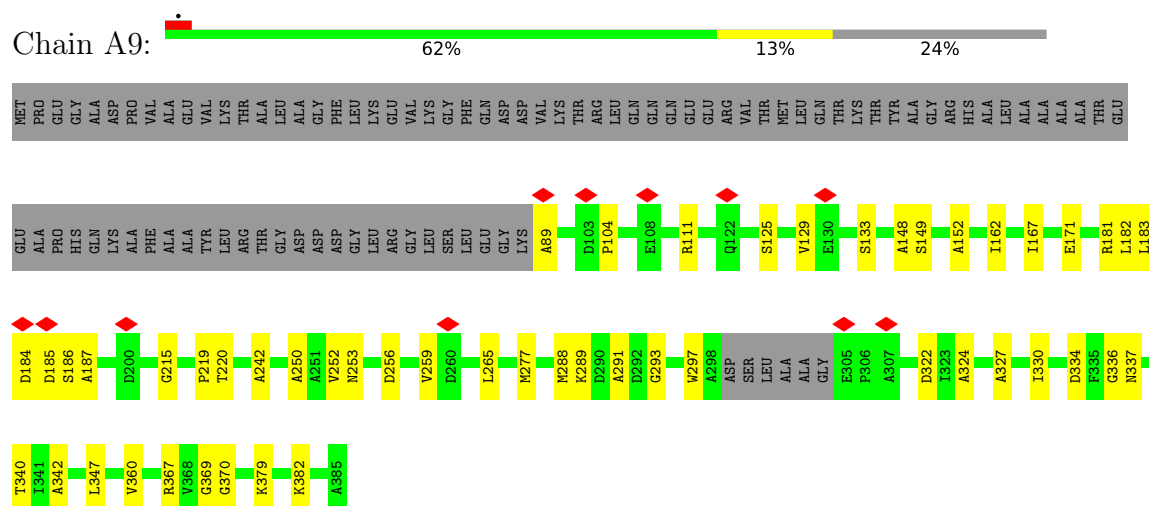


- Molecule 1: Phage major capsid protein, HK97 family



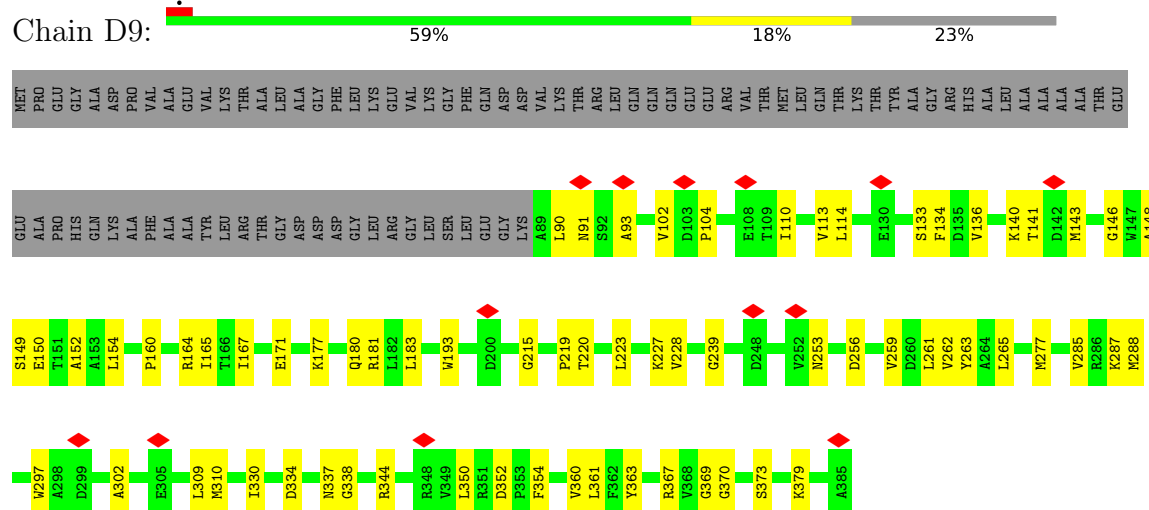
- Molecule 1: Phage major capsid protein, HK97 family

Chain A9:



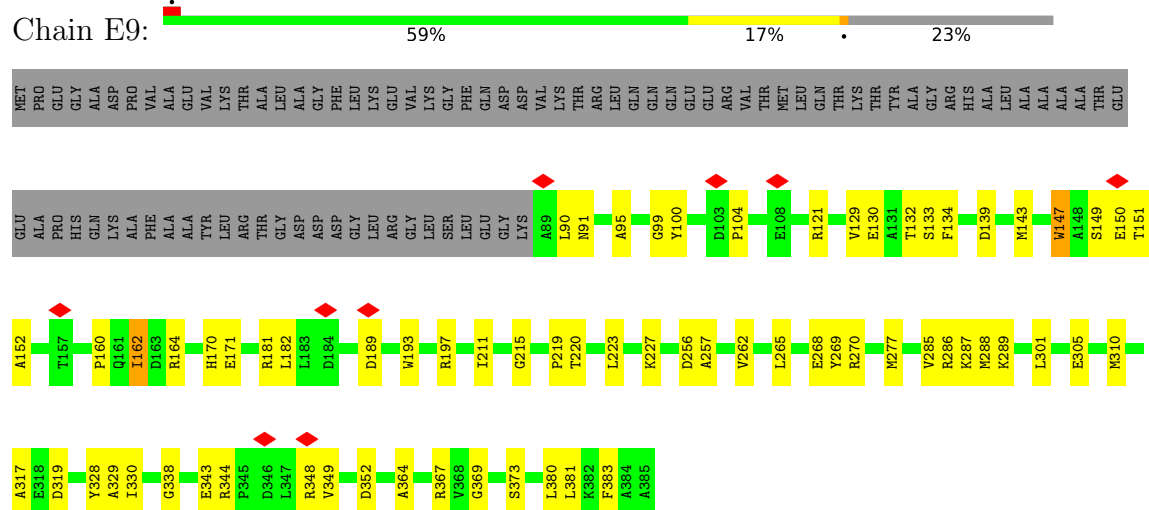
- Molecule 1: Phage major capsid protein, HK97 family

Chain D9:

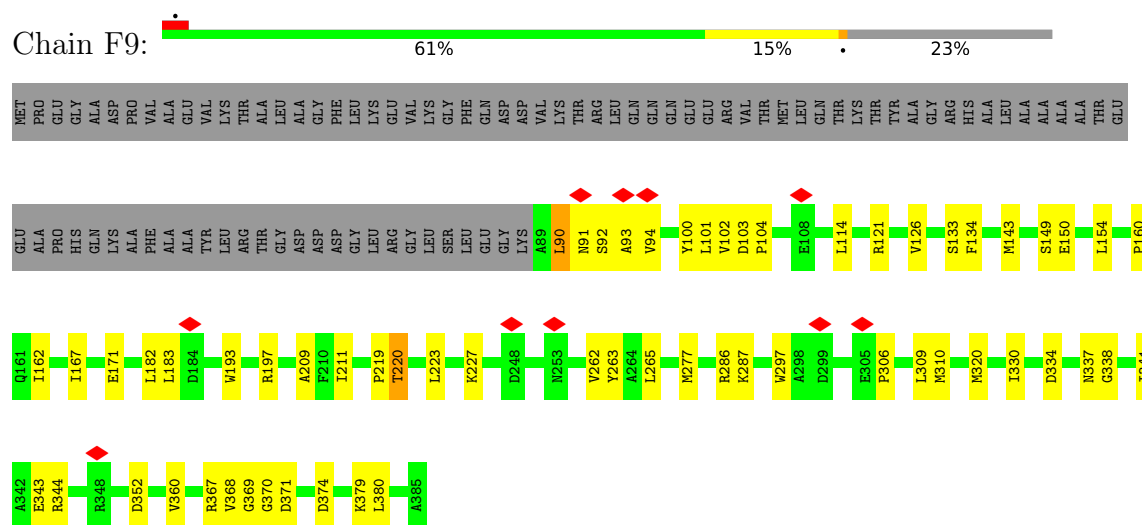


- Molecule 1: Phage major capsid protein, HK97 family

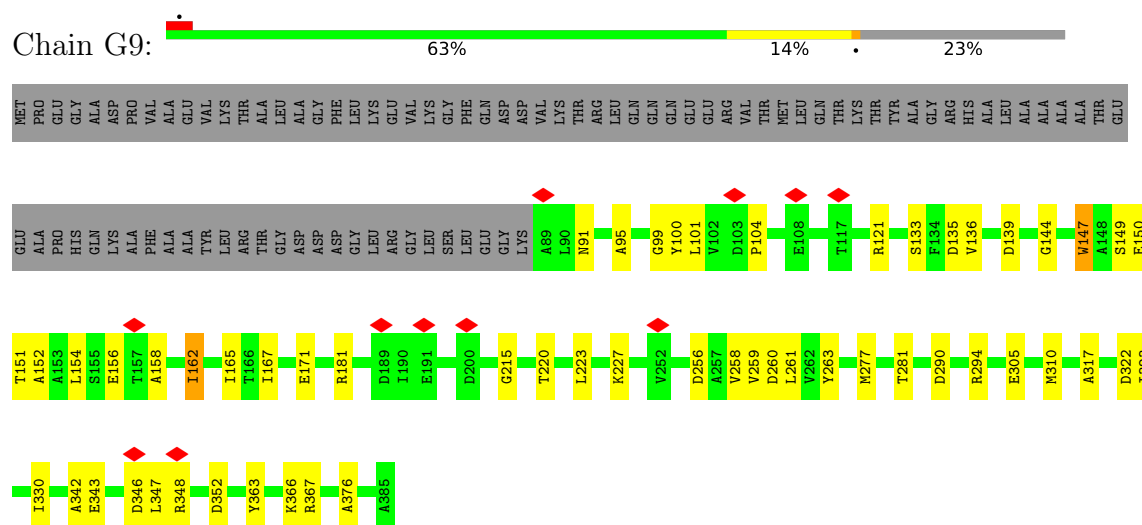
Chain E9:



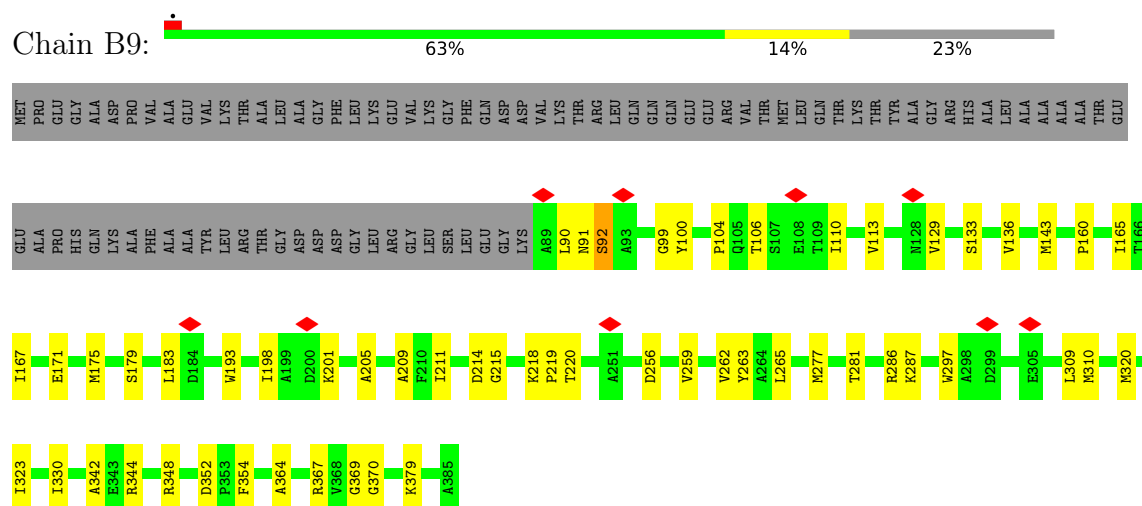
- Molecule 1: Phage major capsid protein, HK97 family



- Molecule 1: Phage major capsid protein, HK97 family

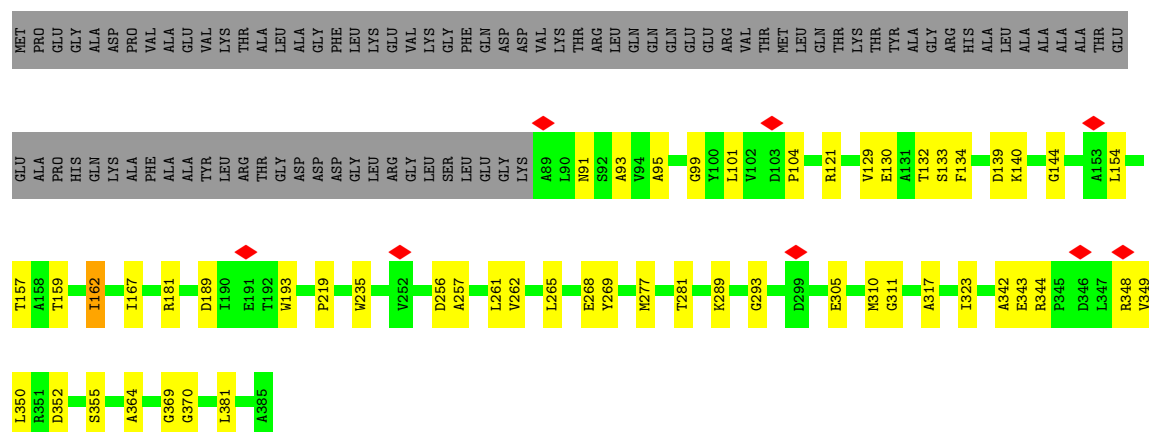


- Molecule 1: Phage major capsid protein, HK97 family



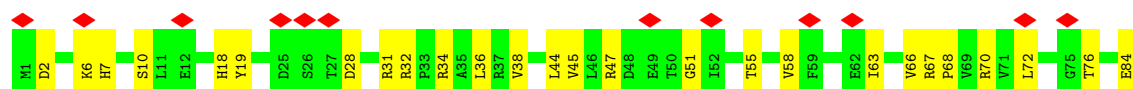
- Molecule 1: Phage major capsid protein, HK97 family

Chain C9:  63% 14% 23%



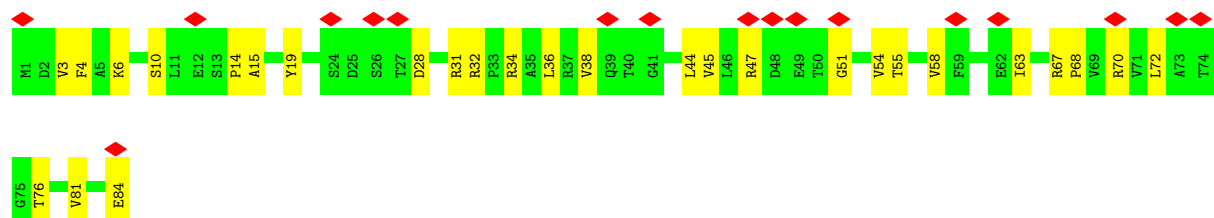
- Molecule 2: Uncharacterized protein

Chain E3:  14% 69% 31%



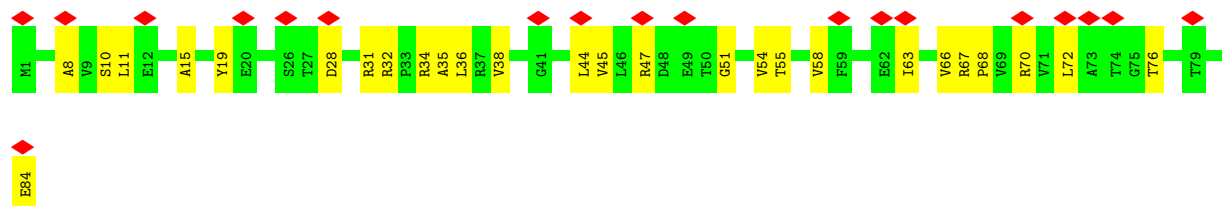
- Molecule 2: Uncharacterized protein

Chain D3:  20% 67% 33%



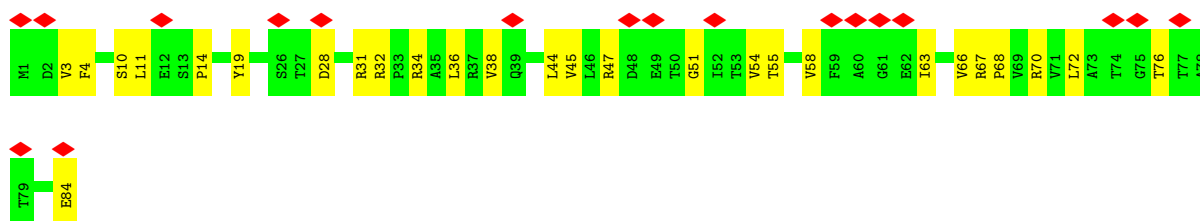
- Molecule 2: Uncharacterized protein

Chain A3:  23% 68% 32%

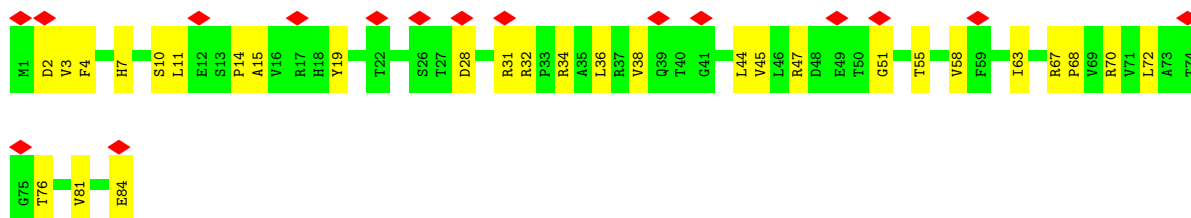


- Molecule 2: Uncharacterized protein

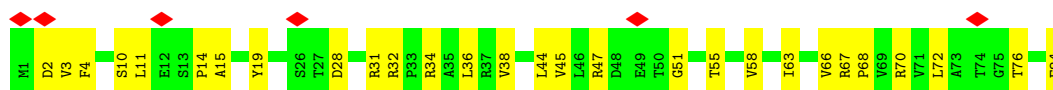
Chain C3:  21% 68% 32%



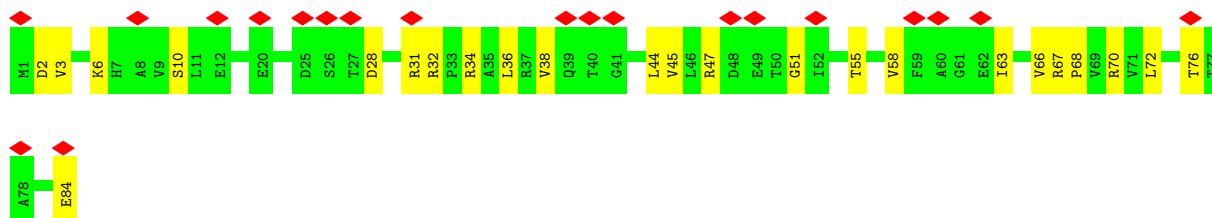
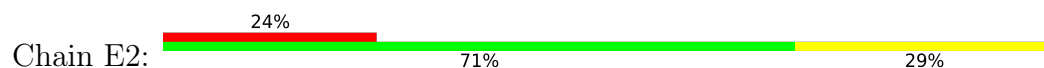
- Molecule 2: Uncharacterized protein



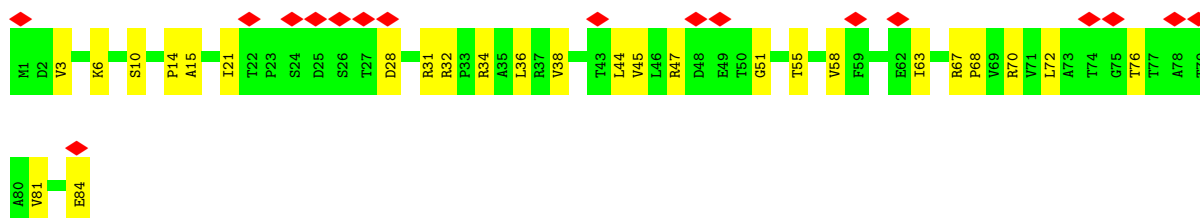
- Molecule 2: Uncharacterized protein



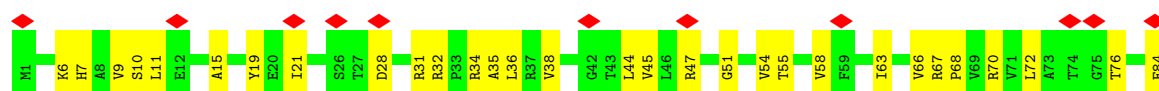
- Molecule 2: Uncharacterized protein



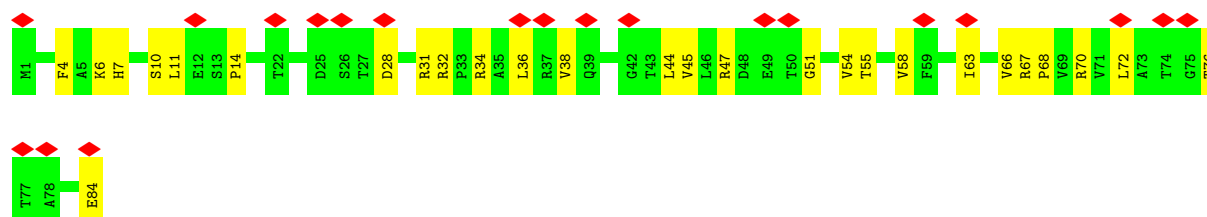
- Molecule 2: Uncharacterized protein



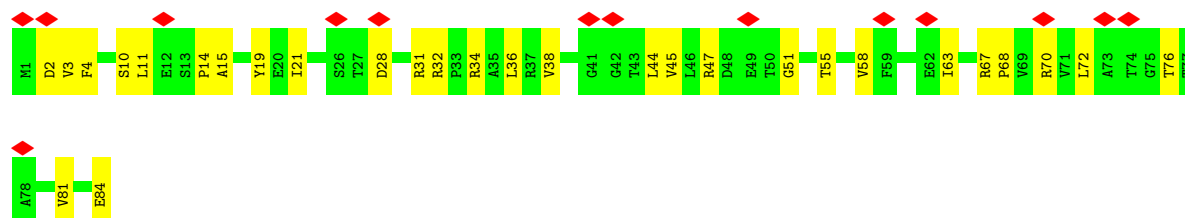
- Molecule 2: Uncharacterized protein



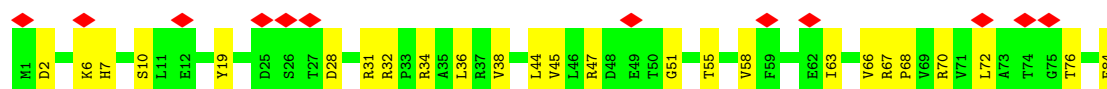
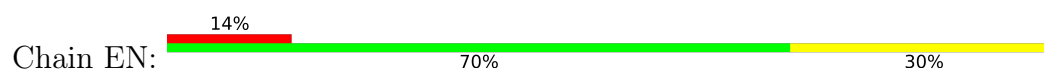
- Molecule 2: Uncharacterized protein



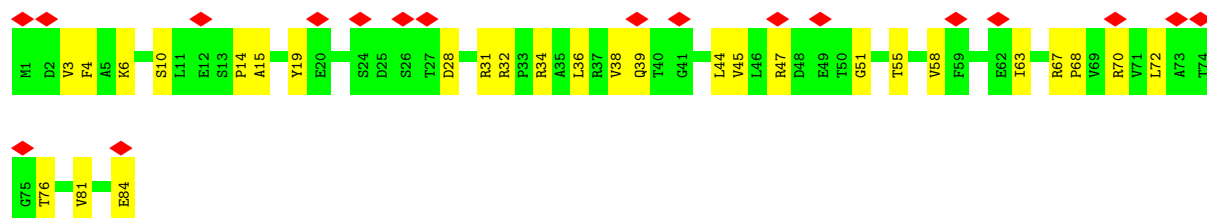
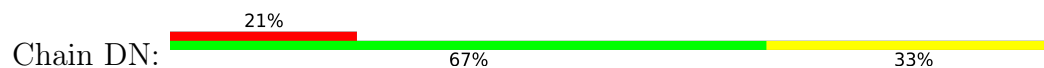
- Molecule 2: Uncharacterized protein



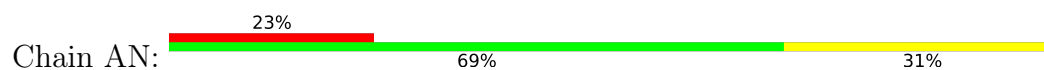
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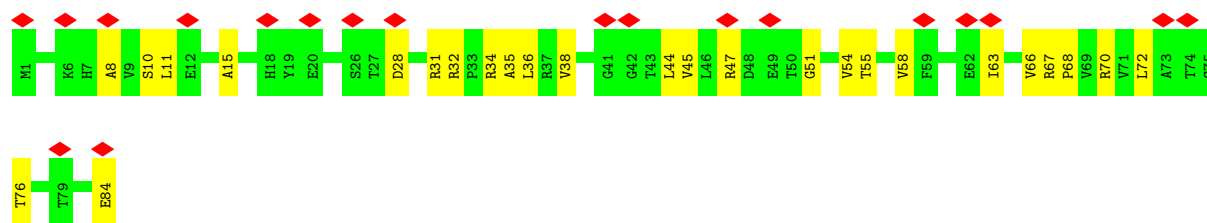


- Molecule 2: Uncharacterized protein

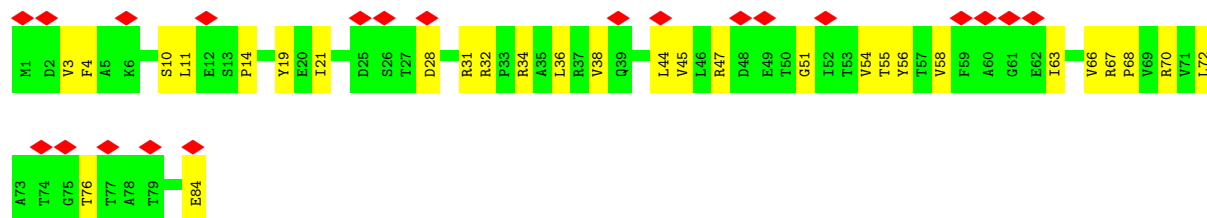


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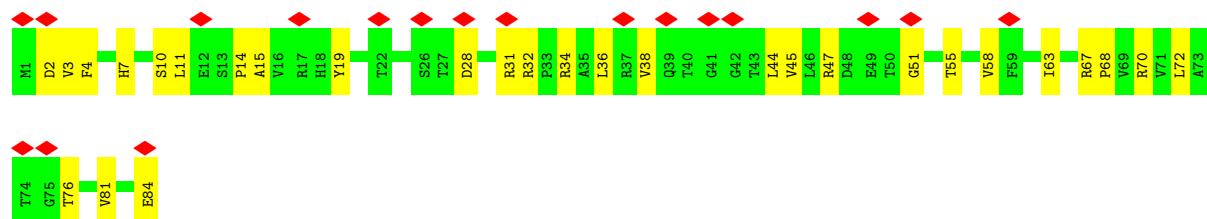




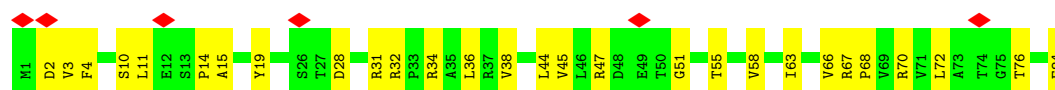
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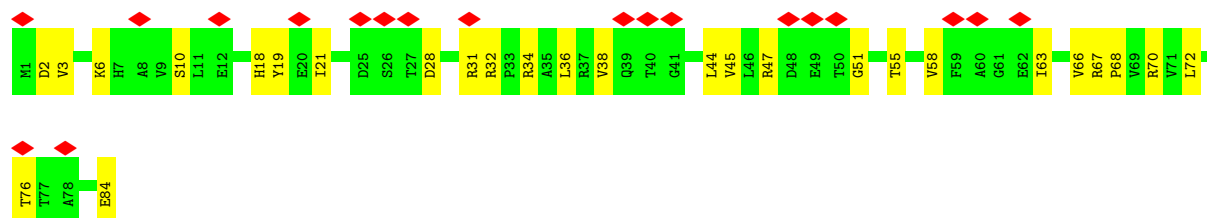
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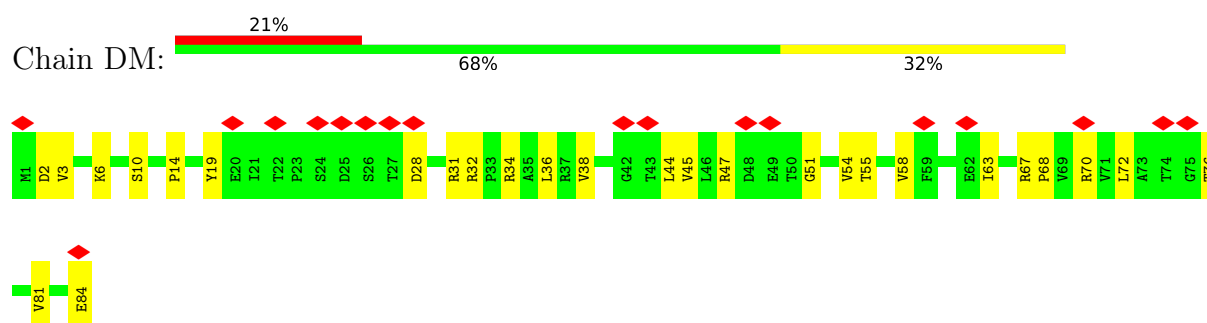
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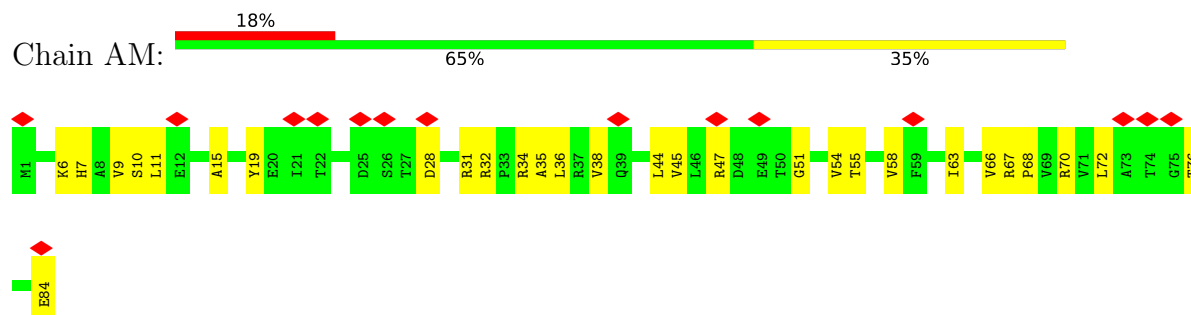
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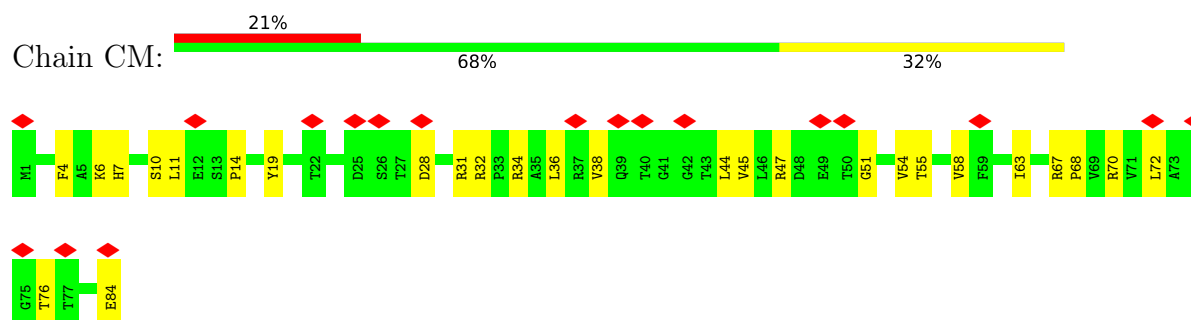
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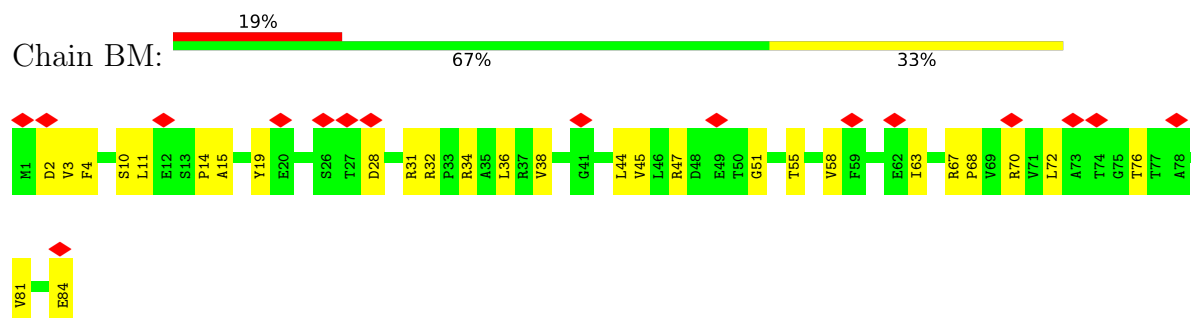
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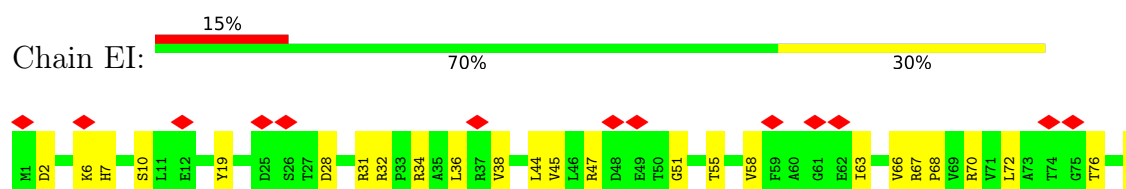
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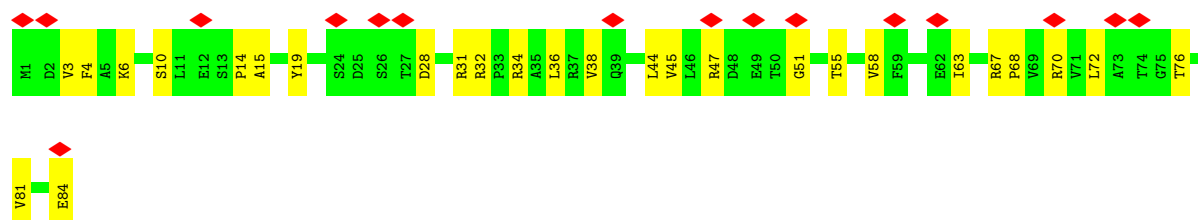
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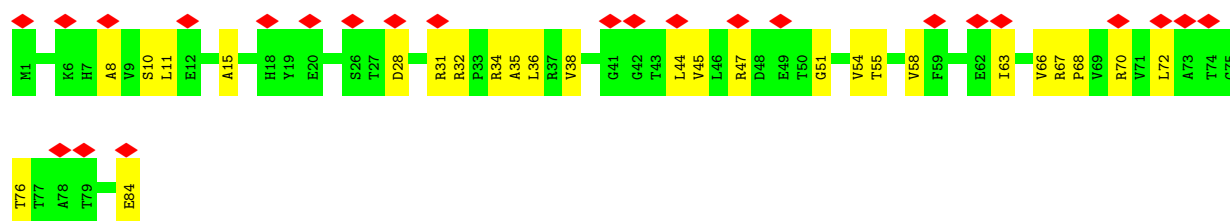
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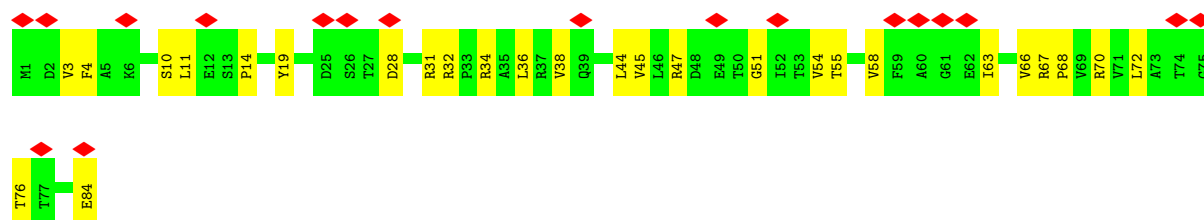
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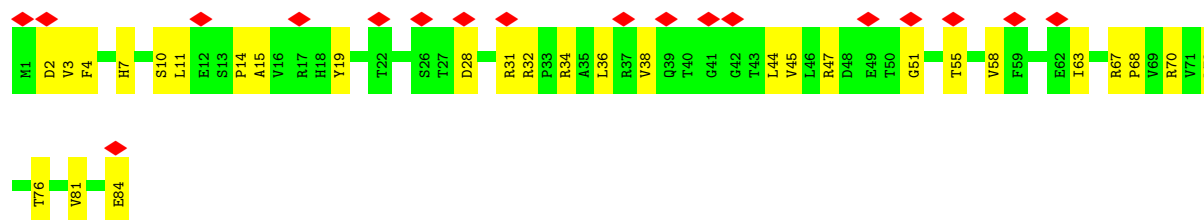
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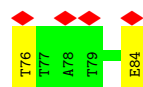
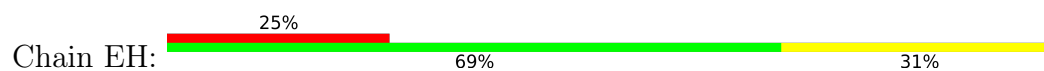


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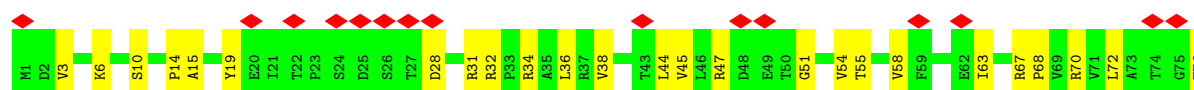




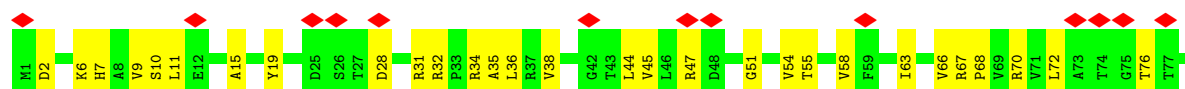
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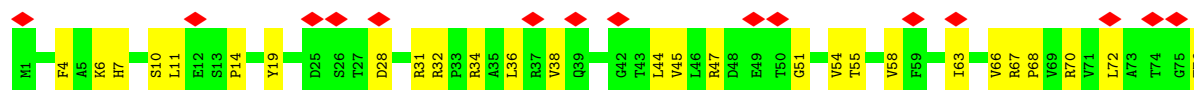
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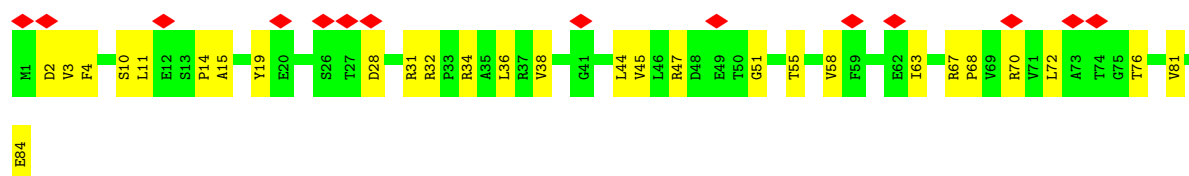
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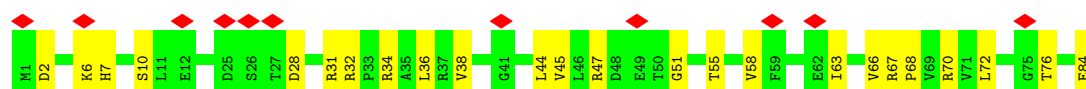
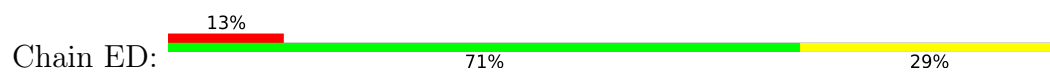
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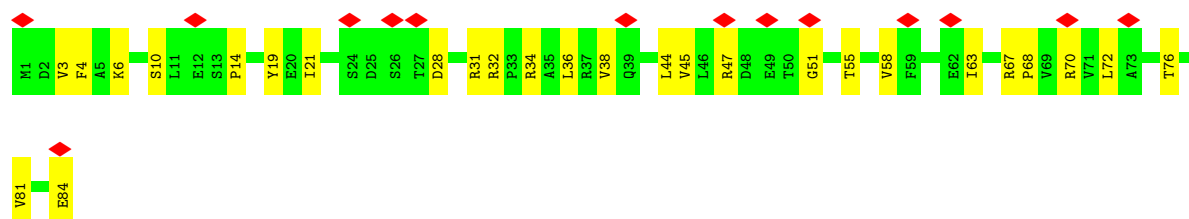
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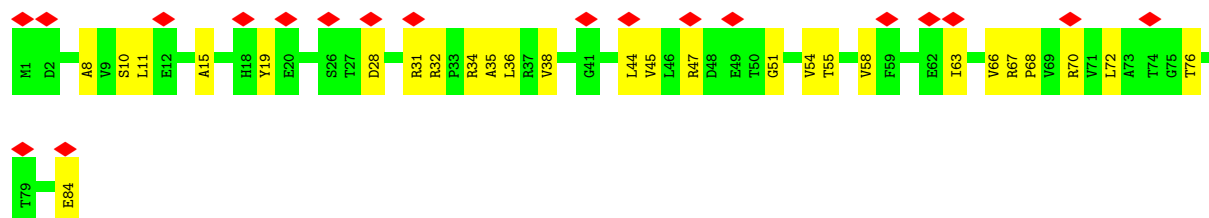
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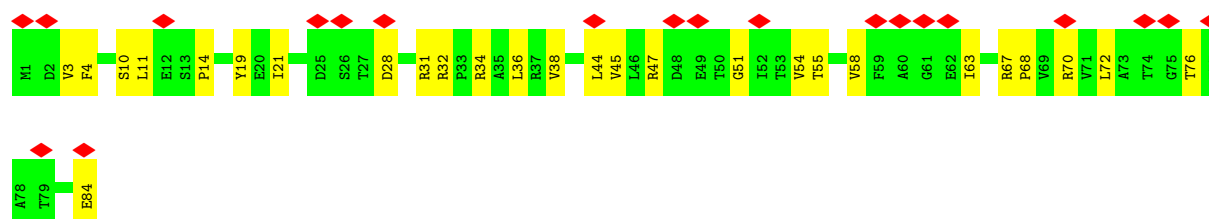
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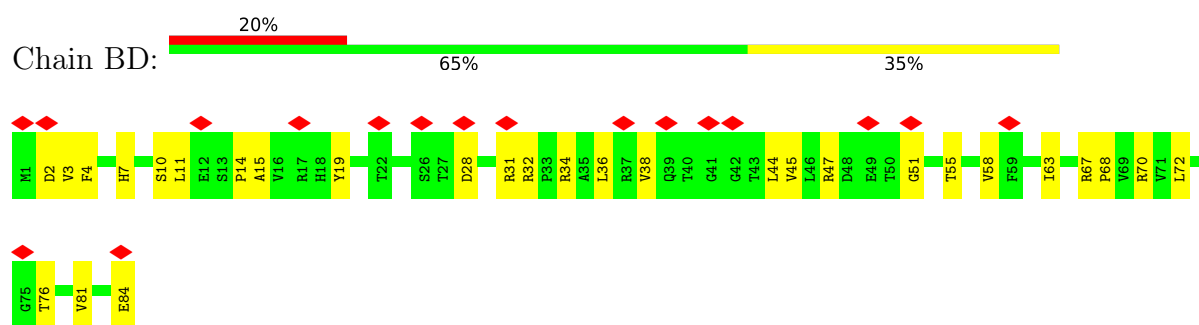
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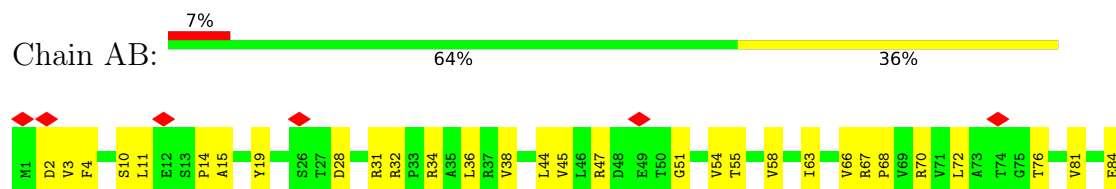
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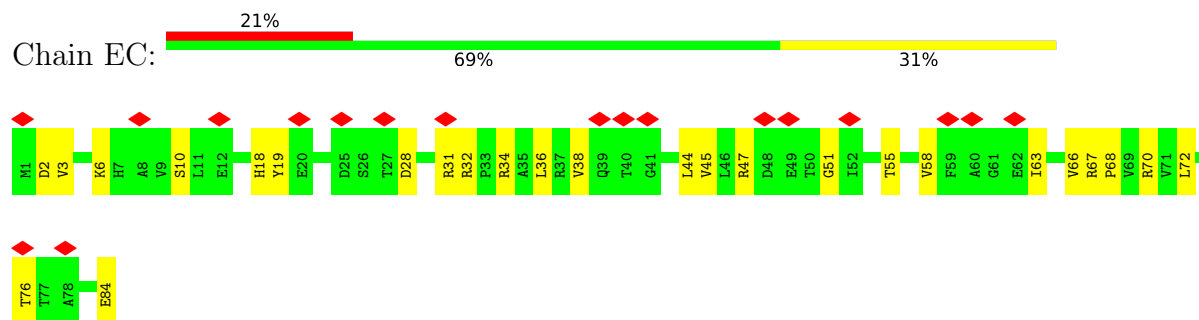
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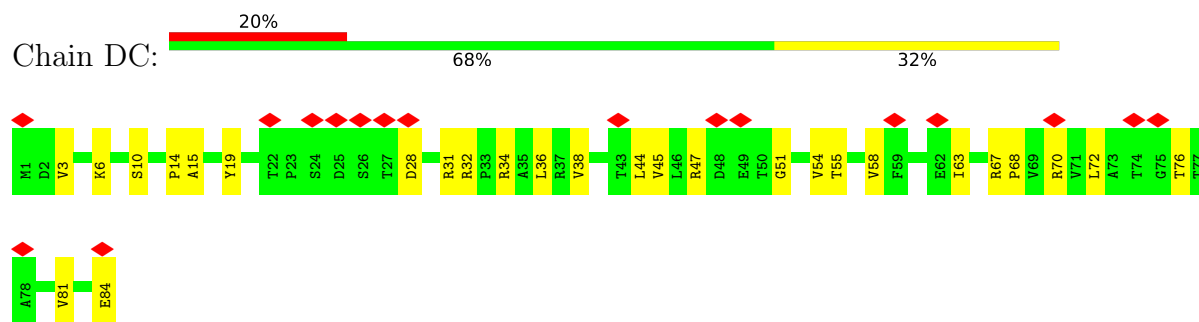
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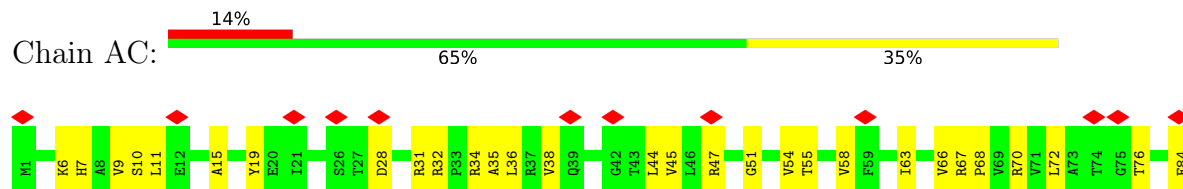
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- Molecule 2: Uncharacterized protein

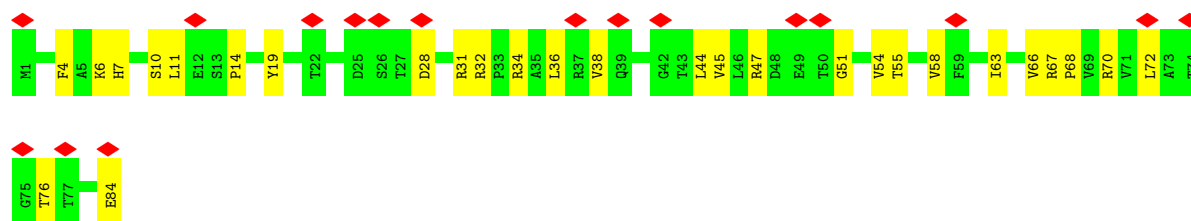


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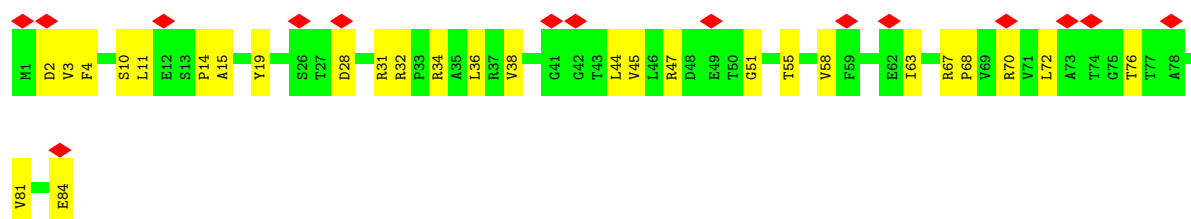


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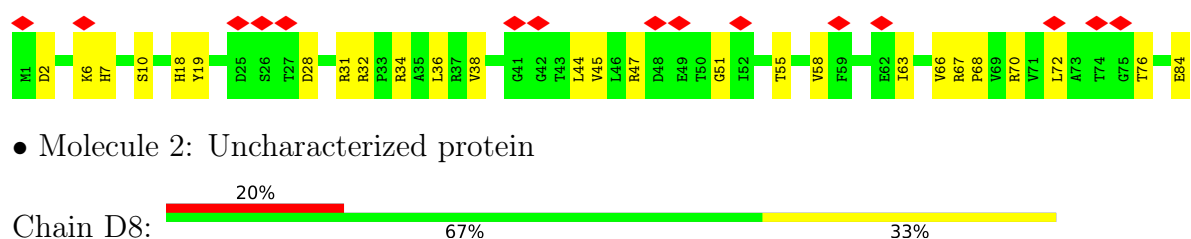




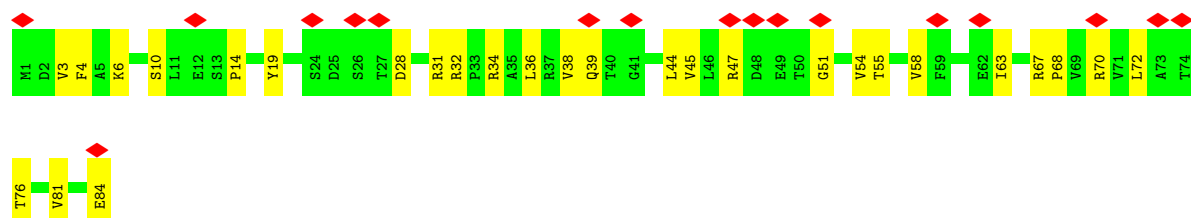
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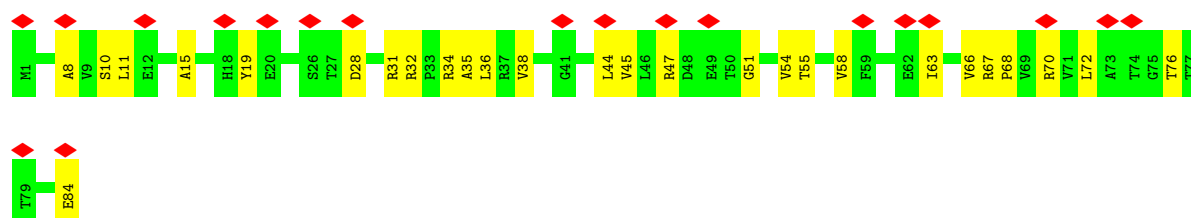
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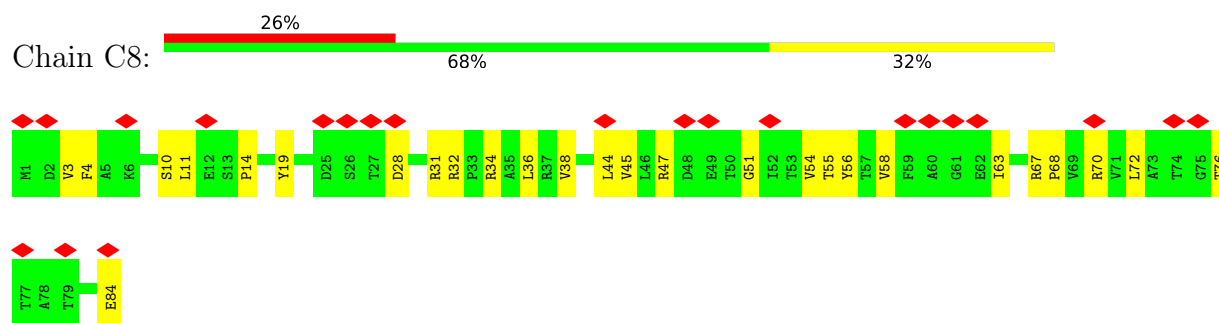
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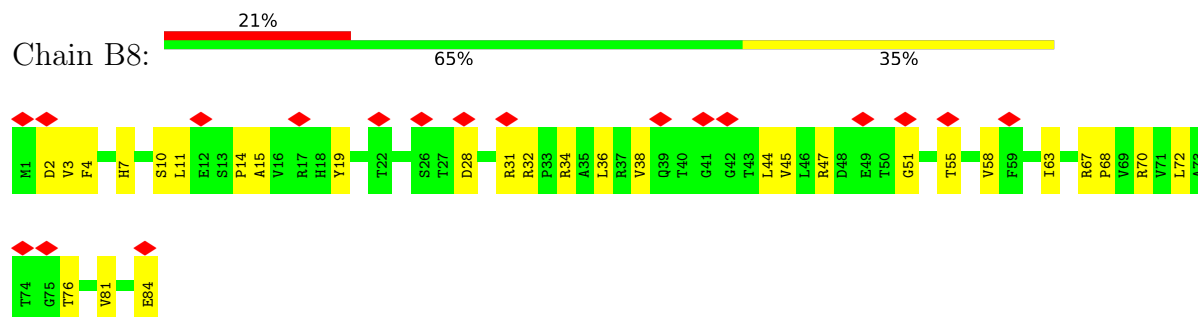
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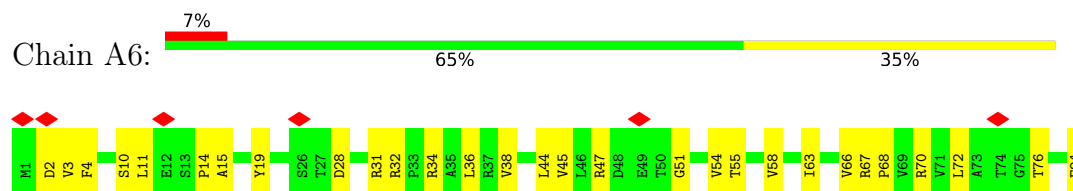
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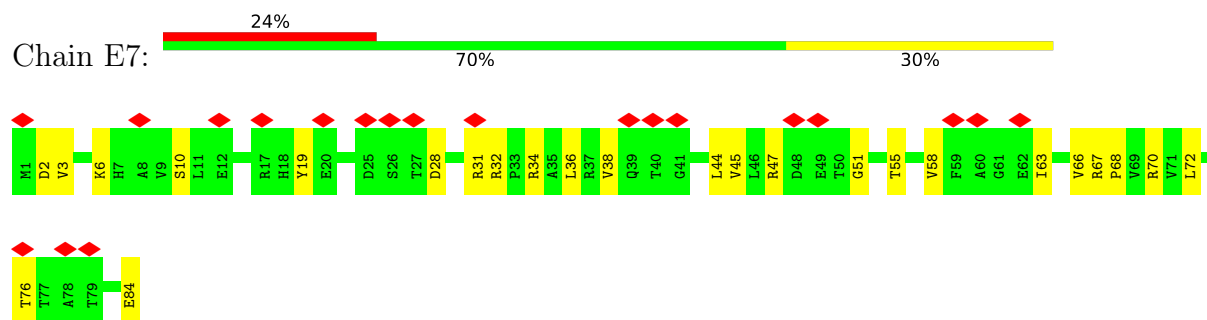
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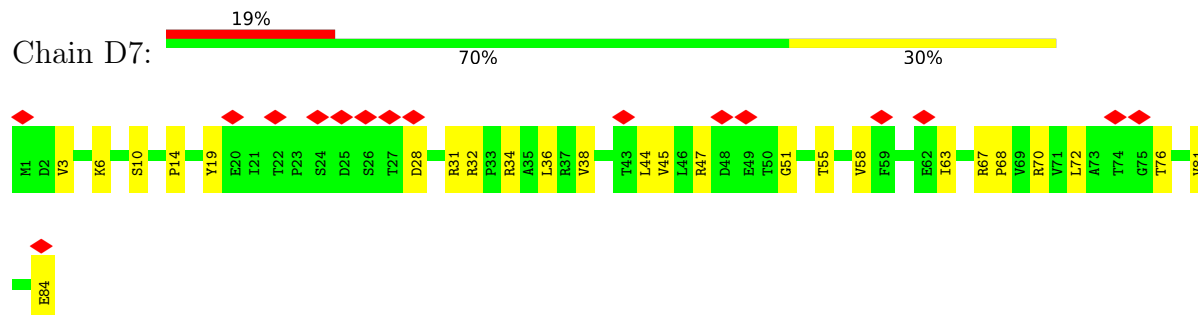
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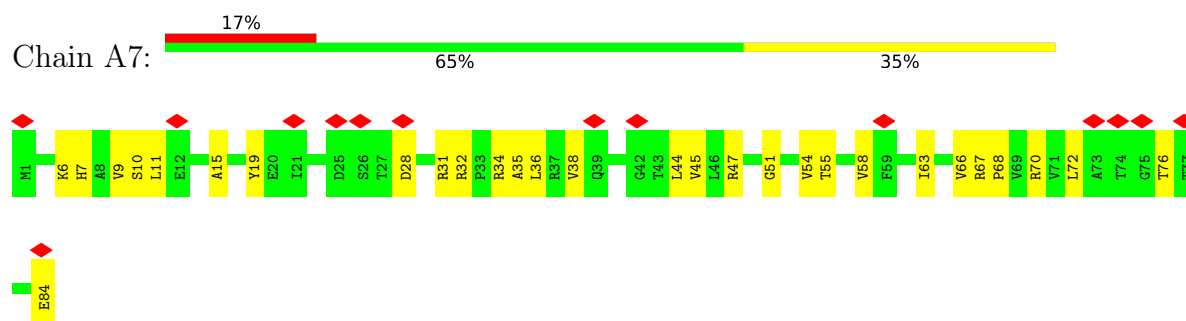
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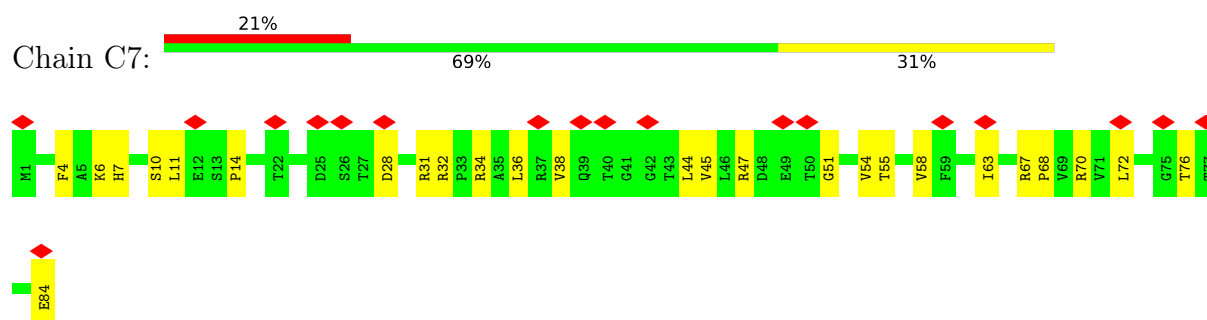
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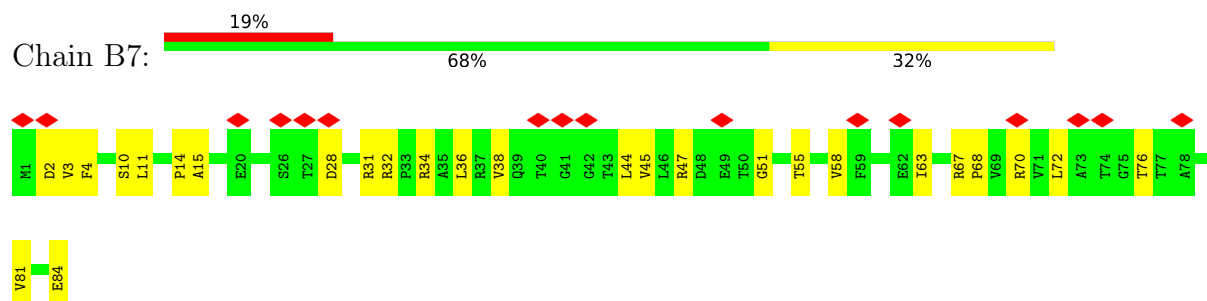
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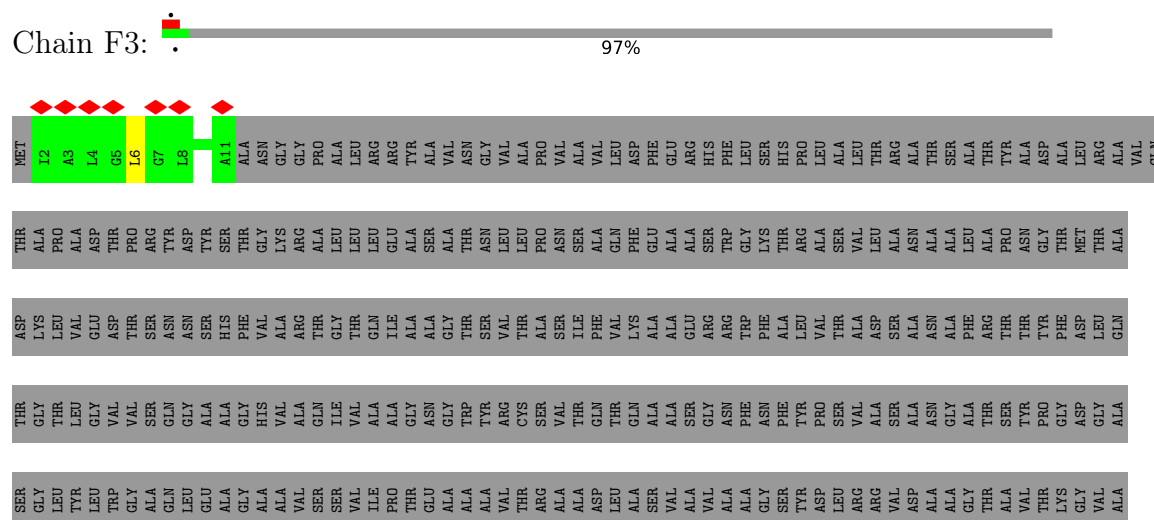
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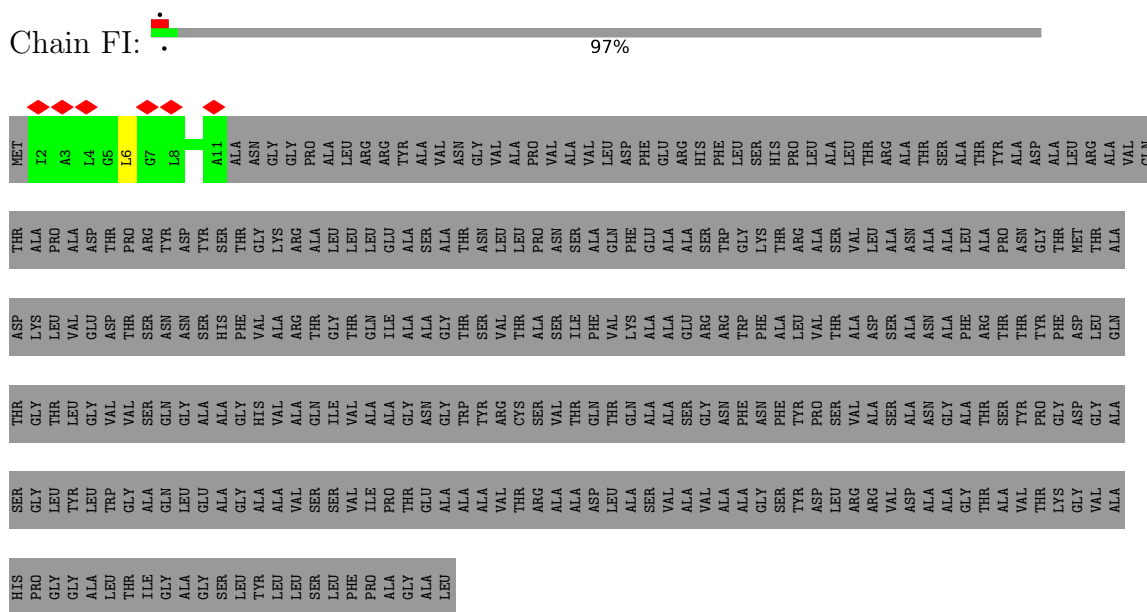
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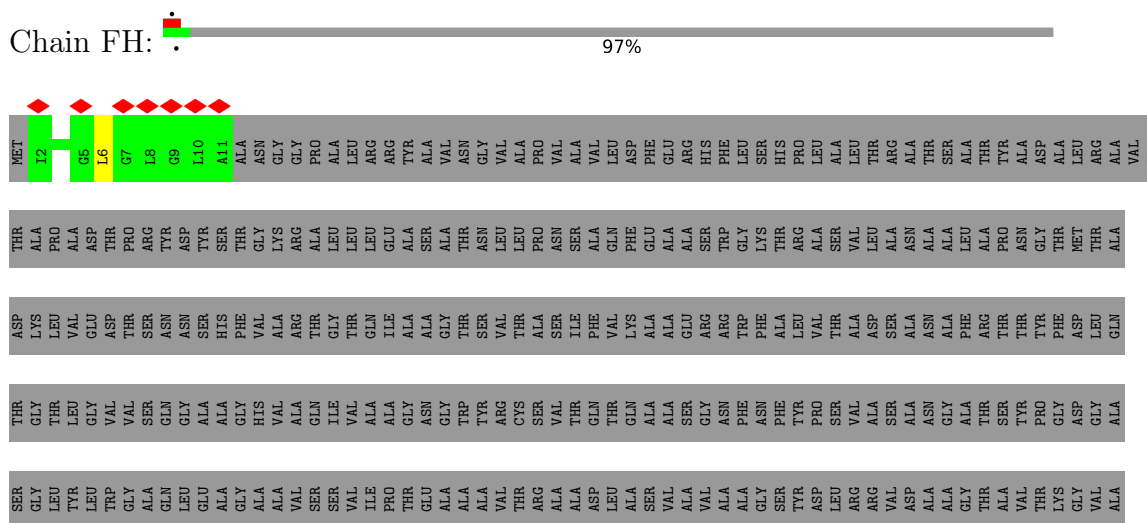
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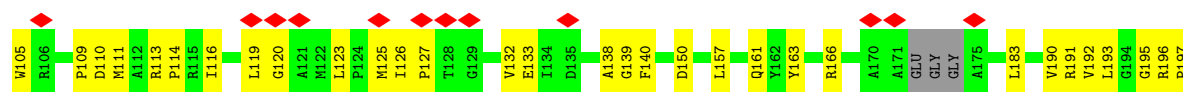


- Molecule 3: Uncharacterized protein

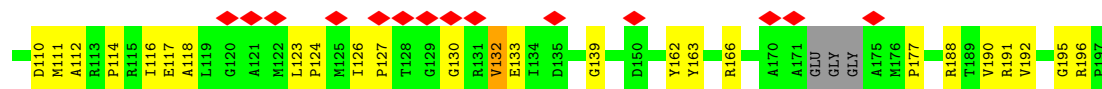
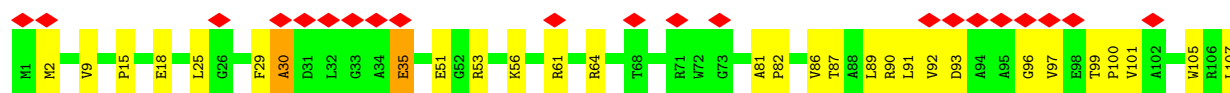
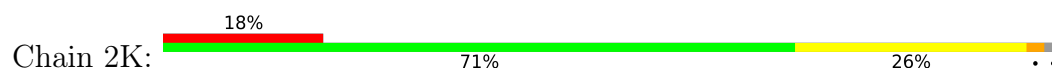


- Molecule 3: Uncharacterized protein

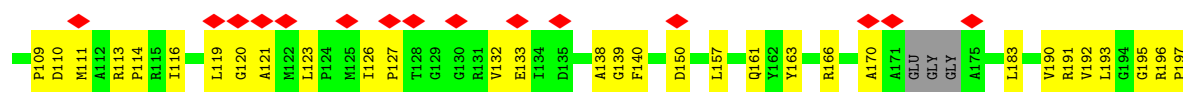
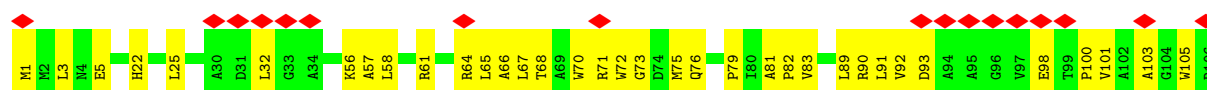




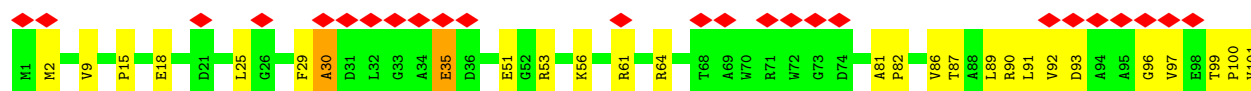
• Molecule 4: Uncharacterized protein



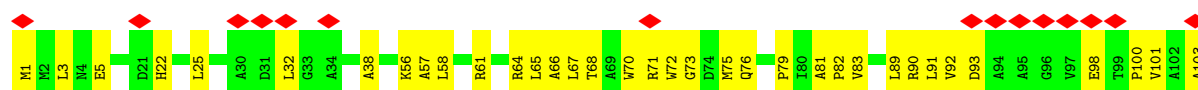
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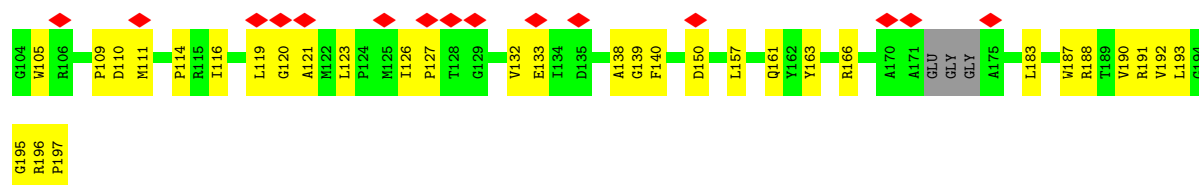


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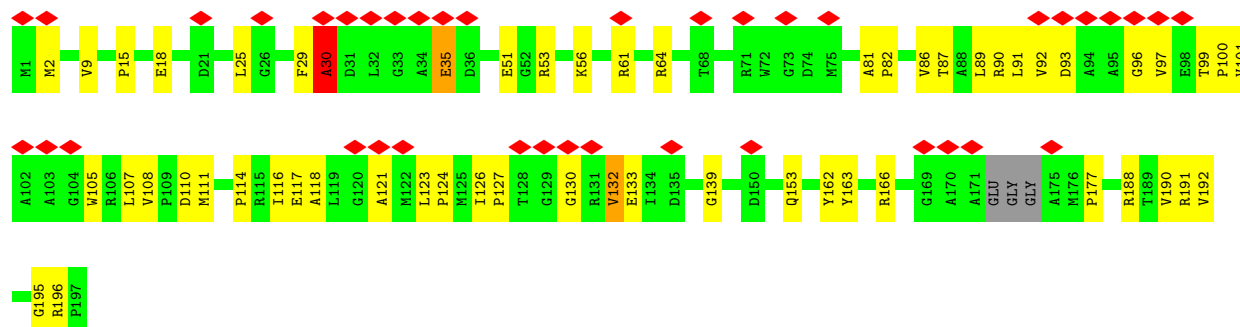


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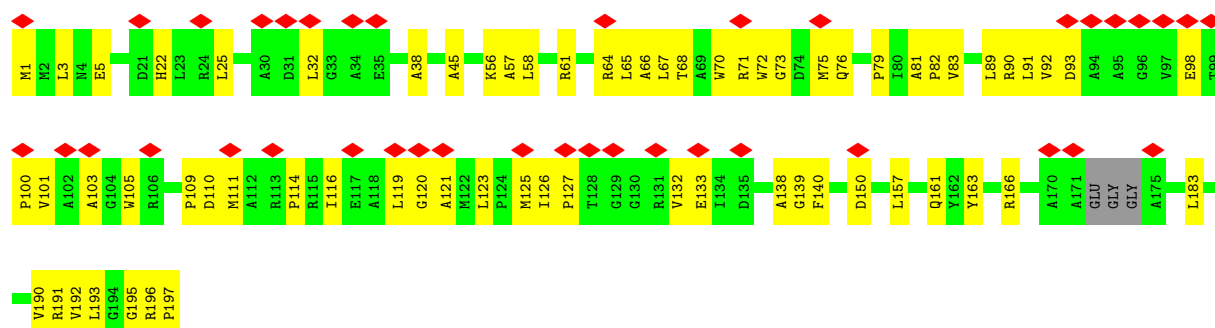




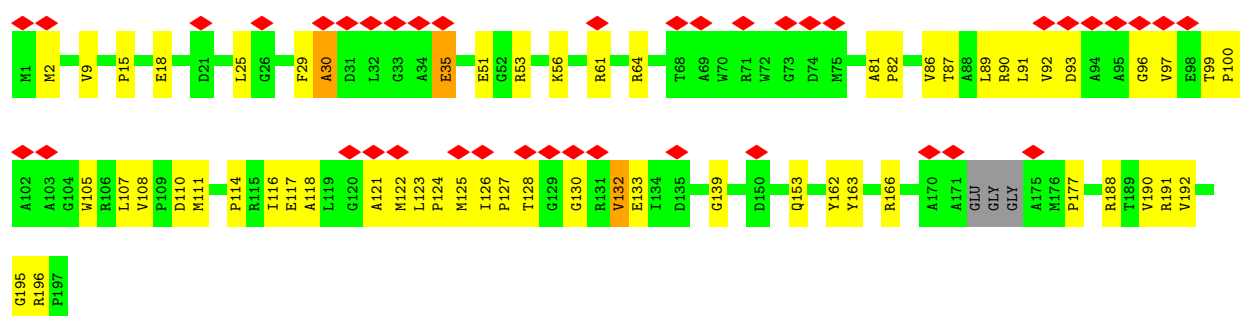
- Molecule 4: Uncharacterized protein



- Molecule 4: Uncharacterized protein



- Molecule 4: Uncharacterized protein



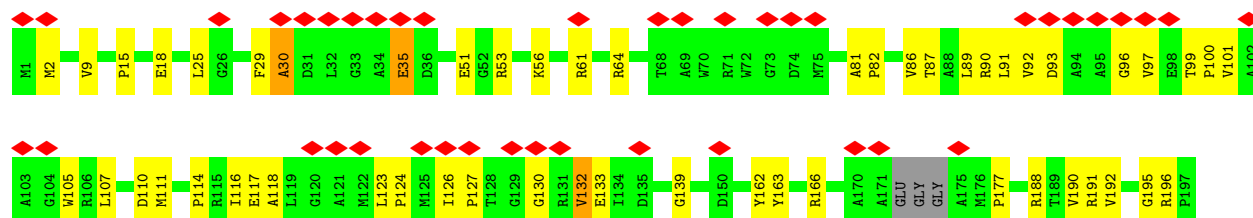
- Molecule 4: Uncharacterized protein

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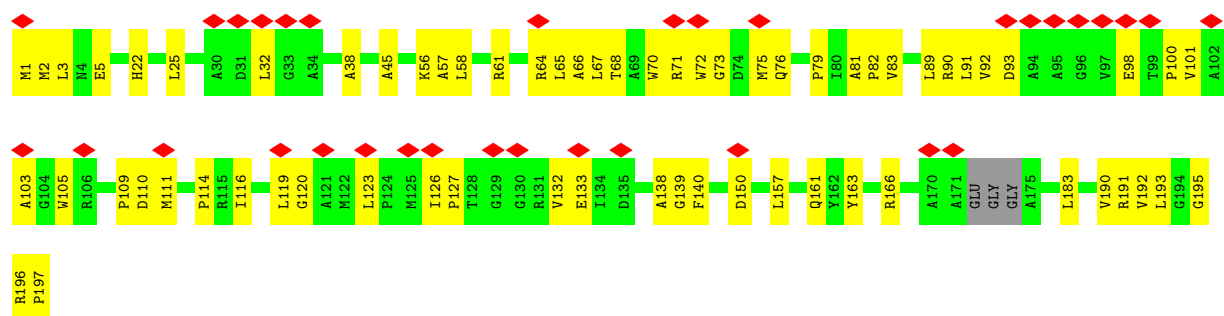
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Chain 2C: 



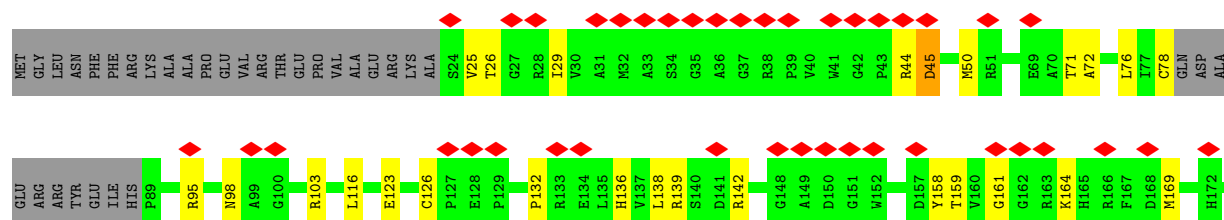
• Molecule 4: Uncharacterized protein

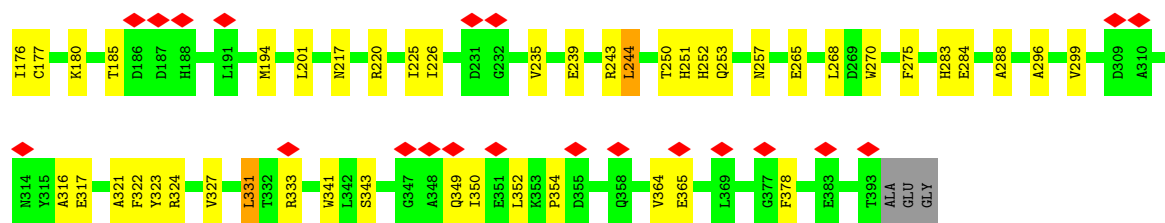
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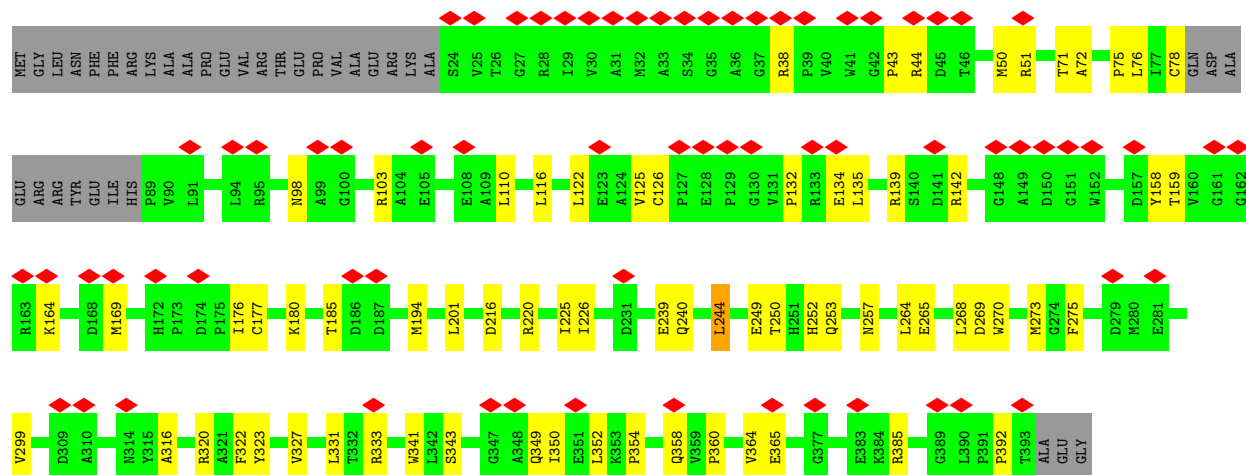
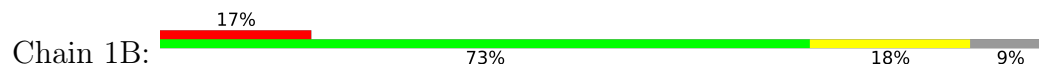
• Molecule 5: Portal protein Rcc01684

Chain 1A: 

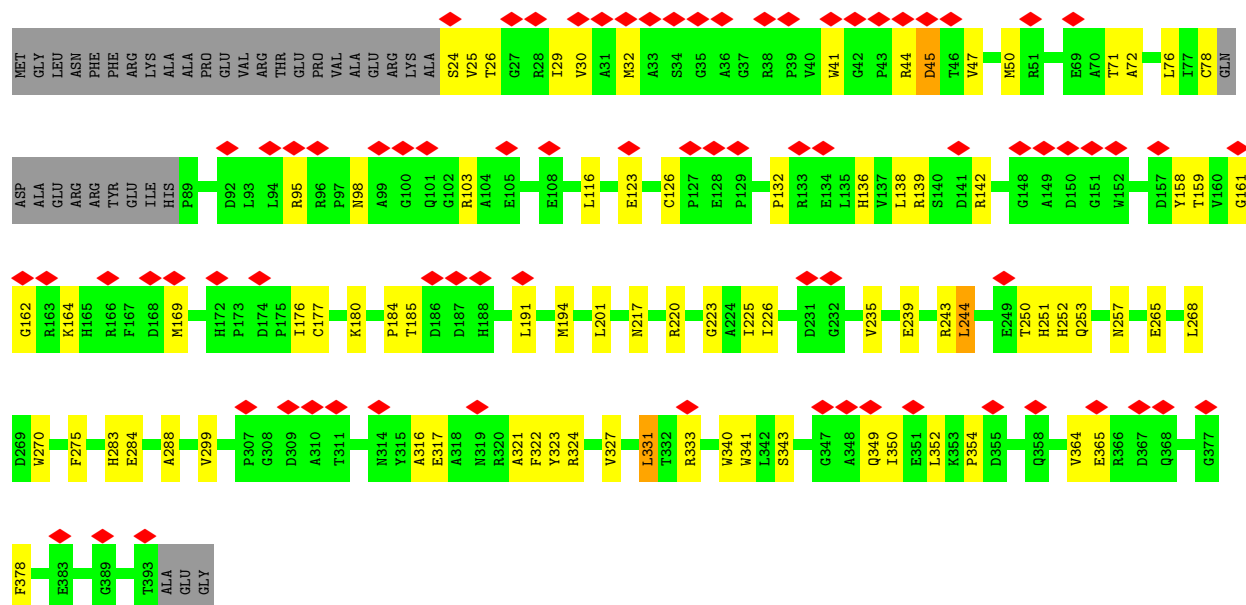




• Molecule 5: Portal protein Rcc01684

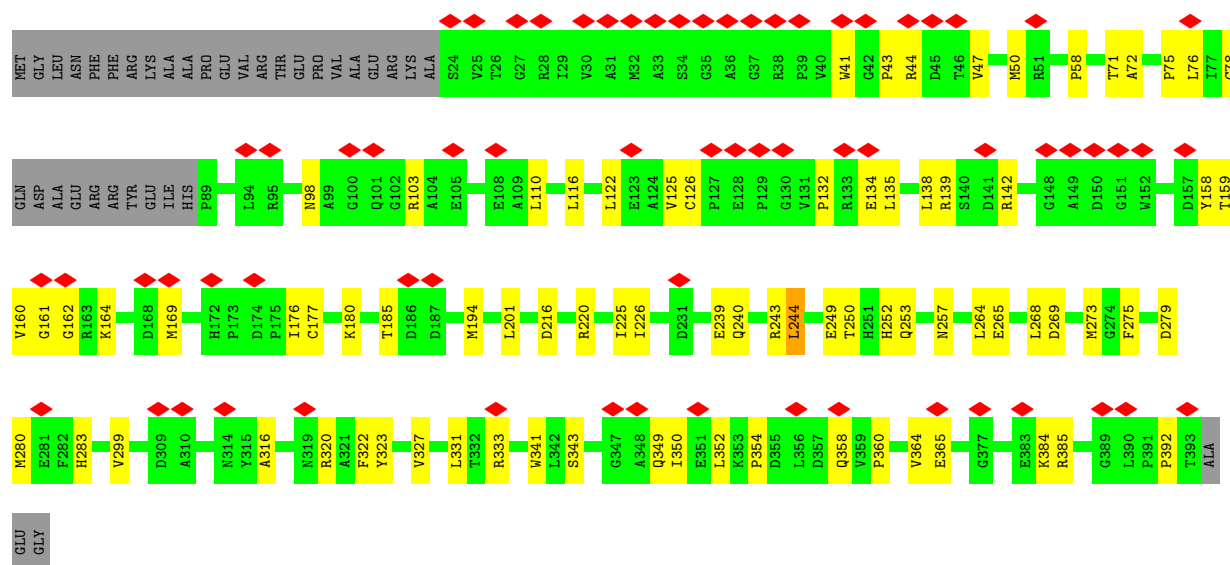


• Molecule 5: Portal protein Rcc01684



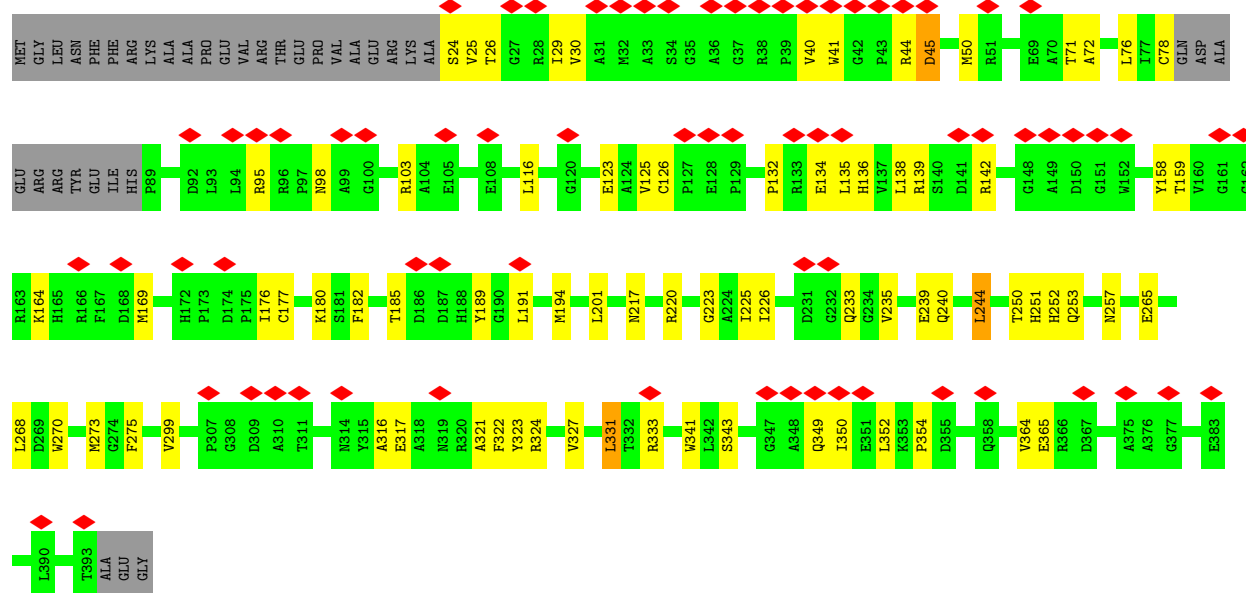
• Molecule 5: Portal protein Rcc01684

Chain 1L: 17% 71% 20% 9%



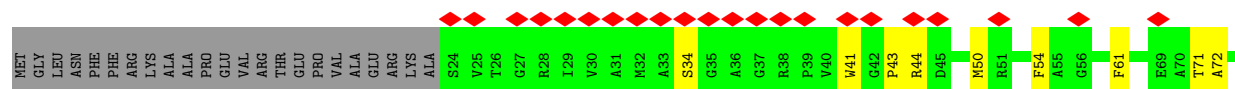
• Molecule 5: Portal protein Rcc01684

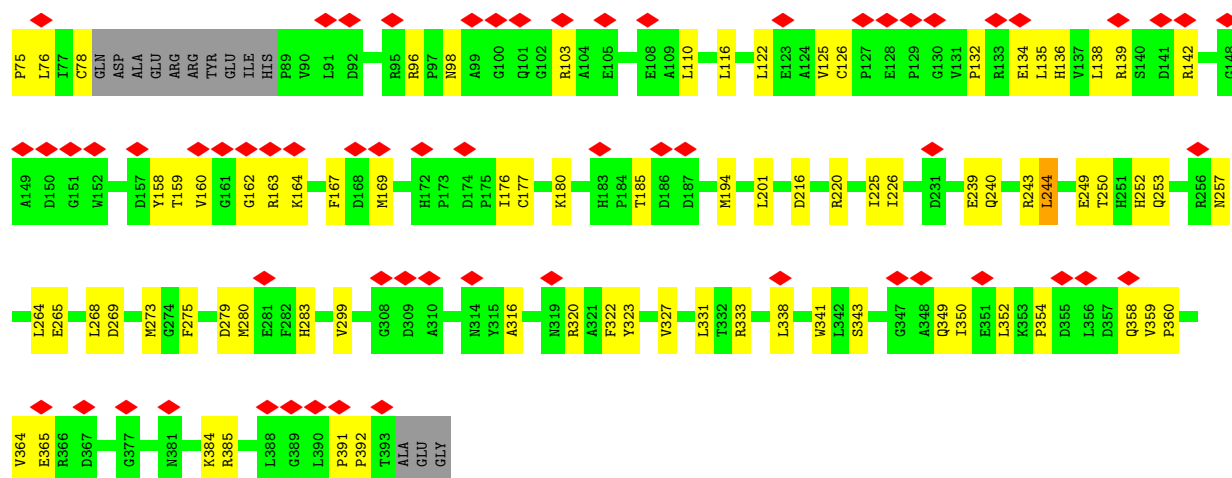
Chain 1I: 18% 71% 19% 9%



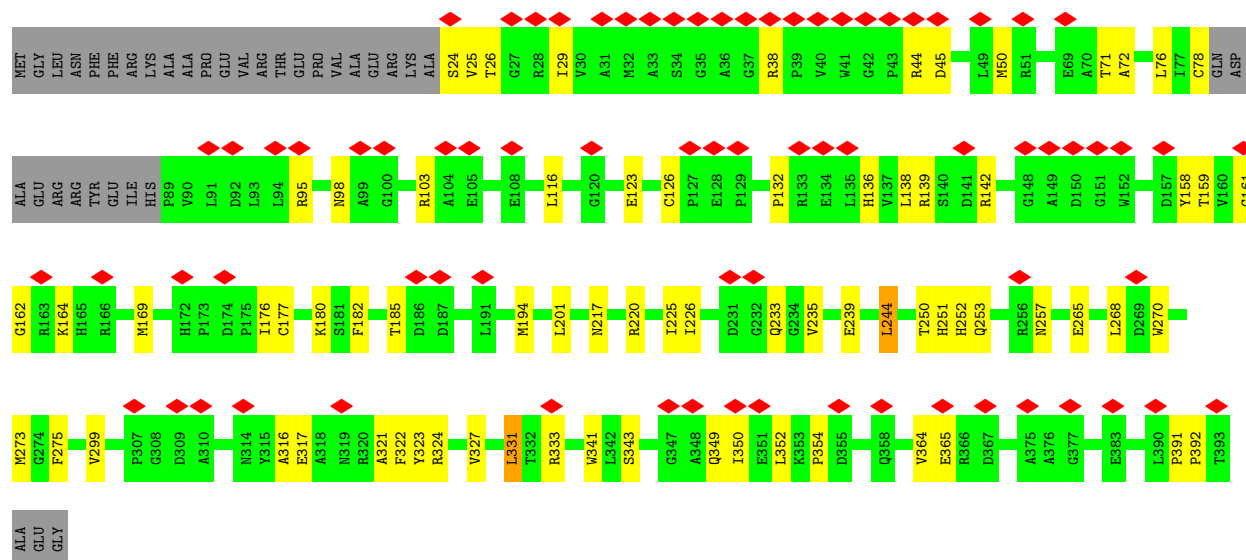
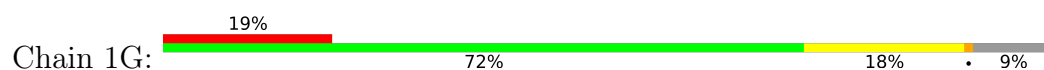
• Molecule 5: Portal protein Rcc01684

Chain 1J: 21% 69% 22% 9%



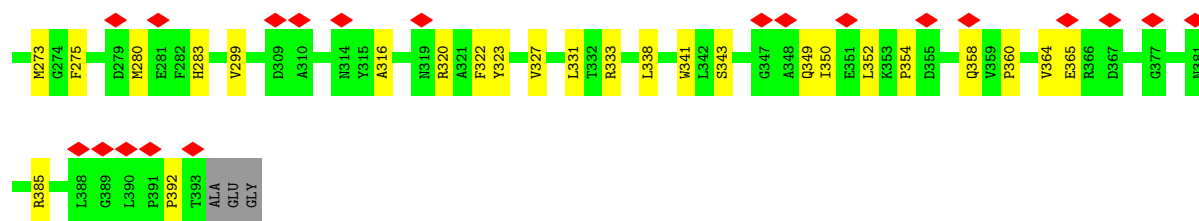


• Molecule 5: Portal protein Rcc01684

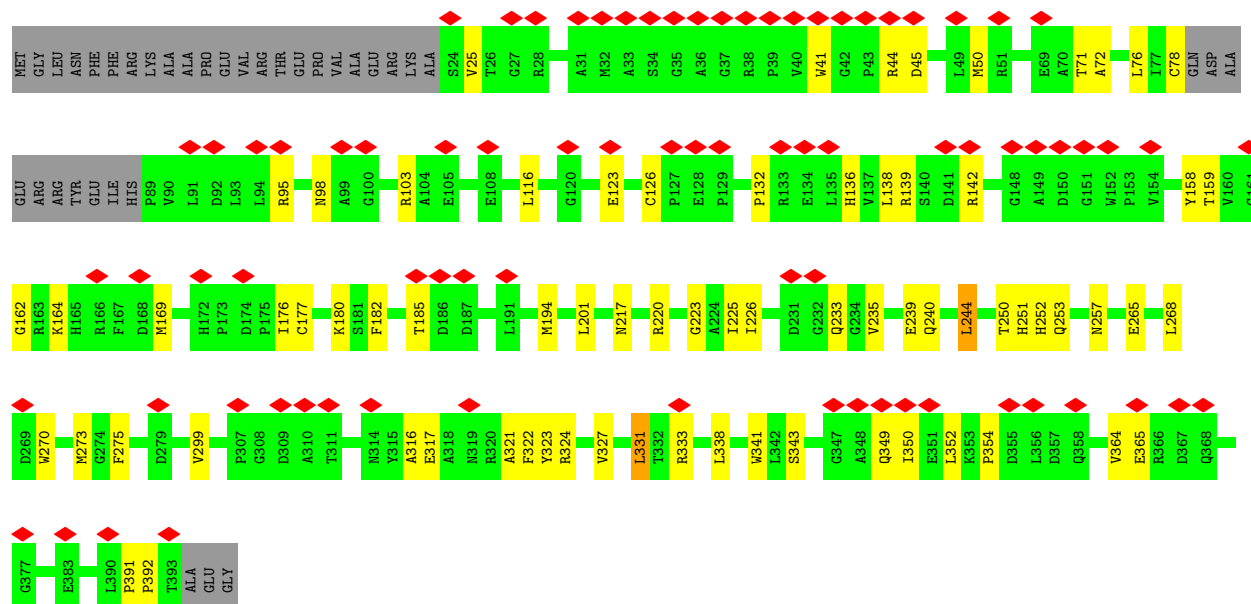
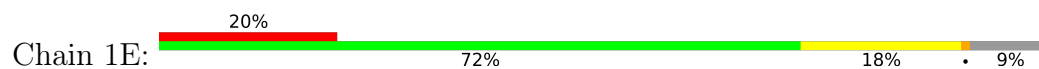


• Molecule 5: Portal protein Rcc01684

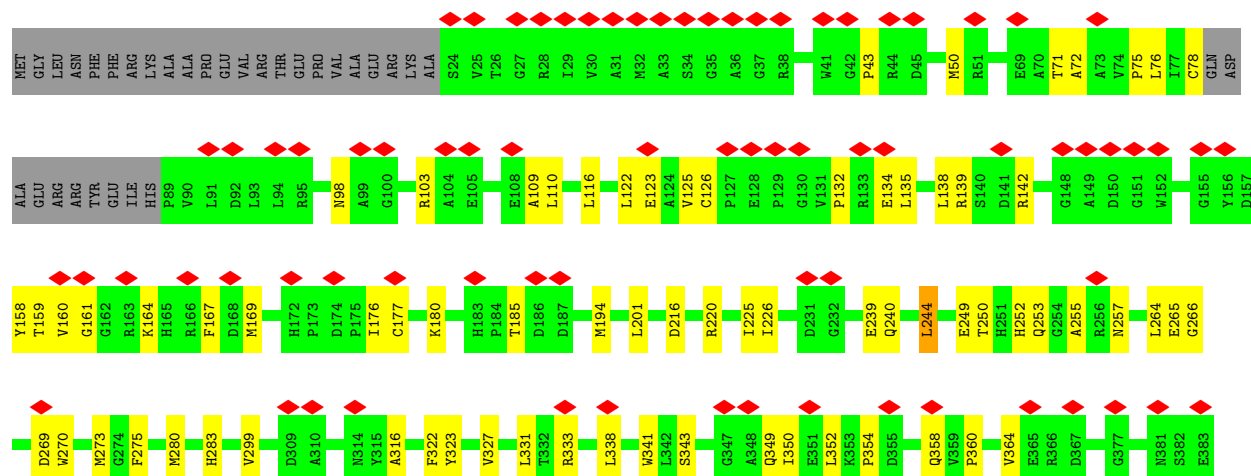
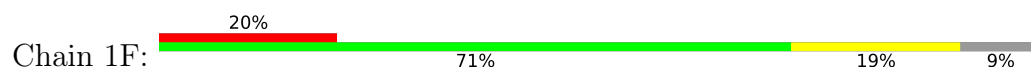


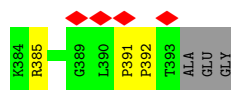


• Molecule 5: Portal protein Rcc01684

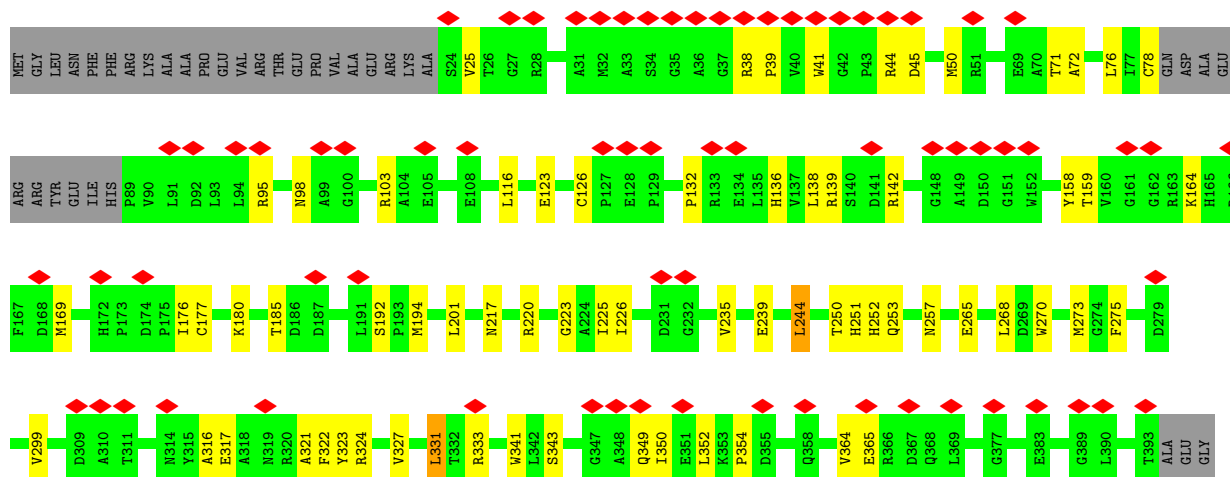
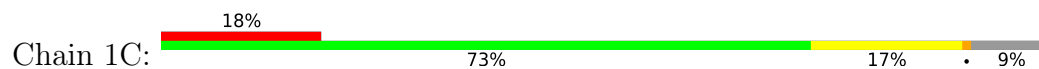


• Molecule 5: Portal protein Rcc01684

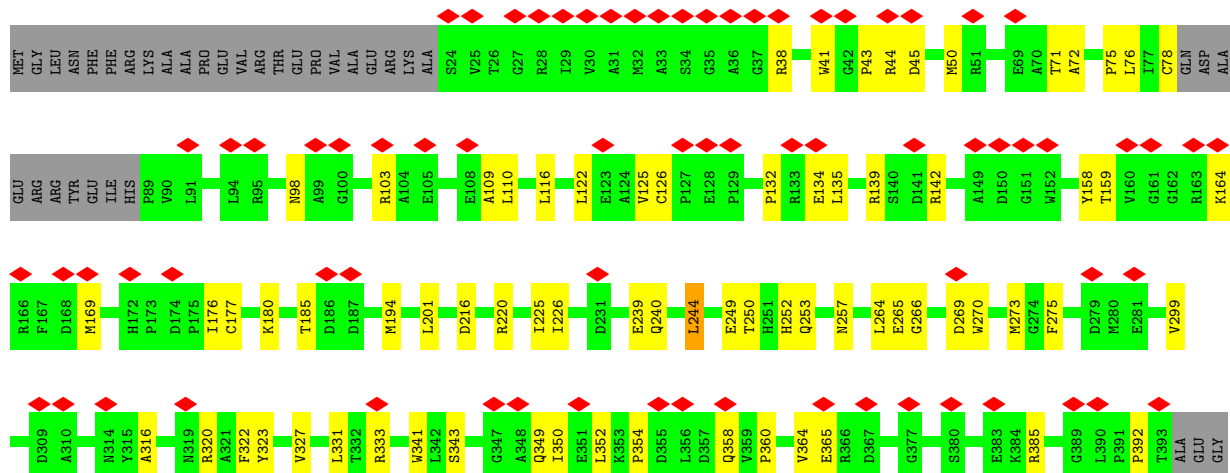
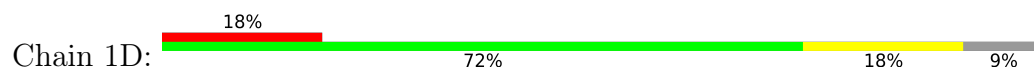




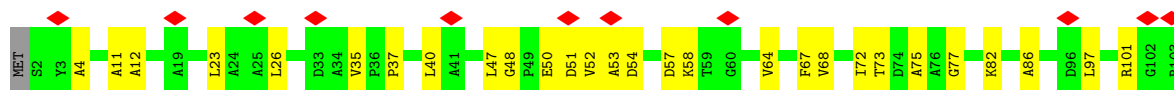
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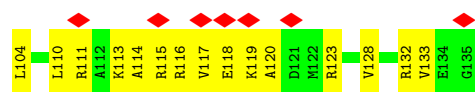


• Molecule 5: Portal protein Rcc01684

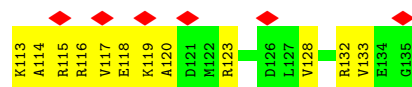
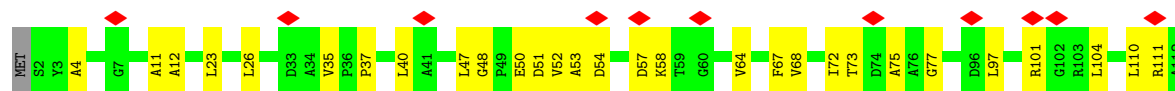


• Molecule 6: Uncharacterized protein

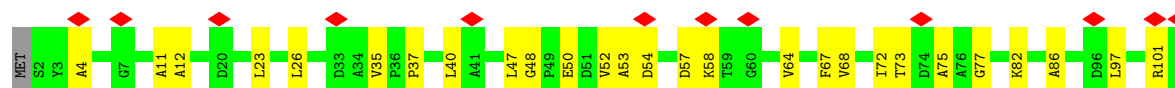




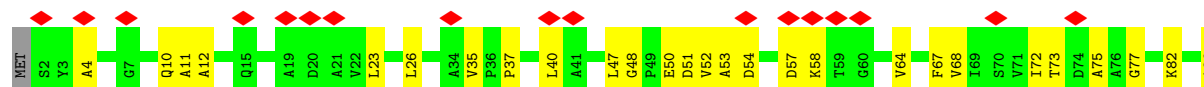
- Molecule 6: Uncharacterized protein



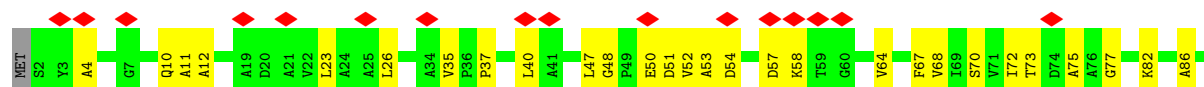
- Molecule 6: Uncharacterized protein



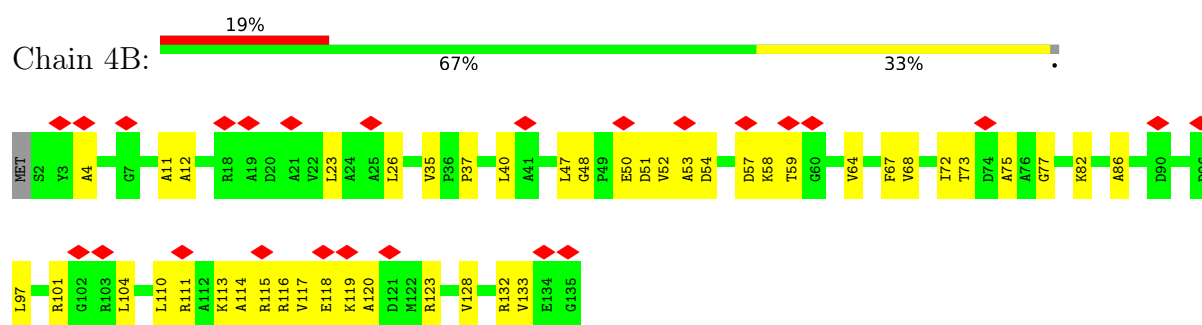
- Molecule 6: Uncharacterized protein



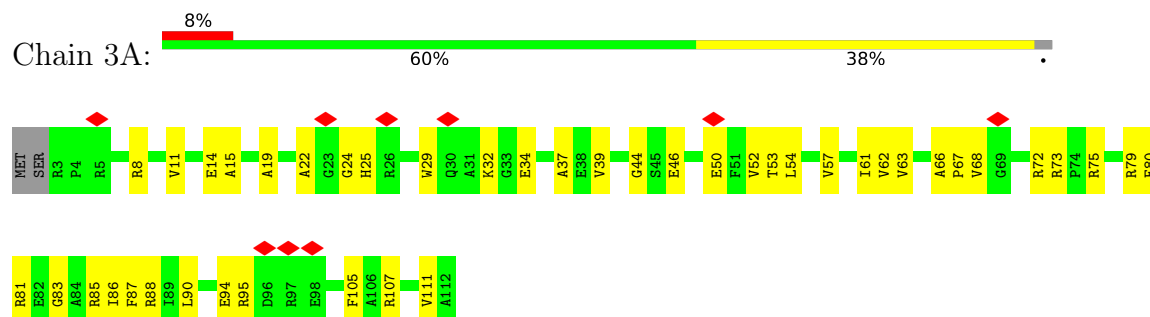
- Molecule 6: Uncharacterized protein



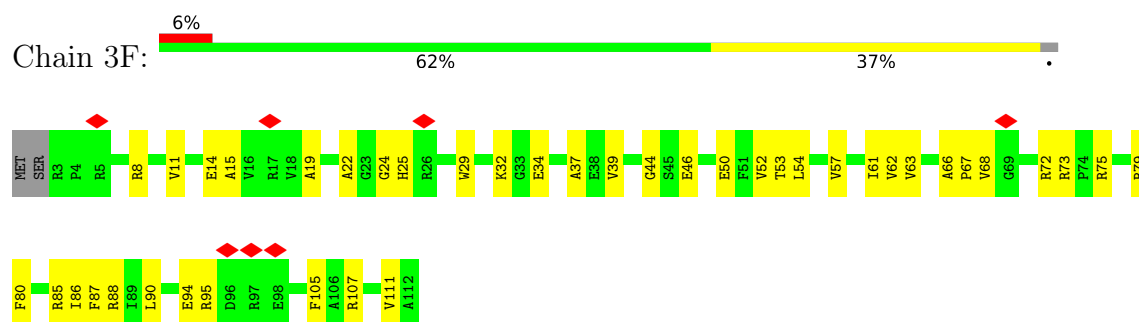
- Molecule 6: Uncharacterized protein



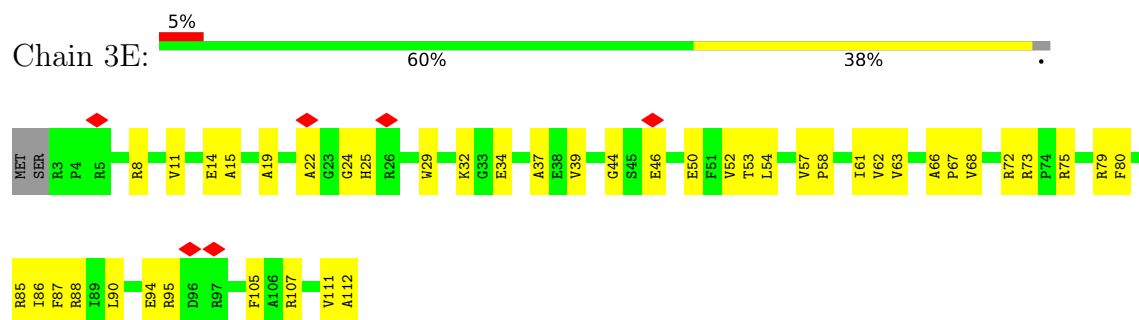
- Molecule 7: Uncharacterized protein



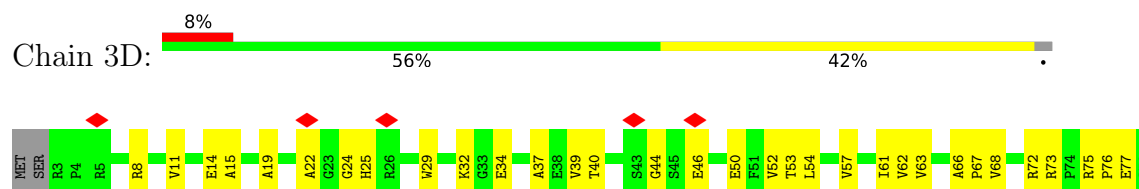
- Molecule 7: Uncharacterized protein

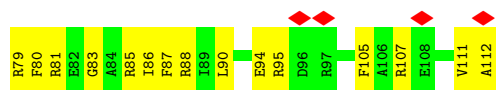


- Molecule 7: Uncharacterized protein

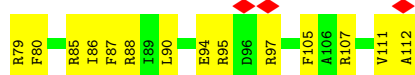


- Molecule 7: Uncharacterized protein





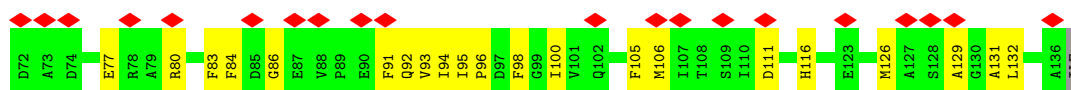
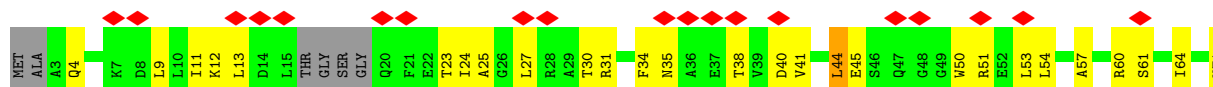
- Molecule 7: Uncharacterized protein



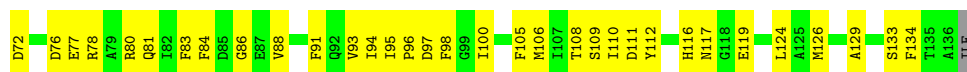
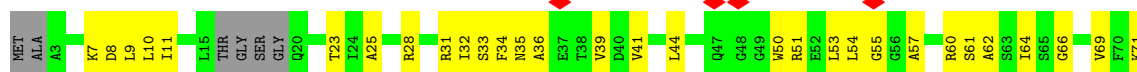
- Molecule 7: Uncharacterized protein



- Molecule 8: Phage major tail protein, TP901-1 family

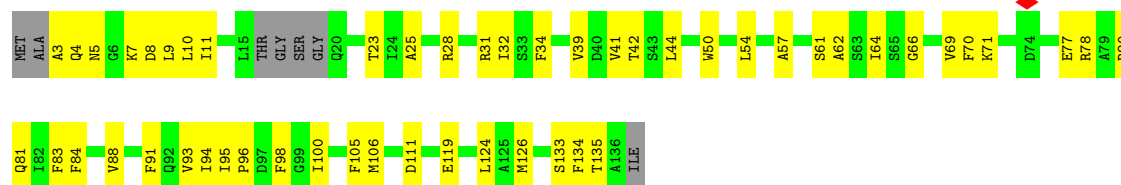


- Molecule 8: Phage major tail protein, TP901-1 family



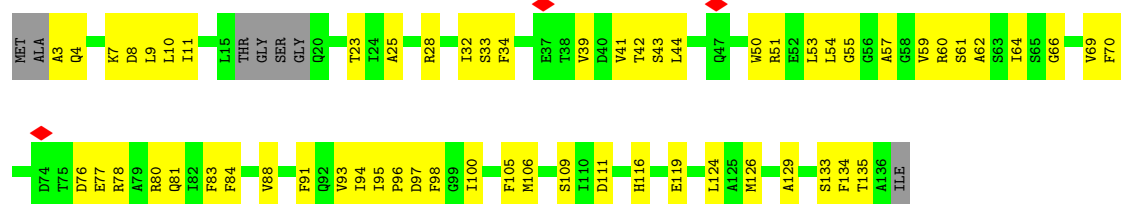
- Molecule 8: Phage major tail protein, TP901-1 family

Chain 5G: 



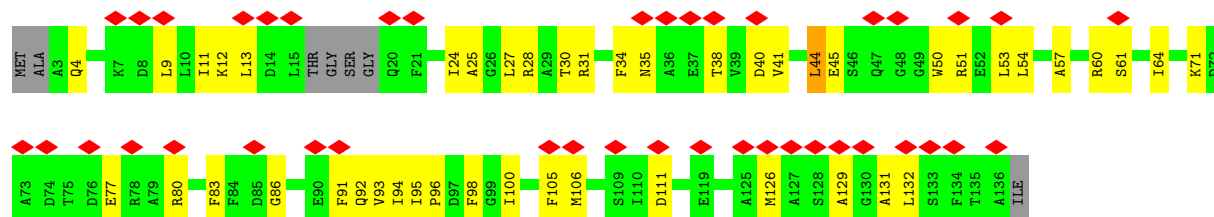
- Molecule 8: Phage major tail protein, TP901-1 family

Chain 5M: 



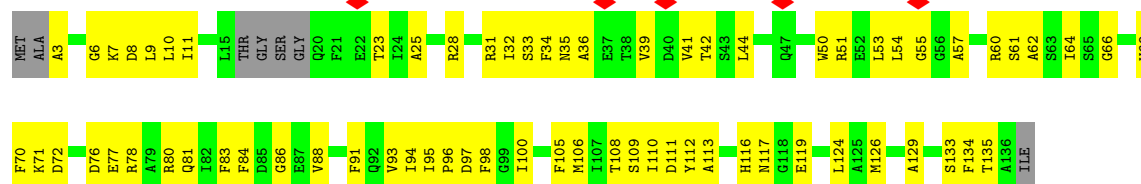
- Molecule 8: Phage major tail protein, TP901-1 family

Chain 5F: 



- Molecule 8: Phage major tail protein, TP901-1 family

Chain 5X: 



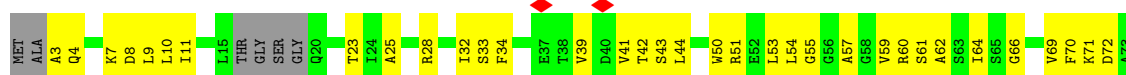
- Molecule 8: Phage major tail protein, TP901-1 family

Chain 5L: 

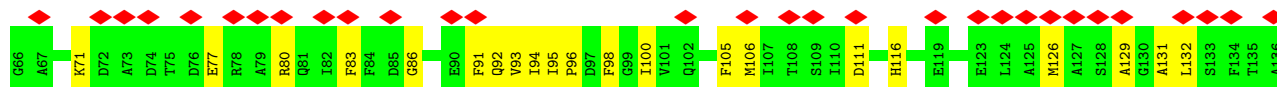
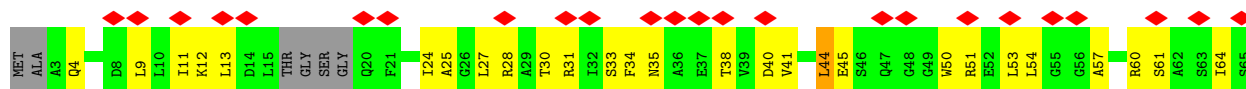
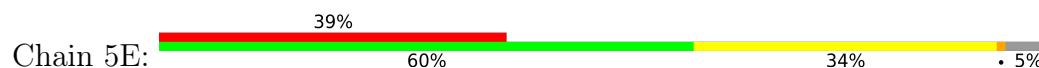




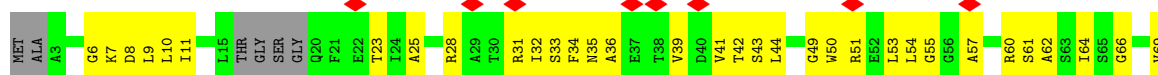
- Molecule 8: Phage major tail protein, TP901-1 family



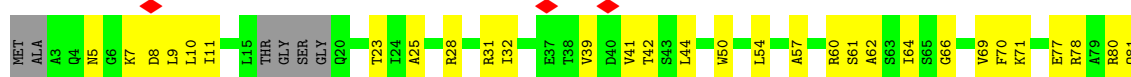
- Molecule 8: Phage major tail protein, TP901-1 family



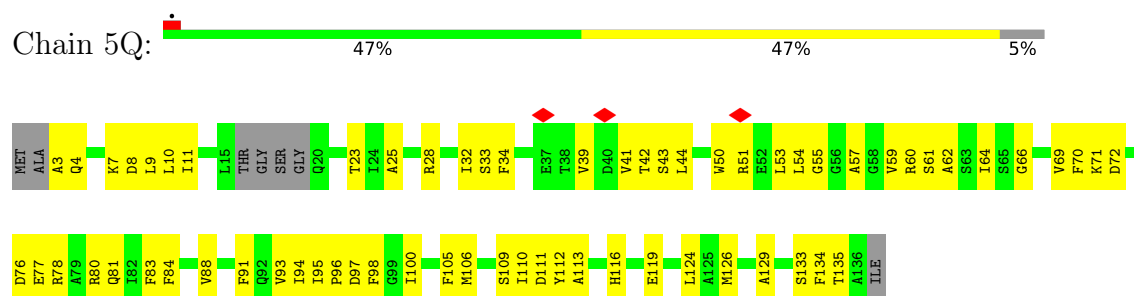
- Molecule 8: Phage major tail protein, TP901-1 family



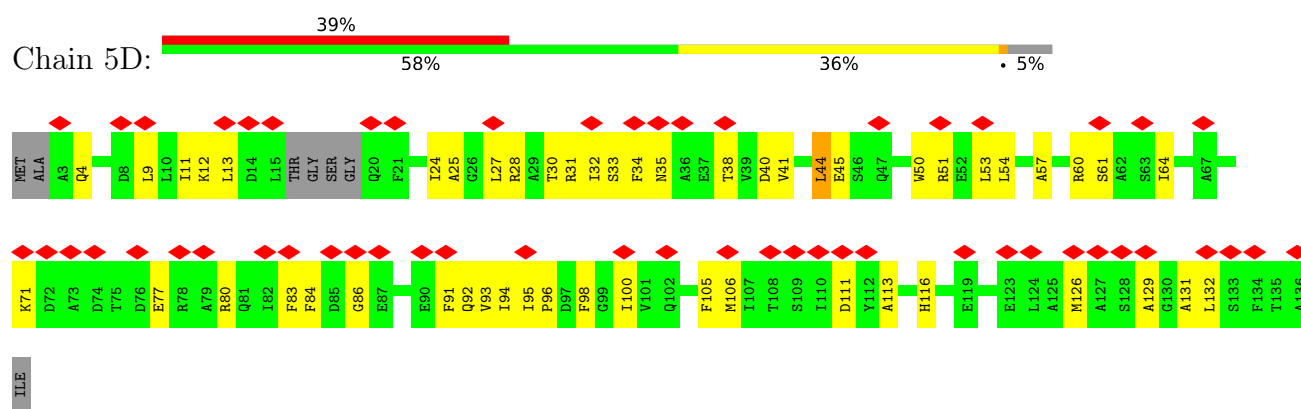
- Molecule 8: Phage major tail protein, TP901-1 family



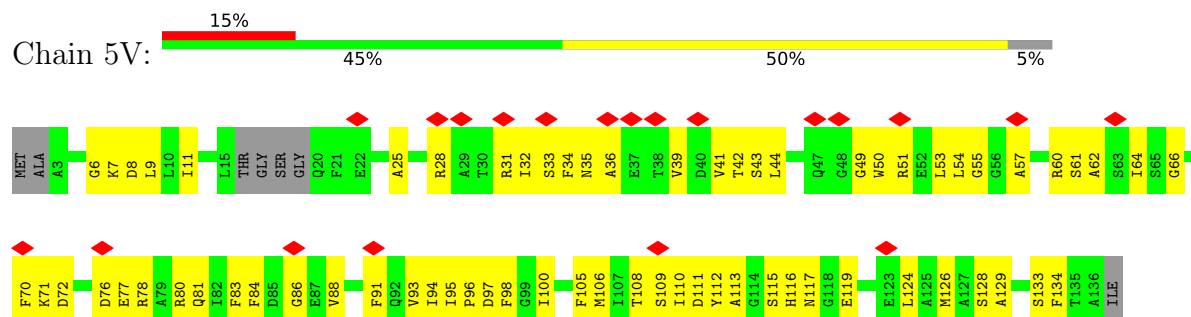
- Molecule 8: Phage major tail protein, TP901-1 family



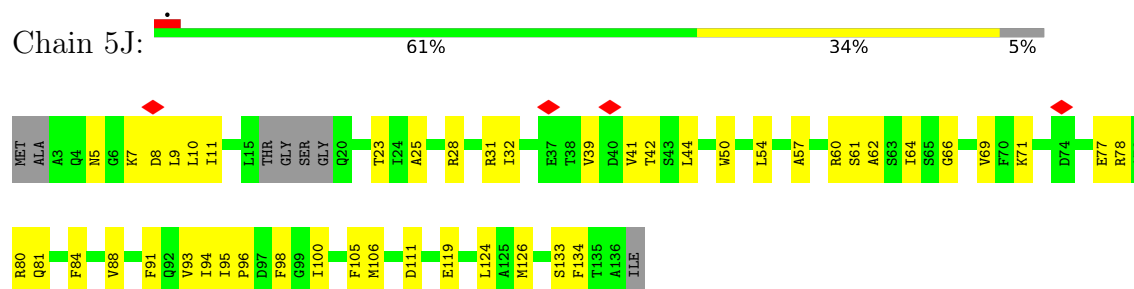
- Molecule 8: Phage major tail protein, TP901-1 family



- Molecule 8: Phage major tail protein, TP901-1 family

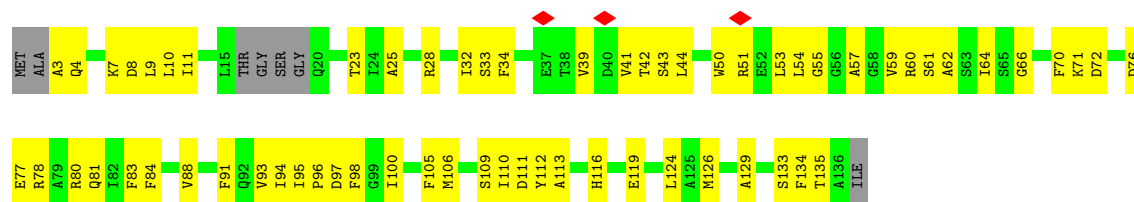


- Molecule 8: Phage major tail protein, TP901-1 family

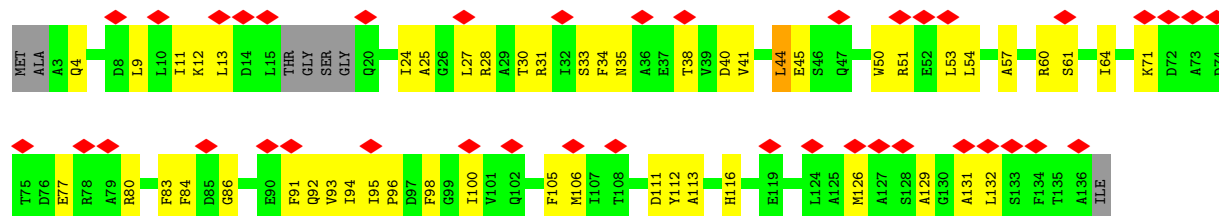


- Molecule 8: Phage major tail protein, TP901-1 family

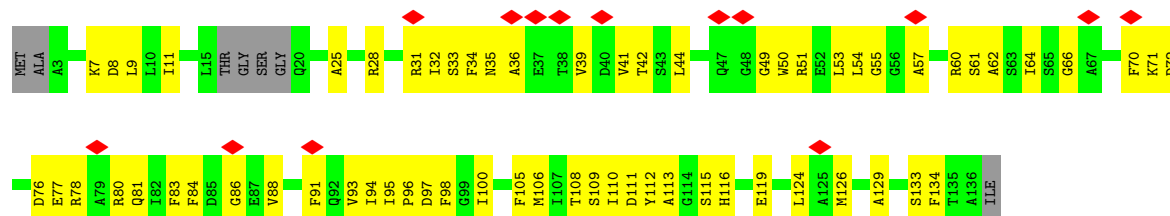




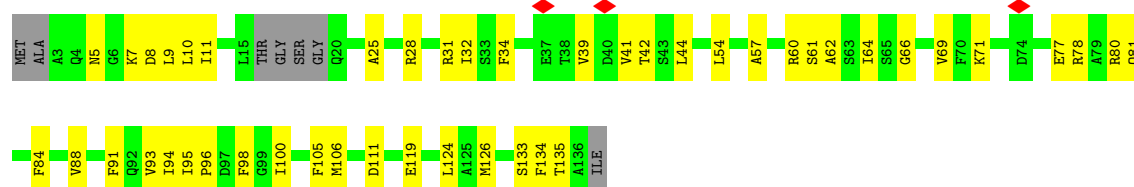
- Molecule 8: Phage major tail protein, TP901-1 family



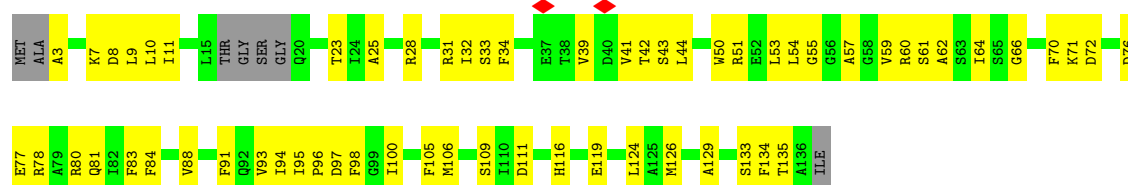
- Molecule 8: Phage major tail protein, TP901-1 family



- Molecule 8: Phage major tail protein, TP901-1 family



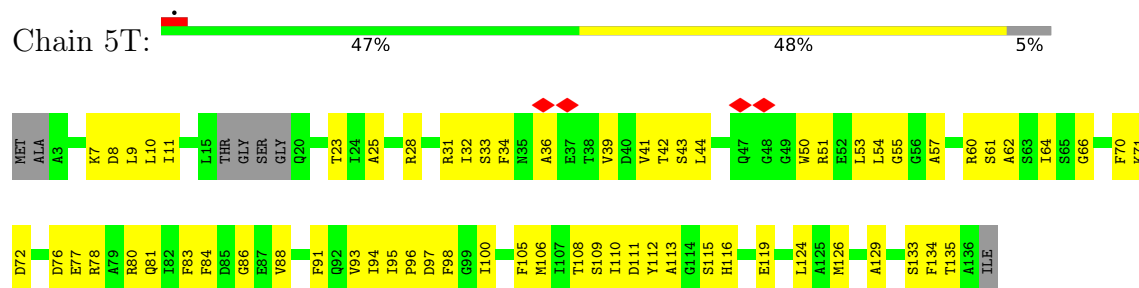
- Molecule 8: Phage major tail protein, TP901-1 family



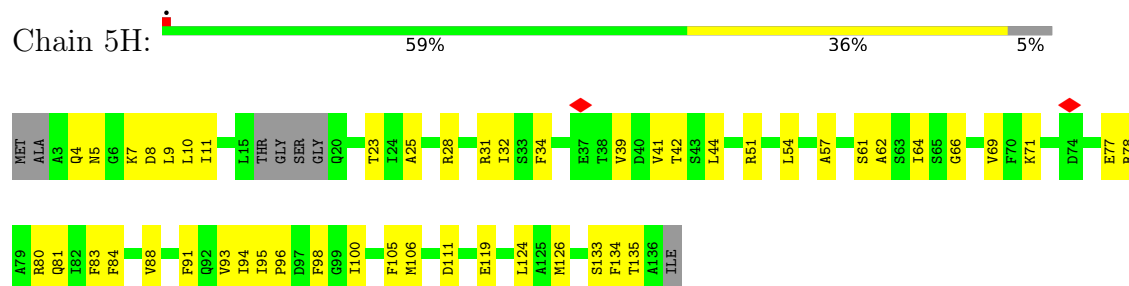
- Molecule 8: Phage major tail protein, TP901-1 family



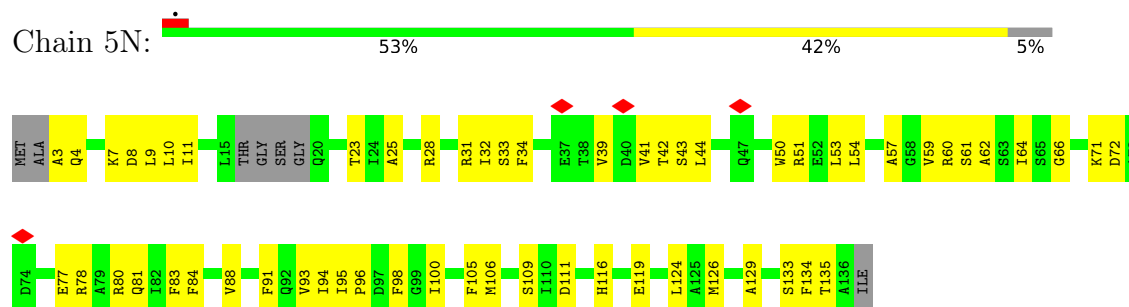
- Molecule 8: Phage major tail protein, TP901-1 family



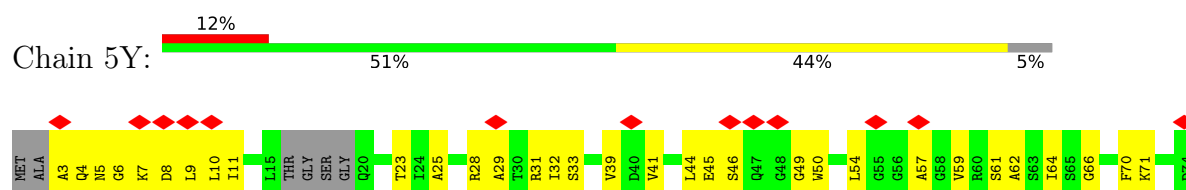
- Molecule 8: Phage major tail protein, TP901-1 family



- Molecule 8: Phage major tail protein, TP901-1 family

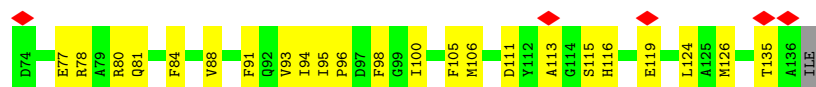
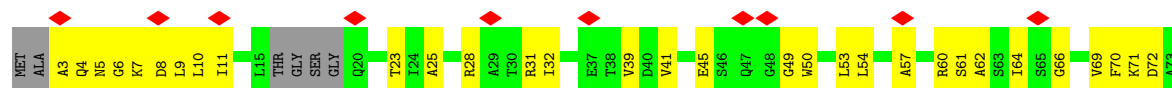


- Molecule 8: Phage major tail protein, TP901-1 family

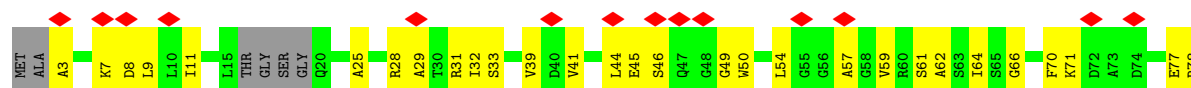




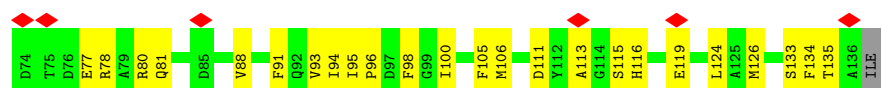
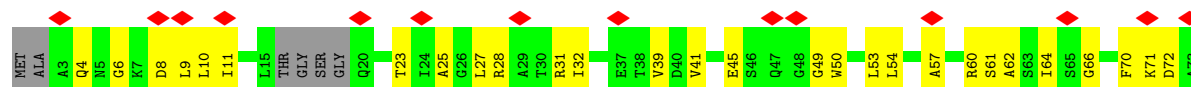
- Molecule 8: Phage major tail protein, TP901-1 family



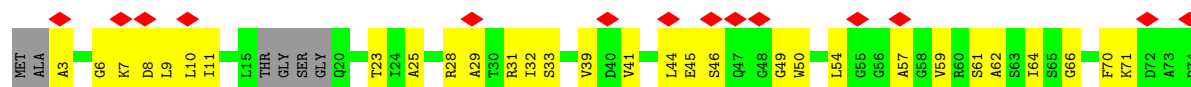
- Molecule 8: Phage major tail protein, TP901-1 family



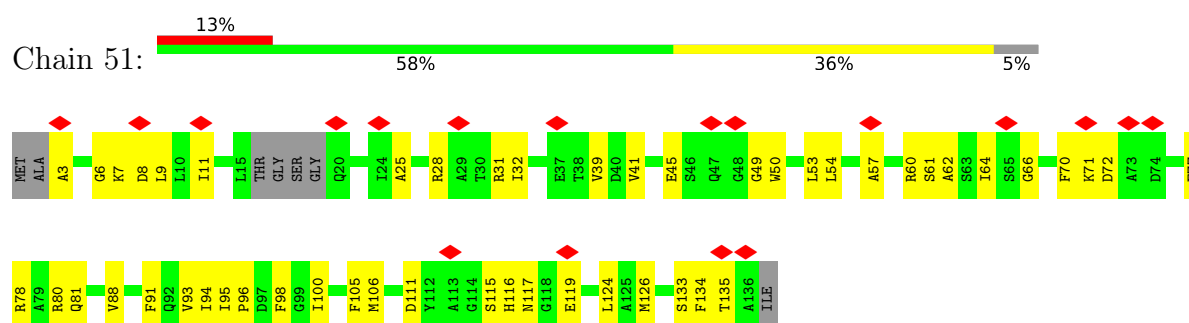
- Molecule 8: Phage major tail protein, TP901-1 family



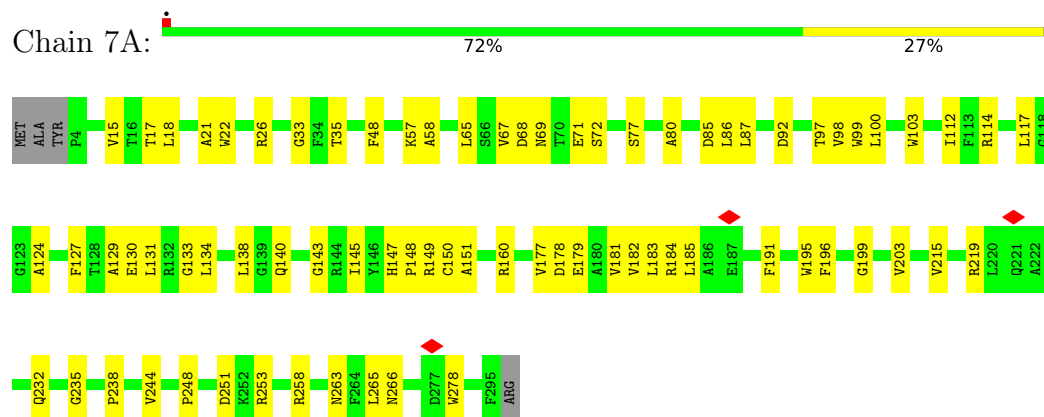
- Molecule 8: Phage major tail protein, TP901-1 family



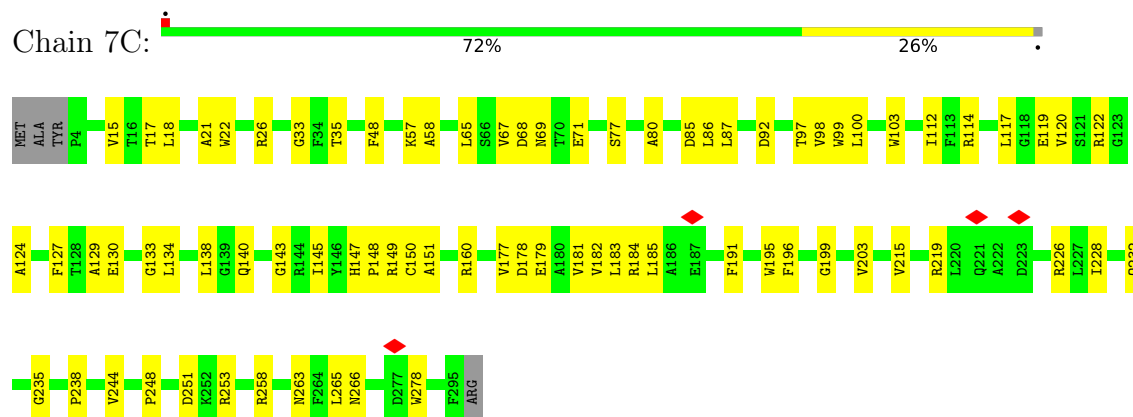
- Molecule 8: Phage major tail protein, TP901-1 family



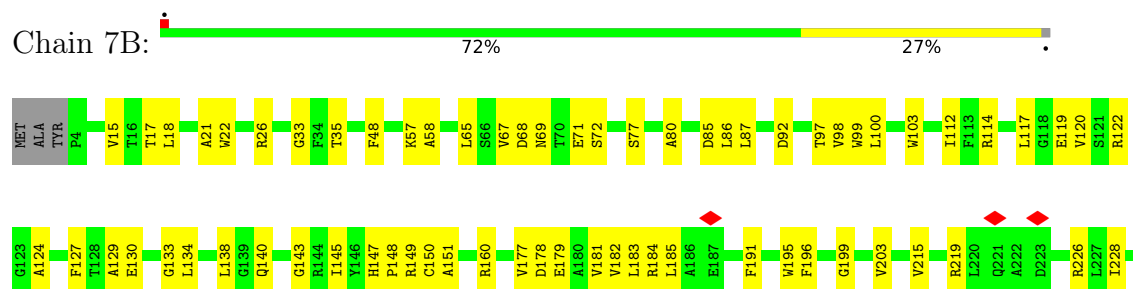
• Molecule 9: Uncharacterized protein

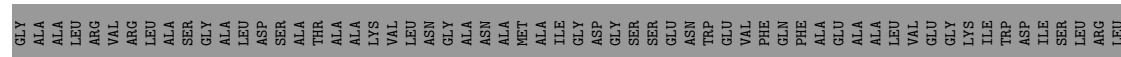


• Molecule 9: Uncharacterized protein



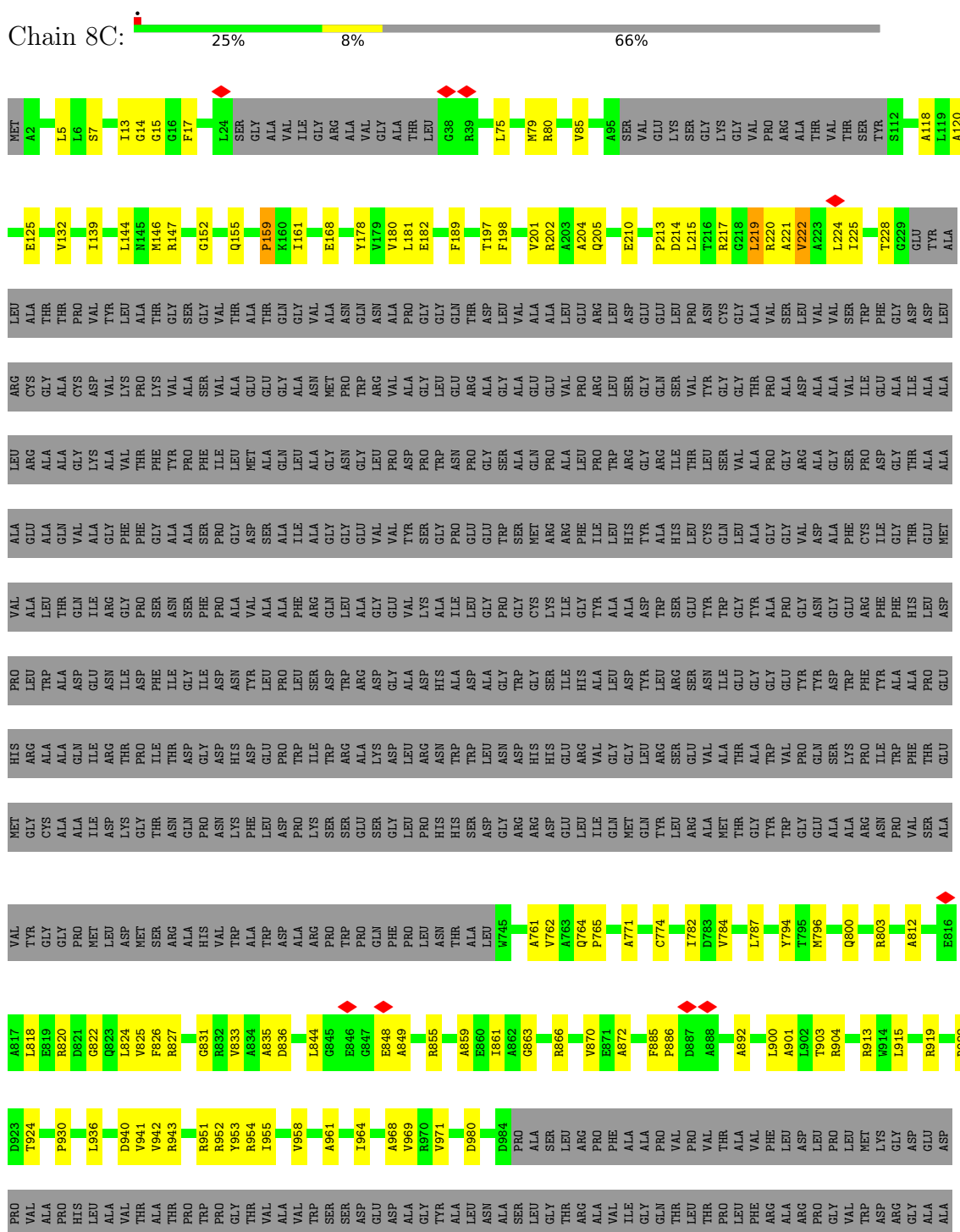
• Molecule 9: Uncharacterized protein





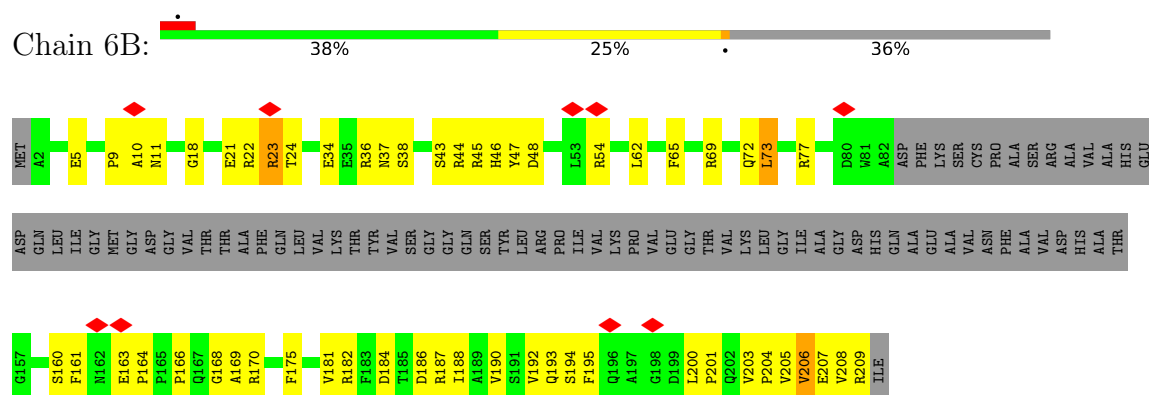
GLU GLY THR THR ALA VAL LYS ARG GLU GLU VAL VAL VAL GLY GLU GLU ALA ALA ALA ASP GLY ILE ALA ALA GLY ALA PHE THR THR LEU LEU GLU VAL VAL ALA ALA GLN VAL VAL ASP SER ASP VAL THR TYR GLY GLY GLY LEU ALA ALA ARG ILE THR THR VAL GLY ALA

- Molecule 10: Uncharacterized protein

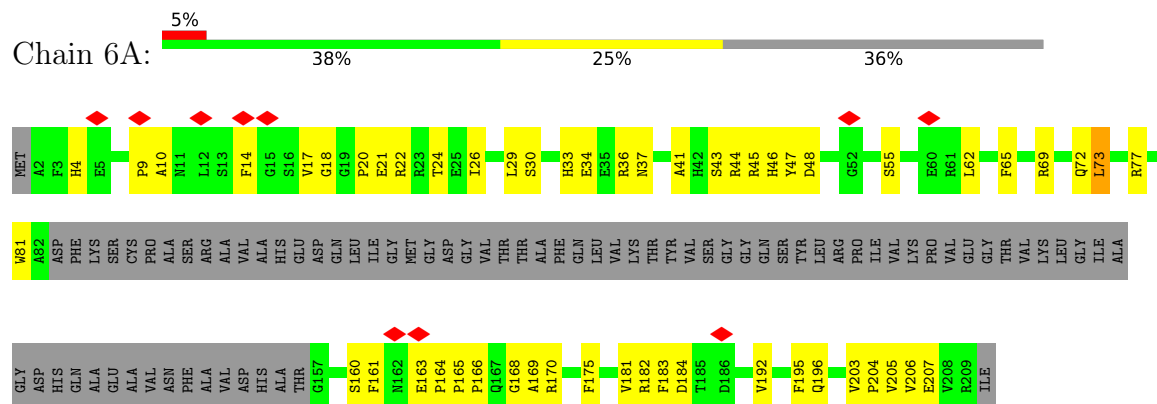




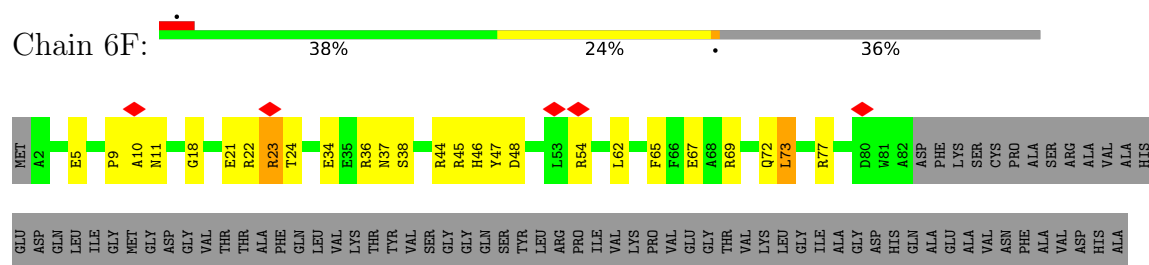
- Molecule 11: Uncharacterized protein



- Molecule 11: Uncharacterized protein

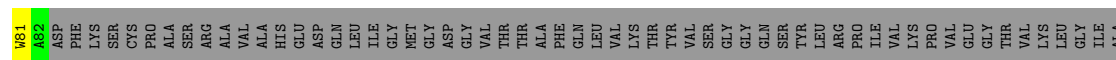
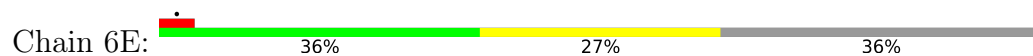


- Molecule 11: Uncharacterized protein

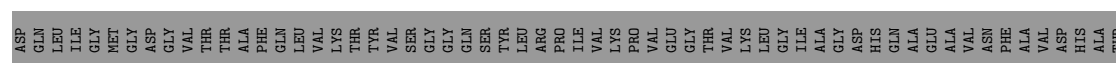




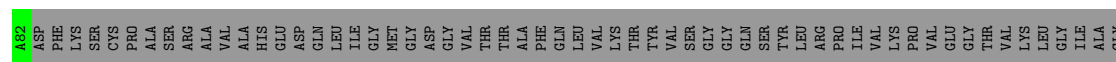
- Molecule 11: Uncharacterized protein



- Molecule 11: Uncharacterized protein



- Molecule 11: Uncharacterized protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27724	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 ($e^-/\text{\AA}^2$)	42.75	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	37.206	Depositor
Minimum map value	0.000	Depositor
Average map value	0.034	Depositor
Map value standard deviation	0.417	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	1020.48, 1020.48, 1020.48	wwPDB
Map dimensions	960, 960, 960	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.063, 1.063, 1.063	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4

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	A4	0.41	0/2216	0.67	0/3012
1	A5	0.32	0/2243	0.66	2/3051 (0.1%)
1	A9	0.41	0/2216	0.67	0/3012
1	AA	0.32	0/2249	0.66	2/3059 (0.1%)
1	AE	0.41	0/2216	0.67	0/3012
1	AF	0.32	0/2253	0.65	2/3064 (0.1%)
1	AJ	0.41	0/2216	0.67	0/3012
1	AK	0.32	0/2253	0.65	2/3064 (0.1%)
1	AO	0.41	0/2216	0.67	0/3012
1	AP	0.32	0/2245	0.66	2/3054 (0.1%)
1	B4	0.38	0/2253	0.68	0/3064
1	B5	0.44	0/2049	0.75	7/2785 (0.3%)
1	B9	0.38	0/2253	0.68	0/3064
1	BA	0.44	0/2055	0.75	7/2793 (0.3%)
1	BE	0.38	0/2253	0.68	0/3064
1	BF	0.44	0/2056	0.75	7/2793 (0.3%)
1	BJ	0.38	0/2253	0.68	0/3064
1	BK	0.44	0/2049	0.75	7/2785 (0.3%)
1	BO	0.38	0/2253	0.68	0/3064
1	BP	0.44	0/2050	0.75	7/2786 (0.3%)
1	C4	0.38	0/2253	0.65	0/3064
1	C5	0.35	0/2253	0.68	1/3064 (0.0%)
1	C9	0.38	0/2253	0.65	0/3064
1	CA	0.35	0/2253	0.68	1/3064 (0.0%)
1	CE	0.38	0/2253	0.65	0/3064
1	CF	0.35	0/2253	0.68	1/3064 (0.0%)
1	CJ	0.38	0/2253	0.65	0/3064
1	CK	0.35	0/2253	0.68	1/3064 (0.0%)
1	CO	0.38	0/2253	0.65	0/3064
1	CP	0.35	0/2253	0.68	1/3064 (0.0%)
1	D4	0.39	0/2253	0.70	0/3064
1	D9	0.39	0/2253	0.70	0/3064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	DE	0.39	0/2253	0.70	0/3064
1	DJ	0.39	0/2253	0.70	0/3064
1	DO	0.39	0/2253	0.70	0/3064
1	E4	0.39	0/2253	0.68	0/3064
1	E9	0.39	0/2253	0.68	0/3064
1	EE	0.39	0/2253	0.68	0/3064
1	EJ	0.39	0/2253	0.68	0/3064
1	EO	0.39	0/2253	0.68	0/3064
1	F4	0.39	0/2253	0.69	1/3064 (0.0%)
1	F9	0.39	0/2253	0.69	1/3064 (0.0%)
1	FE	0.40	0/2253	0.69	1/3064 (0.0%)
1	FJ	0.39	0/2253	0.69	1/3064 (0.0%)
1	FO	0.39	0/2253	0.69	1/3064 (0.0%)
1	G4	0.40	0/2253	0.70	2/3064 (0.1%)
1	G9	0.40	0/2253	0.70	2/3064 (0.1%)
1	GE	0.40	0/2253	0.70	2/3064 (0.1%)
1	GJ	0.40	0/2253	0.70	2/3064 (0.1%)
1	GO	0.40	0/2253	0.70	2/3064 (0.1%)
1	H4	0.39	0/2216	0.66	0/3012
1	H9	0.39	0/2216	0.66	0/3012
1	HE	0.39	0/2216	0.66	0/3012
1	HJ	0.39	0/2216	0.66	0/3012
1	HO	0.39	0/2216	0.66	0/3012
1	I4	0.38	0/2216	0.67	0/3012
1	I9	0.38	0/2216	0.67	0/3012
1	IE	0.38	0/2216	0.67	0/3012
1	IJ	0.38	0/2216	0.67	0/3012
1	IO	0.38	0/2216	0.67	0/3012
1	J4	0.39	0/2216	0.67	0/3012
1	J9	0.39	0/2216	0.67	0/3012
1	JE	0.40	0/2216	0.67	0/3012
1	JJ	0.39	0/2216	0.67	0/3012
1	JO	0.40	0/2216	0.67	0/3012
1	K4	0.42	1/2216 (0.0%)	0.67	0/3012
1	K9	0.42	1/2216 (0.0%)	0.67	0/3012
1	KE	0.42	1/2216 (0.0%)	0.67	0/3012
1	KJ	0.42	1/2216 (0.0%)	0.67	0/3012
1	KO	0.42	1/2216 (0.0%)	0.67	0/3012
1	L4	0.40	0/2216	0.69	1/3012 (0.0%)
1	L9	0.41	0/2216	0.69	1/3012 (0.0%)
1	LE	0.41	0/2216	0.69	1/3012 (0.0%)
1	LJ	0.40	0/2216	0.69	1/3012 (0.0%)
1	LO	0.41	0/2216	0.69	1/3012 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	M4	0.37	0/2253	0.72	0/3064
1	M9	0.37	0/2253	0.72	0/3064
1	ME	0.37	0/2253	0.72	0/3064
1	MJ	0.37	0/2253	0.72	0/3064
1	MO	0.37	0/2253	0.72	0/3064
1	N4	0.39	0/2253	0.73	3/3064 (0.1%)
1	N9	0.39	0/2253	0.74	3/3064 (0.1%)
1	NE	0.39	0/2253	0.73	1/3064 (0.0%)
1	NJ	0.39	0/2253	0.74	3/3064 (0.1%)
1	NO	0.39	0/2253	0.74	3/3064 (0.1%)
1	O4	0.37	0/2253	0.72	0/3064
1	O9	0.38	0/2253	0.72	0/3064
1	OE	0.38	0/2253	0.72	0/3064
1	OJ	0.37	0/2253	0.72	0/3064
1	OO	0.37	0/2253	0.72	0/3064
1	P4	0.38	0/2253	0.77	4/3064 (0.1%)
1	P9	0.38	0/2253	0.77	4/3064 (0.1%)
1	PE	0.38	0/2253	0.77	4/3064 (0.1%)
1	PJ	0.38	0/2253	0.77	4/3064 (0.1%)
1	PO	0.38	0/2253	0.77	4/3064 (0.1%)
1	Q4	0.37	0/2253	0.74	3/3064 (0.1%)
1	Q9	0.37	0/2253	0.74	3/3064 (0.1%)
1	QE	0.37	0/2253	0.74	3/3064 (0.1%)
1	QJ	0.37	0/2253	0.74	3/3064 (0.1%)
1	QO	0.37	0/2253	0.74	3/3064 (0.1%)
1	R4	0.37	0/2253	0.71	0/3064
1	R9	0.37	0/2253	0.71	0/3064
1	RE	0.37	0/2253	0.71	0/3064
1	RJ	0.37	0/2253	0.71	0/3064
1	RO	0.37	0/2253	0.71	0/3064
1	S4	0.40	0/2216	0.74	3/3012 (0.1%)
1	S9	0.41	0/2216	0.74	3/3012 (0.1%)
1	SE	0.41	0/2216	0.74	3/3012 (0.1%)
1	SJ	0.41	0/2216	0.74	3/3012 (0.1%)
1	SO	0.41	0/2216	0.74	3/3012 (0.1%)
1	T4	0.37	0/2216	0.65	0/3012
1	T9	0.37	0/2216	0.65	0/3012
1	TE	0.37	0/2216	0.65	0/3012
1	TJ	0.37	0/2216	0.65	0/3012
1	TO	0.37	0/2216	0.65	0/3012
1	U4	0.40	0/2216	0.67	1/3012 (0.0%)
1	U9	0.40	0/2216	0.67	1/3012 (0.0%)
1	UE	0.40	0/2216	0.67	1/3012 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	UJ	0.40	0/2216	0.67	1/3012 (0.0%)
1	UO	0.40	0/2216	0.67	1/3012 (0.0%)
1	V4	0.39	0/2216	0.69	0/3012
1	V9	0.39	0/2216	0.69	0/3012
1	VE	0.39	0/2216	0.69	0/3012
1	VJ	0.39	0/2216	0.69	0/3012
1	VO	0.39	0/2216	0.69	0/3012
1	W4	0.39	0/2216	0.71	2/3012 (0.1%)
1	W9	0.39	0/2216	0.71	2/3012 (0.1%)
1	WE	0.39	0/2216	0.71	2/3012 (0.1%)
1	WJ	0.39	0/2216	0.71	2/3012 (0.1%)
1	WO	0.39	0/2216	0.71	2/3012 (0.1%)
1	X4	0.35	0/2253	0.65	0/3064
1	X9	0.35	0/2253	0.65	0/3064
1	XE	0.35	0/2253	0.65	0/3064
1	XJ	0.35	0/2253	0.65	0/3064
1	XO	0.35	0/2253	0.65	0/3064
1	Y4	0.35	0/2253	0.63	0/3064
1	Y9	0.36	0/2253	0.63	0/3064
1	YE	0.36	0/2253	0.63	0/3064
1	YJ	0.36	0/2253	0.63	0/3064
1	YO	0.36	0/2253	0.63	0/3064
1	Z4	0.37	0/2251	0.67	0/3061
1	Z9	0.37	0/2251	0.67	0/3061
1	ZE	0.37	0/2251	0.67	0/3061
1	ZJ	0.37	0/2251	0.67	0/3061
1	ZO	0.37	0/2251	0.67	0/3061
2	A1	0.40	0/652	0.65	2/892 (0.2%)
2	A2	0.40	0/652	0.65	2/892 (0.2%)
2	A3	0.39	0/652	0.65	2/892 (0.2%)
2	A6	0.40	0/652	0.65	2/892 (0.2%)
2	A7	0.40	0/652	0.65	2/892 (0.2%)
2	A8	0.40	0/652	0.65	2/892 (0.2%)
2	AB	0.40	0/652	0.65	2/892 (0.2%)
2	AC	0.40	0/652	0.65	2/892 (0.2%)
2	AD	0.40	0/652	0.65	2/892 (0.2%)
2	AG	0.40	0/652	0.65	2/892 (0.2%)
2	AH	0.40	0/652	0.65	2/892 (0.2%)
2	AI	0.40	0/652	0.65	2/892 (0.2%)
2	AL	0.40	0/652	0.65	2/892 (0.2%)
2	AM	0.39	0/652	0.65	2/892 (0.2%)
2	AN	0.40	0/652	0.65	2/892 (0.2%)
2	B2	0.40	0/652	0.65	2/892 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	B3	0.40	0/652	0.65	2/892 (0.2%)
2	B7	0.39	0/652	0.65	2/892 (0.2%)
2	B8	0.40	0/652	0.65	2/892 (0.2%)
2	BC	0.40	0/652	0.65	2/892 (0.2%)
2	BD	0.40	0/652	0.65	2/892 (0.2%)
2	BH	0.40	0/652	0.65	2/892 (0.2%)
2	BI	0.40	0/652	0.65	2/892 (0.2%)
2	BM	0.39	0/652	0.65	2/892 (0.2%)
2	BN	0.40	0/652	0.65	2/892 (0.2%)
2	C2	0.40	0/652	0.65	2/892 (0.2%)
2	C3	0.40	0/652	0.65	2/892 (0.2%)
2	C7	0.40	0/652	0.65	2/892 (0.2%)
2	C8	0.40	0/652	0.65	2/892 (0.2%)
2	CC	0.40	0/652	0.65	2/892 (0.2%)
2	CD	0.40	0/652	0.65	2/892 (0.2%)
2	CH	0.40	0/652	0.65	2/892 (0.2%)
2	CI	0.40	0/652	0.65	2/892 (0.2%)
2	CM	0.40	0/652	0.65	2/892 (0.2%)
2	CN	0.40	0/652	0.65	2/892 (0.2%)
2	D2	0.39	0/652	0.65	2/892 (0.2%)
2	D3	0.40	0/652	0.65	2/892 (0.2%)
2	D7	0.40	0/652	0.65	2/892 (0.2%)
2	D8	0.40	0/652	0.65	2/892 (0.2%)
2	DC	0.40	0/652	0.65	2/892 (0.2%)
2	DD	0.40	0/652	0.65	2/892 (0.2%)
2	DH	0.39	0/652	0.65	2/892 (0.2%)
2	DI	0.40	0/652	0.65	2/892 (0.2%)
2	DM	0.39	0/652	0.65	2/892 (0.2%)
2	DN	0.40	0/652	0.65	2/892 (0.2%)
2	E2	0.39	0/652	0.65	2/892 (0.2%)
2	E3	0.40	0/652	0.65	2/892 (0.2%)
2	E7	0.39	0/652	0.65	2/892 (0.2%)
2	E8	0.40	0/652	0.65	2/892 (0.2%)
2	EC	0.40	0/652	0.65	2/892 (0.2%)
2	ED	0.40	0/652	0.65	2/892 (0.2%)
2	EH	0.40	0/652	0.65	2/892 (0.2%)
2	EI	0.40	0/652	0.65	2/892 (0.2%)
2	EM	0.40	0/652	0.65	2/892 (0.2%)
2	EN	0.40	0/652	0.65	2/892 (0.2%)
3	F2	0.42	0/61	1.07	0/81
3	F3	0.43	0/61	1.06	0/81
3	F7	0.42	0/61	1.07	0/81
3	F8	0.43	0/61	1.06	0/81

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	FC	0.43	0/61	1.07	0/81
3	FD	0.42	0/61	1.07	0/81
3	FH	0.42	0/61	1.07	0/81
3	FI	0.43	0/61	1.07	0/81
3	FM	0.43	0/61	1.07	0/81
3	FN	0.43	0/61	1.07	0/81
4	2A	0.59	1/1482 (0.1%)	0.95	5/2021 (0.2%)
4	2B	0.52	0/1485	0.77	1/2024 (0.0%)
4	2C	0.59	1/1482 (0.1%)	0.95	5/2021 (0.2%)
4	2D	0.52	0/1488	0.77	1/2028 (0.0%)
4	2E	0.59	1/1482 (0.1%)	0.95	5/2021 (0.2%)
4	2F	0.52	0/1488	0.77	1/2028 (0.0%)
4	2G	0.59	1/1479 (0.1%)	0.95	6/2018 (0.3%)
4	2H	0.53	0/1485	0.77	1/2025 (0.0%)
4	2I	0.59	1/1482 (0.1%)	0.95	5/2021 (0.2%)
4	2J	0.52	0/1488	0.77	1/2028 (0.0%)
4	2K	0.59	1/1479 (0.1%)	0.95	5/2016 (0.2%)
4	2L	0.52	0/1488	0.77	1/2028 (0.0%)
5	1A	0.49	0/2785	0.68	1/3794 (0.0%)
5	1B	0.49	0/2794	0.68	1/3804 (0.0%)
5	1C	0.49	0/2782	0.67	1/3790 (0.0%)
5	1D	0.49	0/2791	0.68	1/3801 (0.0%)
5	1E	0.49	0/2788	0.67	1/3797 (0.0%)
5	1F	0.49	0/2788	0.68	1/3797 (0.0%)
5	1G	0.49	0/2794	0.68	1/3804 (0.0%)
5	1H	0.49	0/2788	0.68	1/3797 (0.0%)
5	1I	0.49	0/2788	0.67	1/3797 (0.0%)
5	1J	0.49	0/2788	0.68	1/3797 (0.0%)
5	1K	0.49	0/2788	0.68	1/3797 (0.0%)
5	1L	0.49	0/2788	0.68	1/3797 (0.0%)
6	4A	0.50	0/982	0.80	1/1337 (0.1%)
6	4B	0.50	0/982	0.80	1/1337 (0.1%)
6	4C	0.50	0/982	0.80	1/1337 (0.1%)
6	4D	0.50	0/982	0.80	1/1337 (0.1%)
6	4E	0.50	0/982	0.80	1/1337 (0.1%)
6	4F	0.50	0/982	0.80	1/1337 (0.1%)
7	3A	0.51	0/875	0.77	0/1182
7	3B	0.51	0/875	0.77	0/1182
7	3C	0.51	0/875	0.77	0/1182
7	3D	0.51	0/875	0.77	0/1182
7	3E	0.51	0/875	0.77	0/1182
7	3F	0.51	0/875	0.77	0/1182
8	50	0.38	0/987	0.75	0/1332

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	5I	0.39	0/987	0.75	0/1332
8	52	0.38	0/987	0.75	0/1332
8	53	0.39	0/987	0.74	0/1332
8	5A	0.46	0/987	0.82	0/1332
8	5B	0.46	0/987	0.82	0/1332
8	5C	0.46	0/987	0.82	0/1332
8	5D	0.46	0/987	0.82	0/1332
8	5E	0.46	0/987	0.82	0/1332
8	5F	0.47	0/987	0.82	0/1332
8	5G	0.38	0/987	0.74	0/1332
8	5H	0.38	0/987	0.75	0/1332
8	5I	0.38	0/987	0.75	0/1332
8	5J	0.38	0/987	0.74	0/1332
8	5K	0.38	0/987	0.74	0/1332
8	5L	0.38	0/987	0.75	0/1332
8	5M	0.38	0/987	0.75	0/1332
8	5N	0.38	0/987	0.75	0/1332
8	5O	0.38	0/987	0.75	0/1332
8	5P	0.38	0/987	0.74	0/1332
8	5Q	0.38	0/987	0.75	0/1332
8	5R	0.38	0/987	0.75	0/1332
8	5S	0.38	0/987	0.75	0/1332
8	5T	0.38	0/987	0.75	0/1332
8	5U	0.38	0/987	0.75	0/1332
8	5V	0.38	0/987	0.75	0/1332
8	5W	0.38	0/987	0.75	0/1332
8	5X	0.38	0/987	0.75	0/1332
8	5Y	0.38	0/987	0.75	0/1332
8	5Z	0.39	0/987	0.75	0/1332
9	7A	0.51	0/2222	0.83	0/3010
9	7B	0.51	0/2222	0.83	0/3010
9	7C	0.52	0/2222	0.82	0/3010
10	8A	0.52	0/3292	0.79	4/4459 (0.1%)
10	8B	0.52	0/3292	0.79	4/4459 (0.1%)
10	8C	0.52	0/3292	0.79	4/4459 (0.1%)
11	6A	0.27	0/1085	0.58	0/1472
11	6B	0.28	0/1085	0.58	0/1472
11	6C	0.28	0/1085	0.57	0/1472
11	6D	0.28	0/1085	0.59	0/1472
11	6E	0.28	0/1085	0.57	0/1472
11	6F	0.28	0/1085	0.59	0/1472
All	All	0.41	11/475156 (0.0%)	0.71	325/646033 (0.1%)

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K9	251	ALA	C-N	-8.73	1.21	1.33
1	KE	251	ALA	C-N	-8.72	1.21	1.33
1	KJ	251	ALA	C-N	-8.71	1.21	1.33
1	K4	251	ALA	C-N	-8.71	1.21	1.33
1	KO	251	ALA	C-N	-8.66	1.21	1.33

The worst 5 of 325 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QE	181	ARG	N-CA-C	-9.23	103.12	114.75
1	QJ	181	ARG	N-CA-C	-9.22	103.13	114.75
1	QO	181	ARG	N-CA-C	-9.21	103.14	114.75
1	Q4	181	ARG	N-CA-C	-9.21	103.15	114.75
1	Q9	181	ARG	N-CA-C	-9.20	103.15	114.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A4	2173	0	2142	39	0
1	A5	2199	0	2160	77	0
1	A9	2173	0	2142	38	0
1	AA	2205	0	2172	68	0
1	AE	2173	0	2142	40	0
1	AF	2209	0	2176	56	0
1	AJ	2173	0	2142	42	0
1	AK	2209	0	2176	70	0
1	AO	2173	0	2142	40	0
1	AP	2201	0	2168	93	0
1	B4	2209	0	2176	40	0
1	B5	2009	0	1979	71	0
1	B9	2209	0	2176	42	0
1	BA	2014	0	1984	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BE	2209	0	2176	41	0
1	BF	2015	0	1991	71	0
1	BJ	2209	0	2176	38	0
1	BK	2009	0	1977	80	0
1	BO	2209	0	2176	36	0
1	BP	2009	0	1982	74	0
1	C4	2209	0	2176	37	0
1	C5	2209	0	2176	37	0
1	C9	2209	0	2176	42	0
1	CA	2209	0	2176	36	0
1	CE	2209	0	2176	43	0
1	CF	2209	0	2176	37	0
1	CJ	2209	0	2176	43	0
1	CK	2209	0	2176	39	0
1	CO	2209	0	2176	40	0
1	CP	2209	0	2176	37	0
1	D4	2209	0	2176	52	0
1	D9	2209	0	2176	52	0
1	DE	2209	0	2176	52	0
1	DJ	2209	0	2176	52	0
1	DO	2209	0	2176	50	0
1	E4	2209	0	2176	61	0
1	E9	2209	0	2176	59	0
1	EE	2209	0	2176	59	0
1	EJ	2209	0	2176	58	0
1	EO	2209	0	2176	58	0
1	F4	2209	0	2176	58	0
1	F9	2209	0	2176	60	0
1	FE	2209	0	2176	59	0
1	FJ	2209	0	2176	59	0
1	FO	2209	0	2176	59	0
1	G4	2209	0	2176	44	0
1	G9	2209	0	2176	45	0
1	GE	2209	0	2176	46	0
1	GJ	2209	0	2176	43	0
1	GO	2209	0	2176	46	0
1	H4	2173	0	2142	37	0
1	H9	2173	0	2142	37	0
1	HE	2173	0	2142	38	0
1	HJ	2173	0	2142	38	0
1	HO	2173	0	2142	36	0
1	I4	2173	0	2142	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I9	2173	0	2142	52	0
1	IE	2173	0	2142	54	0
1	IJ	2173	0	2142	54	0
1	IO	2173	0	2142	56	0
1	J4	2173	0	2142	58	0
1	J9	2173	0	2142	54	0
1	JE	2173	0	2142	56	0
1	JJ	2173	0	2142	57	0
1	JO	2173	0	2142	59	0
1	K4	2173	0	2142	49	0
1	K9	2173	0	2142	50	0
1	KE	2173	0	2142	47	0
1	KJ	2173	0	2142	46	0
1	KO	2173	0	2142	48	0
1	L4	2173	0	2142	53	0
1	L9	2173	0	2142	51	0
1	LE	2173	0	2142	52	0
1	LJ	2173	0	2142	49	0
1	LO	2173	0	2142	52	0
1	M4	2209	0	2176	44	0
1	M9	2209	0	2176	42	0
1	ME	2209	0	2176	41	0
1	MJ	2209	0	2176	48	0
1	MO	2209	0	2176	49	0
1	N4	2209	0	2176	46	0
1	N9	2209	0	2176	46	0
1	NE	2209	0	2176	46	0
1	NJ	2209	0	2176	47	0
1	NO	2209	0	2176	47	0
1	O4	2209	0	2176	46	0
1	O9	2209	0	2176	47	0
1	OE	2209	0	2176	48	0
1	OJ	2209	0	2176	46	0
1	OO	2209	0	2176	47	0
1	P4	2209	0	2176	43	0
1	P9	2209	0	2176	46	0
1	PE	2209	0	2176	47	0
1	PJ	2209	0	2176	43	0
1	PO	2209	0	2176	43	0
1	Q4	2209	0	2176	47	0
1	Q9	2209	0	2176	48	0
1	QE	2209	0	2176	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QJ	2209	0	2176	47	0
1	QO	2209	0	2176	50	0
1	R4	2209	0	2176	37	0
1	R9	2209	0	2176	38	0
1	RE	2209	0	2176	39	0
1	RJ	2209	0	2176	39	0
1	RO	2209	0	2176	41	0
1	S4	2173	0	2142	48	0
1	S9	2173	0	2142	47	0
1	SE	2173	0	2142	49	0
1	SJ	2173	0	2142	48	0
1	SO	2173	0	2142	49	0
1	T4	2173	0	2142	44	0
1	T9	2173	0	2142	46	0
1	TE	2173	0	2142	44	0
1	TJ	2173	0	2142	43	0
1	TO	2173	0	2142	43	0
1	U4	2173	0	2142	45	0
1	U9	2173	0	2142	48	0
1	UE	2173	0	2142	44	0
1	UJ	2173	0	2142	41	0
1	UO	2173	0	2142	46	0
1	V4	2173	0	2142	46	0
1	V9	2173	0	2142	44	0
1	VE	2173	0	2142	48	0
1	VJ	2173	0	2142	44	0
1	VO	2173	0	2142	47	0
1	W4	2173	0	2142	50	0
1	W9	2173	0	2142	49	0
1	WE	2173	0	2142	48	0
1	WJ	2173	0	2142	51	0
1	WO	2173	0	2142	49	0
1	X4	2209	0	2176	36	0
1	X9	2209	0	2176	34	0
1	XE	2209	0	2176	36	0
1	XJ	2209	0	2176	35	0
1	XO	2209	0	2176	33	0
1	Y4	2209	0	2176	38	0
1	Y9	2209	0	2176	40	0
1	YE	2209	0	2176	36	0
1	YJ	2209	0	2176	38	0
1	YO	2209	0	2176	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z4	2207	0	2171	49	0
1	Z9	2207	0	2171	46	0
1	ZE	2207	0	2171	42	0
1	ZJ	2207	0	2171	44	0
1	ZO	2207	0	2171	51	0
2	A1	640	0	653	27	0
2	A2	640	0	653	24	0
2	A3	640	0	653	20	0
2	A6	640	0	653	27	0
2	A7	640	0	653	23	0
2	A8	640	0	653	20	0
2	AB	640	0	653	29	0
2	AC	640	0	653	23	0
2	AD	640	0	653	20	0
2	AG	640	0	653	28	0
2	AH	640	0	653	24	0
2	AI	640	0	653	19	0
2	AL	640	0	653	27	0
2	AM	640	0	653	23	0
2	AN	640	0	653	19	0
2	B2	640	0	653	24	0
2	B3	640	0	653	23	0
2	B7	640	0	653	23	0
2	B8	640	0	653	23	0
2	BC	640	0	653	23	0
2	BD	640	0	653	23	0
2	BH	640	0	653	24	0
2	BI	640	0	653	23	0
2	BM	640	0	653	23	0
2	BN	640	0	653	23	0
2	C2	640	0	653	19	0
2	C3	640	0	653	20	0
2	C7	640	0	653	17	0
2	C8	640	0	653	20	0
2	CC	640	0	653	19	0
2	CD	640	0	653	20	0
2	CH	640	0	653	19	0
2	CI	640	0	653	20	0
2	CM	640	0	653	18	0
2	CN	640	0	653	22	0
2	D2	640	0	653	20	0
2	D3	640	0	653	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D7	640	0	653	19	0
2	D8	640	0	653	23	0
2	DC	640	0	653	21	0
2	DD	640	0	653	22	0
2	DH	640	0	653	22	0
2	DI	640	0	653	22	0
2	DM	640	0	653	21	0
2	DN	640	0	653	23	0
2	E2	640	0	653	17	0
2	E3	640	0	653	17	0
2	E7	640	0	653	18	0
2	E8	640	0	653	17	0
2	EC	640	0	653	20	0
2	ED	640	0	653	15	0
2	EH	640	0	653	19	0
2	EI	640	0	653	17	0
2	EM	640	0	653	20	0
2	EN	640	0	653	17	0
3	F2	62	0	73	1	0
3	F3	62	0	73	1	0
3	F7	62	0	73	1	0
3	F8	62	0	73	1	0
3	FC	62	0	73	1	0
3	FD	62	0	73	1	0
3	FH	62	0	73	1	0
3	FI	62	0	73	1	0
3	FM	62	0	73	1	0
3	FN	62	0	73	1	0
4	2A	1450	0	1474	73	0
4	2B	1453	0	1481	77	0
4	2C	1450	0	1474	51	0
4	2D	1456	0	1490	71	0
4	2E	1450	0	1474	65	0
4	2F	1456	0	1490	78	0
4	2G	1447	0	1467	58	0
4	2H	1453	0	1483	73	0
4	2I	1450	0	1474	71	0
4	2J	1456	0	1490	69	0
4	2K	1448	0	1468	57	0
4	2L	1456	0	1490	90	0
5	1A	2714	0	2688	53	0
5	1B	2723	0	2706	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	1C	2711	0	2684	48	0
5	1D	2720	0	2695	63	0
5	1E	2717	0	2695	67	0
5	1F	2717	0	2695	59	0
5	1G	2723	0	2706	69	0
5	1H	2717	0	2695	76	0
5	1I	2717	0	2695	76	0
5	1J	2717	0	2695	96	0
5	1K	2717	0	2695	98	0
5	1L	2717	0	2694	75	0
6	4A	968	0	987	46	0
6	4B	968	0	987	52	0
6	4C	968	0	987	53	0
6	4D	968	0	987	50	0
6	4E	968	0	987	46	0
6	4F	968	0	987	45	0
7	3A	859	0	861	40	0
7	3B	859	0	861	46	0
7	3C	859	0	861	50	0
7	3D	859	0	861	47	0
7	3E	859	0	861	43	0
7	3F	859	0	861	39	0
8	50	972	0	938	132	0
8	51	972	0	938	101	0
8	52	972	0	938	63	0
8	53	972	0	938	62	0
8	5A	972	0	938	94	0
8	5B	972	0	938	103	0
8	5C	972	0	938	112	0
8	5D	972	0	938	103	0
8	5E	972	0	938	93	0
8	5F	972	0	938	86	0
8	5G	972	0	938	50	0
8	5H	972	0	938	44	0
8	5I	972	0	938	42	0
8	5J	972	0	938	45	0
8	5K	972	0	938	56	0
8	5L	972	0	938	58	0
8	5M	972	0	938	101	0
8	5N	972	0	938	87	0
8	5O	972	0	938	89	0
8	5P	972	0	938	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	5Q	972	0	938	124	0
8	5R	972	0	938	119	0
8	5S	972	0	938	126	0
8	5T	972	0	938	150	0
8	5U	972	0	938	183	0
8	5V	972	0	938	233	0
8	5W	972	0	938	248	0
8	5X	972	0	938	178	0
8	5Y	972	0	938	83	0
8	5Z	972	0	938	113	0
9	7A	2179	0	2125	71	0
9	7B	2179	0	2125	68	0
9	7C	2179	0	2125	67	0
10	8A	3246	0	3223	98	0
10	8B	3246	0	3223	99	0
10	8C	3246	0	3223	98	0
11	6A	1056	0	1000	69	0
11	6B	1056	0	1000	70	0
11	6C	1056	0	1000	71	0
11	6D	1056	0	1000	68	0
11	6E	1056	0	1000	72	0
11	6F	1056	0	1000	68	0
12	7A	8	0	0	0	0
12	7B	8	0	0	0	0
12	7C	8	0	0	0	0
All	All	465916	0	460645	10633	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 11.

The worst 5 of 10633 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)
8:5V:42:THR:HG23	8:5Z:116:HIS:CE1	1.14	1.65
1:Z4:151:THR:CB	4:2K:127:PRO:CA	1.75	1.61
1:AP:126:VAL:HG23	5:1K:161:GLY:C	1.27	1.60
1:BA:192:THR:HG23	5:1E:41:TRP:CD1	1.11	1.58
1:BA:192:THR:CG2	5:1E:41:TRP:CD1	1.80	1.55

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A4	287/385 (74%)	258 (90%)	28 (10%)	1 (0%)	36	71
1	A5	295/385 (77%)	273 (92%)	21 (7%)	1 (0%)	36	71
1	A9	287/385 (74%)	258 (90%)	28 (10%)	1 (0%)	36	71
1	AA	295/385 (77%)	273 (92%)	21 (7%)	1 (0%)	36	71
1	AE	287/385 (74%)	258 (90%)	28 (10%)	1 (0%)	36	71
1	AF	295/385 (77%)	273 (92%)	21 (7%)	1 (0%)	36	71
1	AJ	287/385 (74%)	258 (90%)	28 (10%)	1 (0%)	36	71
1	AK	295/385 (77%)	273 (92%)	21 (7%)	1 (0%)	36	71
1	AO	287/385 (74%)	258 (90%)	28 (10%)	1 (0%)	36	71
1	AP	295/385 (77%)	273 (92%)	21 (7%)	1 (0%)	36	71
1	B4	295/385 (77%)	264 (90%)	30 (10%)	1 (0%)	36	71
1	B5	267/385 (69%)	242 (91%)	22 (8%)	3 (1%)	11	45
1	B9	295/385 (77%)	264 (90%)	30 (10%)	1 (0%)	36	71
1	BA	267/385 (69%)	242 (91%)	22 (8%)	3 (1%)	11	45
1	BE	295/385 (77%)	264 (90%)	30 (10%)	1 (0%)	36	71
1	BF	267/385 (69%)	242 (91%)	22 (8%)	3 (1%)	11	45
1	BJ	295/385 (77%)	264 (90%)	30 (10%)	1 (0%)	36	71
1	BK	267/385 (69%)	242 (91%)	22 (8%)	3 (1%)	11	45
1	BO	295/385 (77%)	264 (90%)	30 (10%)	1 (0%)	36	71
1	BP	267/385 (69%)	242 (91%)	22 (8%)	3 (1%)	11	45
1	C4	295/385 (77%)	266 (90%)	29 (10%)	0	100	100
1	C5	295/385 (77%)	264 (90%)	31 (10%)	0	100	100
1	C9	295/385 (77%)	266 (90%)	29 (10%)	0	100	100
1	CA	295/385 (77%)	264 (90%)	31 (10%)	0	100	100
1	CE	295/385 (77%)	266 (90%)	29 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CF	295/385 (77%)	264 (90%)	31 (10%)	0	100	100
1	CJ	295/385 (77%)	266 (90%)	29 (10%)	0	100	100
1	CK	295/385 (77%)	264 (90%)	31 (10%)	0	100	100
1	CO	295/385 (77%)	266 (90%)	29 (10%)	0	100	100
1	CP	295/385 (77%)	264 (90%)	31 (10%)	0	100	100
1	D4	295/385 (77%)	264 (90%)	31 (10%)	0	100	100
1	D9	295/385 (77%)	264 (90%)	31 (10%)	0	100	100
1	DE	295/385 (77%)	264 (90%)	31 (10%)	0	100	100
1	DJ	295/385 (77%)	264 (90%)	31 (10%)	0	100	100
1	DO	295/385 (77%)	264 (90%)	31 (10%)	0	100	100
1	E4	295/385 (77%)	258 (88%)	36 (12%)	1 (0%)	36	71
1	E9	295/385 (77%)	258 (88%)	36 (12%)	1 (0%)	36	71
1	EE	295/385 (77%)	258 (88%)	36 (12%)	1 (0%)	36	71
1	EJ	295/385 (77%)	258 (88%)	36 (12%)	1 (0%)	36	71
1	EO	295/385 (77%)	258 (88%)	36 (12%)	1 (0%)	36	71
1	F4	295/385 (77%)	264 (90%)	29 (10%)	2 (1%)	18	55
1	F9	295/385 (77%)	264 (90%)	29 (10%)	2 (1%)	18	55
1	FE	295/385 (77%)	264 (90%)	29 (10%)	2 (1%)	18	55
1	FJ	295/385 (77%)	264 (90%)	29 (10%)	2 (1%)	18	55
1	FO	295/385 (77%)	264 (90%)	29 (10%)	2 (1%)	18	55
1	G4	295/385 (77%)	263 (89%)	31 (10%)	1 (0%)	36	71
1	G9	295/385 (77%)	263 (89%)	31 (10%)	1 (0%)	36	71
1	GE	295/385 (77%)	263 (89%)	31 (10%)	1 (0%)	36	71
1	GJ	295/385 (77%)	263 (89%)	31 (10%)	1 (0%)	36	71
1	GO	295/385 (77%)	263 (89%)	31 (10%)	1 (0%)	36	71
1	H4	287/385 (74%)	252 (88%)	34 (12%)	1 (0%)	36	71
1	H9	287/385 (74%)	252 (88%)	34 (12%)	1 (0%)	36	71
1	HE	287/385 (74%)	253 (88%)	33 (12%)	1 (0%)	36	71
1	HJ	287/385 (74%)	252 (88%)	34 (12%)	1 (0%)	36	71
1	HO	287/385 (74%)	252 (88%)	34 (12%)	1 (0%)	36	71
1	I4	287/385 (74%)	251 (88%)	35 (12%)	1 (0%)	36	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I9	287/385 (74%)	250 (87%)	36 (12%)	1 (0%)	36	71
1	IE	287/385 (74%)	250 (87%)	36 (12%)	1 (0%)	36	71
1	IJ	287/385 (74%)	251 (88%)	35 (12%)	1 (0%)	36	71
1	IO	287/385 (74%)	250 (87%)	36 (12%)	1 (0%)	36	71
1	J4	287/385 (74%)	256 (89%)	29 (10%)	2 (1%)	18	55
1	J9	287/385 (74%)	256 (89%)	29 (10%)	2 (1%)	18	55
1	JE	287/385 (74%)	256 (89%)	29 (10%)	2 (1%)	18	55
1	JJ	287/385 (74%)	256 (89%)	29 (10%)	2 (1%)	18	55
1	JO	287/385 (74%)	256 (89%)	29 (10%)	2 (1%)	18	55
1	K4	287/385 (74%)	246 (86%)	40 (14%)	1 (0%)	36	71
1	K9	287/385 (74%)	247 (86%)	39 (14%)	1 (0%)	36	71
1	KE	287/385 (74%)	246 (86%)	40 (14%)	1 (0%)	36	71
1	KJ	287/385 (74%)	247 (86%)	39 (14%)	1 (0%)	36	71
1	KO	287/385 (74%)	247 (86%)	39 (14%)	1 (0%)	36	71
1	L4	287/385 (74%)	255 (89%)	31 (11%)	1 (0%)	36	71
1	L9	287/385 (74%)	255 (89%)	31 (11%)	1 (0%)	36	71
1	LE	287/385 (74%)	255 (89%)	31 (11%)	1 (0%)	36	71
1	LJ	287/385 (74%)	255 (89%)	31 (11%)	1 (0%)	36	71
1	LO	287/385 (74%)	255 (89%)	31 (11%)	1 (0%)	36	71
1	M4	295/385 (77%)	254 (86%)	41 (14%)	0	100	100
1	M9	295/385 (77%)	254 (86%)	41 (14%)	0	100	100
1	ME	295/385 (77%)	254 (86%)	41 (14%)	0	100	100
1	MJ	295/385 (77%)	254 (86%)	41 (14%)	0	100	100
1	MO	295/385 (77%)	253 (86%)	42 (14%)	0	100	100
1	N4	295/385 (77%)	264 (90%)	30 (10%)	1 (0%)	36	71
1	N9	295/385 (77%)	264 (90%)	30 (10%)	1 (0%)	36	71
1	NE	295/385 (77%)	264 (90%)	30 (10%)	1 (0%)	36	71
1	NJ	295/385 (77%)	264 (90%)	30 (10%)	1 (0%)	36	71
1	NO	295/385 (77%)	264 (90%)	30 (10%)	1 (0%)	36	71
1	O4	295/385 (77%)	257 (87%)	37 (12%)	1 (0%)	36	71
1	O9	295/385 (77%)	258 (88%)	36 (12%)	1 (0%)	36	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	OE	295/385 (77%)	257 (87%)	37 (12%)	1 (0%)	36	71
1	OJ	295/385 (77%)	258 (88%)	36 (12%)	1 (0%)	36	71
1	OO	295/385 (77%)	257 (87%)	37 (12%)	1 (0%)	36	71
1	P4	295/385 (77%)	256 (87%)	38 (13%)	1 (0%)	36	71
1	P9	295/385 (77%)	256 (87%)	38 (13%)	1 (0%)	36	71
1	PE	295/385 (77%)	256 (87%)	38 (13%)	1 (0%)	36	71
1	PJ	295/385 (77%)	256 (87%)	38 (13%)	1 (0%)	36	71
1	PO	295/385 (77%)	256 (87%)	38 (13%)	1 (0%)	36	71
1	Q4	295/385 (77%)	260 (88%)	34 (12%)	1 (0%)	36	71
1	Q9	295/385 (77%)	260 (88%)	34 (12%)	1 (0%)	36	71
1	QE	295/385 (77%)	260 (88%)	34 (12%)	1 (0%)	36	71
1	QJ	295/385 (77%)	259 (88%)	35 (12%)	1 (0%)	36	71
1	QO	295/385 (77%)	259 (88%)	35 (12%)	1 (0%)	36	71
1	R4	295/385 (77%)	261 (88%)	33 (11%)	1 (0%)	36	71
1	R9	295/385 (77%)	261 (88%)	33 (11%)	1 (0%)	36	71
1	RE	295/385 (77%)	261 (88%)	33 (11%)	1 (0%)	36	71
1	RJ	295/385 (77%)	261 (88%)	33 (11%)	1 (0%)	36	71
1	RO	295/385 (77%)	261 (88%)	33 (11%)	1 (0%)	36	71
1	S4	287/385 (74%)	257 (90%)	29 (10%)	1 (0%)	36	71
1	S9	287/385 (74%)	257 (90%)	29 (10%)	1 (0%)	36	71
1	SE	287/385 (74%)	257 (90%)	29 (10%)	1 (0%)	36	71
1	SJ	287/385 (74%)	257 (90%)	29 (10%)	1 (0%)	36	71
1	SO	287/385 (74%)	257 (90%)	29 (10%)	1 (0%)	36	71
1	T4	287/385 (74%)	255 (89%)	32 (11%)	0	100	100
1	T9	287/385 (74%)	255 (89%)	32 (11%)	0	100	100
1	TE	287/385 (74%)	256 (89%)	31 (11%)	0	100	100
1	TJ	287/385 (74%)	255 (89%)	32 (11%)	0	100	100
1	TO	287/385 (74%)	255 (89%)	32 (11%)	0	100	100
1	U4	287/385 (74%)	253 (88%)	33 (12%)	1 (0%)	36	71
1	U9	287/385 (74%)	253 (88%)	33 (12%)	1 (0%)	36	71
1	UE	287/385 (74%)	253 (88%)	33 (12%)	1 (0%)	36	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	UJ	287/385 (74%)	253 (88%)	33 (12%)	1 (0%)	36	71
1	UO	287/385 (74%)	253 (88%)	33 (12%)	1 (0%)	36	71
1	V4	287/385 (74%)	258 (90%)	28 (10%)	1 (0%)	36	71
1	V9	287/385 (74%)	258 (90%)	28 (10%)	1 (0%)	36	71
1	VE	287/385 (74%)	258 (90%)	28 (10%)	1 (0%)	36	71
1	VJ	287/385 (74%)	258 (90%)	28 (10%)	1 (0%)	36	71
1	VO	287/385 (74%)	258 (90%)	28 (10%)	1 (0%)	36	71
1	W4	287/385 (74%)	251 (88%)	35 (12%)	1 (0%)	36	71
1	W9	287/385 (74%)	251 (88%)	35 (12%)	1 (0%)	36	71
1	WE	287/385 (74%)	252 (88%)	34 (12%)	1 (0%)	36	71
1	WJ	287/385 (74%)	251 (88%)	35 (12%)	1 (0%)	36	71
1	WO	287/385 (74%)	251 (88%)	35 (12%)	1 (0%)	36	71
1	X4	295/385 (77%)	259 (88%)	36 (12%)	0	100	100
1	X9	295/385 (77%)	259 (88%)	36 (12%)	0	100	100
1	XE	295/385 (77%)	259 (88%)	36 (12%)	0	100	100
1	XJ	295/385 (77%)	259 (88%)	36 (12%)	0	100	100
1	XO	295/385 (77%)	259 (88%)	36 (12%)	0	100	100
1	Y4	295/385 (77%)	264 (90%)	31 (10%)	0	100	100
1	Y9	295/385 (77%)	264 (90%)	31 (10%)	0	100	100
1	YE	295/385 (77%)	264 (90%)	31 (10%)	0	100	100
1	YJ	295/385 (77%)	264 (90%)	31 (10%)	0	100	100
1	YO	295/385 (77%)	264 (90%)	31 (10%)	0	100	100
1	Z4	295/385 (77%)	269 (91%)	26 (9%)	0	100	100
1	Z9	295/385 (77%)	269 (91%)	26 (9%)	0	100	100
1	ZE	295/385 (77%)	269 (91%)	26 (9%)	0	100	100
1	ZJ	295/385 (77%)	269 (91%)	26 (9%)	0	100	100
1	ZO	295/385 (77%)	269 (91%)	26 (9%)	0	100	100
2	A1	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	A2	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	A3	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	A6	82/84 (98%)	77 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A7	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	A8	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	AB	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	AC	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	AD	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	AG	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	AH	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	AI	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	AL	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	AM	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	AN	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	B2	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	B3	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	B7	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	B8	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	BC	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	BD	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	BH	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	BI	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	BM	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	BN	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	C2	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	C3	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	C7	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	C8	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	CC	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	CD	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	CH	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	CI	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	CM	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	CN	82/84 (98%)	77 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D2	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	D3	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	D7	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	D8	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	DC	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	DD	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	DH	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	DI	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	DM	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	DN	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	E2	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	E3	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	E7	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	E8	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	EC	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	ED	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	EH	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	EI	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	EM	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	EN	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
3	F2	8/325 (2%)	5 (62%)	3 (38%)	0	100	100
3	F3	8/325 (2%)	5 (62%)	3 (38%)	0	100	100
3	F7	8/325 (2%)	5 (62%)	3 (38%)	0	100	100
3	F8	8/325 (2%)	5 (62%)	3 (38%)	0	100	100
3	FC	8/325 (2%)	5 (62%)	3 (38%)	0	100	100
3	FD	8/325 (2%)	5 (62%)	3 (38%)	0	100	100
3	FH	8/325 (2%)	5 (62%)	3 (38%)	0	100	100
3	FI	8/325 (2%)	5 (62%)	3 (38%)	0	100	100
3	FM	8/325 (2%)	5 (62%)	3 (38%)	0	100	100
3	FN	8/325 (2%)	5 (62%)	3 (38%)	0	100	100
4	2A	190/197 (96%)	161 (85%)	28 (15%)	1 (0%)	24	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	2B	190/197 (96%)	164 (86%)	26 (14%)	0	100	100
4	2C	190/197 (96%)	161 (85%)	28 (15%)	1 (0%)	24	63
4	2D	190/197 (96%)	164 (86%)	26 (14%)	0	100	100
4	2E	190/197 (96%)	161 (85%)	28 (15%)	1 (0%)	24	63
4	2F	190/197 (96%)	164 (86%)	26 (14%)	0	100	100
4	2G	190/197 (96%)	161 (85%)	28 (15%)	1 (0%)	24	63
4	2H	190/197 (96%)	164 (86%)	26 (14%)	0	100	100
4	2I	190/197 (96%)	161 (85%)	28 (15%)	1 (0%)	24	63
4	2J	190/197 (96%)	164 (86%)	26 (14%)	0	100	100
4	2K	190/197 (96%)	161 (85%)	28 (15%)	1 (0%)	24	63
4	2L	190/197 (96%)	164 (86%)	26 (14%)	0	100	100
5	1A	356/396 (90%)	328 (92%)	28 (8%)	0	100	100
5	1B	356/396 (90%)	328 (92%)	28 (8%)	0	100	100
5	1C	356/396 (90%)	328 (92%)	28 (8%)	0	100	100
5	1D	356/396 (90%)	328 (92%)	28 (8%)	0	100	100
5	1E	356/396 (90%)	328 (92%)	28 (8%)	0	100	100
5	1F	356/396 (90%)	328 (92%)	28 (8%)	0	100	100
5	1G	356/396 (90%)	328 (92%)	28 (8%)	0	100	100
5	1H	356/396 (90%)	328 (92%)	28 (8%)	0	100	100
5	1I	356/396 (90%)	328 (92%)	28 (8%)	0	100	100
5	1J	356/396 (90%)	328 (92%)	28 (8%)	0	100	100
5	1K	356/396 (90%)	328 (92%)	28 (8%)	0	100	100
5	1L	356/396 (90%)	328 (92%)	28 (8%)	0	100	100
6	4A	132/135 (98%)	118 (89%)	14 (11%)	0	100	100
6	4B	132/135 (98%)	118 (89%)	14 (11%)	0	100	100
6	4C	132/135 (98%)	118 (89%)	14 (11%)	0	100	100
6	4D	132/135 (98%)	118 (89%)	14 (11%)	0	100	100
6	4E	132/135 (98%)	118 (89%)	14 (11%)	0	100	100
6	4F	132/135 (98%)	118 (89%)	14 (11%)	0	100	100
7	3A	108/112 (96%)	98 (91%)	10 (9%)	0	100	100
7	3B	108/112 (96%)	98 (91%)	10 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	3C	108/112 (96%)	98 (91%)	10 (9%)	0	100	100
7	3D	108/112 (96%)	98 (91%)	10 (9%)	0	100	100
7	3E	108/112 (96%)	98 (91%)	10 (9%)	0	100	100
7	3F	108/112 (96%)	98 (91%)	10 (9%)	0	100	100
8	50	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	51	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	52	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	53	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	5A	126/137 (92%)	115 (91%)	11 (9%)	0	100	100
8	5B	126/137 (92%)	115 (91%)	11 (9%)	0	100	100
8	5C	126/137 (92%)	115 (91%)	11 (9%)	0	100	100
8	5D	126/137 (92%)	115 (91%)	11 (9%)	0	100	100
8	5E	126/137 (92%)	115 (91%)	11 (9%)	0	100	100
8	5F	126/137 (92%)	115 (91%)	11 (9%)	0	100	100
8	5G	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	5H	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	5I	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	5J	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	5K	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	5L	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	5M	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	5N	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	5O	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	5P	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	5Q	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	5R	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	5S	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	5T	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	5U	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	5V	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	5W	126/137 (92%)	111 (88%)	15 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	5X	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	5Y	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
8	5Z	126/137 (92%)	111 (88%)	15 (12%)	0	100	100
9	7A	290/296 (98%)	254 (88%)	36 (12%)	0	100	100
9	7B	290/296 (98%)	255 (88%)	35 (12%)	0	100	100
9	7C	290/296 (98%)	254 (88%)	36 (12%)	0	100	100
10	8A	431/1304 (33%)	375 (87%)	55 (13%)	1 (0%)	43	77
10	8B	431/1304 (33%)	375 (87%)	55 (13%)	1 (0%)	43	77
10	8C	431/1304 (33%)	375 (87%)	55 (13%)	1 (0%)	43	77
11	6A	130/210 (62%)	101 (78%)	29 (22%)	0	100	100
11	6B	130/210 (62%)	102 (78%)	27 (21%)	1 (1%)	16	53
11	6C	130/210 (62%)	101 (78%)	29 (22%)	0	100	100
11	6D	130/210 (62%)	102 (78%)	27 (21%)	1 (1%)	16	53
11	6E	130/210 (62%)	101 (78%)	29 (22%)	0	100	100
11	6F	130/210 (62%)	102 (78%)	27 (21%)	1 (1%)	16	53
All	All	61500/82463 (75%)	54790 (89%)	6573 (11%)	137 (0%)	44	77

5 of 137 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E4	147	TRP
1	F4	93	ALA
1	G4	147	TRP
1	EO	147	TRP
1	FO	93	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A4	215/284 (76%)	214 (100%)	1 (0%)	81	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A5	215/284 (76%)	209 (97%)	6 (3%)	38	59
1	A9	215/284 (76%)	214 (100%)	1 (0%)	81	81
1	AA	217/284 (76%)	211 (97%)	6 (3%)	38	59
1	AE	215/284 (76%)	213 (99%)	2 (1%)	70	76
1	AF	218/284 (77%)	212 (97%)	6 (3%)	38	59
1	AJ	215/284 (76%)	214 (100%)	1 (0%)	81	81
1	AK	218/284 (77%)	212 (97%)	6 (3%)	38	59
1	AO	215/284 (76%)	213 (99%)	2 (1%)	70	76
1	AP	216/284 (76%)	210 (97%)	6 (3%)	38	59
1	B4	218/284 (77%)	218 (100%)	0	100	100
1	B5	196/284 (69%)	193 (98%)	3 (2%)	57	70
1	B9	218/284 (77%)	218 (100%)	0	100	100
1	BA	197/284 (69%)	194 (98%)	3 (2%)	57	70
1	BE	218/284 (77%)	218 (100%)	0	100	100
1	BF	197/284 (69%)	194 (98%)	3 (2%)	57	70
1	BJ	218/284 (77%)	218 (100%)	0	100	100
1	BK	196/284 (69%)	193 (98%)	3 (2%)	57	70
1	BO	218/284 (77%)	218 (100%)	0	100	100
1	BP	196/284 (69%)	193 (98%)	3 (2%)	57	70
1	C4	218/284 (77%)	215 (99%)	3 (1%)	59	71
1	C5	218/284 (77%)	216 (99%)	2 (1%)	70	76
1	C9	218/284 (77%)	215 (99%)	3 (1%)	59	71
1	CA	218/284 (77%)	216 (99%)	2 (1%)	70	76
1	CE	218/284 (77%)	215 (99%)	3 (1%)	59	71
1	CF	218/284 (77%)	216 (99%)	2 (1%)	70	76
1	CJ	218/284 (77%)	215 (99%)	3 (1%)	59	71
1	CK	218/284 (77%)	216 (99%)	2 (1%)	70	76
1	CO	218/284 (77%)	215 (99%)	3 (1%)	59	71
1	CP	218/284 (77%)	216 (99%)	2 (1%)	70	76
1	D4	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	D9	218/284 (77%)	217 (100%)	1 (0%)	81	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DE	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	DJ	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	DO	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	E4	218/284 (77%)	216 (99%)	2 (1%)	70	76
1	E9	218/284 (77%)	216 (99%)	2 (1%)	70	76
1	EE	218/284 (77%)	216 (99%)	2 (1%)	70	76
1	EJ	218/284 (77%)	216 (99%)	2 (1%)	70	76
1	EO	218/284 (77%)	216 (99%)	2 (1%)	70	76
1	F4	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	F9	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	FE	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	FJ	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	FO	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	G4	218/284 (77%)	215 (99%)	3 (1%)	59	71
1	G9	218/284 (77%)	215 (99%)	3 (1%)	59	71
1	GE	218/284 (77%)	215 (99%)	3 (1%)	59	71
1	GJ	218/284 (77%)	215 (99%)	3 (1%)	59	71
1	GO	218/284 (77%)	215 (99%)	3 (1%)	59	71
1	H4	215/284 (76%)	215 (100%)	0	100	100
1	H9	215/284 (76%)	215 (100%)	0	100	100
1	HE	215/284 (76%)	215 (100%)	0	100	100
1	HJ	215/284 (76%)	215 (100%)	0	100	100
1	HO	215/284 (76%)	215 (100%)	0	100	100
1	I4	215/284 (76%)	215 (100%)	0	100	100
1	I9	215/284 (76%)	215 (100%)	0	100	100
1	IE	215/284 (76%)	215 (100%)	0	100	100
1	IJ	215/284 (76%)	215 (100%)	0	100	100
1	IO	215/284 (76%)	215 (100%)	0	100	100
1	J4	215/284 (76%)	215 (100%)	0	100	100
1	J9	215/284 (76%)	215 (100%)	0	100	100
1	JE	215/284 (76%)	215 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	JJ	215/284 (76%)	215 (100%)	0	100	100
1	JO	215/284 (76%)	215 (100%)	0	100	100
1	K4	215/284 (76%)	213 (99%)	2 (1%)	70	76
1	K9	215/284 (76%)	213 (99%)	2 (1%)	70	76
1	KE	215/284 (76%)	213 (99%)	2 (1%)	70	76
1	KJ	215/284 (76%)	213 (99%)	2 (1%)	70	76
1	KO	215/284 (76%)	213 (99%)	2 (1%)	70	76
1	L4	215/284 (76%)	214 (100%)	1 (0%)	81	81
1	L9	215/284 (76%)	214 (100%)	1 (0%)	81	81
1	LE	215/284 (76%)	214 (100%)	1 (0%)	81	81
1	LJ	215/284 (76%)	214 (100%)	1 (0%)	81	81
1	LO	215/284 (76%)	214 (100%)	1 (0%)	81	81
1	M4	218/284 (77%)	216 (99%)	2 (1%)	70	76
1	M9	218/284 (77%)	216 (99%)	2 (1%)	70	76
1	ME	218/284 (77%)	216 (99%)	2 (1%)	70	76
1	MJ	218/284 (77%)	216 (99%)	2 (1%)	70	76
1	MO	218/284 (77%)	216 (99%)	2 (1%)	70	76
1	N4	218/284 (77%)	214 (98%)	4 (2%)	51	66
1	N9	218/284 (77%)	214 (98%)	4 (2%)	51	66
1	NE	218/284 (77%)	214 (98%)	4 (2%)	51	66
1	NJ	218/284 (77%)	214 (98%)	4 (2%)	51	66
1	NO	218/284 (77%)	214 (98%)	4 (2%)	51	66
1	O4	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	O9	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	OE	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	OJ	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	OO	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	P4	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	P9	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	PE	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	PJ	218/284 (77%)	217 (100%)	1 (0%)	81	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	PO	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	Q4	218/284 (77%)	215 (99%)	3 (1%)	59	71
1	Q9	218/284 (77%)	215 (99%)	3 (1%)	59	71
1	QE	218/284 (77%)	215 (99%)	3 (1%)	59	71
1	QJ	218/284 (77%)	215 (99%)	3 (1%)	59	71
1	QO	218/284 (77%)	215 (99%)	3 (1%)	59	71
1	R4	218/284 (77%)	215 (99%)	3 (1%)	59	71
1	R9	218/284 (77%)	215 (99%)	3 (1%)	59	71
1	RE	218/284 (77%)	215 (99%)	3 (1%)	59	71
1	RJ	218/284 (77%)	215 (99%)	3 (1%)	59	71
1	RO	218/284 (77%)	215 (99%)	3 (1%)	59	71
1	S4	215/284 (76%)	215 (100%)	0	100	100
1	S9	215/284 (76%)	215 (100%)	0	100	100
1	SE	215/284 (76%)	215 (100%)	0	100	100
1	SJ	215/284 (76%)	215 (100%)	0	100	100
1	SO	215/284 (76%)	215 (100%)	0	100	100
1	T4	215/284 (76%)	214 (100%)	1 (0%)	81	81
1	T9	215/284 (76%)	214 (100%)	1 (0%)	81	81
1	TE	215/284 (76%)	214 (100%)	1 (0%)	81	81
1	TJ	215/284 (76%)	214 (100%)	1 (0%)	81	81
1	TO	215/284 (76%)	214 (100%)	1 (0%)	81	81
1	U4	215/284 (76%)	214 (100%)	1 (0%)	81	81
1	U9	215/284 (76%)	213 (99%)	2 (1%)	70	76
1	UE	215/284 (76%)	214 (100%)	1 (0%)	81	81
1	UJ	215/284 (76%)	214 (100%)	1 (0%)	81	81
1	UO	215/284 (76%)	214 (100%)	1 (0%)	81	81
1	V4	215/284 (76%)	215 (100%)	0	100	100
1	V9	215/284 (76%)	215 (100%)	0	100	100
1	VE	215/284 (76%)	215 (100%)	0	100	100
1	VJ	215/284 (76%)	215 (100%)	0	100	100
1	VO	215/284 (76%)	215 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W4	215/284 (76%)	214 (100%)	1 (0%)	81	81
1	W9	215/284 (76%)	214 (100%)	1 (0%)	81	81
1	WE	215/284 (76%)	214 (100%)	1 (0%)	81	81
1	WJ	215/284 (76%)	214 (100%)	1 (0%)	81	81
1	WO	215/284 (76%)	214 (100%)	1 (0%)	81	81
1	X4	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	X9	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	XE	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	XJ	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	XO	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	Y4	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	Y9	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	YE	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	YJ	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	YO	218/284 (77%)	217 (100%)	1 (0%)	81	81
1	Z4	217/284 (76%)	217 (100%)	0	100	100
1	Z9	217/284 (76%)	217 (100%)	0	100	100
1	ZE	217/284 (76%)	217 (100%)	0	100	100
1	ZJ	217/284 (76%)	217 (100%)	0	100	100
1	ZO	217/284 (76%)	217 (100%)	0	100	100
2	A1	69/69 (100%)	69 (100%)	0	100	100
2	A2	69/69 (100%)	69 (100%)	0	100	100
2	A3	69/69 (100%)	69 (100%)	0	100	100
2	A6	69/69 (100%)	69 (100%)	0	100	100
2	A7	69/69 (100%)	69 (100%)	0	100	100
2	A8	69/69 (100%)	69 (100%)	0	100	100
2	AB	69/69 (100%)	69 (100%)	0	100	100
2	AC	69/69 (100%)	69 (100%)	0	100	100
2	AD	69/69 (100%)	69 (100%)	0	100	100
2	AG	69/69 (100%)	69 (100%)	0	100	100
2	AH	69/69 (100%)	69 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AI	69/69 (100%)	69 (100%)	0	100	100
2	AL	69/69 (100%)	69 (100%)	0	100	100
2	AM	69/69 (100%)	69 (100%)	0	100	100
2	AN	69/69 (100%)	69 (100%)	0	100	100
2	B2	69/69 (100%)	69 (100%)	0	100	100
2	B3	69/69 (100%)	69 (100%)	0	100	100
2	B7	69/69 (100%)	69 (100%)	0	100	100
2	B8	69/69 (100%)	69 (100%)	0	100	100
2	BC	69/69 (100%)	69 (100%)	0	100	100
2	BD	69/69 (100%)	69 (100%)	0	100	100
2	BH	69/69 (100%)	69 (100%)	0	100	100
2	BI	69/69 (100%)	69 (100%)	0	100	100
2	BM	69/69 (100%)	69 (100%)	0	100	100
2	BN	69/69 (100%)	69 (100%)	0	100	100
2	C2	69/69 (100%)	69 (100%)	0	100	100
2	C3	69/69 (100%)	69 (100%)	0	100	100
2	C7	69/69 (100%)	69 (100%)	0	100	100
2	C8	69/69 (100%)	69 (100%)	0	100	100
2	CC	69/69 (100%)	69 (100%)	0	100	100
2	CD	69/69 (100%)	69 (100%)	0	100	100
2	CH	69/69 (100%)	69 (100%)	0	100	100
2	CI	69/69 (100%)	69 (100%)	0	100	100
2	CM	69/69 (100%)	69 (100%)	0	100	100
2	CN	69/69 (100%)	69 (100%)	0	100	100
2	D2	69/69 (100%)	69 (100%)	0	100	100
2	D3	69/69 (100%)	69 (100%)	0	100	100
2	D7	69/69 (100%)	69 (100%)	0	100	100
2	D8	69/69 (100%)	69 (100%)	0	100	100
2	DC	69/69 (100%)	69 (100%)	0	100	100
2	DD	69/69 (100%)	69 (100%)	0	100	100
2	DH	69/69 (100%)	69 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	DI	69/69 (100%)	69 (100%)	0	100	100
2	DM	69/69 (100%)	69 (100%)	0	100	100
2	DN	69/69 (100%)	69 (100%)	0	100	100
2	E2	69/69 (100%)	69 (100%)	0	100	100
2	E3	69/69 (100%)	69 (100%)	0	100	100
2	E7	69/69 (100%)	69 (100%)	0	100	100
2	E8	69/69 (100%)	69 (100%)	0	100	100
2	EC	69/69 (100%)	69 (100%)	0	100	100
2	ED	69/69 (100%)	69 (100%)	0	100	100
2	EH	69/69 (100%)	69 (100%)	0	100	100
2	EI	69/69 (100%)	69 (100%)	0	100	100
2	EM	69/69 (100%)	69 (100%)	0	100	100
2	EN	69/69 (100%)	69 (100%)	0	100	100
3	F2	5/224 (2%)	5 (100%)	0	100	100
3	F3	5/224 (2%)	5 (100%)	0	100	100
3	F7	5/224 (2%)	5 (100%)	0	100	100
3	F8	5/224 (2%)	5 (100%)	0	100	100
3	FC	5/224 (2%)	5 (100%)	0	100	100
3	FD	5/224 (2%)	5 (100%)	0	100	100
3	FH	5/224 (2%)	5 (100%)	0	100	100
3	FI	5/224 (2%)	5 (100%)	0	100	100
3	FM	5/224 (2%)	5 (100%)	0	100	100
3	FN	5/224 (2%)	5 (100%)	0	100	100
4	2A	138/141 (98%)	137 (99%)	1 (1%)	76	79
4	2B	139/141 (99%)	139 (100%)	0	100	100
4	2C	138/141 (98%)	137 (99%)	1 (1%)	76	79
4	2D	140/141 (99%)	140 (100%)	0	100	100
4	2E	138/141 (98%)	137 (99%)	1 (1%)	76	79
4	2F	140/141 (99%)	140 (100%)	0	100	100
4	2G	137/141 (97%)	136 (99%)	1 (1%)	76	79
4	2H	139/141 (99%)	139 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	2I	138/141 (98%)	137 (99%)	1 (1%)	76	79
4	2J	140/141 (99%)	140 (100%)	0	100	100
4	2K	137/141 (97%)	136 (99%)	1 (1%)	76	79
4	2L	140/141 (99%)	140 (100%)	0	100	100
5	1A	272/302 (90%)	268 (98%)	4 (2%)	57	70
5	1B	274/302 (91%)	272 (99%)	2 (1%)	76	79
5	1C	272/302 (90%)	268 (98%)	4 (2%)	57	70
5	1D	273/302 (90%)	271 (99%)	2 (1%)	76	79
5	1E	273/302 (90%)	269 (98%)	4 (2%)	57	70
5	1F	273/302 (90%)	271 (99%)	2 (1%)	76	79
5	1G	274/302 (91%)	270 (98%)	4 (2%)	57	70
5	1H	273/302 (90%)	271 (99%)	2 (1%)	76	79
5	1I	273/302 (90%)	269 (98%)	4 (2%)	57	70
5	1J	273/302 (90%)	271 (99%)	2 (1%)	76	79
5	1K	273/302 (90%)	269 (98%)	4 (2%)	57	70
5	1L	273/302 (90%)	271 (99%)	2 (1%)	76	79
6	4A	91/92 (99%)	91 (100%)	0	100	100
6	4B	91/92 (99%)	91 (100%)	0	100	100
6	4C	91/92 (99%)	91 (100%)	0	100	100
6	4D	91/92 (99%)	91 (100%)	0	100	100
6	4E	91/92 (99%)	91 (100%)	0	100	100
6	4F	91/92 (99%)	91 (100%)	0	100	100
7	3A	83/85 (98%)	83 (100%)	0	100	100
7	3B	83/85 (98%)	83 (100%)	0	100	100
7	3C	83/85 (98%)	83 (100%)	0	100	100
7	3D	83/85 (98%)	83 (100%)	0	100	100
7	3E	83/85 (98%)	83 (100%)	0	100	100
7	3F	83/85 (98%)	83 (100%)	0	100	100
8	50	99/103 (96%)	99 (100%)	0	100	100
8	51	99/103 (96%)	99 (100%)	0	100	100
8	52	99/103 (96%)	99 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	53	99/103 (96%)	99 (100%)	0	100	100
8	5A	99/103 (96%)	97 (98%)	2 (2%)	48	65
8	5B	99/103 (96%)	97 (98%)	2 (2%)	48	65
8	5C	99/103 (96%)	97 (98%)	2 (2%)	48	65
8	5D	99/103 (96%)	97 (98%)	2 (2%)	48	65
8	5E	99/103 (96%)	97 (98%)	2 (2%)	48	65
8	5F	99/103 (96%)	97 (98%)	2 (2%)	48	65
8	5G	99/103 (96%)	99 (100%)	0	100	100
8	5H	99/103 (96%)	99 (100%)	0	100	100
8	5I	99/103 (96%)	99 (100%)	0	100	100
8	5J	99/103 (96%)	99 (100%)	0	100	100
8	5K	99/103 (96%)	99 (100%)	0	100	100
8	5L	99/103 (96%)	99 (100%)	0	100	100
8	5M	99/103 (96%)	99 (100%)	0	100	100
8	5N	99/103 (96%)	99 (100%)	0	100	100
8	5O	99/103 (96%)	99 (100%)	0	100	100
8	5P	99/103 (96%)	99 (100%)	0	100	100
8	5Q	99/103 (96%)	99 (100%)	0	100	100
8	5R	99/103 (96%)	99 (100%)	0	100	100
8	5S	99/103 (96%)	99 (100%)	0	100	100
8	5T	99/103 (96%)	99 (100%)	0	100	100
8	5U	99/103 (96%)	99 (100%)	0	100	100
8	5V	99/103 (96%)	99 (100%)	0	100	100
8	5W	99/103 (96%)	99 (100%)	0	100	100
8	5X	99/103 (96%)	99 (100%)	0	100	100
8	5Y	99/103 (96%)	99 (100%)	0	100	100
8	5Z	99/103 (96%)	99 (100%)	0	100	100
9	7A	212/218 (97%)	212 (100%)	0	100	100
9	7B	212/218 (97%)	212 (100%)	0	100	100
9	7C	212/218 (97%)	212 (100%)	0	100	100
10	8A	310/952 (33%)	307 (99%)	3 (1%)	68	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	8B	310/952 (33%)	307 (99%)	3 (1%)	68	76
10	8C	310/952 (33%)	307 (99%)	3 (1%)	68	76
11	6A	109/169 (64%)	107 (98%)	2 (2%)	51	66
11	6B	109/169 (64%)	106 (97%)	3 (3%)	38	59
11	6C	109/169 (64%)	107 (98%)	2 (2%)	51	66
11	6D	109/169 (64%)	106 (97%)	3 (3%)	38	59
11	6E	109/169 (64%)	107 (98%)	2 (2%)	51	66
11	6F	109/169 (64%)	106 (97%)	3 (3%)	38	59
All	All	46345/61207 (76%)	46044 (99%)	301 (1%)	76	80

5 of 301 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	5A	45	GLU
10	8C	219	LEU
5	1L	244	LEU
5	1E	25	VAL
11	6C	203	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 439 such sidechains are listed below:

Mol	Chain	Res	Type
2	BD	39	GLN
2	A8	7	HIS
8	51	116	HIS
8	5N	102	GLN
2	AC	39	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	SF4	7C	301	-	0,12,12	-	-	-		
12	SF4	7A	301	-	0,12,12	-	-	-		
12	SF4	7B	301	-	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	SF4	7C	301	-	-	-	0/6/5/5
12	SF4	7A	301	-	-	-	0/6/5/5
12	SF4	7B	301	-	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

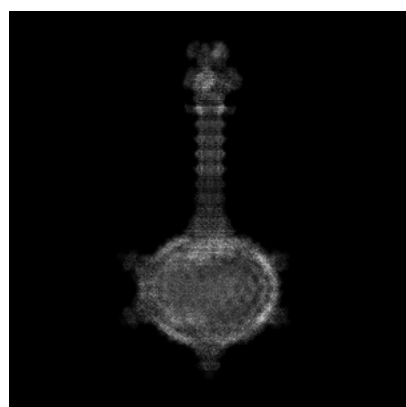
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10443. These allow visual inspection of the internal detail of the map and identification of artifacts.

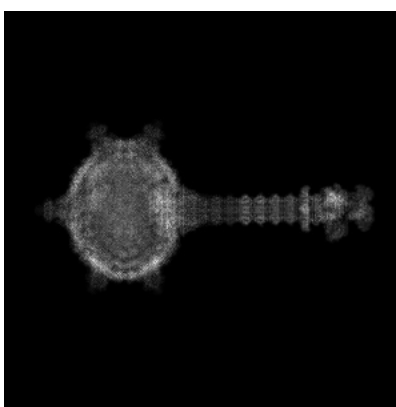
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

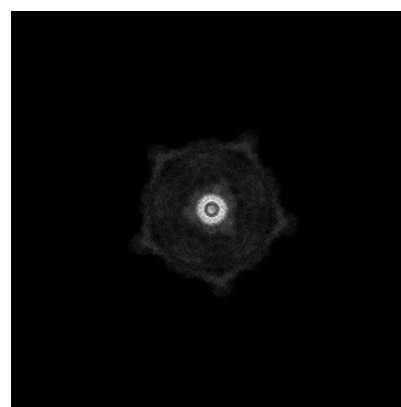
6.1.1 Primary map



X



Y

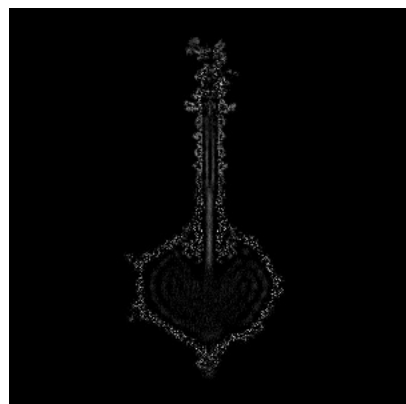


Z

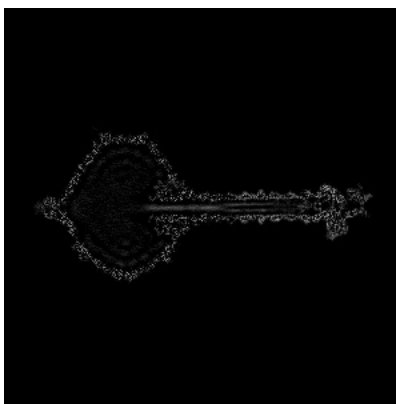
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

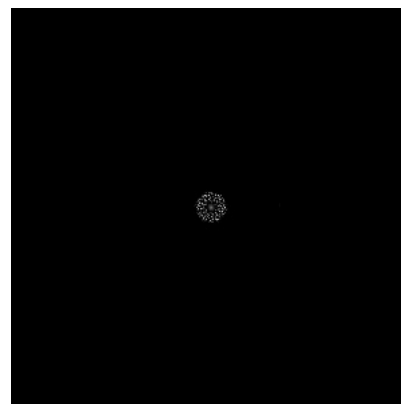
6.2.1 Primary map



X Index: 480



Y Index: 480

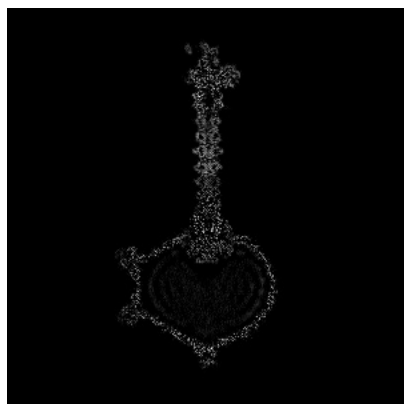


Z Index: 480

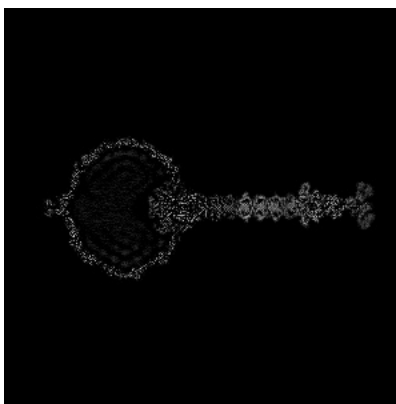
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

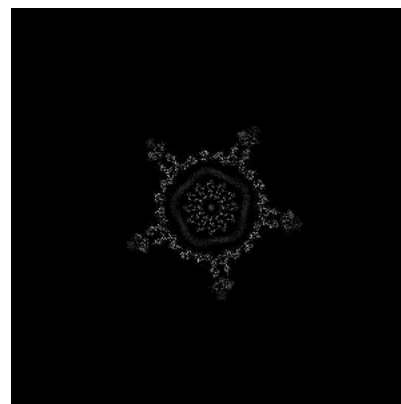
6.3.1 Primary map



X Index: 501



Y Index: 503

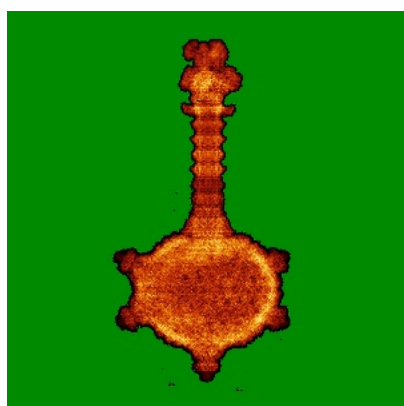


Z Index: 371

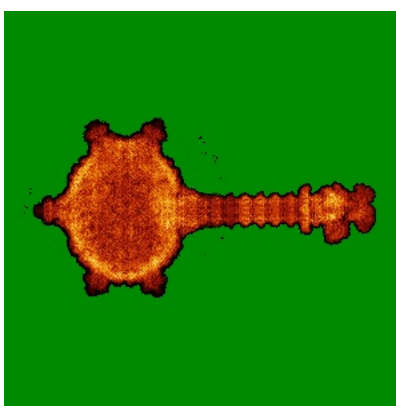
The images above show the largest variance slices of the map in three orthogonal directions.

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

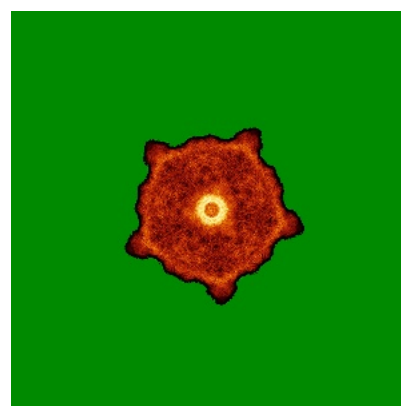
6.4.1 Primary map



X



Y

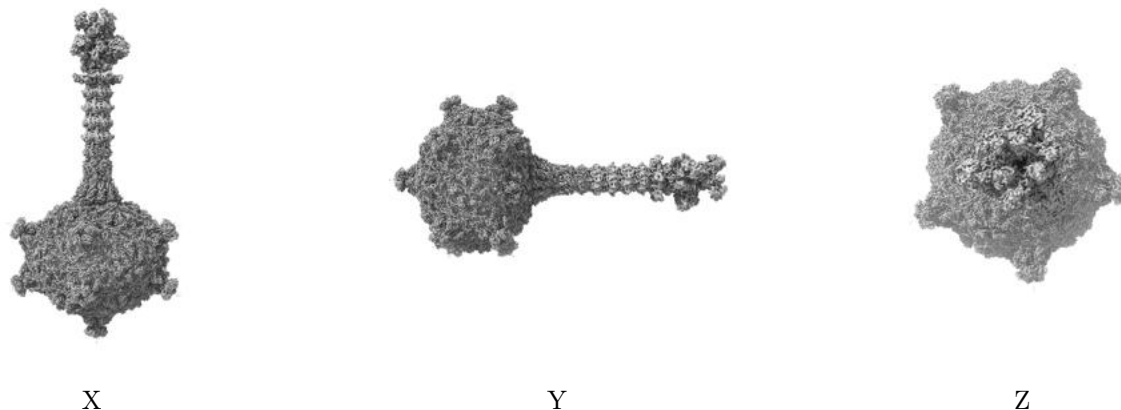


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

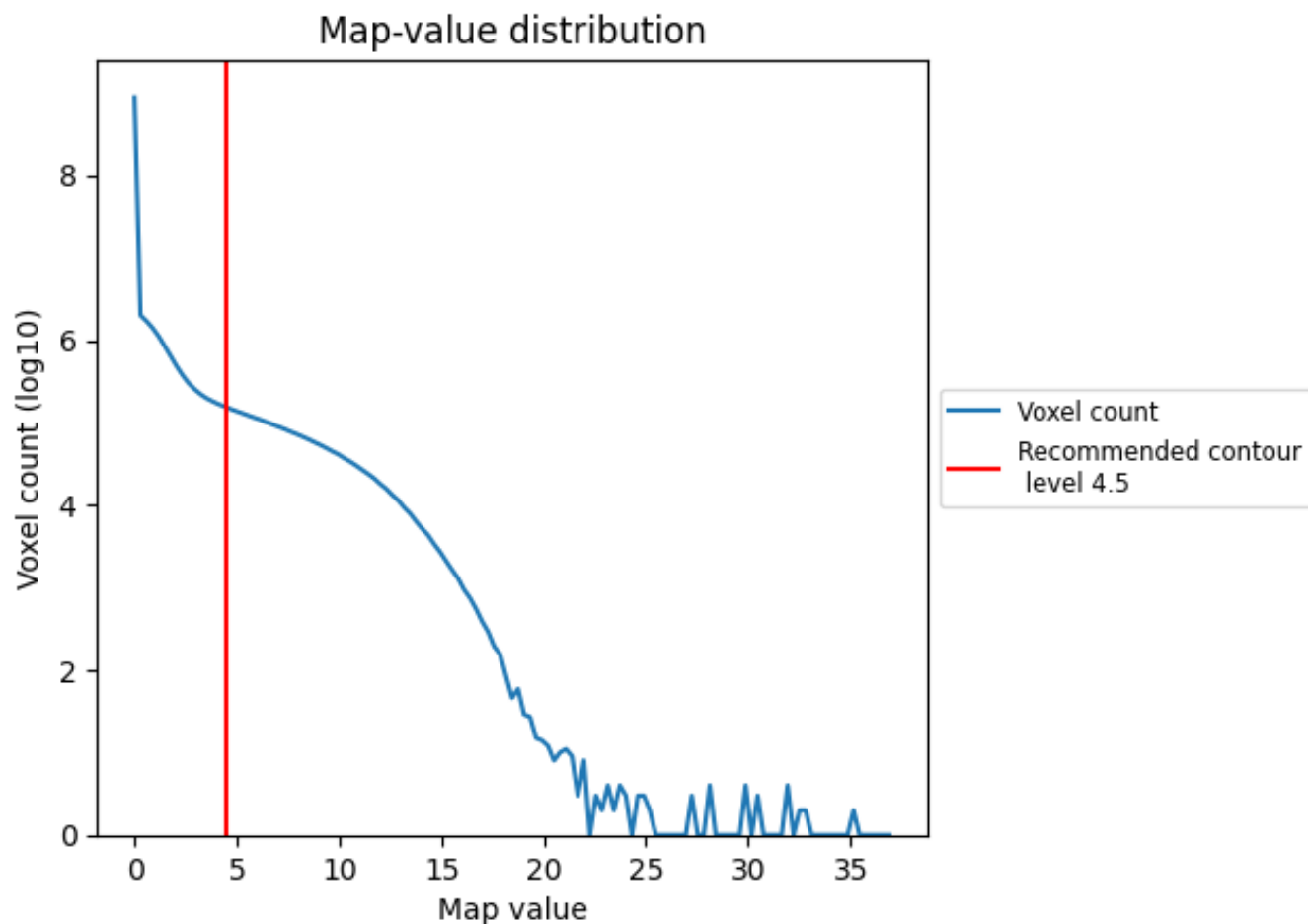
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

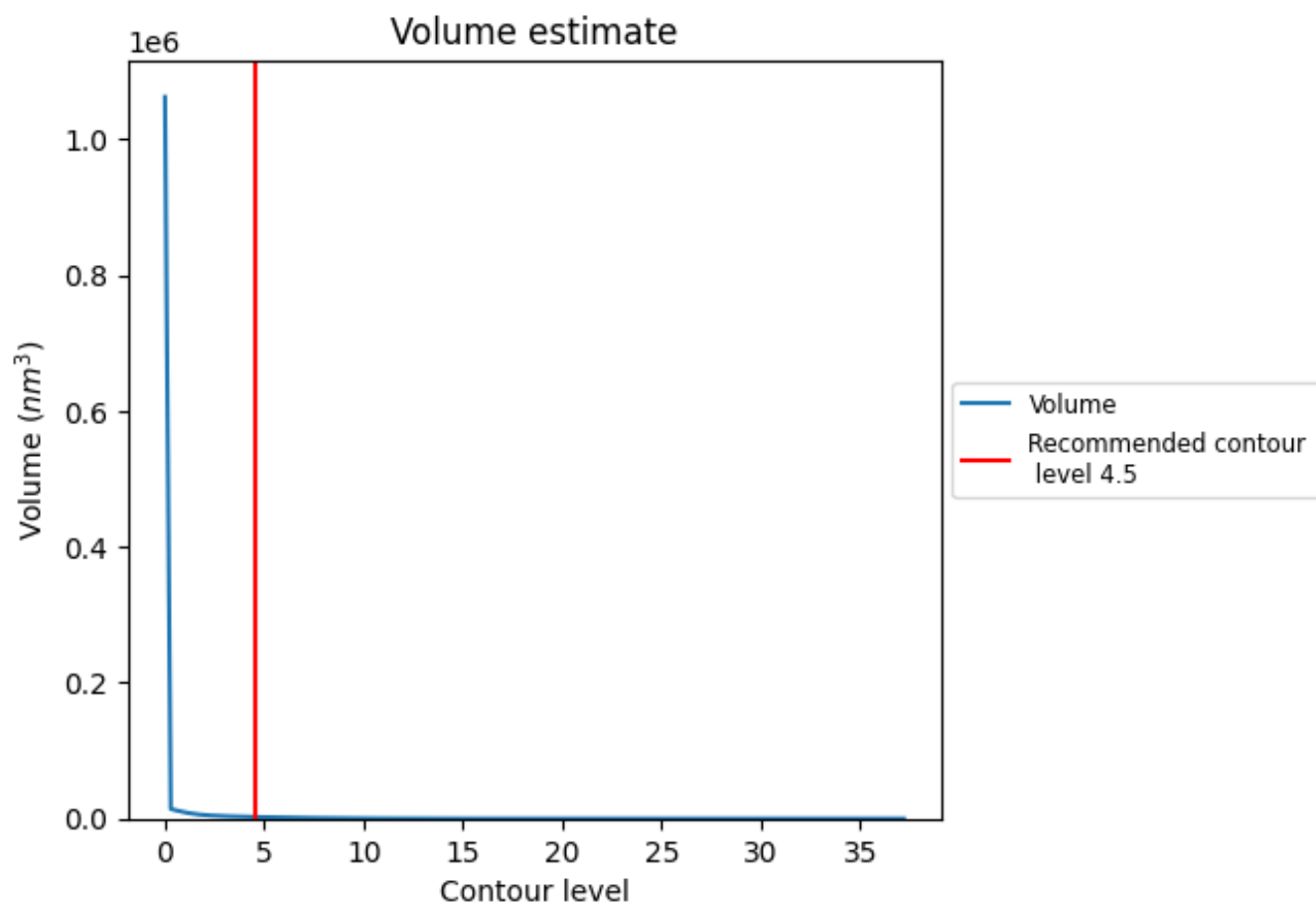
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

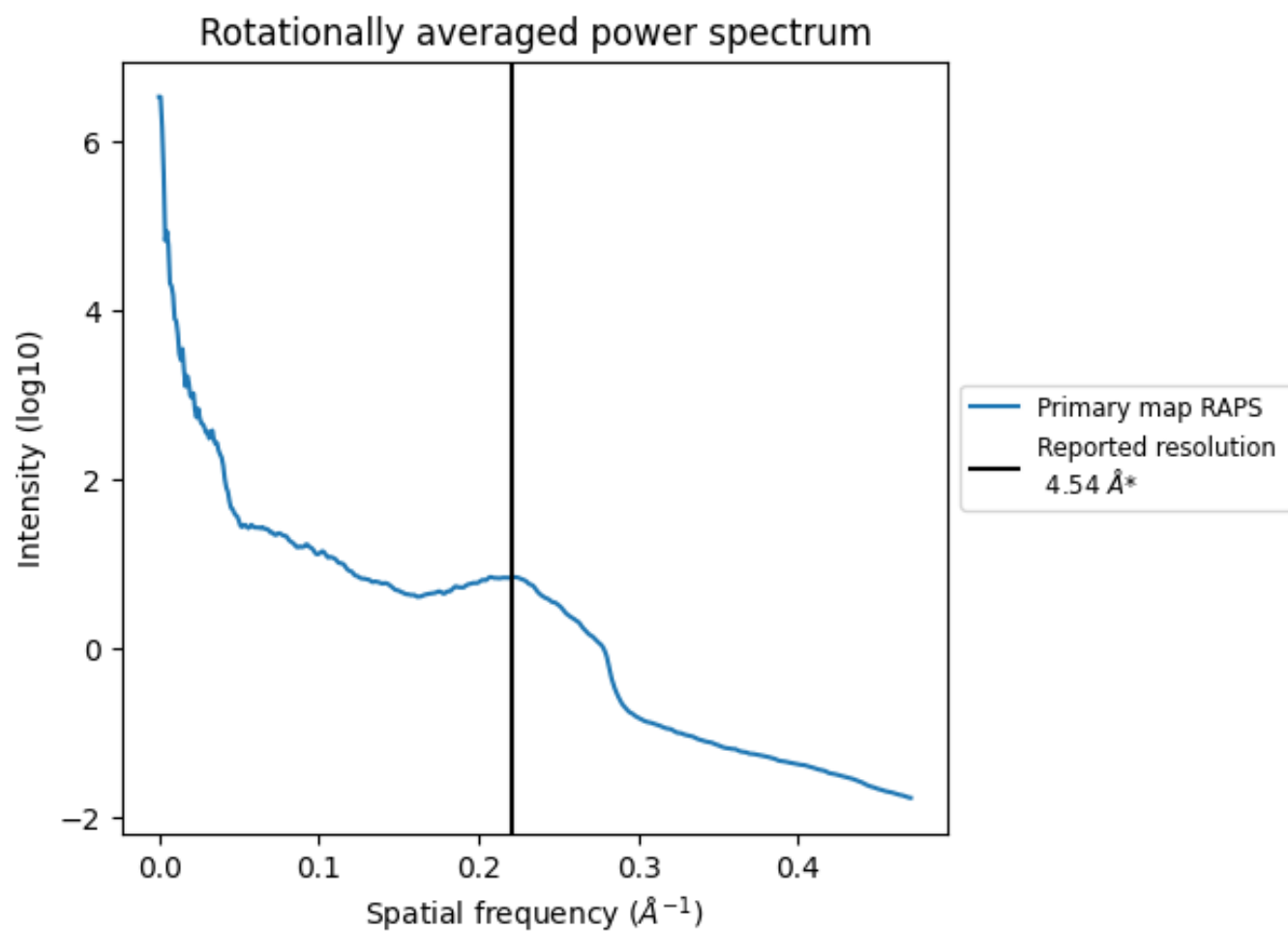
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2436 nm³; this corresponds to an approximate mass of 2201 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

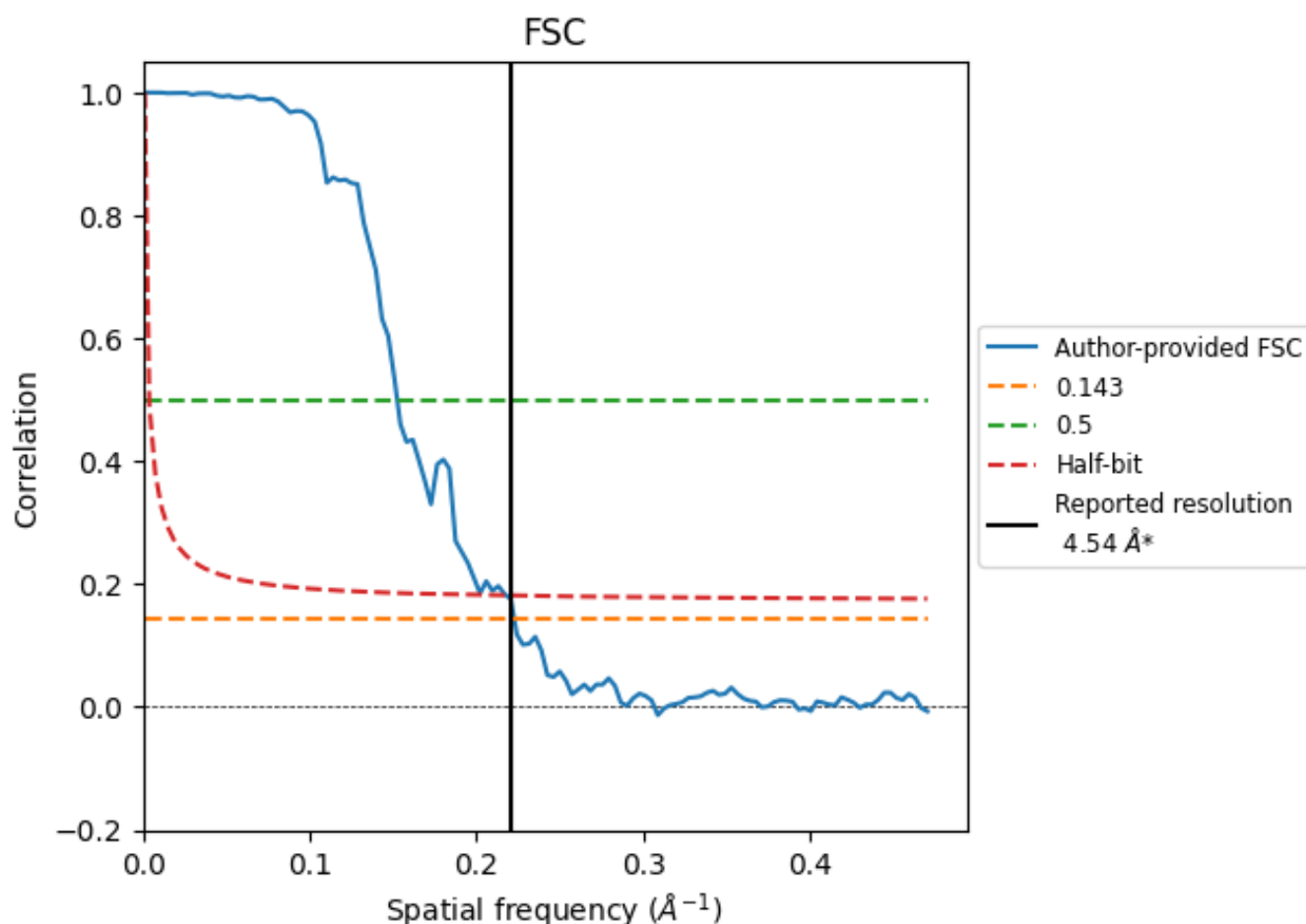


*Reported resolution corresponds to spatial frequency of 0.220 Å⁻¹

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 0.220 Å⁻¹

8.2 Resolution estimates [i](#)

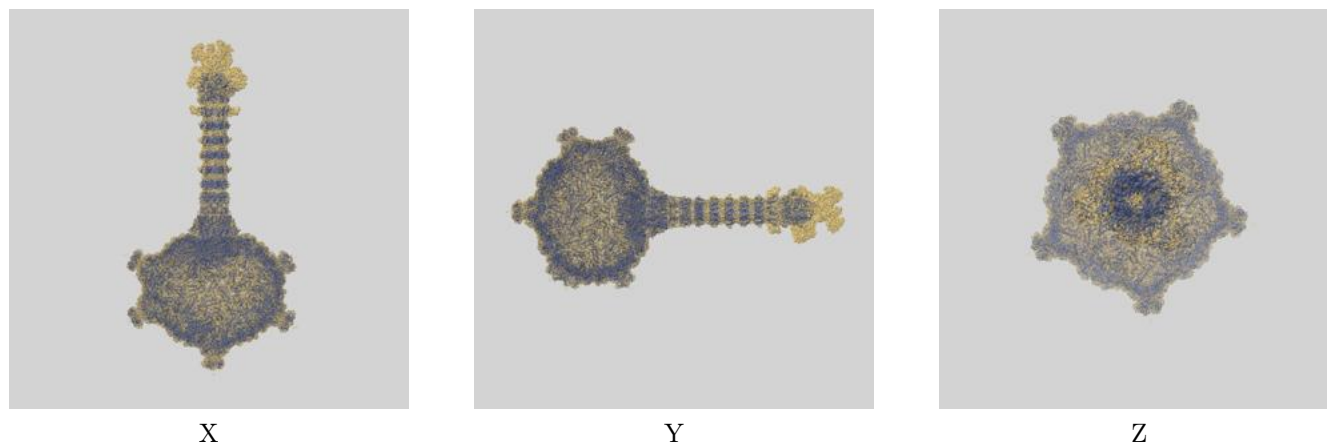
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.54	-	-
Author-provided FSC curve	4.49	6.56	4.59
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

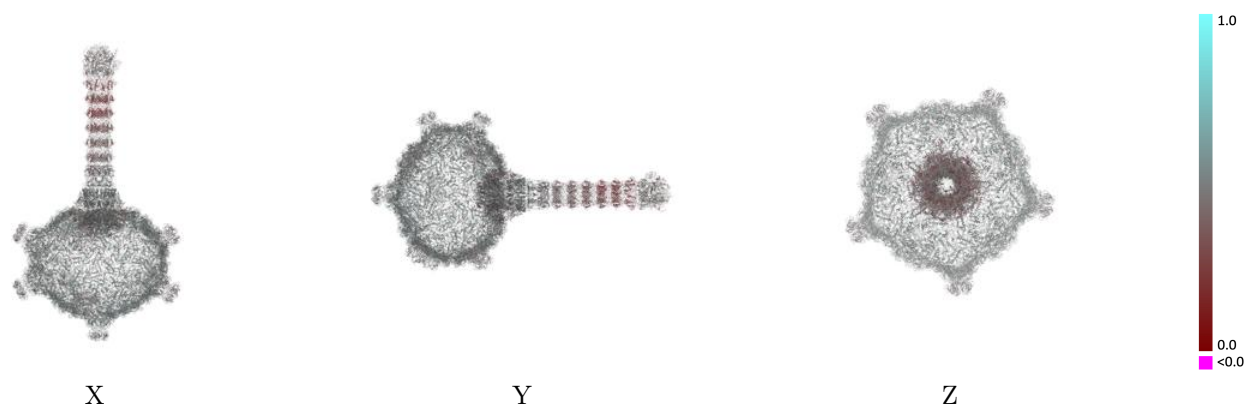
This section contains information regarding the fit between EMDB map EMD-10443 and PDB model 6TBA. Per-residue inclusion information can be found in section [3](#) on page [31](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

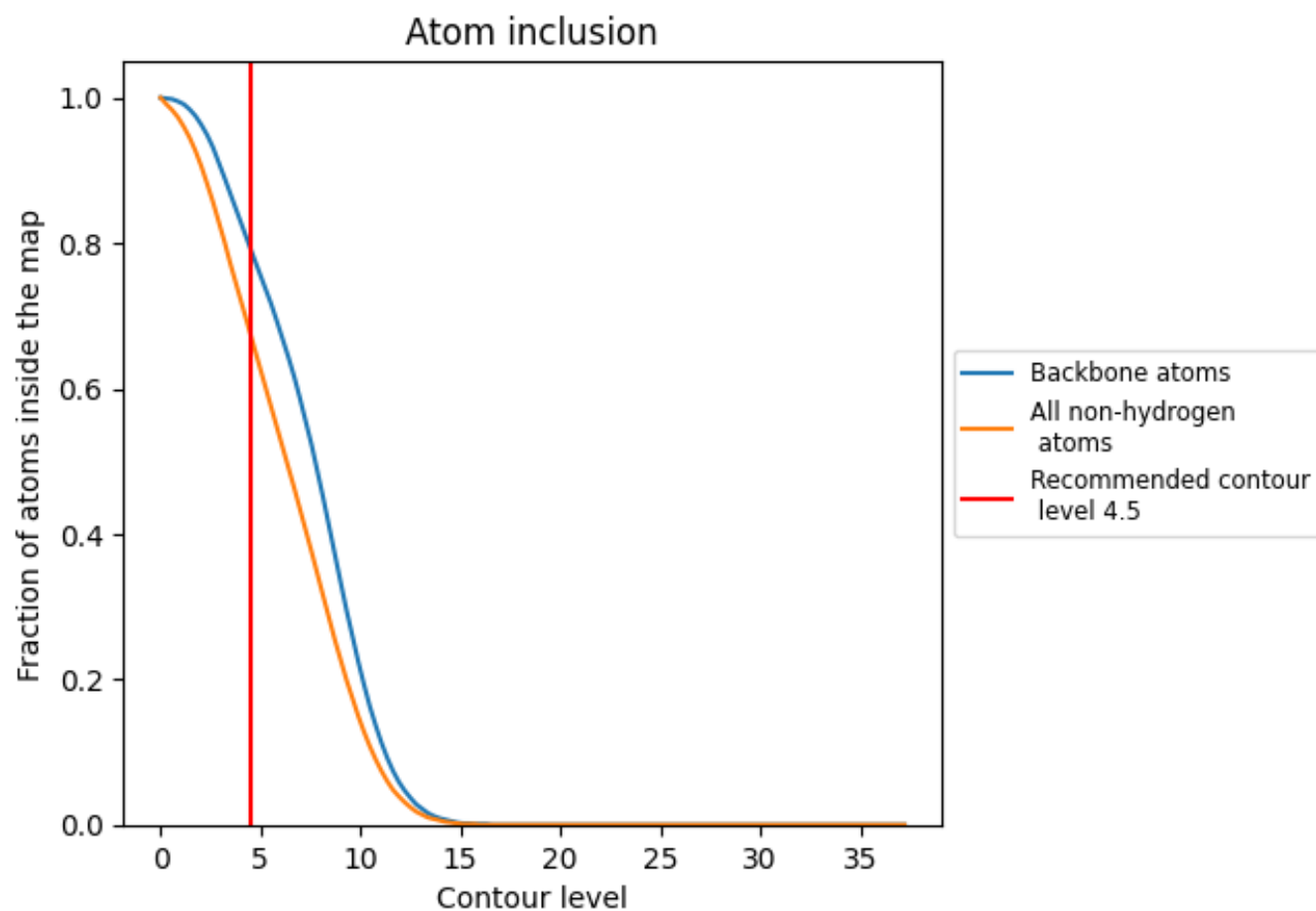


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 67% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6740	 0.4720
1A	 0.5900	 0.4690
1B	 0.5820	 0.4650
1C	 0.5760	 0.4640
1D	 0.5670	 0.4590
1E	 0.5550	 0.4510
1F	 0.5620	 0.4540
1G	 0.5580	 0.4480
1H	 0.5660	 0.4570
1I	 0.5630	 0.4550
1J	 0.5530	 0.4600
1K	 0.5580	 0.4660
1L	 0.5670	 0.4630
2A	 0.6070	 0.4800
2B	 0.6190	 0.4820
2C	 0.6260	 0.4780
2D	 0.6130	 0.4730
2E	 0.6210	 0.4760
2F	 0.5930	 0.4720
2G	 0.5890	 0.4700
2H	 0.5830	 0.4700
2I	 0.5990	 0.4730
2J	 0.6200	 0.4750
2K	 0.6230	 0.4780
2L	 0.5990	 0.4750
3A	 0.6450	 0.5030
3B	 0.6640	 0.4980
3C	 0.6350	 0.4850
3D	 0.6420	 0.4770
3E	 0.6630	 0.4830
3F	 0.6580	 0.4940
4A	 0.6090	 0.4710
4B	 0.5980	 0.4430
4C	 0.5790	 0.4090
4D	 0.5770	 0.4050



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Chain	Atom inclusion	Q-score
4E	 0.6120	 0.4300
4F	 0.6210	 0.4590
50	 0.6280	 0.3020
51	 0.6360	 0.3070
52	 0.6240	 0.3030
53	 0.6320	 0.3080
5A	 0.5030	 0.4340
5B	 0.4800	 0.4130
5C	 0.4900	 0.3650
5D	 0.4730	 0.3460
5E	 0.4460	 0.3780
5F	 0.4970	 0.4170
5G	 0.7870	 0.3970
5H	 0.7840	 0.3930
5I	 0.7780	 0.3880
5J	 0.7660	 0.3890
5K	 0.7830	 0.3870
5L	 0.7770	 0.3890
5M	 0.7830	 0.3960
5N	 0.7650	 0.3780
5O	 0.7550	 0.3400
5P	 0.7410	 0.3230
5Q	 0.7360	 0.3410
5R	 0.7740	 0.3790
5S	 0.7420	 0.3630
5T	 0.7230	 0.3220
5U	 0.6950	 0.2530
5V	 0.6560	 0.2150
5W	 0.6840	 0.2460
5X	 0.7180	 0.3260
5Y	 0.6260	 0.3010
5Z	 0.6370	 0.3010
6A	 0.7240	 0.3420
6B	 0.7210	 0.3480
6C	 0.7210	 0.3410
6D	 0.7180	 0.3480
6E	 0.7180	 0.3420
6F	 0.7230	 0.3480
7A	 0.7960	 0.4420
7B	 0.8000	 0.4440
7C	 0.7920	 0.4390
8A	 0.7600	 0.4460

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Chain	Atom inclusion	Q-score
8B	 0.7560	 0.4430
8C	 0.7580	 0.4460
A1	 0.6670	 0.4560
A2	 0.5800	 0.4560
A3	 0.5300	 0.4390
A4	 0.7360	 0.5020
A5	 0.6250	 0.4590
A6	 0.6620	 0.4500
A7	 0.5810	 0.4590
A8	 0.5350	 0.4380
A9	 0.7300	 0.4990
AA	 0.6230	 0.4570
AB	 0.6630	 0.4550
AC	 0.5810	 0.4570
AD	 0.5310	 0.4390
AE	 0.7350	 0.4980
AF	 0.6230	 0.4560
AG	 0.6680	 0.4580
AH	 0.5850	 0.4600
AI	 0.5220	 0.4380
AJ	 0.7320	 0.4960
AK	 0.6240	 0.4560
AL	 0.6630	 0.4560
AM	 0.5830	 0.4550
AN	 0.5410	 0.4360
AO	 0.7350	 0.4980
AP	 0.6250	 0.4590
B2	 0.5590	 0.4570
B3	 0.5520	 0.4360
B4	 0.7320	 0.5010
B5	 0.6490	 0.4750
B7	 0.5600	 0.4540
B8	 0.5520	 0.4380
B9	 0.7340	 0.5000
BA	 0.6440	 0.4720
BC	 0.5570	 0.4540
BD	 0.5560	 0.4360
BE	 0.7320	 0.5000
BF	 0.6430	 0.4700
BH	 0.5670	 0.4540
BI	 0.5520	 0.4380
BJ	 0.7290	 0.4980

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Chain	Atom inclusion	Q-score
BK	 0.6500	 0.4740
BM	 0.5570	 0.4560
BN	 0.5490	 0.4350
BO	 0.7330	 0.4980
BP	 0.6520	 0.4750
C2	 0.5440	 0.4400
C3	 0.5560	 0.4470
C4	 0.7330	 0.4960
C5	 0.7100	 0.4950
C7	 0.5470	 0.4400
C8	 0.5410	 0.4450
C9	 0.7330	 0.4950
CA	 0.7080	 0.4930
CC	 0.5570	 0.4410
CD	 0.5540	 0.4460
CE	 0.7320	 0.4960
CF	 0.7120	 0.4920
CH	 0.5460	 0.4370
CI	 0.5570	 0.4460
CJ	 0.7350	 0.4950
CK	 0.7090	 0.4930
CM	 0.5460	 0.4390
CN	 0.5570	 0.4480
CO	 0.7300	 0.4950
CP	 0.7090	 0.4910
D2	 0.5590	 0.4620
D3	 0.5540	 0.4440
D4	 0.7120	 0.5000
D7	 0.5670	 0.4650
D8	 0.5520	 0.4410
D9	 0.7110	 0.4980
DC	 0.5600	 0.4640
DD	 0.5570	 0.4430
DE	 0.7130	 0.4970
DH	 0.5570	 0.4630
DI	 0.5510	 0.4440
DJ	 0.7140	 0.4960
DM	 0.5560	 0.4600
DN	 0.5460	 0.4450
DO	 0.7110	 0.4970
E2	 0.5470	 0.4480
E3	 0.5670	 0.4580

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Chain	Atom inclusion	Q-score
E4	 0.7220	 0.5020
E7	 0.5430	 0.4520
E8	 0.5620	 0.4600
E9	 0.7230	 0.5010
EC	 0.5470	 0.4540
ED	 0.5670	 0.4600
EE	 0.7180	 0.5000
EH	 0.5430	 0.4540
EI	 0.5640	 0.4620
EJ	 0.7200	 0.5010
EM	 0.5440	 0.4480
EN	 0.5680	 0.4610
EO	 0.7160	 0.5020
F2	 0.3390	 0.3790
F3	 0.2740	 0.3470
F4	 0.7180	 0.5010
F7	 0.3710	 0.3790
F8	 0.2900	 0.3370
F9	 0.7150	 0.4980
FC	 0.3550	 0.3960
FD	 0.2740	 0.3370
FE	 0.7170	 0.4980
FH	 0.3390	 0.3870
FI	 0.3060	 0.3290
FJ	 0.7150	 0.4980
FM	 0.3550	 0.3890
FN	 0.2900	 0.3260
FO	 0.7180	 0.4970
G4	 0.7300	 0.5050
G9	 0.7270	 0.5030
GE	 0.7270	 0.5020
GJ	 0.7250	 0.5020
GO	 0.7240	 0.5010
H4	 0.6940	 0.4920
H9	 0.6960	 0.4880
HE	 0.6960	 0.4900
HJ	 0.6990	 0.4890
HO	 0.6980	 0.4880
I4	 0.6780	 0.4910
I9	 0.6770	 0.4910
IE	 0.6760	 0.4910
IJ	 0.6800	 0.4910

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Chain	Atom inclusion	Q-score
IO	 0.6750	 0.4900
J4	 0.6870	 0.4940
J9	 0.6830	 0.4910
JE	 0.6850	 0.4940
JJ	 0.6880	 0.4920
JO	 0.6830	 0.4930
K4	 0.6820	 0.4900
K9	 0.6820	 0.4890
KE	 0.6850	 0.4880
KJ	 0.6830	 0.4880
KO	 0.6830	 0.4900
L4	 0.6960	 0.4980
L9	 0.6930	 0.4960
LE	 0.6930	 0.4950
LJ	 0.6910	 0.4970
LO	 0.6860	 0.4980
M4	 0.7030	 0.4970
M9	 0.6960	 0.4960
ME	 0.7010	 0.4940
MJ	 0.6990	 0.4950
MO	 0.6960	 0.4950
N4	 0.7060	 0.4910
N9	 0.7010	 0.4900
NE	 0.7040	 0.4890
NJ	 0.7040	 0.4890
NO	 0.6980	 0.4880
O4	 0.7130	 0.4970
O9	 0.6990	 0.4950
OE	 0.7040	 0.4950
OJ	 0.7030	 0.4940
OO	 0.7030	 0.4930
P4	 0.7030	 0.4950
P9	 0.6980	 0.4930
PE	 0.6990	 0.4920
PJ	 0.6980	 0.4910
PO	 0.6950	 0.4930
Q4	 0.7040	 0.4910
Q9	 0.7030	 0.4880
QE	 0.6990	 0.4890
QJ	 0.7020	 0.4850
QO	 0.6980	 0.4890
R4	 0.7050	 0.4940

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Chain	Atom inclusion	Q-score
R9	 0.6980	 0.4930
RE	 0.7010	 0.4930
RJ	 0.7000	 0.4940
RO	 0.7010	 0.4930
S4	 0.6810	 0.4890
S9	 0.6800	 0.4860
SE	 0.6770	 0.4830
SJ	 0.6830	 0.4860
SO	 0.6740	 0.4880
T4	 0.6850	 0.4900
T9	 0.6850	 0.4890
TE	 0.6800	 0.4890
TJ	 0.6830	 0.4880
TO	 0.6800	 0.4880
U4	 0.6780	 0.5010
U9	 0.6800	 0.4980
UE	 0.6790	 0.4990
UJ	 0.6800	 0.5000
UO	 0.6800	 0.4980
V4	 0.6890	 0.4900
V9	 0.6870	 0.4850
VE	 0.6910	 0.4850
VJ	 0.6860	 0.4850
VO	 0.6870	 0.4870
W4	 0.6840	 0.4860
W9	 0.6810	 0.4820
WE	 0.6820	 0.4820
WJ	 0.6860	 0.4820
WO	 0.6770	 0.4830
X4	 0.7000	 0.4990
X9	 0.7020	 0.4970
XE	 0.6960	 0.4980
XJ	 0.6960	 0.4980
XO	 0.6930	 0.4970
Y4	 0.7140	 0.4990
Y9	 0.7090	 0.4960
YE	 0.7120	 0.4940
YJ	 0.7110	 0.4950
YO	 0.7090	 0.4970
Z4	 0.7070	 0.4970
Z9	 0.7060	 0.4930
ZE	 0.7040	 0.4950

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Chain	Atom inclusion	Q-score
ZJ	 0.7050	 0.4970
ZO	 0.7040	 0.4950