wwPDB EM Validation Summary Report (i)

May 18, 2024 – 11:56 pm BST

PDB ID	:	6TBA
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 (i) 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 (i)) were used in the production of this report:

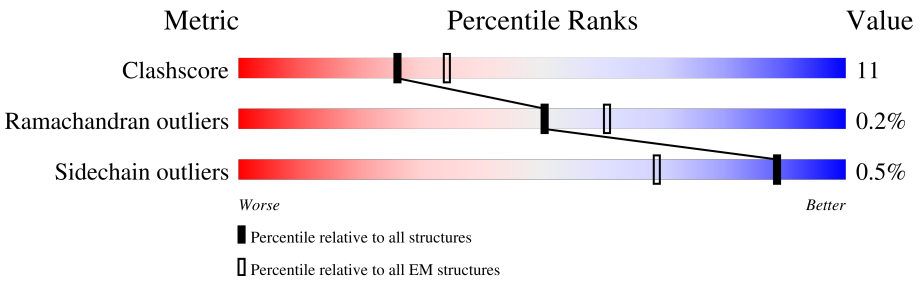
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	• 62% 13% 24%
1	A5	385	13% 61% 16% 23%
1	A9	385	• 62% 13% 24%
1	AA	385	13% 61% 16% 23%
1	AE	385	• 62% 14% 24%
1	AF	385	12% 61% 16% 23%
1	AJ	385	• 61% 14% 24%
1	AK	385	12% 62% 15% 23%

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Mol	Chain	Length	Quality of chain
1	AO	385	62% 13% 24%
1	AP	385	11% 61% 16% 23%
1	B4	385	64% 13% 23%
1	B5	385	8% 55% 15% 30%
1	B9	385	64% 13% 23%
1	BA	385	9% 55% 15% 30%
1	BE	385	64% 12% 23%
1	BF	385	9% 53% 16% 30%
1	BJ	385	64% 12% 23%
1	BK	385	8% 54% 15% 30%
1	BO	385	65% 11% 23%
1	BP	385	8% 53% 17% 30%
1	C4	385	64% 13% 23%
1	C5	385	65% 12% 23%
1	C9	385	64% 14% 23%
1	CA	385	5% 65% 12% 23%
1	CE	385	64% 14% 23%
1	CF	385	65% 12% 23%
1	CJ	385	63% 15% 23%
1	CK	385	65% 12% 23%
1	CO	385	64% 13% 23%
1	CP	385	65% 11% 23%
1	D4	385	60% 17% 23%
1	D9	385	60% 17% 23%
1	DE	385	60% 17% 23%

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Mol	Chain	Length	Quality of chain
1	DJ	385	60% 17% 23%
1	DO	385	60% 17% 23%
1	E4	385	60% 17% 23%
1	E9	385	60% 17% 23%
1	EE	385	60% 17% 23%
1	EJ	385	60% 17% 23%
1	EO	385	60% 17% 23%
1	F4	385	62% 15% 23%
1	F9	385	61% 16% 23%
1	FE	385	61% 16% 23%
1	FJ	385	62% 15% 23%
1	FO	385	61% 16% 23%
1	G4	385	64% 12% 23%
1	G9	385	64% 13% 23%
1	GE	385	64% 13% 23%
1	GJ	385	64% 12% 23%
1	GO	385	63% 13% 23%
1	H4	385	63% 12% 24%
1	H9	385	62% 13% 24%
1	HE	385	62% 13% 24%
1	HJ	385	62% 13% 24%
1	HO	385	62% 13% 24%
1	I4	385	5% 58% 17% 24%
1	I9	385	5% 59% 16% 24%
1	IE	385	5% 59% 16% 24%

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Mol	Chain	Length	Quality of chain
1	IJ	385	5% 59% 17% 24%
1	IO	385	5% 58% 17% 24%
1	J4	385	5% 57% 18% 24%
1	J9	385	5% 58% 17% 24%
1	JE	385	5% 58% 17% 24%
1	JJ	385	57% 18% 24%
1	JO	385	5% 57% 18% 24%
1	K4	385	59% 16% 24%
1	K9	385	59% 17% 24%
1	KE	385	60% 15% 24%
1	KJ	385	60% 15% 24%
1	KO	385	59% 16% 24%
1	L4	385	59% 16% 24%
1	L9	385	60% 16% 24%
1	LE	385	60% 16% 24%
1	LJ	385	61% 15% 24%
1	LO	385	60% 15% 24%
1	M4	385	63% 15% 23%
1	M9	385	63% 15% 23%
1	ME	385	63% 14% 23%
1	MJ	385	62% 15% 23%
1	MO	385	61% 16% 23%
1	N4	385	62% 15% 23%
1	N9	385	62% 15% 23%
1	NE	385	62% 15% 23%

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Mol	Chain	Length	Quality of chain
1	NJ	385	62% 14% 23%
1	NO	385	62% 15% 23%
1	O4	385	61% 16% 23%
1	O9	385	5% 60% 17% 23%
1	OE	385	60% 17% 23%
1	OJ	385	5% 61% 16% 23%
1	OO	385	61% 16% 23%
1	P4	385	63% 14% 23%
1	P9	385	62% 14% 23%
1	PE	385	62% 15% 23%
1	PJ	385	63% 14% 23%
1	PO	385	63% 14% 23%
1	Q4	385	61% 15% 23%
1	Q9	385	61% 15% 23%
1	QE	385	61% 15% 23%
1	QJ	385	61% 15% 23%
1	QO	385	60% 16% 23%
1	R4	385	65% 12% 23%
1	R9	385	64% 13% 23%
1	RE	385	63% 14% 23%
1	RJ	385	64% 13% 23%
1	RO	385	63% 14% 23%
1	S4	385	5% 60% 15% 24%
1	S9	385	5% 61% 14% 24%
1	SE	385	61% 15% 24%

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Mol	Chain	Length	Quality of chain
1	SJ	385	5% 61% 14% 24%
1	SO	385	5% 61% 15% 24%
1	T4	385	5% 61% 15% 24%
1	T9	385	61% 15% 24%
1	TE	385	5% 61% 14% 24%
1	TJ	385	5% 62% 14% 24%
1	TO	385	61% 15% 24%
1	U4	385	5% 61% 14% 24%
1	U9	385	5% 61% 15% 24%
1	UE	385	5% 61% 14% 24%
1	UJ	385	5% 61% 14% 24%
1	UO	385	5% 61% 15% 24%
1	V4	385	61% 15% 24%
1	V9	385	62% 14% 24%
1	VE	385	60% 15% 24%
1	VJ	385	61% 14% 24%
1	VO	385	61% 15% 24%
1	W4	385	5% 59% 16% 24%
1	W9	385	5% 59% 16% 24%
1	WE	385	6% 59% 16% 24%
1	WJ	385	5% 59% 16% 24%
1	WO	385	5% 60% 16% 24%
1	X4	385	67% 10% 23%
1	X9	385	67% 10% 23%
1	XE	385	66% 11% 23%

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Mol	Chain	Length	Quality of chain
1	XJ	385	66% 11% 23%
1	XO	385	67% 10% 23%
1	Y4	385	65% 12% 23%
1	Y9	385	64% 13% 23%
1	YE	385	65% 12% 23%
1	YJ	385	65% 12% 23%
1	YO	385	65% 12% 23%
1	Z4	385	62% 15% 23%
1	Z9	385	63% 14% 23%
1	ZE	385	63% 14% 23%
1	ZJ	385	63% 14% 23%
1	ZO	385	62% 14% 23%
2	A1	84	7% 67% 33%
2	A2	84	13% 64% 36%
2	A3	84	23% 68% 32%
2	A6	84	7% 65% 35%
2	A7	84	17% 65% 35%
2	A8	84	24% 68% 32%
2	AB	84	7% 64% 36%
2	AC	84	14% 65% 35%
2	AD	84	23% 68% 32%
2	AG	84	7% 65% 35%
2	AH	84	17% 64% 36%
2	AI	84	29% 69% 31%
2	AL	84	7% 67% 33%

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Mol	Chain	Length	Quality of chain
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%
2	CN	84	25% 65% 35%
2	D2	84	20% 69% 31%
2	D3	84	20% 67% 33%
2	D7	84	19% 70% 30%

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Mol	Chain	Length	Quality of chain
2	D8	84	20% 67% 33%
2	DC	84	20% 68% 32%
2	DD	84	17% 68% 32%
2	DH	84	19% 68% 32%
2	DI	84	19% 68% 32%
2	DM	84	21% 68% 32%
2	DN	84	21% 67% 33%
2	E2	84	24% 71% 29%
2	E3	84	14% 69% 31%
2	E7	84	24% 70% 30%
2	E8	84	18% 69% 31%
2	EC	84	21% 69% 31%
2	ED	84	13% 71% 29%
2	EH	84	25% 69% 31%
2	EI	84	15% 70% 30%
2	EM	84	23% 68% 32%
2	EN	84	14% 70% 30%
3	F2	325	97%
3	F3	325	97%
3	F7	325	97%
3	F8	325	97%
3	FC	325	97%
3	FD	325	97%
3	FH	325	97%
3	FI	325	97%

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Mol	Chain	Length	Quality of chain
3	FM	325	97%
3	FN	325	97%
4	2A	197	20% 70% 28%
4	2B	197	15% 66% 31%
4	2C	197	21% 72% 25%
4	2D	197	17% 66% 31%
4	2E	197	20% 69% 28%
4	2F	197	19% 64% 34%
4	2G	197	20% 71% 26%
4	2H	197	20% 65% 32%
4	2I	197	20% 70% 27%
4	2J	197	15% 66% 32%
4	2K	197	18% 72% 25%
4	2L	197	16% 66% 31%
5	1A	396	15% 74% 17% 9%
5	1B	396	17% 74% 17% 9%
5	1C	396	18% 74% 16% 9%
5	1D	396	18% 73% 18% 9%
5	1E	396	20% 73% 17% 9%
5	1F	396	20% 72% 19% 9%
5	1G	396	19% 73% 17% 9%
5	1H	396	19% 70% 21% 9%
5	1I	396	18% 71% 19% 9%
5	1J	396	21% 70% 21% 9%
5	1K	396	19% 71% 20% 9%

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Mol	Chain	Length	Quality of chain
5	1L	396	17% 71% 19% 9%
6	4A	135	13% 69% 28%
6	4B	135	19% 68% 29%
6	4C	135	21% 68% 29%
6	4D	135	21% 68% 29%
6	4E	135	13% 70% 27%
6	4F	135	13% 70% 27%
7	3A	112	8% 61% 38%
7	3B	112	6% 59% 39%
7	3C	112	6% 57% 41%
7	3D	112	8% 56% 42%
7	3E	112	5% 60% 38%
7	3F	112	6% 62% 36%
8	50	137	12% 50% 44% 5%
8	51	137	13% 58% 36% 5%
8	52	137	14% 54% 40% 5%
8	53	137	15% 58% 36% 5%
8	5A	137	28% 60% 34% 5%
8	5B	137	33% 59% 34% 5%
8	5C	137	29% 58% 36% 5%
8	5D	137	39% 58% 36% 5%
8	5E	137	39% 60% 34% 5%
8	5F	137	30% 61% 32% 5%
8	5G	137	57% 37% 5%
8	5H	137	58% 36% 5%

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Mol	Chain	Length	Quality of chain
8	5I	137	61% 34% 5%
8	5J	137	61% 34% 5%
8	5K	137	58% 36% 5%
8	5L	137	57% 37% 5%
8	5M	137	50% 44% 5%
8	5N	137	52% 42% 5%
8	5O	137	50% 44% 5%
8	5P	137	47% 47% 5%
8	5Q	137	47% 47% 5%
8	5R	137	47% 47% 5%
8	5S	137	50% 45% 5%
8	5T	137	46% 48% 5%
8	5U	137	10% 48% 46% 5%
8	5V	137	15% 45% 50% 5%
8	5W	137	7% 43% 51% 5%
8	5X	137	44% 50% 5%
8	5Y	137	12% 51% 43% 5%
8	5Z	137	11% 53% 41% 5%
9	7A	296	70% 28%
9	7B	296	71% 27%
9	7C	296	71% 27%
10	8A	1304	25% 9% 66%
10	8B	1304	25% 9% 66%
10	8C	1304	25% 8% 66%
11	6A	210	5% 38% 25% 36%

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Mol	Chain	Length	Quality of chain
11	6B	210	37% 24% • 36%
11	6C	210	36% 27% • 36%
11	6D	210	5% 37% 23% • 36%
11	6E	210	37% 26% • 36%
11	6F	210	37% 23% • 36%

2 Entry composition (i)

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

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

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

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

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

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

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

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

- Molecule 2 is a protein called Uncharacterized protein.

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

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

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

- Molecule 3 is a protein called Uncharacterized protein.

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

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

- Molecule 4 is a protein called Uncharacterized protein.

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

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

- Molecule 5 is a protein called Portal protein Rcc01684.

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

- Molecule 6 is a protein called Uncharacterized protein.

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

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

- Molecule 7 is a protein called Uncharacterized protein.

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

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

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

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

- Molecule 9 is a protein called Uncharacterized protein.

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

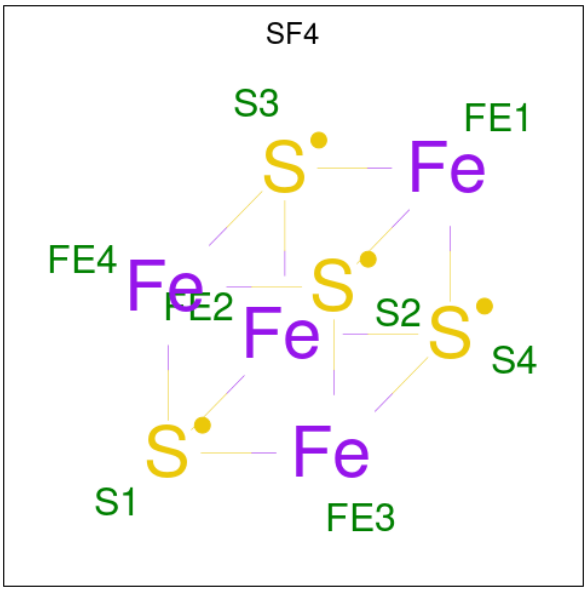
- Molecule 10 is a protein called Uncharacterized protein.

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

- Molecule 11 is a protein called Uncharacterized protein.

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

- Molecule 12 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



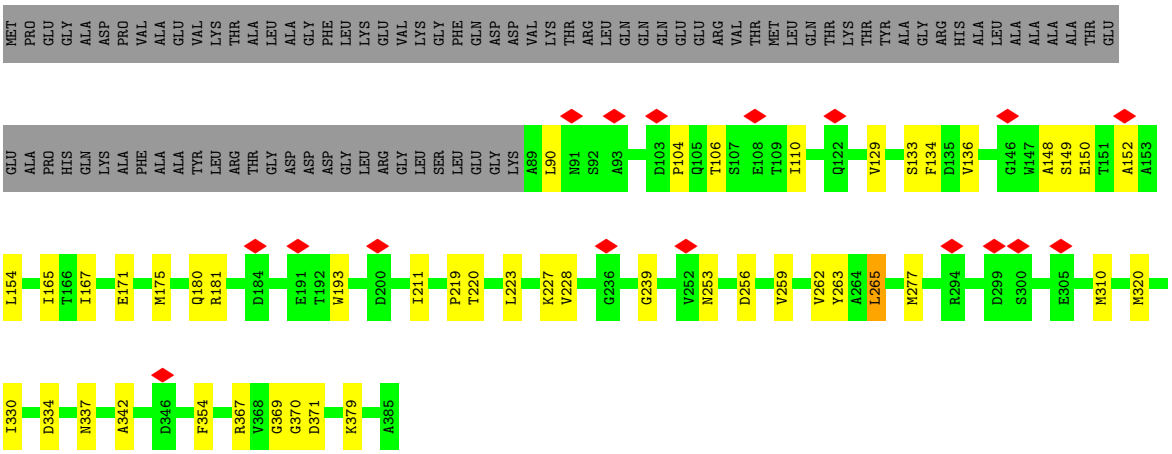
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
12	7A	1	8	4	4	0
			Total	Fe	S	
12	7C	1	8	4	4	0
			Total	Fe	S	
12	7B	1	8	4	4	0

3 Residue-property plots (i)

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

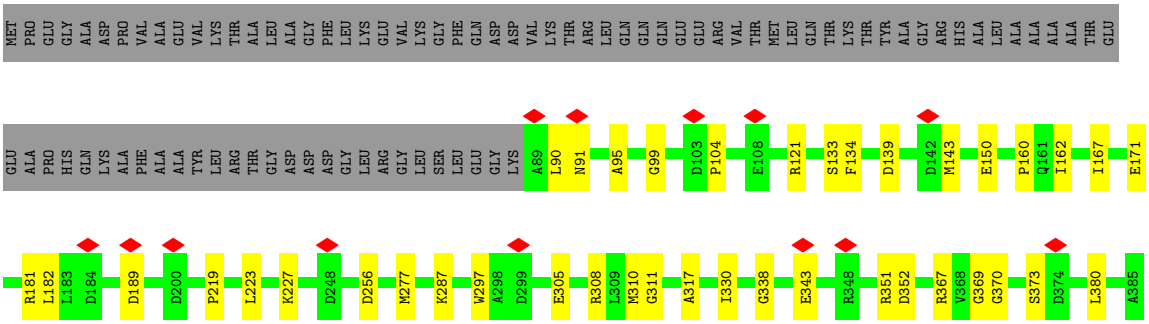
• Molecule 1: Phage major capsid protein, HK97 family

Chain C5:



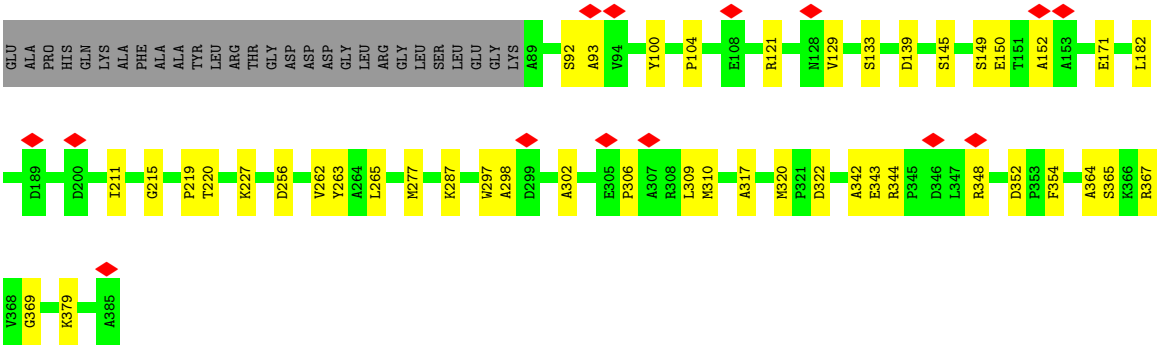
• Molecule 1: Phage major capsid protein, HK97 family

Chain X4:



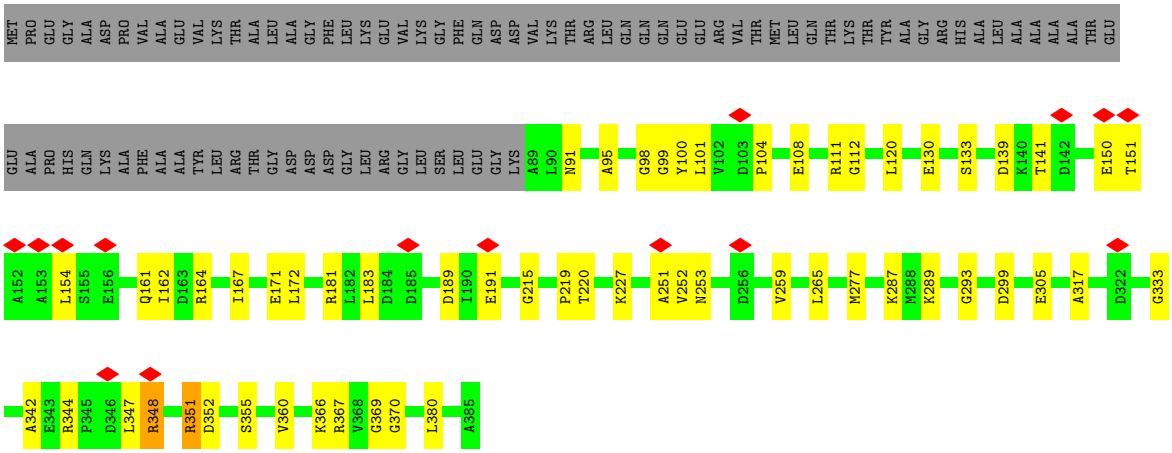
• Molecule 1: Phage major capsid protein, HK97 family

Chain Y4:



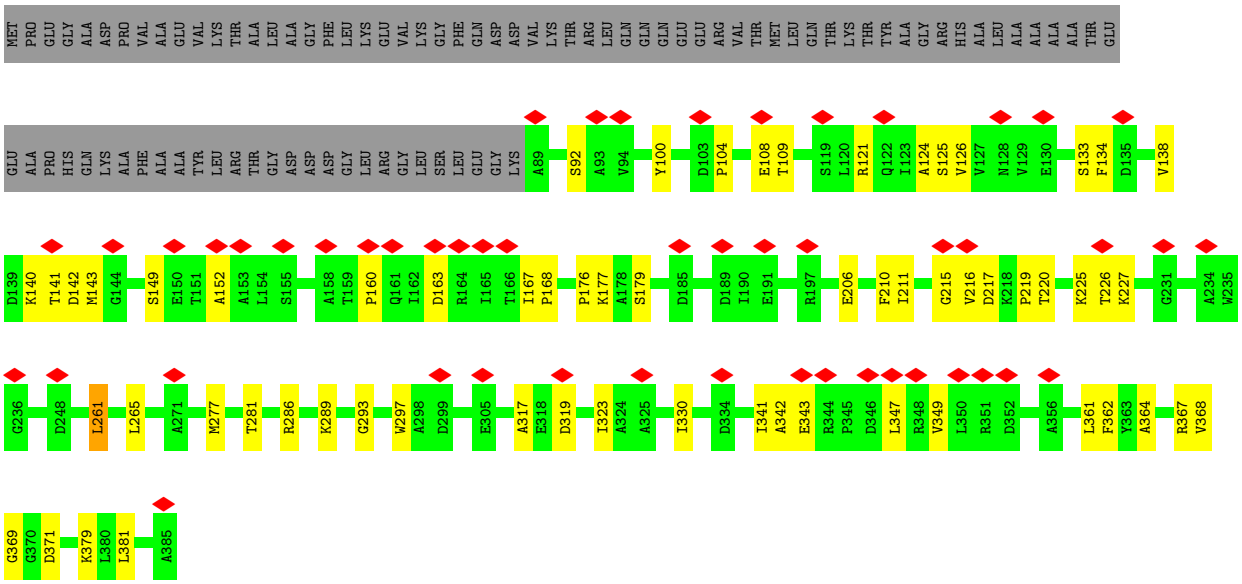
• Molecule 1: Phage major capsid protein, HK97 family

Chain Z4:



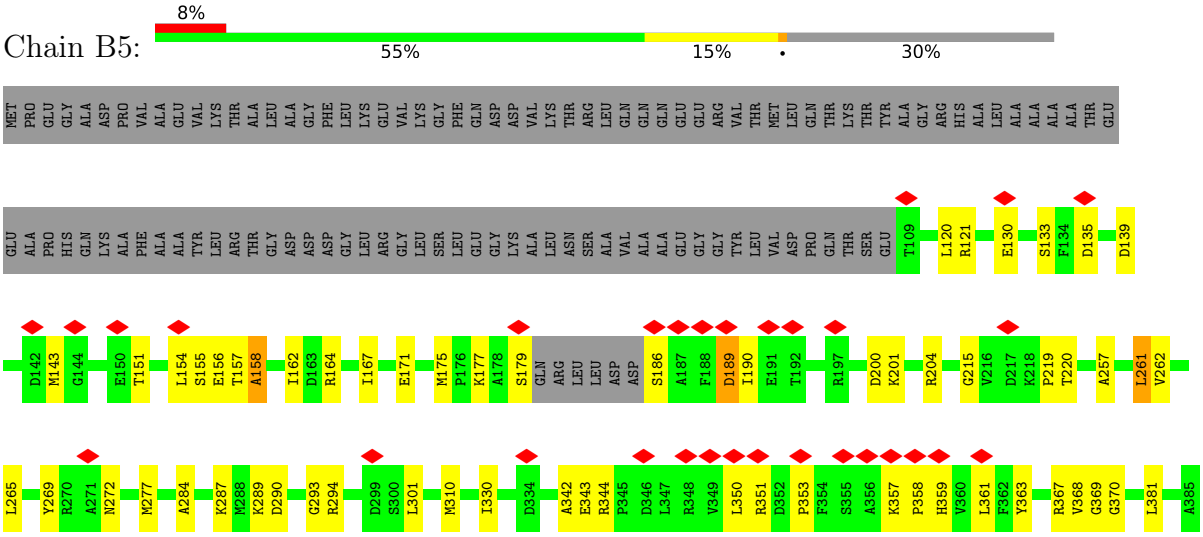
• Molecule 1: Phage major capsid protein, HK97 family

Chain A5:



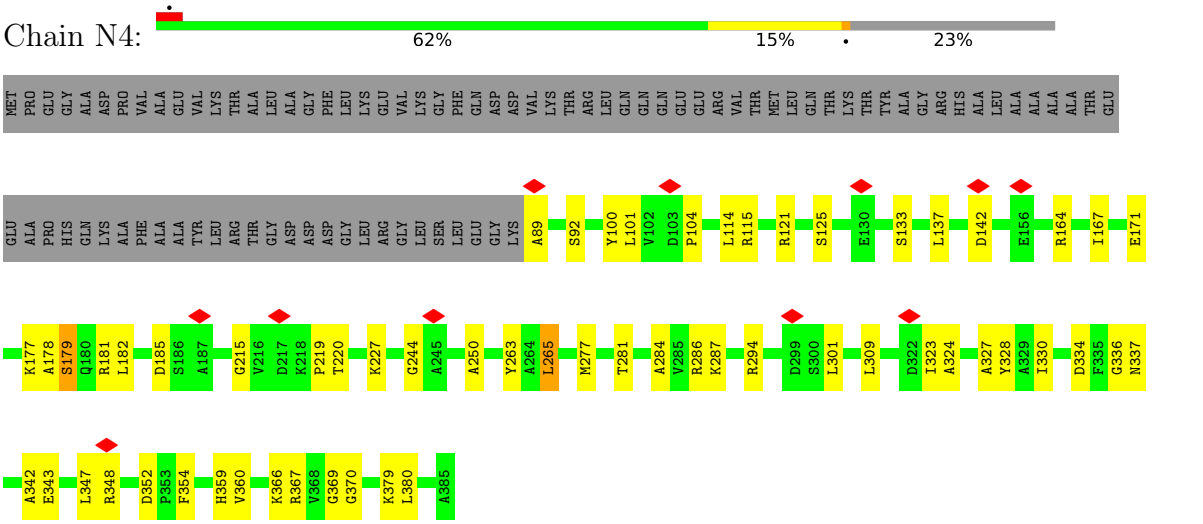
• Molecule 1: Phage major capsid protein, HK97 family

Chain B5:



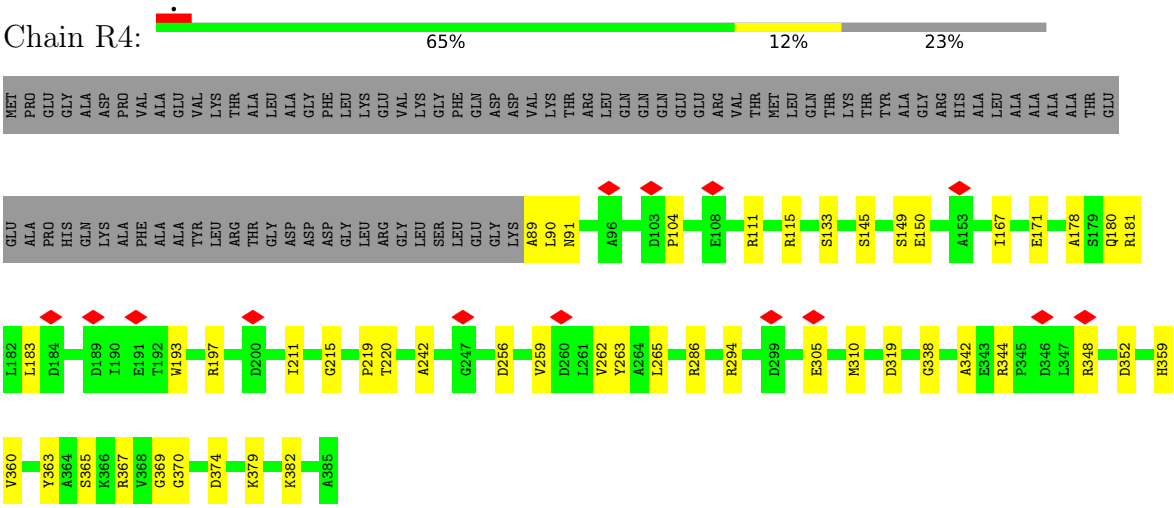
• Molecule 1: Phage major capsid protein, HK97 family

Chain N4:



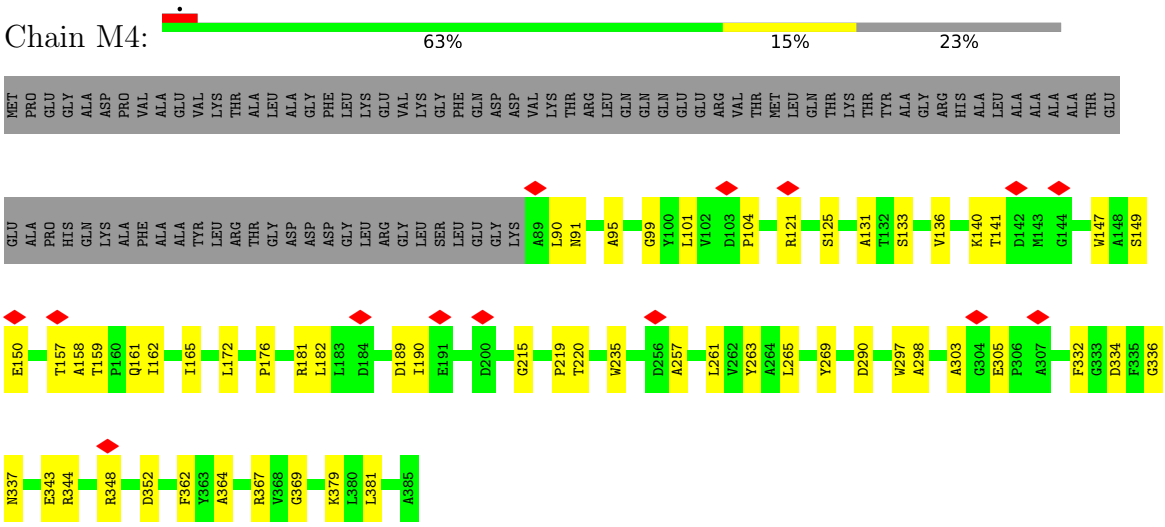
• Molecule 1: Phage major capsid protein, HK97 family

Chain R4:



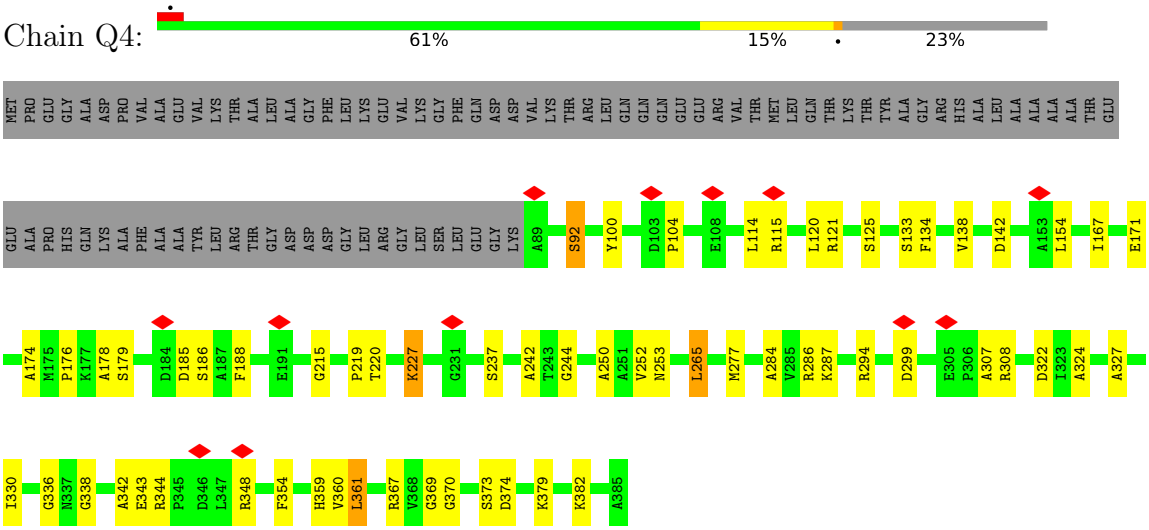
• Molecule 1: Phage major capsid protein, HK97 family

Chain M4:



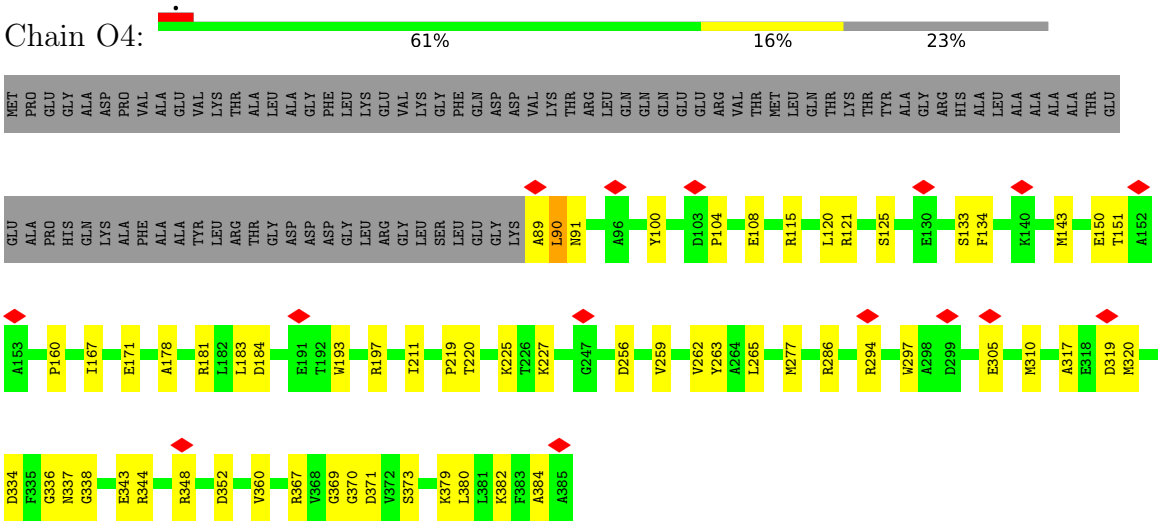
• Molecule 1: Phage major capsid protein, HK97 family

Chain Q4:



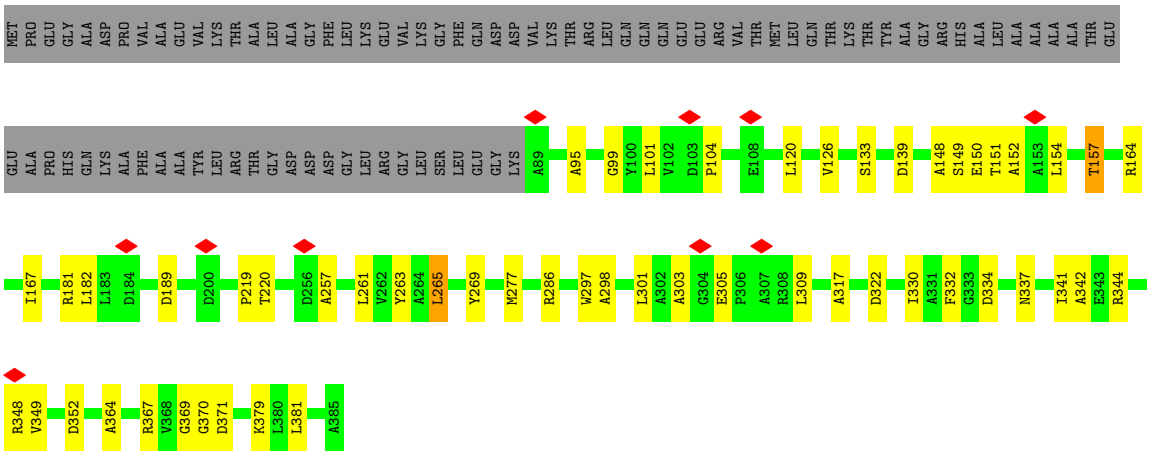
• Molecule 1: Phage major capsid protein, HK97 family

Chain O4:



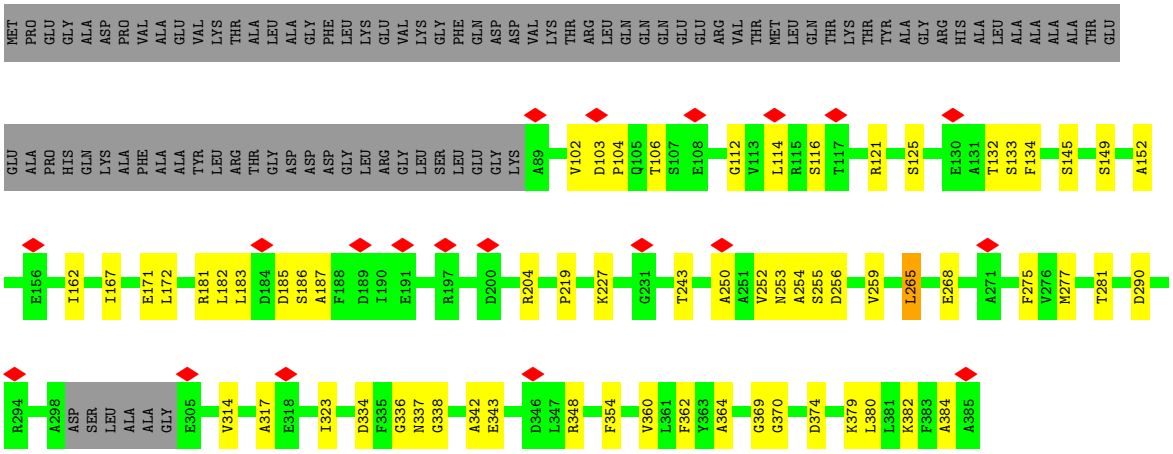
• Molecule 1: Phage major capsid protein, HK97 family

Chain P4:



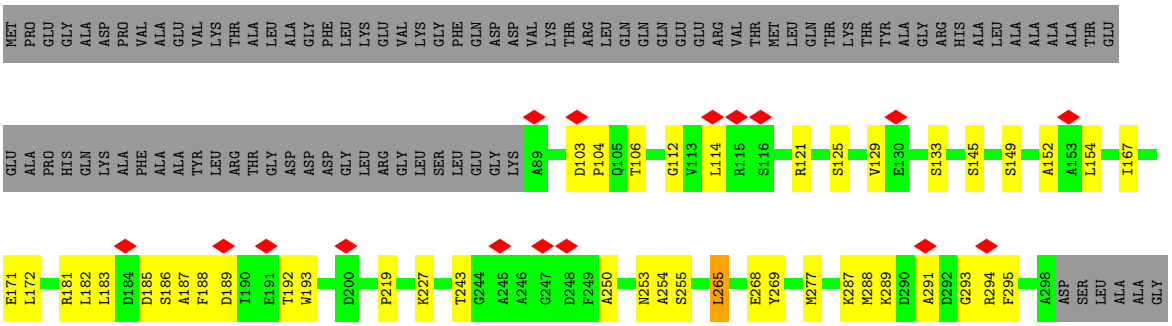
• Molecule 1: Phage major capsid protein, HK97 family

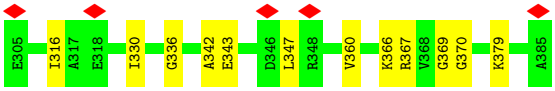
Chain W4:



• Molecule 1: Phage major capsid protein, HK97 family

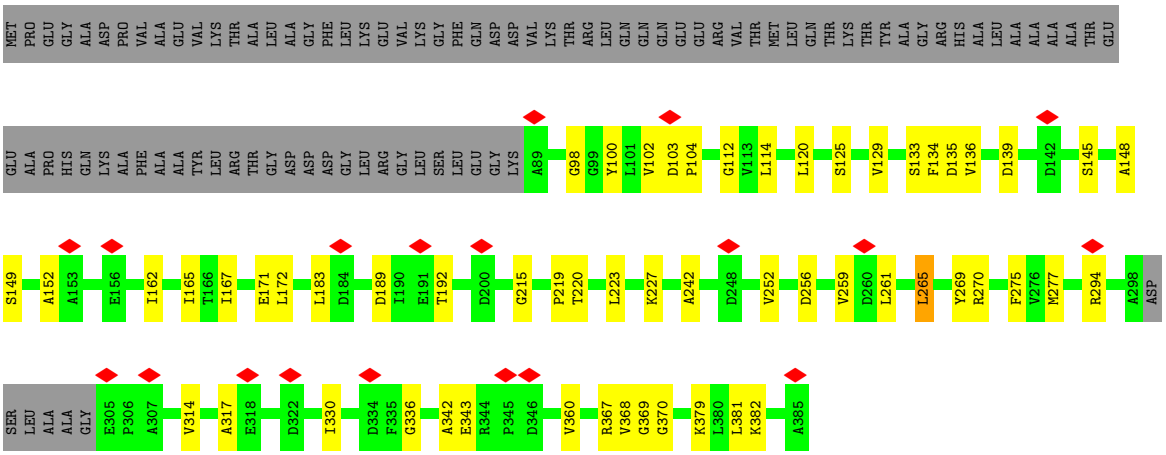
Chain U4:





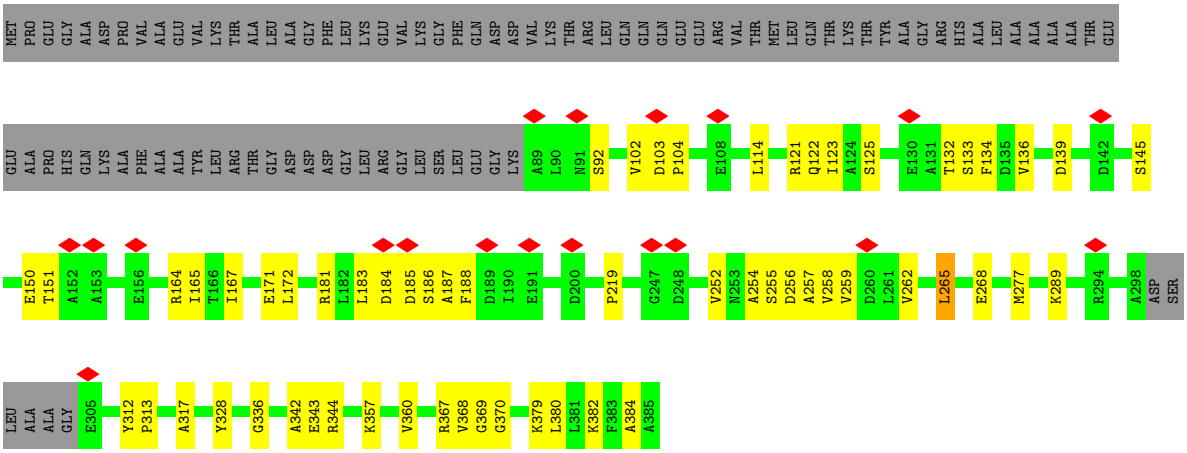
• Molecule 1: Phage major capsid protein, HK97 family

Chain T4:



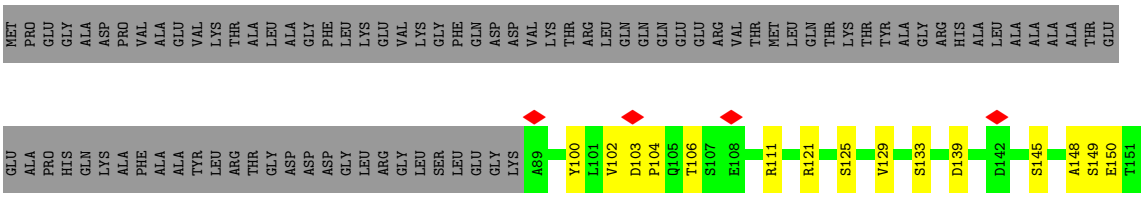
• Molecule 1: Phage major capsid protein, HK97 family

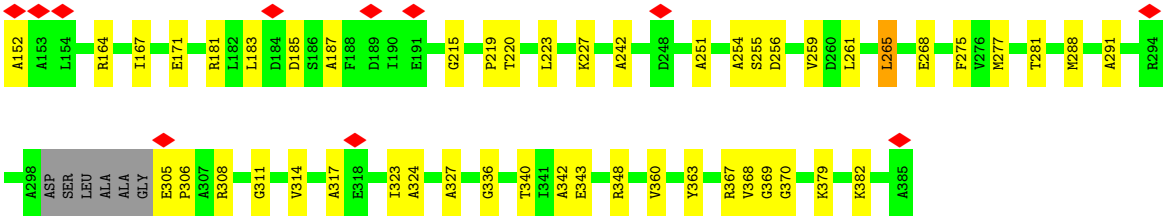
Chain S4:



• Molecule 1: Phage major capsid protein, HK97 family

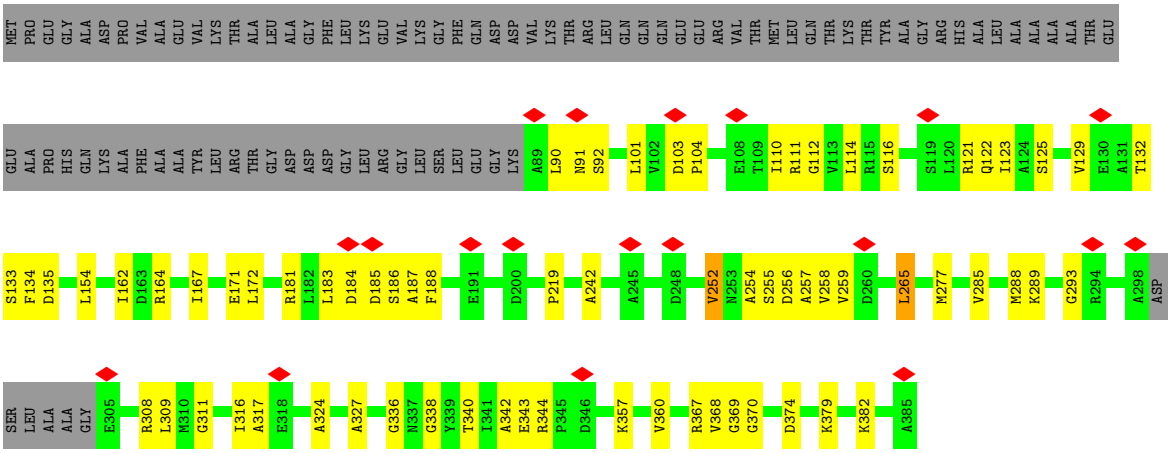
Chain K4:





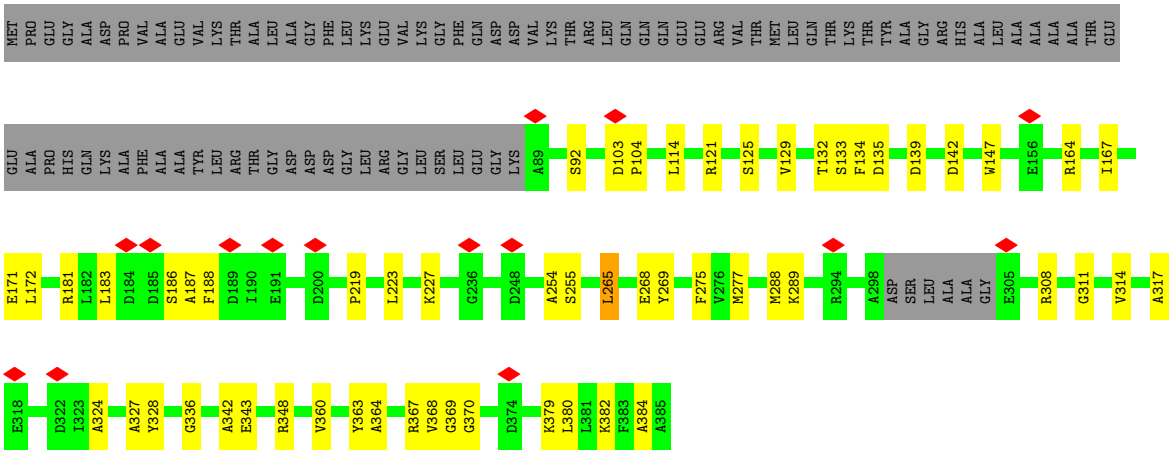
• Molecule 1: Phage major capsid protein, HK97 family

Chain J4:



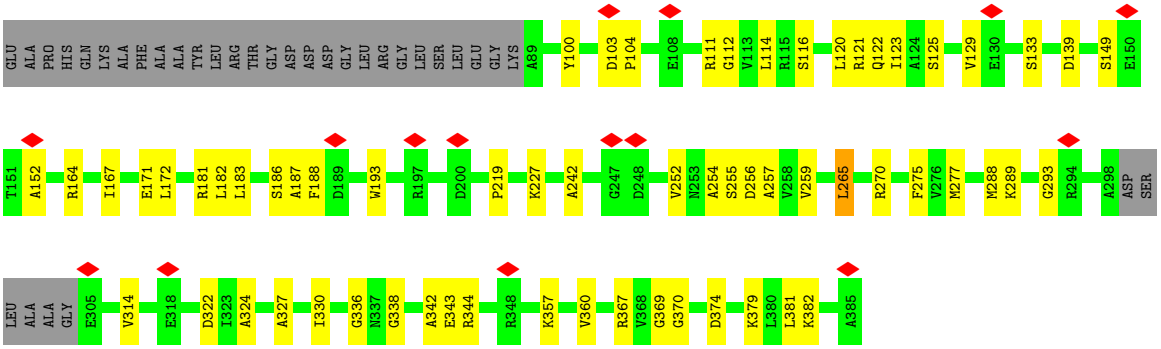
• Molecule 1: Phage major capsid protein, HK97 family

Chain V4:



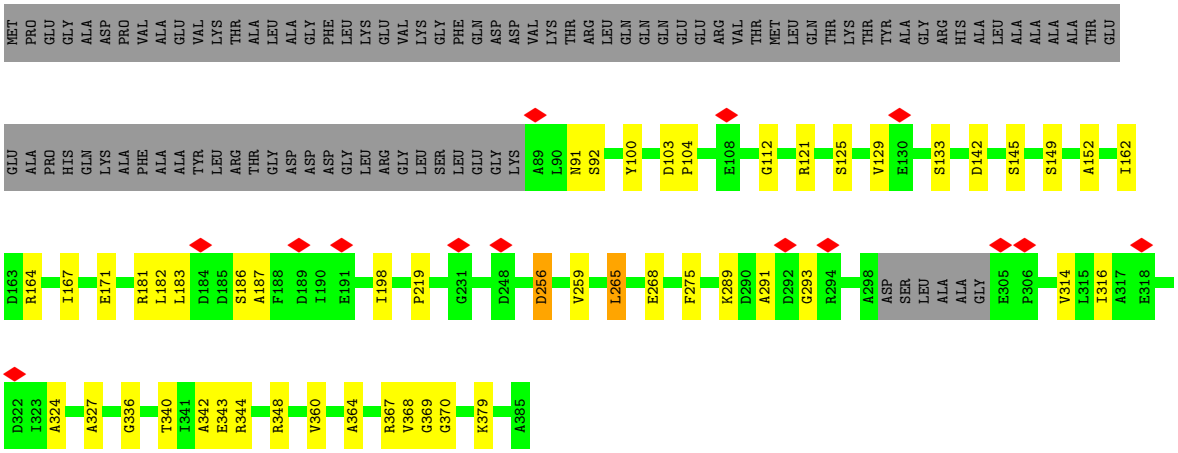
• Molecule 1: Phage major capsid protein, HK97 family

Chain L4:



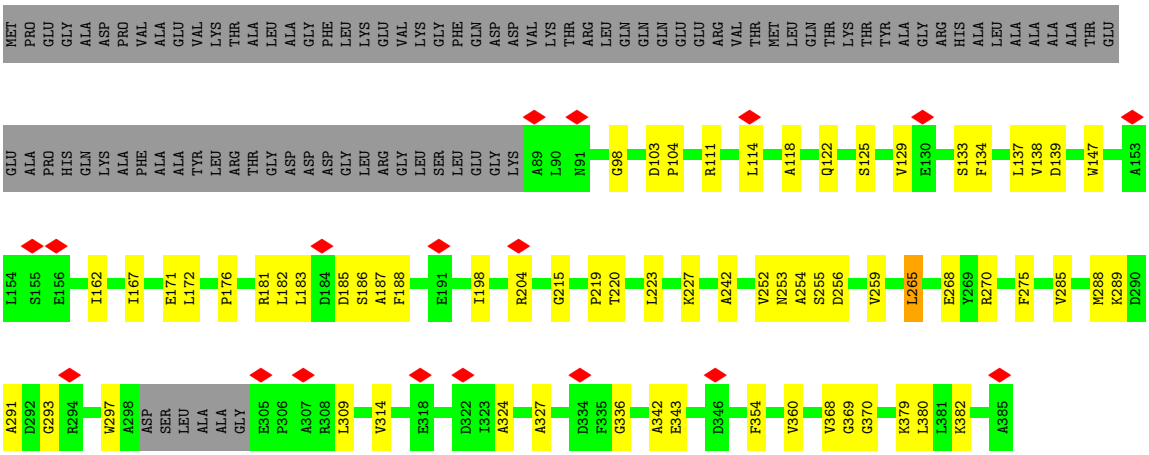
• Molecule 1: Phage major capsid protein, HK97 family

Chain H4:



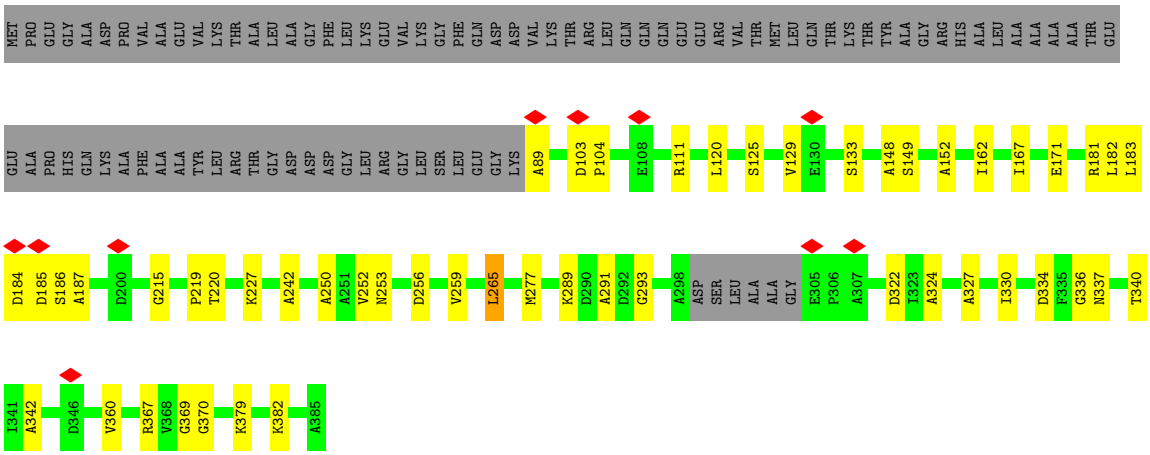
• Molecule 1: Phage major capsid protein, HK97 family

Chain I4:



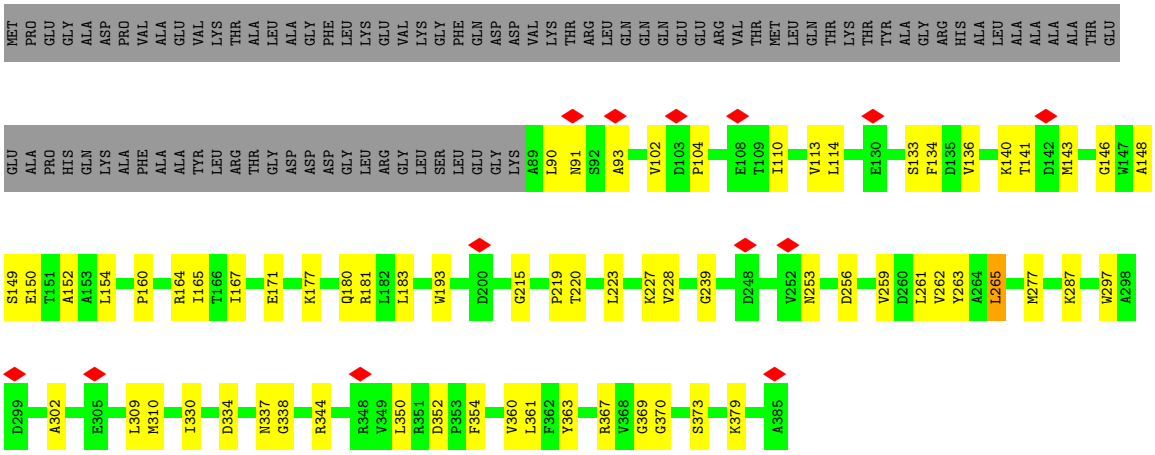
• Molecule 1: Phage major capsid protein, HK97 family

Chain A4:



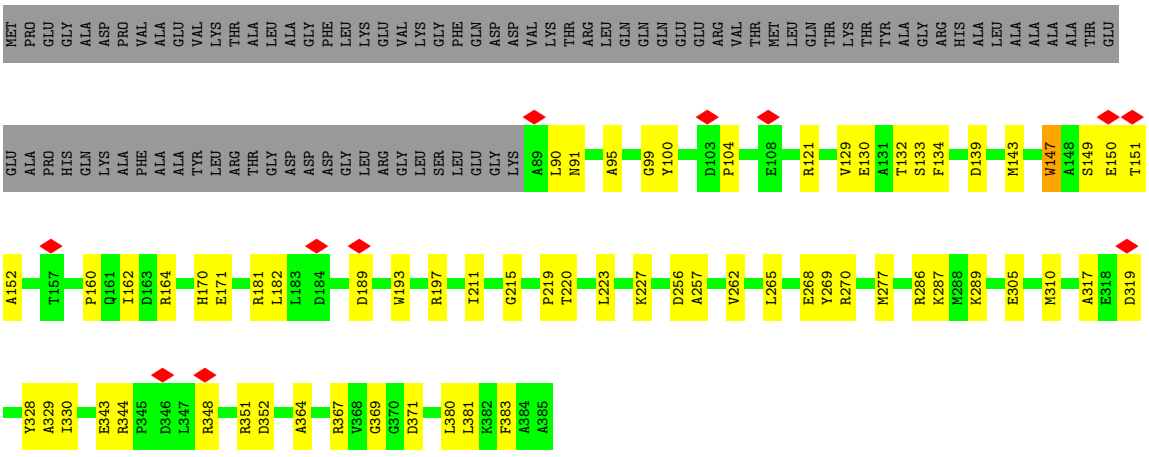
• Molecule 1: Phage major capsid protein, HK97 family

Chain D4:



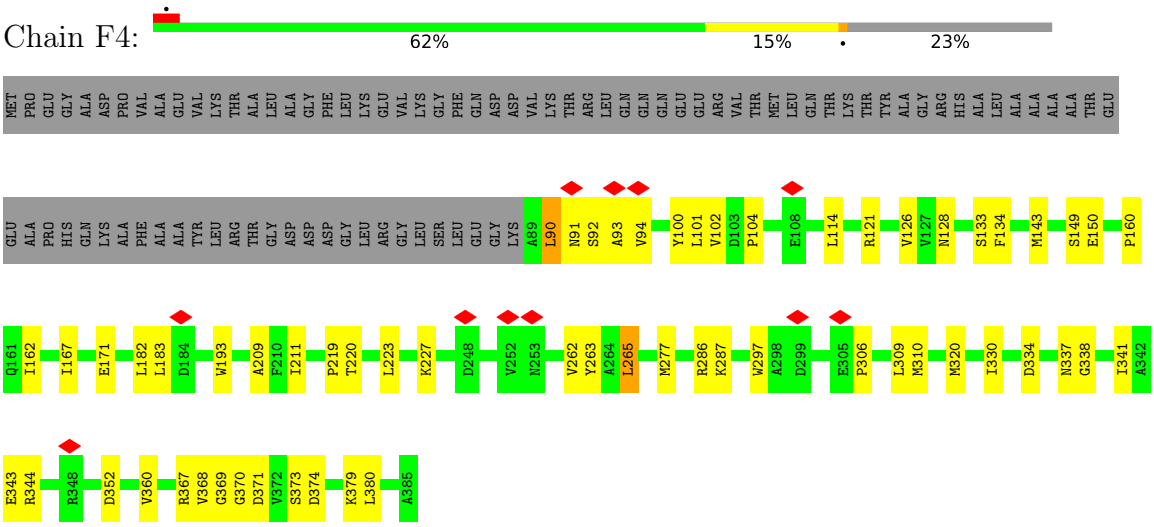
• Molecule 1: Phage major capsid protein, HK97 family

Chain E4:



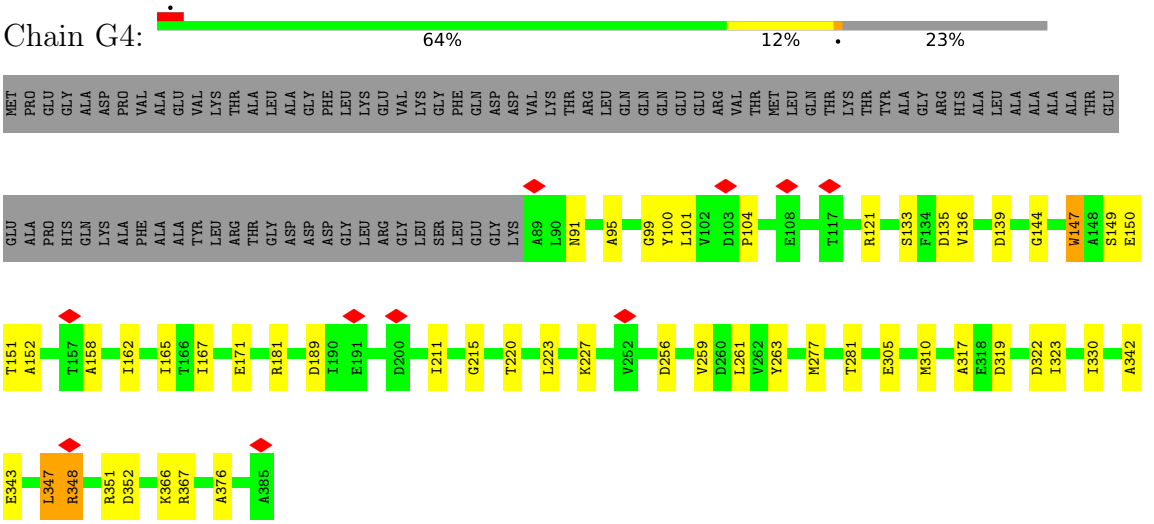
• Molecule 1: Phage major capsid protein, HK97 family

Chain F4:



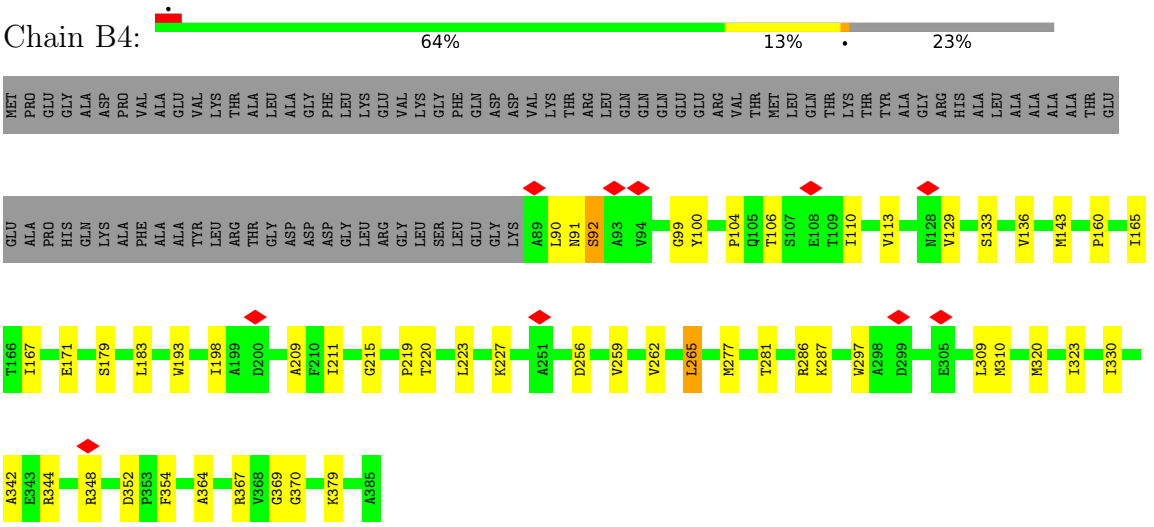
- Molecule 1: Phage major capsid protein, HK97 family

Chain G4:



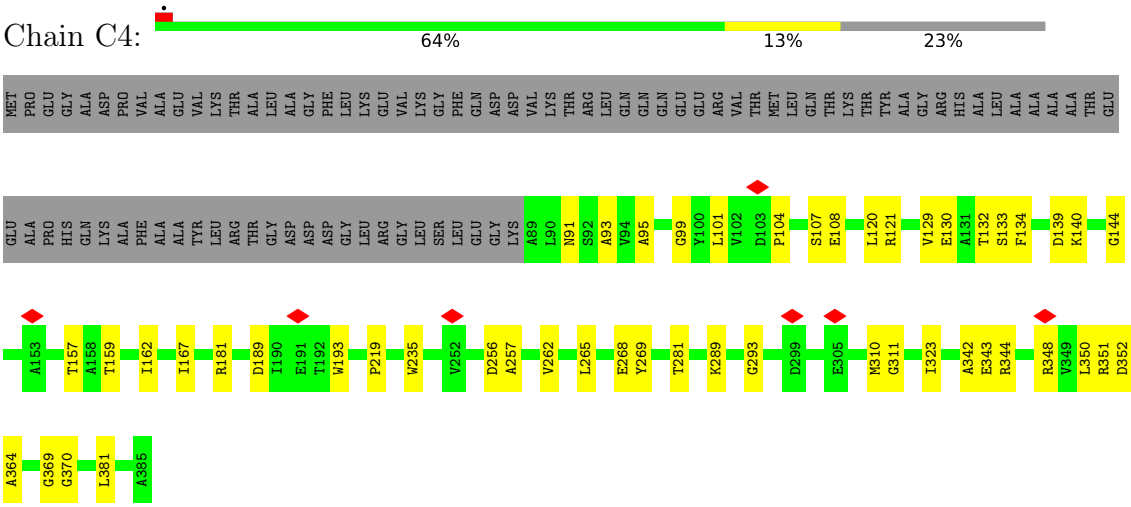
- Molecule 1: Phage major capsid protein, HK97 family

Chain B4:



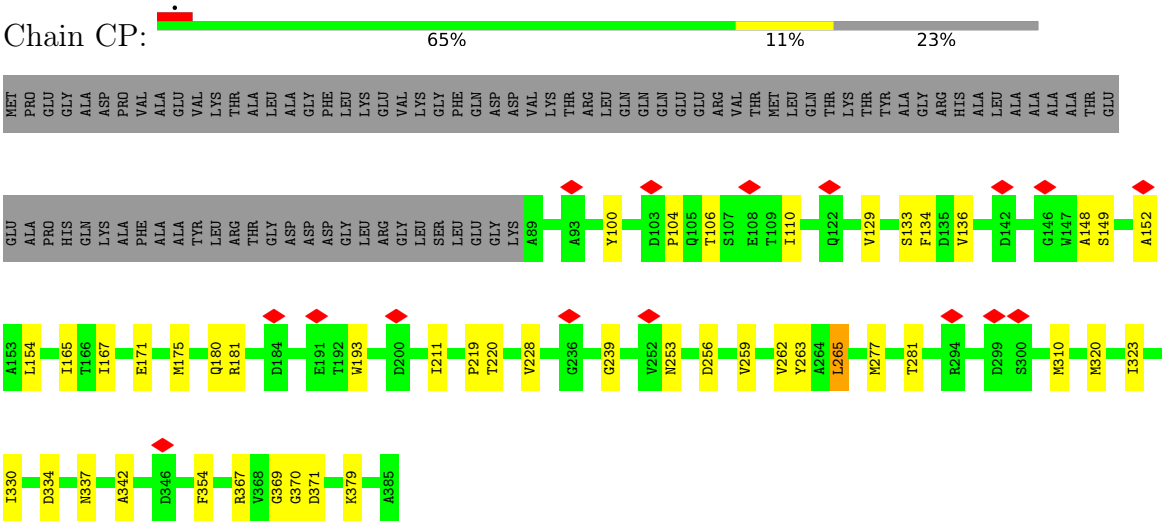
• Molecule 1: Phage major capsid protein, HK97 family

Chain C4:



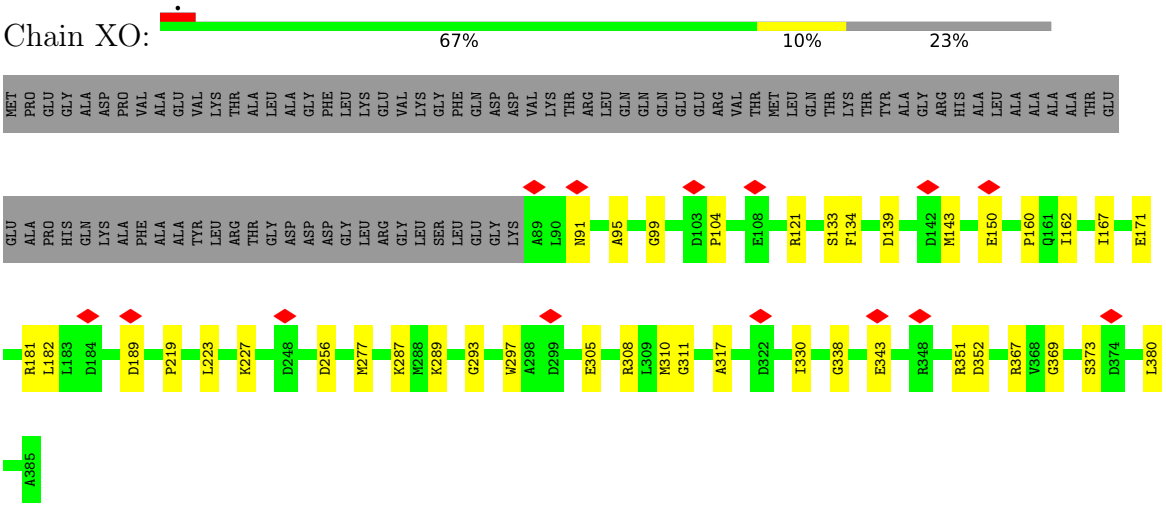
• Molecule 1: Phage major capsid protein, HK97 family

Chain CP:



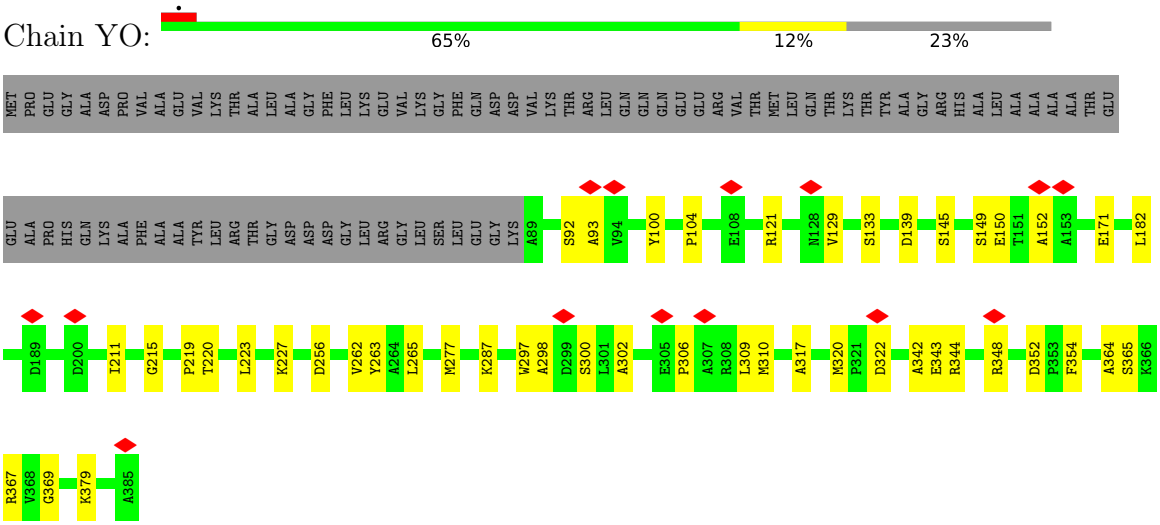
• Molecule 1: Phage major capsid protein, HK97 family

Chain XO:



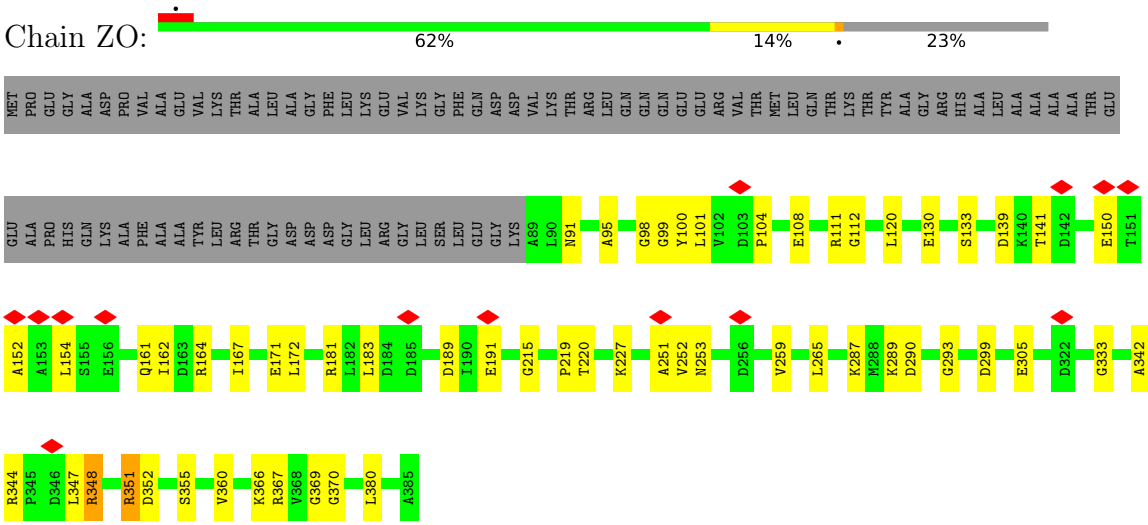
- Molecule 1: Phage major capsid protein, HK97 family

Chain YO:



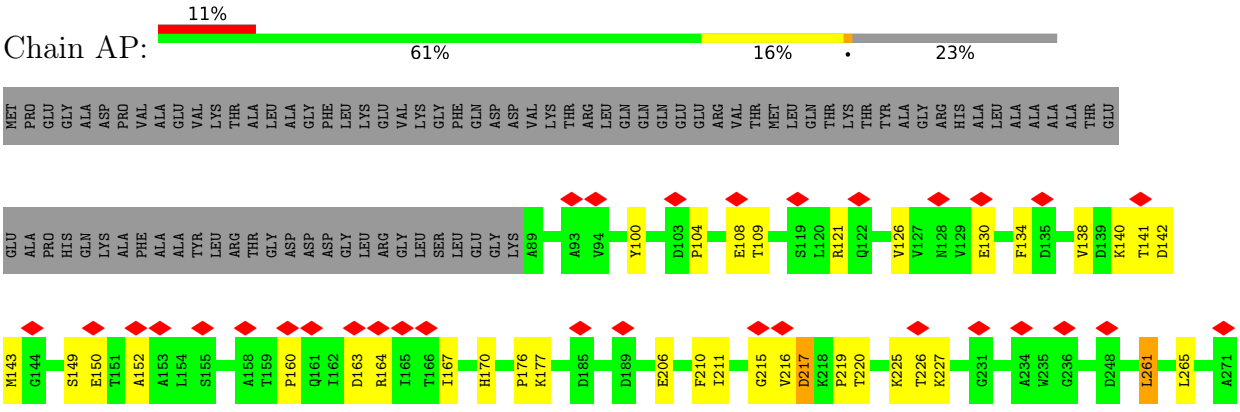
- Molecule 1: Phage major capsid protein, HK97 family

Chain ZO:



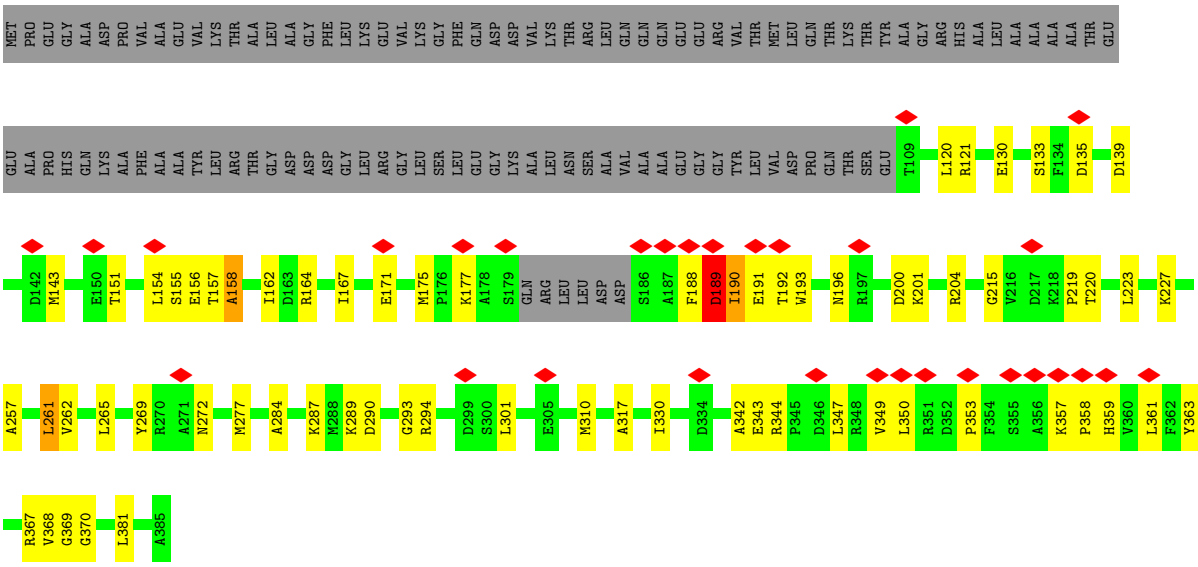
- Molecule 1: Phage major capsid protein, HK97 family

Chain AP:



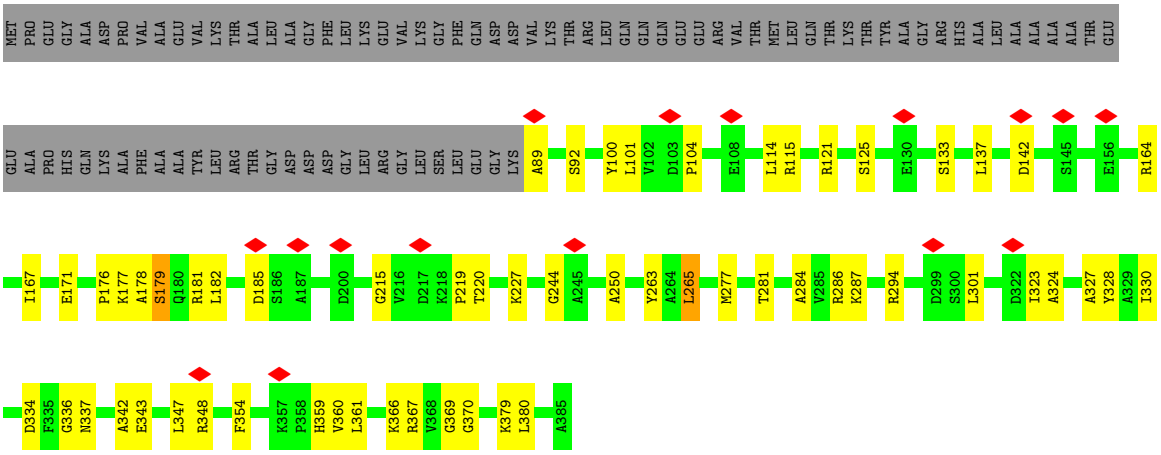
• Molecule 1: Phage major capsid protein, HK97 family

Chain BP:



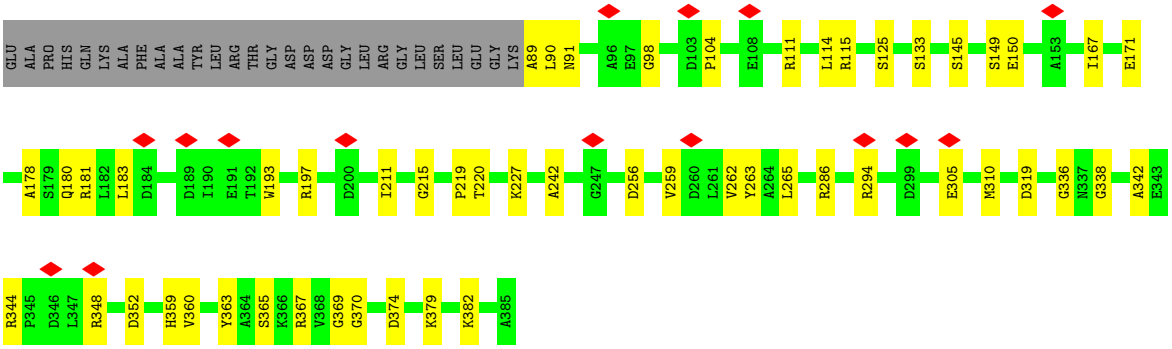
• Molecule 1: Phage major capsid protein, HK97 family

Chain NO:



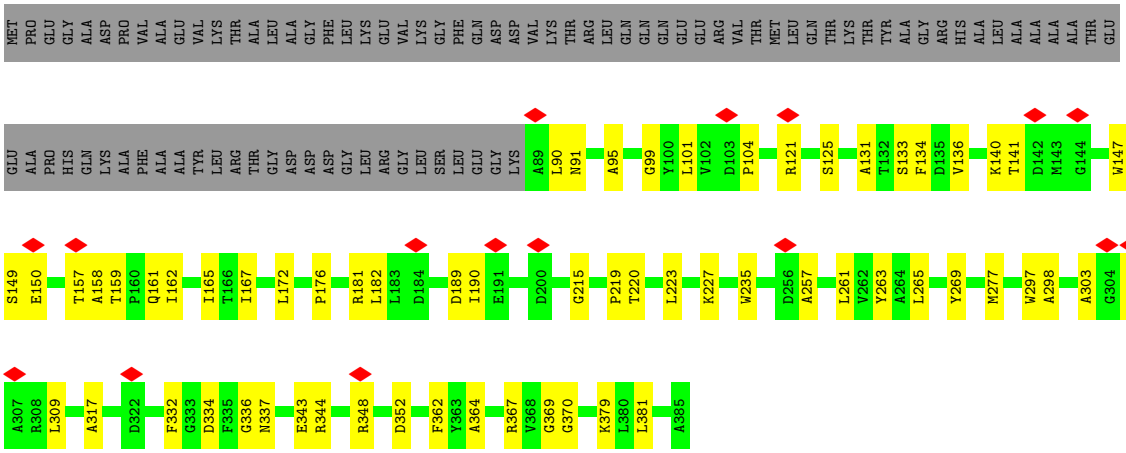
• Molecule 1: Phage major capsid protein, HK97 family

Chain RO:



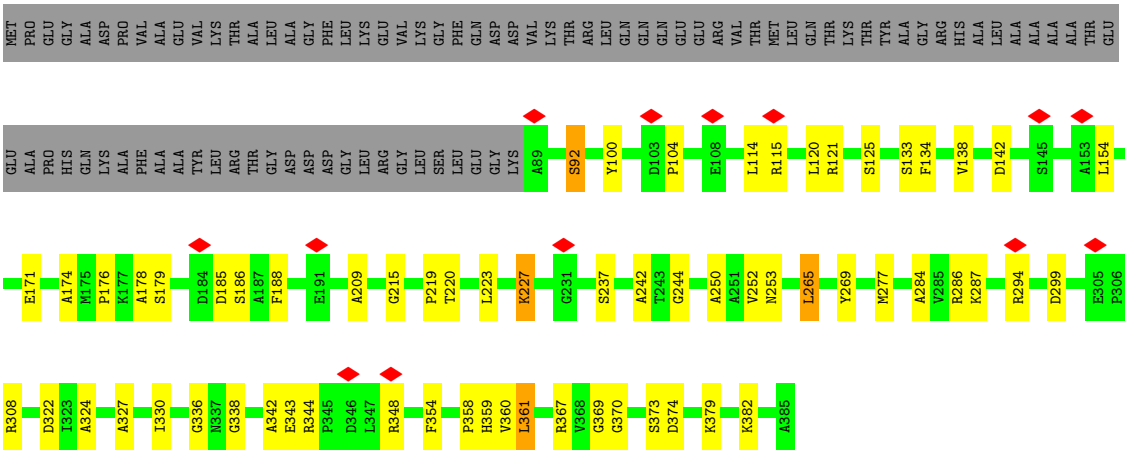
• Molecule 1: Phage major capsid protein, HK97 family

Chain MO:



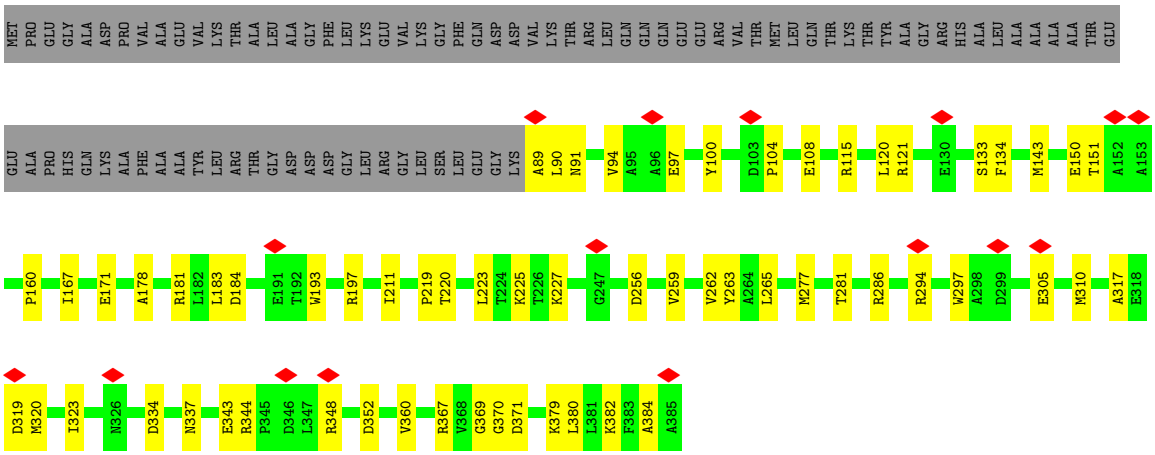
• Molecule 1: Phage major capsid protein, HK97 family

Chain QO:



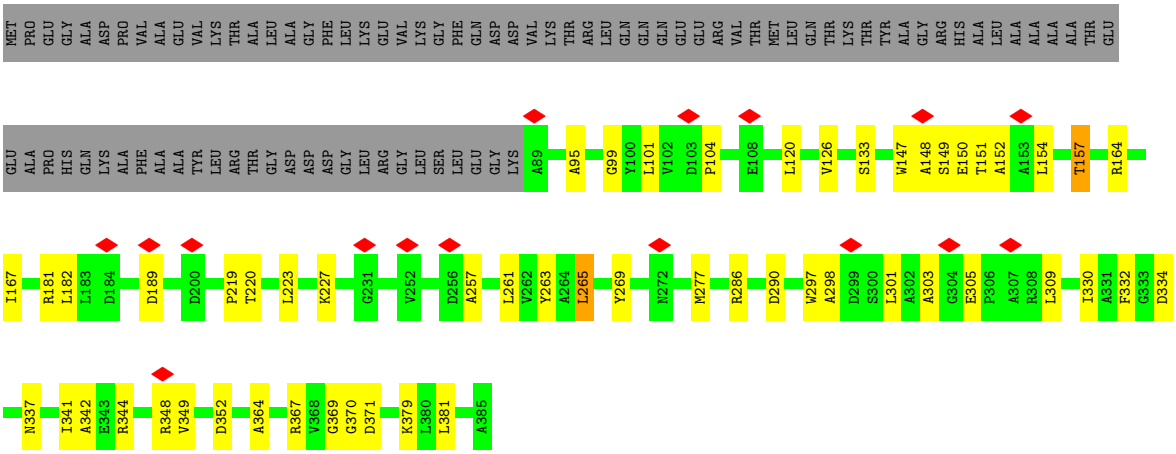
• Molecule 1: Phage major capsid protein, HK97 family

Chain OO:



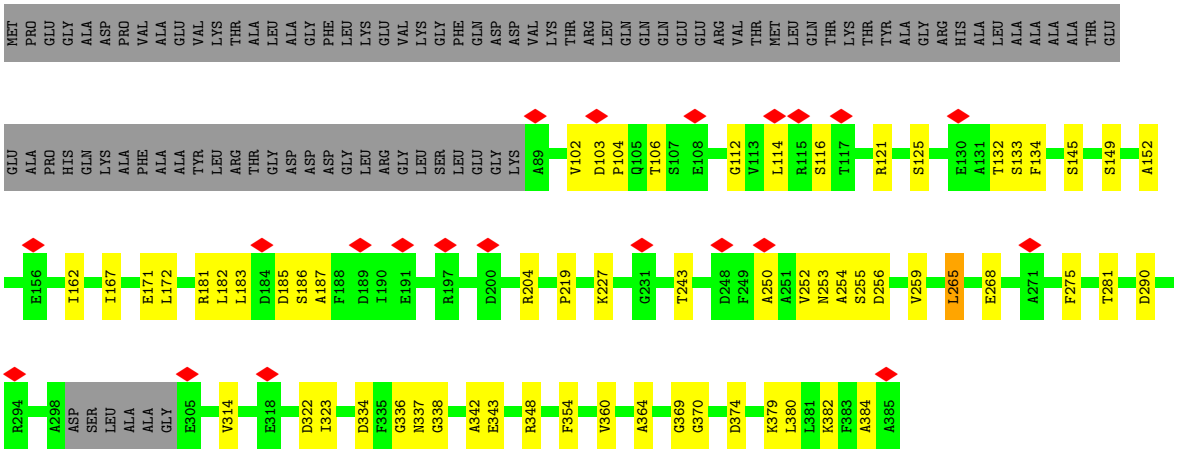
• Molecule 1: Phage major capsid protein, HK97 family

Chain PO:



• Molecule 1: Phage major capsid protein, HK97 family

Chain WO:



• Molecule 1: Phage major capsid protein, HK97 family

Chain UO: 5% 61% 15% 24%

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

GLU ALA PRO HIS GLN LYS ALA PHE ALA ALA TYR LEU ARG THR GLY ASP ASP ASP GLY LEU ARG GLY LEU SER LEU GLU GLU GLY LYS A89 D103 P104 Q105 T106 G112 V113 L114 R115 S116 R121 S125 V129 S133 S145 G146 W147 A148 S149 E150 T151 A152 A153 L154

R164 I167 E171 L172 R181 L182 L183 D184 D185 S186 A187 F188 D189 I190 E191 T192 W193 D200 P219 L223 K227 T243 G244 A245 A246 G247 D248 F249 A250 N253 A254 S255 L265 E268 Y269 M277 K287 M288 K289 D290 A291 D292 G293 R294 F295 A298

ASP SER LEU ALA ALA GLY E305 I316 A317 E318 I330 G336 A342 E343 D346 L347 R348 V360 K366 R367 V368 G369 G370 K379 A385

- Molecule 1: Phage major capsid protein, HK97 family

Chain TO: 61% 15% 24%

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

GLU ALA PRO HIS GLN LYS ALA PHE ALA ALA TYR LEU ARG THR GLY ASP ASP ASP GLY LEU ARG GLY LEU SER LEU GLU GLU GLY LYS A89 G98 G99 Y100 L101 V102 D103 P104 G112 V113 L114 L120 S125 V129 E130 S133 F134 D135 V136 D139 D142 S145

A148 S149 A152 I165 T166 I167 E171 L172 L183 D184 D189 I190 E191 T192 D200 G215 P219 T220 L223 K227 A242 D248 V252 D256 V259 D260 L261 L265 E268 Y269 R270 F275 V276 M277 R294 A298 ASP SER LEU ALA

ALA GLY E305 V314 A317 E318 D322 I330 D334 F335 G336 A342 E343 R344 P345 D346 V360 R367 V368 G369 G370 K379 L380 L381 K382 A385

- Molecule 1: Phage major capsid protein, HK97 family

Chain SO: 5% 61% 15% 24%

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

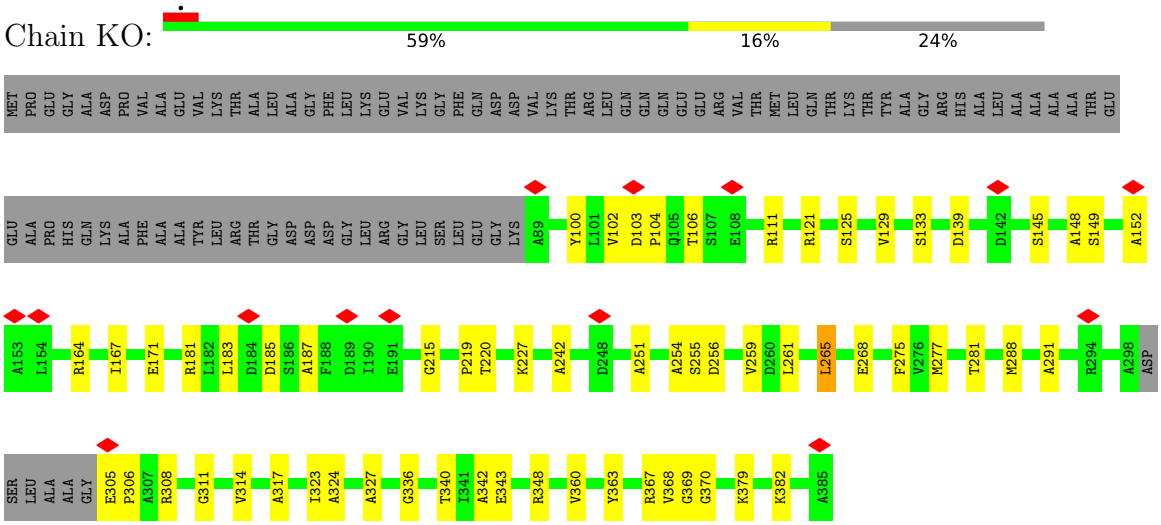
GLU ALA PRO HIS GLN LYS ALA PHE ALA ALA TYR LEU ARG THR GLY ASP ASP ASP GLY LEU ARG GLY LEU SER LEU GLU GLU GLY LYS A89 L90 N91 S92 V102 D103 P104 E108 L114 R121 Q122 I123 A124 S125 E130 A131 T132 S133 F134 D135 V136 D139 S145 E150

T151 A152 A153 E156 R164 I165 T166 I167 E171 L172 R181 L182 L183 D184 D185 S186 A187 F188 D189 I190 E191 D200 P219 K227 G247 D248 V252 N253 A254 S255 D256 A257 V258 V259 D260 L261 V262 L265 E268 K289 D290 A291 R294 A298 ASP SER

LEU ALA ALA GLY E305 E318 D322 Y328 G336 A342 E343 R344 K357 V360 R367 V368 G369 G370 K379 L380 L381 K382 F383 A384 A385

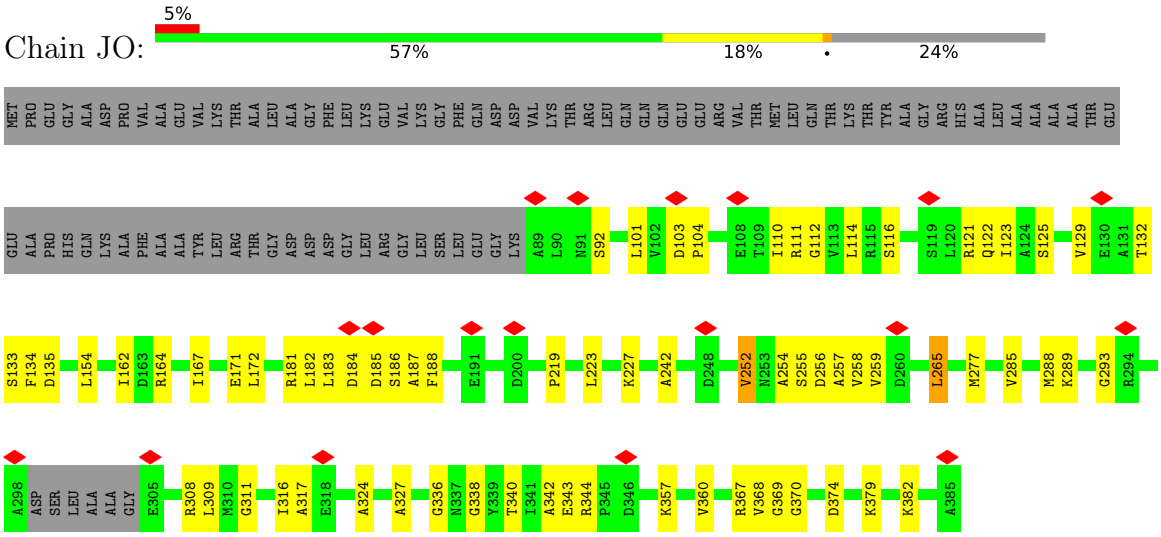
• Molecule 1: Phage major capsid protein, HK97 family

Chain KO:



• Molecule 1: Phage major capsid protein, HK97 family

Chain JO:



• Molecule 1: Phage major capsid protein, HK97 family

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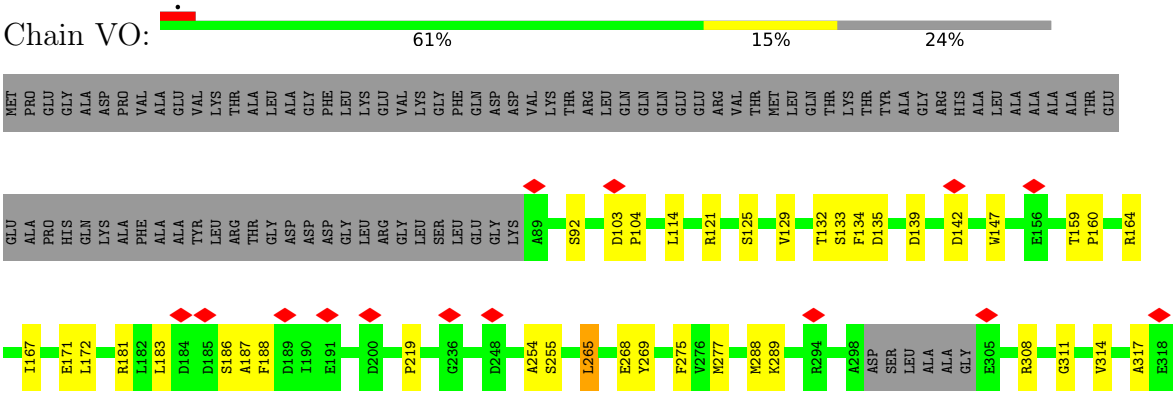
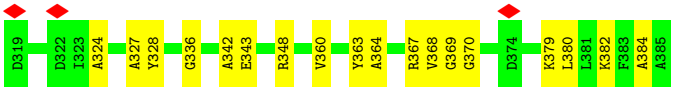
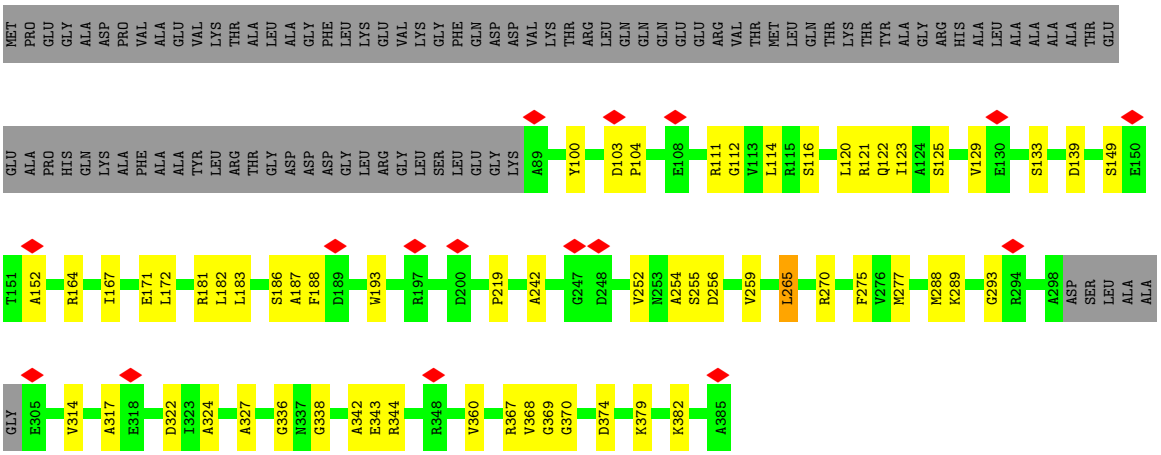




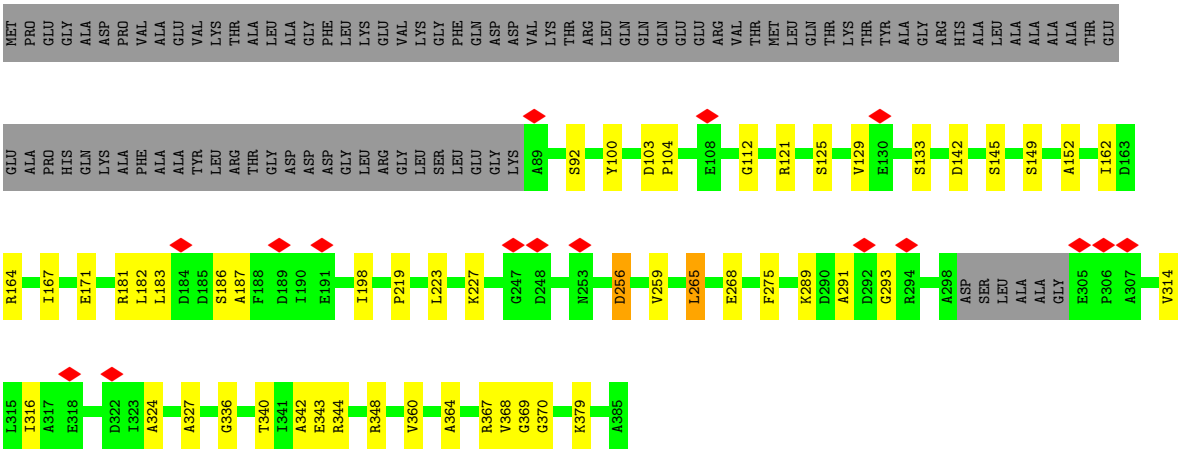
• Molecule 1: Phage major capsid protein, HK97 family

Chain LO:



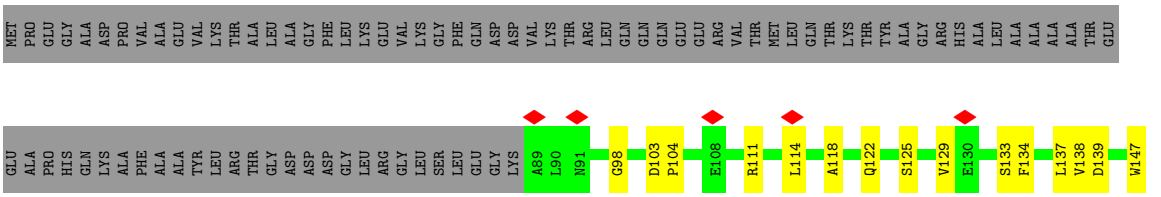
• Molecule 1: Phage major capsid protein, HK97 family

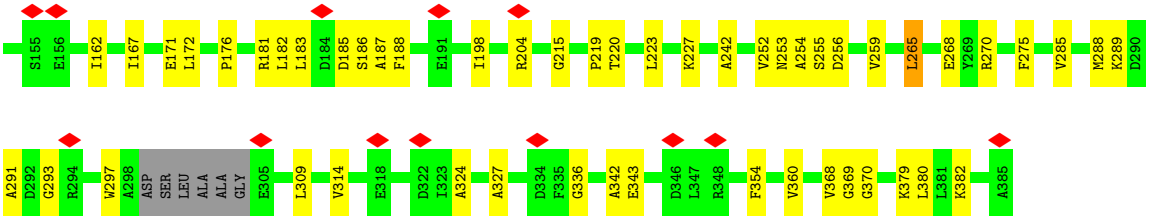
Chain HO:



• Molecule 1: Phage major capsid protein, HK97 family

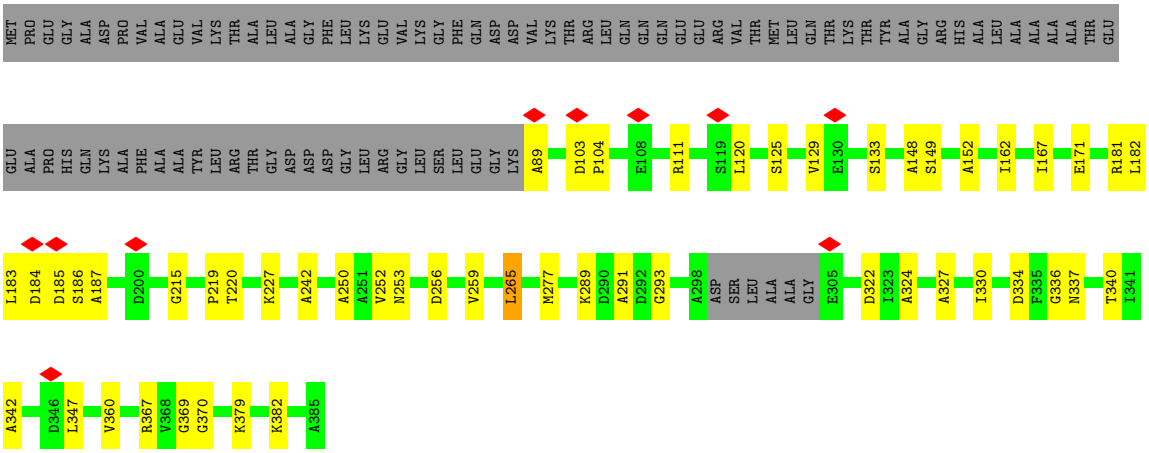
Chain IO:





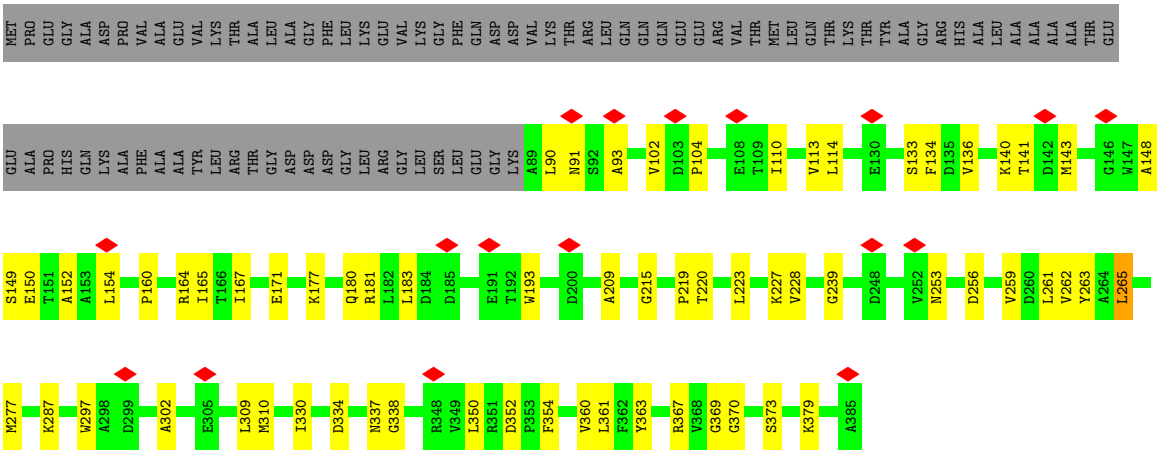
• Molecule 1: Phage major capsid protein, HK97 family

Chain AO:



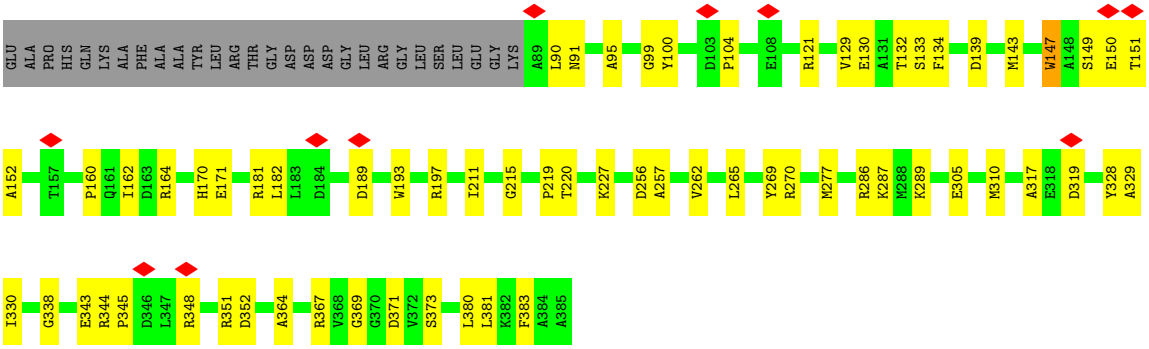
• Molecule 1: Phage major capsid protein, HK97 family

Chain DO:



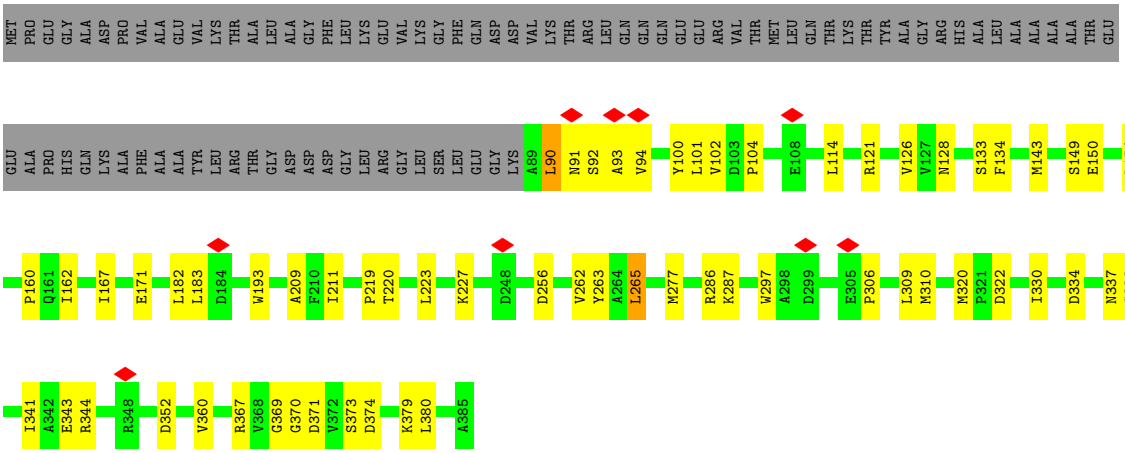
• Molecule 1: Phage major capsid protein, HK97 family

Chain EO:



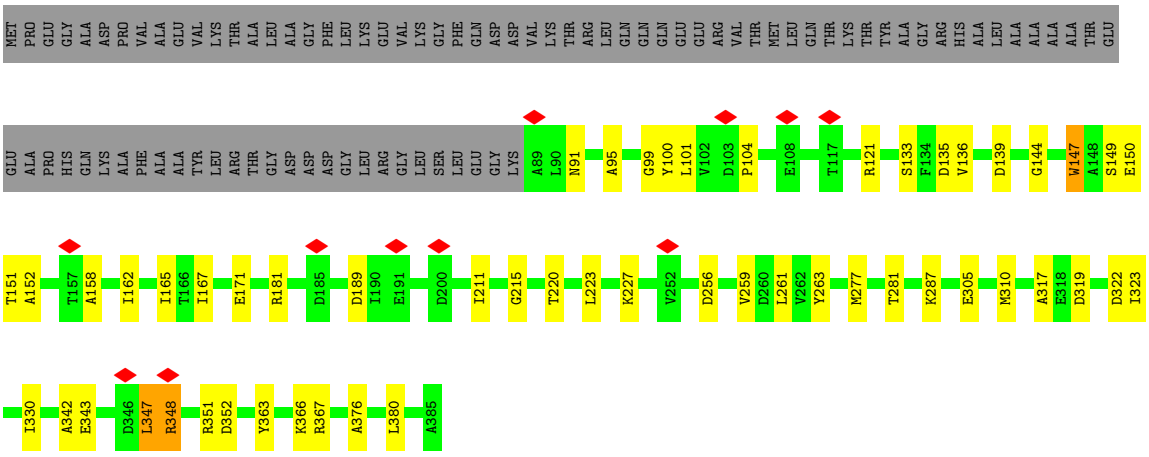
• Molecule 1: Phage major capsid protein, HK97 family

Chain FO:



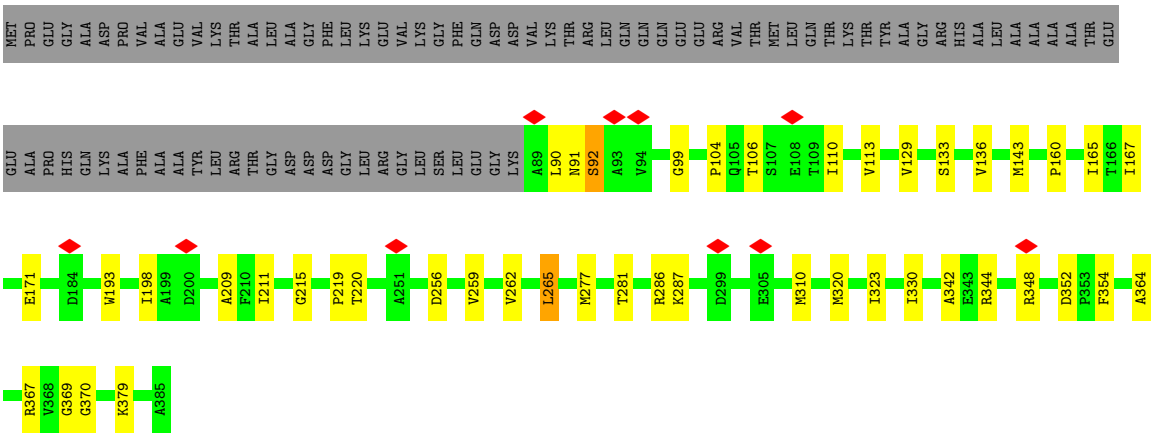
• Molecule 1: Phage major capsid protein, HK97 family

Chain GO:



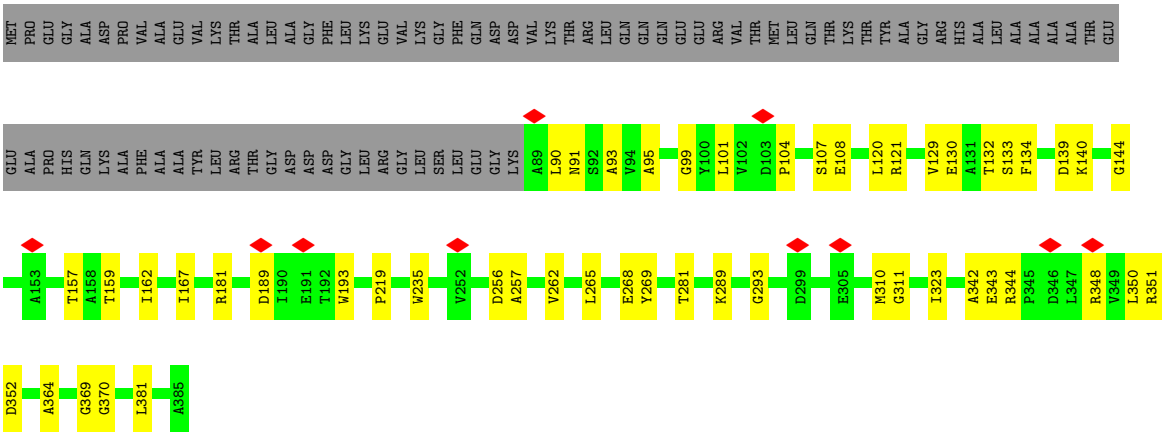
• Molecule 1: Phage major capsid protein, HK97 family

Chain BO:



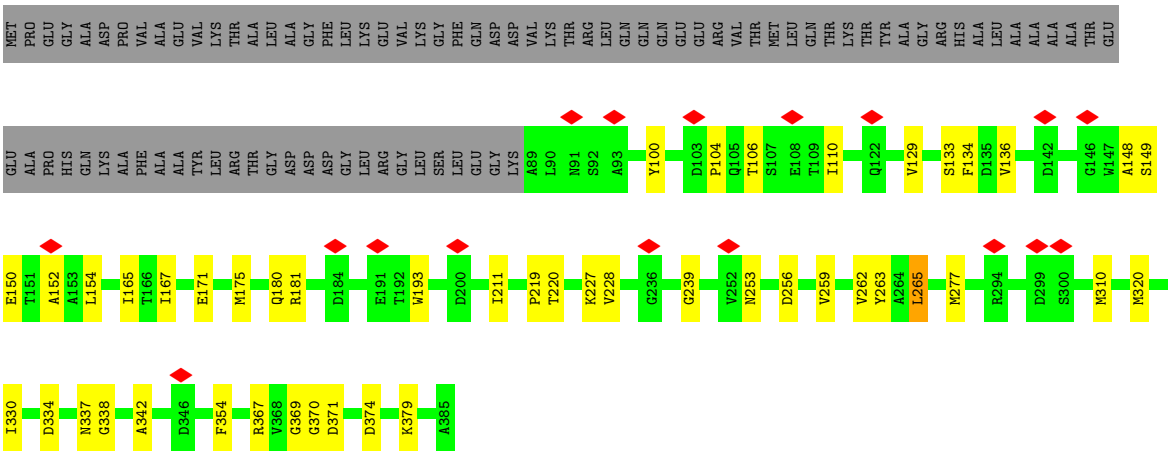
• Molecule 1: Phage major capsid protein, HK97 family

Chain CO:



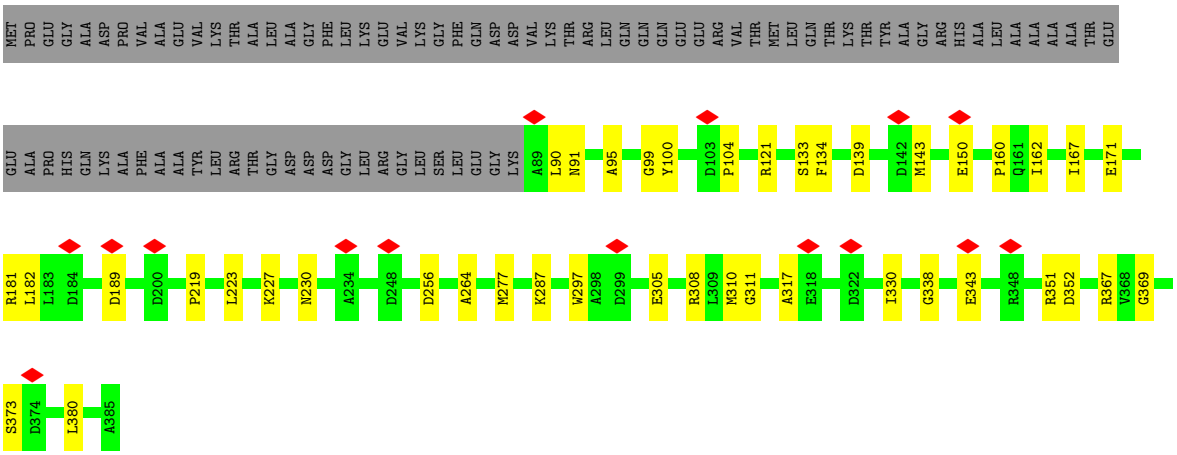
• Molecule 1: Phage major capsid protein, HK97 family

Chain CK:



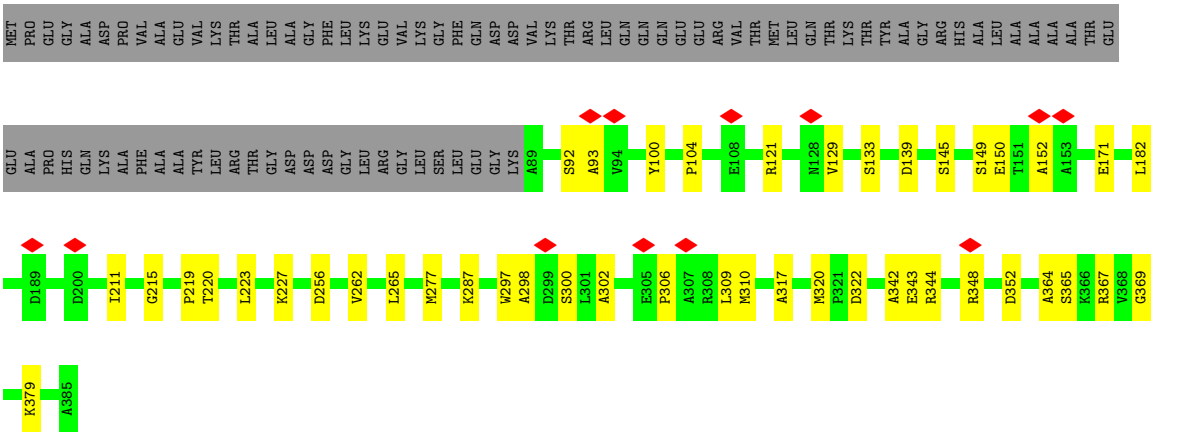
• Molecule 1: Phage major capsid protein, HK97 family

Chain XJ:



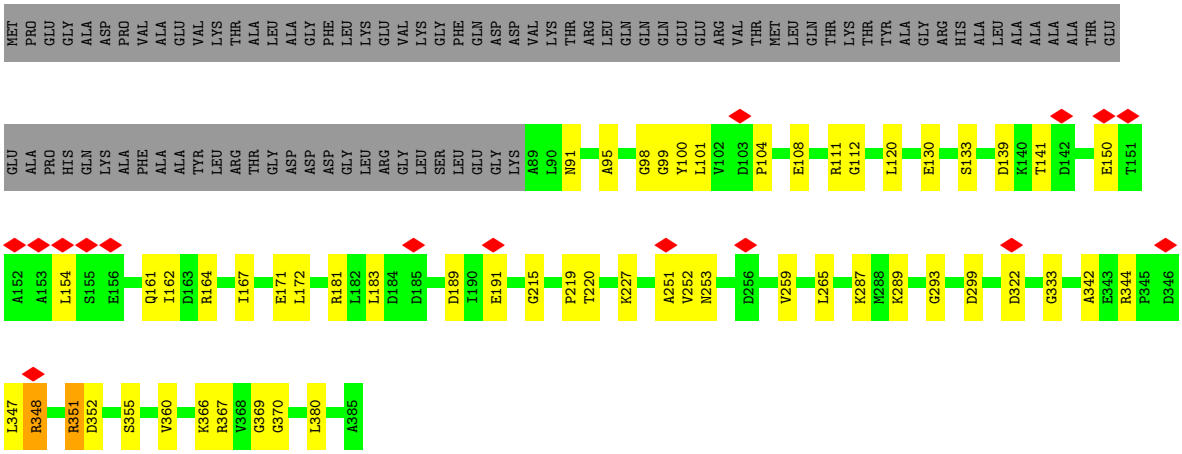
• Molecule 1: Phage major capsid protein, HK97 family

Chain YJ:



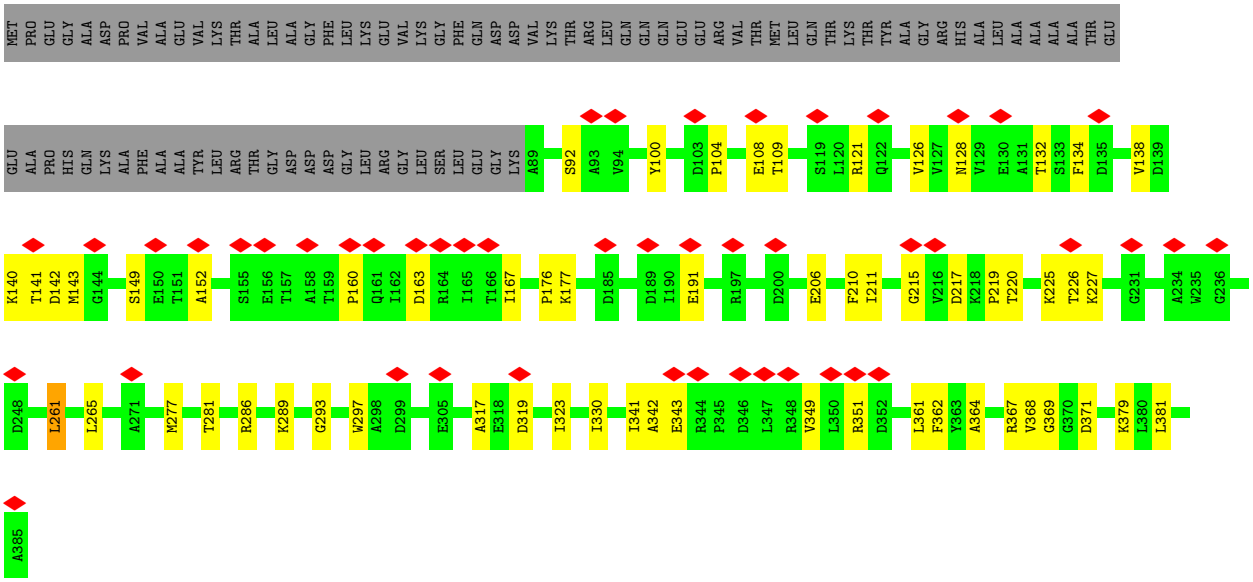
• Molecule 1: Phage major capsid protein, HK97 family

Chain ZJ:



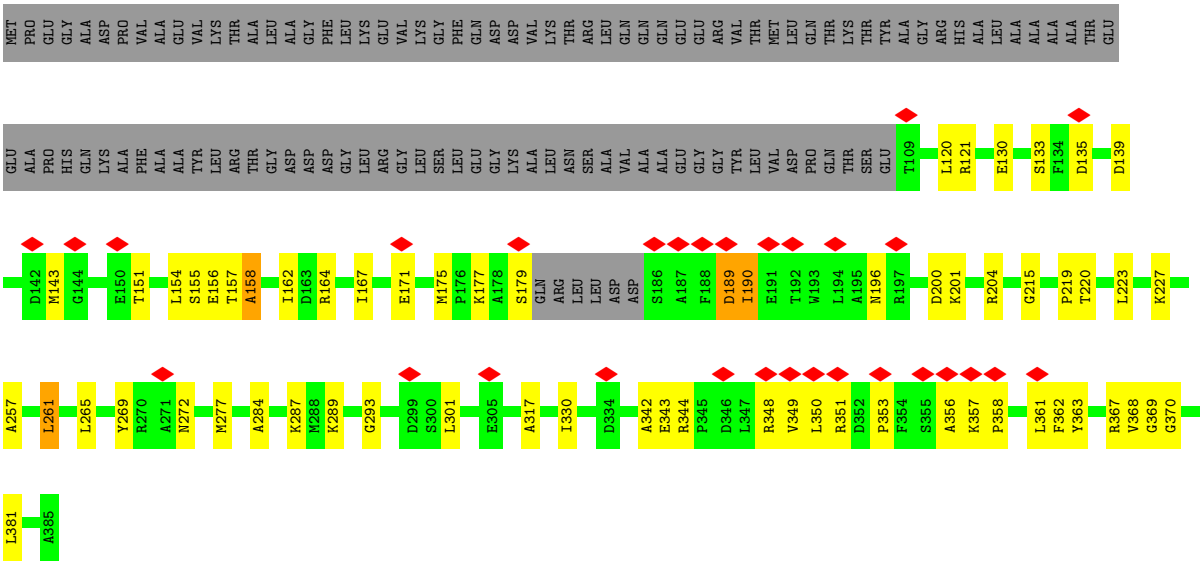
• Molecule 1: Phage major capsid protein, HK97 family

Chain AK:



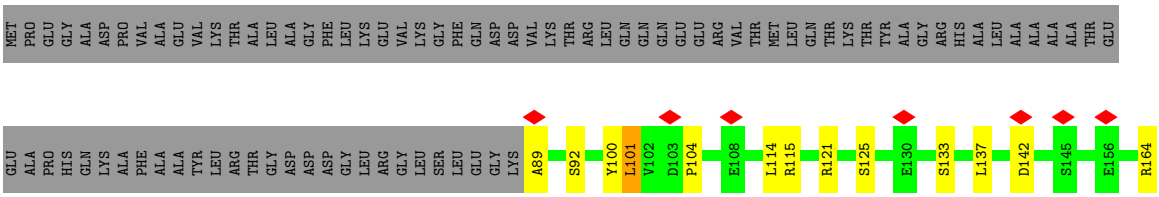
• Molecule 1: Phage major capsid protein, HK97 family

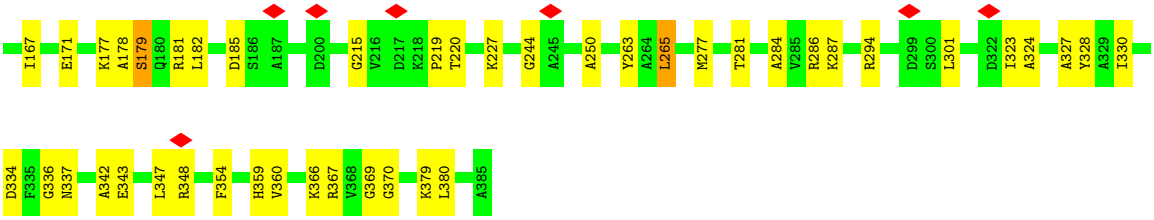
Chain BK:



• Molecule 1: Phage major capsid protein, HK97 family

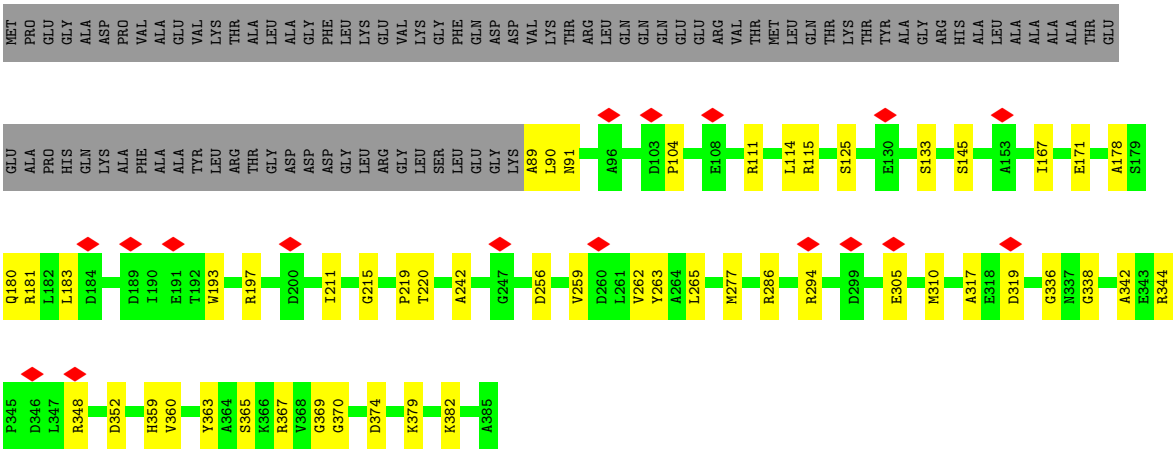
Chain NJ:





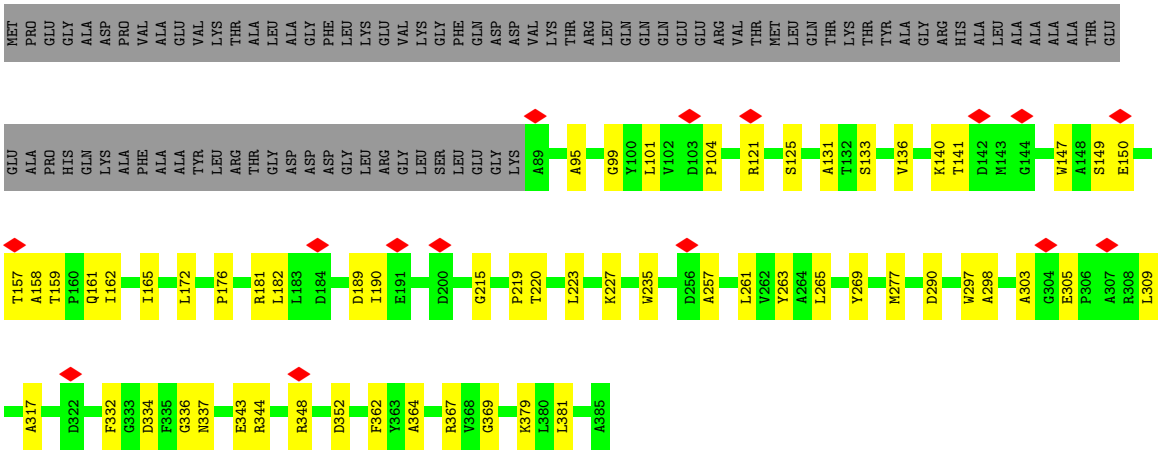
• Molecule 1: Phage major capsid protein, HK97 family

Chain RJ:



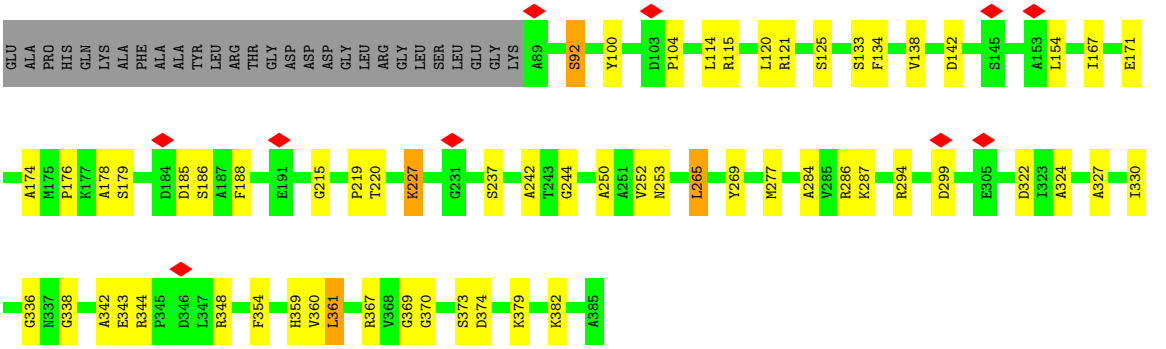
• Molecule 1: Phage major capsid protein, HK97 family

Chain MJ:



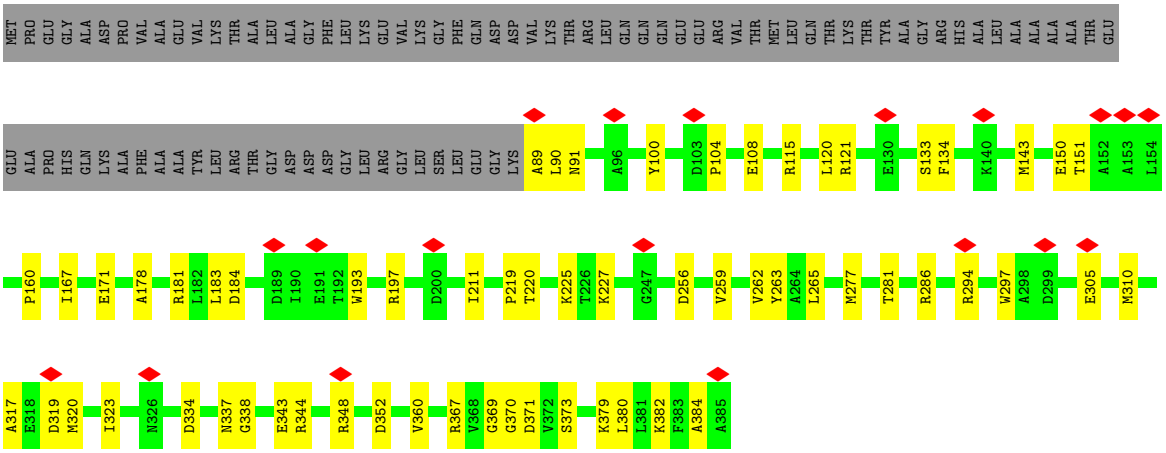
• Molecule 1: Phage major capsid protein, HK97 family

Chain QJ:



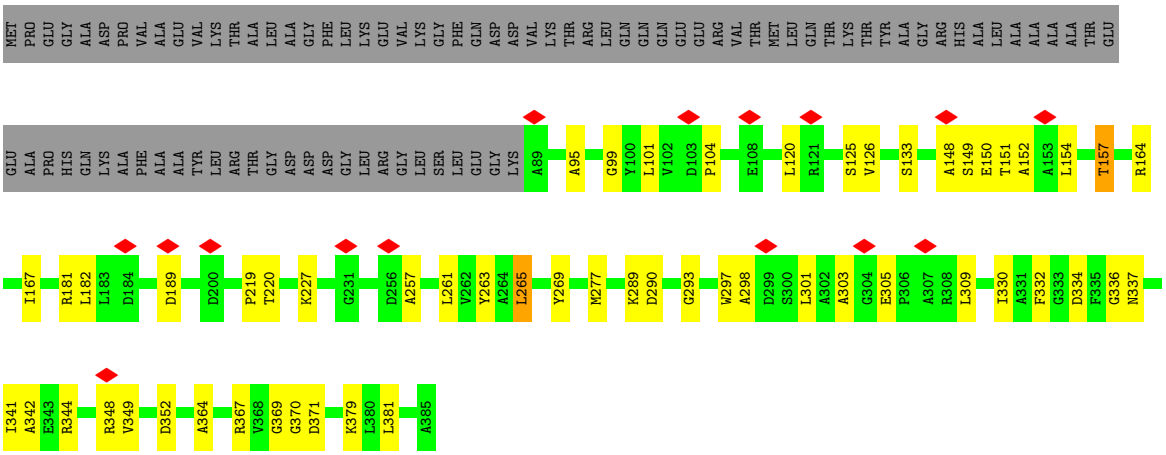
• Molecule 1: Phage major capsid protein, HK97 family

Chain OJ:



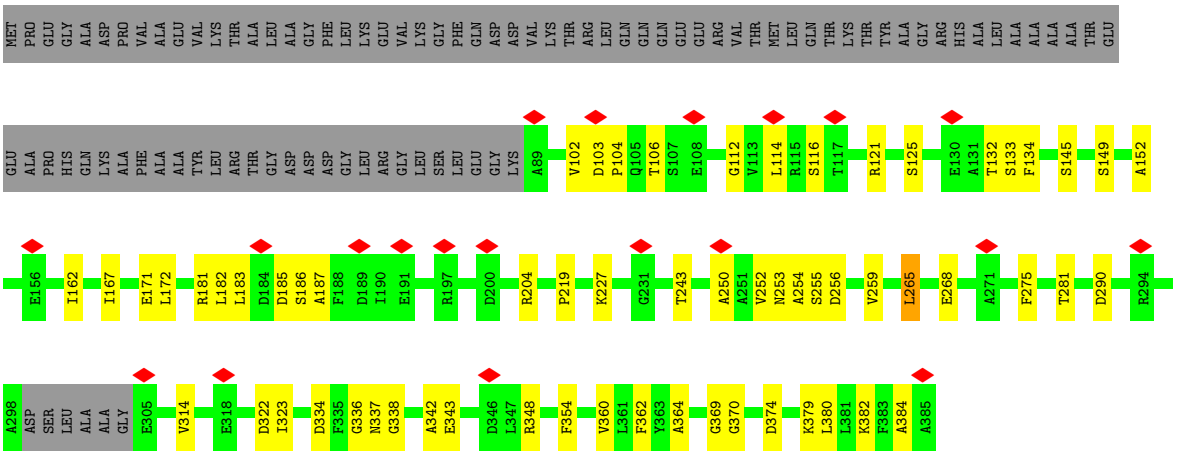
• Molecule 1: Phage major capsid protein, HK97 family

Chain PJ:



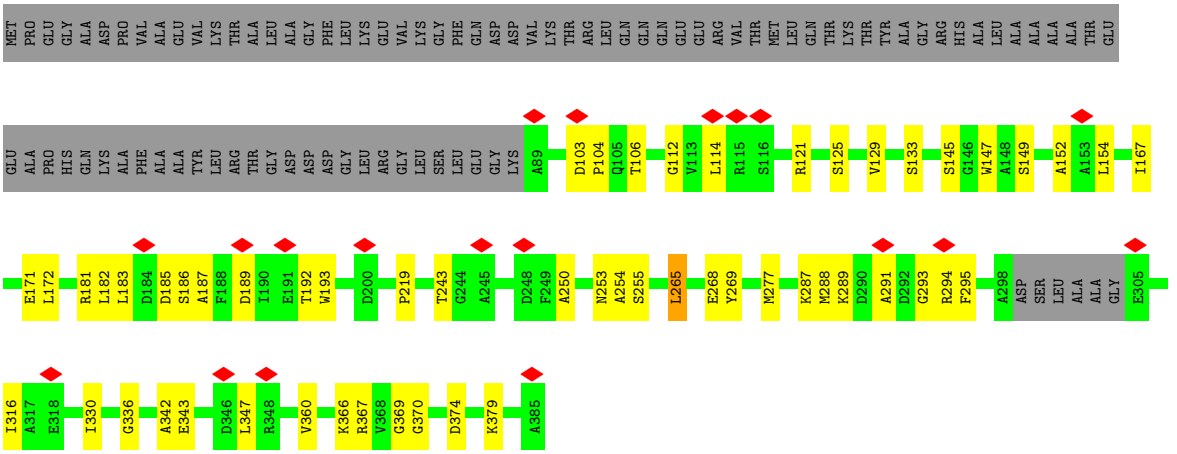
• Molecule 1: Phage major capsid protein, HK97 family

Chain WJ:



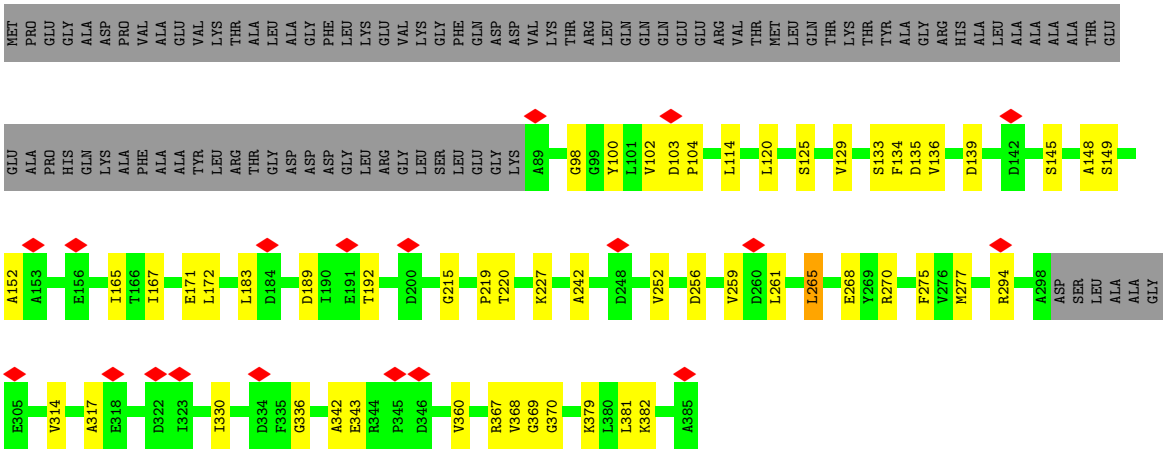
• Molecule 1: Phage major capsid protein, HK97 family

Chain UJ:



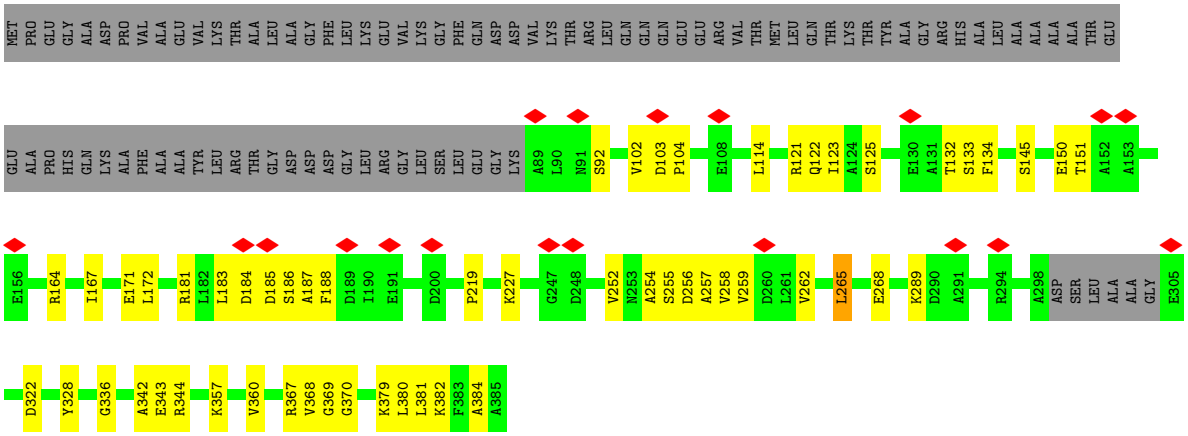
• Molecule 1: Phage major capsid protein, HK97 family

Chain TJ:



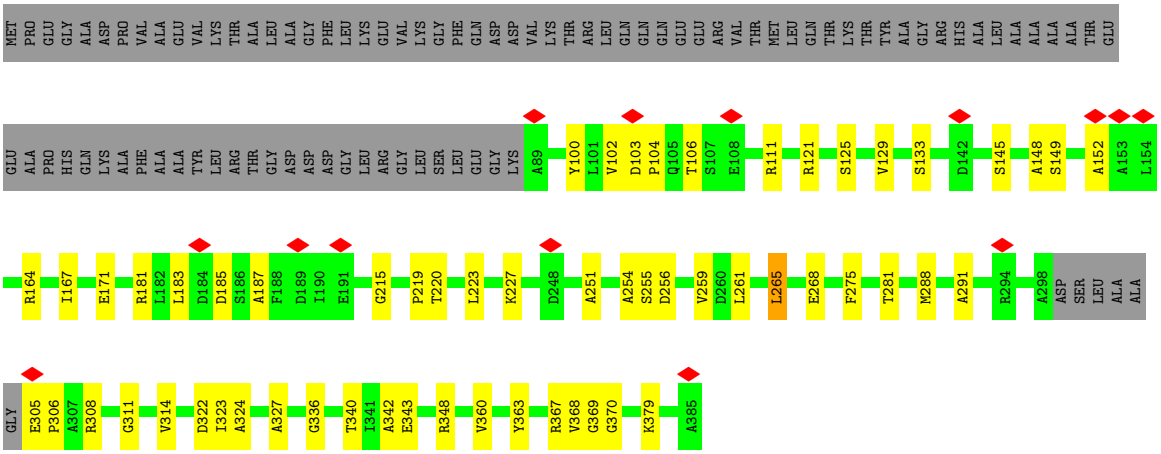
• Molecule 1: Phage major capsid protein, HK97 family

Chain SJ: 5% 61% 14% 24%



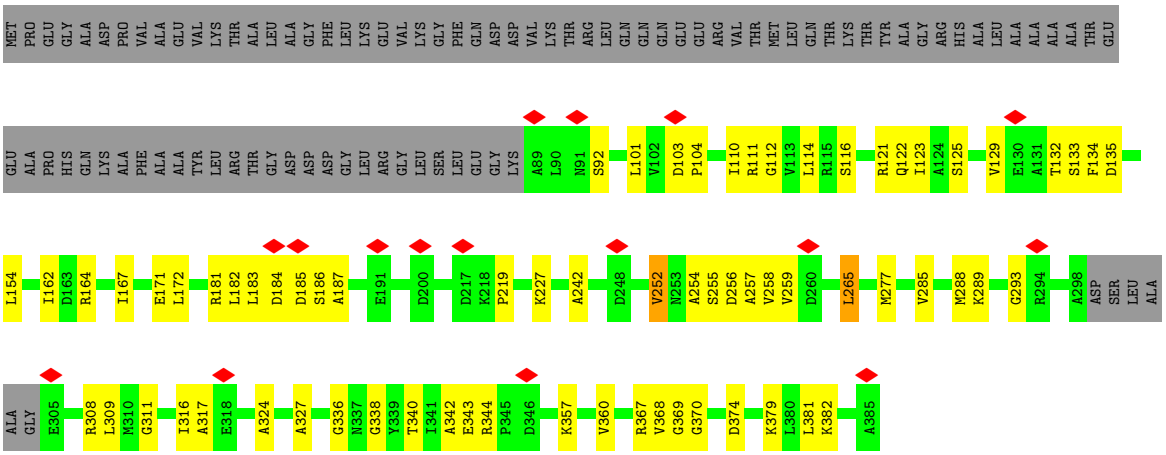
- Molecule 1: Phage major capsid protein, HK97 family

Chain KJ: 60% 15% 24%



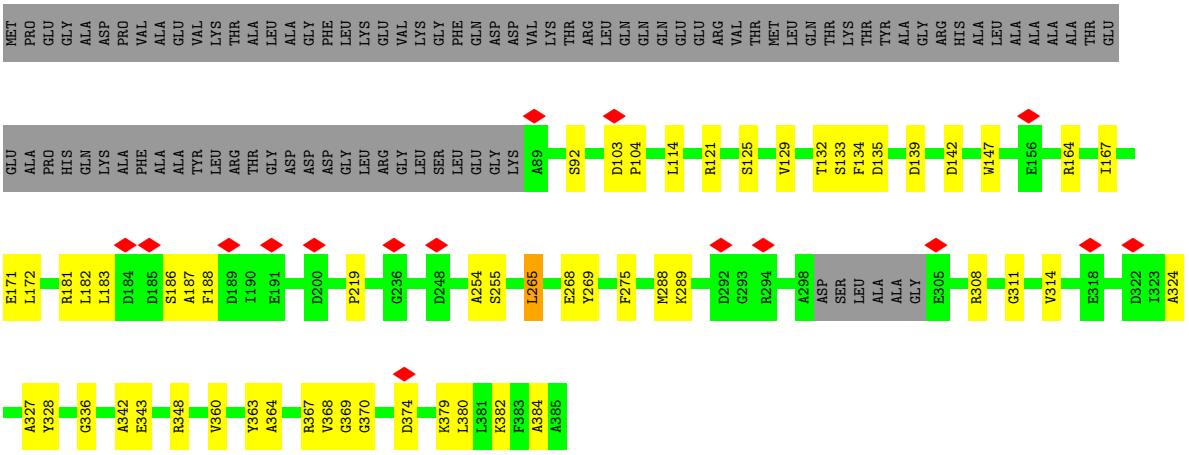
- Molecule 1: Phage major capsid protein, HK97 family

Chain JJ: 57% 18% 24%



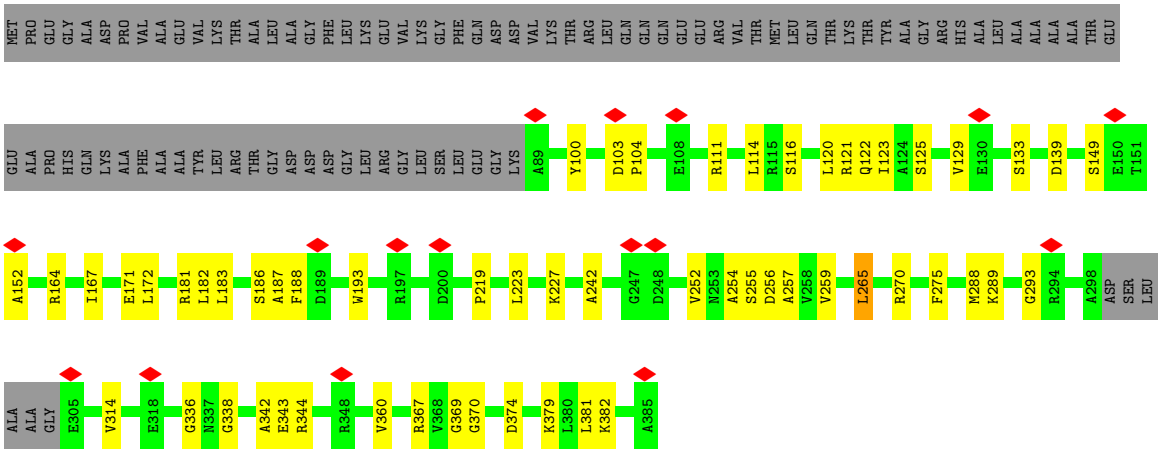
- Molecule 1: Phage major capsid protein, HK97 family

Chain VJ:



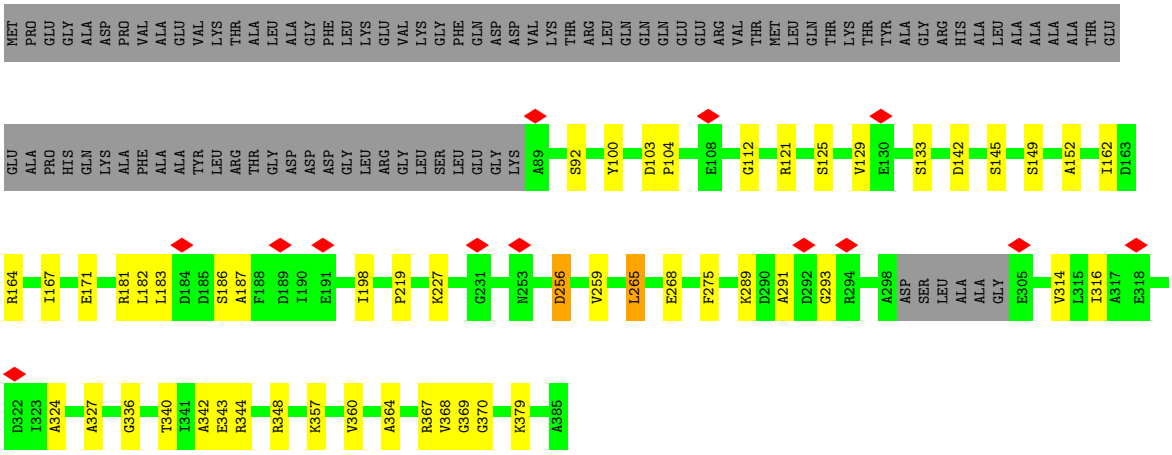
• Molecule 1: Phage major capsid protein, HK97 family

Chain LJ:



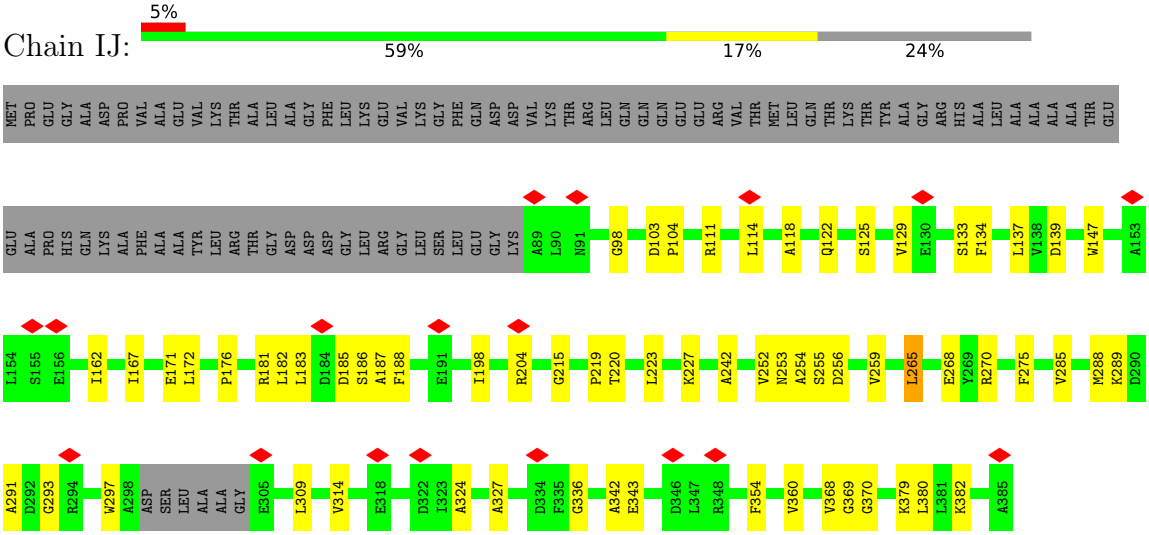
• Molecule 1: Phage major capsid protein, HK97 family

Chain HJ:



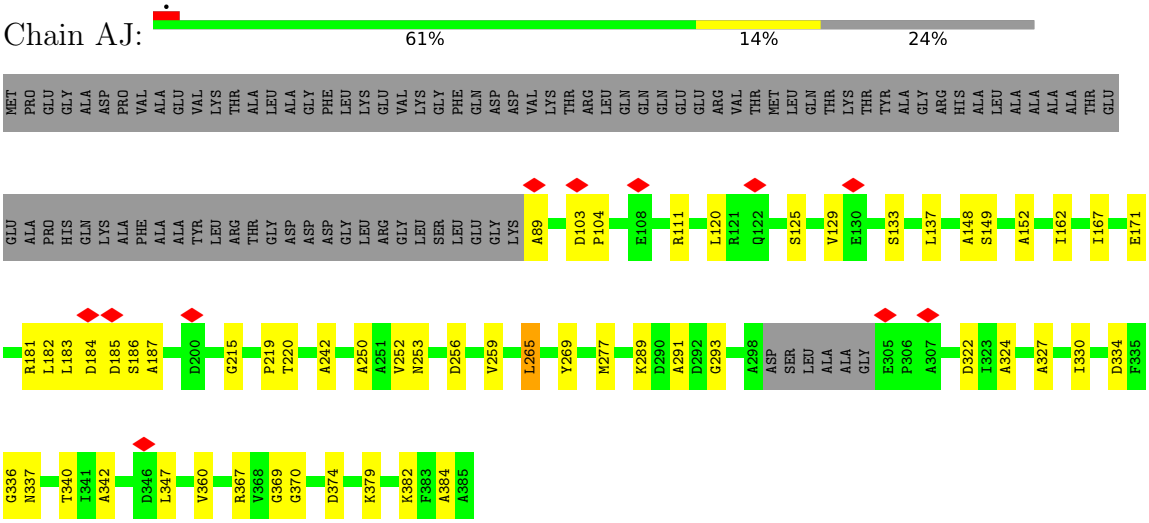
• Molecule 1: Phage major capsid protein, HK97 family

Chain IJ:



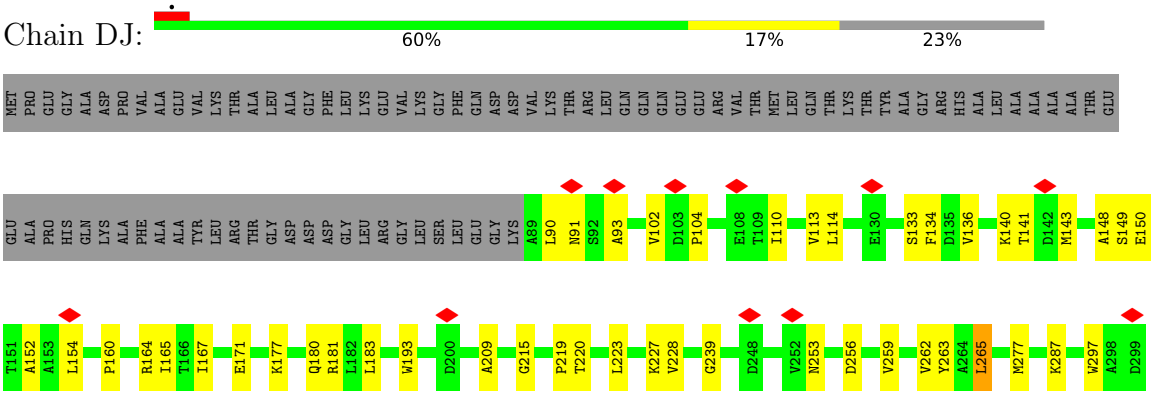
• Molecule 1: Phage major capsid protein, HK97 family

Chain AJ:



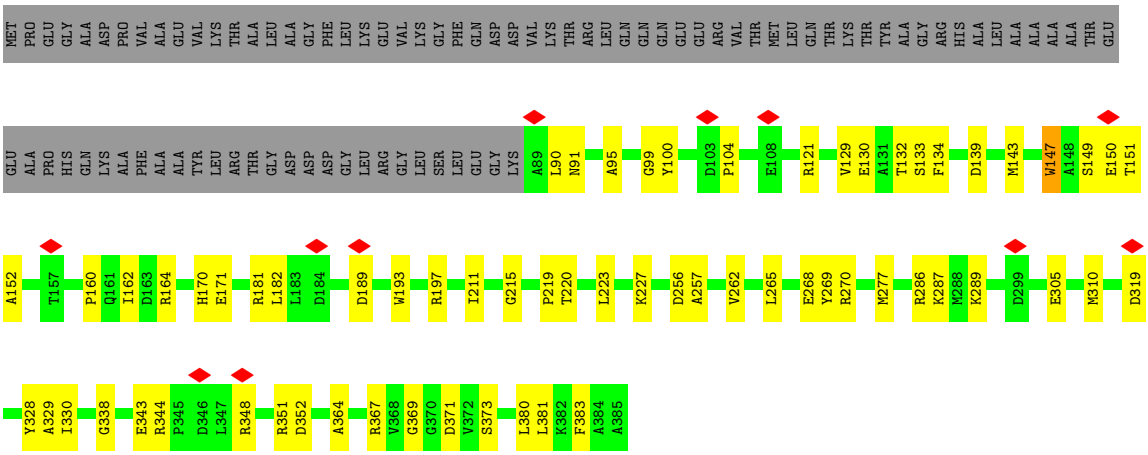
• Molecule 1: Phage major capsid protein, HK97 family

Chain DJ:



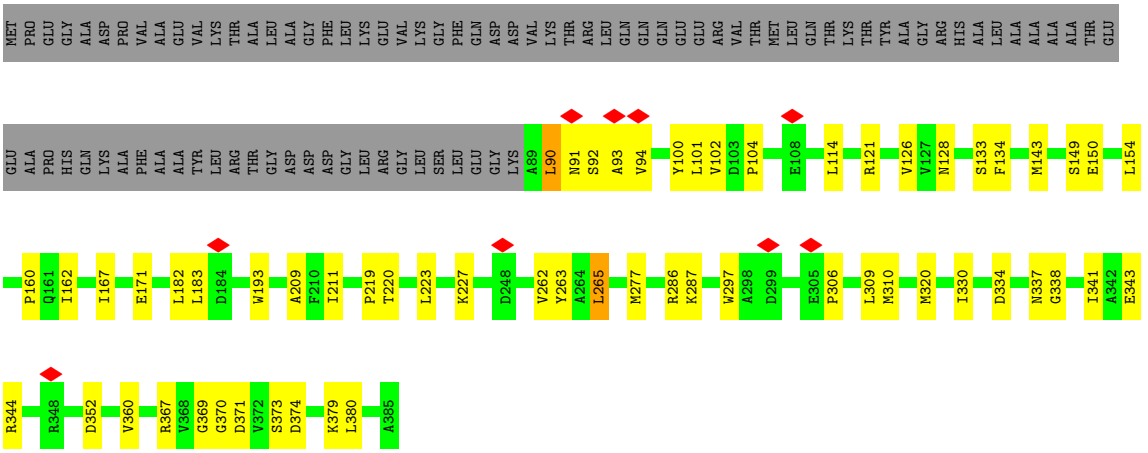
• Molecule 1: Phage major capsid protein, HK97 family

Chain EJ:



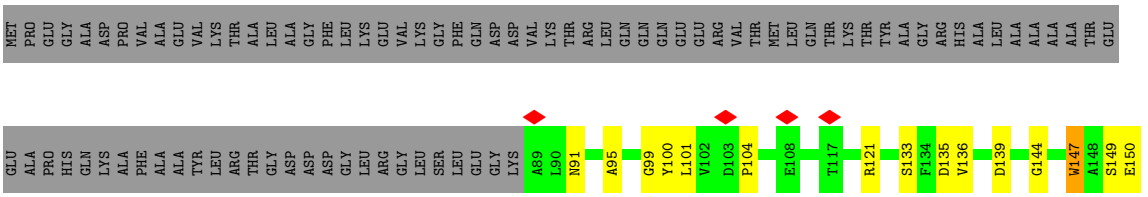
• Molecule 1: Phage major capsid protein, HK97 family

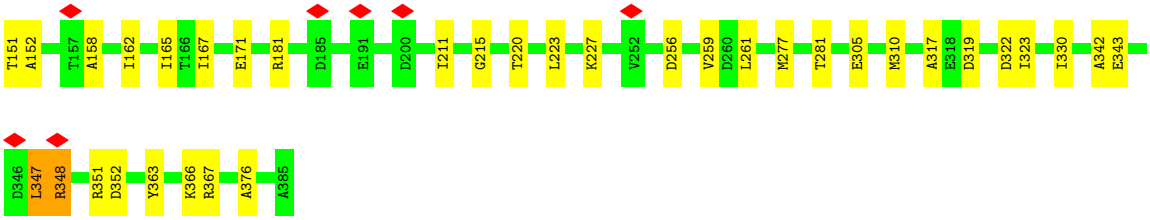
Chain FJ:



• Molecule 1: Phage major capsid protein, HK97 family

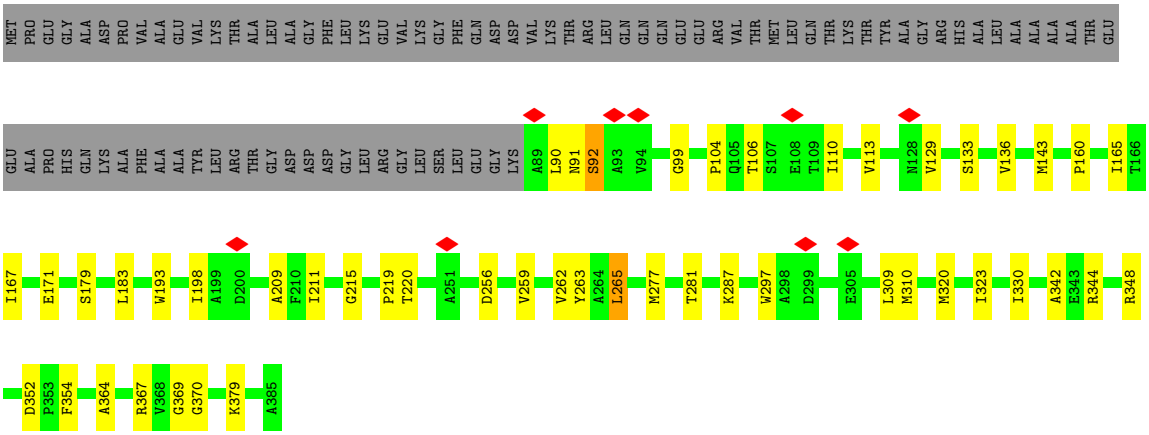
Chain GJ:





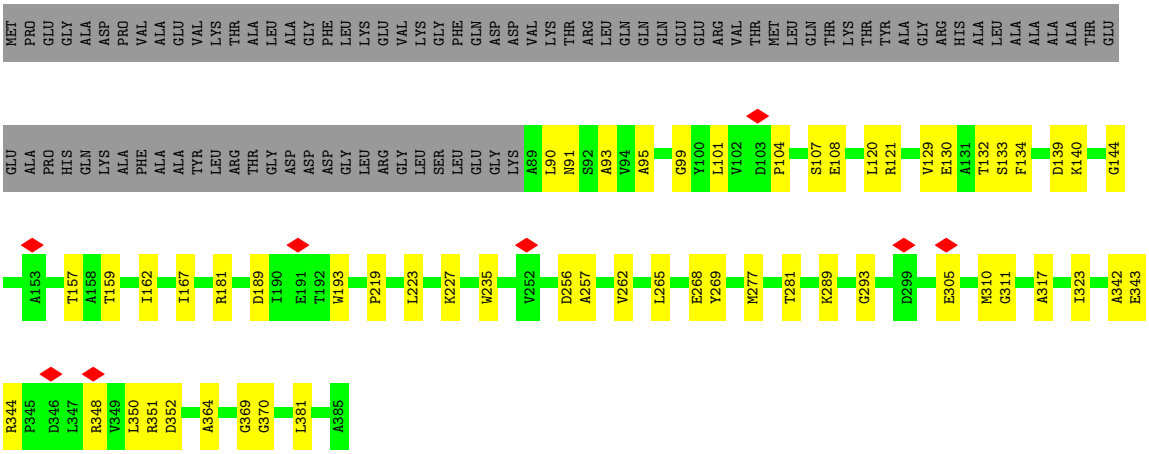
• Molecule 1: Phage major capsid protein, HK97 family

Chain BJ:



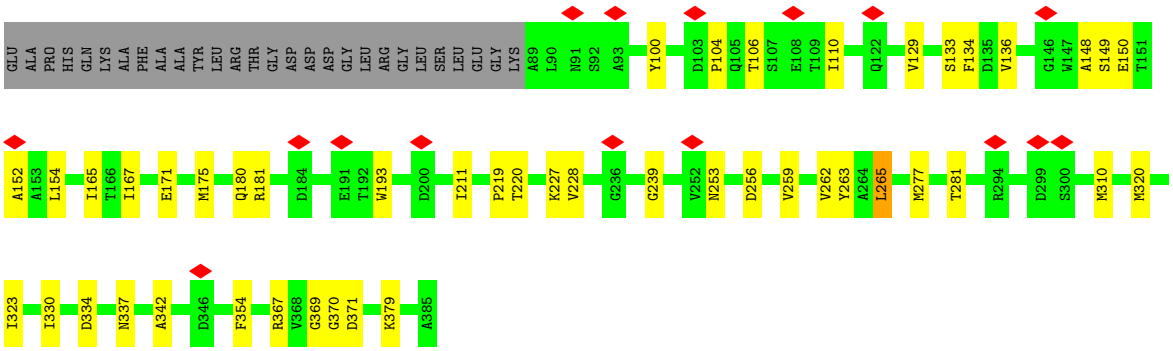
• Molecule 1: Phage major capsid protein, HK97 family

Chain CJ:



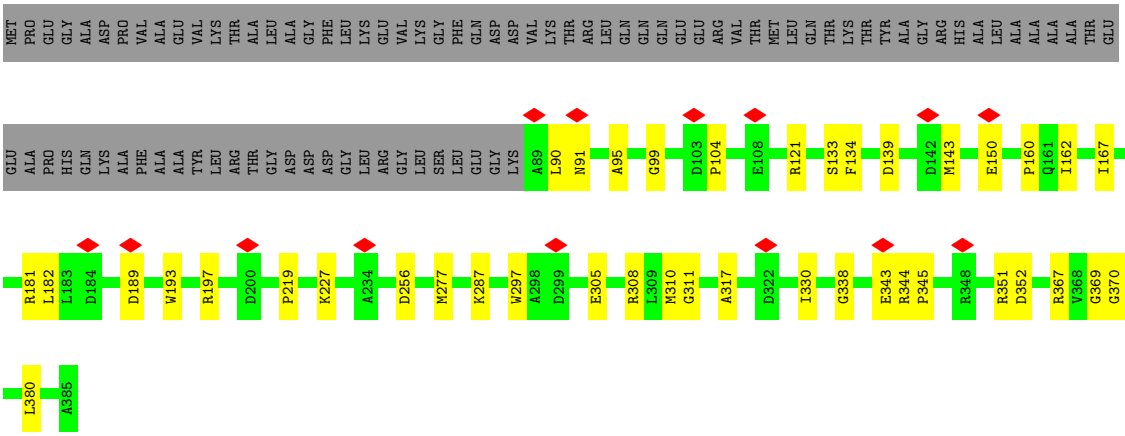
• Molecule 1: Phage major capsid protein, HK97 family

Chain CF:



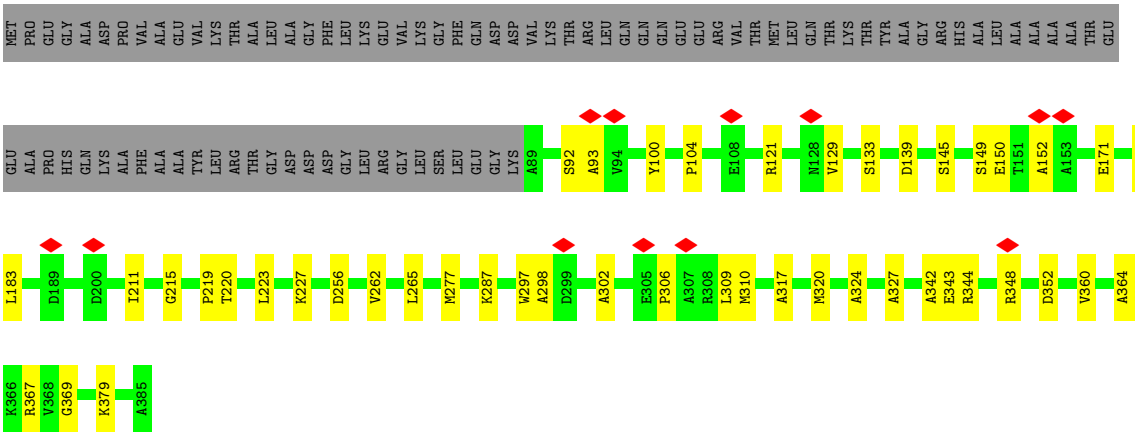
• Molecule 1: Phage major capsid protein, HK97 family

Chain XE:



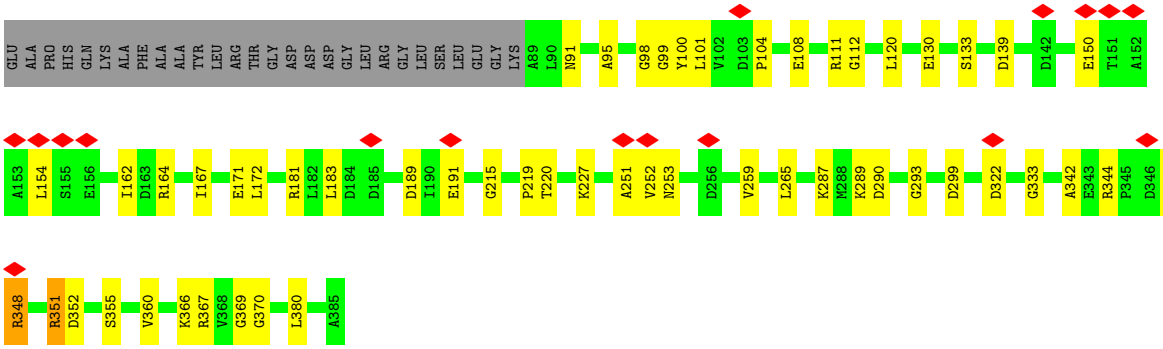
• Molecule 1: Phage major capsid protein, HK97 family

Chain YE:



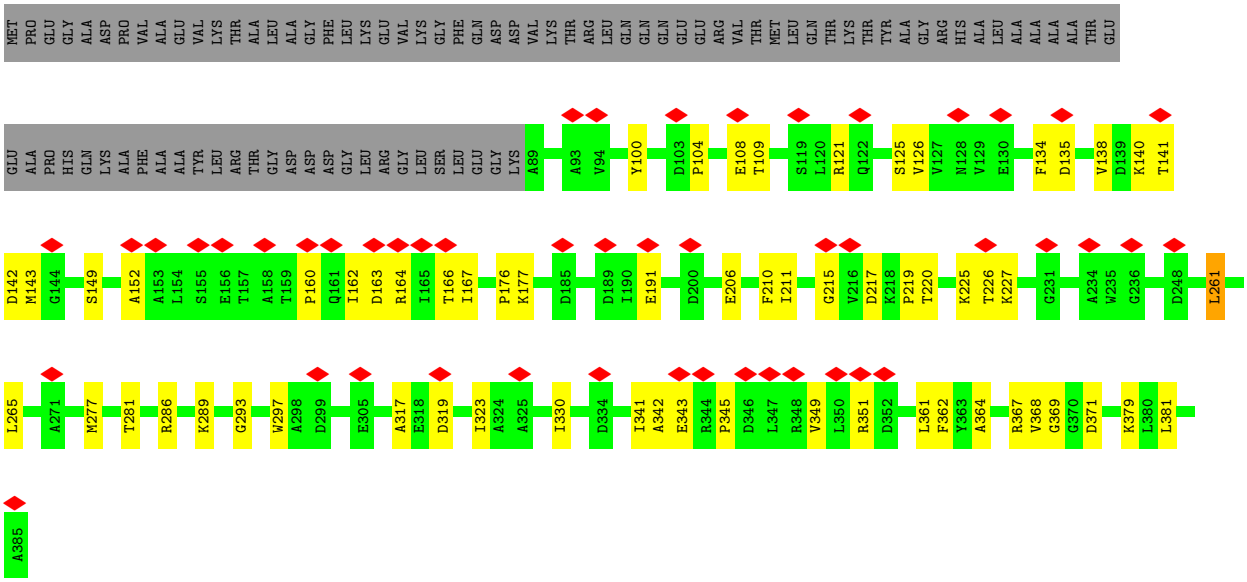
• Molecule 1: Phage major capsid protein, HK97 family

Chain ZE:



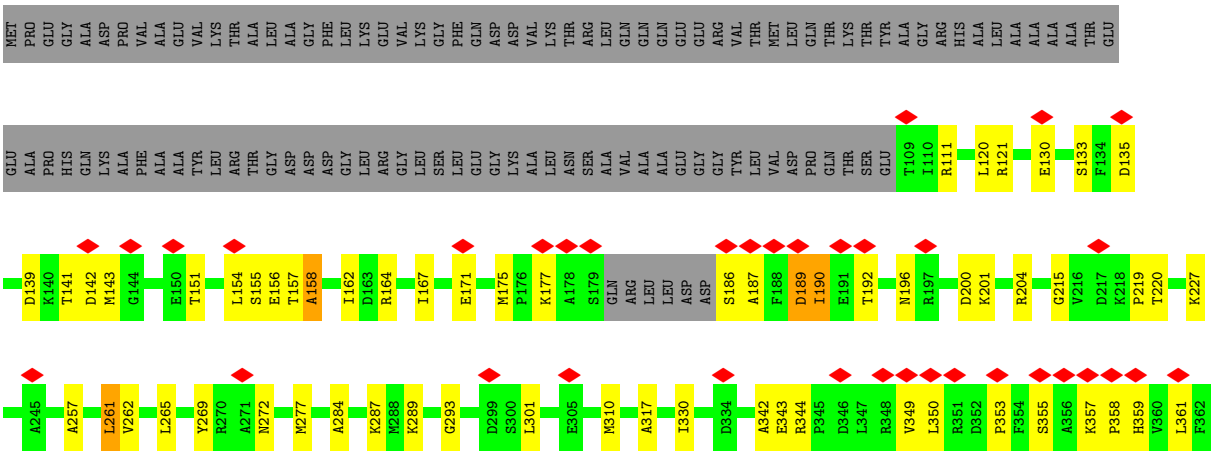
- Molecule 1: Phage major capsid protein, HK97 family

Chain AF:



- Molecule 1: Phage major capsid protein, HK97 family

Chain BF:



• Molecule 1: Phage major capsid protein, HK97 family

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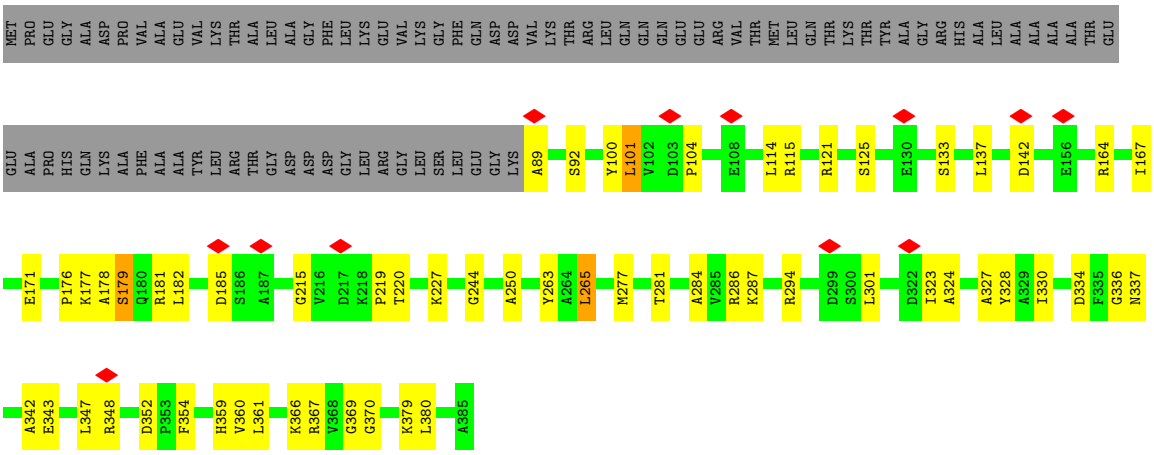
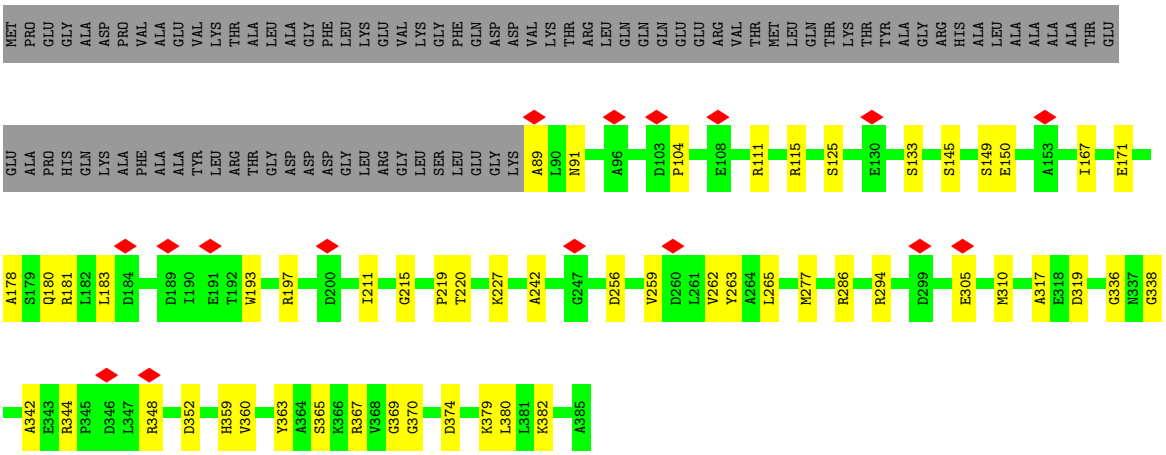


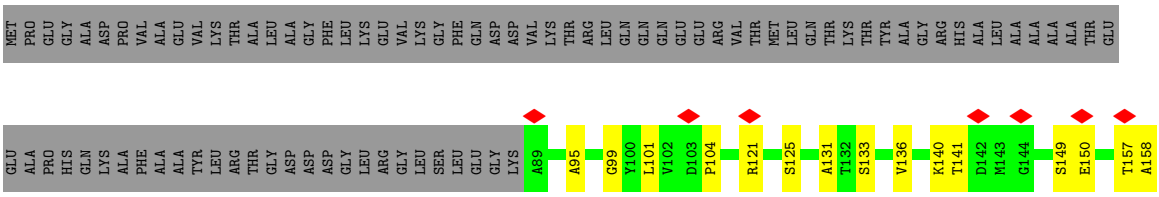
• Molecule 1: Phage major capsid protein, HK97 family

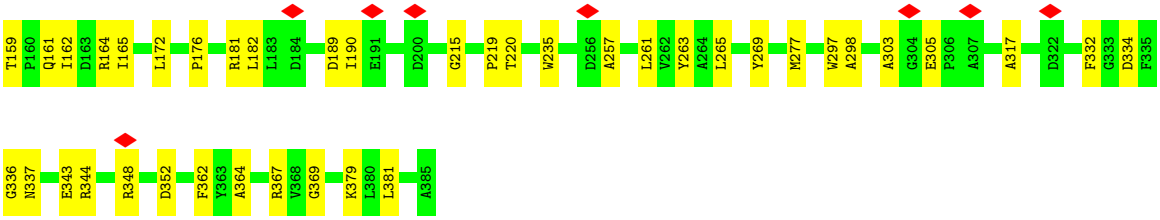
Chain RE:



• Molecule 1: Phage major capsid protein, HK97 family

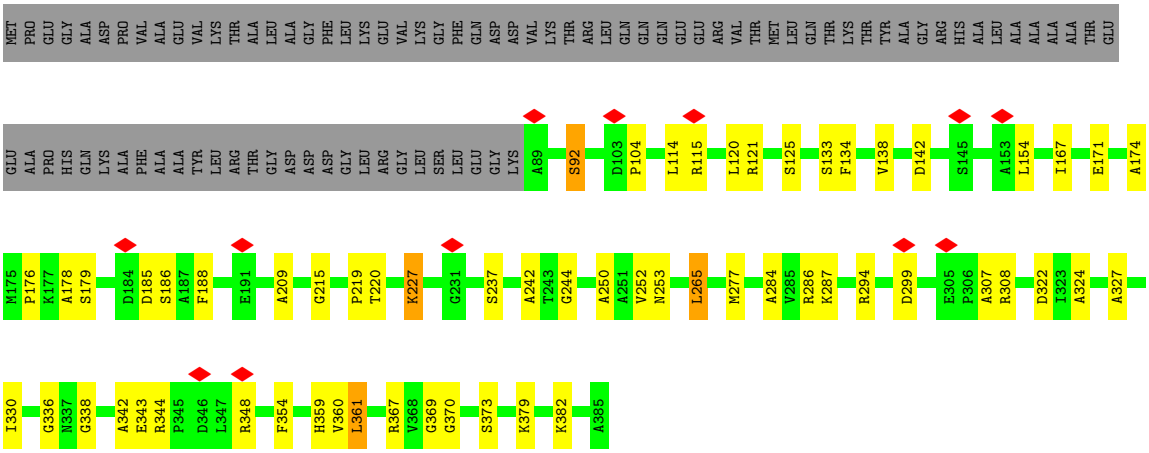
Chain ME:





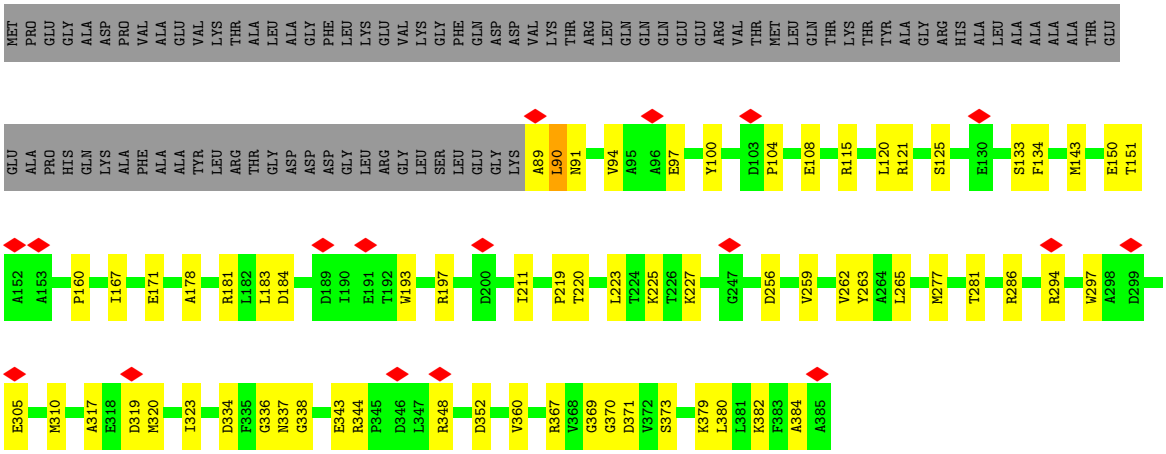
• Molecule 1: Phage major capsid protein, HK97 family

Chain QE:



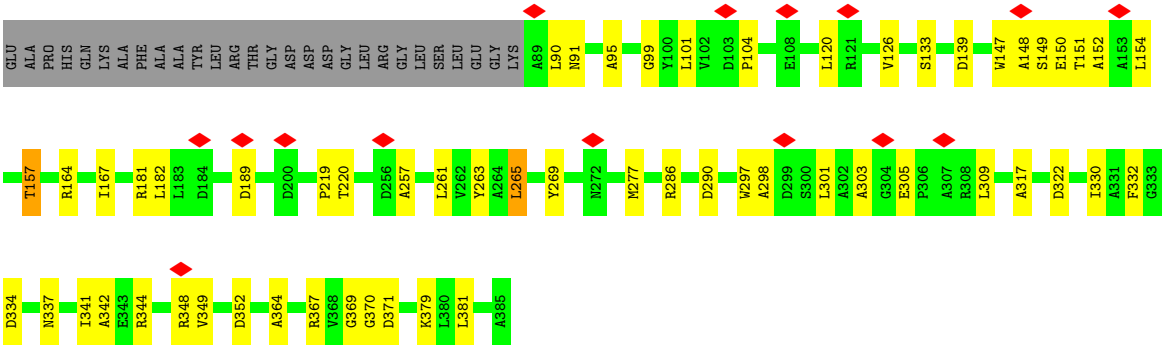
• Molecule 1: Phage major capsid protein, HK97 family

Chain OE:



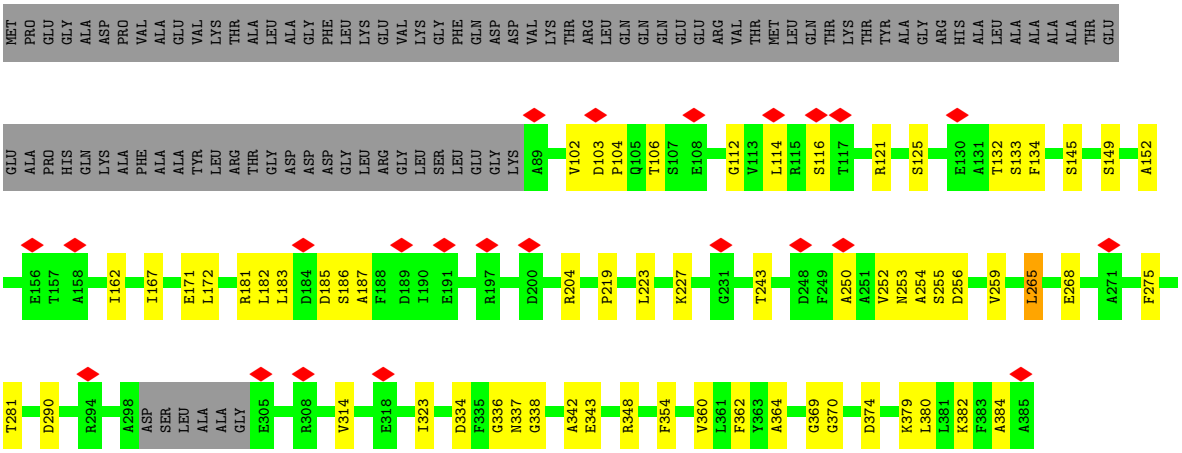
• Molecule 1: Phage major capsid protein, HK97 family

Chain PE:



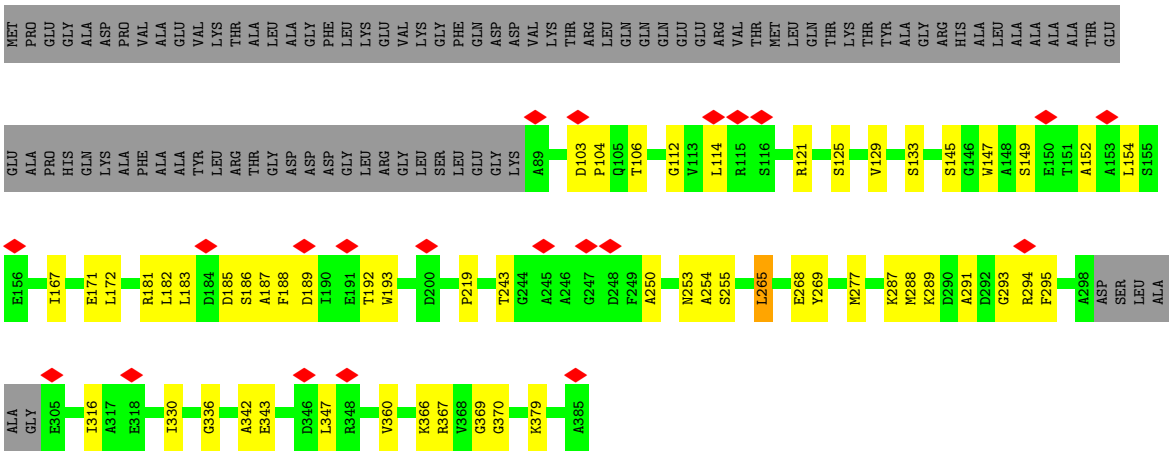
• Molecule 1: Phage major capsid protein, HK97 family

Chain WE:



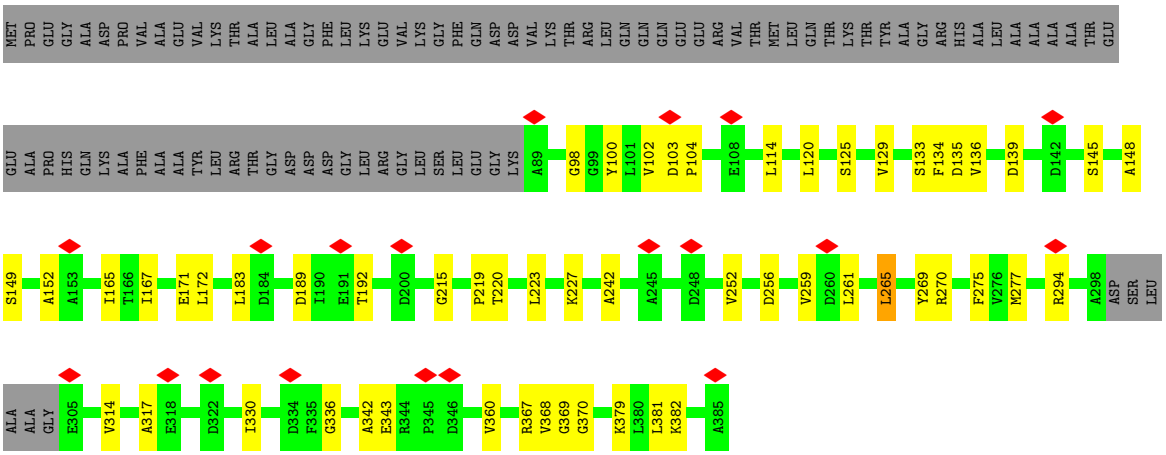
• Molecule 1: Phage major capsid protein, HK97 family

Chain UE:



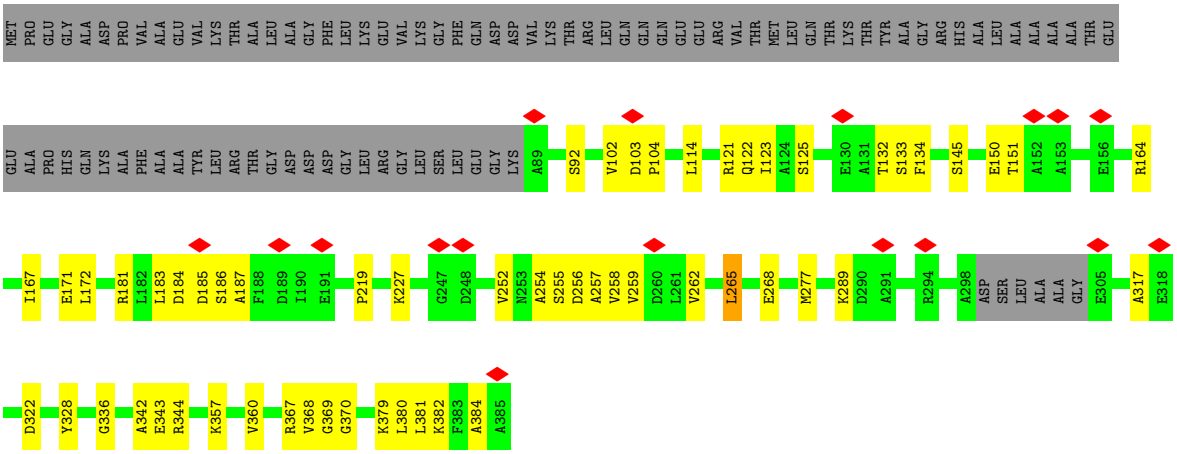
• Molecule 1: Phage major capsid protein, HK97 family

Chain TE:



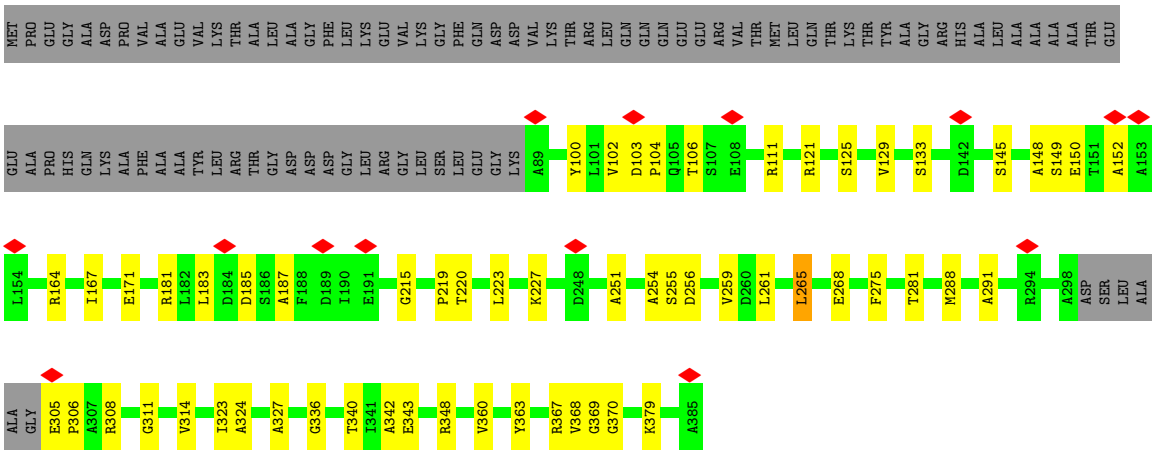
• Molecule 1: Phage major capsid protein, HK97 family

Chain SE:



• Molecule 1: Phage major capsid protein, HK97 family

Chain KE:



• Molecule 1: Phage major capsid protein, HK97 family

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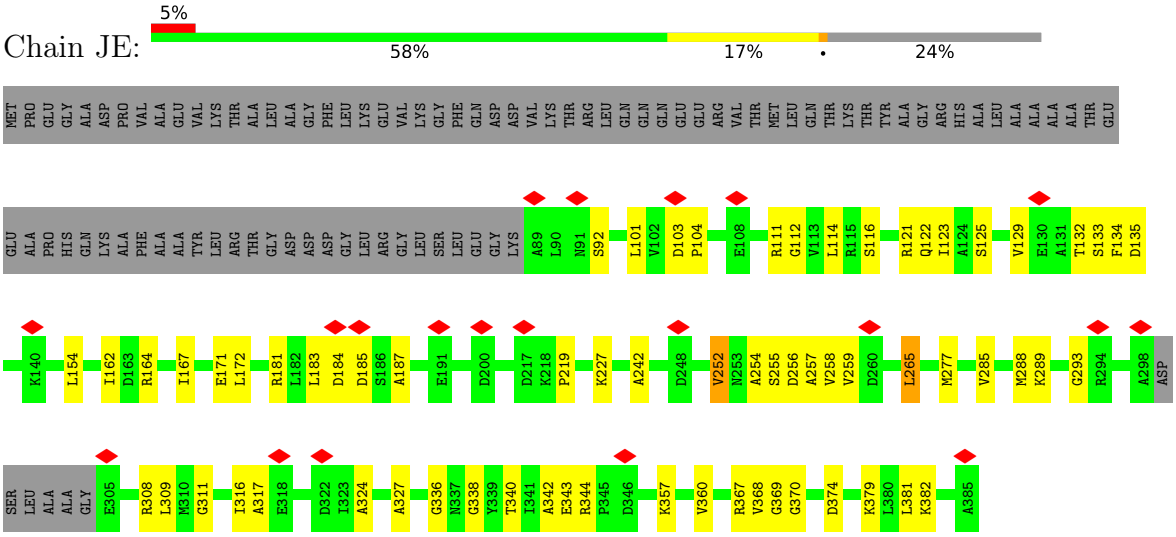
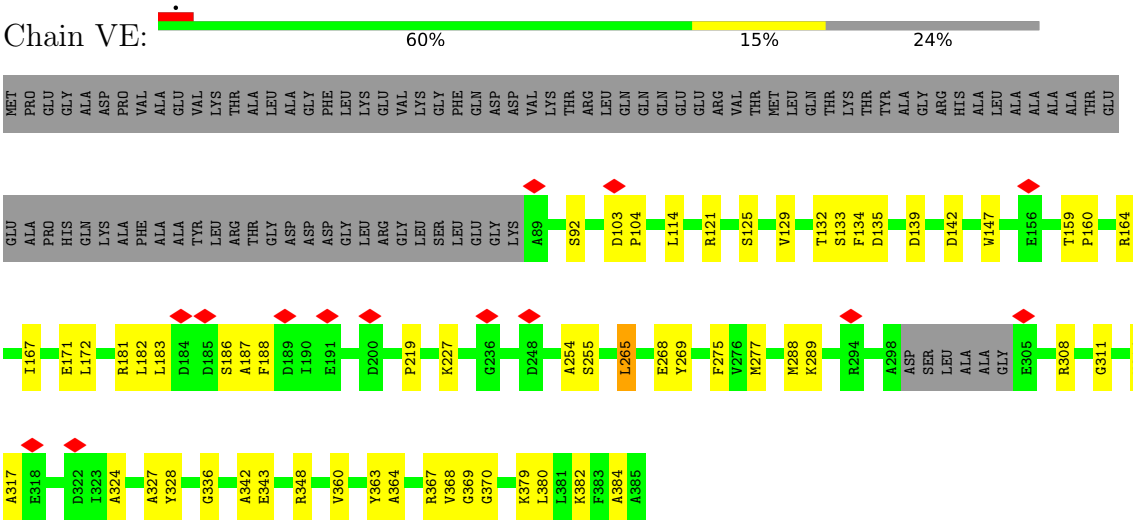


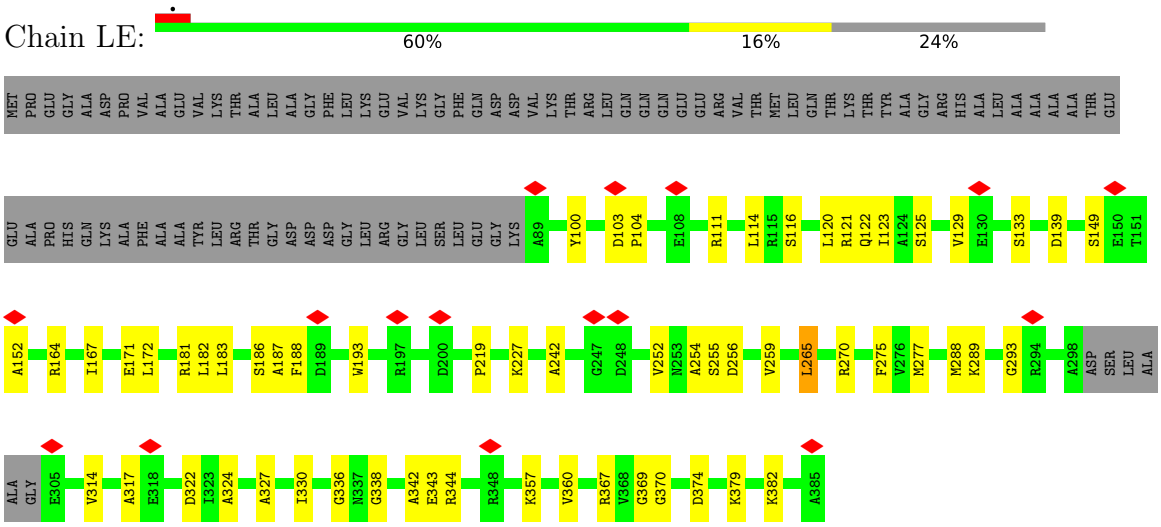
- Molecule 1: Phage major capsid protein, HK97 family

Chain VE:



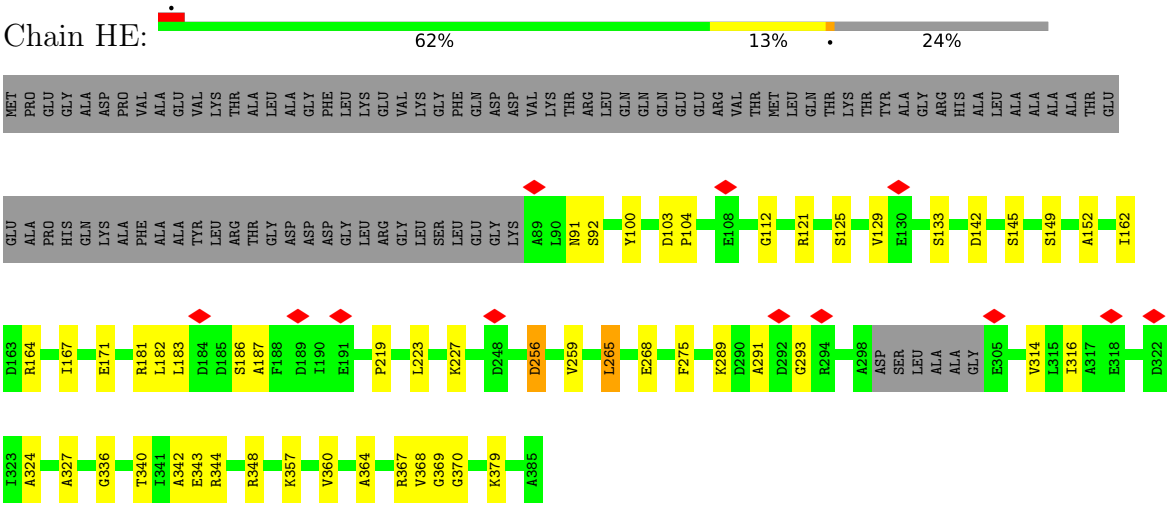
- Molecule 1: Phage major capsid protein, HK97 family

Chain LE:



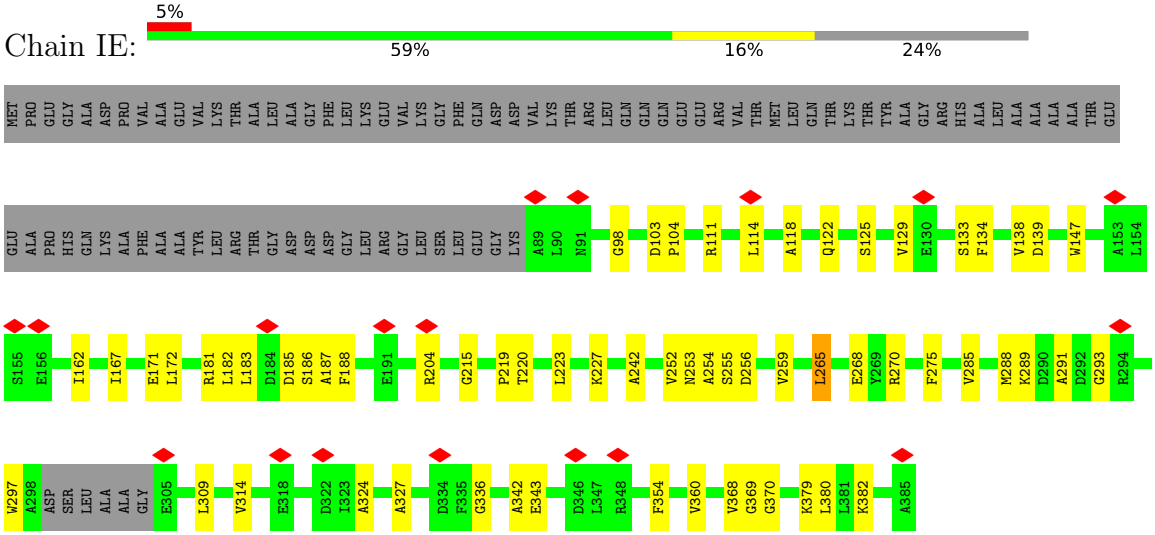
- Molecule 1: Phage major capsid protein, HK97 family

Chain HE:



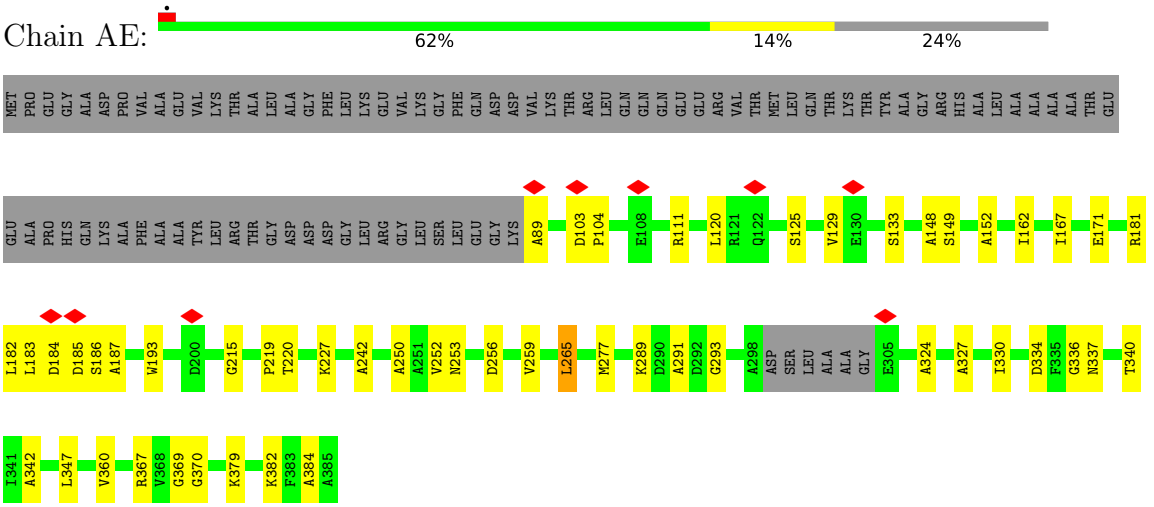
- Molecule 1: Phage major capsid protein, HK97 family

Chain IE:



- Molecule 1: Phage major capsid protein, HK97 family

Chain AE:



• Molecule 1: Phage major capsid protein, HK97 family

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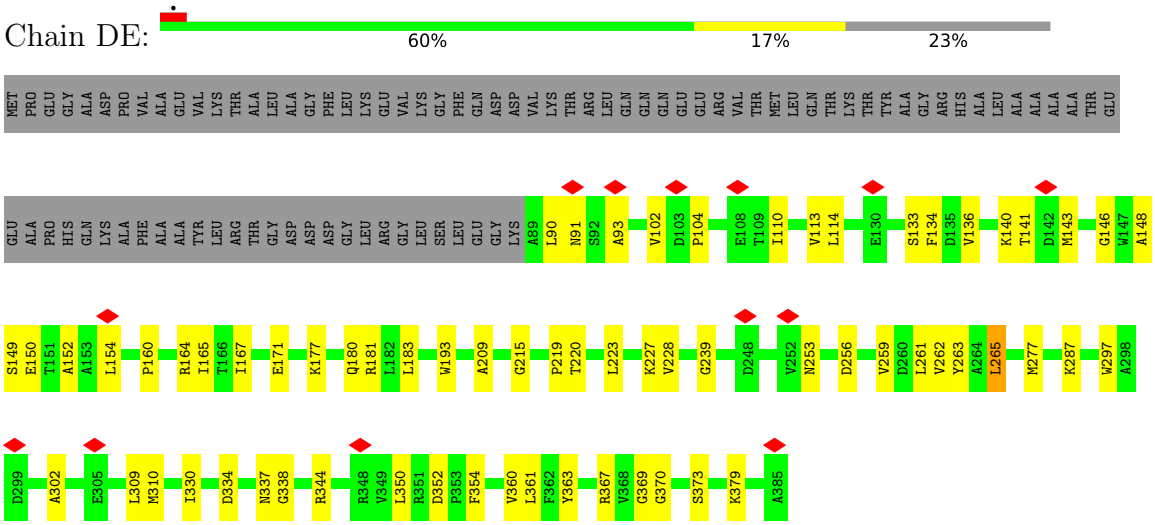
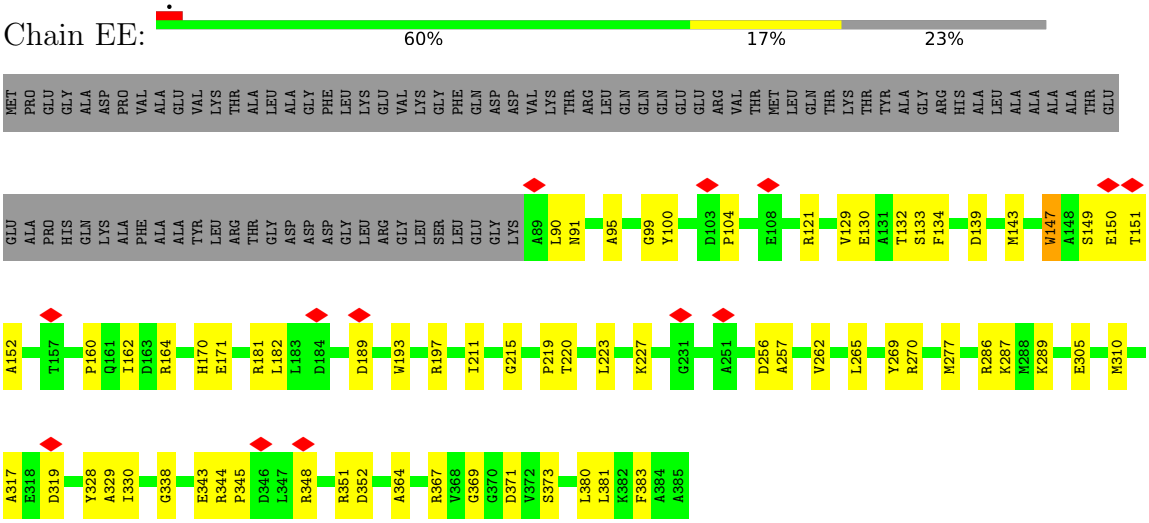


• Molecule 1: Phage major capsid protein, HK97 family

Chain EE:



• Molecule 1: Phage major capsid protein, HK97 family

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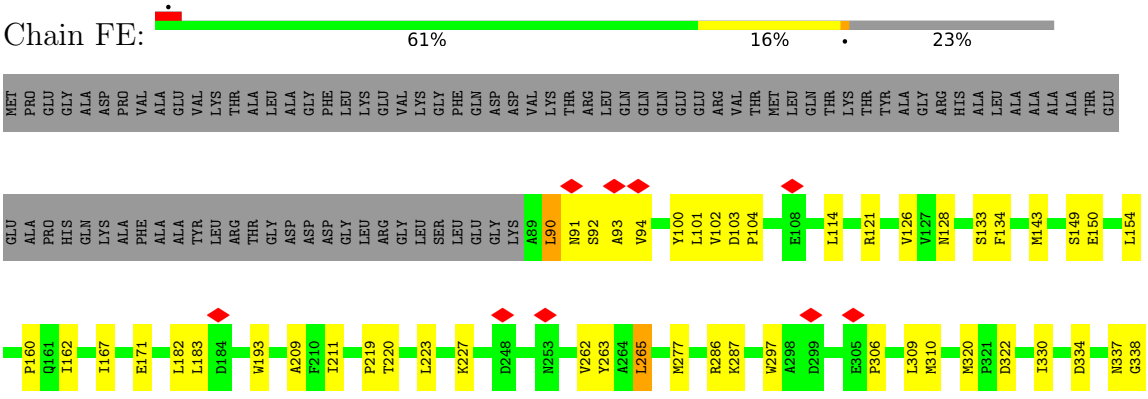

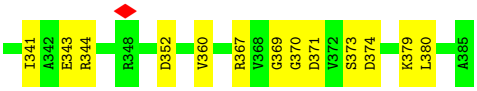

- Molecule 1: Phage major capsid protein, HK97 family

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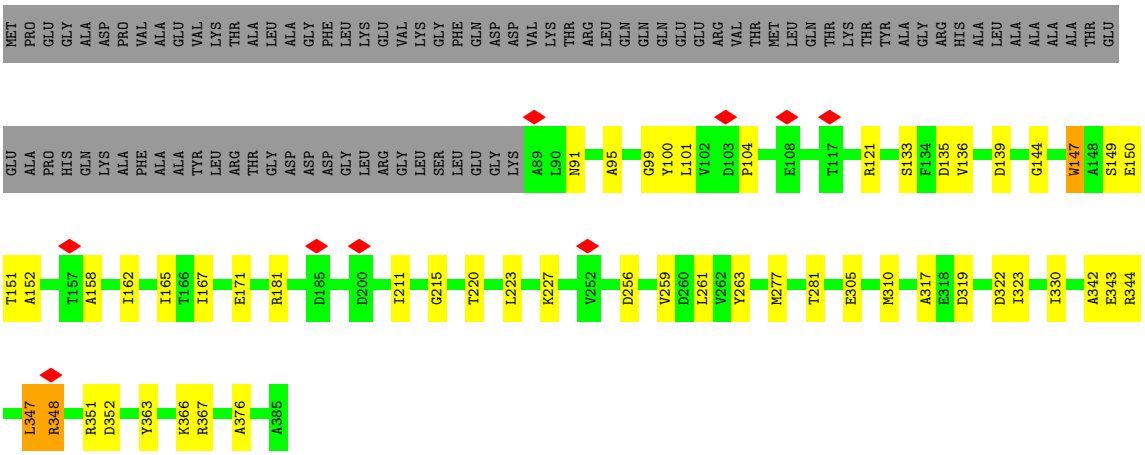
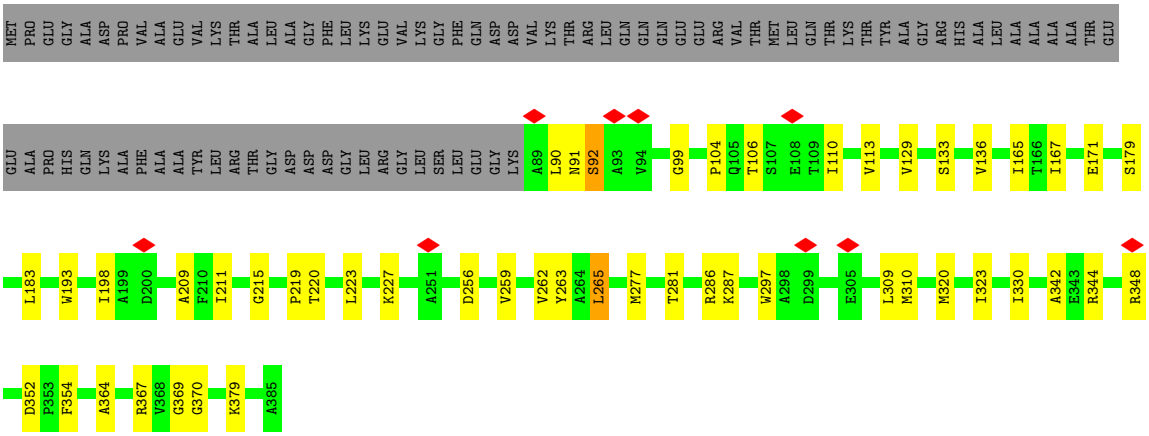


- Molecule 1: Phage major capsid protein, HK97 family

Chain BE:



- Molecule 1: Phage major capsid protein, HK97 family

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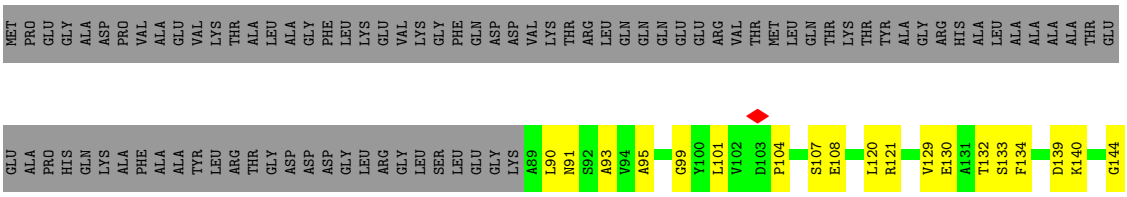
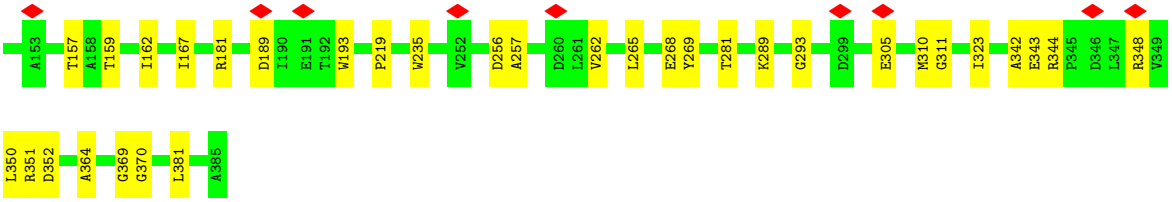
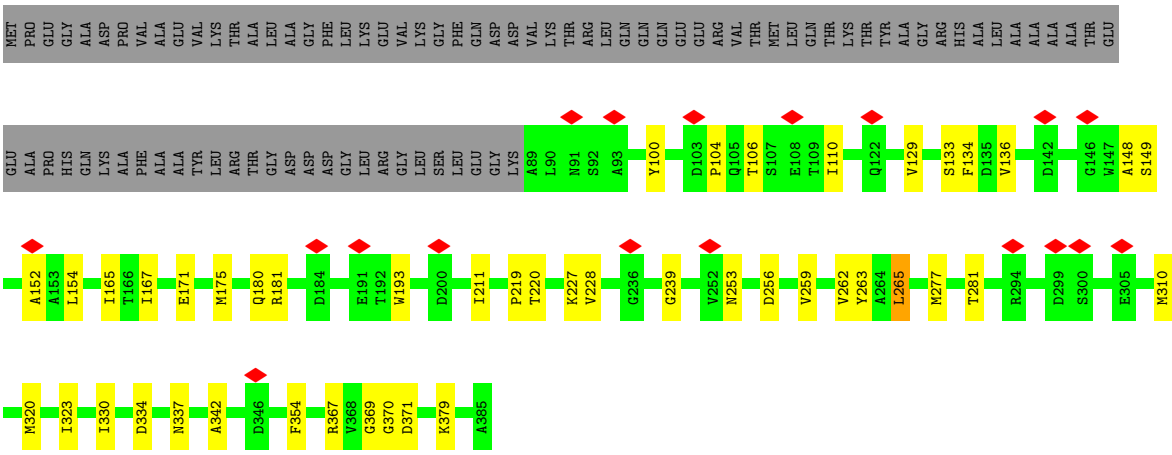




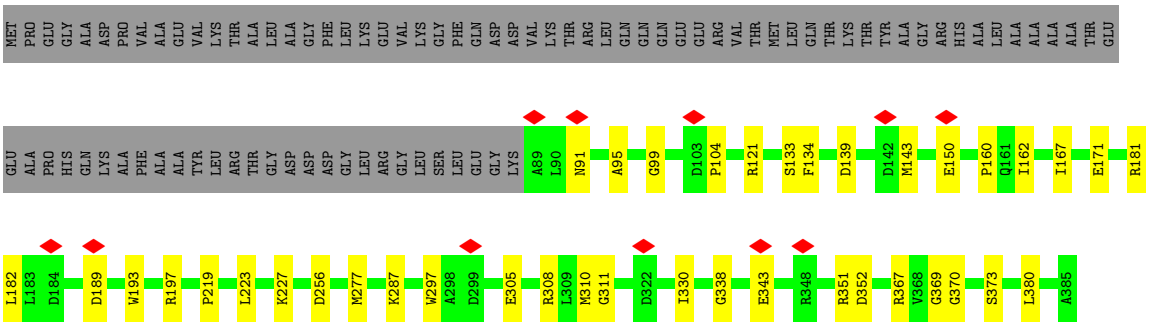
• Molecule 1: Phage major capsid protein, HK97 family

Chain CA:



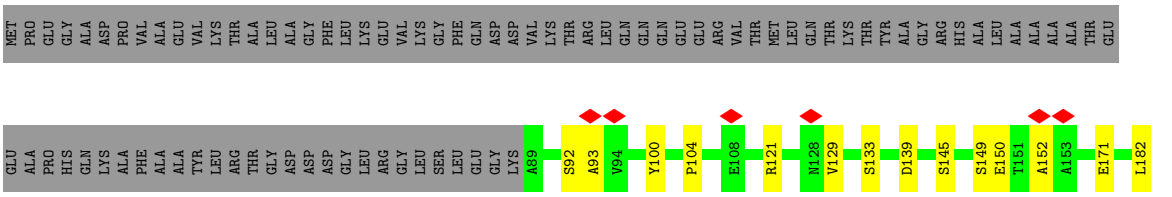
• Molecule 1: Phage major capsid protein, HK97 family

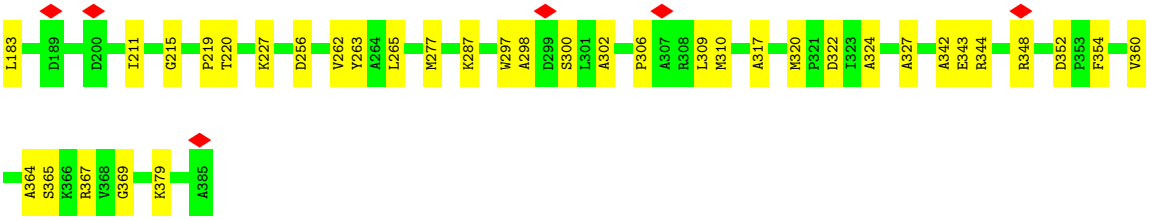
Chain X9:



• Molecule 1: Phage major capsid protein, HK97 family

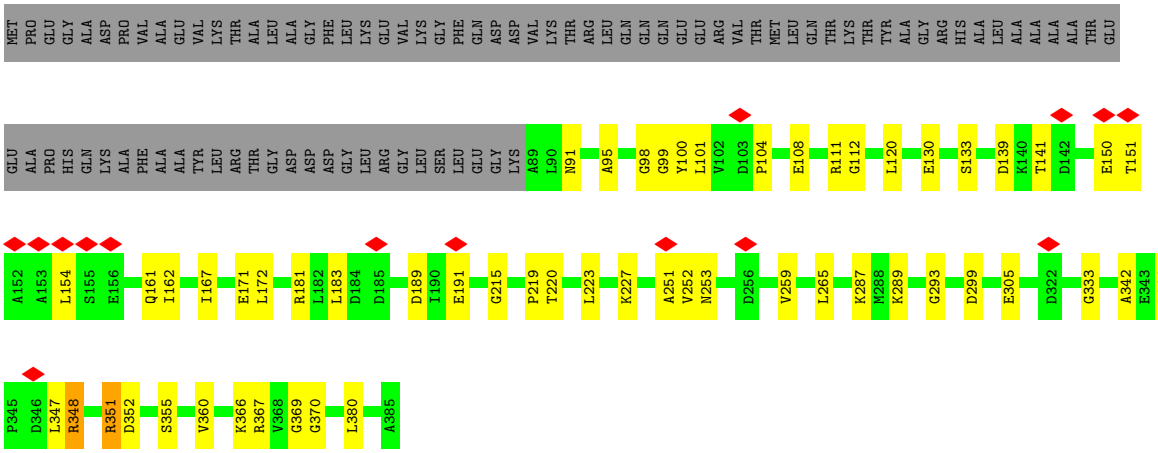
Chain Y9:





• Molecule 1: Phage major capsid protein, HK97 family

Chain Z9:



• Molecule 1: Phage major capsid protein, HK97 family

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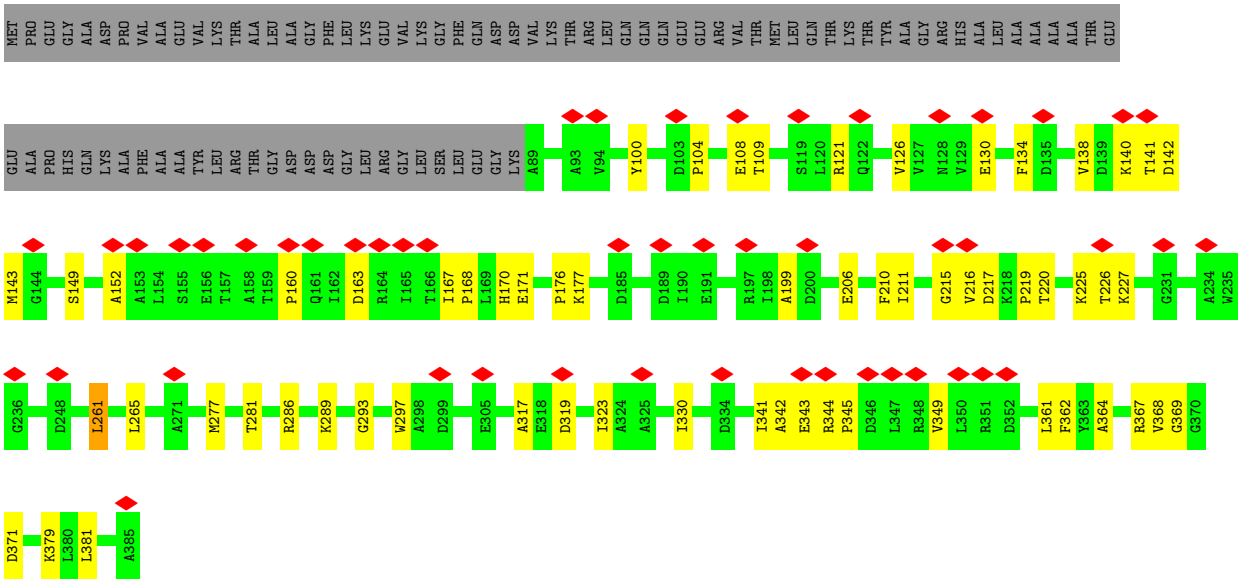
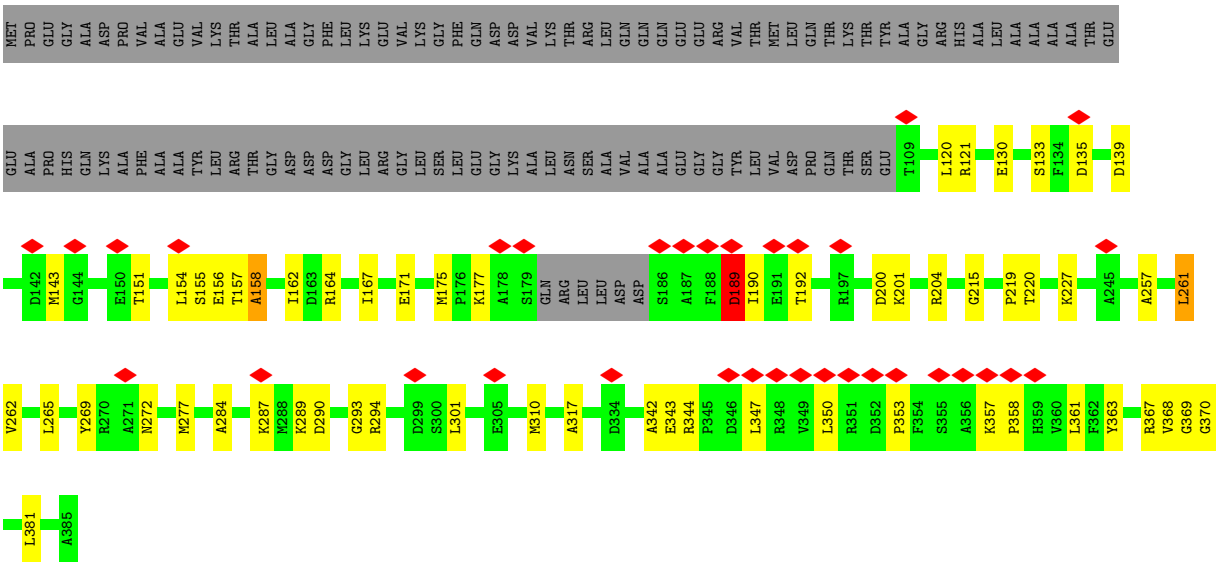


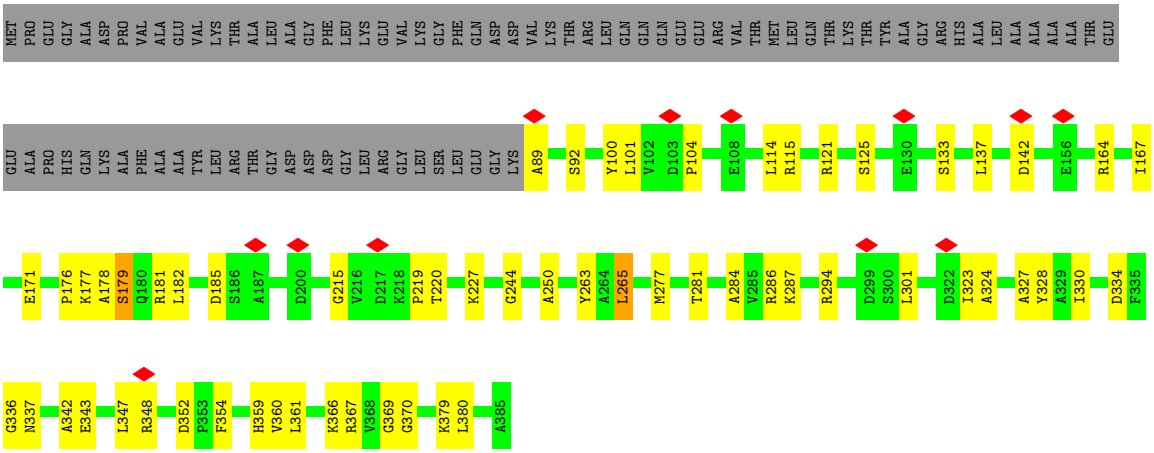
• Molecule 1: Phage major capsid protein, HK97 family

Chain BA:



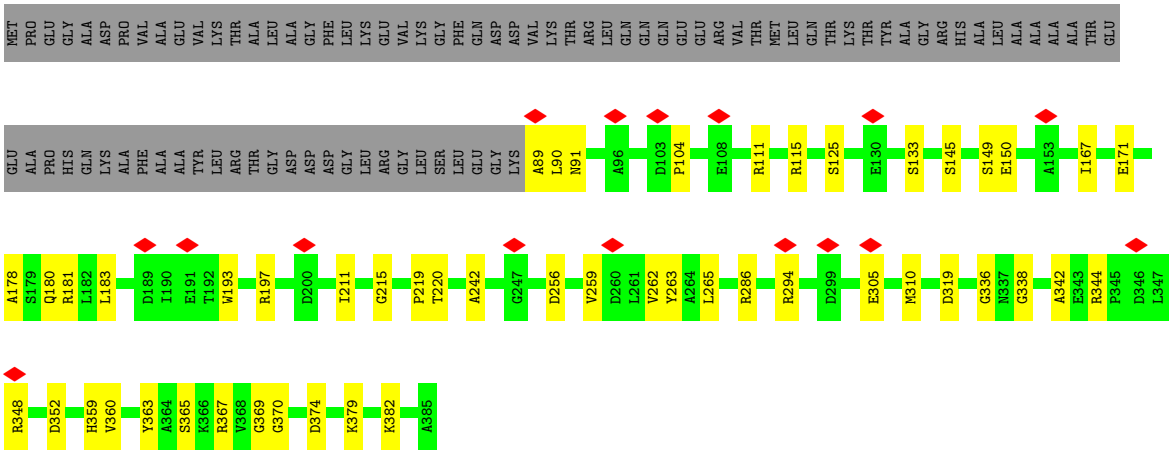
- Molecule 1: Phage major capsid protein, HK97 family

Chain N9:



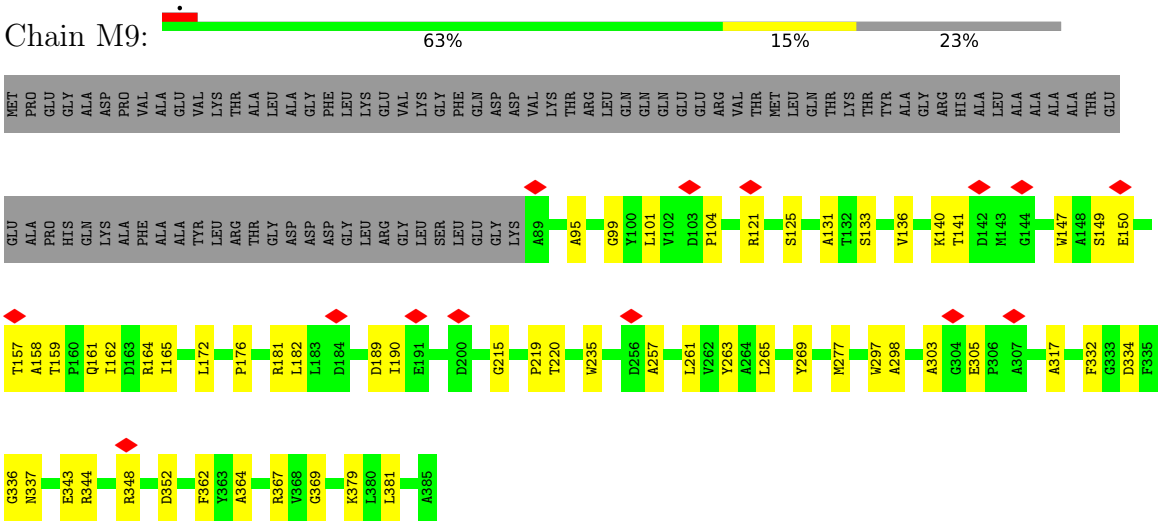
- Molecule 1: Phage major capsid protein, HK97 family

Chain R9:



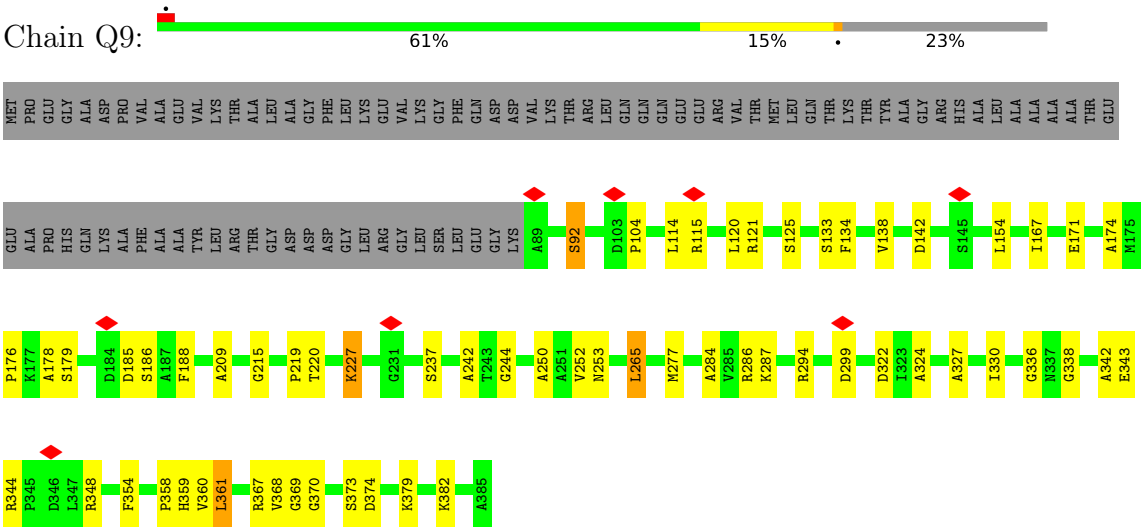
• Molecule 1: Phage major capsid protein, HK97 family

Chain M9:



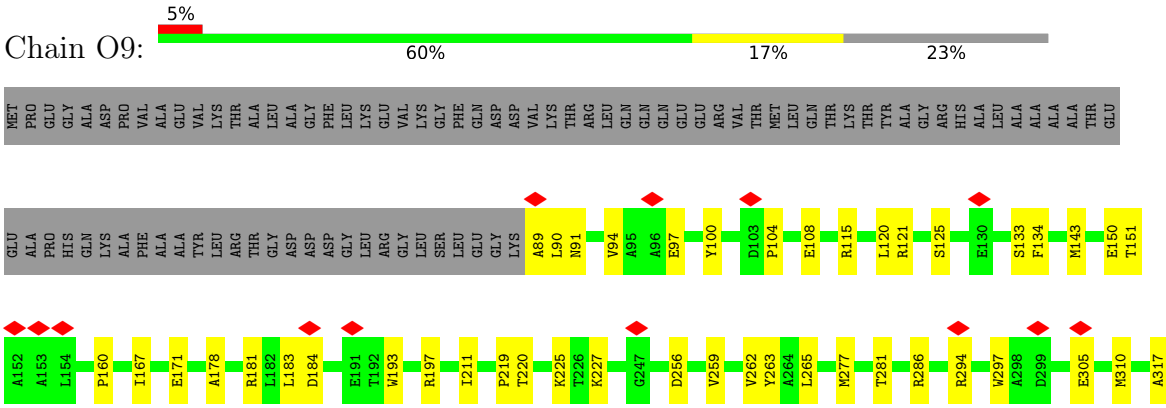
• Molecule 1: Phage major capsid protein, HK97 family

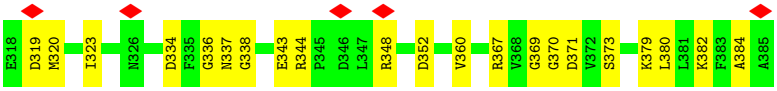
Chain Q9:



• Molecule 1: Phage major capsid protein, HK97 family

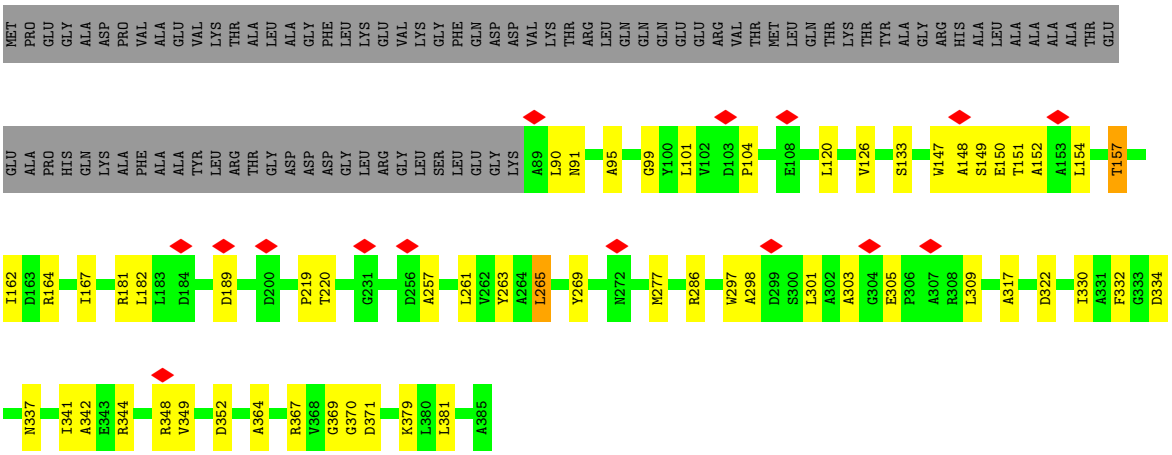
Chain O9:





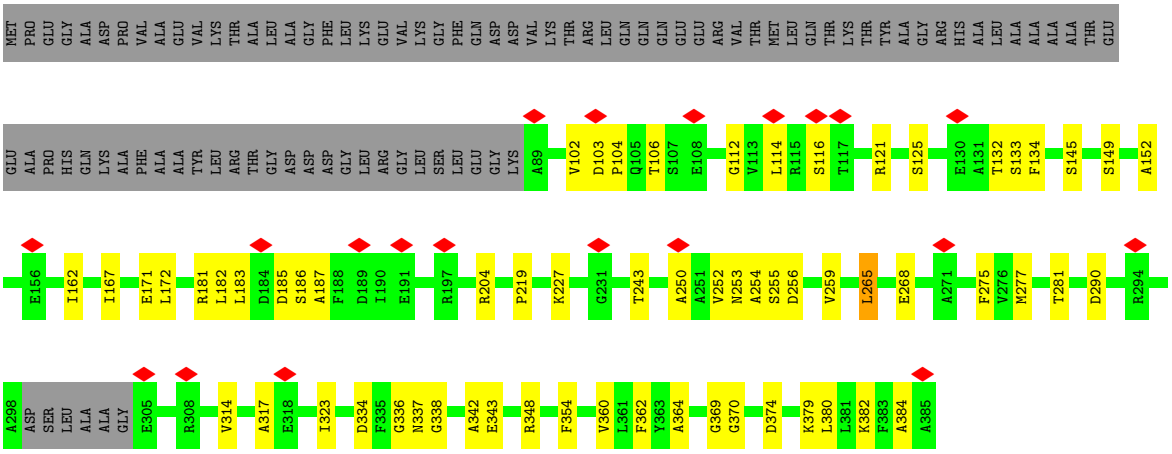
• Molecule 1: Phage major capsid protein, HK97 family

Chain P9:



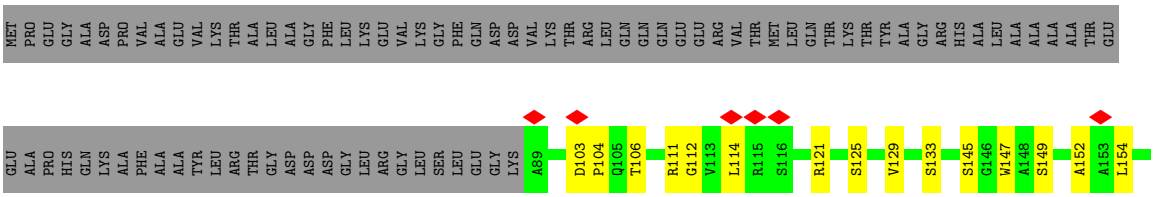
• Molecule 1: Phage major capsid protein, HK97 family

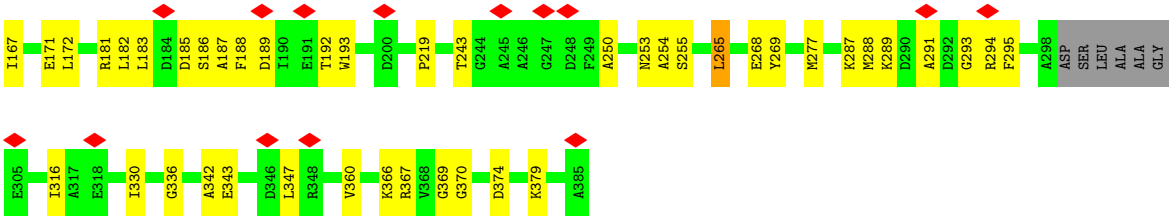
Chain W9:



• Molecule 1: Phage major capsid protein, HK97 family

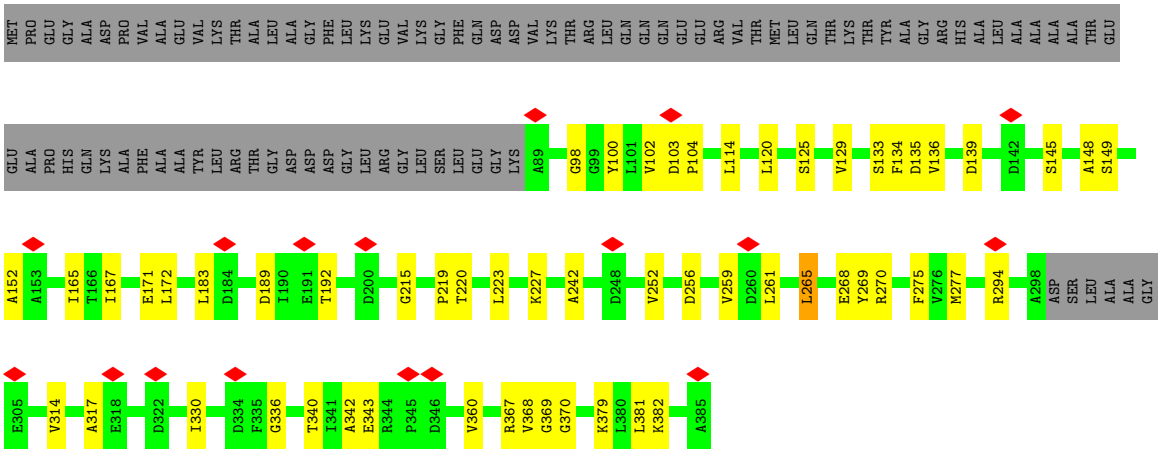
Chain U9:





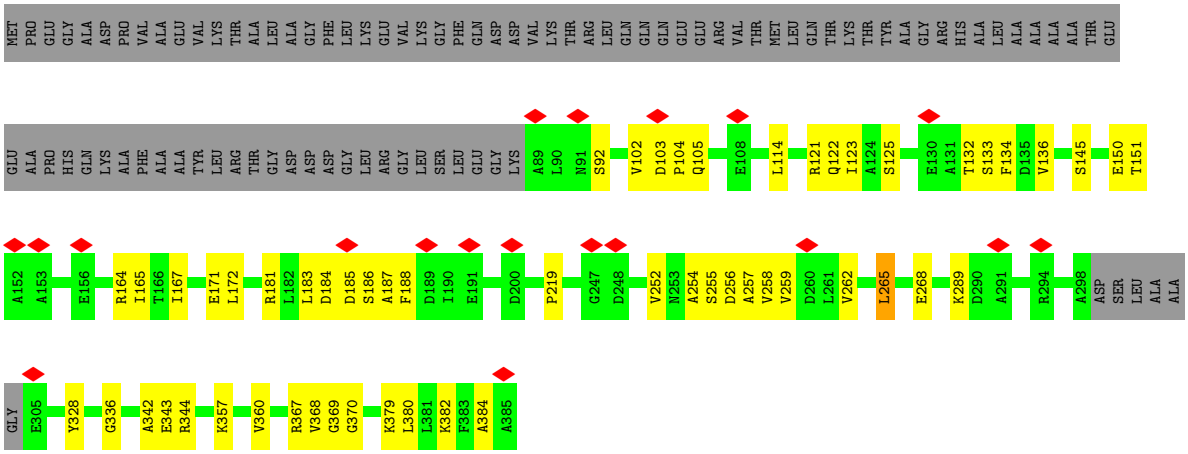
• Molecule 1: Phage major capsid protein, HK97 family

Chain T9:



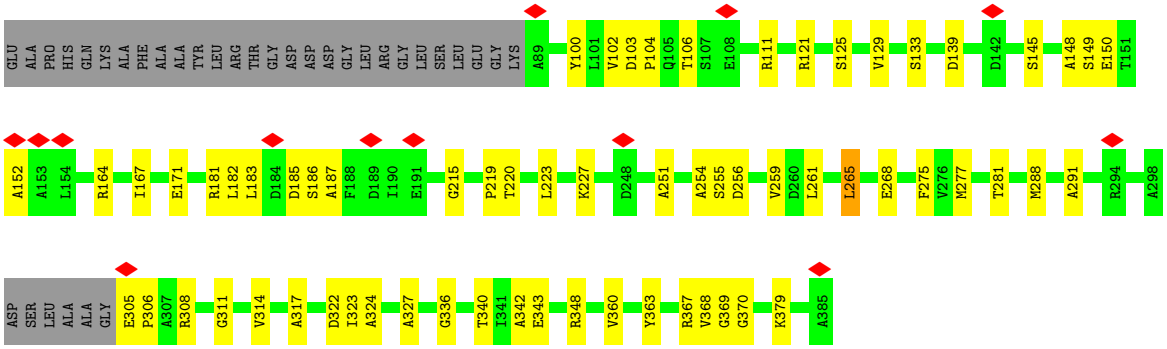
• Molecule 1: Phage major capsid protein, HK97 family

Chain S9:



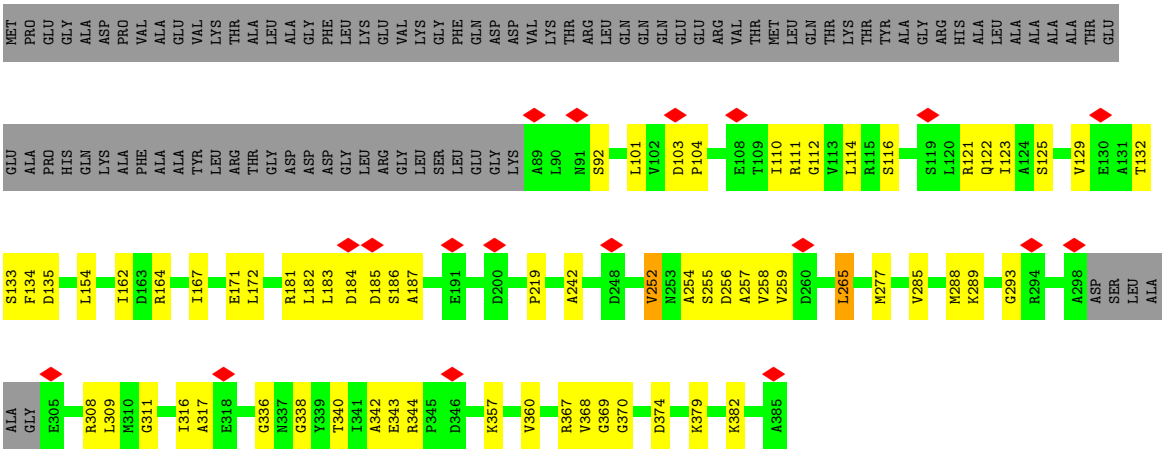
• Molecule 1: Phage major capsid protein, HK97 family

Chain K9:



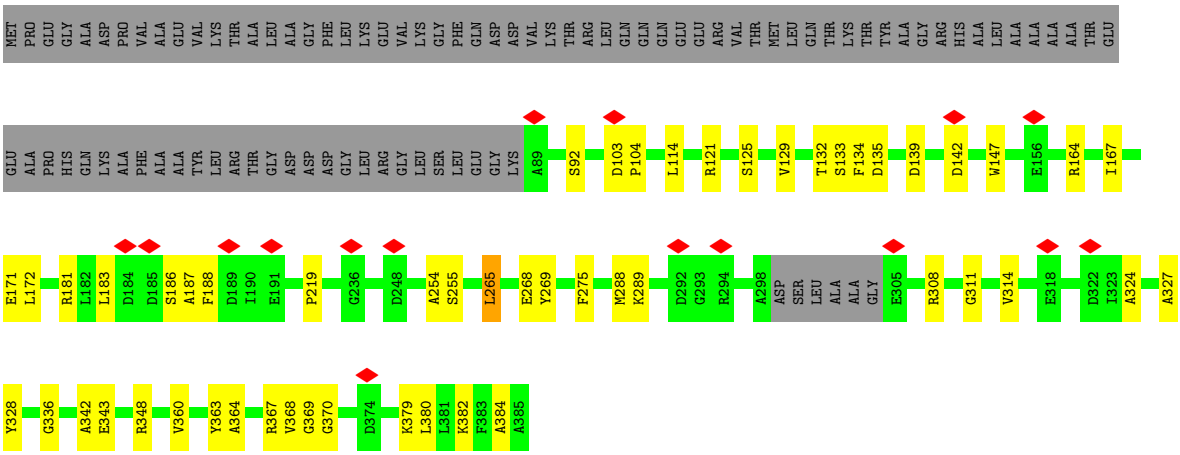
• Molecule 1: Phage major capsid protein, HK97 family

Chain J9:



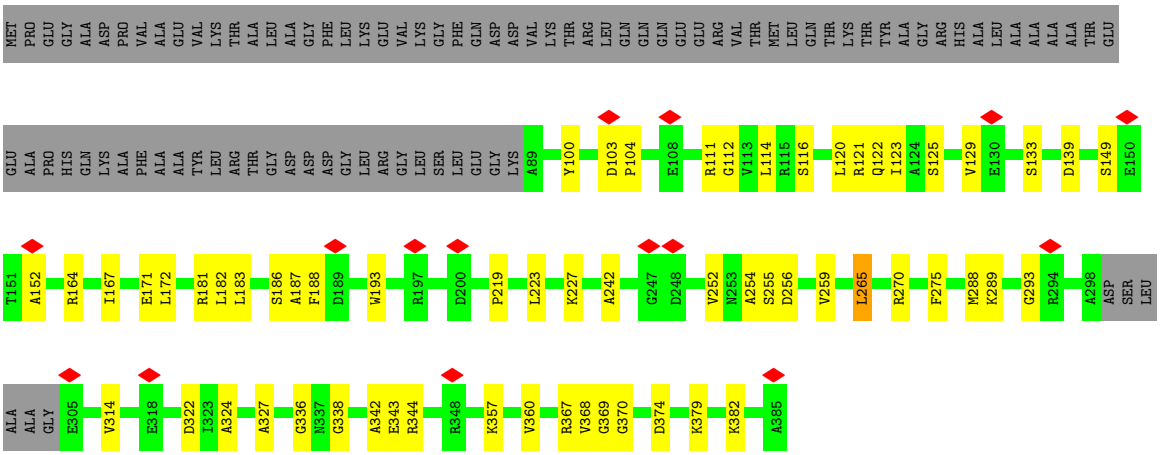
• Molecule 1: Phage major capsid protein, HK97 family

Chain V9:



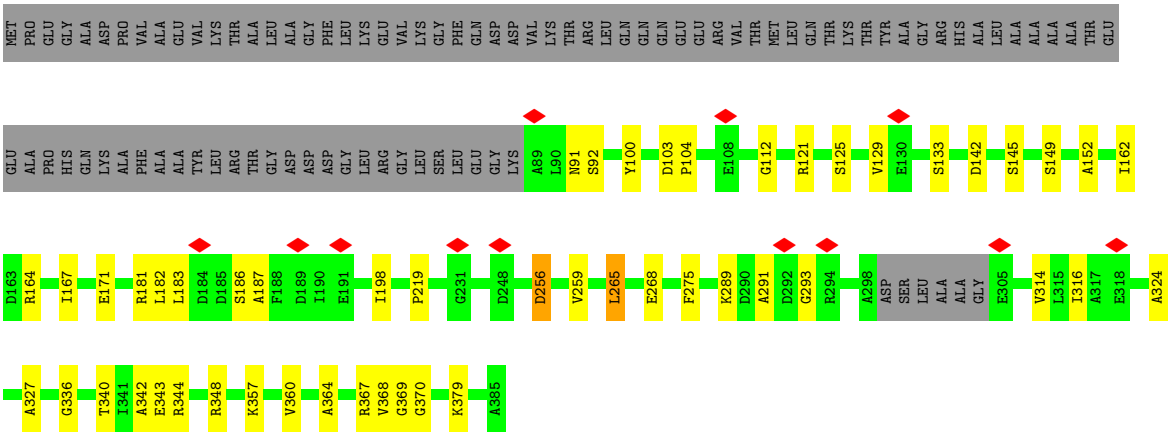
• Molecule 1: Phage major capsid protein, HK97 family

Chain L9:



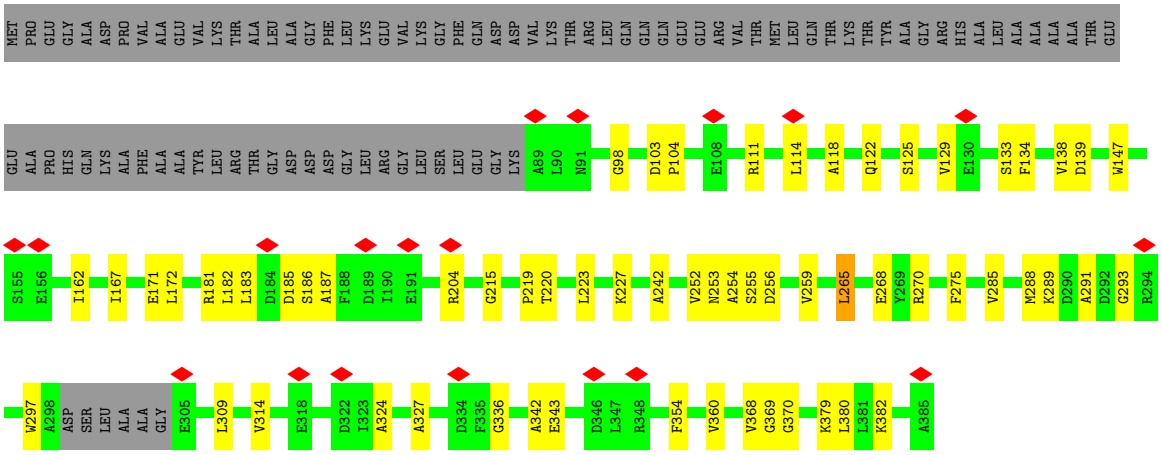
• Molecule 1: Phage major capsid protein, HK97 family

Chain H9:



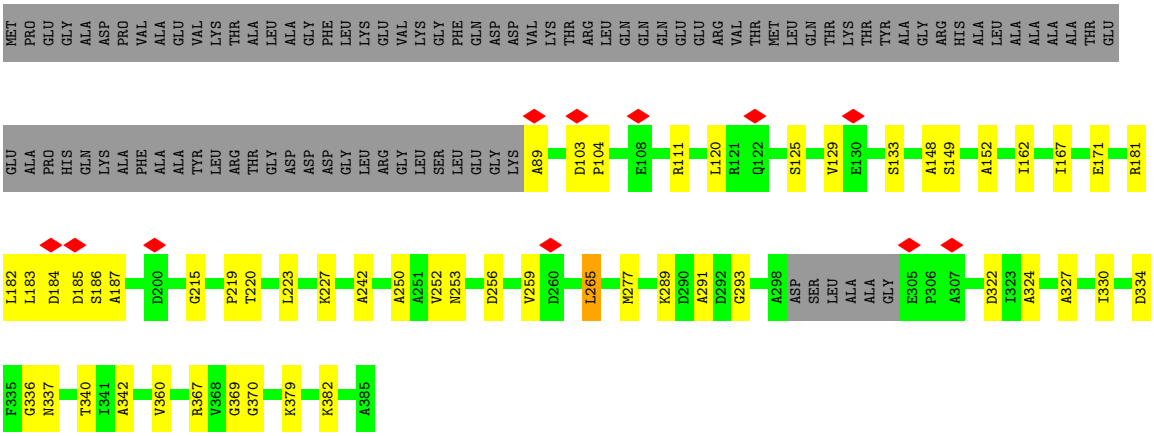
• Molecule 1: Phage major capsid protein, HK97 family

Chain I9:



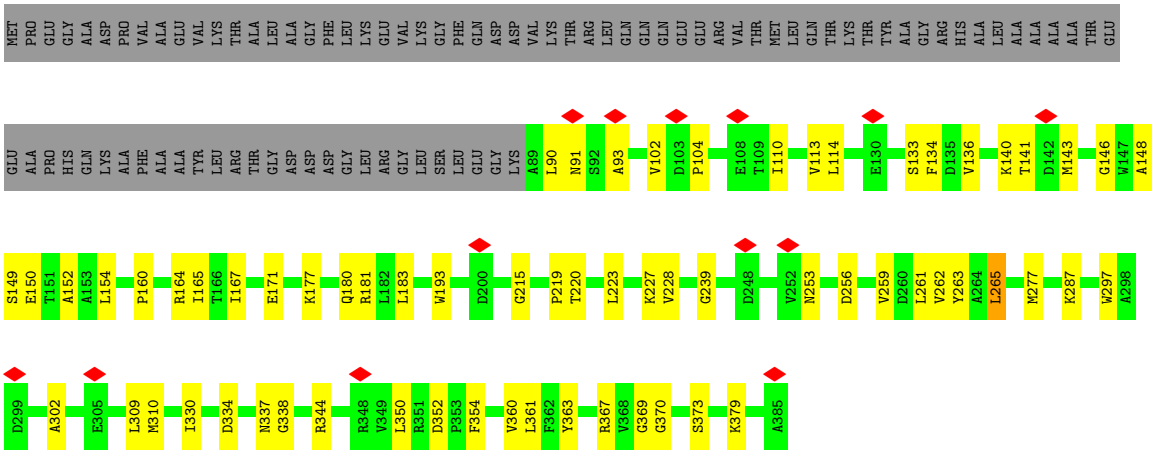
• Molecule 1: Phage major capsid protein, HK97 family

Chain A9: 62% 13% 24%



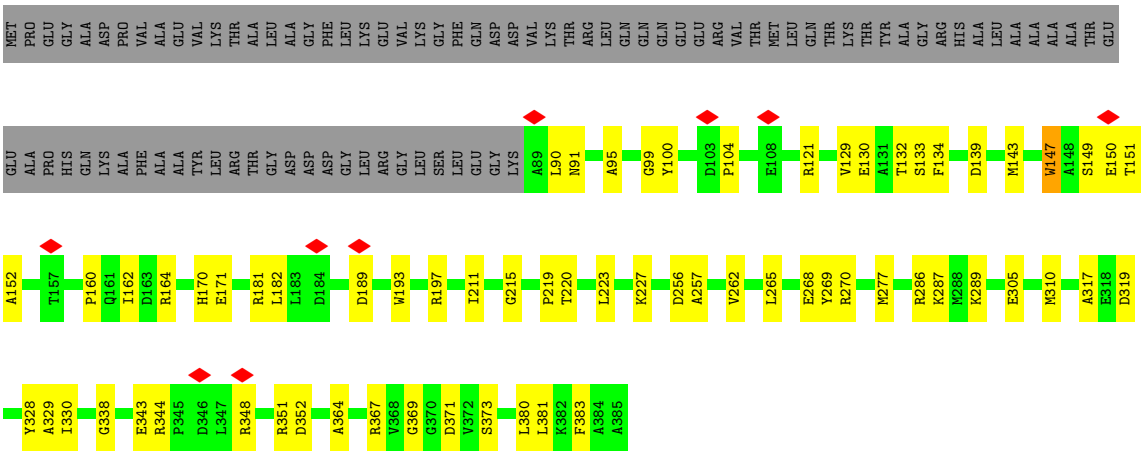
- Molecule 1: Phage major capsid protein, HK97 family

Chain D9: 60% 17% 23%



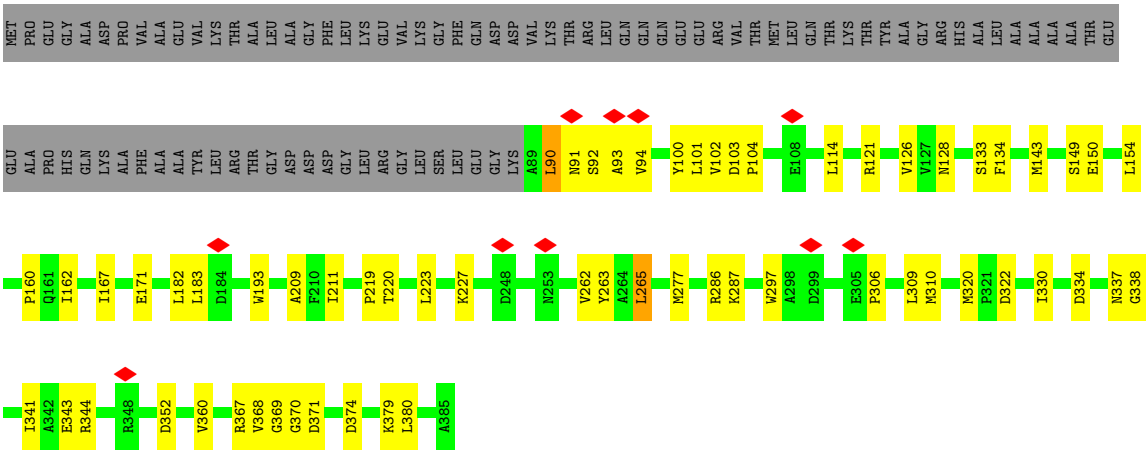
- Molecule 1: Phage major capsid protein, HK97 family

Chain E9: 60% 17% 23%



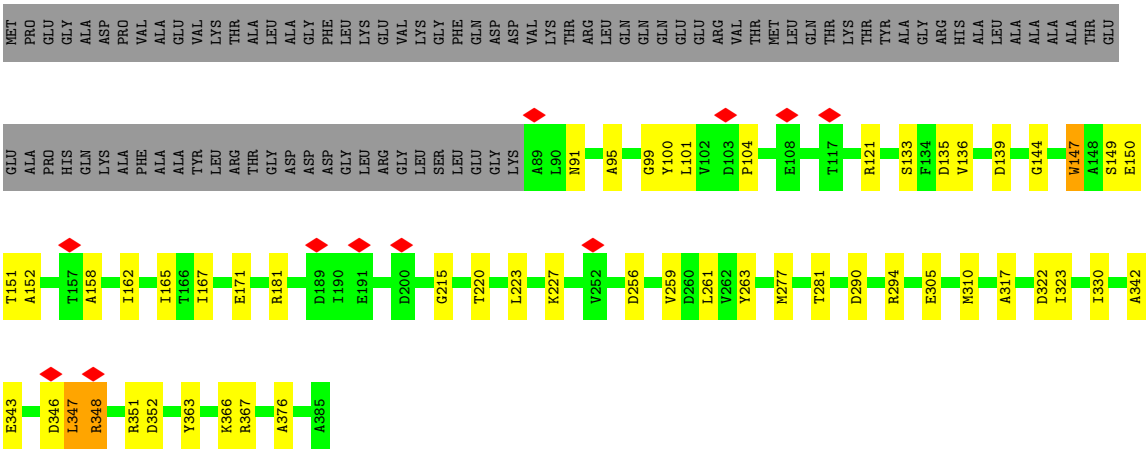
- Molecule 1: Phage major capsid protein, HK97 family

Chain F9:



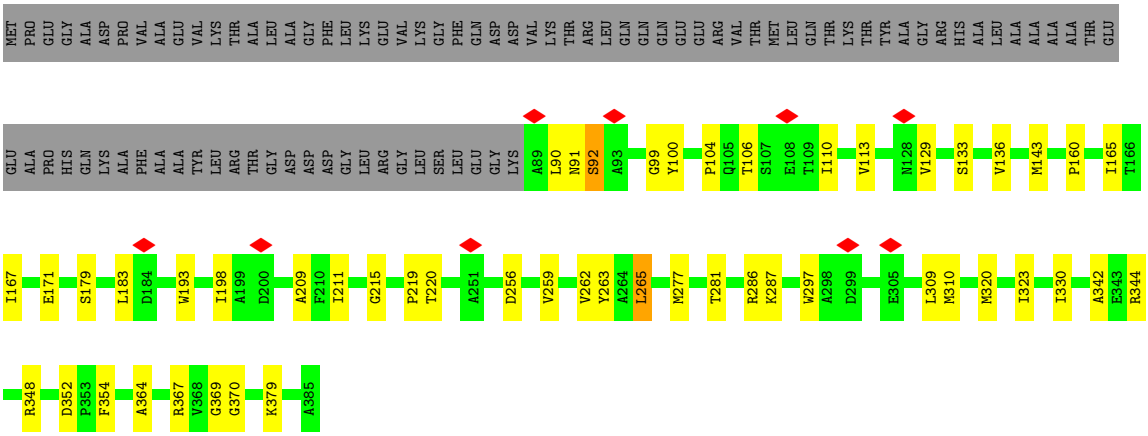
- Molecule 1: Phage major capsid protein, HK97 family

Chain G9:



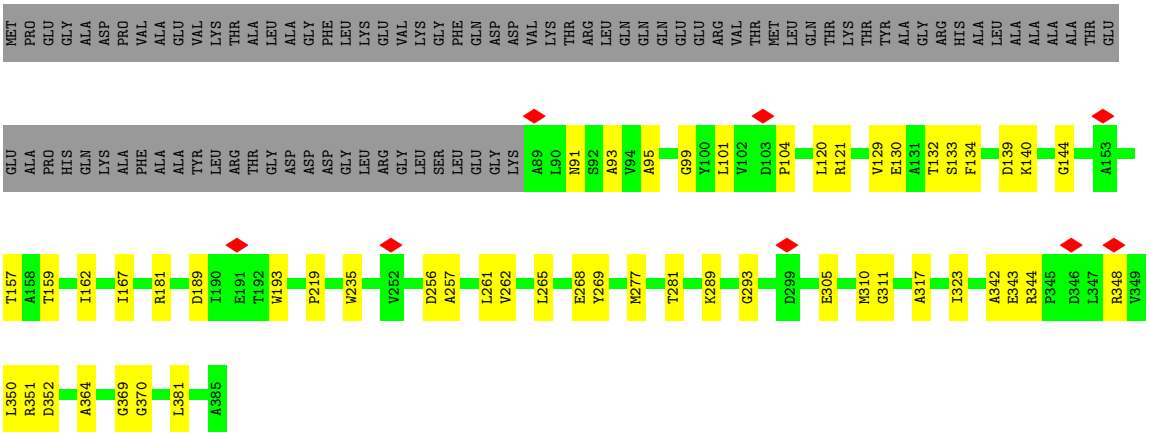
- Molecule 1: Phage major capsid protein, HK97 family

Chain B9:



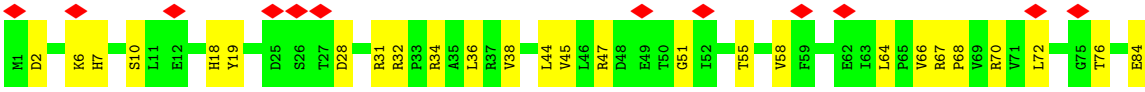
- Molecule 1: Phage major capsid protein, HK97 family

Chain C9:



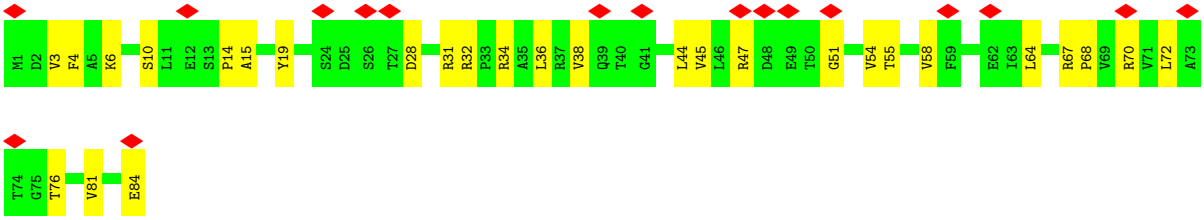
- Molecule 2: Uncharacterized protein

Chain E3:



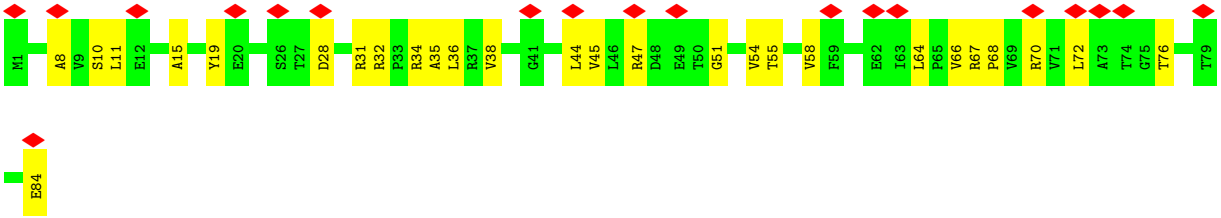
- Molecule 2: Uncharacterized protein

Chain D3:



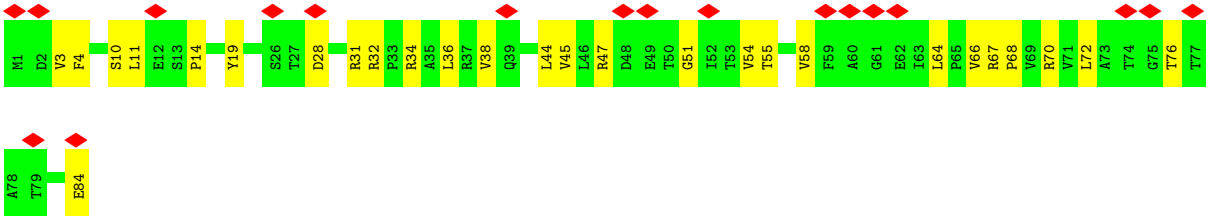
- Molecule 2: Uncharacterized protein

Chain A3:



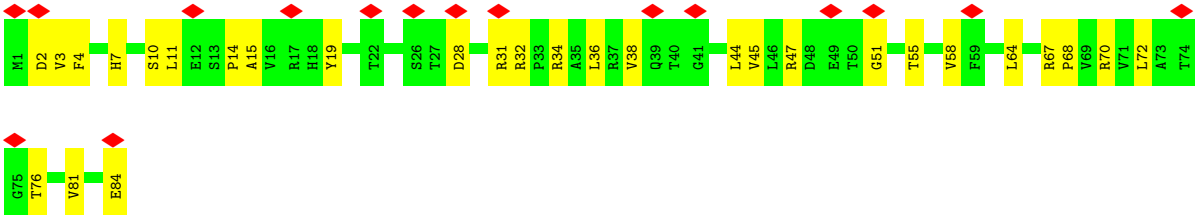
- Molecule 2: Uncharacterized protein

Chain C3:



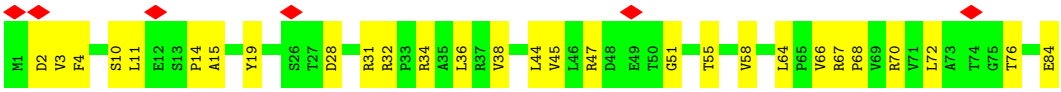
• Molecule 2: Uncharacterized protein

Chain B3:



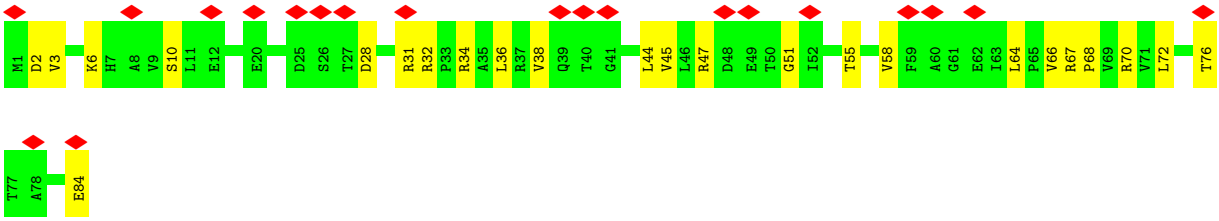
• Molecule 2: Uncharacterized protein

Chain A1:



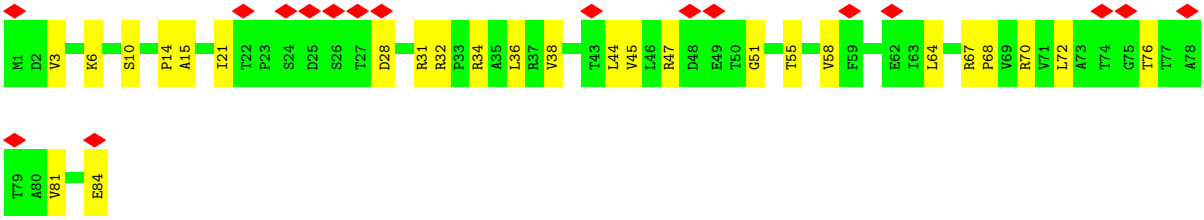
• Molecule 2: Uncharacterized protein

Chain E2:



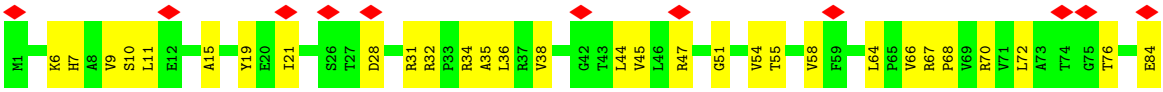
• Molecule 2: Uncharacterized protein

Chain D2:



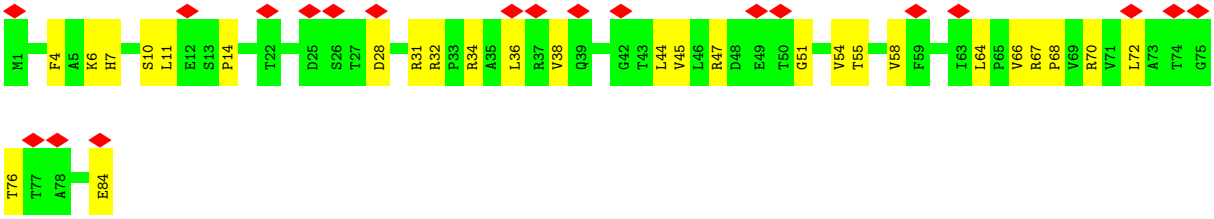
• Molecule 2: Uncharacterized protein

Chain A2: 13% 64% 36%



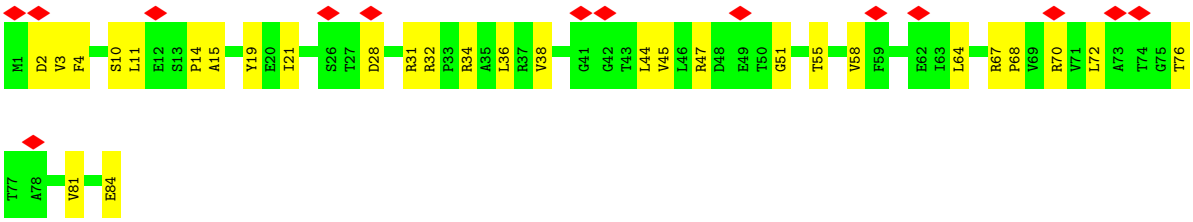
• Molecule 2: Uncharacterized protein

Chain C2: 24% 68% 32%



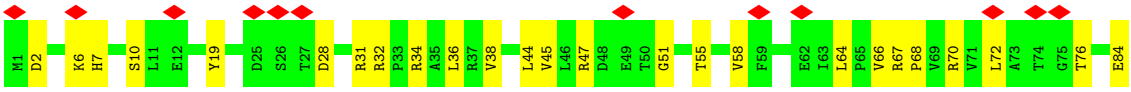
• Molecule 2: Uncharacterized protein

Chain B2: 17% 65% 35%



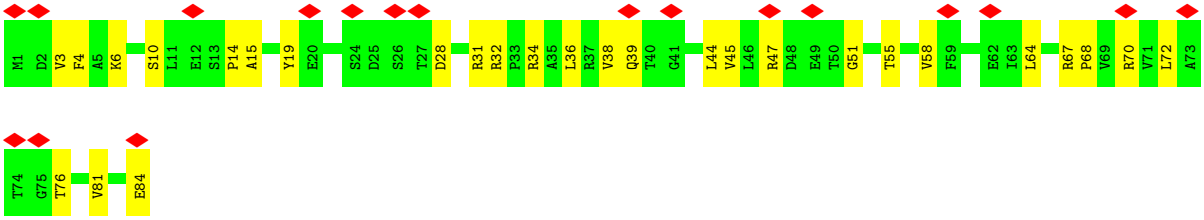
• Molecule 2: Uncharacterized protein

Chain EN: 14% 70% 30%



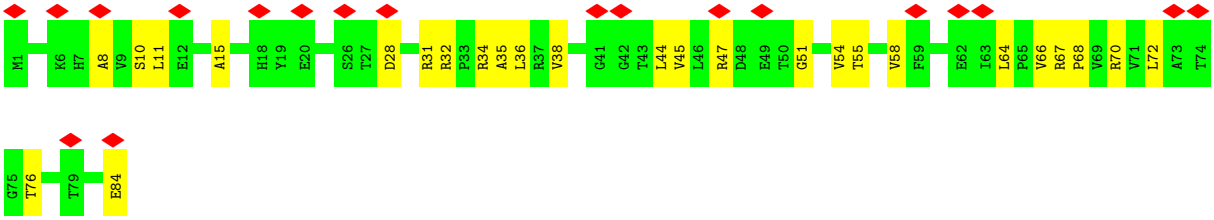
• Molecule 2: Uncharacterized protein

Chain DN: 21% 67% 33%



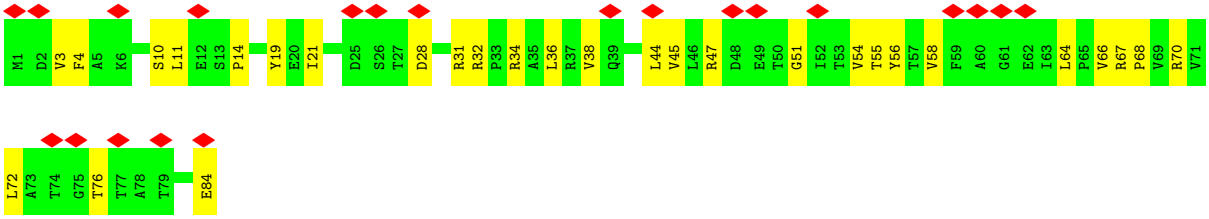
• Molecule 2: Uncharacterized protein

Chain AN: 23% 69% 31%



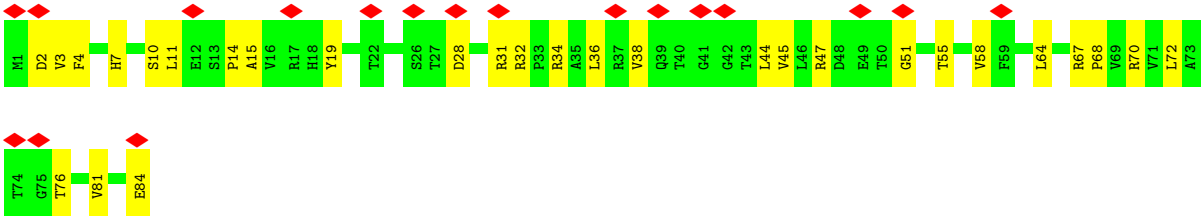
• Molecule 2: Uncharacterized protein

Chain CN:



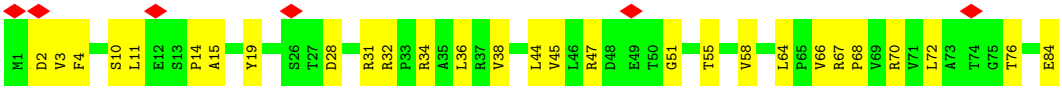
• Molecule 2: Uncharacterized protein

Chain BN:



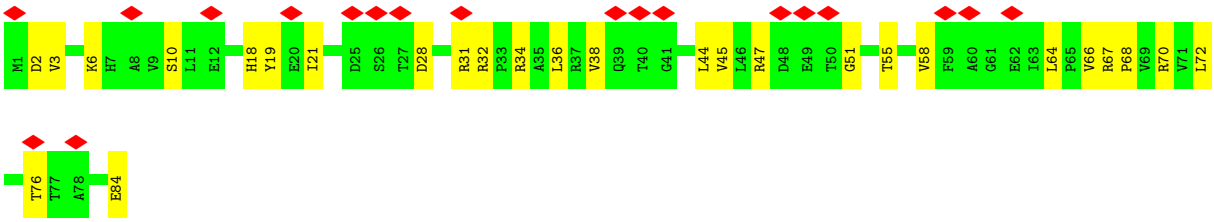
• Molecule 2: Uncharacterized protein

Chain AL:



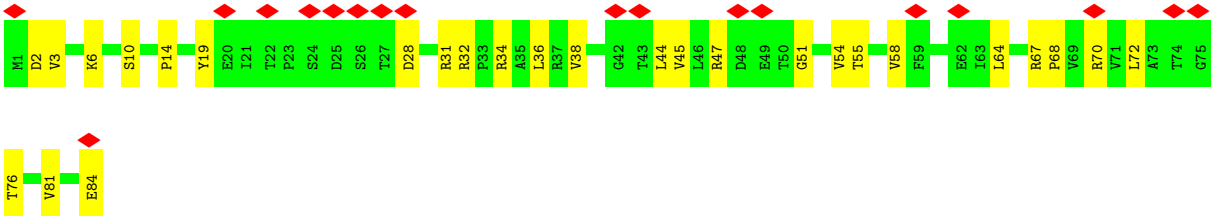
• Molecule 2: Uncharacterized protein

Chain EM:



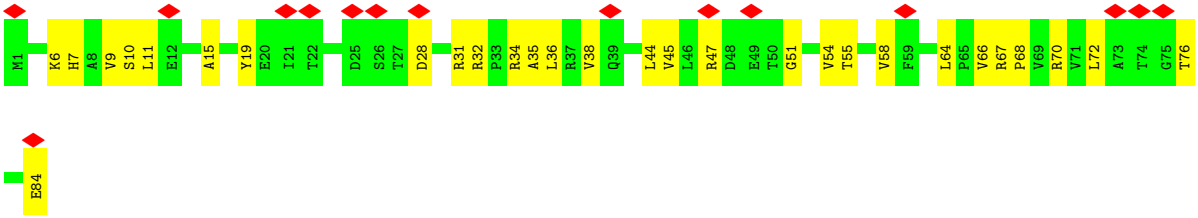
• Molecule 2: Uncharacterized protein

Chain DM: 21% 68% 32%



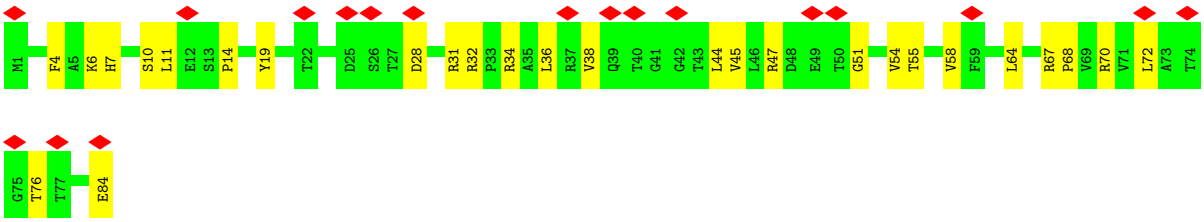
- Molecule 2: Uncharacterized protein

Chain AM: 18% 65% 35%



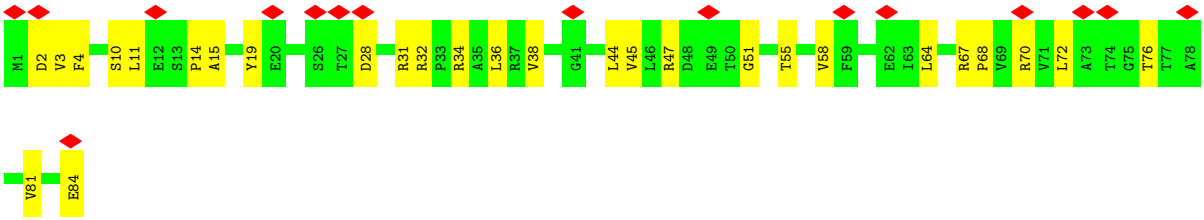
- Molecule 2: Uncharacterized protein

Chain CM: 21% 68% 32%



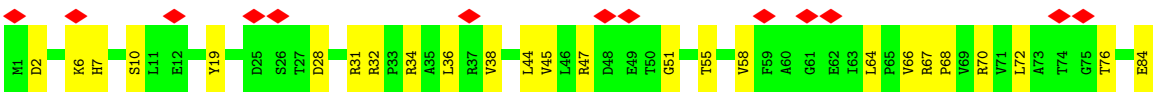
- Molecule 2: Uncharacterized protein

Chain BM: 19% 67% 33%



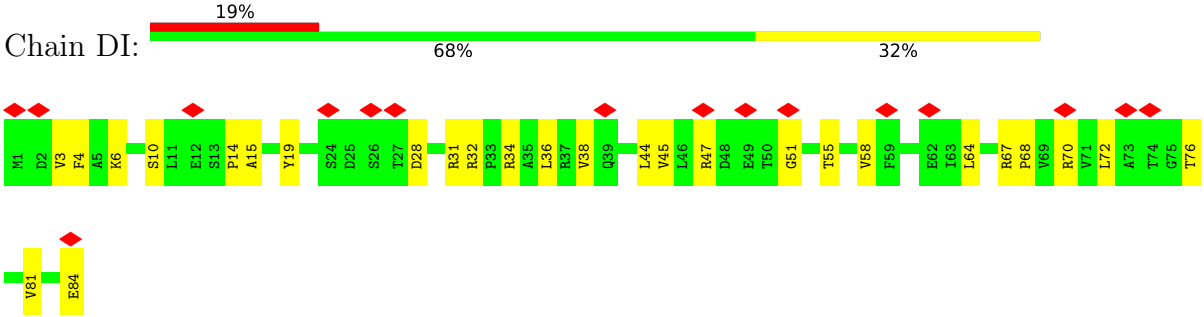
- Molecule 2: Uncharacterized protein

Chain EI: 15% 70% 30%



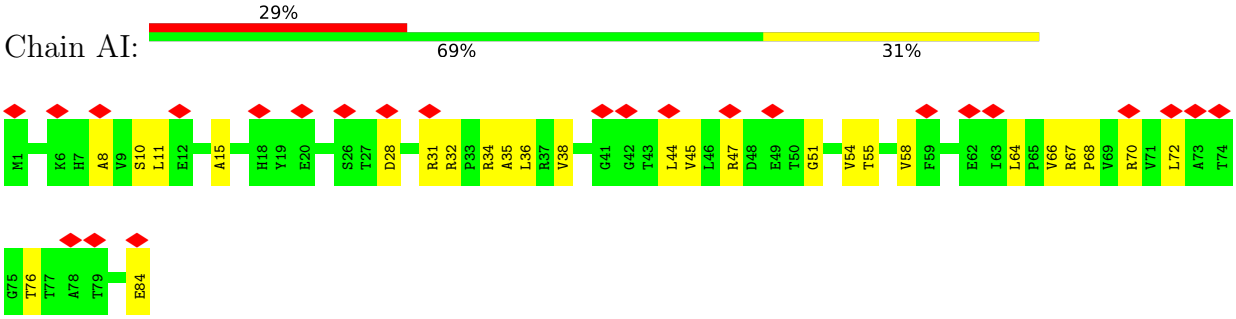
- Molecule 2: Uncharacterized protein

Chain DI:



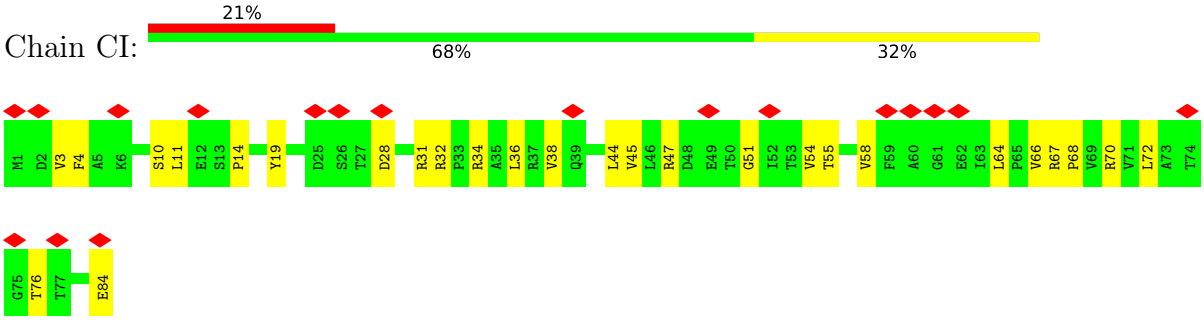
- Molecule 2: Uncharacterized protein

Chain AI:



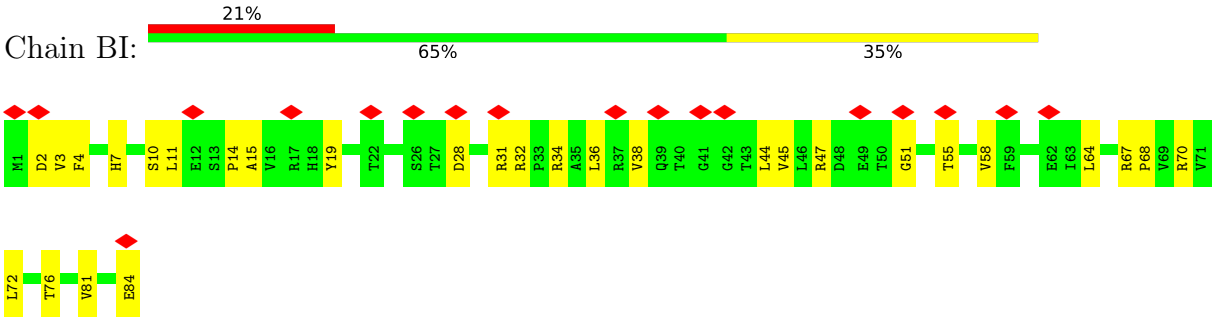
- Molecule 2: Uncharacterized protein

Chain CI:



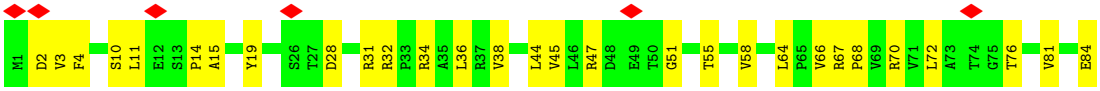
- Molecule 2: Uncharacterized protein

Chain BI:



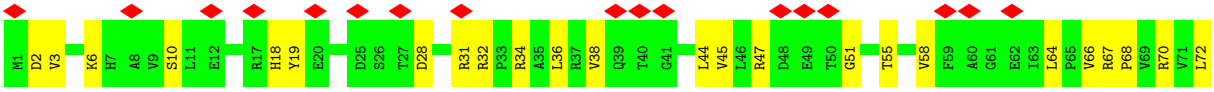
- Molecule 2: Uncharacterized protein

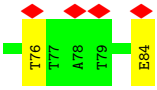
Chain AG:



• Molecule 2: Uncharacterized protein

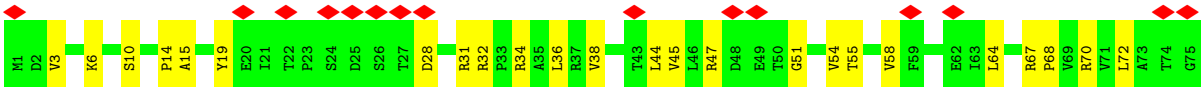
Chain EH:

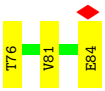




• Molecule 2: Uncharacterized protein

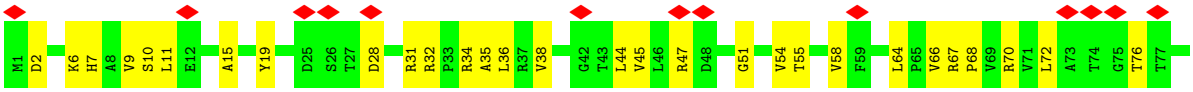
Chain DH:





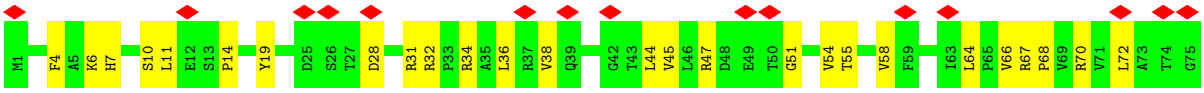
• Molecule 2: Uncharacterized protein

Chain AH:



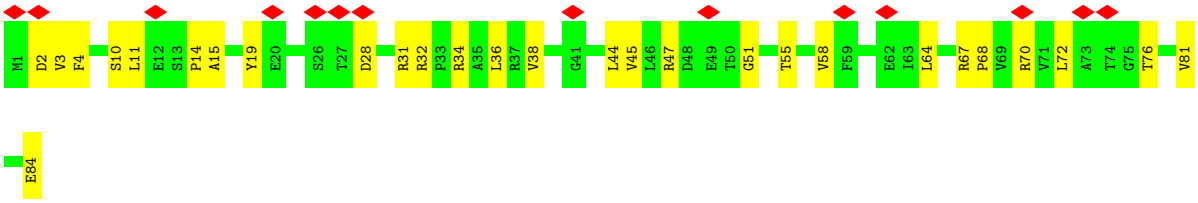
• Molecule 2: Uncharacterized protein

Chain CH:



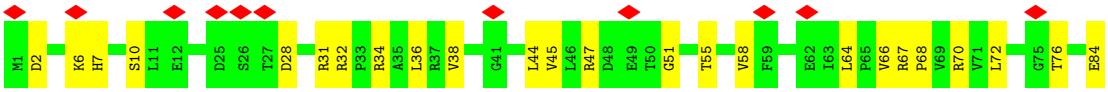
• Molecule 2: Uncharacterized protein

Chain BH: 17% 67% 33%



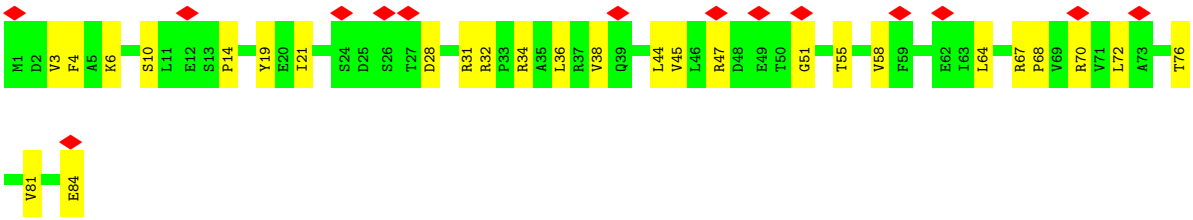
- Molecule 2: Uncharacterized protein

Chain ED: 13% 71% 29%



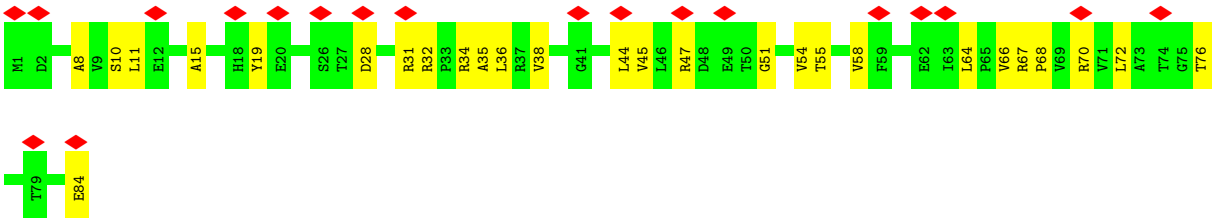
- Molecule 2: Uncharacterized protein

Chain DD: 17% 68% 32%



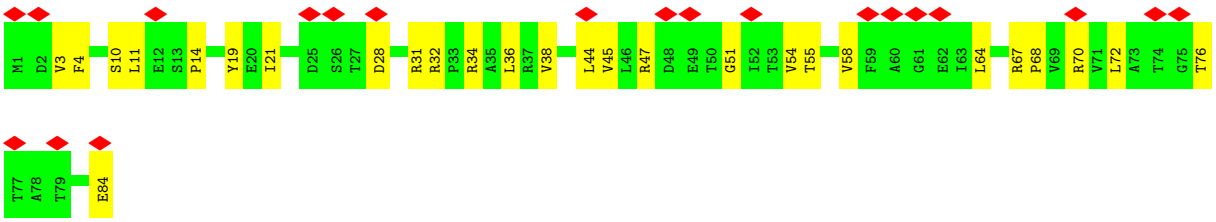
- Molecule 2: Uncharacterized protein

Chain AD: 23% 68% 32%



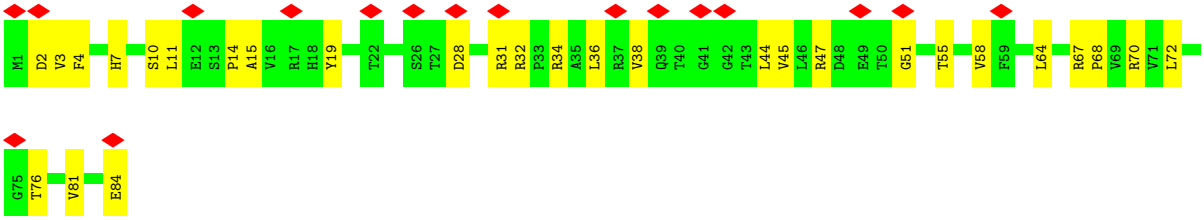
- Molecule 2: Uncharacterized protein

Chain CD: 24% 68% 32%



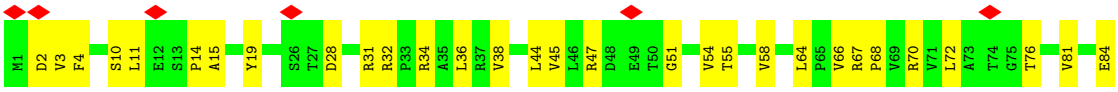
- Molecule 2: Uncharacterized protein

Chain BD:



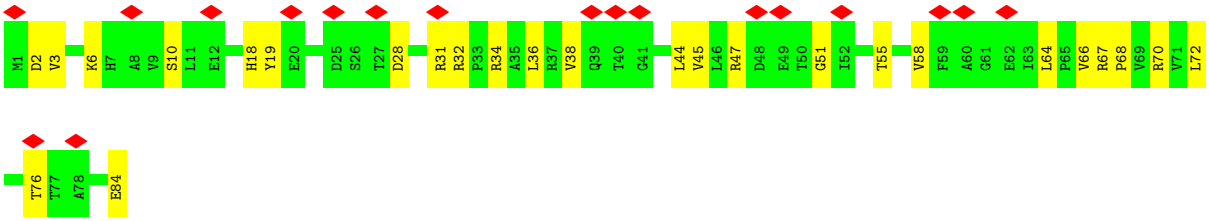
- Molecule 2: Uncharacterized protein

Chain AB:



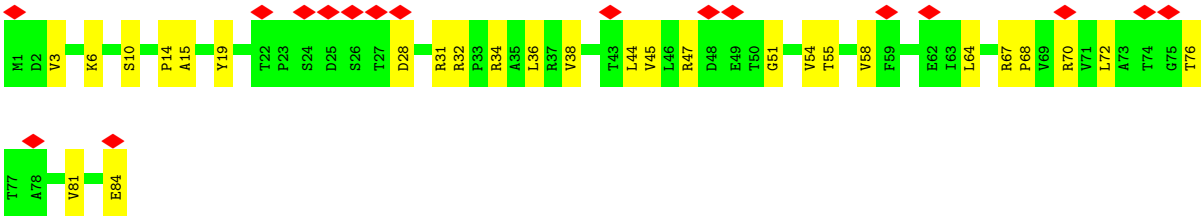
- Molecule 2: Uncharacterized protein

Chain EC:



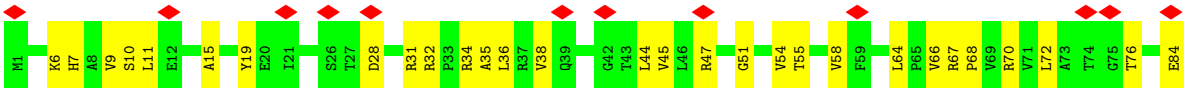
- Molecule 2: Uncharacterized protein

Chain DC:



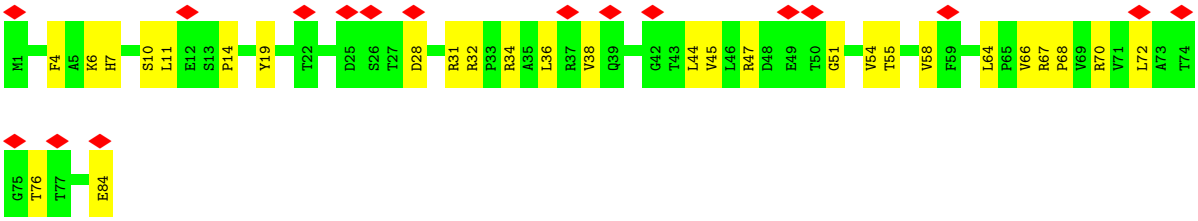
- Molecule 2: Uncharacterized protein

Chain AC:



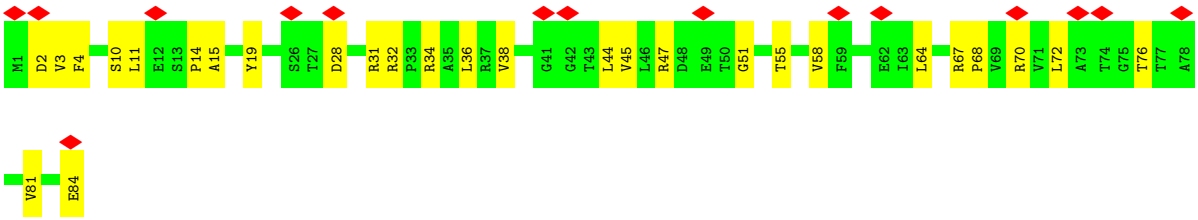
- Molecule 2: Uncharacterized protein

Chain CC:



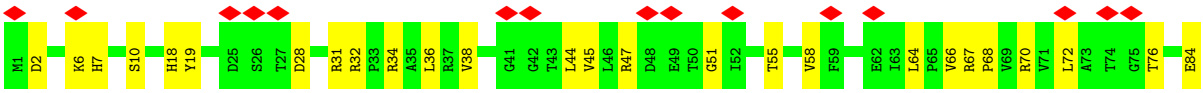
- Molecule 2: Uncharacterized protein

Chain BC:



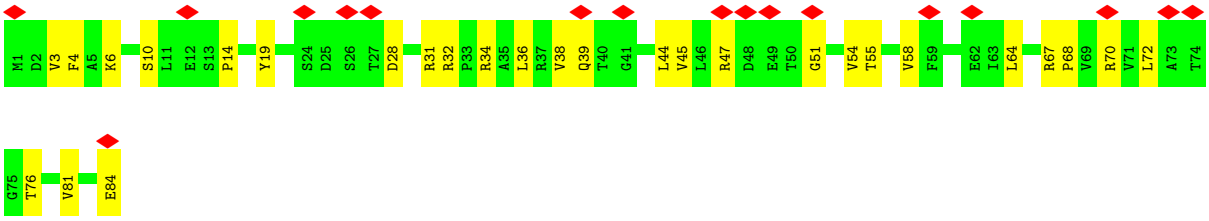
- Molecule 2: Uncharacterized protein

Chain E8:



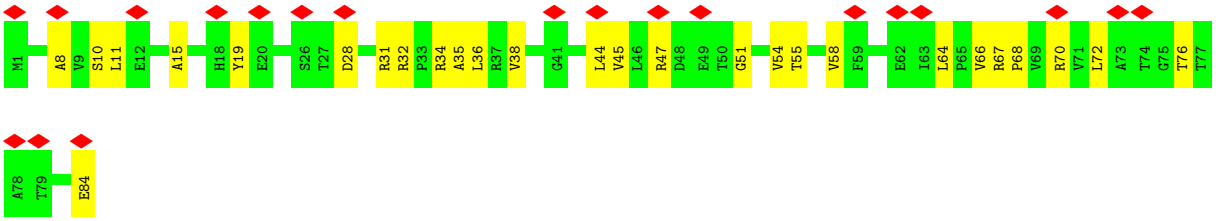
- Molecule 2: Uncharacterized protein

Chain D8:



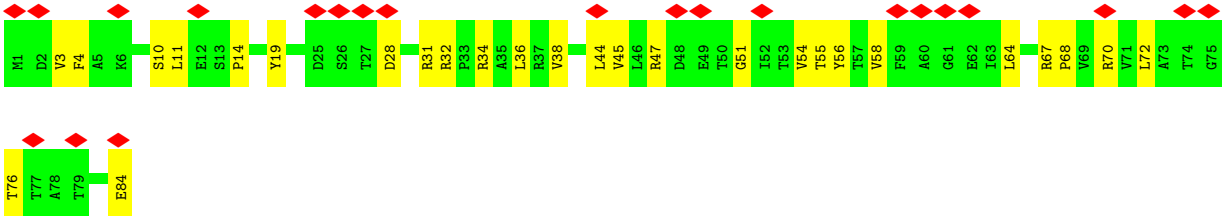
- Molecule 2: Uncharacterized protein

Chain A8:



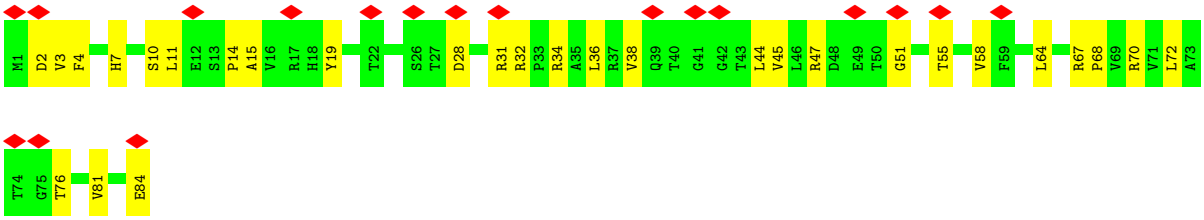
- Molecule 2: Uncharacterized protein

Chain C8:



- Molecule 2: Uncharacterized protein

Chain B8:

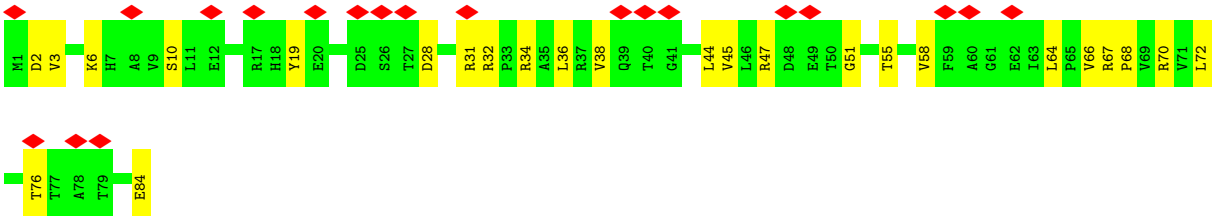


- Molecule 2: Uncharacterized protein

Chain A6:

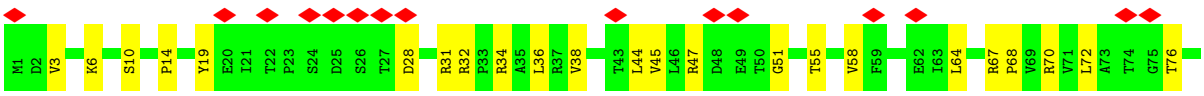
- Molecule 2: Uncharacterized protein

Chain E7:



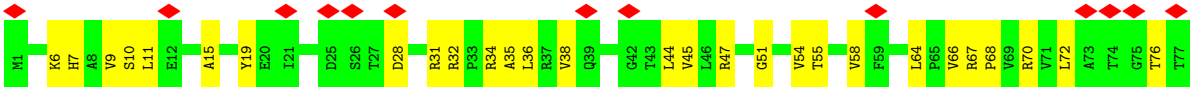
- Molecule 2: Uncharacterized protein

Chain D7:



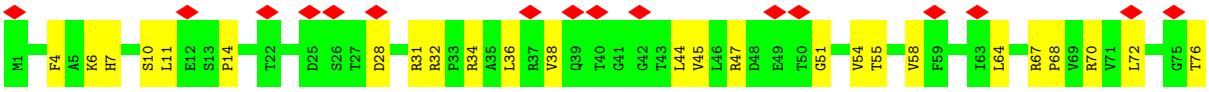
• Molecule 2: Uncharacterized protein

Chain A7:



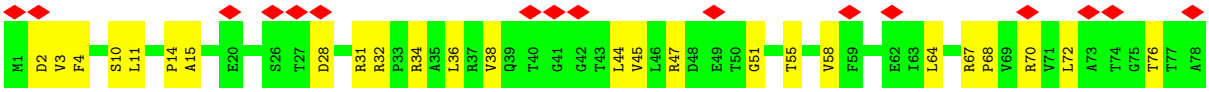
• Molecule 2: Uncharacterized protein

Chain C7:



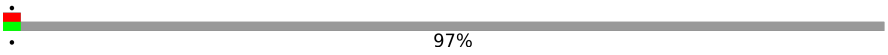
• Molecule 2: Uncharacterized protein

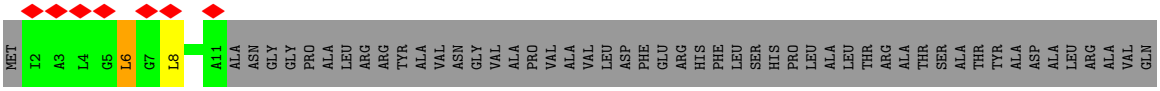
Chain B7:

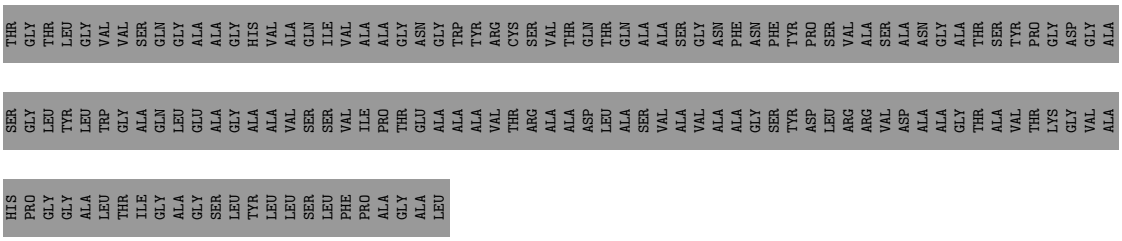


• Molecule 3: Uncharacterized protein

Chain F3:

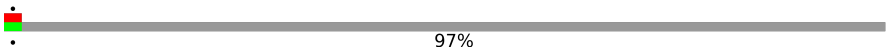


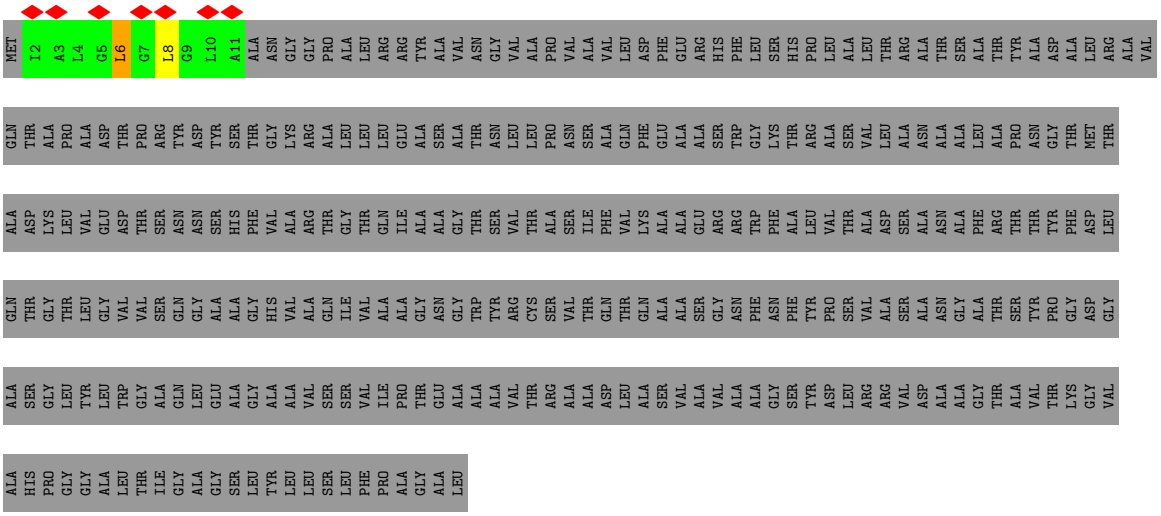




• Molecule 3: Uncharacterized protein

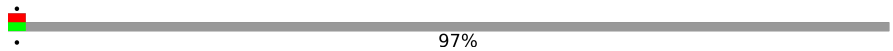
Chain F2:

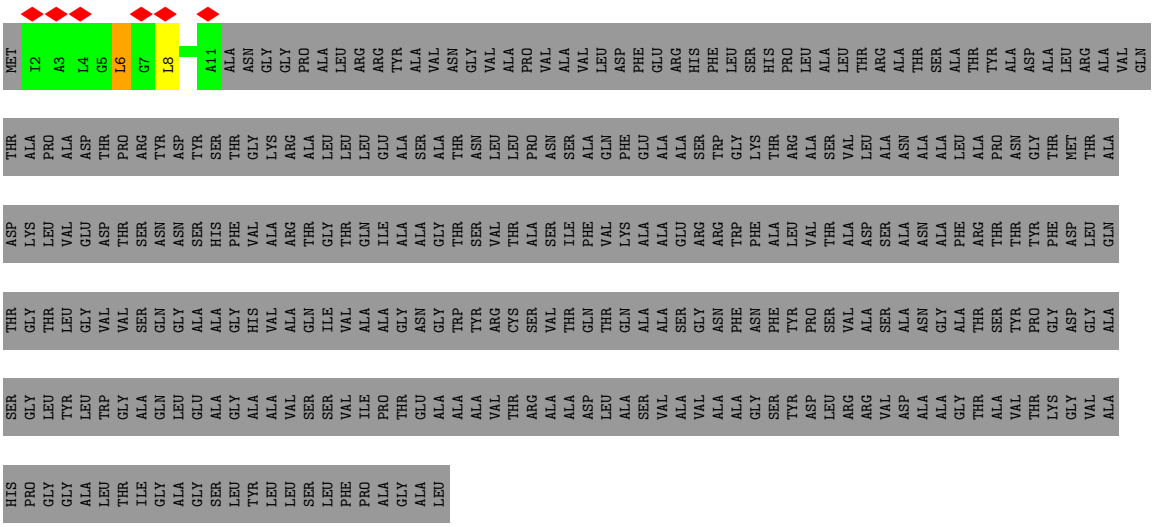




• Molecule 3: Uncharacterized protein

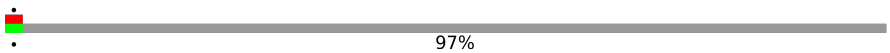
Chain FN:

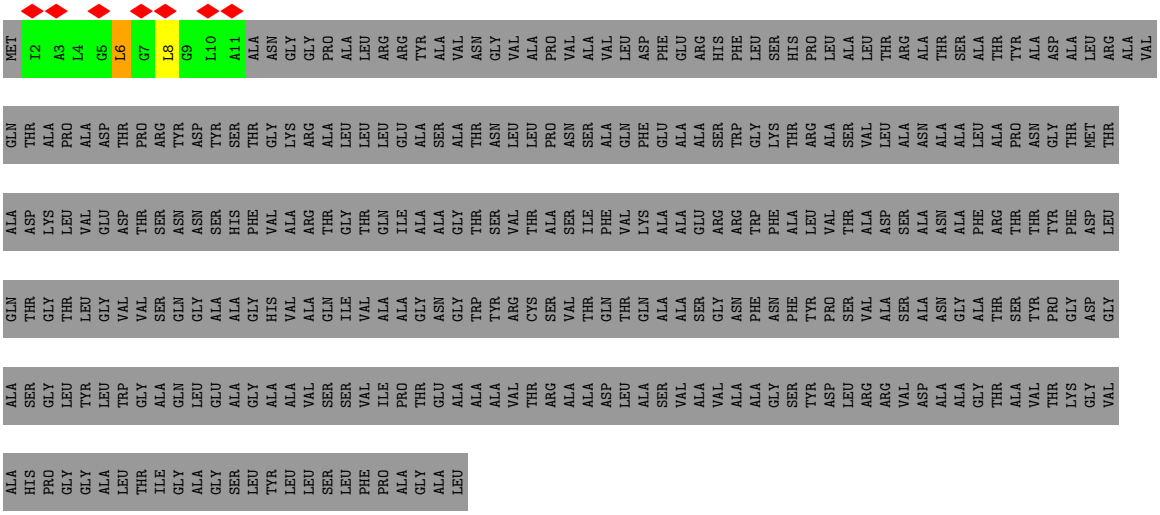




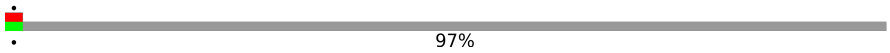
• Molecule 3: Uncharacterized protein

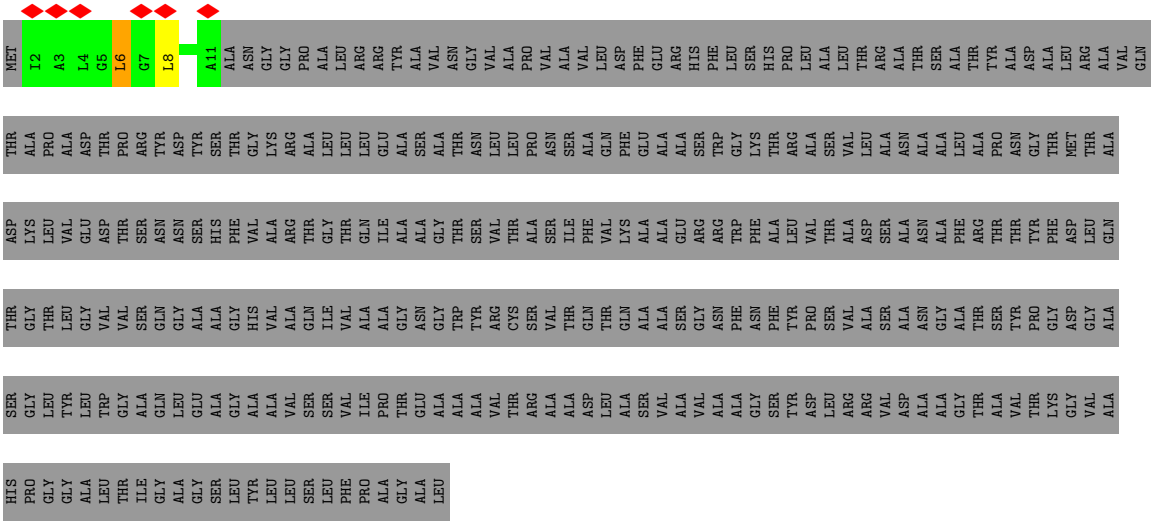
Chain FM:



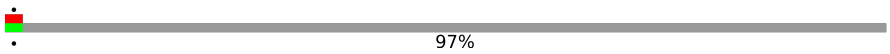


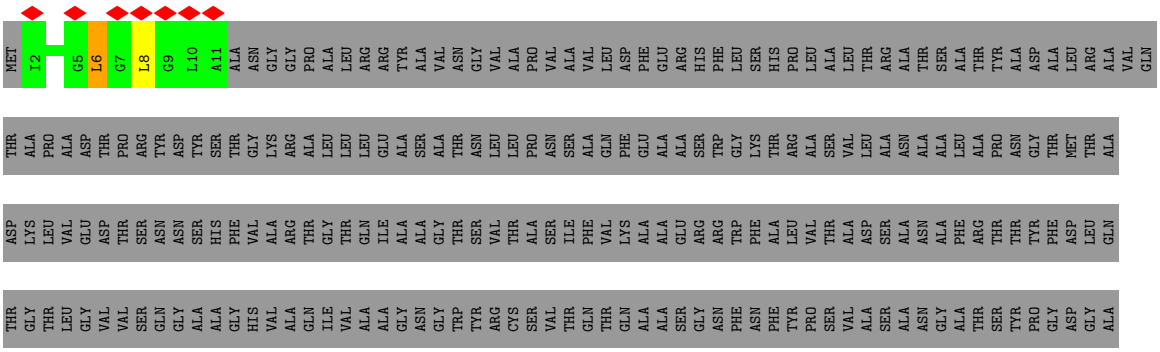
• Molecule 3: Uncharacterized protein

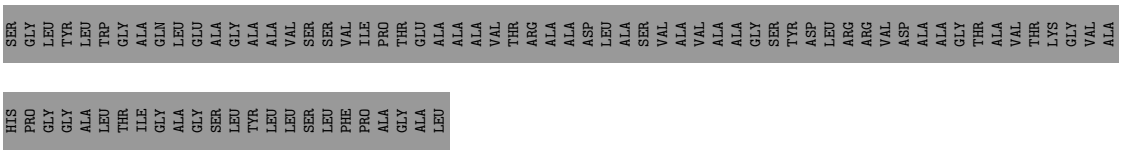
Chain FI: 



• Molecule 3: Uncharacterized protein

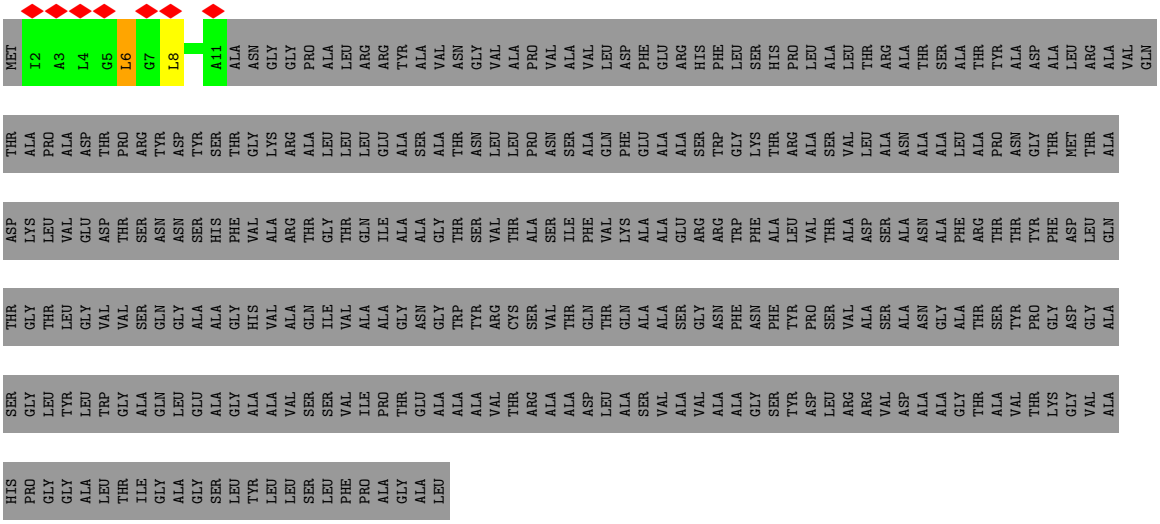
Chain FH: 





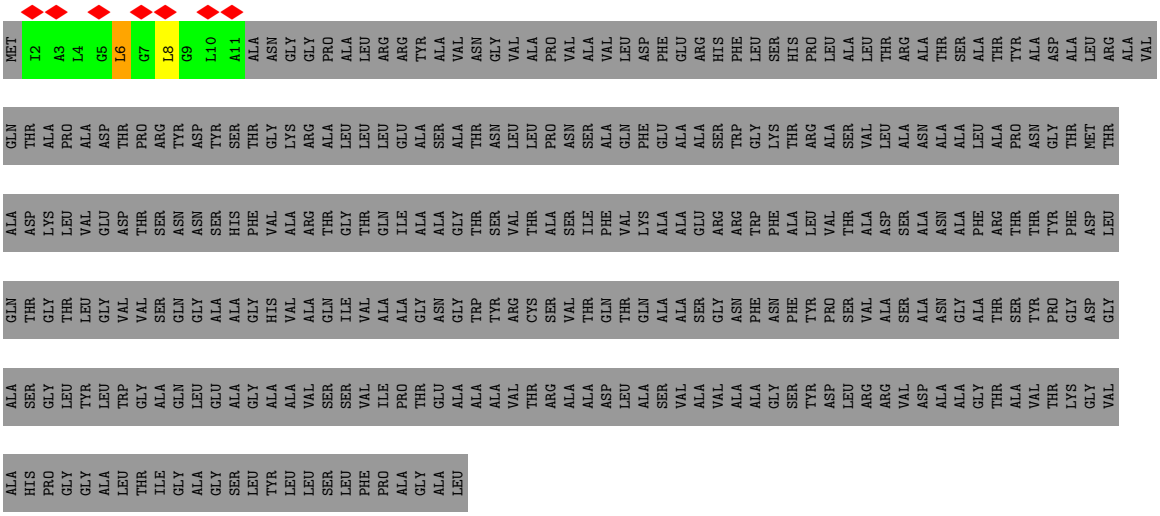
• Molecule 3: Uncharacterized protein

Chain FD: 97%



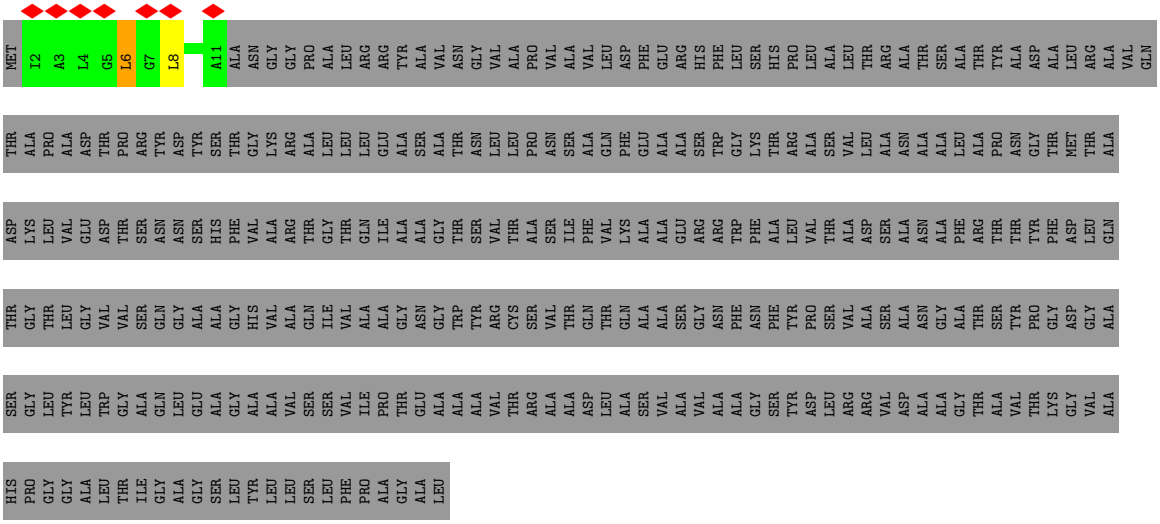
• Molecule 3: Uncharacterized protein

Chain FC: 97%



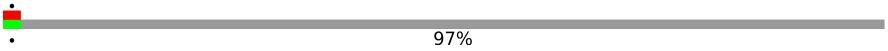
• Molecule 3: Uncharacterized protein

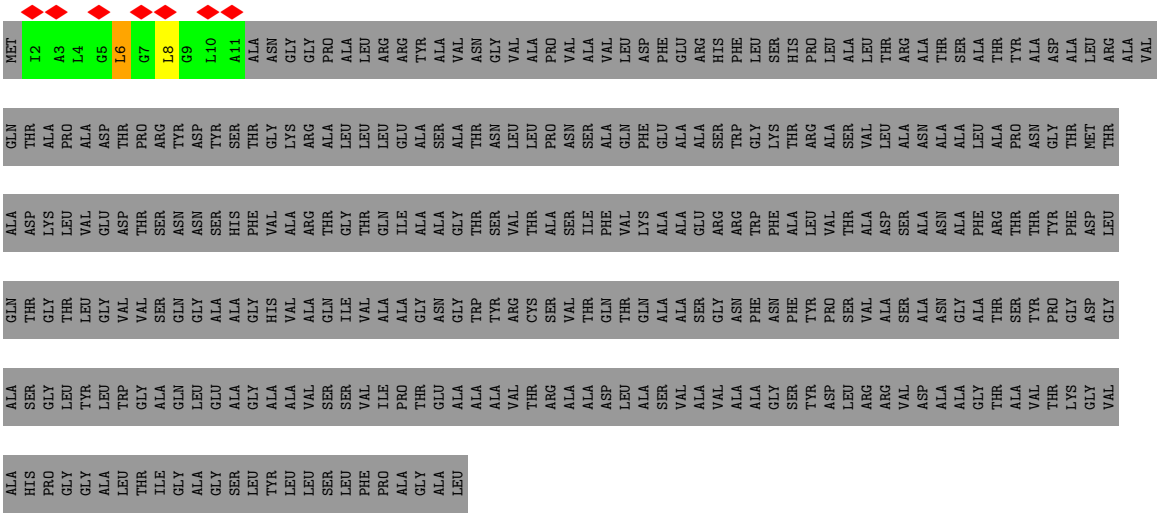
Chain F8: 97%



- Molecule 3: Uncharacterized protein

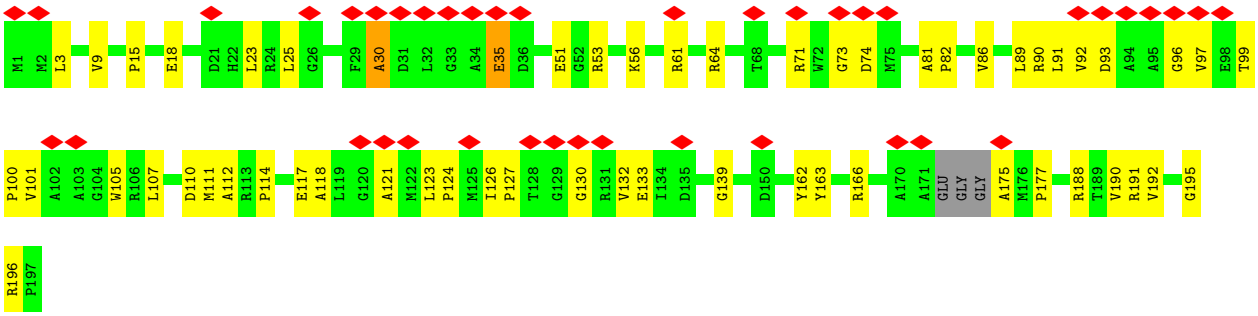
Chain F7:





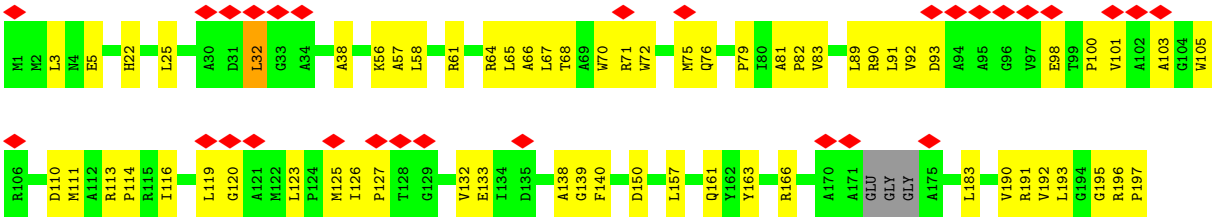
- Molecule 4: Uncharacterized protein

Chain 2A:



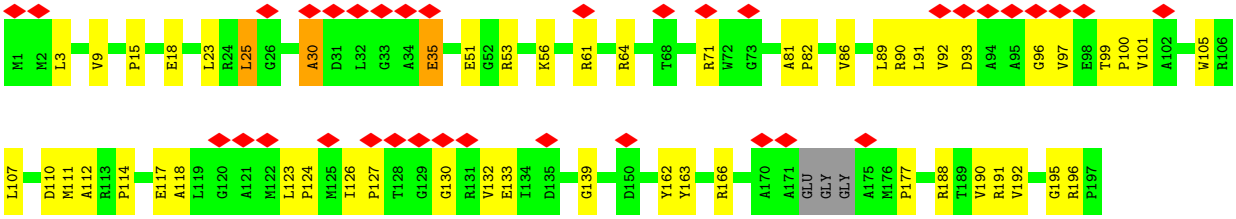
- Molecule 4: Uncharacterized protein

Chain 2B:



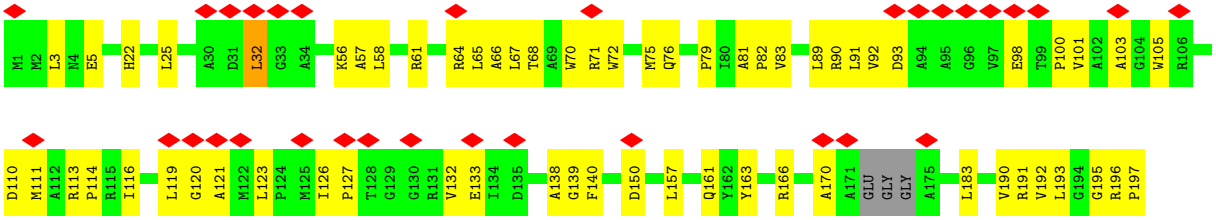
- Molecule 4: Uncharacterized protein

Chain 2K:



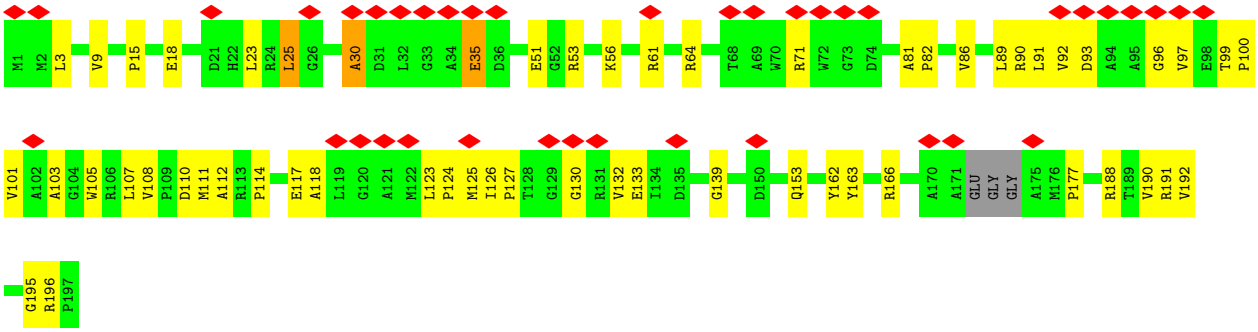
- Molecule 4: Uncharacterized protein

Chain 2L:



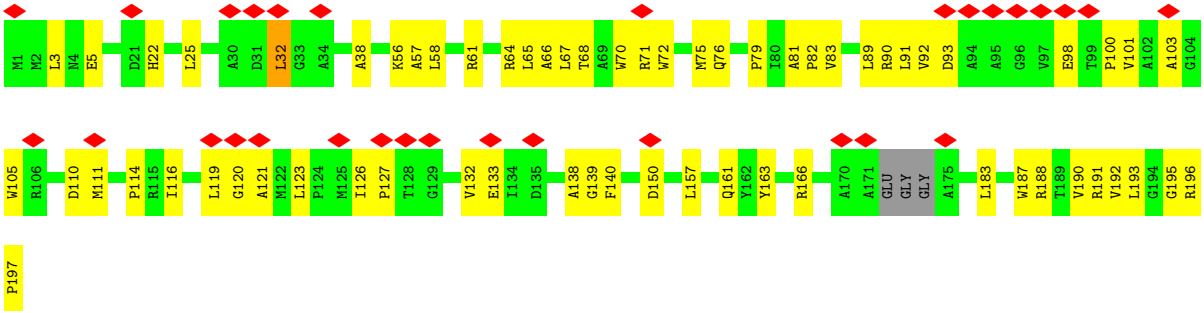
- Molecule 4: Uncharacterized protein

Chain 2I:



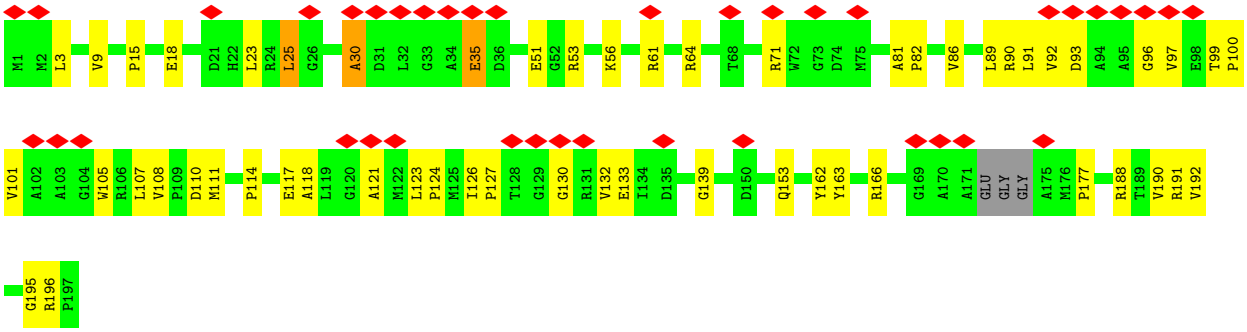
- Molecule 4: Uncharacterized protein

Chain 2J:



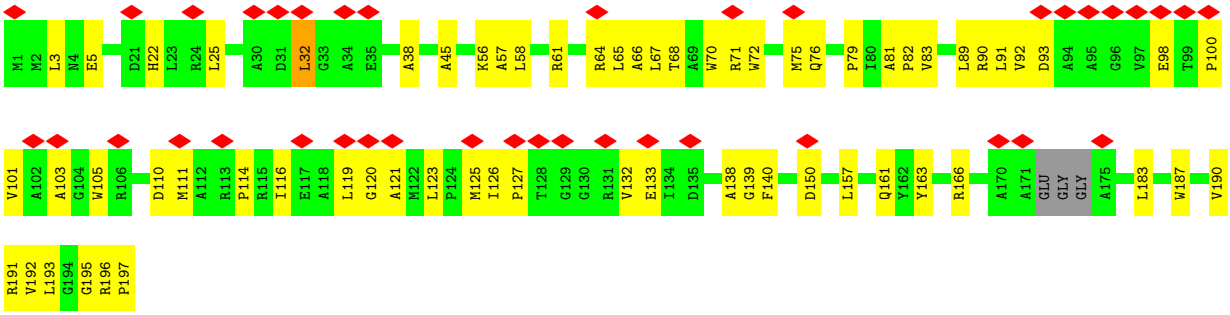
• Molecule 4: Uncharacterized protein

Chain 2G:



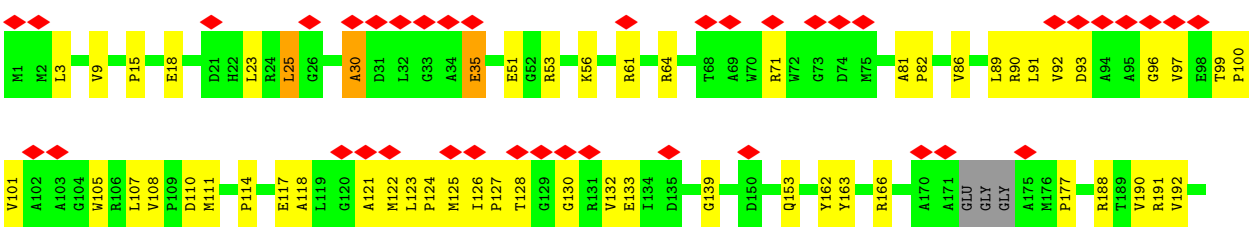
• Molecule 4: Uncharacterized protein

Chain 2H:



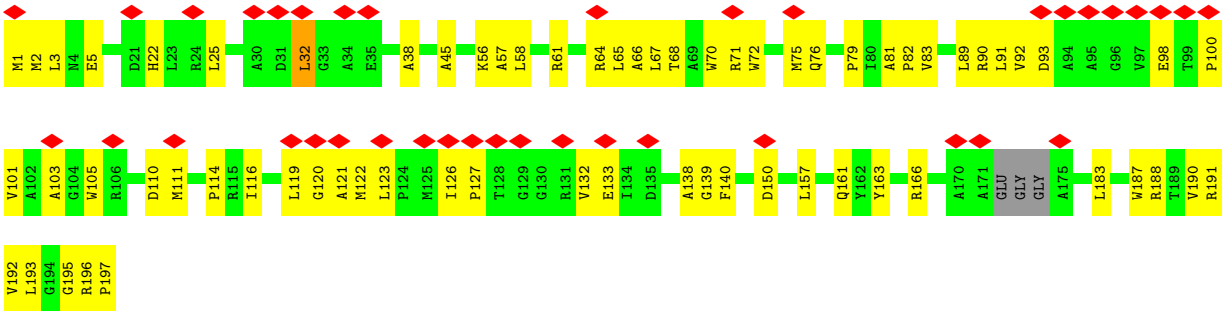
• Molecule 4: Uncharacterized protein

Chain 2E:



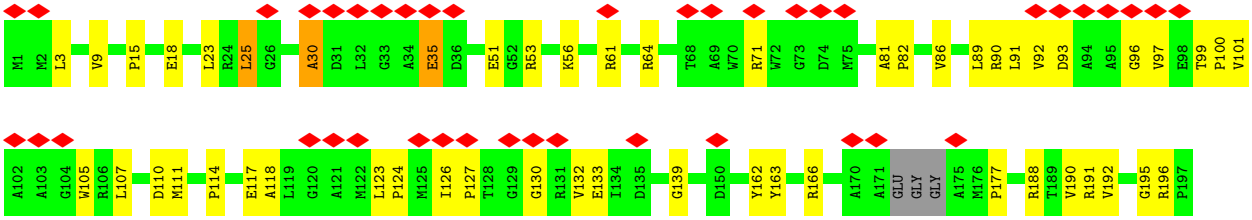
• Molecule 4: Uncharacterized protein

Chain 2F:



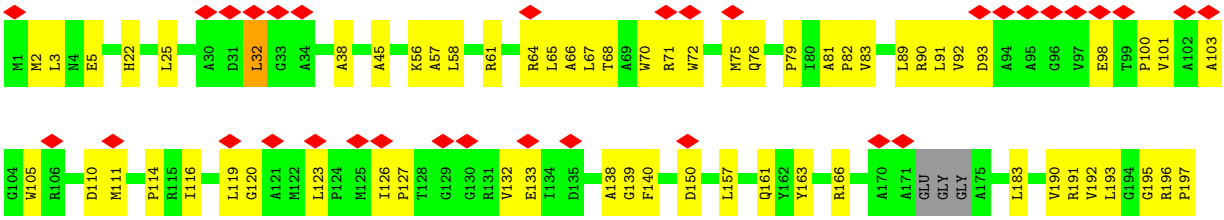
• Molecule 4: Uncharacterized protein

Chain 2C:



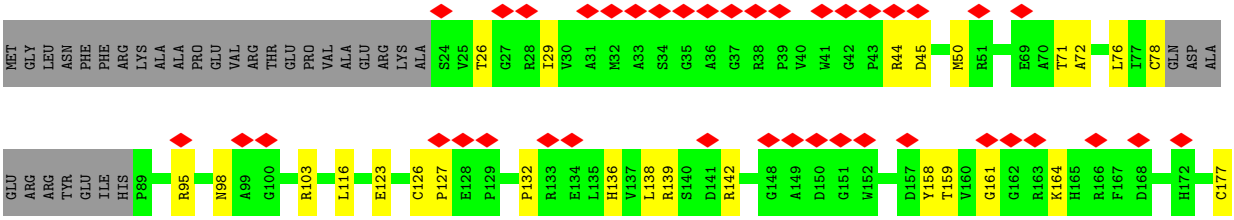
• Molecule 4: Uncharacterized protein

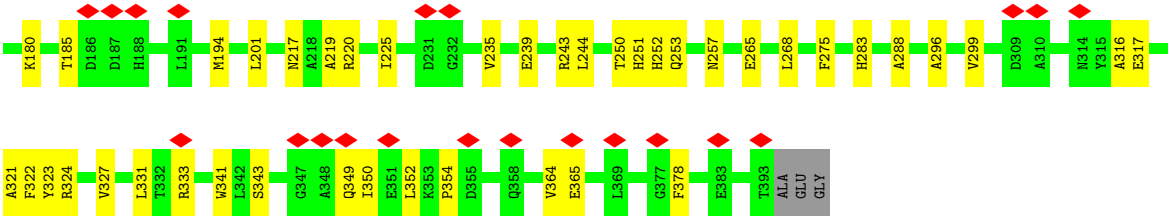
Chain 2D:



• Molecule 5: Portal protein Rcc01684

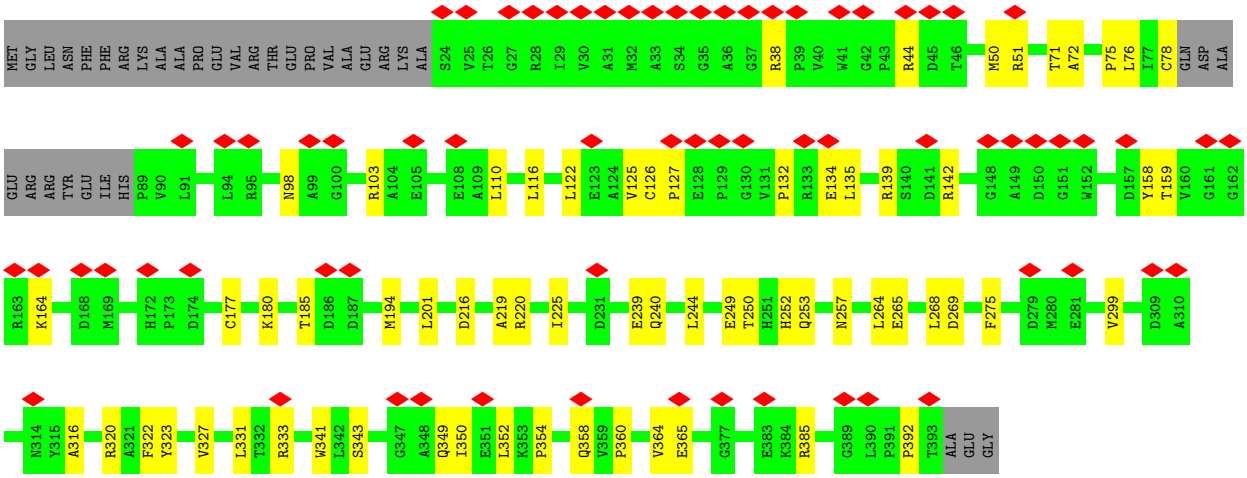
Chain 1A:





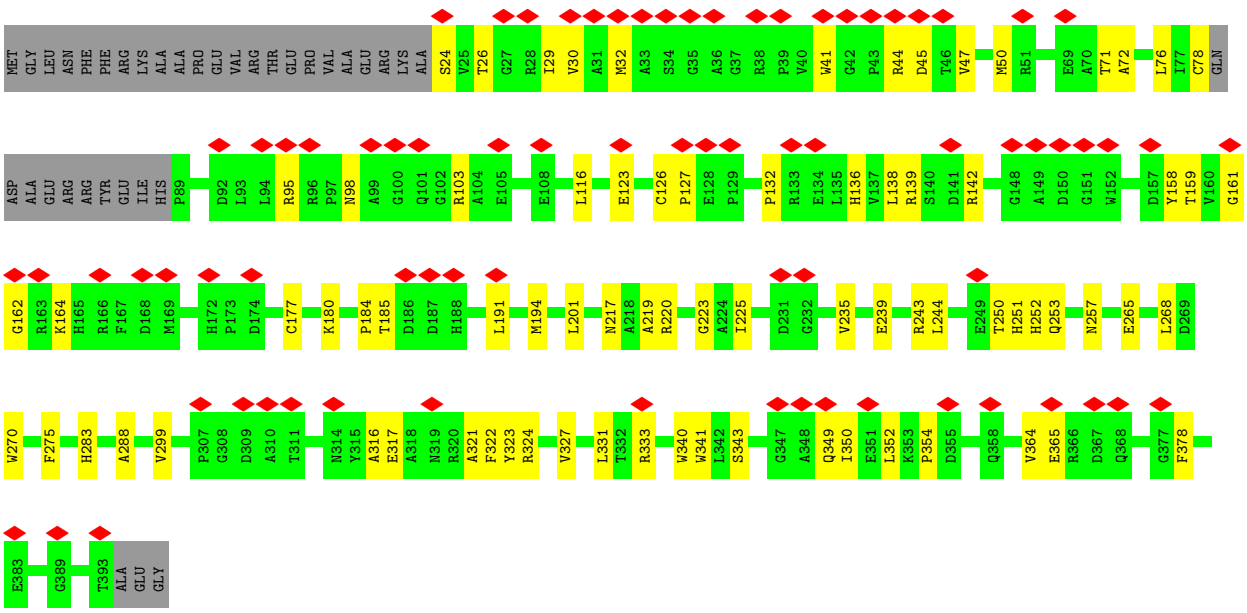
• Molecule 5: Portal protein Rcc01684

Chain 1B:



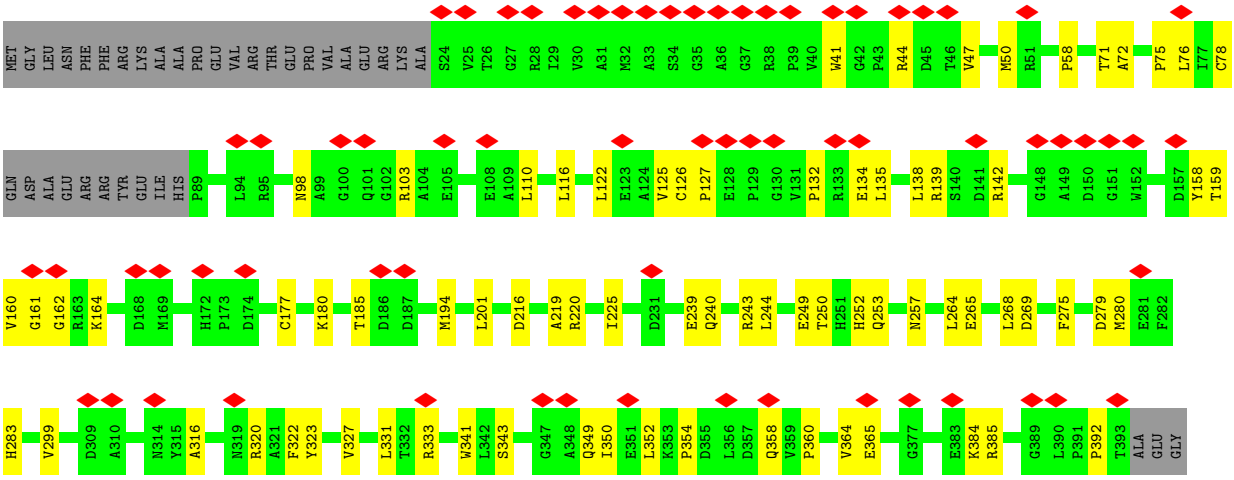
• Molecule 5: Portal protein Rcc01684

Chain 1K:



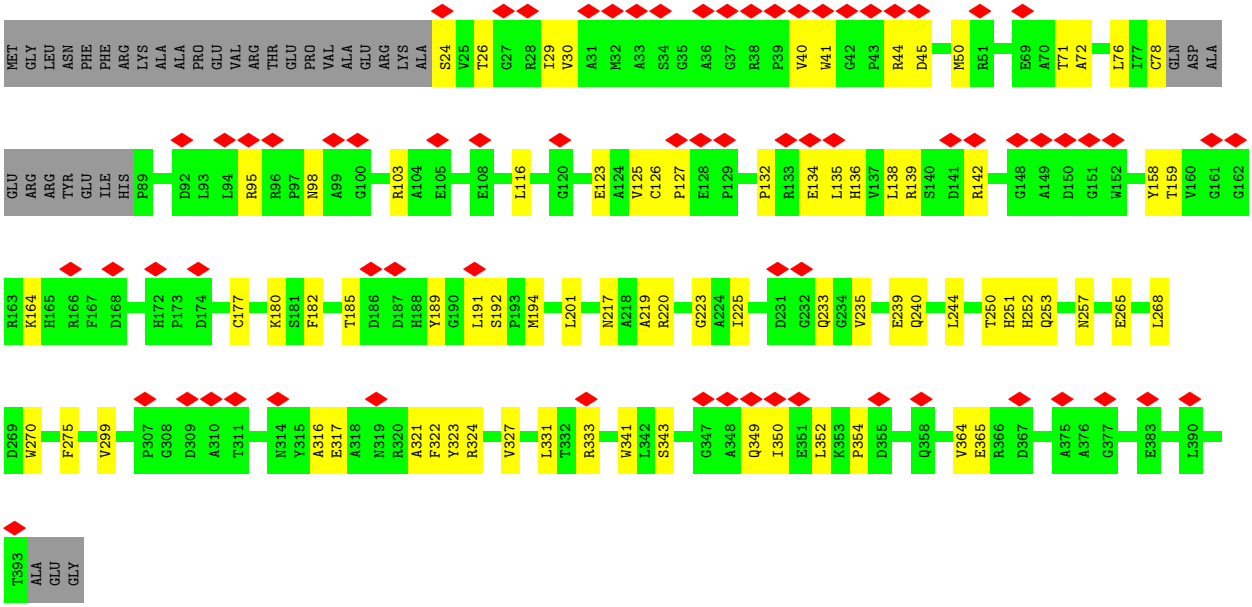
• Molecule 5: Portal protein Rcc01684

Chain 1L:



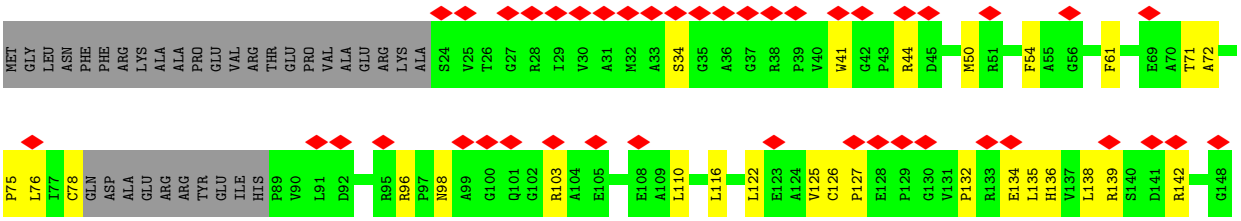
- Molecule 5: Portal protein Rcc01684

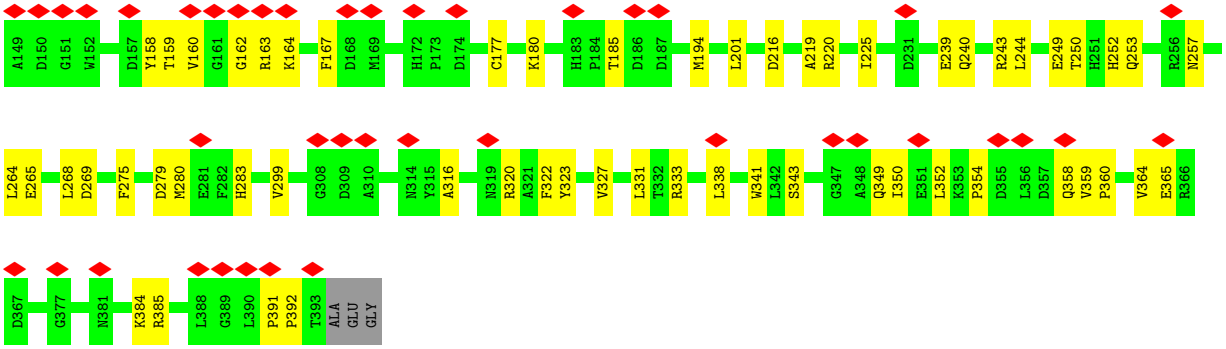
Chain 1I:



- Molecule 5: Portal protein Rcc01684

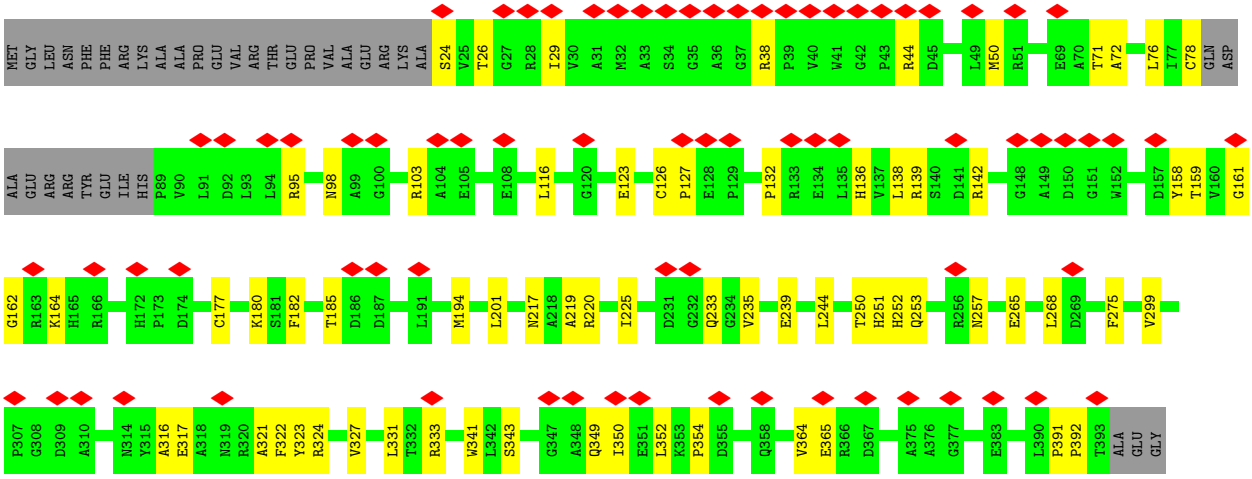
Chain 1J:





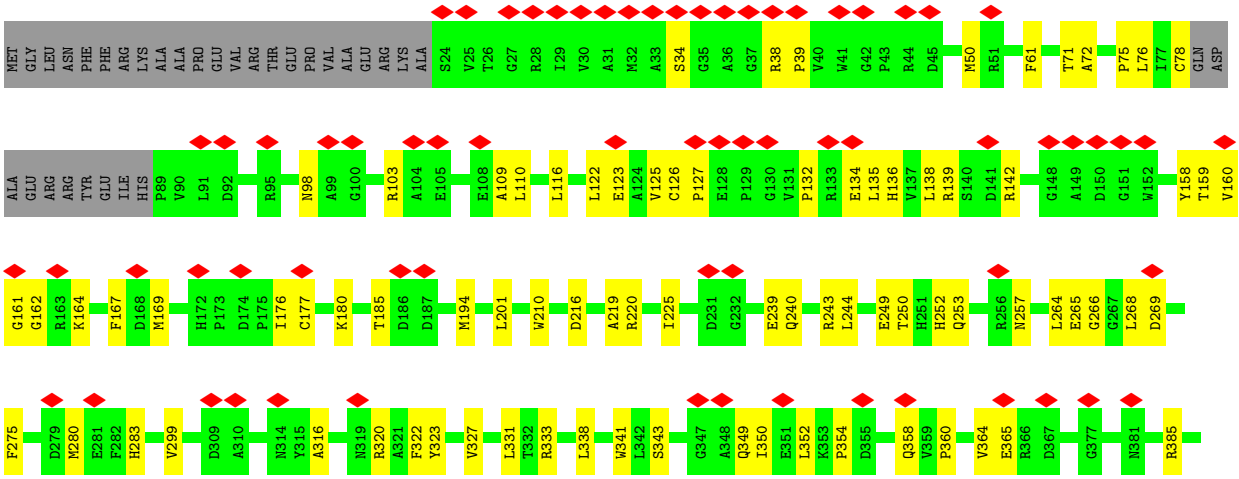
- Molecule 5: Portal protein Rcc01684

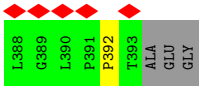
Chain 1G:



- Molecule 5: Portal protein Rcc01684

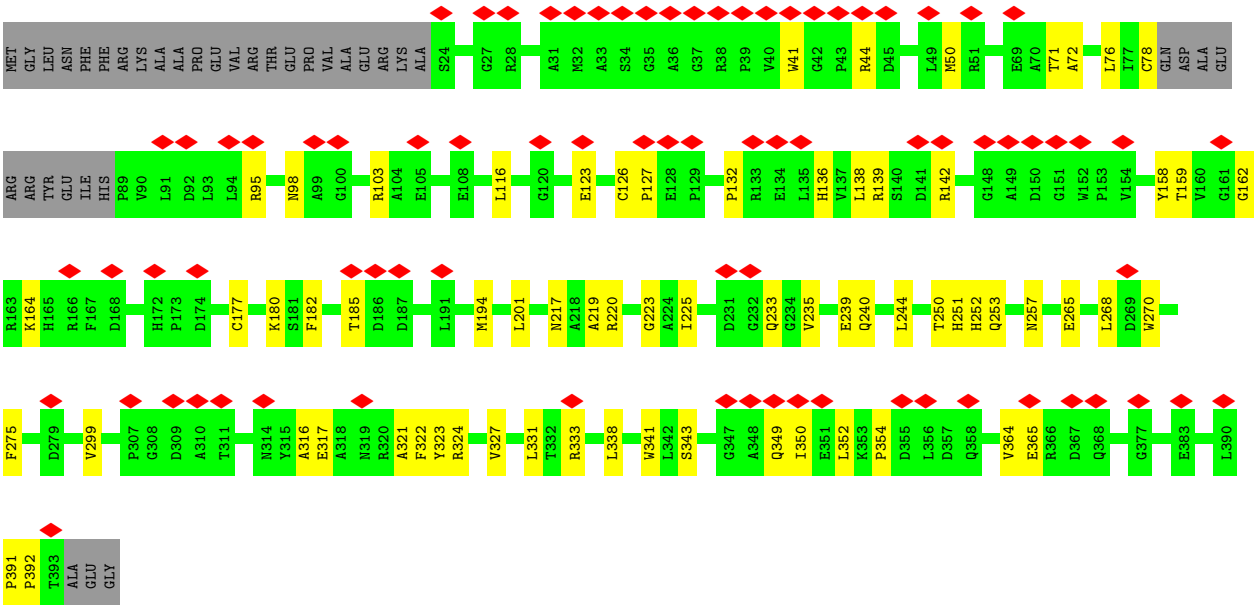
Chain 1H:





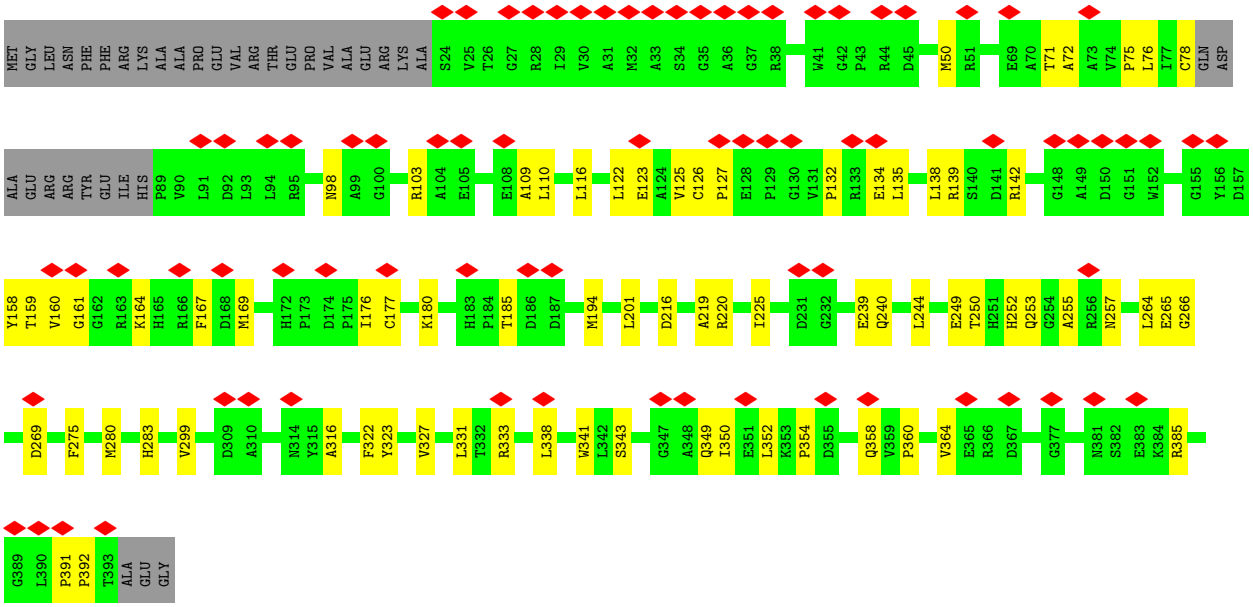
• Molecule 5: Portal protein Rcc01684

Chain 1E:



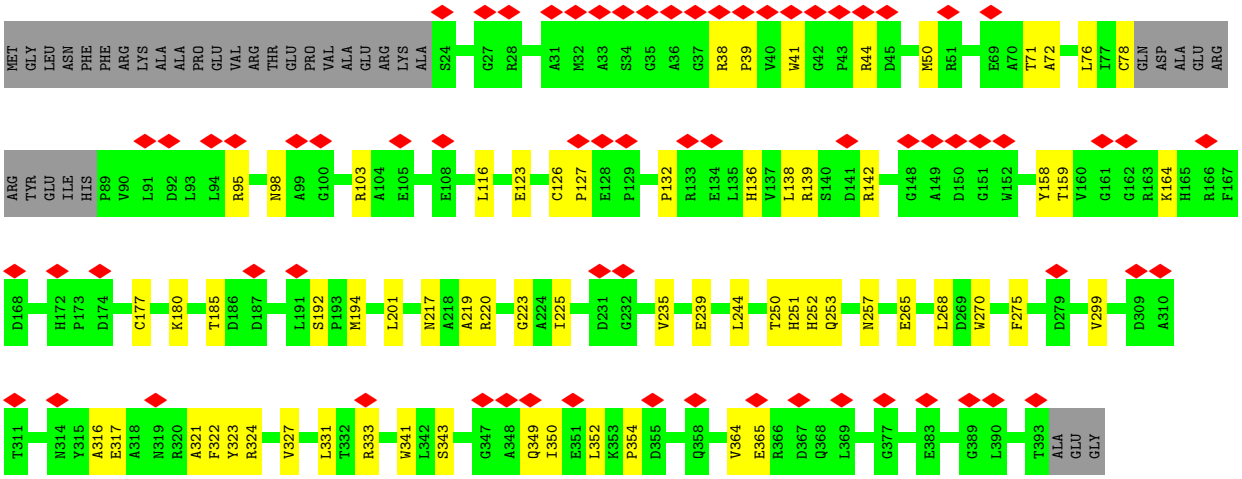
• Molecule 5: Portal protein Rcc01684

Chain 1F:



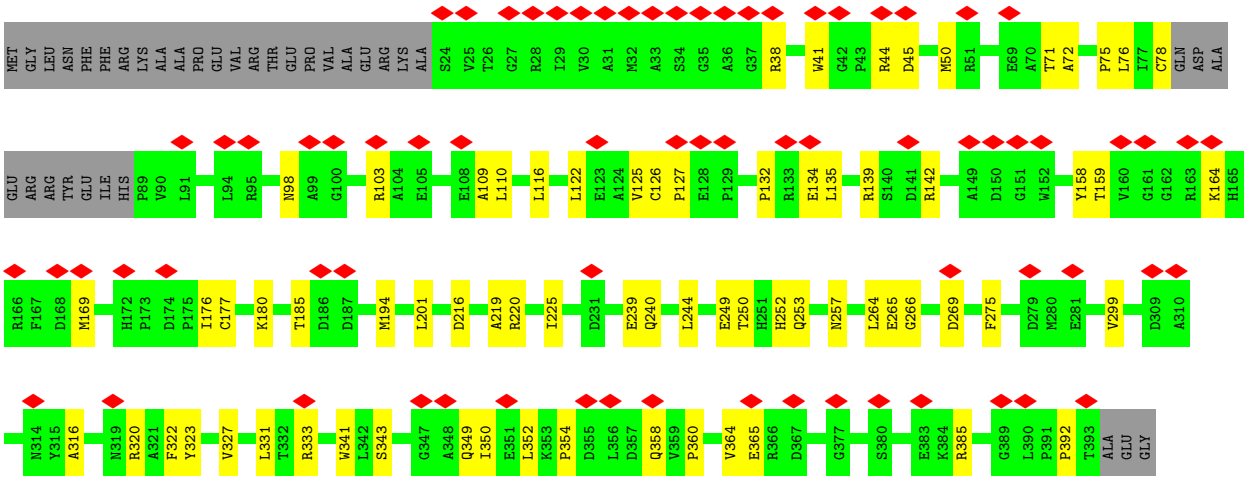
• Molecule 5: Portal protein Rcc01684

Chain 1C:



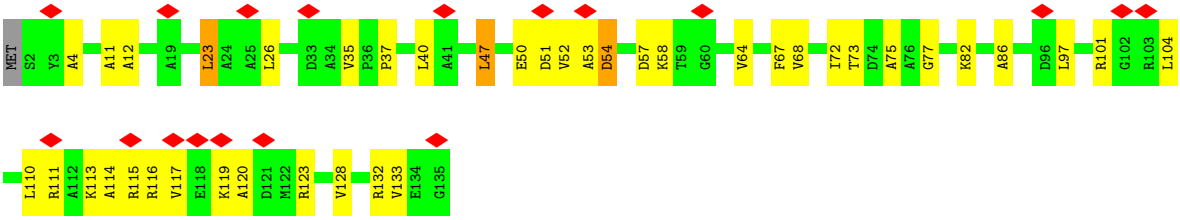
- Molecule 5: Portal protein Rcc01684

Chain 1D:



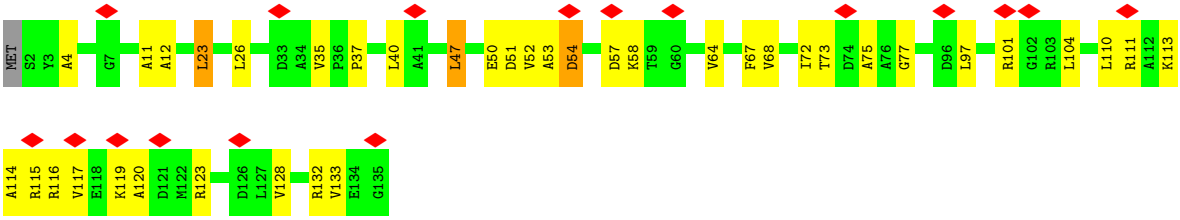
- Molecule 6: Uncharacterized protein

Chain 4A:



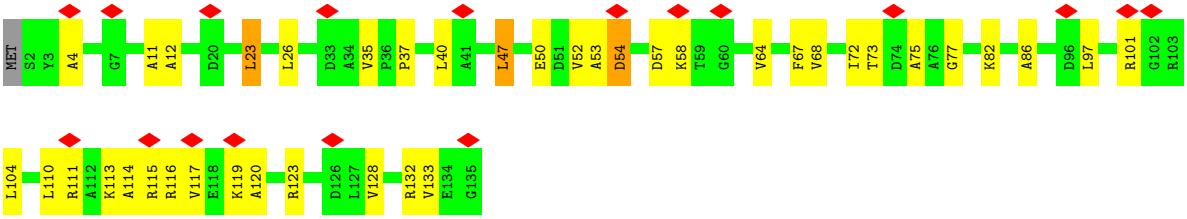
- Molecule 6: Uncharacterized protein

Chain 4F:



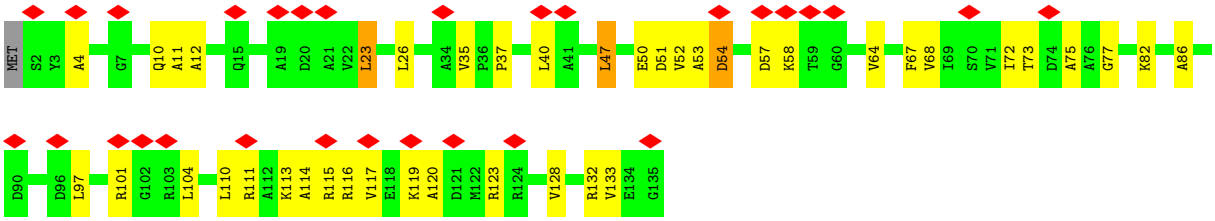
• Molecule 6: Uncharacterized protein

Chain 4E:



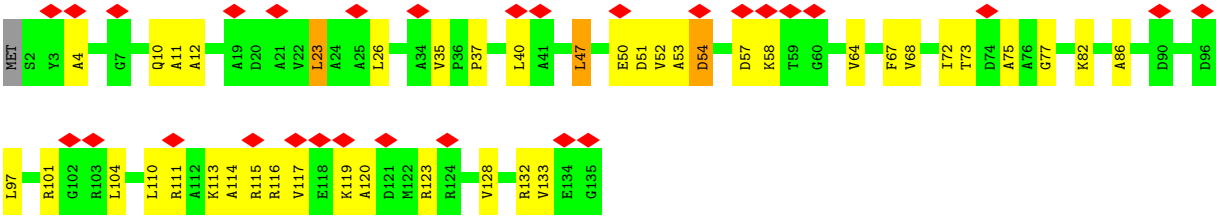
• Molecule 6: Uncharacterized protein

Chain 4D:



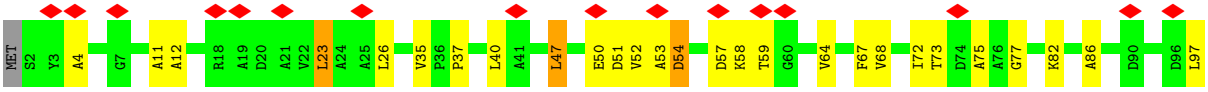
• Molecule 6: Uncharacterized protein

Chain 4C:



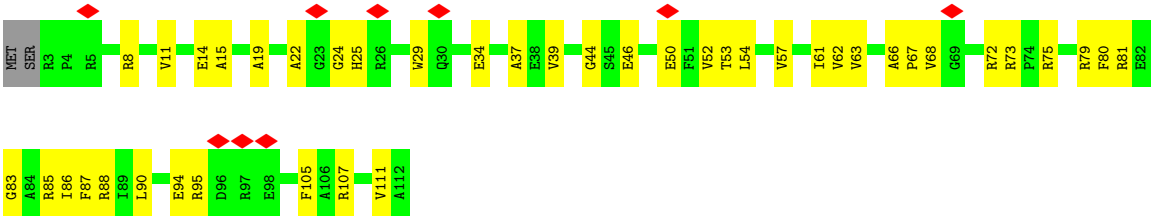
• Molecule 6: Uncharacterized protein

Chain 4B:



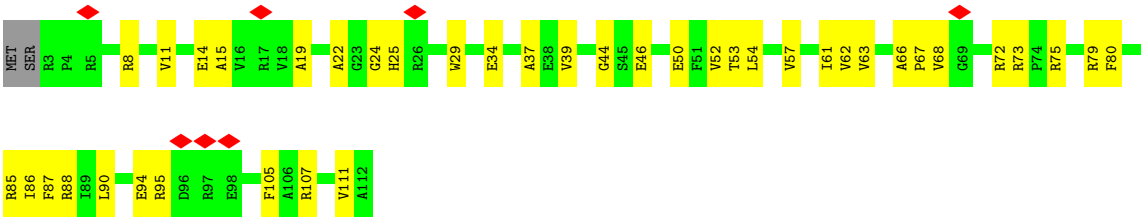
• Molecule 7: Uncharacterized protein

Chain 3A:



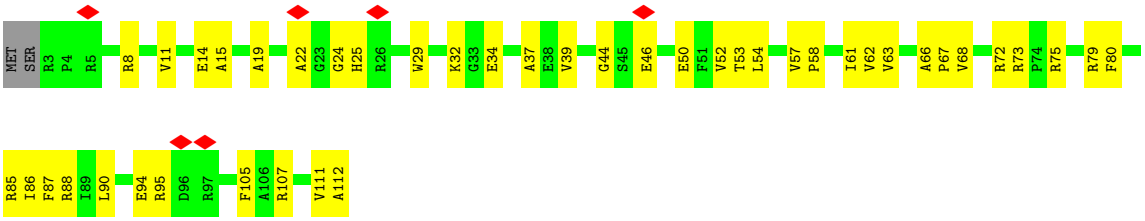
• Molecule 7: Uncharacterized protein

Chain 3F:



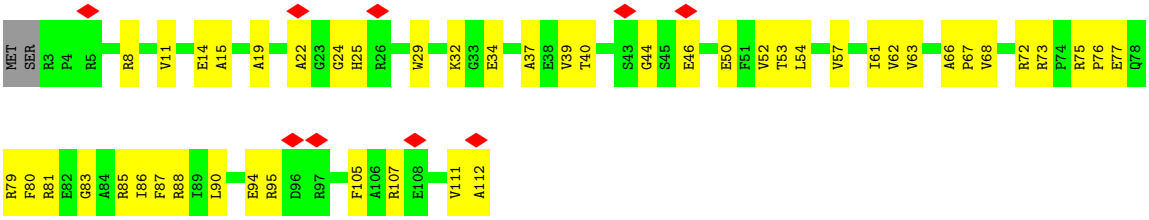
• Molecule 7: Uncharacterized protein

Chain 3E:



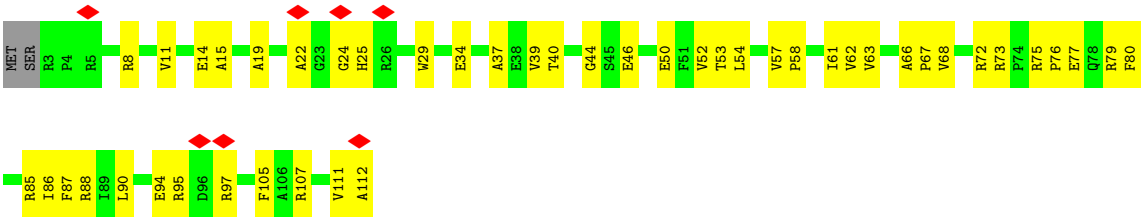
• Molecule 7: Uncharacterized protein

Chain 3D:



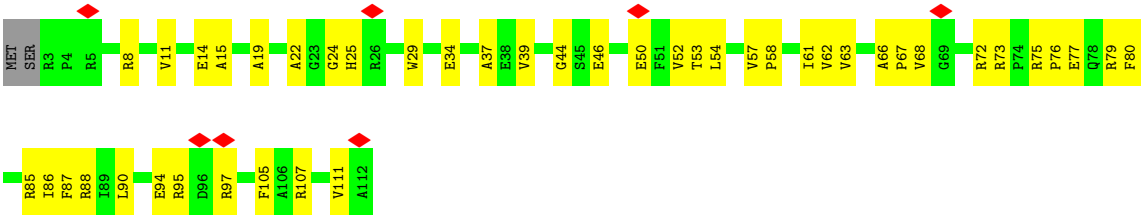
• Molecule 7: Uncharacterized protein

Chain 3C:



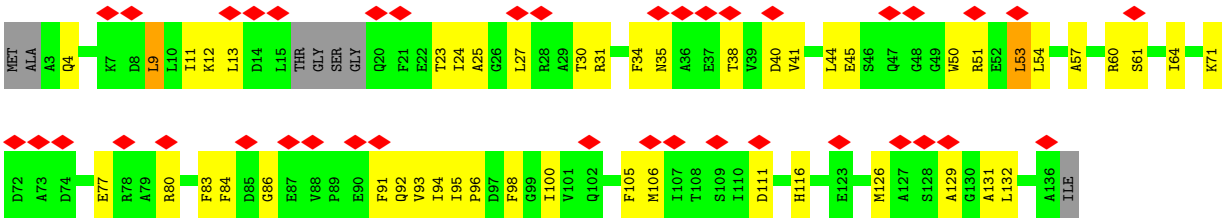
- Molecule 7: Uncharacterized protein

Chain 3B:



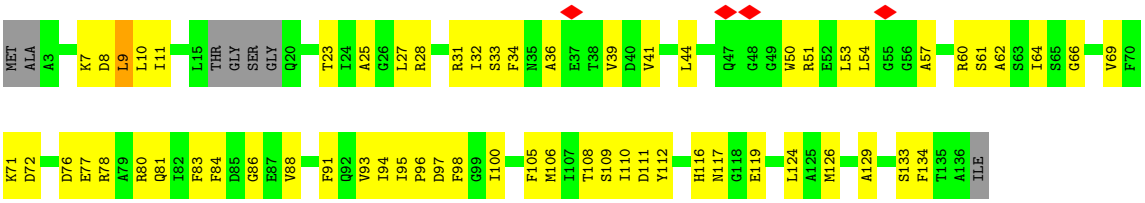
- Molecule 8: Phage major tail protein, TP901-1 family

Chain 5A:



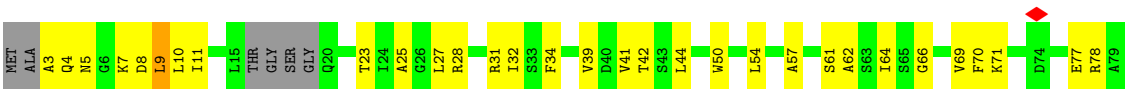
- Molecule 8: Phage major tail protein, TP901-1 family

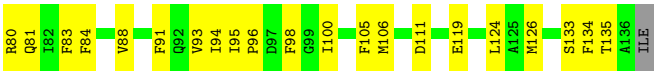
Chain 5S:



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

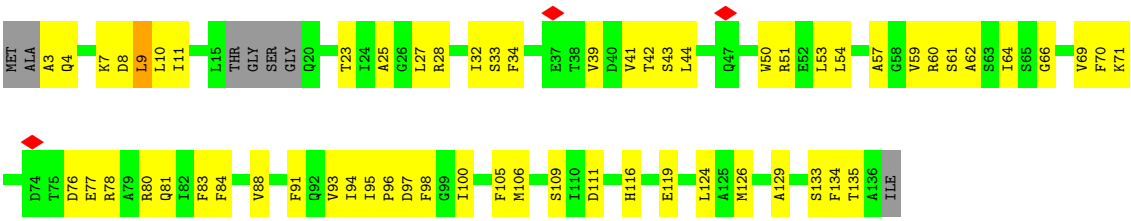
Chain 5G:





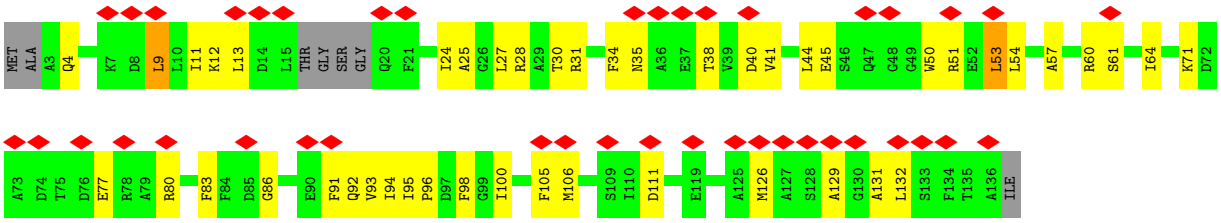
• Molecule 8: Phage major tail protein, TP901-1 family

Chain 5M:



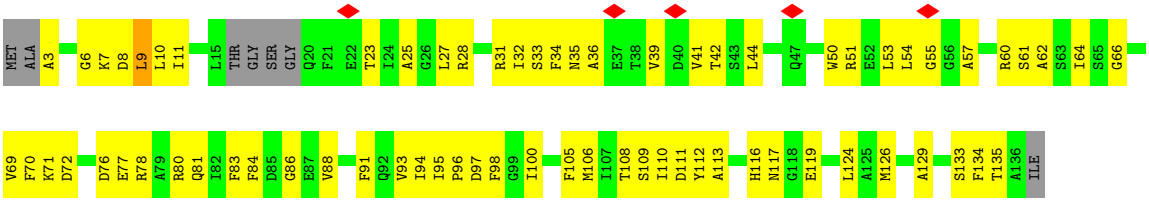
• Molecule 8: Phage major tail protein, TP901-1 family

Chain 5F:



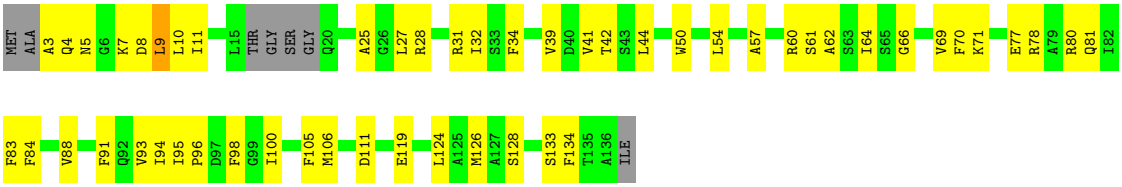
• Molecule 8: Phage major tail protein, TP901-1 family

Chain 5X:



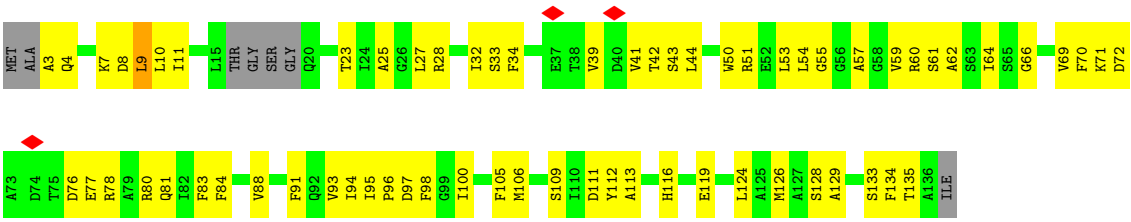
• Molecule 8: Phage major tail protein, TP901-1 family

Chain 5L:



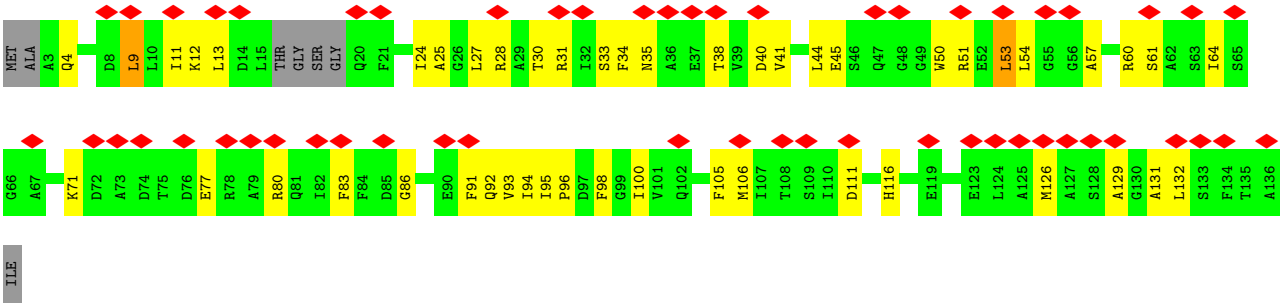
• Molecule 8: Phage major tail protein, TP901-1 family

Chain 5R:



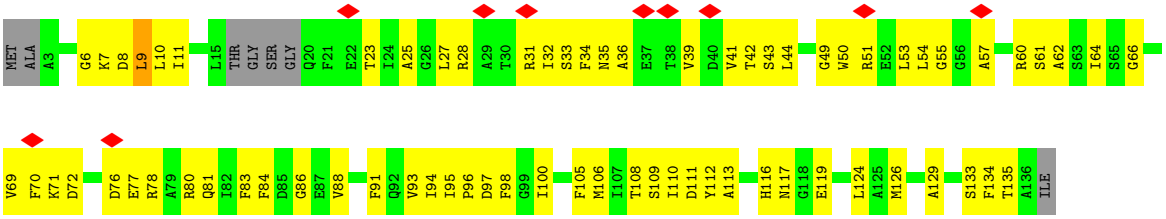
• Molecule 8: Phage major tail protein, TP901-1 family

Chain 5E:



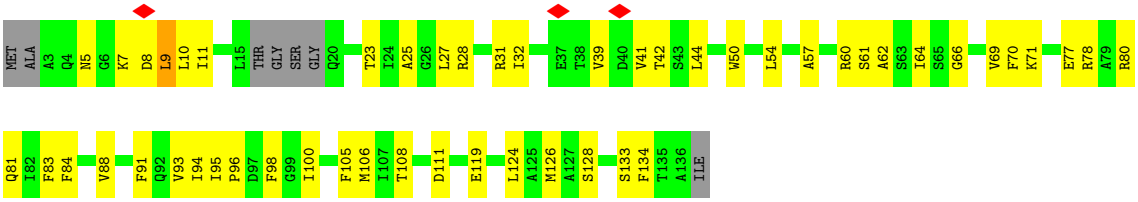
• Molecule 8: Phage major tail protein, TP901-1 family

Chain 5W:



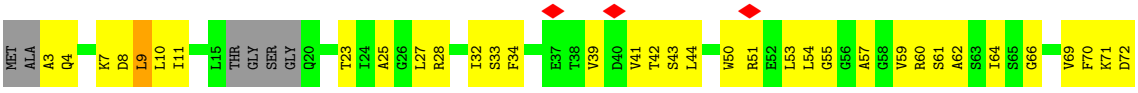
• Molecule 8: Phage major tail protein, TP901-1 family

Chain 5K:



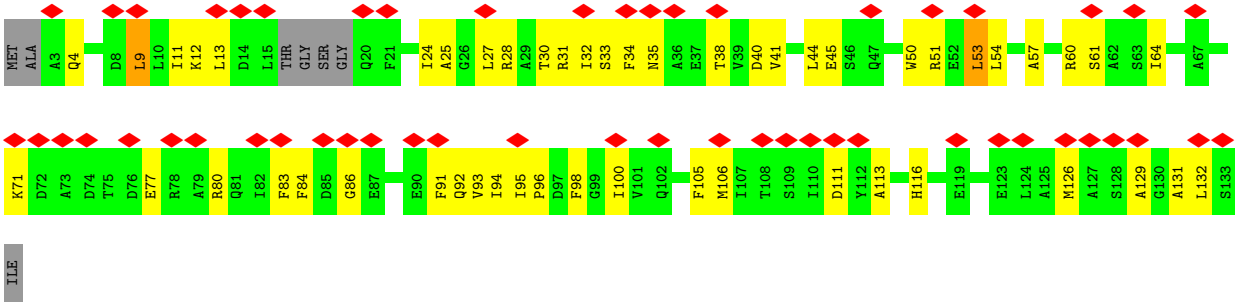
• Molecule 8: Phage major tail protein, TP901-1 family

Chain 5Q:



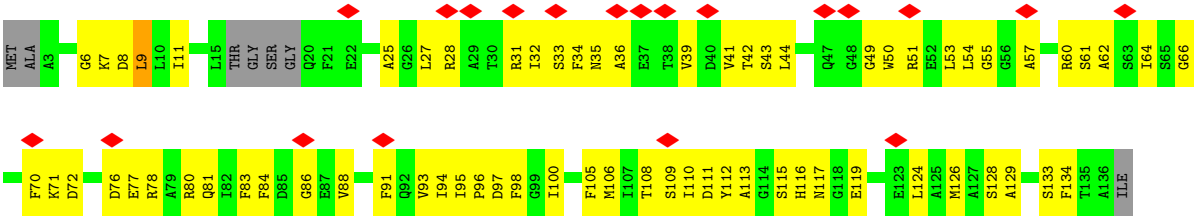
• Molecule 8: Phage major tail protein, TP901-1 family

Chain 5D:



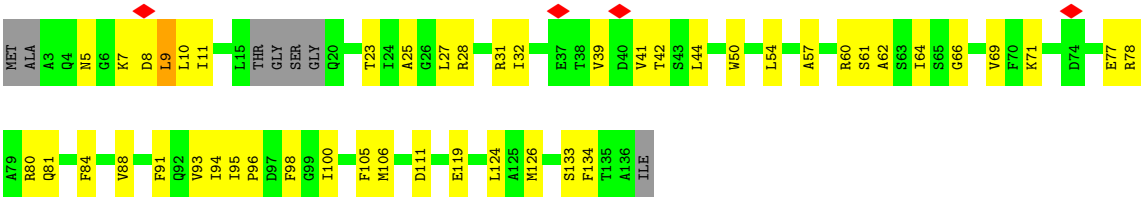
• Molecule 8: Phage major tail protein, TP901-1 family

Chain 5V:



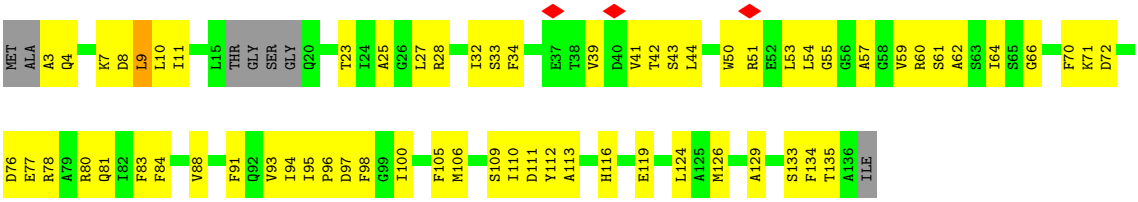
• Molecule 8: Phage major tail protein, TP901-1 family

Chain 5J:



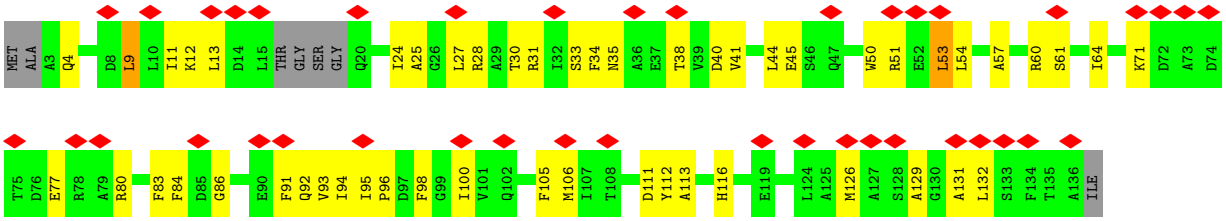
• Molecule 8: Phage major tail protein, TP901-1 family

Chain 5P:



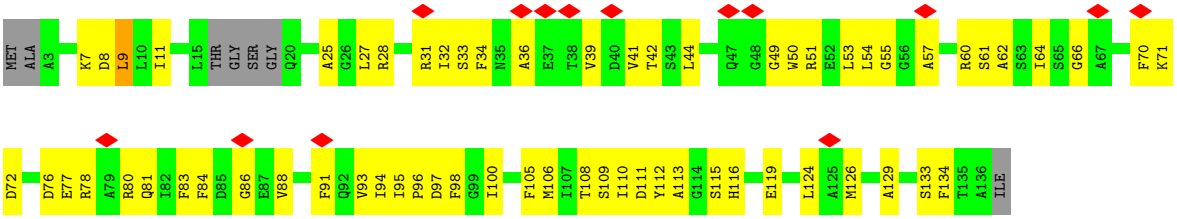
• Molecule 8: Phage major tail protein, TP901-1 family

Chain 5C:



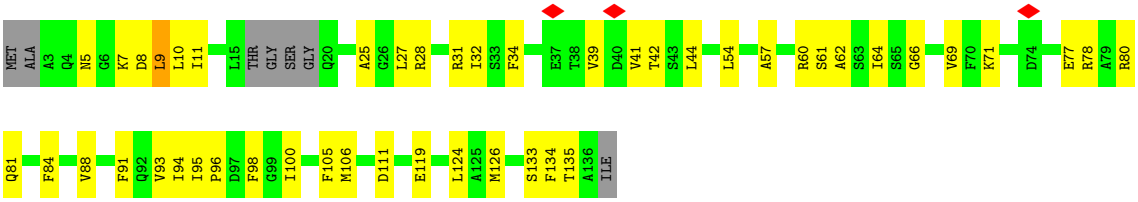
• Molecule 8: Phage major tail protein, TP901-1 family

Chain 5U:



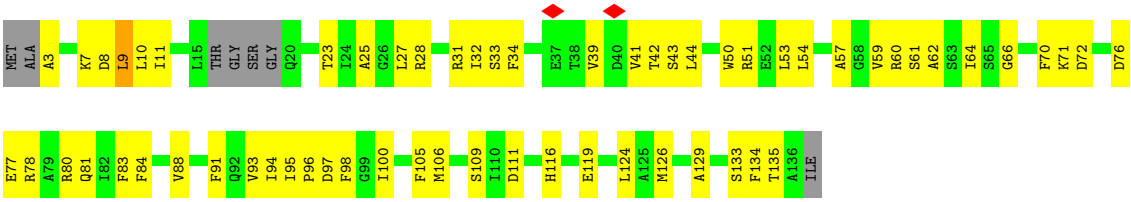
• Molecule 8: Phage major tail protein, TP901-1 family

Chain 5I:



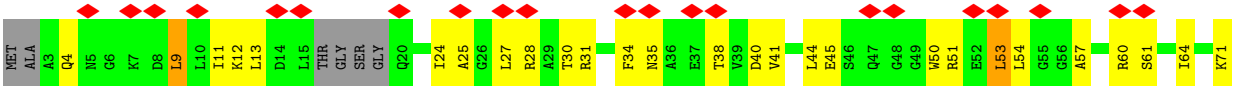
• Molecule 8: Phage major tail protein, TP901-1 family

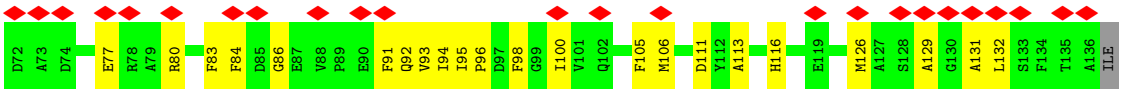
Chain 5O:



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

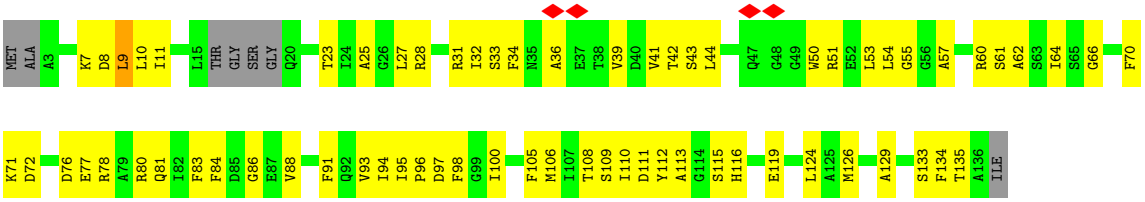
Chain 5B:





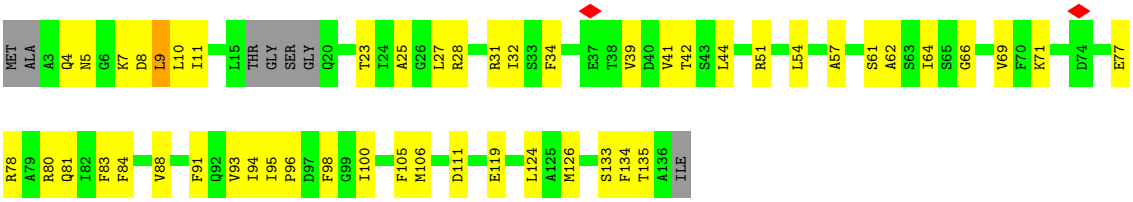
• Molecule 8: Phage major tail protein, TP901-1 family

Chain 5T:



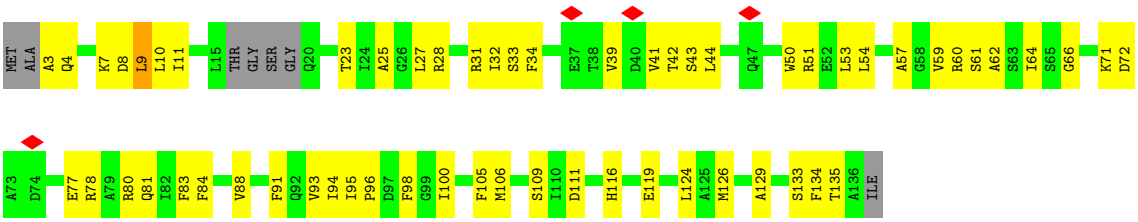
• Molecule 8: Phage major tail protein, TP901-1 family

Chain 5H:



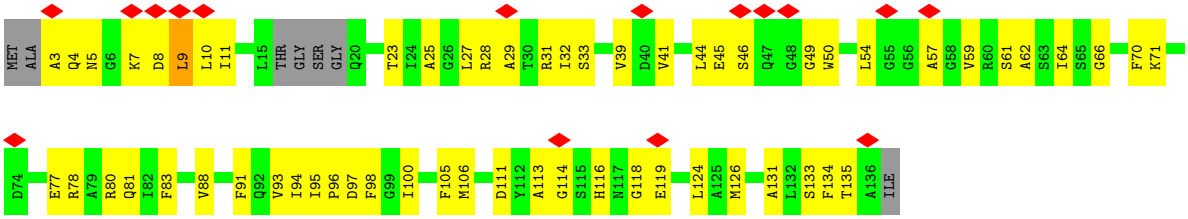
• Molecule 8: Phage major tail protein, TP901-1 family

Chain 5N:



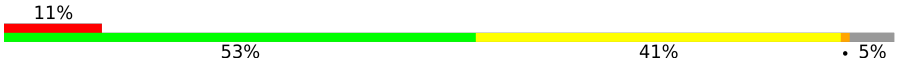
• Molecule 8: Phage major tail protein, TP901-1 family

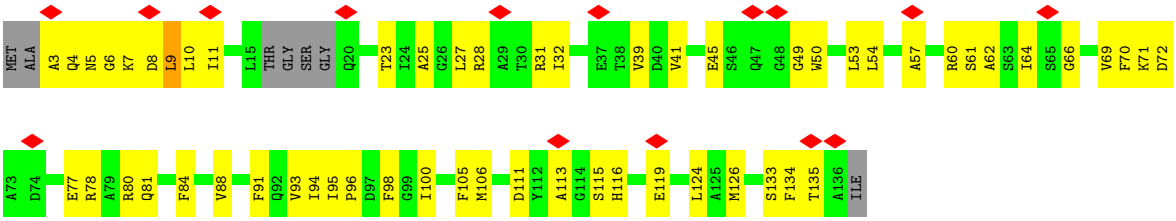
Chain 5Y:



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

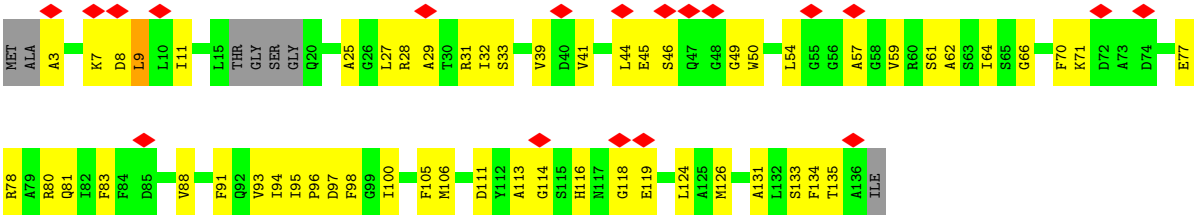
Chain 5Z:





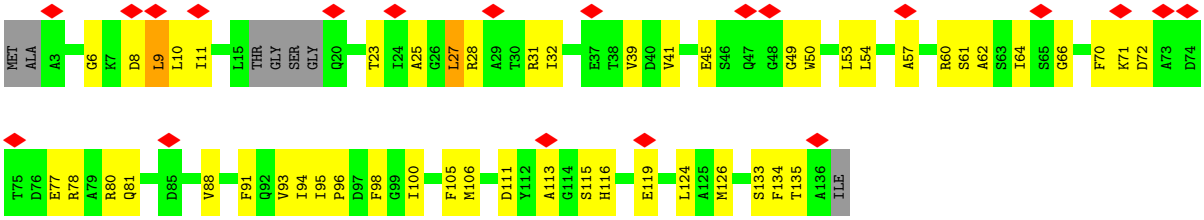
- Molecule 8: Phage major tail protein, TP901-1 family

Chain 52:



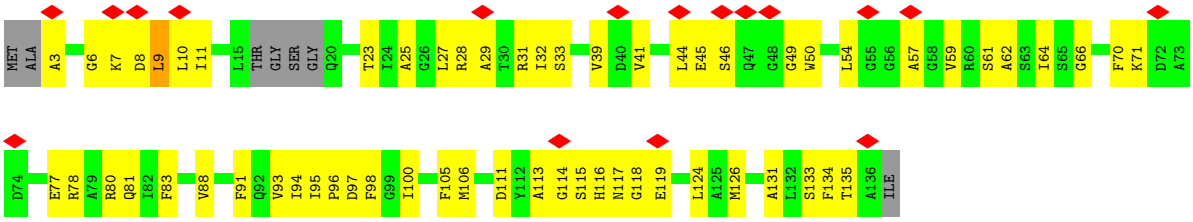
- Molecule 8: Phage major tail protein, TP901-1 family

Chain 53:



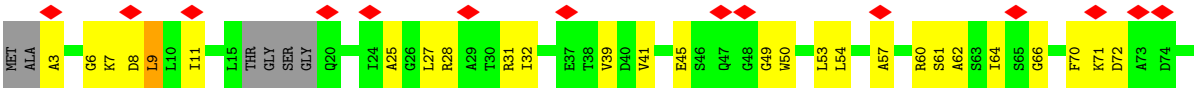
- Molecule 8: Phage major tail protein, TP901-1 family

Chain 50:



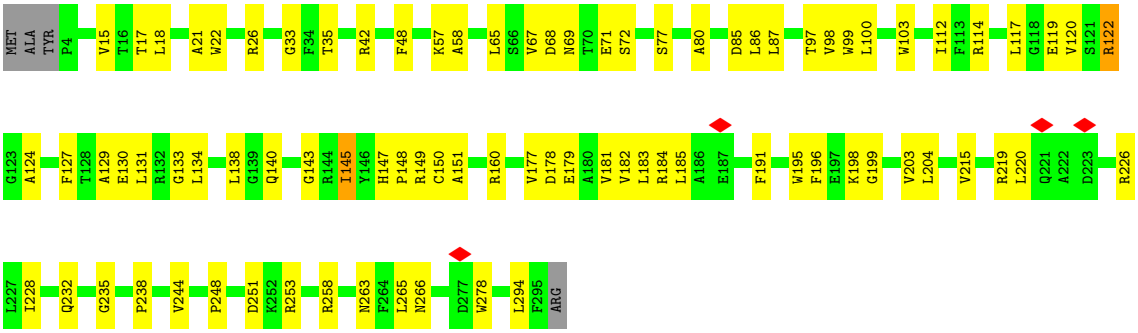
- Molecule 8: Phage major tail protein, TP901-1 family

Chain 51:



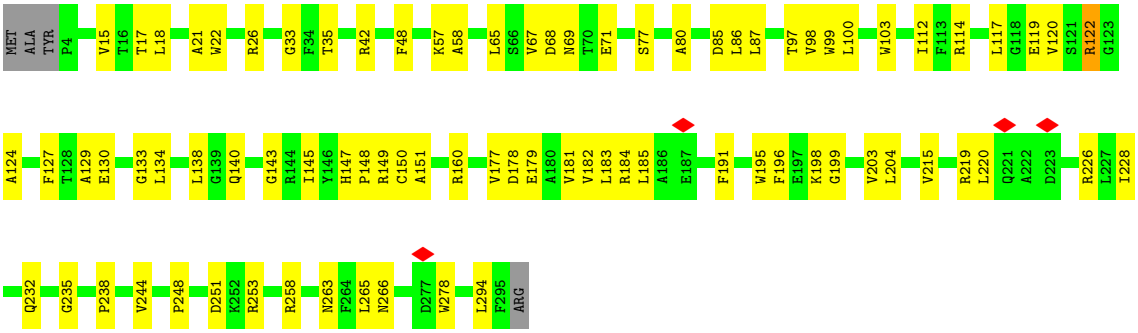
• Molecule 9: Uncharacterized protein

Chain 7A:



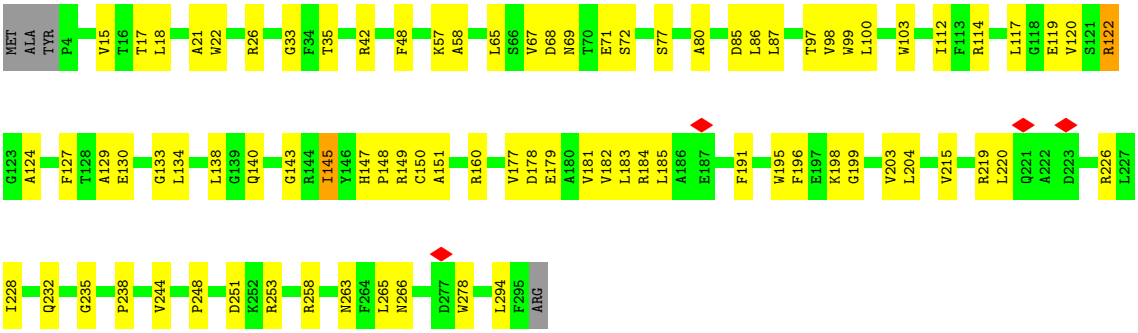
• Molecule 9: Uncharacterized protein

Chain 7C:



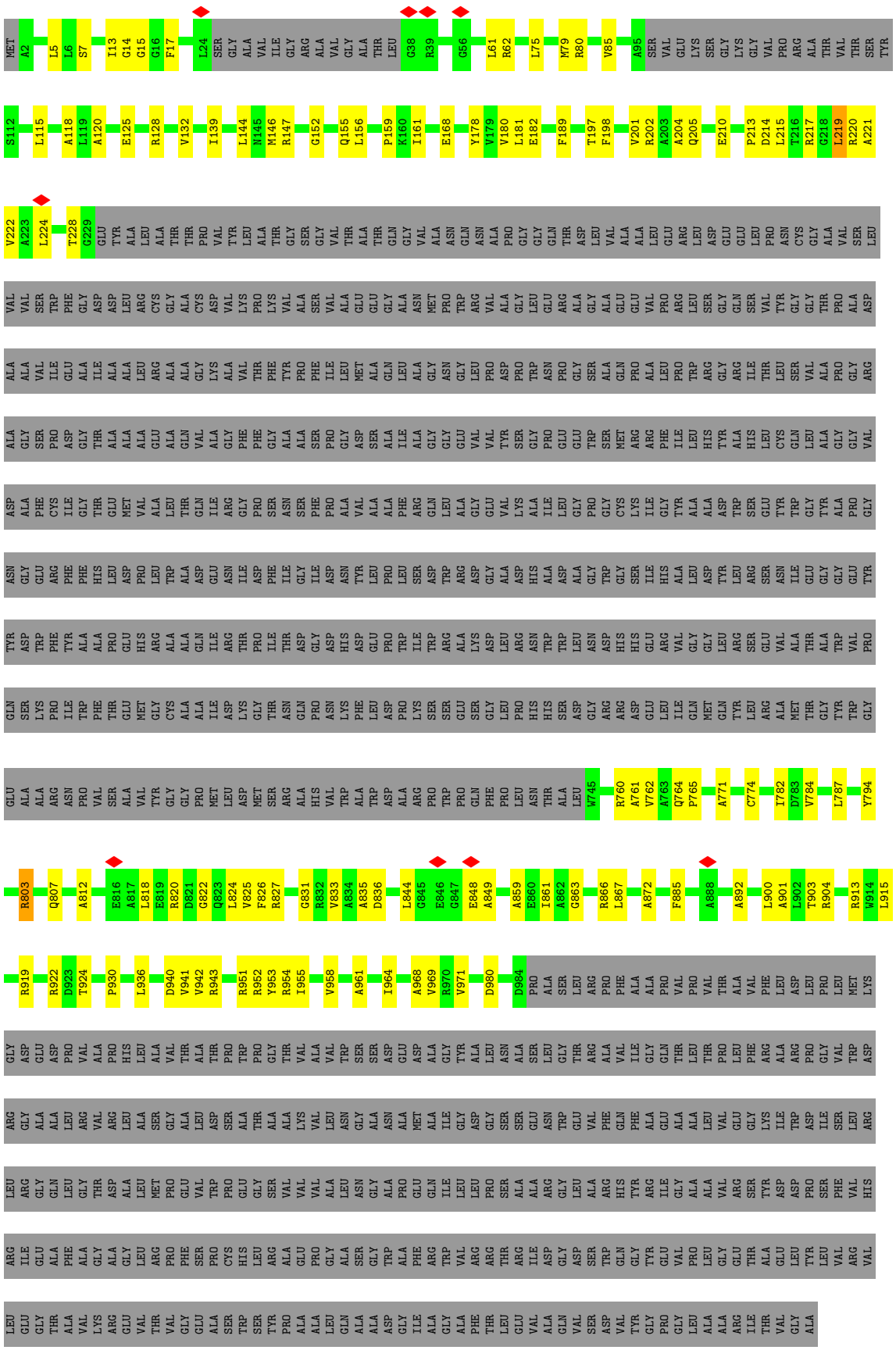
• Molecule 9: Uncharacterized protein

Chain 7B:



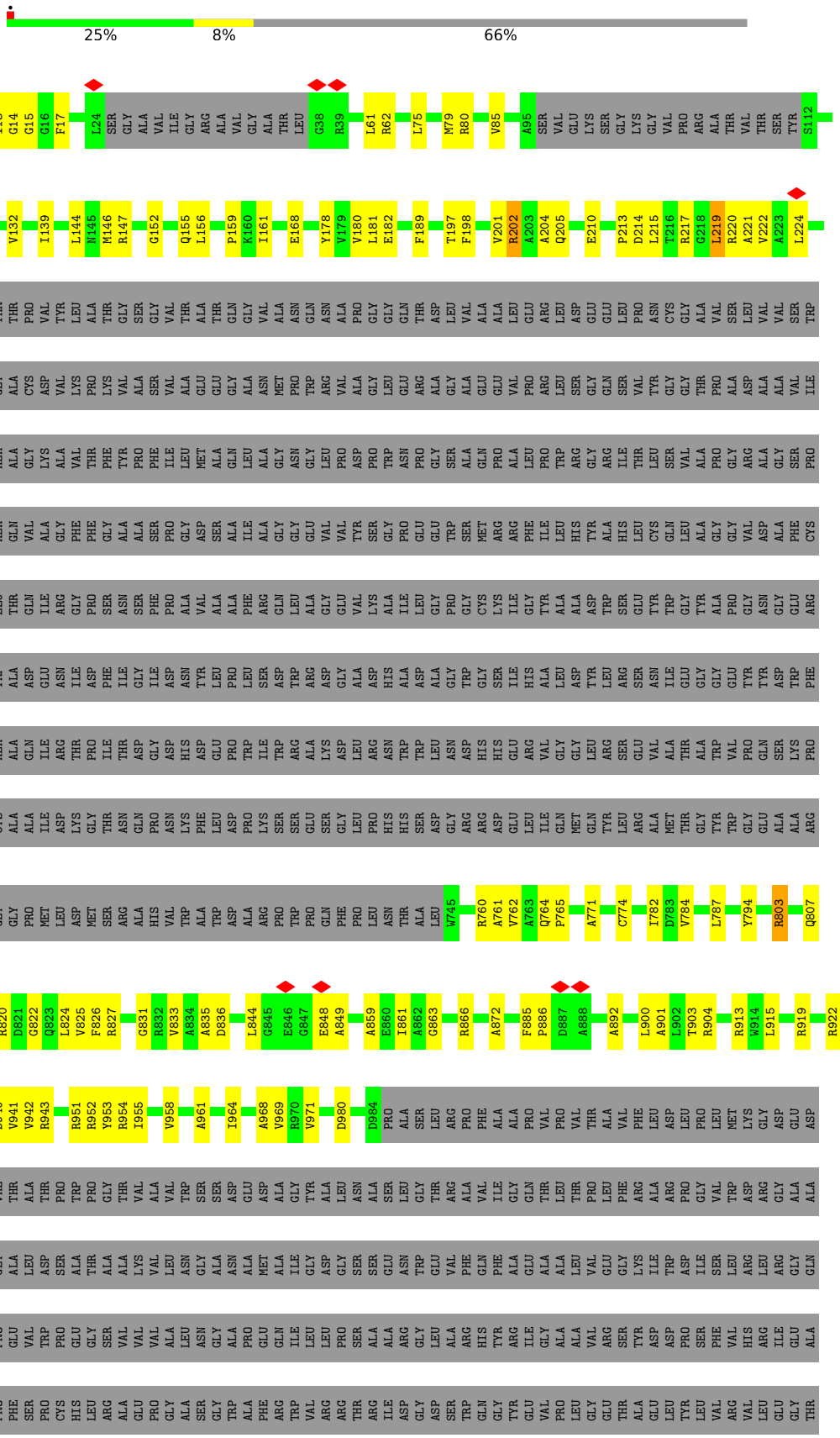
• Molecule 10: Uncharacterized protein

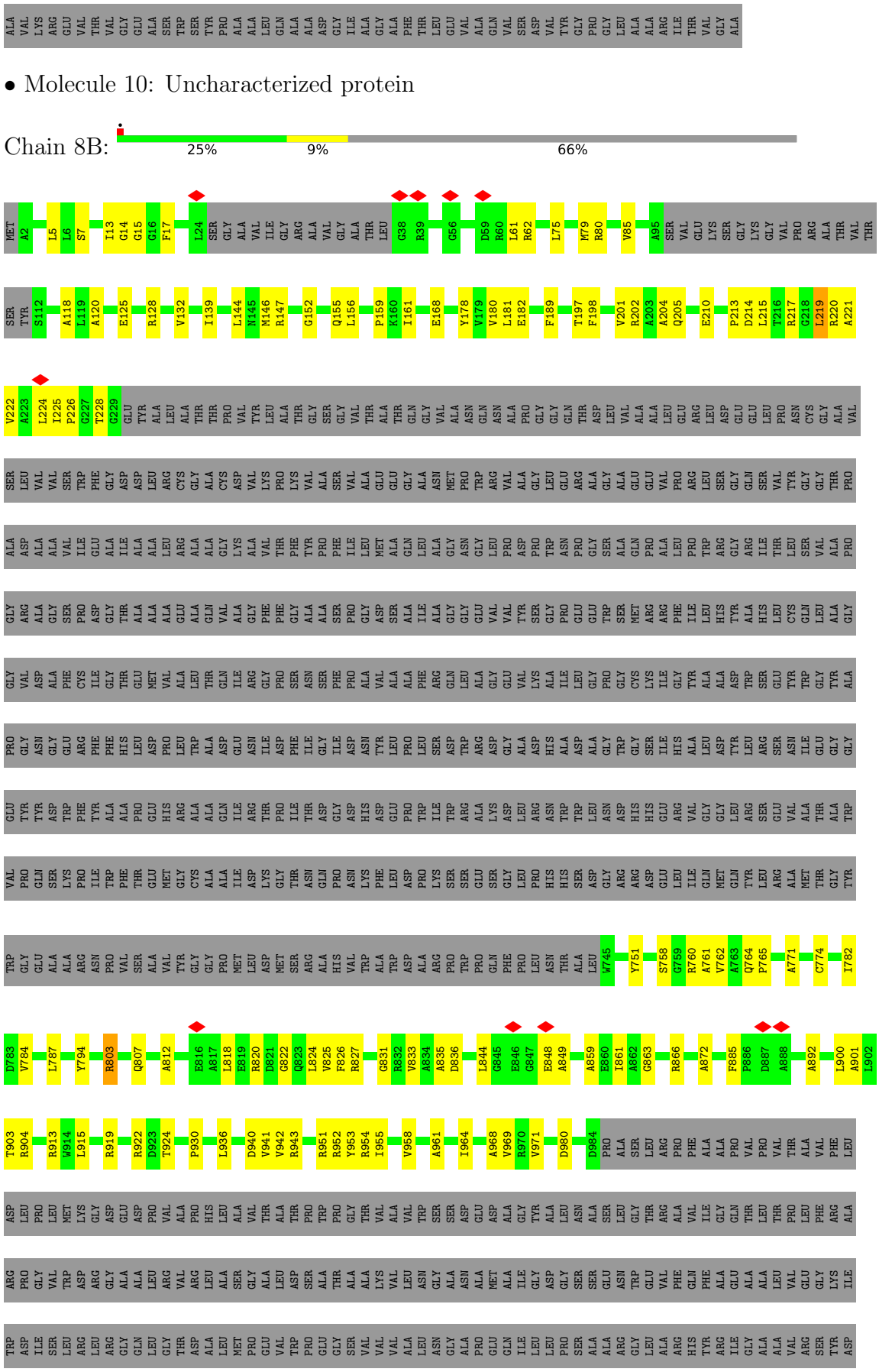
Chain 8A:



- Molecule 10: Uncharacterized protein

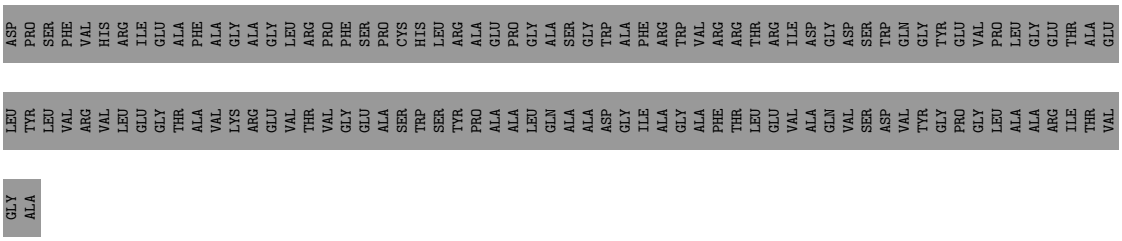
Chain 8C:





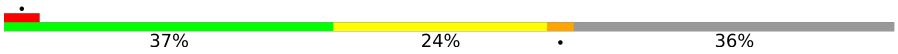
• Molecule 10: Uncharacterized protein

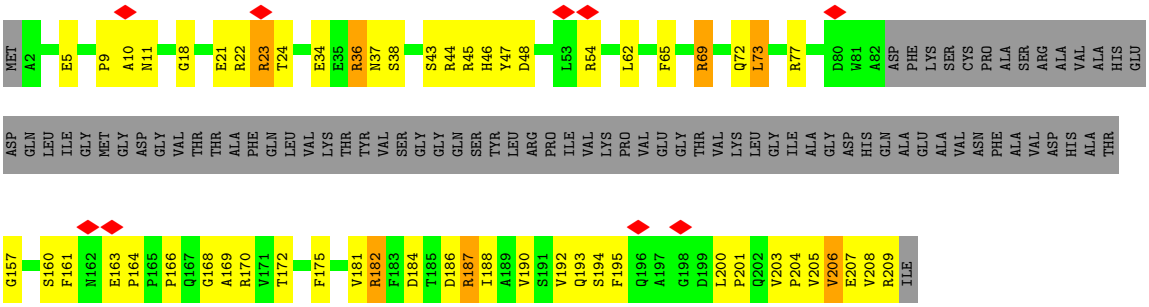
Chain 8B: 25% 9% 66%



• Molecule 11: Uncharacterized protein

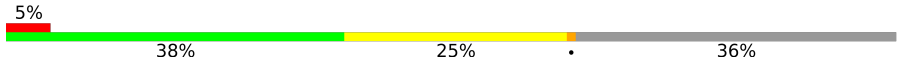
Chain 6B:

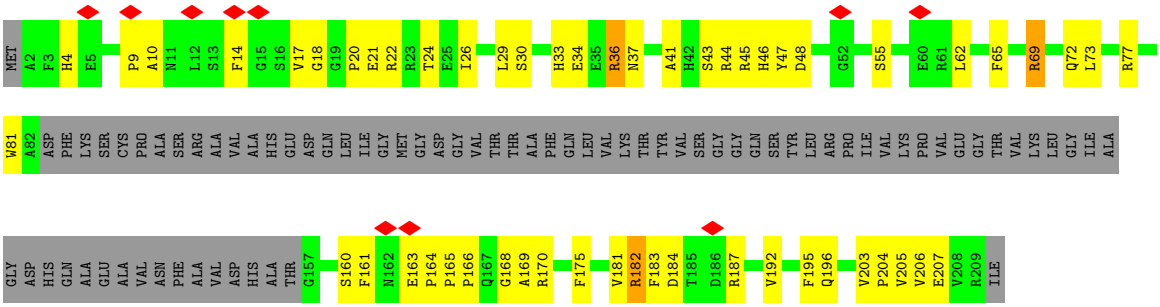




• Molecule 11: Uncharacterized protein

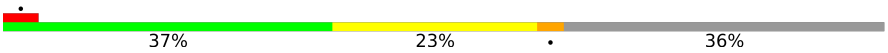
Chain 6A:

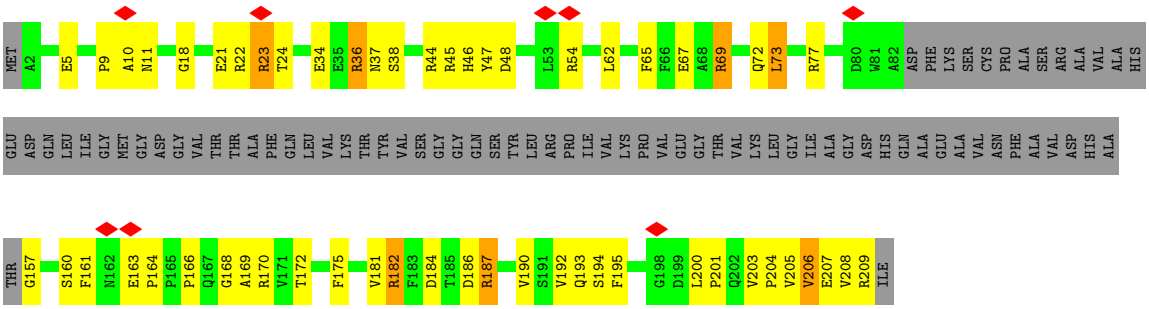




• Molecule 11: Uncharacterized protein

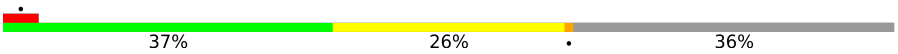
Chain 6F:

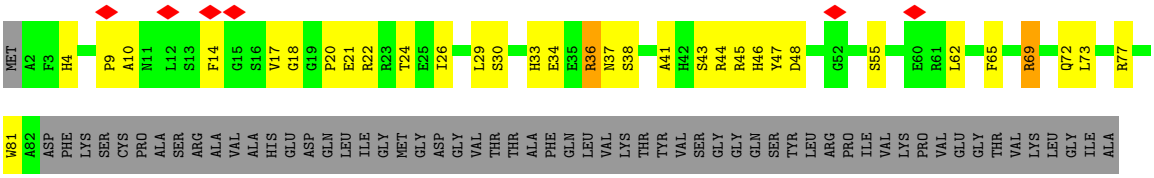




• Molecule 11: Uncharacterized protein

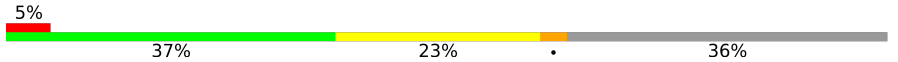
Chain 6E:

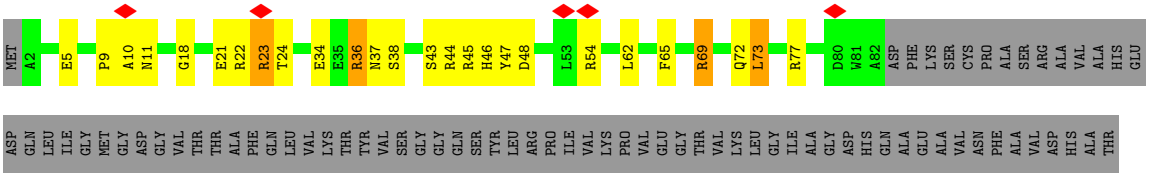


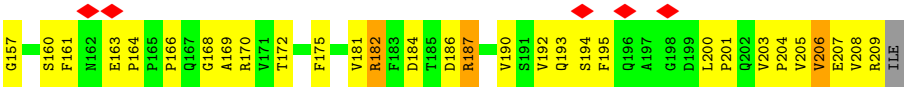


- Molecule 11: Uncharacterized protein

Chain 6D:

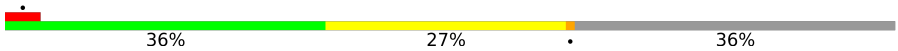


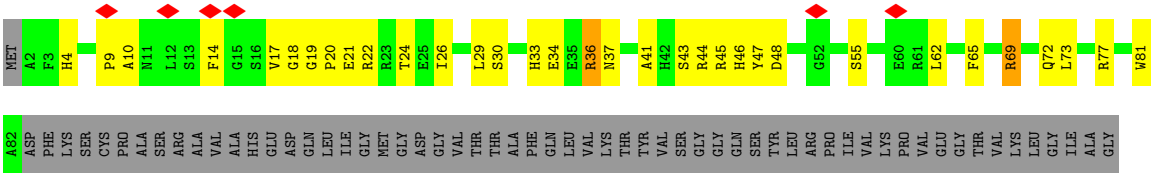


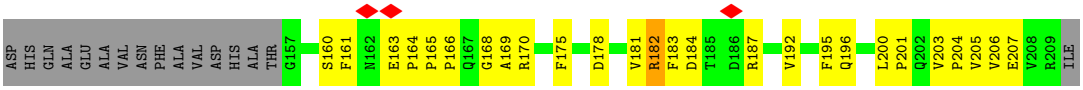


- Molecule 11: Uncharacterized protein

Chain 6C:







4 Experimental information (i)

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 ($e^-/Å^2$)	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 (i)

5.1 Standard geometry (i)

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	0.44	0/2216	0.67	3/3012 (0.1%)
1	A5	0.38	0/2243	0.67	1/3051 (0.0%)
1	A9	0.44	0/2216	0.67	3/3012 (0.1%)
1	AA	0.38	0/2249	0.67	1/3059 (0.0%)
1	AE	0.44	0/2216	0.67	3/3012 (0.1%)
1	AF	0.38	0/2253	0.67	1/3064 (0.0%)
1	AJ	0.44	0/2216	0.67	3/3012 (0.1%)
1	AK	0.38	0/2253	0.67	1/3064 (0.0%)
1	AO	0.44	0/2216	0.67	3/3012 (0.1%)
1	AP	0.38	0/2245	0.67	1/3054 (0.0%)
1	B4	0.42	0/2253	0.66	1/3064 (0.0%)
1	B5	0.44	0/2049	0.66	1/2785 (0.0%)
1	B9	0.42	0/2253	0.66	1/3064 (0.0%)
1	BA	0.44	0/2055	0.66	1/2793 (0.0%)
1	BE	0.42	0/2253	0.66	1/3064 (0.0%)
1	BF	0.43	0/2056	0.66	1/2793 (0.0%)
1	BJ	0.42	0/2253	0.66	1/3064 (0.0%)
1	BK	0.44	0/2049	0.66	1/2785 (0.0%)
1	BO	0.42	0/2253	0.66	1/3064 (0.0%)
1	BP	0.44	0/2050	0.66	1/2786 (0.0%)
1	C4	0.43	0/2253	0.65	1/3064 (0.0%)
1	C5	0.40	0/2253	0.67	1/3064 (0.0%)
1	C9	0.43	0/2253	0.65	1/3064 (0.0%)
1	CA	0.40	0/2253	0.67	1/3064 (0.0%)
1	CE	0.43	0/2253	0.65	1/3064 (0.0%)
1	CF	0.40	0/2253	0.67	1/3064 (0.0%)
1	CJ	0.43	0/2253	0.65	1/3064 (0.0%)
1	CK	0.40	0/2253	0.67	1/3064 (0.0%)
1	CO	0.43	0/2253	0.65	1/3064 (0.0%)
1	CP	0.40	0/2253	0.67	1/3064 (0.0%)
1	D4	0.43	0/2253	0.68	1/3064 (0.0%)
1	D9	0.43	0/2253	0.68	1/3064 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	DE	0.43	0/2253	0.68	1/3064 (0.0%)
1	DJ	0.43	0/2253	0.68	1/3064 (0.0%)
1	DO	0.42	0/2253	0.68	1/3064 (0.0%)
1	E4	0.43	0/2253	0.65	1/3064 (0.0%)
1	E9	0.43	0/2253	0.65	1/3064 (0.0%)
1	EE	0.43	0/2253	0.65	1/3064 (0.0%)
1	EJ	0.43	0/2253	0.65	1/3064 (0.0%)
1	EO	0.43	0/2253	0.65	1/3064 (0.0%)
1	F4	0.42	0/2253	0.66	2/3064 (0.1%)
1	F9	0.42	0/2253	0.66	2/3064 (0.1%)
1	FE	0.42	0/2253	0.66	2/3064 (0.1%)
1	FJ	0.42	0/2253	0.66	2/3064 (0.1%)
1	FO	0.42	0/2253	0.66	2/3064 (0.1%)
1	G4	0.42	0/2253	0.66	1/3064 (0.0%)
1	G9	0.42	0/2253	0.66	1/3064 (0.0%)
1	GE	0.42	0/2253	0.66	1/3064 (0.0%)
1	GJ	0.42	0/2253	0.66	1/3064 (0.0%)
1	GO	0.42	0/2253	0.66	1/3064 (0.0%)
1	H4	0.42	0/2216	0.65	2/3012 (0.1%)
1	H9	0.42	0/2216	0.65	2/3012 (0.1%)
1	HE	0.42	0/2216	0.65	2/3012 (0.1%)
1	HJ	0.42	0/2216	0.65	2/3012 (0.1%)
1	HO	0.42	0/2216	0.65	2/3012 (0.1%)
1	I4	0.41	0/2216	0.66	2/3012 (0.1%)
1	I9	0.41	0/2216	0.66	2/3012 (0.1%)
1	IE	0.41	0/2216	0.66	2/3012 (0.1%)
1	IJ	0.41	0/2216	0.66	2/3012 (0.1%)
1	IO	0.41	0/2216	0.66	2/3012 (0.1%)
1	J4	0.41	0/2216	0.65	2/3012 (0.1%)
1	J9	0.41	0/2216	0.65	2/3012 (0.1%)
1	JE	0.41	0/2216	0.65	2/3012 (0.1%)
1	JJ	0.41	0/2216	0.65	2/3012 (0.1%)
1	JO	0.41	0/2216	0.65	2/3012 (0.1%)
1	K4	0.42	1/2216 (0.0%)	0.66	2/3012 (0.1%)
1	K9	0.42	1/2216 (0.0%)	0.66	2/3012 (0.1%)
1	KE	0.42	1/2216 (0.0%)	0.66	2/3012 (0.1%)
1	KJ	0.42	1/2216 (0.0%)	0.66	2/3012 (0.1%)
1	KO	0.42	1/2216 (0.0%)	0.66	2/3012 (0.1%)
1	L4	0.42	0/2216	0.67	3/3012 (0.1%)
1	L9	0.42	0/2216	0.67	3/3012 (0.1%)
1	LE	0.42	0/2216	0.67	3/3012 (0.1%)
1	LJ	0.42	0/2216	0.67	3/3012 (0.1%)
1	LO	0.42	0/2216	0.67	3/3012 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	M4	0.41	0/2253	0.67	0/3064
1	M9	0.41	0/2253	0.67	0/3064
1	ME	0.41	0/2253	0.67	0/3064
1	MJ	0.41	0/2253	0.67	0/3064
1	MO	0.41	0/2253	0.67	0/3064
1	N4	0.42	0/2253	0.69	1/3064 (0.0%)
1	N9	0.42	0/2253	0.69	1/3064 (0.0%)
1	NE	0.43	0/2253	0.69	1/3064 (0.0%)
1	NJ	0.42	0/2253	0.69	1/3064 (0.0%)
1	NO	0.42	0/2253	0.69	1/3064 (0.0%)
1	O4	0.42	0/2253	0.68	2/3064 (0.1%)
1	O9	0.42	0/2253	0.68	2/3064 (0.1%)
1	OE	0.42	0/2253	0.68	2/3064 (0.1%)
1	OJ	0.42	0/2253	0.68	2/3064 (0.1%)
1	OO	0.42	0/2253	0.68	2/3064 (0.1%)
1	P4	0.40	0/2253	0.70	2/3064 (0.1%)
1	P9	0.40	0/2253	0.70	2/3064 (0.1%)
1	PE	0.40	0/2253	0.70	2/3064 (0.1%)
1	PJ	0.40	0/2253	0.70	2/3064 (0.1%)
1	PO	0.40	0/2253	0.70	2/3064 (0.1%)
1	Q4	0.42	0/2253	0.71	3/3064 (0.1%)
1	Q9	0.42	0/2253	0.71	3/3064 (0.1%)
1	QE	0.42	0/2253	0.71	3/3064 (0.1%)
1	QJ	0.42	0/2253	0.71	3/3064 (0.1%)
1	QO	0.42	0/2253	0.71	3/3064 (0.1%)
1	R4	0.42	0/2253	0.66	0/3064
1	R9	0.42	0/2253	0.66	0/3064
1	RE	0.42	0/2253	0.66	0/3064
1	RJ	0.42	0/2253	0.66	0/3064
1	RO	0.42	0/2253	0.66	0/3064
1	S4	0.41	0/2216	0.68	2/3012 (0.1%)
1	S9	0.41	0/2216	0.68	2/3012 (0.1%)
1	SE	0.41	0/2216	0.68	2/3012 (0.1%)
1	SJ	0.41	0/2216	0.68	2/3012 (0.1%)
1	SO	0.41	0/2216	0.68	2/3012 (0.1%)
1	T4	0.41	0/2216	0.65	3/3012 (0.1%)
1	T9	0.41	0/2216	0.65	3/3012 (0.1%)
1	TE	0.41	0/2216	0.65	3/3012 (0.1%)
1	TJ	0.41	0/2216	0.65	3/3012 (0.1%)
1	TO	0.41	0/2216	0.65	3/3012 (0.1%)
1	U4	0.41	0/2216	0.66	2/3012 (0.1%)
1	U9	0.42	0/2216	0.66	2/3012 (0.1%)
1	UE	0.42	0/2216	0.66	2/3012 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	UJ	0.42	0/2216	0.66	2/3012 (0.1%)
1	UO	0.42	0/2216	0.66	2/3012 (0.1%)
1	V4	0.41	0/2216	0.66	2/3012 (0.1%)
1	V9	0.41	0/2216	0.66	2/3012 (0.1%)
1	VE	0.41	0/2216	0.66	2/3012 (0.1%)
1	VJ	0.41	0/2216	0.66	2/3012 (0.1%)
1	VO	0.41	0/2216	0.66	2/3012 (0.1%)
1	W4	0.41	0/2216	0.66	2/3012 (0.1%)
1	W9	0.41	0/2216	0.66	2/3012 (0.1%)
1	WE	0.41	0/2216	0.66	2/3012 (0.1%)
1	WJ	0.41	0/2216	0.66	2/3012 (0.1%)
1	WO	0.41	0/2216	0.66	2/3012 (0.1%)
1	X4	0.40	0/2253	0.64	0/3064
1	X9	0.40	0/2253	0.64	0/3064
1	XE	0.40	0/2253	0.64	0/3064
1	XJ	0.40	0/2253	0.64	0/3064
1	XO	0.40	0/2253	0.64	0/3064
1	Y4	0.40	0/2253	0.65	0/3064
1	Y9	0.40	0/2253	0.65	0/3064
1	YE	0.40	0/2253	0.65	0/3064
1	YJ	0.40	0/2253	0.65	0/3064
1	YO	0.40	0/2253	0.65	0/3064
1	Z4	0.39	0/2251	0.65	1/3061 (0.0%)
1	Z9	0.39	0/2251	0.65	1/3061 (0.0%)
1	ZE	0.39	0/2251	0.65	1/3061 (0.0%)
1	ZJ	0.39	0/2251	0.65	1/3061 (0.0%)
1	ZO	0.39	0/2251	0.65	1/3061 (0.0%)
2	A1	0.43	0/652	0.65	1/892 (0.1%)
2	A2	0.43	0/652	0.65	1/892 (0.1%)
2	A3	0.43	0/652	0.65	1/892 (0.1%)
2	A6	0.43	0/652	0.65	1/892 (0.1%)
2	A7	0.43	0/652	0.65	1/892 (0.1%)
2	A8	0.43	0/652	0.65	1/892 (0.1%)
2	AB	0.43	0/652	0.65	1/892 (0.1%)
2	AC	0.43	0/652	0.65	1/892 (0.1%)
2	AD	0.43	0/652	0.65	1/892 (0.1%)
2	AG	0.43	0/652	0.65	1/892 (0.1%)
2	AH	0.43	0/652	0.65	1/892 (0.1%)
2	AI	0.43	0/652	0.65	1/892 (0.1%)
2	AL	0.43	0/652	0.65	1/892 (0.1%)
2	AM	0.43	0/652	0.65	1/892 (0.1%)
2	AN	0.43	0/652	0.65	1/892 (0.1%)
2	B2	0.43	0/652	0.65	1/892 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	B3	0.43	0/652	0.65	1/892 (0.1%)
2	B7	0.43	0/652	0.65	1/892 (0.1%)
2	B8	0.43	0/652	0.65	1/892 (0.1%)
2	BC	0.43	0/652	0.65	1/892 (0.1%)
2	BD	0.43	0/652	0.65	1/892 (0.1%)
2	BH	0.43	0/652	0.65	1/892 (0.1%)
2	BI	0.43	0/652	0.65	1/892 (0.1%)
2	BM	0.43	0/652	0.65	1/892 (0.1%)
2	BN	0.43	0/652	0.65	1/892 (0.1%)
2	C2	0.43	0/652	0.65	1/892 (0.1%)
2	C3	0.43	0/652	0.65	1/892 (0.1%)
2	C7	0.43	0/652	0.65	1/892 (0.1%)
2	C8	0.43	0/652	0.65	1/892 (0.1%)
2	CC	0.43	0/652	0.65	1/892 (0.1%)
2	CD	0.43	0/652	0.65	1/892 (0.1%)
2	CH	0.43	0/652	0.65	1/892 (0.1%)
2	CI	0.43	0/652	0.65	1/892 (0.1%)
2	CM	0.43	0/652	0.65	1/892 (0.1%)
2	CN	0.43	0/652	0.65	1/892 (0.1%)
2	D2	0.43	0/652	0.65	1/892 (0.1%)
2	D3	0.43	0/652	0.65	1/892 (0.1%)
2	D7	0.43	0/652	0.65	1/892 (0.1%)
2	D8	0.43	0/652	0.65	1/892 (0.1%)
2	DC	0.43	0/652	0.65	1/892 (0.1%)
2	DD	0.43	0/652	0.65	1/892 (0.1%)
2	DH	0.43	0/652	0.65	1/892 (0.1%)
2	DI	0.43	0/652	0.65	1/892 (0.1%)
2	DM	0.43	0/652	0.65	1/892 (0.1%)
2	DN	0.43	0/652	0.65	1/892 (0.1%)
2	E2	0.43	0/652	0.65	1/892 (0.1%)
2	E3	0.43	0/652	0.65	1/892 (0.1%)
2	E7	0.43	0/652	0.65	1/892 (0.1%)
2	E8	0.43	0/652	0.65	1/892 (0.1%)
2	EC	0.43	0/652	0.65	1/892 (0.1%)
2	ED	0.43	0/652	0.65	1/892 (0.1%)
2	EH	0.43	0/652	0.65	1/892 (0.1%)
2	EI	0.43	0/652	0.65	1/892 (0.1%)
2	EM	0.43	0/652	0.65	1/892 (0.1%)
2	EN	0.43	0/652	0.65	1/892 (0.1%)
3	F2	0.40	0/61	1.43	2/81 (2.5%)
3	F3	0.41	0/61	1.42	2/81 (2.5%)
3	F7	0.40	0/61	1.43	2/81 (2.5%)
3	F8	0.41	0/61	1.42	2/81 (2.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	FC	0.40	0/61	1.43	2/81 (2.5%)
3	FD	0.40	0/61	1.42	2/81 (2.5%)
3	FH	0.40	0/61	1.43	2/81 (2.5%)
3	FI	0.41	0/61	1.42	2/81 (2.5%)
3	FM	0.40	0/61	1.42	2/81 (2.5%)
3	FN	0.40	0/61	1.42	2/81 (2.5%)
4	2A	0.58	1/1482 (0.1%)	0.81	3/2021 (0.1%)
4	2B	0.54	0/1485	0.74	1/2024 (0.0%)
4	2C	0.58	1/1482 (0.1%)	0.81	3/2021 (0.1%)
4	2D	0.54	0/1488	0.74	1/2028 (0.0%)
4	2E	0.58	1/1482 (0.1%)	0.81	3/2021 (0.1%)
4	2F	0.54	0/1488	0.74	1/2028 (0.0%)
4	2G	0.58	1/1479 (0.1%)	0.81	3/2018 (0.1%)
4	2H	0.54	0/1485	0.74	1/2025 (0.0%)
4	2I	0.58	1/1482 (0.1%)	0.81	3/2021 (0.1%)
4	2J	0.54	0/1488	0.74	1/2028 (0.0%)
4	2K	0.57	1/1479 (0.1%)	0.81	3/2016 (0.1%)
4	2L	0.54	0/1488	0.74	1/2028 (0.0%)
5	1A	0.50	0/2785	0.66	2/3794 (0.1%)
5	1B	0.49	0/2794	0.66	2/3804 (0.1%)
5	1C	0.50	0/2782	0.66	2/3790 (0.1%)
5	1D	0.49	0/2791	0.66	2/3801 (0.1%)
5	1E	0.50	0/2788	0.66	2/3797 (0.1%)
5	1F	0.49	0/2788	0.66	2/3797 (0.1%)
5	1G	0.50	0/2794	0.65	2/3804 (0.1%)
5	1H	0.49	0/2788	0.66	2/3797 (0.1%)
5	1I	0.50	0/2788	0.66	2/3797 (0.1%)
5	1J	0.49	0/2788	0.66	2/3797 (0.1%)
5	1K	0.50	0/2788	0.66	2/3797 (0.1%)
5	1L	0.49	0/2788	0.66	2/3797 (0.1%)
6	4A	0.52	0/982	0.76	3/1337 (0.2%)
6	4B	0.52	0/982	0.76	3/1337 (0.2%)
6	4C	0.52	0/982	0.76	3/1337 (0.2%)
6	4D	0.52	0/982	0.76	3/1337 (0.2%)
6	4E	0.52	0/982	0.76	3/1337 (0.2%)
6	4F	0.52	0/982	0.76	3/1337 (0.2%)
7	3A	0.57	0/875	0.69	0/1182
7	3B	0.57	0/875	0.70	0/1182
7	3C	0.57	0/875	0.69	0/1182
7	3D	0.57	0/875	0.69	0/1182
7	3E	0.57	0/875	0.69	0/1182
7	3F	0.57	0/875	0.69	0/1182
8	50	0.45	0/987	0.75	2/1332 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	51	0.45	0/987	0.75	2/1332 (0.2%)
8	52	0.44	0/987	0.75	2/1332 (0.2%)
8	53	0.45	0/987	0.75	2/1332 (0.2%)
8	5A	0.44	0/987	0.74	2/1332 (0.2%)
8	5B	0.44	0/987	0.74	2/1332 (0.2%)
8	5C	0.44	0/987	0.74	2/1332 (0.2%)
8	5D	0.44	0/987	0.74	2/1332 (0.2%)
8	5E	0.44	0/987	0.74	2/1332 (0.2%)
8	5F	0.44	0/987	0.74	2/1332 (0.2%)
8	5G	0.45	0/987	0.75	2/1332 (0.2%)
8	5H	0.45	0/987	0.75	2/1332 (0.2%)
8	5I	0.45	0/987	0.75	2/1332 (0.2%)
8	5J	0.45	0/987	0.75	2/1332 (0.2%)
8	5K	0.45	0/987	0.75	2/1332 (0.2%)
8	5L	0.45	0/987	0.75	2/1332 (0.2%)
8	5M	0.44	0/987	0.75	2/1332 (0.2%)
8	5N	0.45	0/987	0.75	2/1332 (0.2%)
8	5O	0.44	0/987	0.75	2/1332 (0.2%)
8	5P	0.45	0/987	0.75	2/1332 (0.2%)
8	5Q	0.44	0/987	0.75	2/1332 (0.2%)
8	5R	0.45	0/987	0.75	2/1332 (0.2%)
8	5S	0.44	0/987	0.75	2/1332 (0.2%)
8	5T	0.44	0/987	0.75	2/1332 (0.2%)
8	5U	0.44	0/987	0.75	2/1332 (0.2%)
8	5V	0.44	0/987	0.75	2/1332 (0.2%)
8	5W	0.44	0/987	0.75	2/1332 (0.2%)
8	5X	0.44	0/987	0.75	2/1332 (0.2%)
8	5Y	0.44	0/987	0.75	2/1332 (0.2%)
8	5Z	0.45	0/987	0.75	2/1332 (0.2%)
9	7A	0.51	0/2222	0.73	3/3010 (0.1%)
9	7B	0.51	0/2222	0.73	3/3010 (0.1%)
9	7C	0.51	0/2222	0.73	2/3010 (0.1%)
10	8A	0.53	0/3292	0.68	1/4459 (0.0%)
10	8B	0.53	0/3292	0.68	1/4459 (0.0%)
10	8C	0.53	0/3292	0.68	1/4459 (0.0%)
11	6A	0.29	0/1085	0.53	0/1472
11	6B	0.29	0/1085	0.54	0/1472
11	6C	0.29	0/1085	0.53	0/1472
11	6D	0.29	0/1085	0.54	0/1472
11	6E	0.29	0/1085	0.53	0/1472
11	6F	0.29	0/1085	0.54	0/1472
All	All	0.44	11/475156 (0.0%)	0.68	432/646033 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2C	114	PRO	N-CD	-5.97	1.39	1.47
4	2I	114	PRO	N-CD	-5.97	1.39	1.47
4	2A	114	PRO	N-CD	-5.93	1.39	1.47
4	2E	114	PRO	N-CD	-5.93	1.39	1.47
4	2G	114	PRO	N-CD	-5.92	1.39	1.47

The worst 5 of 432 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AK	217	ASP	CB-CG-OD1	8.09	125.58	118.30
1	AF	217	ASP	CB-CG-OD1	8.09	125.58	118.30
1	A5	217	ASP	CB-CG-OD1	8.07	125.56	118.30
1	AP	217	ASP	CB-CG-OD1	8.07	125.56	118.30
1	AA	217	ASP	CB-CG-OD1	8.06	125.55	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A4	2173	0	2142	38	0
1	A5	2199	0	2160	77	0
1	A9	2173	0	2142	38	0
1	AA	2205	0	2172	66	0
1	AE	2173	0	2142	39	0
1	AF	2209	0	2176	57	0
1	AJ	2173	0	2142	42	0
1	AK	2209	0	2176	71	0
1	AO	2173	0	2142	39	0
1	AP	2201	0	2168	92	0
1	B4	2209	0	2176	38	0
1	B5	2009	0	1979	72	0
1	B9	2209	0	2176	39	0
1	BA	2014	0	1984	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BE	2209	0	2176	39	0
1	BF	2015	0	1991	71	0
1	BJ	2209	0	2176	37	0
1	BK	2009	0	1977	80	0
1	BO	2209	0	2176	35	0
1	BP	2009	0	1982	74	0
1	C4	2209	0	2176	38	0
1	C5	2209	0	2176	38	0
1	C9	2209	0	2176	41	0
1	CA	2209	0	2176	35	0
1	CE	2209	0	2176	42	0
1	CF	2209	0	2176	37	0
1	CJ	2209	0	2176	43	0
1	CK	2209	0	2176	38	0
1	CO	2209	0	2176	39	0
1	CP	2209	0	2176	37	0
1	D4	2209	0	2176	49	0
1	D9	2209	0	2176	50	0
1	DE	2209	0	2176	50	0
1	DJ	2209	0	2176	50	0
1	DO	2209	0	2176	47	0
1	E4	2209	0	2176	56	0
1	E9	2209	0	2176	56	0
1	EE	2209	0	2176	56	0
1	EJ	2209	0	2176	55	0
1	EO	2209	0	2176	55	0
1	F4	2209	0	2176	57	0
1	F9	2209	0	2176	60	0
1	FE	2209	0	2176	58	0
1	FJ	2209	0	2176	57	0
1	FO	2209	0	2176	58	0
1	G4	2209	0	2176	44	0
1	G9	2209	0	2176	45	0
1	GE	2209	0	2176	45	0
1	GJ	2209	0	2176	43	0
1	GO	2209	0	2176	47	0
1	H4	2173	0	2142	35	0
1	H9	2173	0	2142	35	0
1	HE	2173	0	2142	37	0
1	HJ	2173	0	2142	36	0
1	HO	2173	0	2142	34	0
1	I4	2173	0	2142	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I9	2173	0	2142	50	0
1	IE	2173	0	2142	53	0
1	IJ	2173	0	2142	53	0
1	IO	2173	0	2142	54	0
1	J4	2173	0	2142	54	0
1	J9	2173	0	2142	51	0
1	JE	2173	0	2142	52	0
1	JJ	2173	0	2142	54	0
1	JO	2173	0	2142	56	0
1	K4	2173	0	2142	47	0
1	K9	2173	0	2142	50	0
1	KE	2173	0	2142	46	0
1	KJ	2173	0	2142	45	0
1	KO	2173	0	2142	46	0
1	L4	2173	0	2142	50	0
1	L9	2173	0	2142	49	0
1	LE	2173	0	2142	49	0
1	LJ	2173	0	2142	44	0
1	LO	2173	0	2142	48	0
1	M4	2209	0	2176	43	0
1	M9	2209	0	2176	42	0
1	ME	2209	0	2176	41	0
1	MJ	2209	0	2176	47	0
1	MO	2209	0	2176	48	0
1	N4	2209	0	2176	45	0
1	N9	2209	0	2176	46	0
1	NE	2209	0	2176	46	0
1	NJ	2209	0	2176	45	0
1	NO	2209	0	2176	45	0
1	O4	2209	0	2176	46	0
1	O9	2209	0	2176	47	0
1	OE	2209	0	2176	49	0
1	OJ	2209	0	2176	45	0
1	OO	2209	0	2176	46	0
1	P4	2209	0	2176	41	0
1	P9	2209	0	2176	43	0
1	PE	2209	0	2176	44	0
1	PJ	2209	0	2176	41	0
1	PO	2209	0	2176	42	0
1	Q4	2209	0	2176	45	0
1	Q9	2209	0	2176	46	0
1	QE	2209	0	2176	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QJ	2209	0	2176	45	0
1	QO	2209	0	2176	49	0
1	R4	2209	0	2176	38	0
1	R9	2209	0	2176	39	0
1	RE	2209	0	2176	40	0
1	RJ	2209	0	2176	40	0
1	RO	2209	0	2176	42	0
1	S4	2173	0	2142	47	0
1	S9	2173	0	2142	46	0
1	SE	2173	0	2142	48	0
1	SJ	2173	0	2142	48	0
1	SO	2173	0	2142	49	0
1	T4	2173	0	2142	42	0
1	T9	2173	0	2142	44	0
1	TE	2173	0	2142	41	0
1	TJ	2173	0	2142	39	0
1	TO	2173	0	2142	41	0
1	U4	2173	0	2142	41	0
1	U9	2173	0	2142	45	0
1	UE	2173	0	2142	41	0
1	UJ	2173	0	2142	40	0
1	UO	2173	0	2142	44	0
1	V4	2173	0	2142	45	0
1	V9	2173	0	2142	42	0
1	VE	2173	0	2142	46	0
1	VJ	2173	0	2142	43	0
1	VO	2173	0	2142	44	0
1	W4	2173	0	2142	49	0
1	W9	2173	0	2142	48	0
1	WE	2173	0	2142	47	0
1	WJ	2173	0	2142	49	0
1	WO	2173	0	2142	47	0
1	X4	2209	0	2176	33	0
1	X9	2209	0	2176	31	0
1	XE	2209	0	2176	33	0
1	XJ	2209	0	2176	33	0
1	XO	2209	0	2176	30	0
1	Y4	2209	0	2176	36	0
1	Y9	2209	0	2176	38	0
1	YE	2209	0	2176	34	0
1	YJ	2209	0	2176	35	0
1	YO	2209	0	2176	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z4	2207	0	2171	50	0
1	Z9	2207	0	2171	45	0
1	ZE	2207	0	2171	42	0
1	ZJ	2207	0	2171	43	0
1	ZO	2207	0	2171	50	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	27	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	23	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	18	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	19	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	72	0
4	2B	1453	0	1481	75	0
4	2C	1450	0	1474	50	0
4	2D	1456	0	1490	69	0
4	2E	1450	0	1474	65	0
4	2F	1456	0	1490	76	0
4	2G	1447	0	1467	58	0
4	2H	1453	0	1483	72	0
4	2I	1450	0	1474	70	0
4	2J	1456	0	1490	67	0
4	2K	1448	0	1468	56	0
4	2L	1456	0	1490	88	0
5	1A	2714	0	2688	50	0
5	1B	2723	0	2706	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	1C	2711	0	2684	44	0
5	1D	2720	0	2695	58	0
5	1E	2717	0	2695	63	0
5	1F	2717	0	2695	55	0
5	1G	2723	0	2706	65	0
5	1H	2717	0	2695	72	0
5	1I	2717	0	2695	72	0
5	1J	2717	0	2695	91	0
5	1K	2717	0	2695	93	0
5	1L	2717	0	2694	71	0
6	4A	968	0	987	46	0
6	4B	968	0	987	50	0
6	4C	968	0	987	52	0
6	4D	968	0	987	51	0
6	4E	968	0	987	46	0
6	4F	968	0	987	44	0
7	3A	859	0	861	39	0
7	3B	859	0	861	45	0
7	3C	859	0	861	49	0
7	3D	859	0	861	47	0
7	3E	859	0	861	43	0
7	3F	859	0	861	38	0
8	50	972	0	938	129	0
8	51	972	0	938	100	0
8	52	972	0	938	62	0
8	53	972	0	938	58	0
8	5A	972	0	938	88	0
8	5B	972	0	938	98	0
8	5C	972	0	938	105	0
8	5D	972	0	938	98	0
8	5E	972	0	938	89	0
8	5F	972	0	938	83	0
8	5G	972	0	938	49	0
8	5H	972	0	938	44	0
8	5I	972	0	938	41	0
8	5J	972	0	938	44	0
8	5K	972	0	938	55	0
8	5L	972	0	938	57	0
8	5M	972	0	938	99	0
8	5N	972	0	938	86	0
8	5O	972	0	938	88	0
8	5P	972	0	938	107	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	5Q	972	0	938	126	0
8	5R	972	0	938	119	0
8	5S	972	0	938	123	0
8	5T	972	0	938	147	0
8	5U	972	0	938	179	0
8	5V	972	0	938	229	0
8	5W	972	0	938	246	0
8	5X	972	0	938	173	0
8	5Y	972	0	938	81	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	66	0
10	8A	3246	0	3223	95	0
10	8B	3246	0	3223	96	0
10	8C	3246	0	3223	95	0
11	6A	1056	0	1000	69	0
11	6B	1056	0	1000	71	0
11	6C	1056	0	1000	71	0
11	6D	1056	0	1000	68	0
11	6E	1056	0	1000	71	0
11	6F	1056	0	1000	70	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	10374	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 10374 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: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
1:AP:126:VAL:HG23	5:1K:161:GLY:C	1.27	1.55

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A4	287/385 (74%)	258 (90%)	28 (10%)	1 (0%)	41	76
1	A5	295/385 (77%)	273 (92%)	21 (7%)	1 (0%)	41	76
1	A9	287/385 (74%)	258 (90%)	28 (10%)	1 (0%)	41	76
1	AA	295/385 (77%)	273 (92%)	21 (7%)	1 (0%)	41	76
1	AE	287/385 (74%)	258 (90%)	28 (10%)	1 (0%)	41	76
1	AF	295/385 (77%)	273 (92%)	21 (7%)	1 (0%)	41	76
1	AJ	287/385 (74%)	258 (90%)	28 (10%)	1 (0%)	41	76
1	AK	295/385 (77%)	273 (92%)	21 (7%)	1 (0%)	41	76
1	AO	287/385 (74%)	258 (90%)	28 (10%)	1 (0%)	41	76
1	AP	295/385 (77%)	273 (92%)	21 (7%)	1 (0%)	41	76
1	B4	295/385 (77%)	264 (90%)	30 (10%)	1 (0%)	41	76
1	B5	267/385 (69%)	242 (91%)	22 (8%)	3 (1%)	14	52
1	B9	295/385 (77%)	264 (90%)	30 (10%)	1 (0%)	41	76
1	BA	267/385 (69%)	242 (91%)	22 (8%)	3 (1%)	14	52
1	BE	295/385 (77%)	264 (90%)	30 (10%)	1 (0%)	41	76
1	BF	267/385 (69%)	242 (91%)	22 (8%)	3 (1%)	14	52
1	BJ	295/385 (77%)	264 (90%)	30 (10%)	1 (0%)	41	76
1	BK	267/385 (69%)	242 (91%)	22 (8%)	3 (1%)	14	52
1	BO	295/385 (77%)	264 (90%)	30 (10%)	1 (0%)	41	76
1	BP	267/385 (69%)	242 (91%)	22 (8%)	3 (1%)	14	52
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%)	41	76
1	E9	295/385 (77%)	258 (88%)	36 (12%)	1 (0%)	41	76
1	EE	295/385 (77%)	258 (88%)	36 (12%)	1 (0%)	41	76
1	EJ	295/385 (77%)	258 (88%)	36 (12%)	1 (0%)	41	76
1	EO	295/385 (77%)	258 (88%)	36 (12%)	1 (0%)	41	76
1	F4	295/385 (77%)	264 (90%)	29 (10%)	2 (1%)	22	62
1	F9	295/385 (77%)	264 (90%)	29 (10%)	2 (1%)	22	62
1	FE	295/385 (77%)	264 (90%)	29 (10%)	2 (1%)	22	62
1	FJ	295/385 (77%)	264 (90%)	29 (10%)	2 (1%)	22	62
1	FO	295/385 (77%)	264 (90%)	29 (10%)	2 (1%)	22	62
1	G4	295/385 (77%)	263 (89%)	31 (10%)	1 (0%)	41	76
1	G9	295/385 (77%)	263 (89%)	31 (10%)	1 (0%)	41	76
1	GE	295/385 (77%)	263 (89%)	31 (10%)	1 (0%)	41	76
1	GJ	295/385 (77%)	263 (89%)	31 (10%)	1 (0%)	41	76
1	GO	295/385 (77%)	263 (89%)	31 (10%)	1 (0%)	41	76
1	H4	287/385 (74%)	252 (88%)	34 (12%)	1 (0%)	41	76
1	H9	287/385 (74%)	252 (88%)	34 (12%)	1 (0%)	41	76
1	HE	287/385 (74%)	253 (88%)	33 (12%)	1 (0%)	41	76
1	HJ	287/385 (74%)	252 (88%)	34 (12%)	1 (0%)	41	76
1	HO	287/385 (74%)	252 (88%)	34 (12%)	1 (0%)	41	76
1	I4	287/385 (74%)	251 (88%)	35 (12%)	1 (0%)	41	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I9	287/385 (74%)	250 (87%)	36 (12%)	1 (0%)	41	76
1	IE	287/385 (74%)	250 (87%)	36 (12%)	1 (0%)	41	76
1	IJ	287/385 (74%)	251 (88%)	35 (12%)	1 (0%)	41	76
1	IO	287/385 (74%)	250 (87%)	36 (12%)	1 (0%)	41	76
1	J4	287/385 (74%)	256 (89%)	29 (10%)	2 (1%)	22	62
1	J9	287/385 (74%)	256 (89%)	29 (10%)	2 (1%)	22	62
1	JE	287/385 (74%)	256 (89%)	29 (10%)	2 (1%)	22	62
1	JJ	287/385 (74%)	256 (89%)	29 (10%)	2 (1%)	22	62
1	JO	287/385 (74%)	256 (89%)	29 (10%)	2 (1%)	22	62
1	K4	287/385 (74%)	246 (86%)	40 (14%)	1 (0%)	41	76
1	K9	287/385 (74%)	247 (86%)	39 (14%)	1 (0%)	41	76
1	KE	287/385 (74%)	246 (86%)	40 (14%)	1 (0%)	41	76
1	KJ	287/385 (74%)	247 (86%)	39 (14%)	1 (0%)	41	76
1	KO	287/385 (74%)	247 (86%)	39 (14%)	1 (0%)	41	76
1	L4	287/385 (74%)	255 (89%)	31 (11%)	1 (0%)	41	76
1	L9	287/385 (74%)	255 (89%)	31 (11%)	1 (0%)	41	76
1	LE	287/385 (74%)	255 (89%)	31 (11%)	1 (0%)	41	76
1	LJ	287/385 (74%)	255 (89%)	31 (11%)	1 (0%)	41	76
1	LO	287/385 (74%)	255 (89%)	31 (11%)	1 (0%)	41	76
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%)	41	76
1	N9	295/385 (77%)	264 (90%)	30 (10%)	1 (0%)	41	76
1	NE	295/385 (77%)	264 (90%)	30 (10%)	1 (0%)	41	76
1	NJ	295/385 (77%)	264 (90%)	30 (10%)	1 (0%)	41	76
1	NO	295/385 (77%)	264 (90%)	30 (10%)	1 (0%)	41	76
1	O4	295/385 (77%)	257 (87%)	37 (12%)	1 (0%)	41	76
1	O9	295/385 (77%)	258 (88%)	36 (12%)	1 (0%)	41	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	OE	295/385 (77%)	257 (87%)	37 (12%)	1 (0%)	41	76
1	OJ	295/385 (77%)	258 (88%)	36 (12%)	1 (0%)	41	76
1	OO	295/385 (77%)	257 (87%)	37 (12%)	1 (0%)	41	76
1	P4	295/385 (77%)	256 (87%)	38 (13%)	1 (0%)	41	76
1	P9	295/385 (77%)	256 (87%)	38 (13%)	1 (0%)	41	76
1	PE	295/385 (77%)	256 (87%)	38 (13%)	1 (0%)	41	76
1	PJ	295/385 (77%)	256 (87%)	38 (13%)	1 (0%)	41	76
1	PO	295/385 (77%)	256 (87%)	38 (13%)	1 (0%)	41	76
1	Q4	295/385 (77%)	260 (88%)	34 (12%)	1 (0%)	41	76
1	Q9	295/385 (77%)	260 (88%)	34 (12%)	1 (0%)	41	76
1	QE	295/385 (77%)	260 (88%)	34 (12%)	1 (0%)	41	76
1	QJ	295/385 (77%)	259 (88%)	35 (12%)	1 (0%)	41	76
1	QO	295/385 (77%)	259 (88%)	35 (12%)	1 (0%)	41	76
1	R4	295/385 (77%)	261 (88%)	33 (11%)	1 (0%)	41	76
1	R9	295/385 (77%)	261 (88%)	33 (11%)	1 (0%)	41	76
1	RE	295/385 (77%)	261 (88%)	33 (11%)	1 (0%)	41	76
1	RJ	295/385 (77%)	261 (88%)	33 (11%)	1 (0%)	41	76
1	RO	295/385 (77%)	261 (88%)	33 (11%)	1 (0%)	41	76
1	S4	287/385 (74%)	257 (90%)	29 (10%)	1 (0%)	41	76
1	S9	287/385 (74%)	257 (90%)	29 (10%)	1 (0%)	41	76
1	SE	287/385 (74%)	257 (90%)	29 (10%)	1 (0%)	41	76
1	SJ	287/385 (74%)	257 (90%)	29 (10%)	1 (0%)	41	76
1	SO	287/385 (74%)	257 (90%)	29 (10%)	1 (0%)	41	76
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%)	41	76
1	U9	287/385 (74%)	253 (88%)	33 (12%)	1 (0%)	41	76
1	UE	287/385 (74%)	253 (88%)	33 (12%)	1 (0%)	41	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	UJ	287/385 (74%)	253 (88%)	33 (12%)	1 (0%)	41	76
1	UO	287/385 (74%)	253 (88%)	33 (12%)	1 (0%)	41	76
1	V4	287/385 (74%)	258 (90%)	28 (10%)	1 (0%)	41	76
1	V9	287/385 (74%)	258 (90%)	28 (10%)	1 (0%)	41	76
1	VE	287/385 (74%)	258 (90%)	28 (10%)	1 (0%)	41	76
1	VJ	287/385 (74%)	258 (90%)	28 (10%)	1 (0%)	41	76
1	VO	287/385 (74%)	258 (90%)	28 (10%)	1 (0%)	41	76
1	W4	287/385 (74%)	251 (88%)	35 (12%)	1 (0%)	41	76
1	W9	287/385 (74%)	251 (88%)	35 (12%)	1 (0%)	41	76
1	WE	287/385 (74%)	252 (88%)	34 (12%)	1 (0%)	41	76
1	WJ	287/385 (74%)	251 (88%)	35 (12%)	1 (0%)	41	76
1	WO	287/385 (74%)	251 (88%)	35 (12%)	1 (0%)	41	76
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%)	29	68

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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%)	29	68
4	2D	190/197 (96%)	164 (86%)	26 (14%)	0	100	100
4	2E	190/197 (96%)	161 (85%)	28 (15%)	1 (0%)	29	68
4	2F	190/197 (96%)	164 (86%)	26 (14%)	0	100	100
4	2G	190/197 (96%)	161 (85%)	28 (15%)	1 (0%)	29	68
4	2H	190/197 (96%)	164 (86%)	26 (14%)	0	100	100
4	2I	190/197 (96%)	161 (85%)	28 (15%)	1 (0%)	29	68
4	2J	190/197 (96%)	164 (86%)	26 (14%)	0	100	100
4	2K	190/197 (96%)	161 (85%)	28 (15%)	1 (0%)	29	68
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%)	47	81
10	8B	431/1304 (33%)	375 (87%)	55 (13%)	1 (0%)	47	81
10	8C	431/1304 (33%)	375 (87%)	55 (13%)	1 (0%)	47	81
11	6A	130/210 (62%)	101 (78%)	29 (22%)	0	100	100
11	6B	130/210 (62%)	102 (78%)	27 (21%)	1 (1%)	19	60
11	6C	130/210 (62%)	101 (78%)	29 (22%)	0	100	100
11	6D	130/210 (62%)	102 (78%)	27 (21%)	1 (1%)	19	60
11	6E	130/210 (62%)	101 (78%)	29 (22%)	0	100	100
11	6F	130/210 (62%)	102 (78%)	27 (21%)	1 (1%)	19	60
All	All	61500/82463 (75%)	54790 (89%)	6573 (11%)	137 (0%)	50	81

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 (i)

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

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A5	215/284 (76%)	211 (98%)	4 (2%)	57	75
1	A9	215/284 (76%)	215 (100%)	0	100	100
1	AA	217/284 (76%)	213 (98%)	4 (2%)	59	77
1	AE	215/284 (76%)	215 (100%)	0	100	100
1	AF	218/284 (77%)	214 (98%)	4 (2%)	59	77
1	AJ	215/284 (76%)	215 (100%)	0	100	100
1	AK	218/284 (77%)	214 (98%)	4 (2%)	59	77
1	AO	215/284 (76%)	215 (100%)	0	100	100
1	AP	216/284 (76%)	212 (98%)	4 (2%)	57	75
1	B4	218/284 (77%)	218 (100%)	0	100	100
1	B5	196/284 (69%)	193 (98%)	3 (2%)	65	80
1	B9	218/284 (77%)	218 (100%)	0	100	100
1	BA	197/284 (69%)	194 (98%)	3 (2%)	65	80
1	BE	218/284 (77%)	218 (100%)	0	100	100
1	BF	197/284 (69%)	194 (98%)	3 (2%)	65	80
1	BJ	218/284 (77%)	218 (100%)	0	100	100
1	BK	196/284 (69%)	193 (98%)	3 (2%)	65	80
1	BO	218/284 (77%)	218 (100%)	0	100	100
1	BP	196/284 (69%)	193 (98%)	3 (2%)	65	80
1	C4	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	C5	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	C9	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	CA	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	CE	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	CF	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	CJ	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	CK	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	CO	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	CP	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	D4	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	D9	218/284 (77%)	217 (100%)	1 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DE	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	DJ	218/284 (77%)	218 (100%)	0	100	100
1	DO	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	E4	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	E9	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	EE	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	EJ	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	EO	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	F4	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	F9	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	FE	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	FJ	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	FO	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	G4	218/284 (77%)	215 (99%)	3 (1%)	67	81
1	G9	218/284 (77%)	215 (99%)	3 (1%)	67	81
1	GE	218/284 (77%)	215 (99%)	3 (1%)	67	81
1	GJ	218/284 (77%)	215 (99%)	3 (1%)	67	81
1	GO	218/284 (77%)	215 (99%)	3 (1%)	67	81
1	H4	215/284 (76%)	214 (100%)	1 (0%)	88	93
1	H9	215/284 (76%)	214 (100%)	1 (0%)	88	93
1	HE	215/284 (76%)	214 (100%)	1 (0%)	88	93
1	HJ	215/284 (76%)	214 (100%)	1 (0%)	88	93
1	HO	215/284 (76%)	214 (100%)	1 (0%)	88	93
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%)	214 (100%)	1 (0%)	88	93
1	K9	215/284 (76%)	214 (100%)	1 (0%)	88	93
1	KE	215/284 (76%)	214 (100%)	1 (0%)	88	93
1	KJ	215/284 (76%)	214 (100%)	1 (0%)	88	93
1	KO	215/284 (76%)	214 (100%)	1 (0%)	88	93
1	L4	215/284 (76%)	215 (100%)	0	100	100
1	L9	215/284 (76%)	215 (100%)	0	100	100
1	LE	215/284 (76%)	215 (100%)	0	100	100
1	LJ	215/284 (76%)	215 (100%)	0	100	100
1	LO	215/284 (76%)	215 (100%)	0	100	100
1	M4	218/284 (77%)	218 (100%)	0	100	100
1	M9	218/284 (77%)	218 (100%)	0	100	100
1	ME	218/284 (77%)	218 (100%)	0	100	100
1	MJ	218/284 (77%)	218 (100%)	0	100	100
1	MO	218/284 (77%)	218 (100%)	0	100	100
1	N4	218/284 (77%)	214 (98%)	4 (2%)	59	77
1	N9	218/284 (77%)	214 (98%)	4 (2%)	59	77
1	NE	218/284 (77%)	214 (98%)	4 (2%)	59	77
1	NJ	218/284 (77%)	214 (98%)	4 (2%)	59	77
1	NO	218/284 (77%)	214 (98%)	4 (2%)	59	77
1	O4	218/284 (77%)	218 (100%)	0	100	100
1	O9	218/284 (77%)	218 (100%)	0	100	100
1	OE	218/284 (77%)	218 (100%)	0	100	100
1	OJ	218/284 (77%)	218 (100%)	0	100	100
1	OO	218/284 (77%)	218 (100%)	0	100	100
1	P4	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	P9	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	PE	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	PJ	218/284 (77%)	217 (100%)	1 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	PO	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	Q4	218/284 (77%)	215 (99%)	3 (1%)	67	81
1	Q9	218/284 (77%)	215 (99%)	3 (1%)	67	81
1	QE	218/284 (77%)	215 (99%)	3 (1%)	67	81
1	QJ	218/284 (77%)	215 (99%)	3 (1%)	67	81
1	QO	218/284 (77%)	215 (99%)	3 (1%)	67	81
1	R4	218/284 (77%)	218 (100%)	0	100	100
1	R9	218/284 (77%)	218 (100%)	0	100	100
1	RE	218/284 (77%)	218 (100%)	0	100	100
1	RJ	218/284 (77%)	218 (100%)	0	100	100
1	RO	218/284 (77%)	218 (100%)	0	100	100
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%)	215 (100%)	0	100	100
1	T9	215/284 (76%)	215 (100%)	0	100	100
1	TE	215/284 (76%)	215 (100%)	0	100	100
1	TJ	215/284 (76%)	215 (100%)	0	100	100
1	TO	215/284 (76%)	215 (100%)	0	100	100
1	U4	215/284 (76%)	215 (100%)	0	100	100
1	U9	215/284 (76%)	215 (100%)	0	100	100
1	UE	215/284 (76%)	215 (100%)	0	100	100
1	UJ	215/284 (76%)	215 (100%)	0	100	100
1	UO	215/284 (76%)	215 (100%)	0	100	100
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%)	215 (100%)	0	100	100
1	W9	215/284 (76%)	215 (100%)	0	100	100
1	WE	215/284 (76%)	215 (100%)	0	100	100
1	WJ	215/284 (76%)	215 (100%)	0	100	100
1	WO	215/284 (76%)	215 (100%)	0	100	100
1	X4	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	X9	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	XE	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	XJ	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	XO	218/284 (77%)	217 (100%)	1 (0%)	88	93
1	Y4	218/284 (77%)	218 (100%)	0	100	100
1	Y9	218/284 (77%)	218 (100%)	0	100	100
1	YE	218/284 (77%)	218 (100%)	0	100	100
1	YJ	218/284 (77%)	218 (100%)	0	100	100
1	YO	218/284 (77%)	218 (100%)	0	100	100
1	Z4	217/284 (76%)	215 (99%)	2 (1%)	78	87
1	Z9	217/284 (76%)	215 (99%)	2 (1%)	78	87
1	ZE	217/284 (76%)	215 (99%)	2 (1%)	78	87
1	ZJ	217/284 (76%)	215 (99%)	2 (1%)	78	87
1	ZO	217/284 (76%)	215 (99%)	2 (1%)	78	87
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%)	136 (99%)	2 (1%)	67	81
4	2B	139/141 (99%)	139 (100%)	0	100	100
4	2C	138/141 (98%)	136 (99%)	2 (1%)	67	81
4	2D	140/141 (99%)	140 (100%)	0	100	100
4	2E	138/141 (98%)	136 (99%)	2 (1%)	67	81
4	2F	140/141 (99%)	140 (100%)	0	100	100
4	2G	137/141 (97%)	135 (98%)	2 (2%)	65	80
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%)	136 (99%)	2 (1%)	67	81
4	2J	140/141 (99%)	140 (100%)	0	100	100
4	2K	137/141 (97%)	135 (98%)	2 (2%)	65	80
4	2L	140/141 (99%)	140 (100%)	0	100	100
5	1A	272/302 (90%)	272 (100%)	0	100	100
5	1B	274/302 (91%)	274 (100%)	0	100	100
5	1C	272/302 (90%)	272 (100%)	0	100	100
5	1D	273/302 (90%)	273 (100%)	0	100	100
5	1E	273/302 (90%)	273 (100%)	0	100	100
5	1F	273/302 (90%)	273 (100%)	0	100	100
5	1G	274/302 (91%)	274 (100%)	0	100	100
5	1H	273/302 (90%)	273 (100%)	0	100	100
5	1I	273/302 (90%)	273 (100%)	0	100	100
5	1J	273/302 (90%)	273 (100%)	0	100	100
5	1K	273/302 (90%)	273 (100%)	0	100	100
5	1L	273/302 (90%)	273 (100%)	0	100	100
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%)	98 (99%)	1 (1%)	76	86
8	5B	99/103 (96%)	98 (99%)	1 (1%)	76	86
8	5C	99/103 (96%)	98 (99%)	1 (1%)	76	86
8	5D	99/103 (96%)	98 (99%)	1 (1%)	76	86
8	5E	99/103 (96%)	98 (99%)	1 (1%)	76	86
8	5F	99/103 (96%)	98 (99%)	1 (1%)	76	86
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%)	208 (98%)	4 (2%)	57	75
9	7B	212/218 (97%)	208 (98%)	4 (2%)	57	75
9	7C	212/218 (97%)	208 (98%)	4 (2%)	57	75
10	8A	310/952 (33%)	301 (97%)	9 (3%)	42	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	8B	310/952 (33%)	301 (97%)	9 (3%)	42	64
10	8C	310/952 (33%)	301 (97%)	9 (3%)	42	64
11	6A	109/169 (64%)	104 (95%)	5 (5%)	27	53
11	6B	109/169 (64%)	102 (94%)	7 (6%)	17	44
11	6C	109/169 (64%)	104 (95%)	5 (5%)	27	53
11	6D	109/169 (64%)	102 (94%)	7 (6%)	17	44
11	6E	109/169 (64%)	104 (95%)	5 (5%)	27	53
11	6F	109/169 (64%)	102 (94%)	7 (6%)	17	44
All	All	46345/61207 (76%)	46113 (100%)	232 (0%)	89	93

5 of 232 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	140	LYS
11	6D	36	ARG
4	2K	71	ARG
10	8B	807	GLN
11	6F	182	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 196 such sidechains are listed below:

Mol	Chain	Res	Type
5	1A	253	GLN
5	1G	253	GLN
4	2B	161	GLN
8	5X	116	HIS
8	5P	116	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	7B	301	-	0,12,12	-	-	-		
12	SF4	7C	301	-	0,12,12	-	-	-		
12	SF4	7A	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	7B	301	-	-	-	0/6/5/5
12	SF4	7C	301	-	-	-	0/6/5/5
12	SF4	7A	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 (i)

There are no chain breaks in this entry.

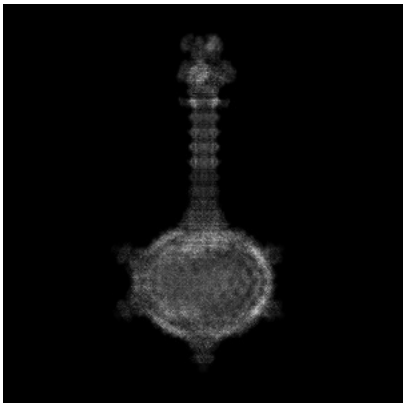
6 Map visualisation (i)

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.

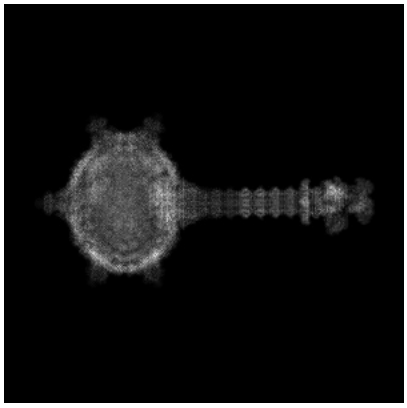
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

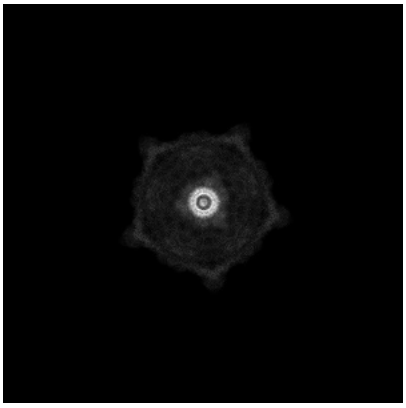
6.1.1 Primary map



X



Y

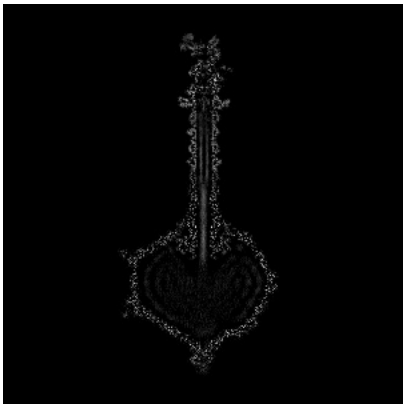


Z

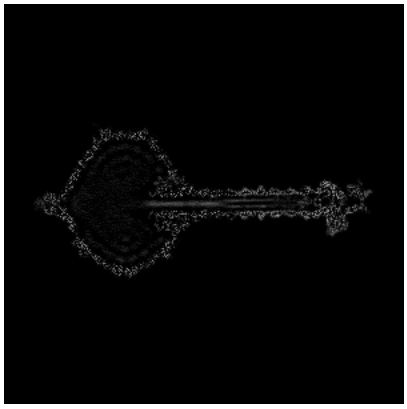
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

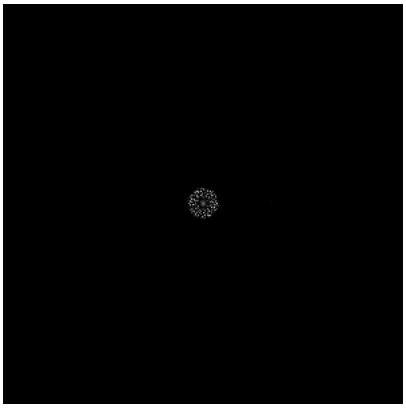
6.2.1 Primary map



X Index: 480



Y Index: 480

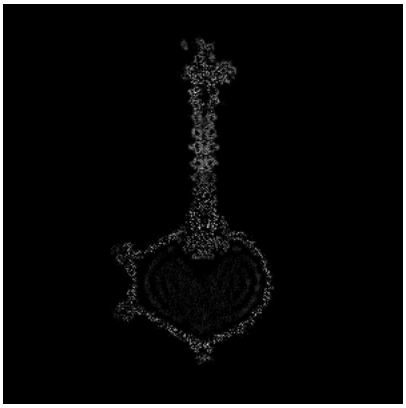


Z Index: 480

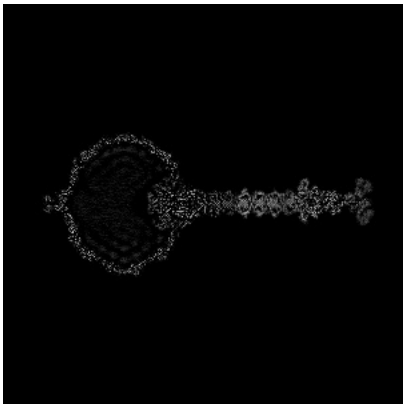
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

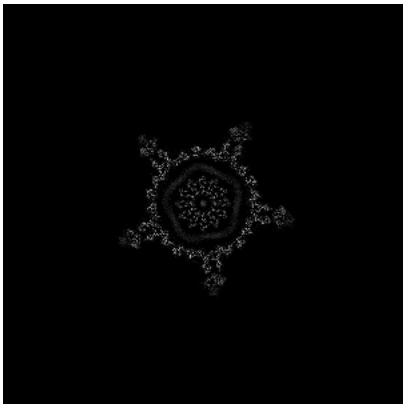
6.3.1 Primary map



X Index: 501



Y Index: 503

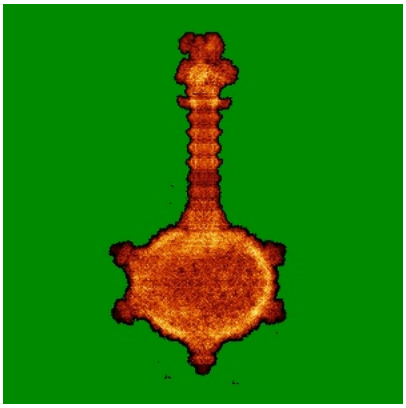


Z Index: 371

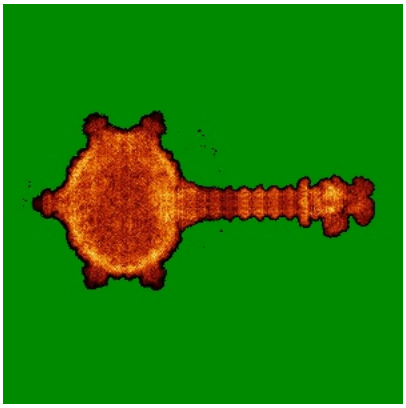
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

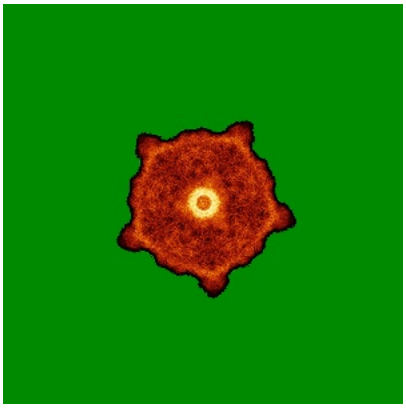
6.4.1 Primary map



X



Y

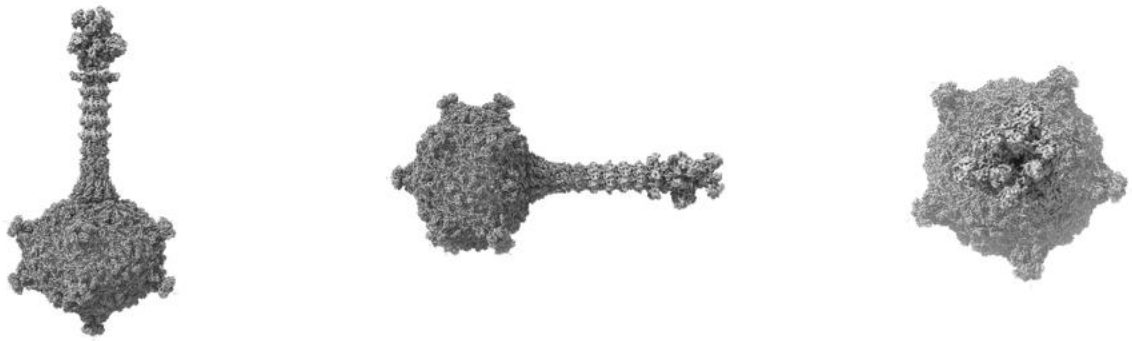


Z

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



X Y Z

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.

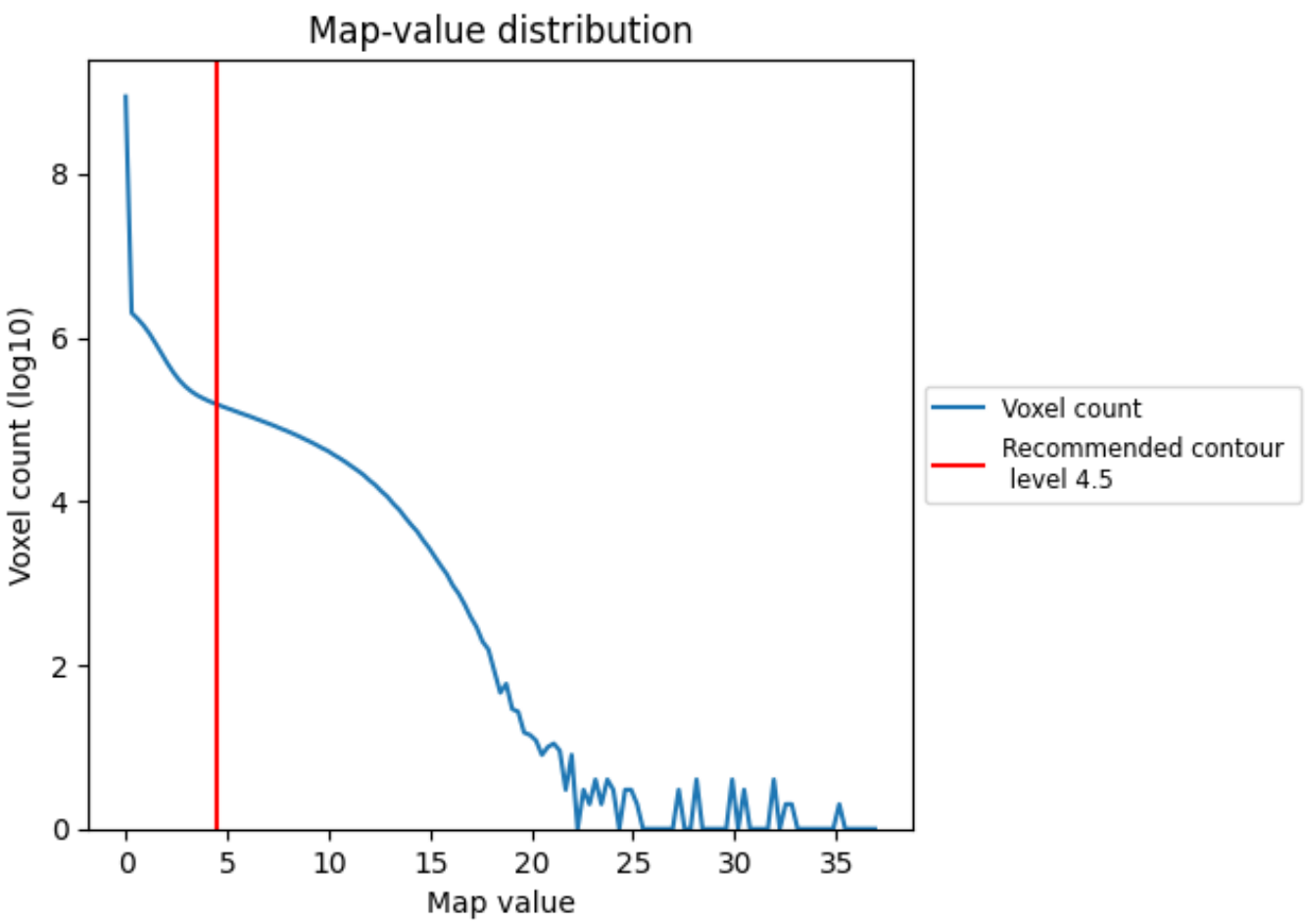
6.6 Mask visualisation (i)

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

7 Map analysis (i)

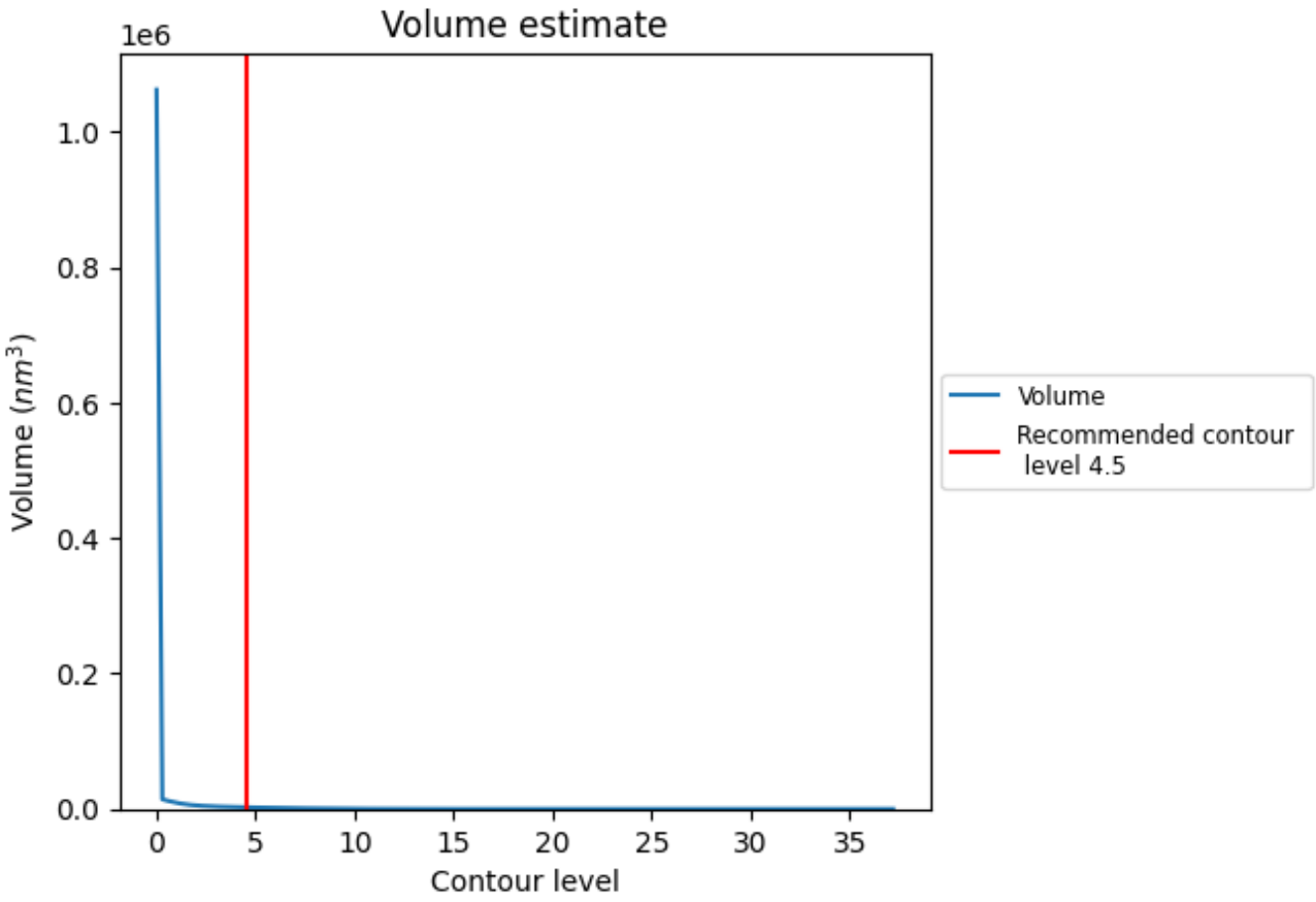
This section contains the results of statistical analysis of the map.

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.

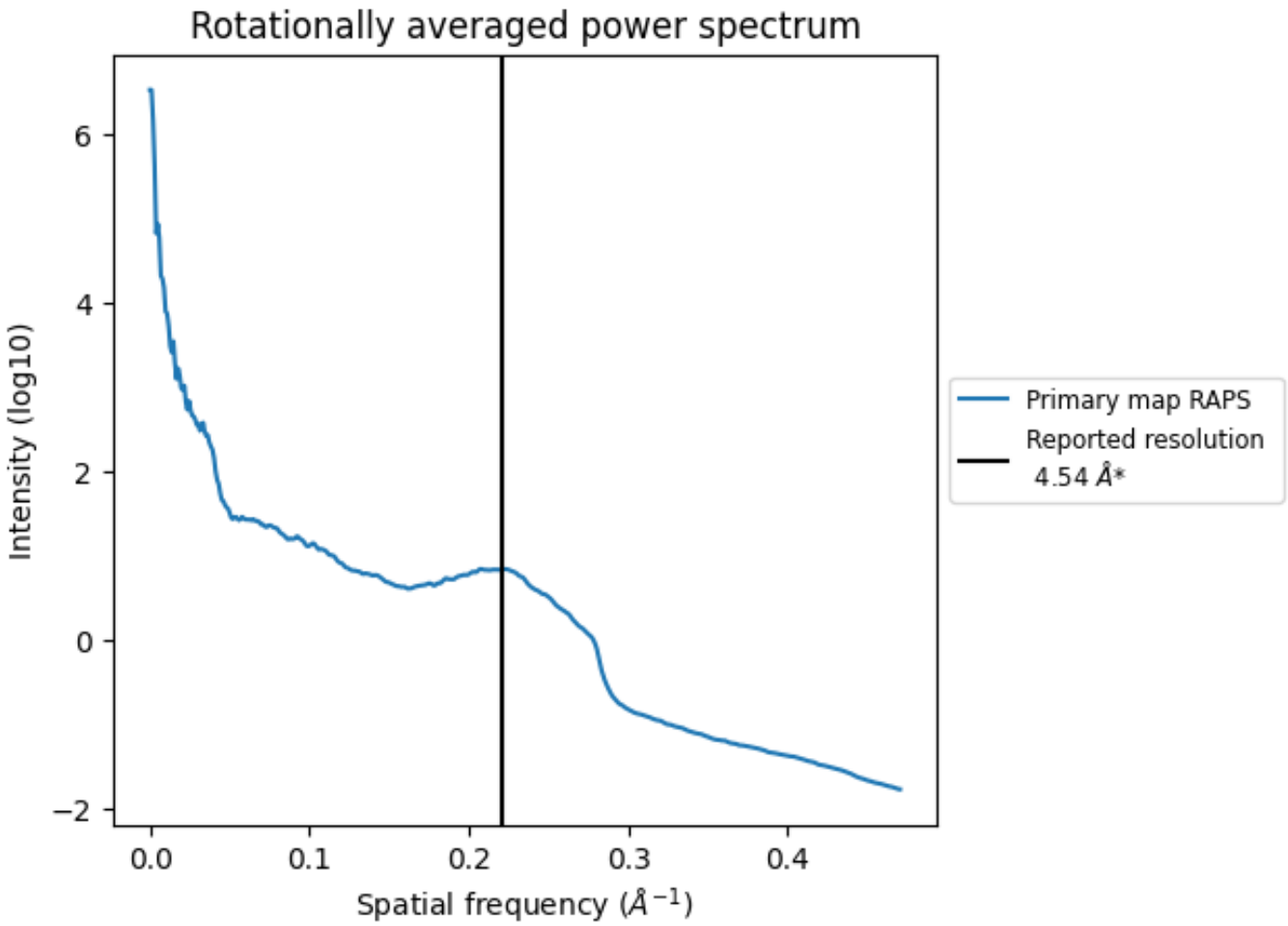
7.2 Volume estimate (i)



The volume at the recommended contour level is 2436 nm^3; 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 (i)

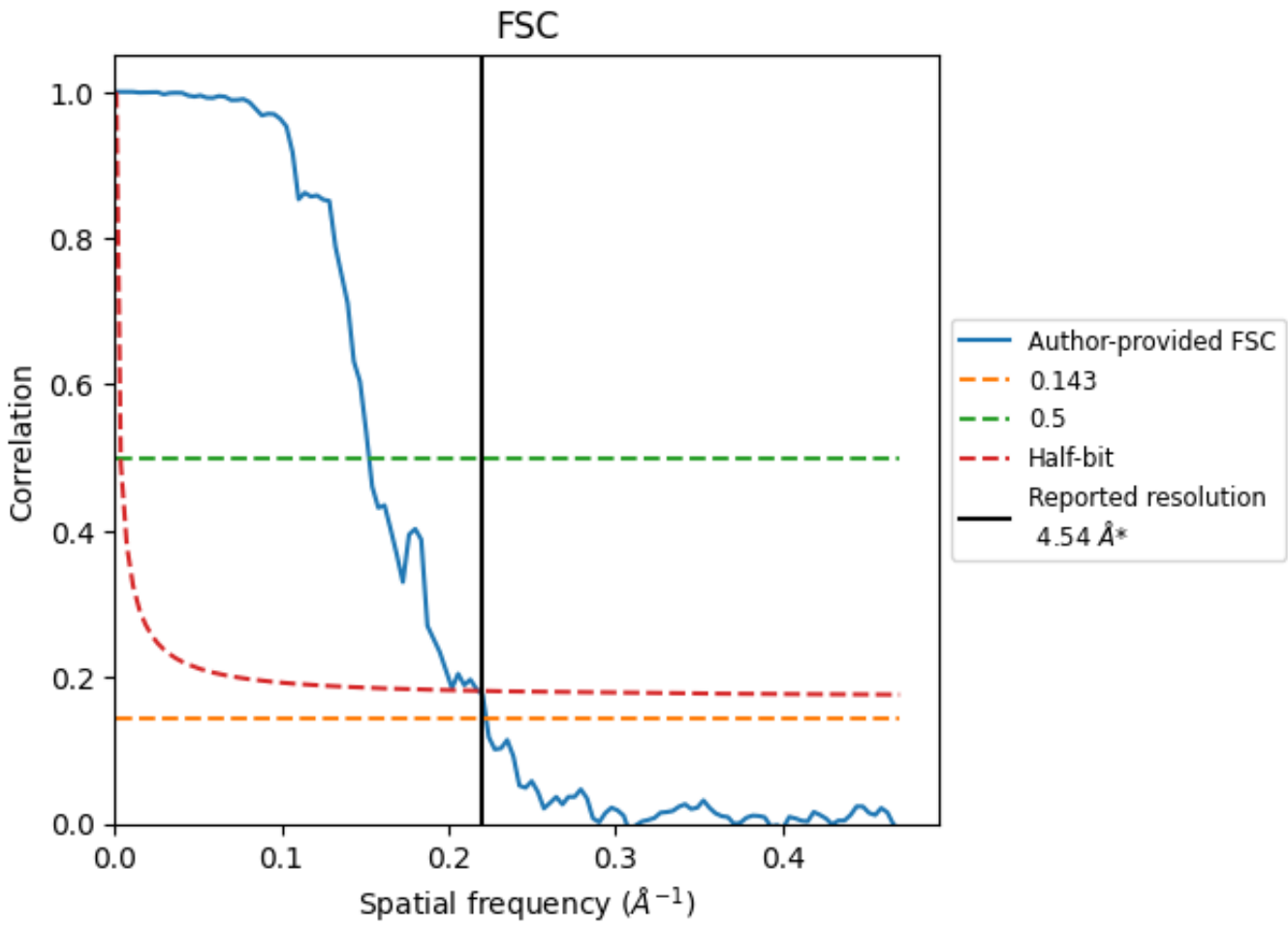


*Reported resolution corresponds to spatial frequency of 0.220 Å^{-1}

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)

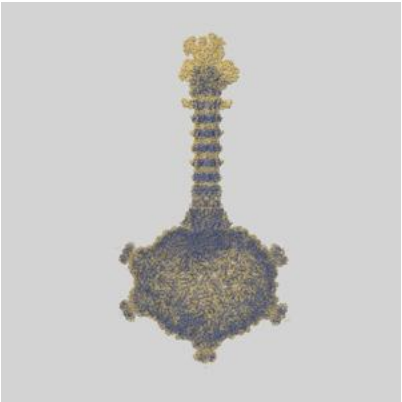
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.54	-	-
Author-provided FSC curve	4.49	6.56	4.59
Unmasked-calculated*	-	-	-

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

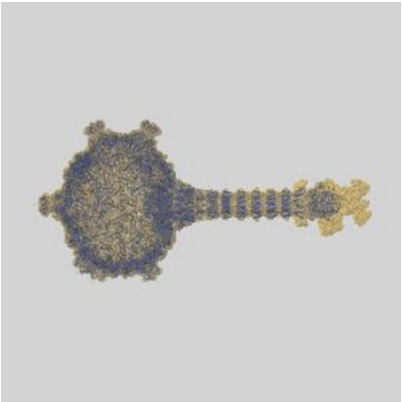
9 Map-model fit (i)

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.

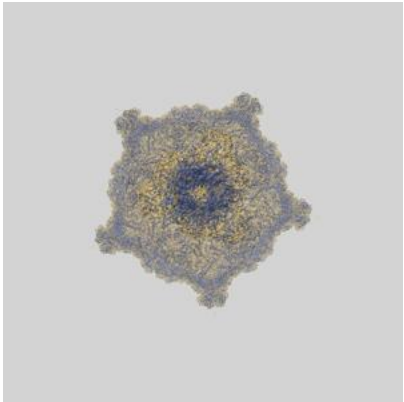
9.1 Map-model overlay (i)



X



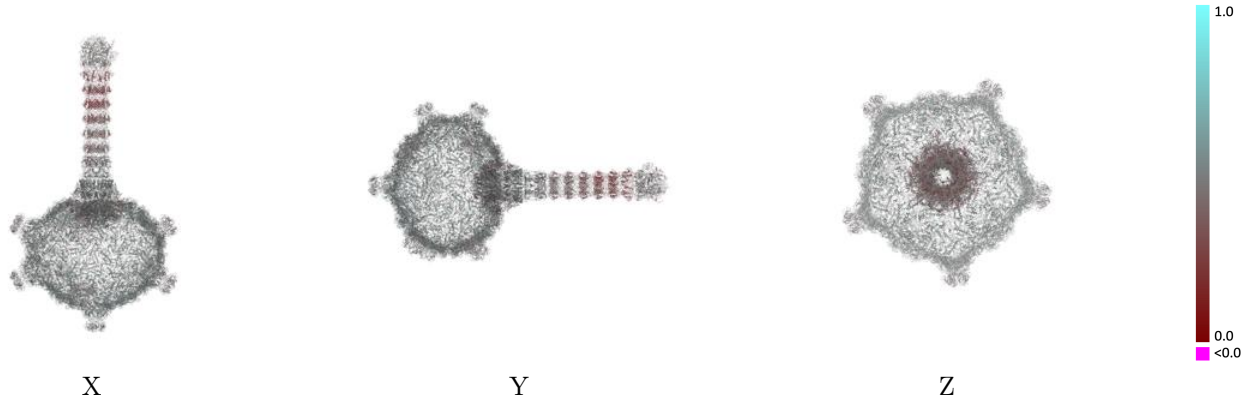
Y



Z

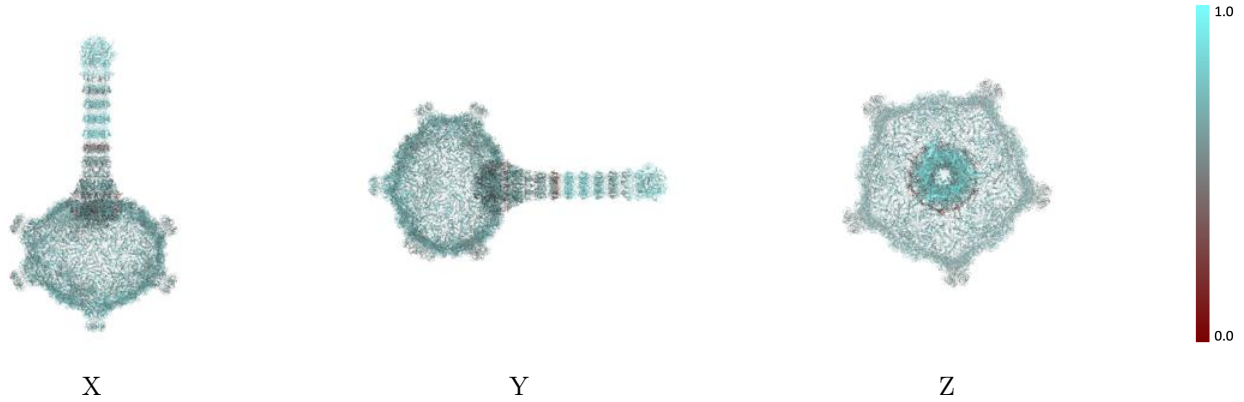
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



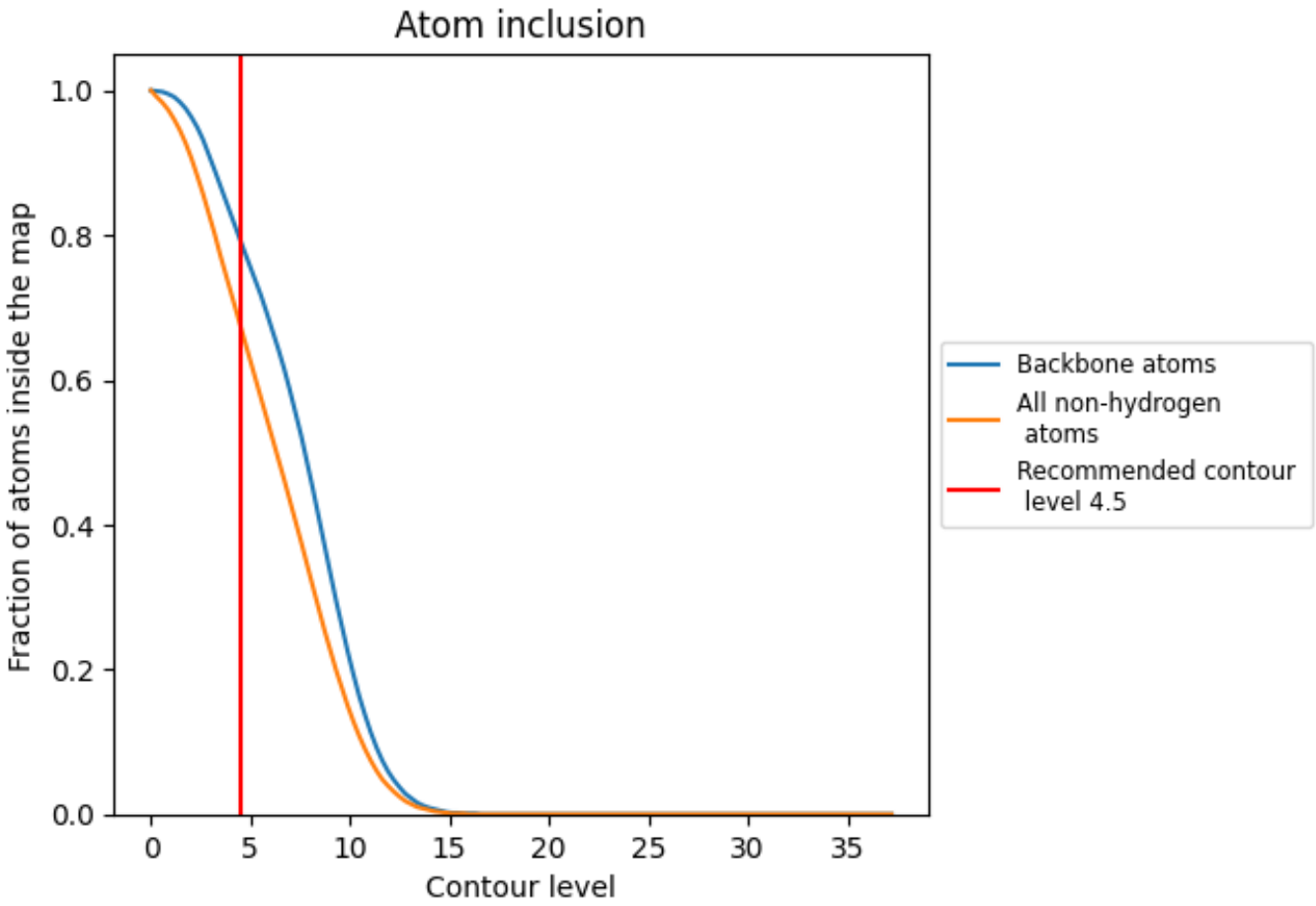
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.5).

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 (i)

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