wwPDB EM Validation Summary Report

Nov 27, 2022 – 02:50 PM EST

PDB ID	:	6V8I
EMDB ID	:	EMD-20872
Title	:	Composite atomic model of the Staphylococcus aureus phage 80alpha baseplate
Authors	:	Kizziah, J.L.; Dokland, T.
Deposited on	:	2019-12-11
Resolution	:	3.70 Å(reported)
Based on initial model	:	5EFV

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:

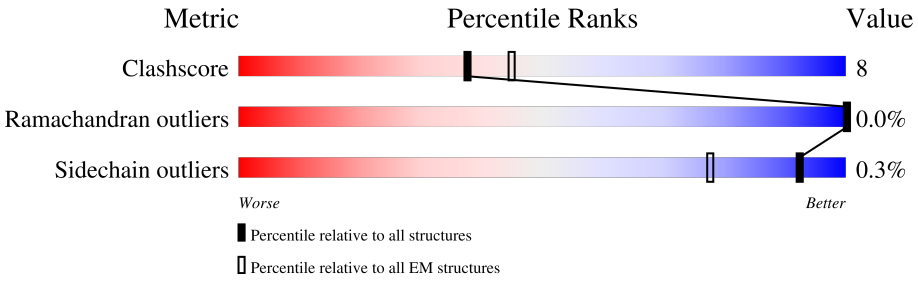
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.70 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	AC	315	82% 18%
1	AD	315	79% 21%
1	BC	315	7% 81% 18%
1	BD	315	80% 20%
1	CC	315	81% 19%
1	CD	315	81% 18%
2	AE	633	17% 54% 7% 39%
2	BE	633	17% 54% 7% 39%

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Mol	Chain	Length	Quality of chain
2	CE	633	18% 54% 8% 39%
3	AF	1154	98%
3	BF	1154	98%
3	CF	1154	98%
4	AJ	607	20% 7% 72%
4	AK	607	24% 7% 69%
4	AL	607	8% 22% 8% 70%
4	BJ	607	20% 8% 72%
4	BK	607	24% 7% 69%
4	BL	607	9% 23% 7% 70%
4	CJ	607	20% 8% 72%
4	CK	607	24% 7% 69%
4	CL	607	8% 23% 7% 70%
4	DJ	607	20% 7% 72%
4	DK	607	5% 24% 7% 69%
4	DL	607	9% 23% 6% 70%
4	EJ	607	20% 8% 72%
4	EK	607	5% 23% 8% 69%
4	EL	607	8% 22% 7% 70%
4	FJ	607	20% 7% 72%
4	FK	607	25% 7% 69%
4	FL	607	8% 23% 6% 70%
5	AM	390	5% 23% 8% 68%
5	AN	390	26% 5% 69%
5	BM	390	6% 24% 8% 68%

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Mol	Chain	Length	Quality of chain
5	BN	390	25% 6% 69%
5	CM	390	5% 23% 8% 68%
5	CN	390	26% 5% 69%
5	DM	390	5% 23% 8% 68%
5	DN	390	24% 7% 69%
5	EM	390	5% 23% 9% 68%
5	EN	390	26% 5% 69%
5	FM	390	6% 23% 8% 68%
5	FN	390	26% 5% 69%
6	AA	193	10% 52% 24% 24%
6	AB	193	5% 58% 28% 14%
6	BA	193	9% 52% 24% 24%
6	BB	193	53% 33% 14%
6	CA	193	9% 57% 19% 24%
6	CB	193	5% 55% 31% 14%
6	DA	193	9% 55% 21% 24%
6	DB	193	5% 52% 34% 14%
6	EA	193	11% 53% 23% 24%
6	EB	193	5% 55% 31% 14%
6	FA	193	8% 51% 25% 24%
6	FB	193	5% 54% 32% 14%
7	AG	636	89% 11%
7	AH	636	86% 14%
7	AI	636	85% 14%
7	BG	636	88% 12%

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Mol	Chain	Length	Quality of chain
7	BH	636	85% 14%
7	BI	636	87% 12%
7	CG	636	88% 12%
7	CH	636	86% 14%
7	CI	636	86% 14%
7	DG	636	89% 11%
7	DH	636	87% 12%
7	DI	636	87% 13%
7	EG	636	88% 11%
7	EH	636	87% 13%
7	EI	636	86% 14%
7	FG	636	88% 11%
7	FH	636	87% 13%
7	FI	636	87% 12%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 171102 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 Distal Tail Protein, gp58.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AC	314	Total	C	N	O	S	0	0
			2601	1666	428	497	10		
1	AD	314	Total	C	N	O	S	0	0
			2601	1666	428	497	10		
1	CC	314	Total	C	N	O	S	0	0
			2601	1666	428	497	10		
1	CD	314	Total	C	N	O	S	0	0
			2601	1666	428	497	10		
1	BC	314	Total	C	N	O	S	0	0
			2601	1666	428	497	10		
1	BD	314	Total	C	N	O	S	0	0
			2601	1666	428	497	10		

- Molecule 2 is a protein called Tail-Associated Lysin, gp59.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AE	387	Total	C	N	O	S	0	0
			3068	1944	518	598	8		
2	CE	387	Total	C	N	O	S	0	0
			3068	1944	518	598	8		
2	BE	387	Total	C	N	O	S	0	0
			3068	1944	518	598	8		

- Molecule 3 is a protein called Tape Measure Protein, gp57.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	CF	20	Total	C	N	O	0	0
			160	98	30	32		
3	BF	20	Total	C	N	O	0	0
			160	98	30	32		
3	AF	20	Total	C	N	O	0	0
			160	98	30	32		

- Molecule 4 is a protein called Fiber Lower, gp62.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BJ	167	Total	C	N	O	S	0	0
			1331	839	223	268	1		
4	BK	189	Total	C	N	O	S	0	0
			1496	941	252	302	1		
4	BL	181	Total	C	N	O	S	0	0
			1430	899	243	287	1		
4	DJ	167	Total	C	N	O	S	0	0
			1331	839	223	268	1		
4	DK	189	Total	C	N	O	S	0	0
			1496	941	252	302	1		
4	DL	181	Total	C	N	O	S	0	0
			1430	899	243	287	1		
4	AJ	167	Total	C	N	O	S	0	0
			1331	839	223	268	1		
4	AK	189	Total	C	N	O	S	0	0
			1496	941	252	302	1		
4	AL	181	Total	C	N	O	S	0	0
			1430	899	243	287	1		
4	FJ	167	Total	C	N	O	S	0	0
			1331	839	223	268	1		
4	FK	189	Total	C	N	O	S	0	0
			1496	941	252	302	1		
4	FL	181	Total	C	N	O	S	0	0
			1430	899	243	287	1		
4	CJ	167	Total	C	N	O	S	0	0
			1331	839	223	268	1		
4	CK	189	Total	C	N	O	S	0	0
			1496	941	252	302	1		
4	CL	181	Total	C	N	O	S	0	0
			1430	899	243	287	1		
4	EJ	167	Total	C	N	O	S	0	0
			1331	839	223	268	1		
4	EK	189	Total	C	N	O	S	0	0
			1496	941	252	302	1		
4	EL	181	Total	C	N	O	S	0	0
			1430	899	243	287	1		

- Molecule 5 is a protein called Fiber Upper, gp68.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BN	121	Total	C	N	O	S	0	0
			981	629	168	180	4		
5	BM	123	Total	C	N	O	S	0	0
			991	634	170	183	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	DN	121	Total	C	N	O	S	0	0
			981	629	168	180	4		
5	DM	123	Total	C	N	O	S	0	0
			991	634	170	183	4		
5	AN	121	Total	C	N	O	S	0	0
			981	629	168	180	4		
5	AM	123	Total	C	N	O	S	0	0
			991	634	170	183	4		
5	FN	121	Total	C	N	O	S	0	0
			981	629	168	180	4		
5	FM	123	Total	C	N	O	S	0	0
			991	634	170	183	4		
5	CN	121	Total	C	N	O	S	0	0
			981	629	168	180	4		
5	CM	123	Total	C	N	O	S	0	0
			991	634	170	183	4		
5	EN	121	Total	C	N	O	S	0	0
			981	629	168	180	4		
5	EM	123	Total	C	N	O	S	0	0
			991	634	170	183	4		

- Molecule 6 is a protein called Major Tail Protein, gp53.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	EB	166	Total	C	N	O	S	0	0
			1320	828	218	269	5		
6	EA	147	Total	C	N	O	S	0	0
			1165	731	190	239	5		
6	BB	166	Total	C	N	O	S	0	0
			1320	828	218	269	5		
6	BA	147	Total	C	N	O	S	0	0
			1165	731	190	239	5		
6	DB	166	Total	C	N	O	S	0	0
			1320	828	218	269	5		
6	DA	147	Total	C	N	O	S	0	0
			1165	731	190	239	5		
6	AB	166	Total	C	N	O	S	0	0
			1320	828	218	269	5		
6	AA	147	Total	C	N	O	S	0	0
			1165	731	190	239	5		
6	FB	166	Total	C	N	O	S	0	0
			1320	828	218	269	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	FA	147	Total	C	N	O	S	0	0
			1165	731	190	239	5		
6	CB	166	Total	C	N	O	S	0	0
			1320	828	218	269	5		
6	CA	147	Total	C	N	O	S	0	0
			1165	731	190	239	5		

- Molecule 7 is a protein called Receptor Binding Protein, gp61.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BH	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		
7	BG	635	Total	C	N	O	S	0	0
			5201	3308	895	983	15		
7	BI	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		
7	DH	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		
7	DG	635	Total	C	N	O	S	0	0
			5201	3308	895	983	15		
7	DI	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		
7	AH	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		
7	AG	635	Total	C	N	O	S	0	0
			5201	3308	895	983	15		
7	AI	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		
7	FH	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		
7	FG	635	Total	C	N	O	S	0	0
			5201	3308	895	983	15		
7	FI	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		
7	CH	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		
7	CG	635	Total	C	N	O	S	0	0
			5201	3308	895	983	15		
7	CI	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		
7	EH	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	EG	635	Total	C	N	O	S	0	0
			5201	3308	895	983	15		
7	EI	634	Total	C	N	O	S	0	0
			5193	3304	894	980	15		

- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

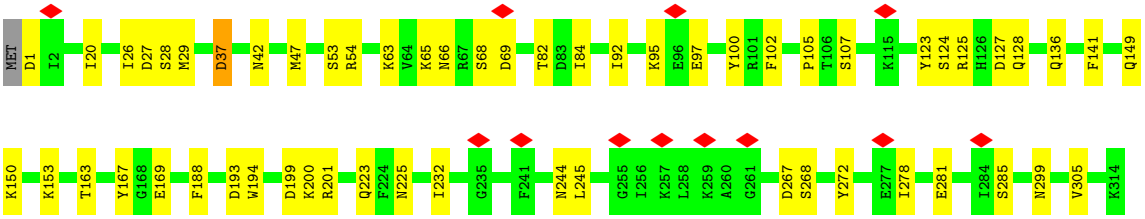
Mol	Chain	Residues	Atoms		AltConf
8	BH	1	Total	Fe	0
			1	1	
8	DH	1	Total	Fe	0
			1	1	
8	AH	1	Total	Fe	0
			1	1	
8	FH	1	Total	Fe	0
			1	1	
8	CH	1	Total	Fe	0
			1	1	
8	EH	1	Total	Fe	0
			1	1	

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.

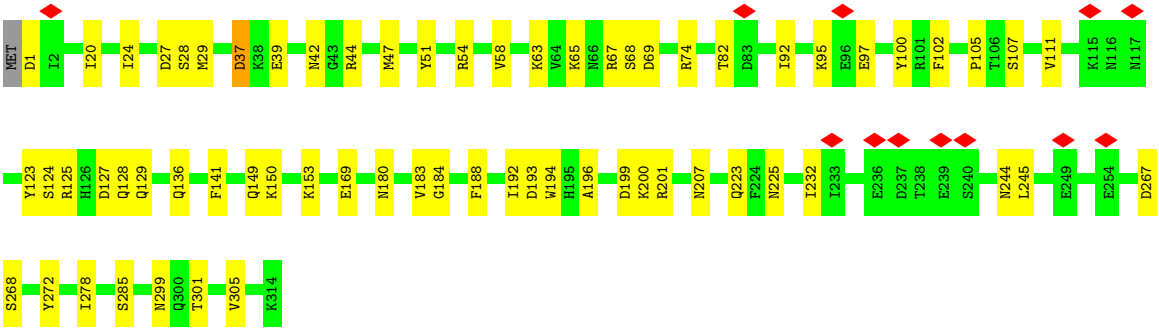
• Molecule 1: Distal Tail Protein, gp58

Chain AC:



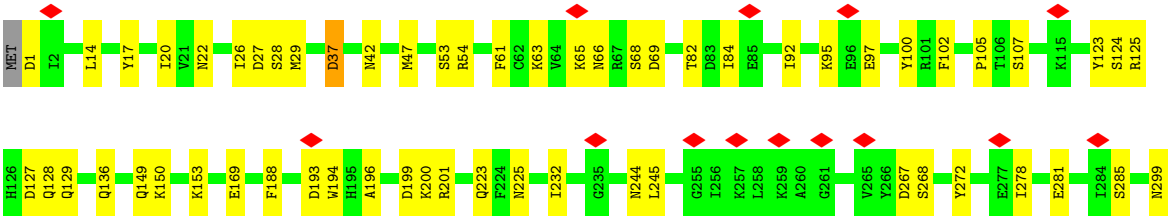
• Molecule 1: Distal Tail Protein, gp58

Chain AD:



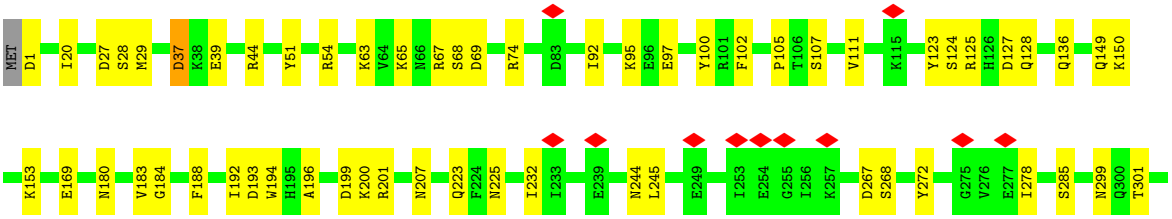
• Molecule 1: Distal Tail Protein, gp58

Chain CC:



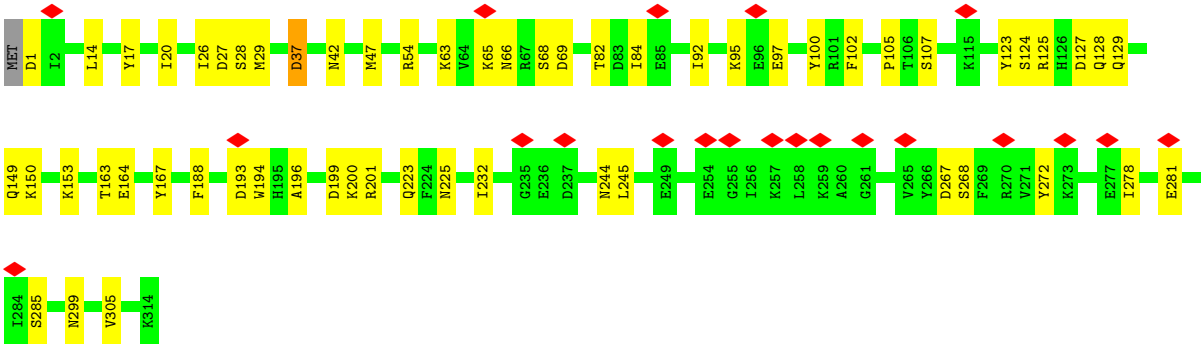
• Molecule 1: Distal Tail Protein, gp58

Chain CD:



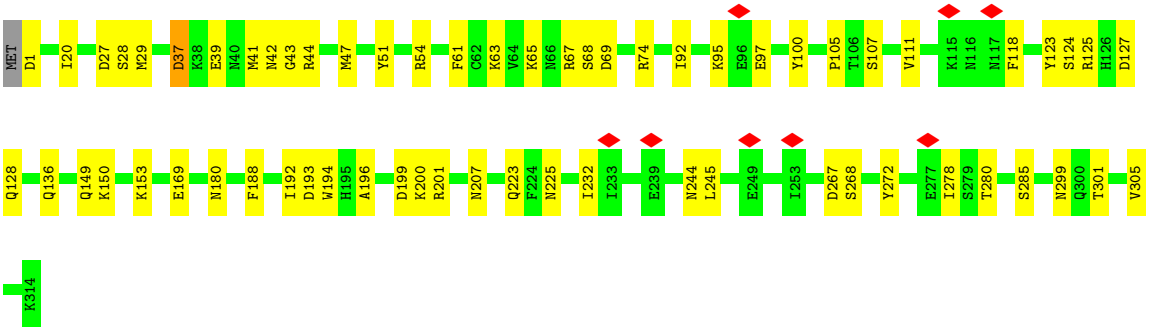
• Molecule 1: Distal Tail Protein, gp58

Chain BC:



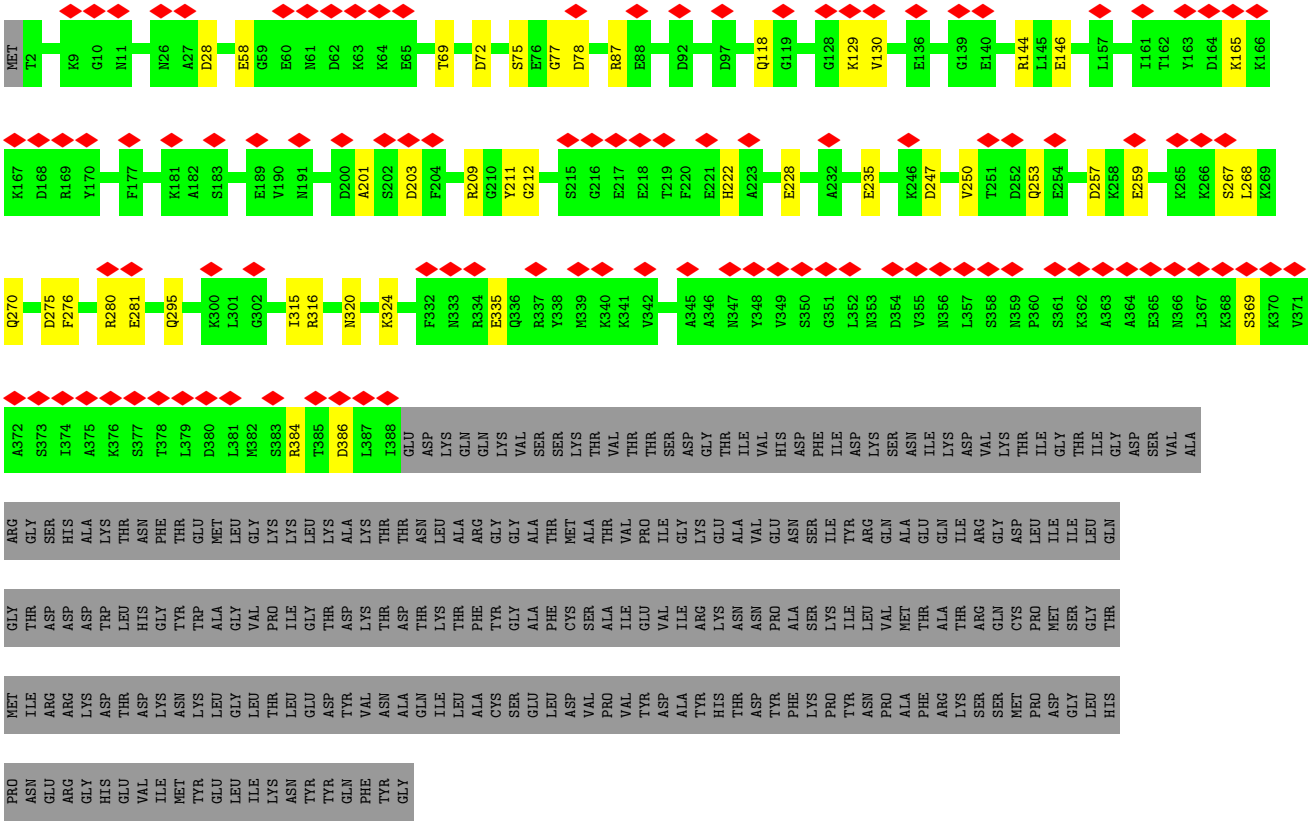
• Molecule 1: Distal Tail Protein, gp58

Chain BD:



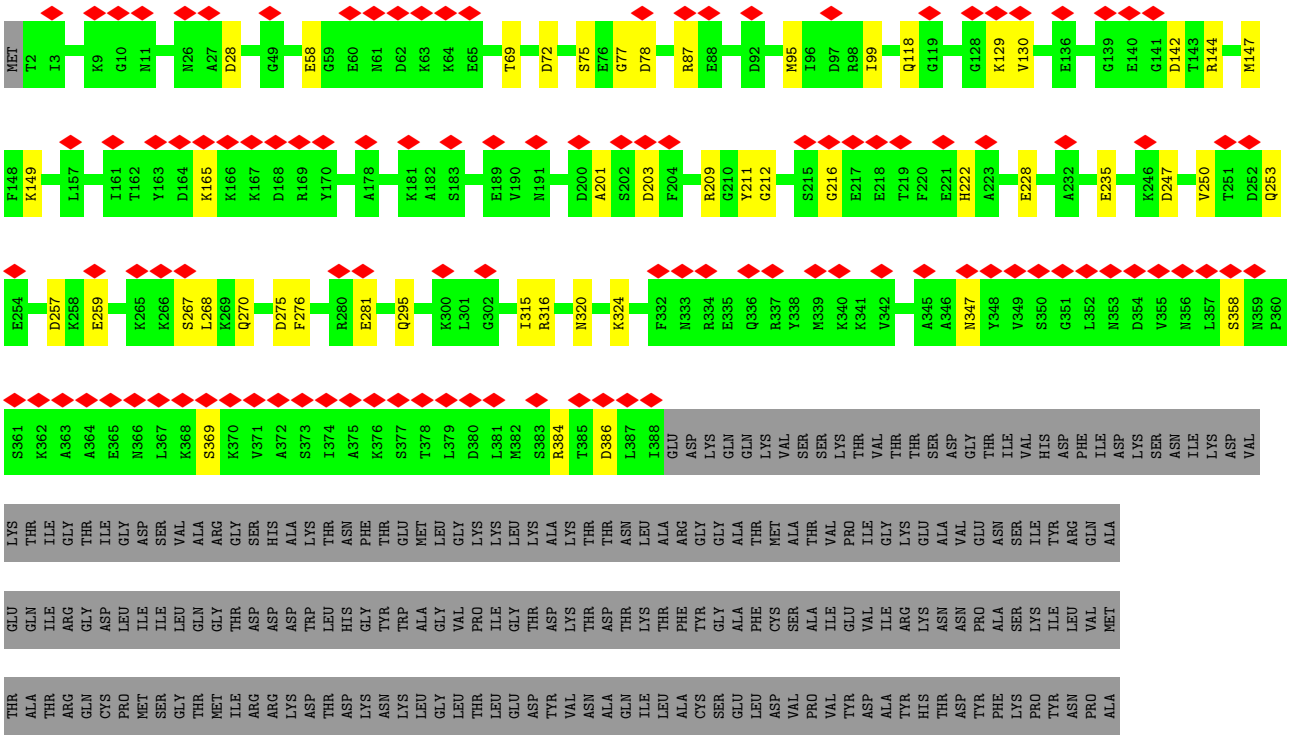
• Molecule 2: Tail-Associated Lysin, gp59

Chain AE:



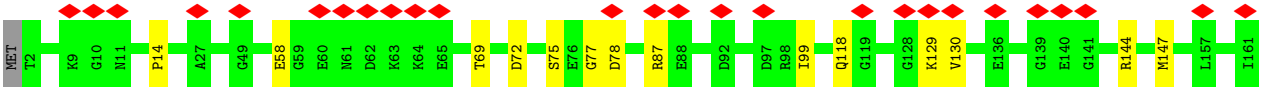
• Molecule 2: Tail-Associated Lysin, gp59

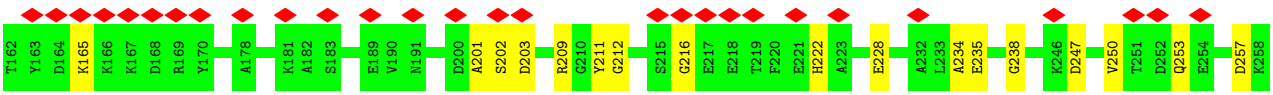
Chain CE:

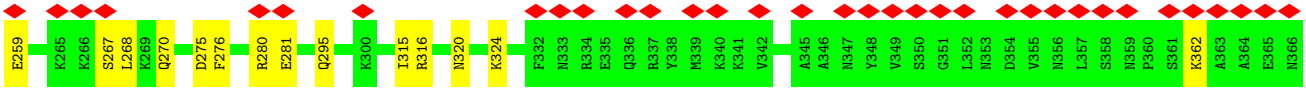


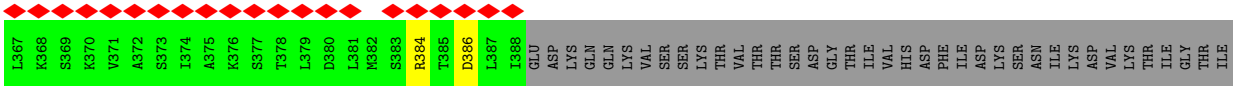
• Molecule 2: Tail-Associated Lysin, gp59

Chain BE:



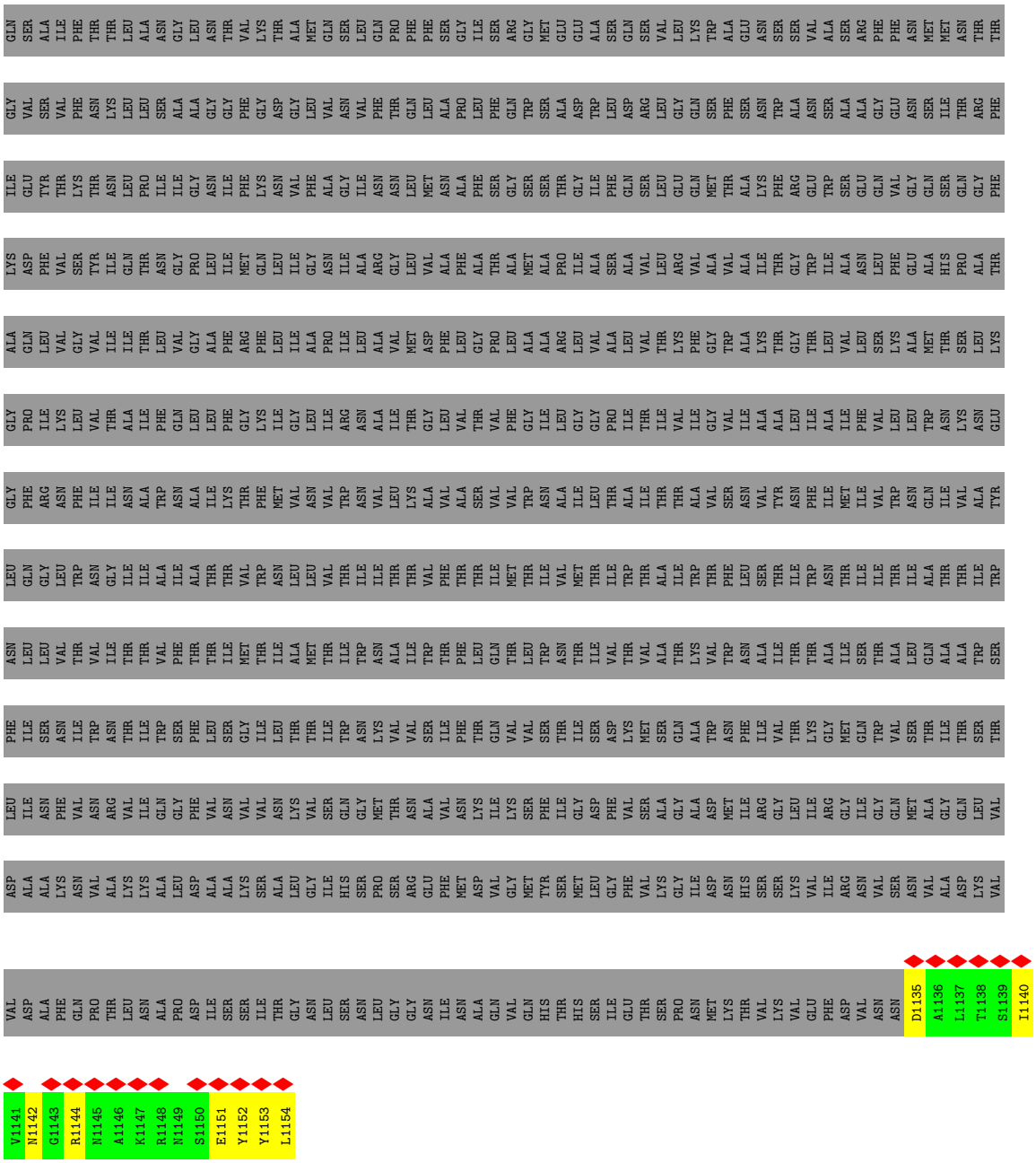






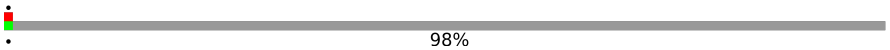
• Molecule 3: Tape Measure Protein, gp57

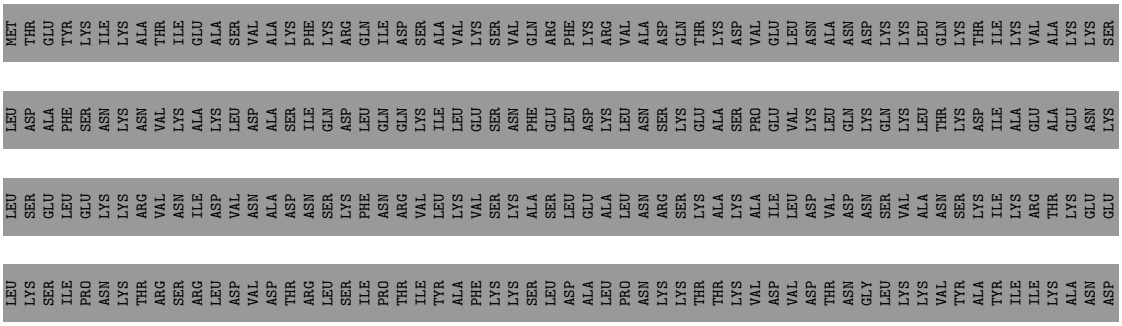
Chain CF:

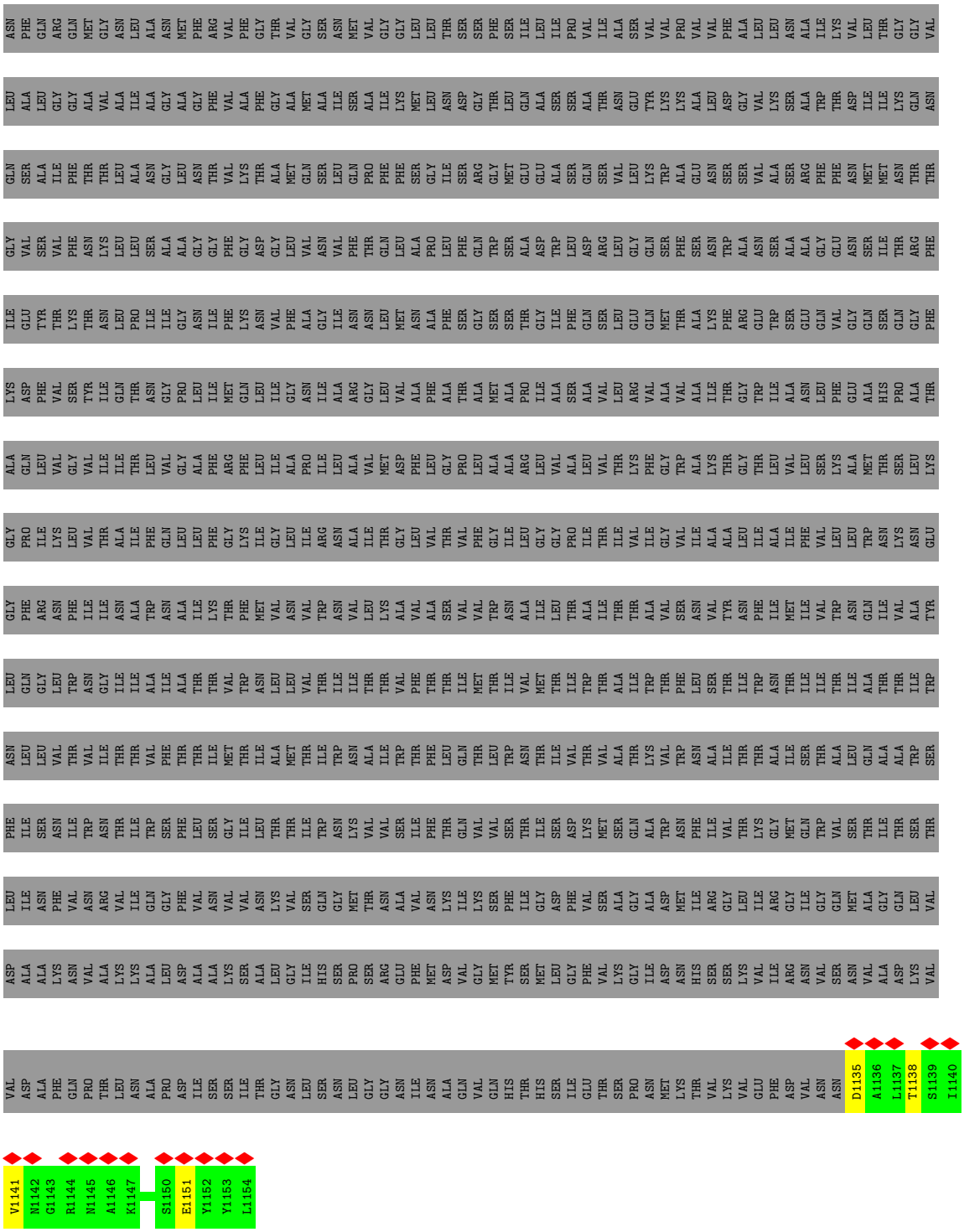


• Molecule 3: Tape Measure Protein, gp57

Chain BF:

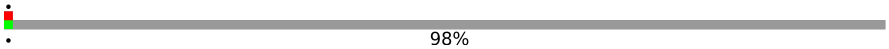


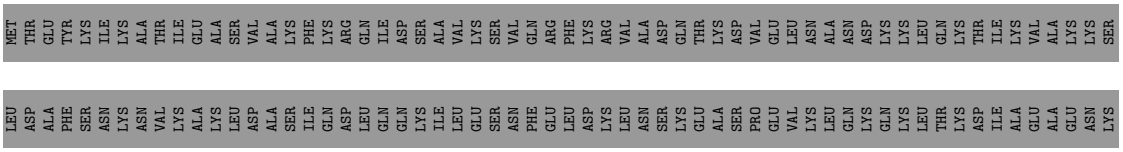


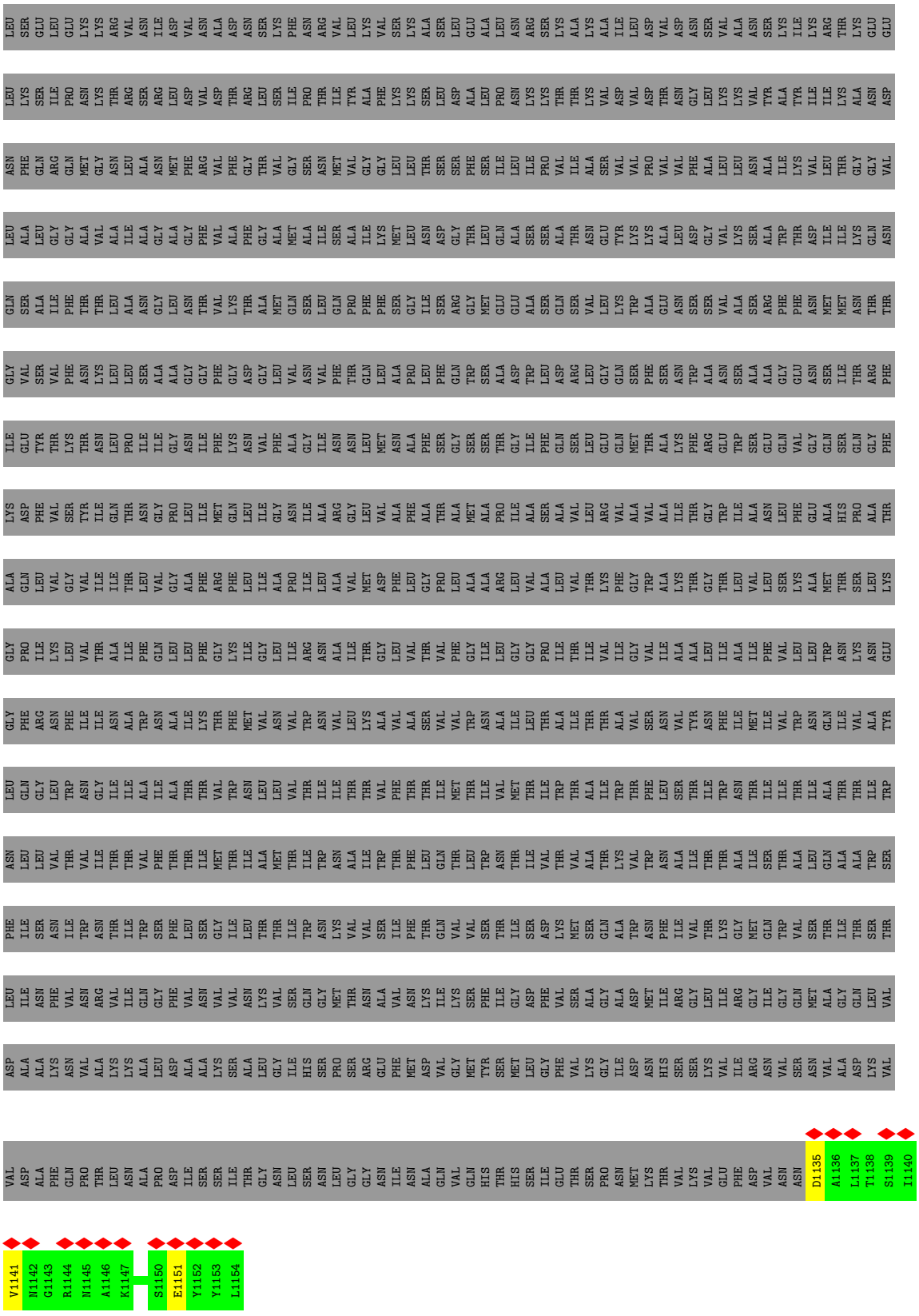


• Molecule 3: Tape Measure Protein, gp57

Chain AF:

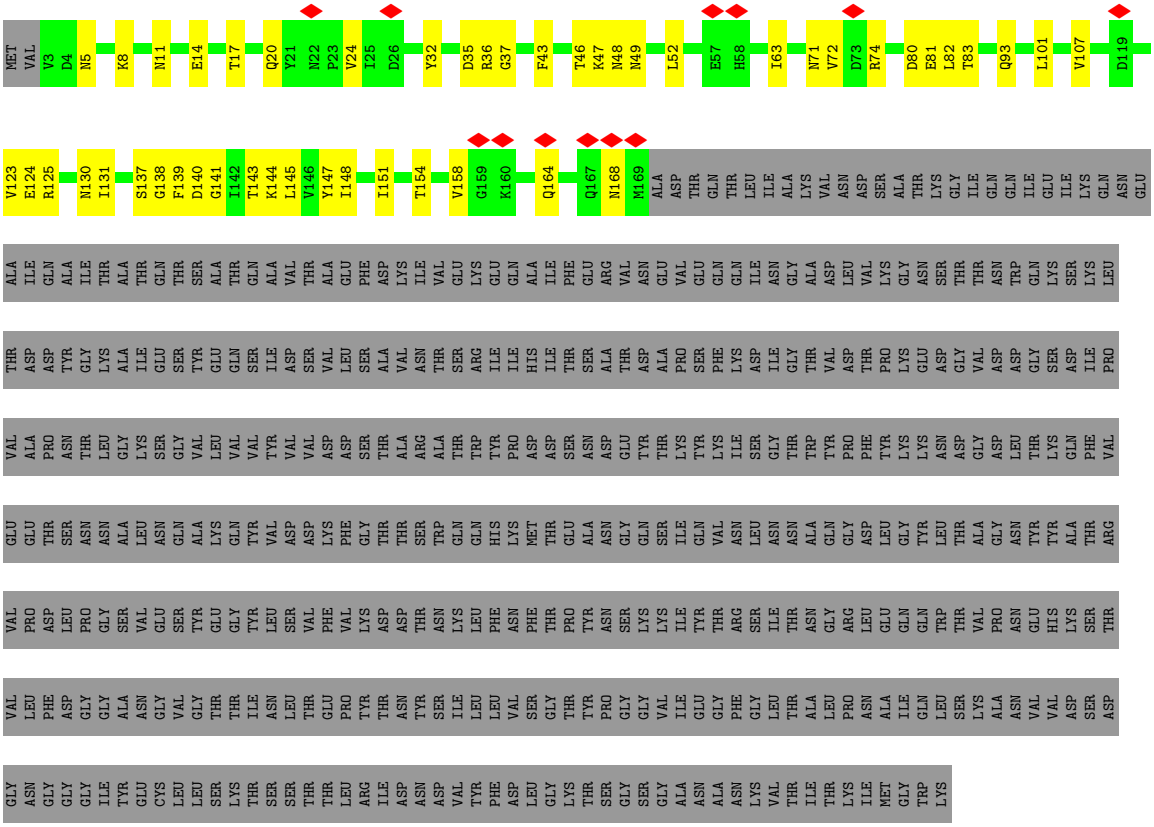






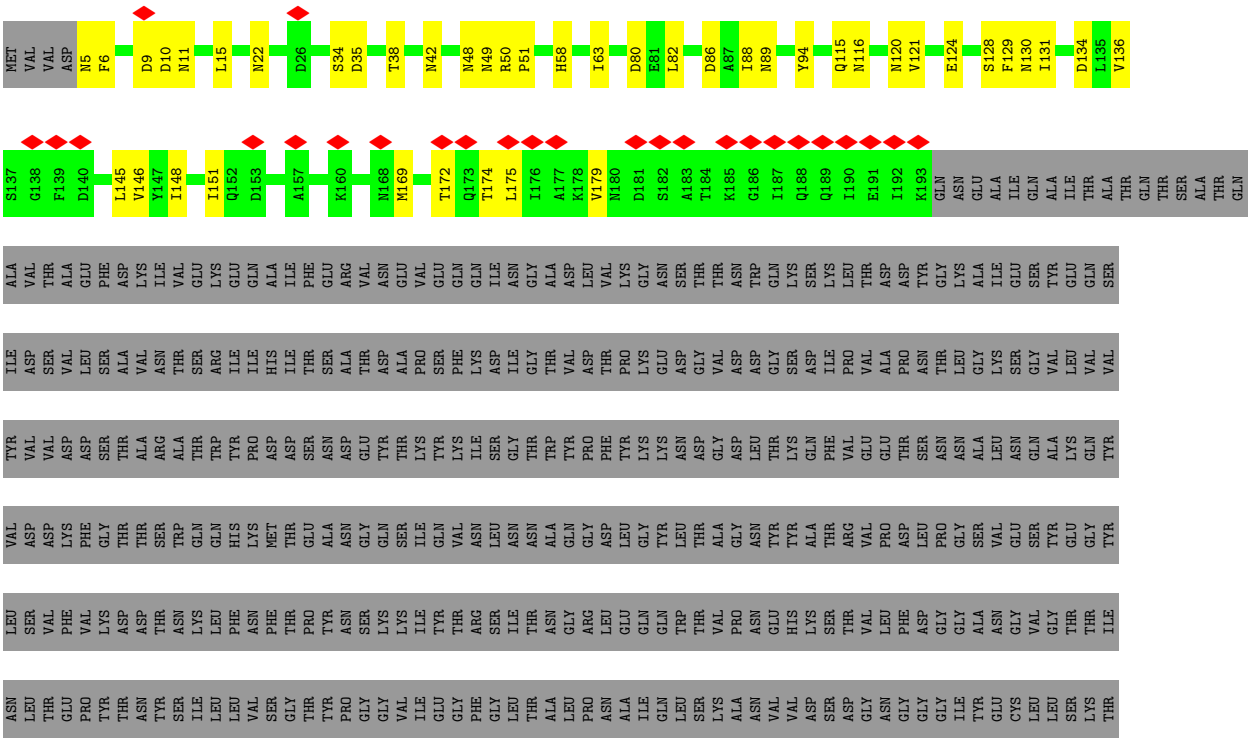
• Molecule 4: Fiber Lower, gp62

Chain BJ: 20% 8% 72%



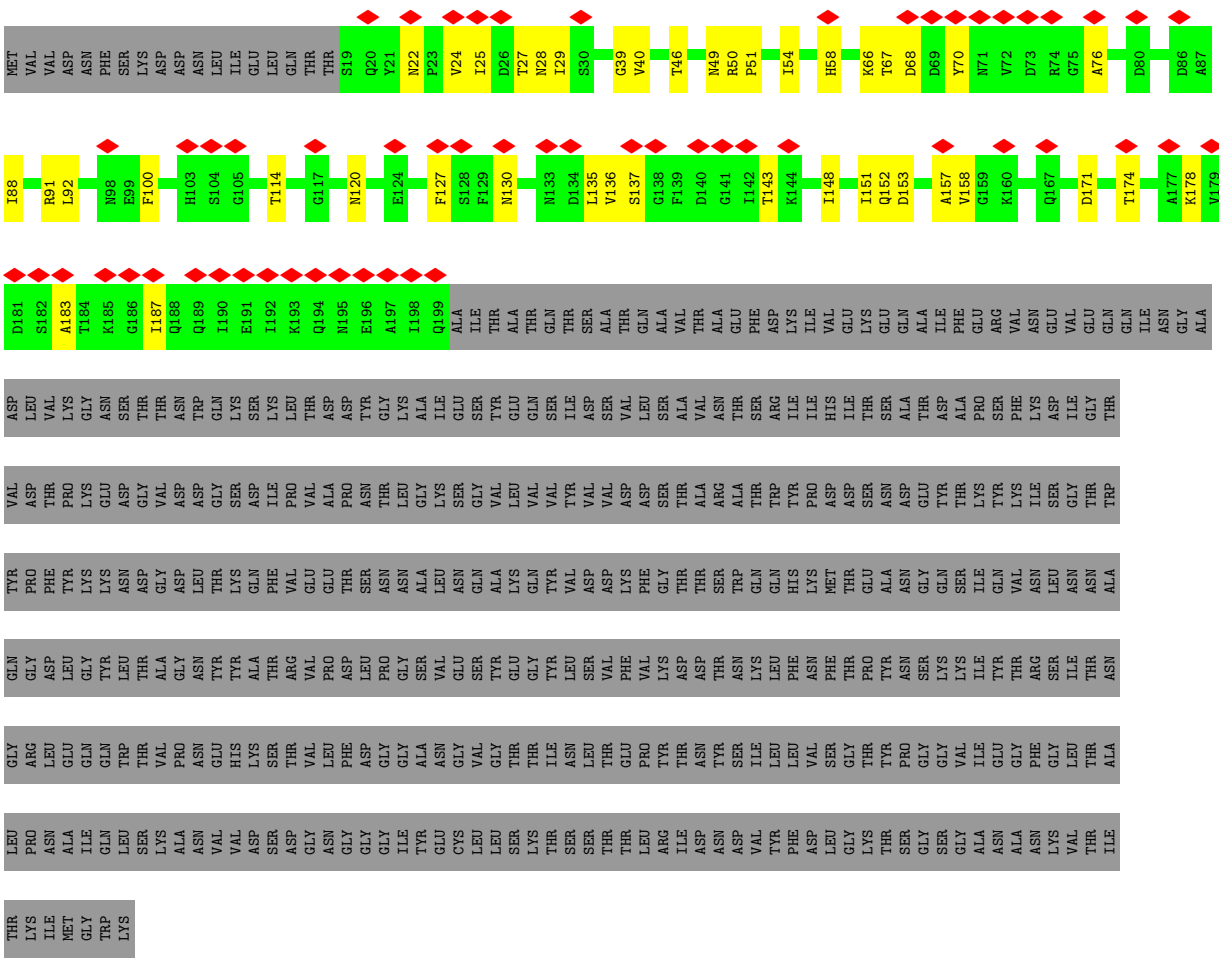
• Molecule 4: Fiber Lower, gp62

Chain BK:



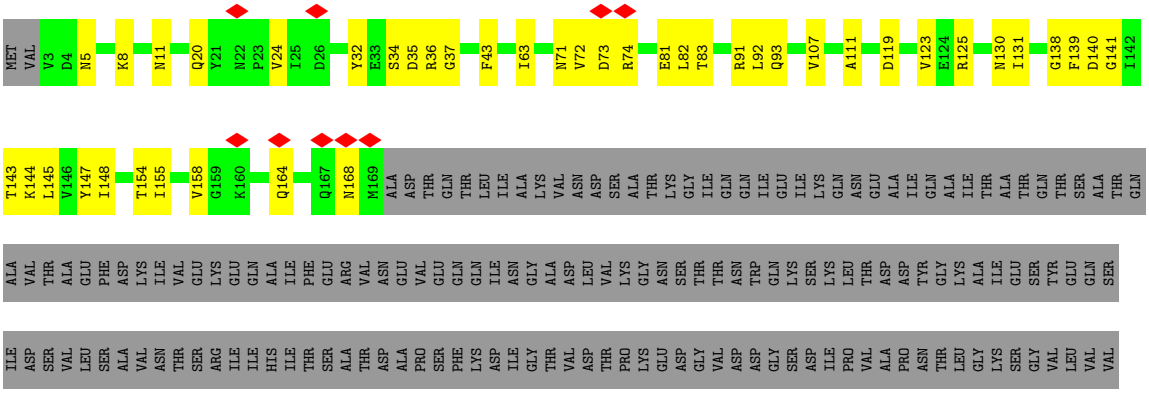
• Molecule 4: Fiber Lower, gp62

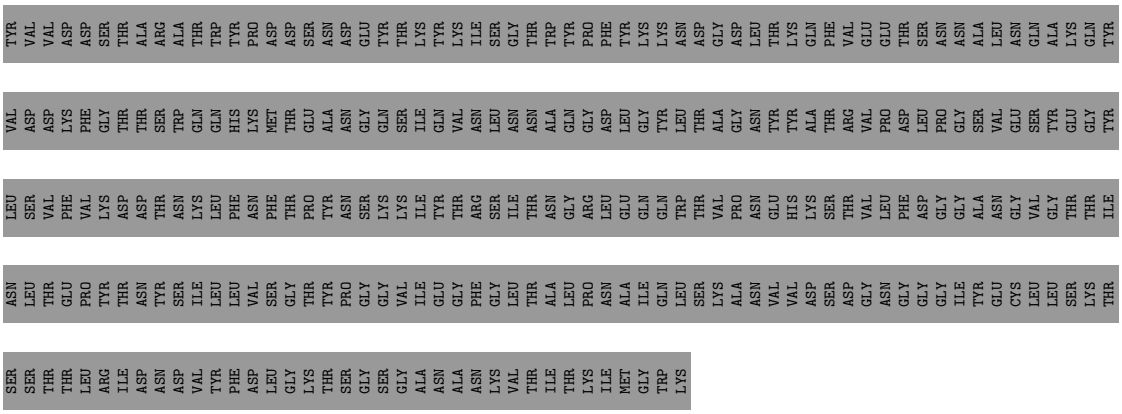
Chain BL:



• Molecule 4: Fiber Lower, gp62

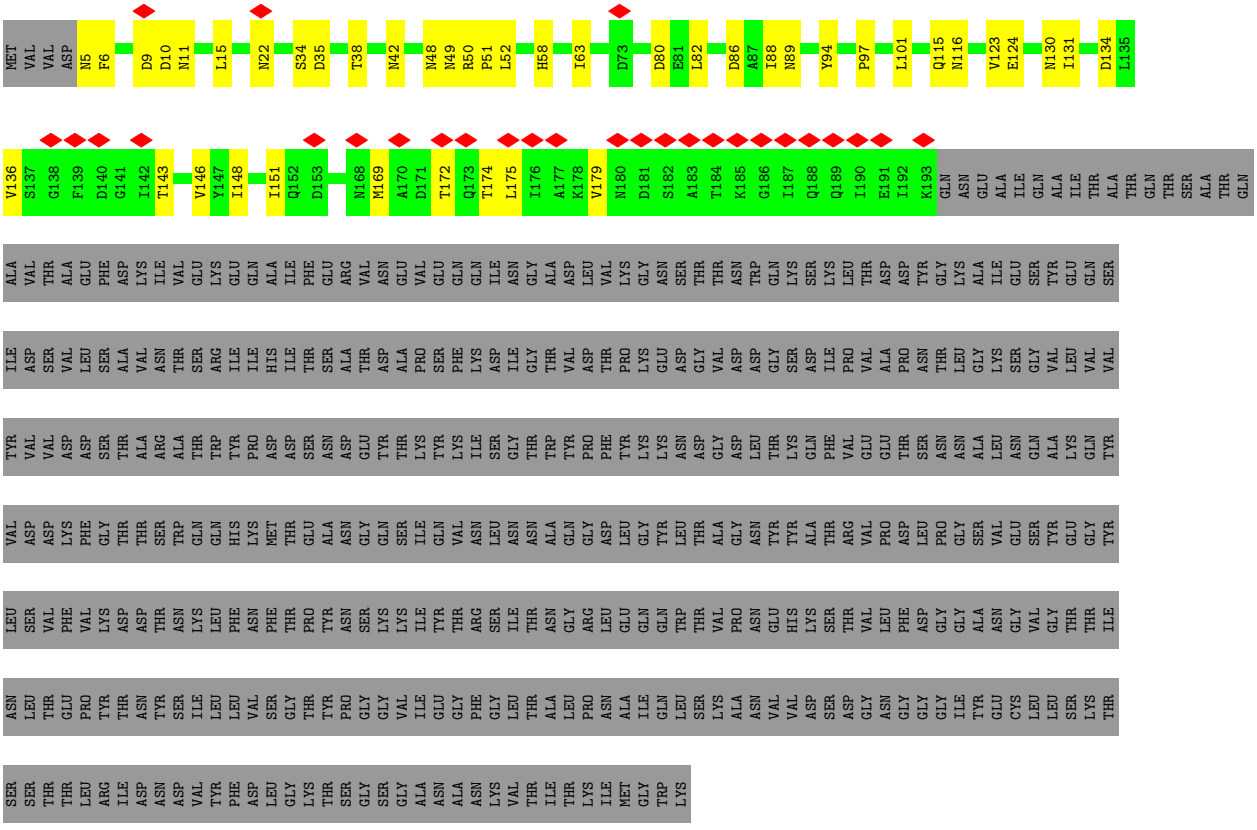
Chain DJ:





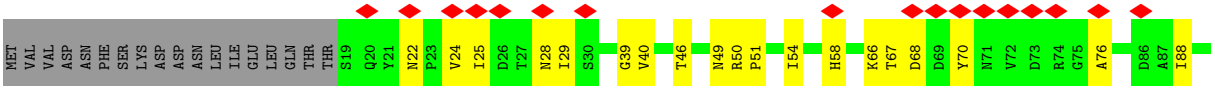
• Molecule 4: Fiber Lower, gp62

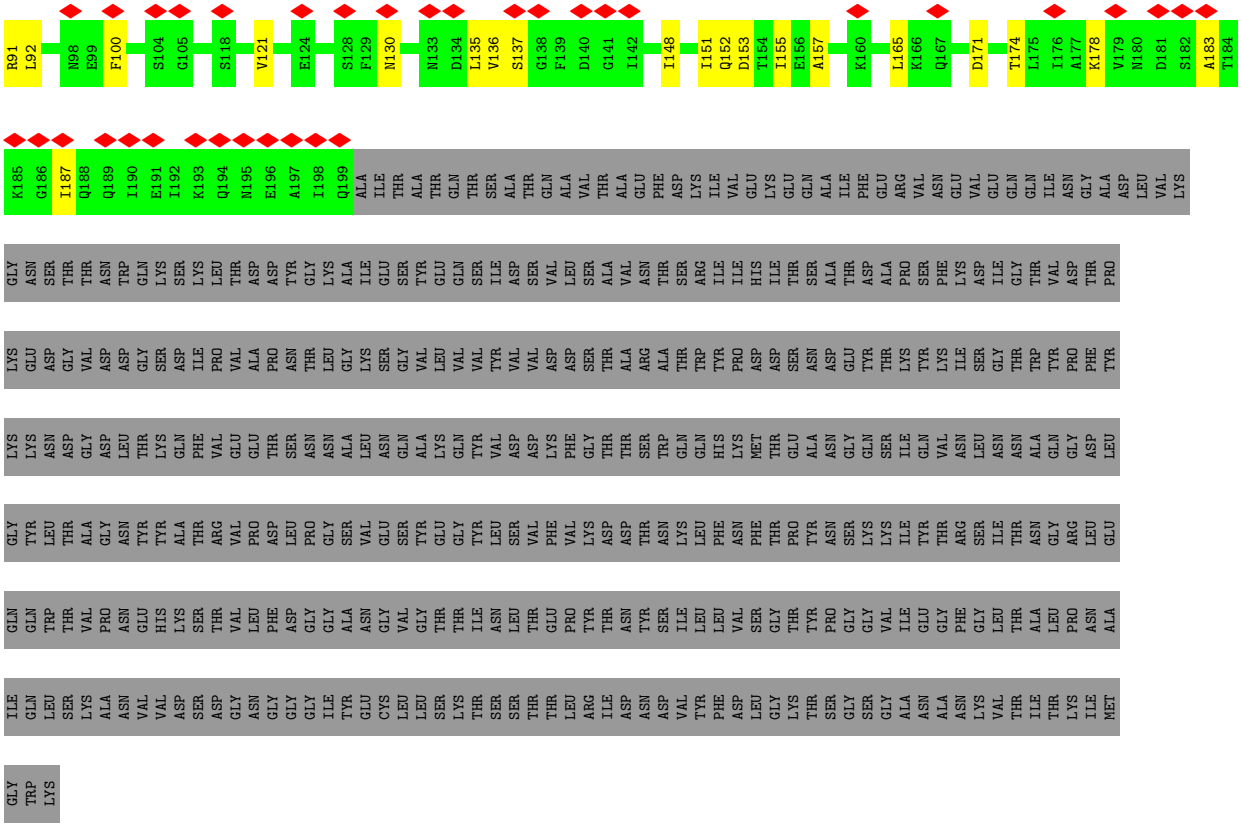
Chain DK:



• Molecule 4: Fiber Lower, gp62

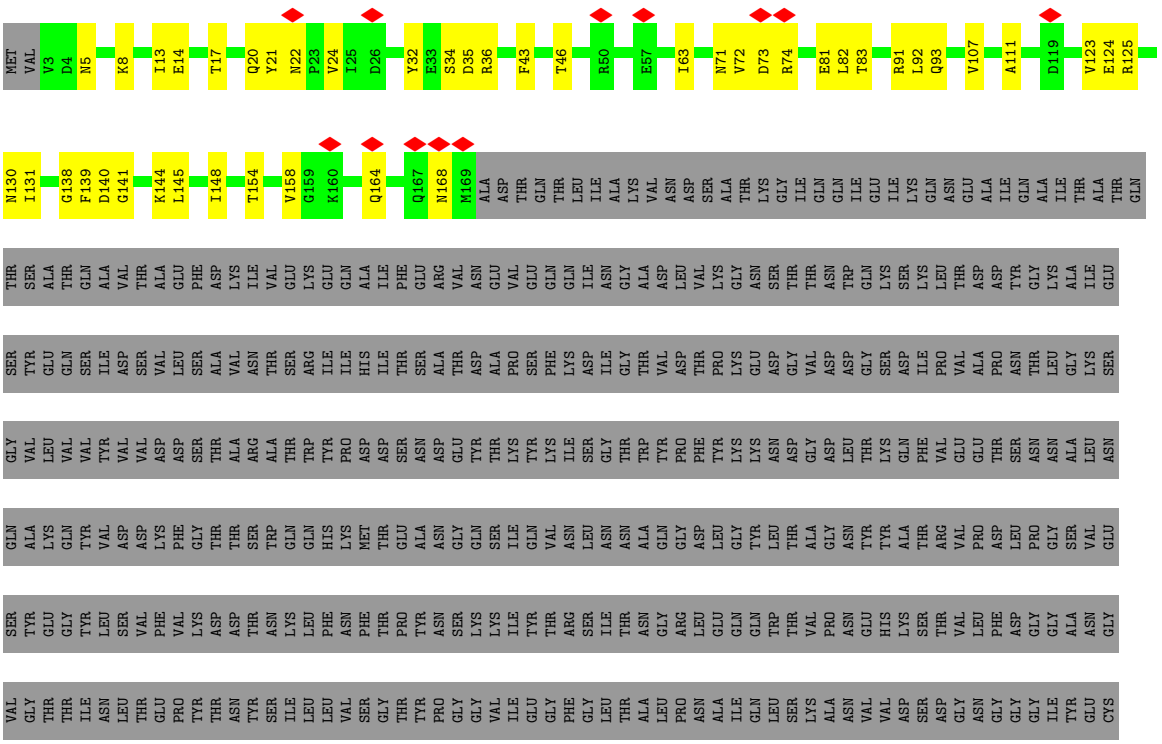
Chain DL:





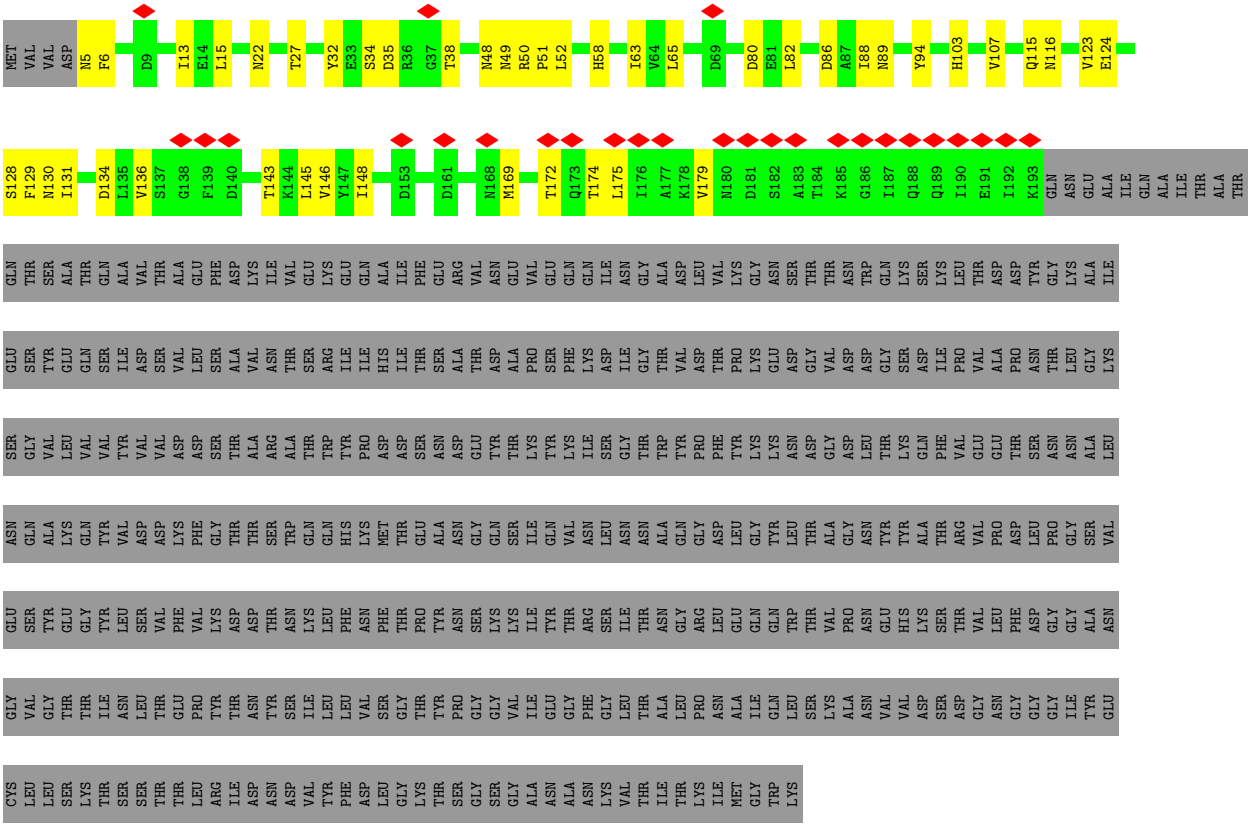
• Molecule 4: Fiber Lower, gp62

Chain AJ:



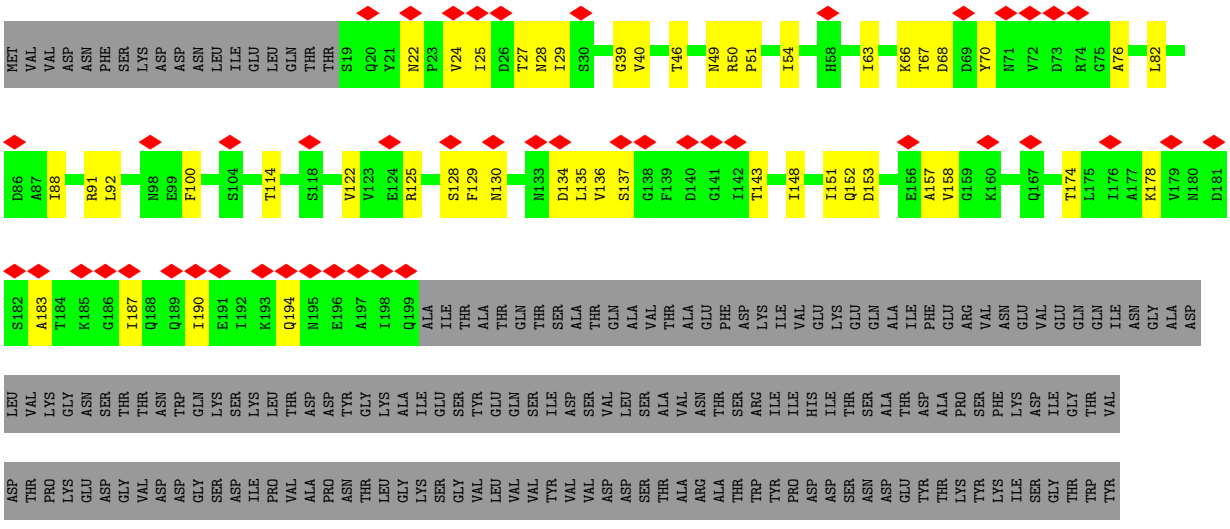
• Molecule 4: Fiber Lower, gp62

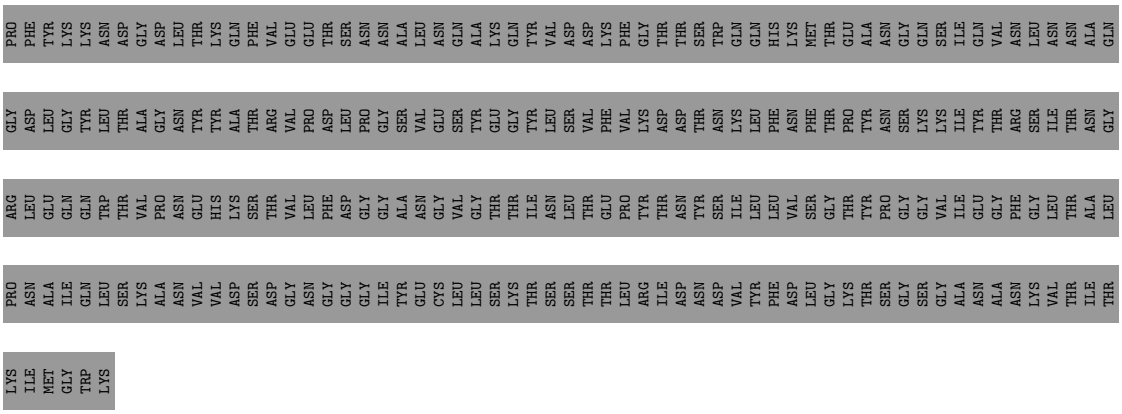
Chain AK:



• Molecule 4: Fiber Lower, gp62

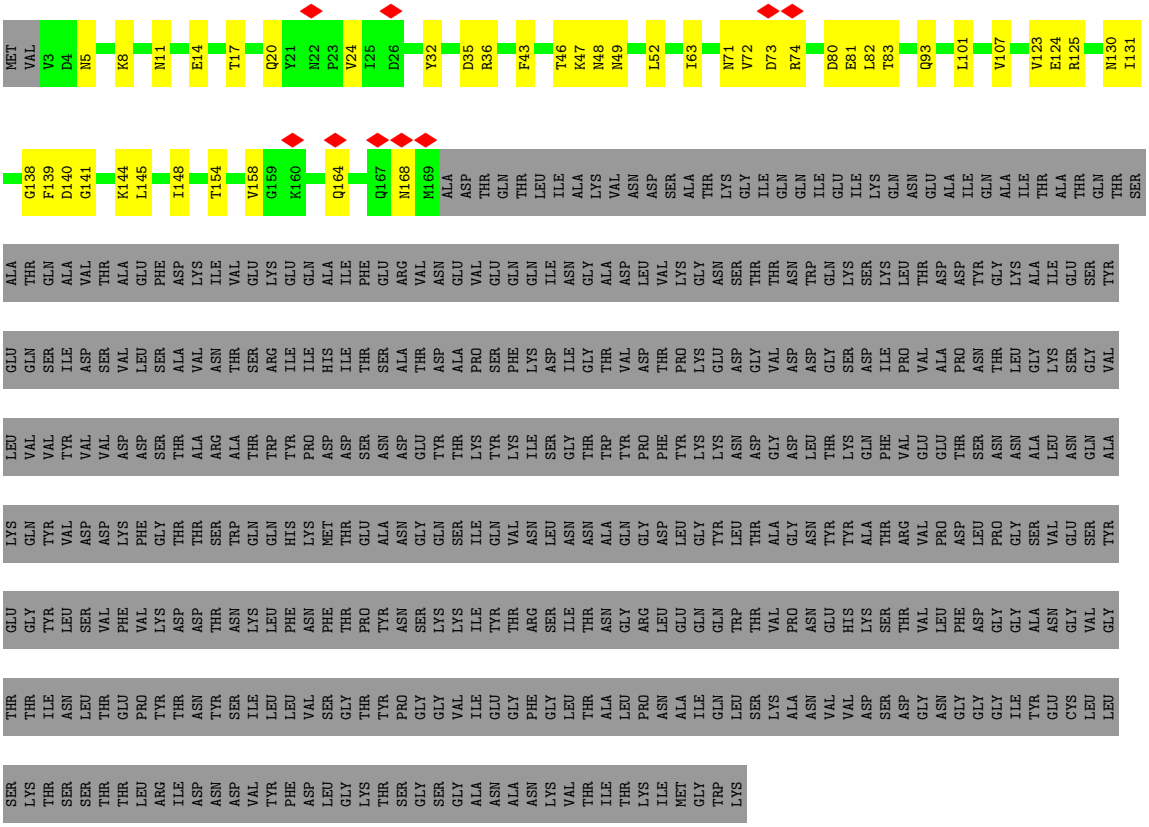
Chain AL:





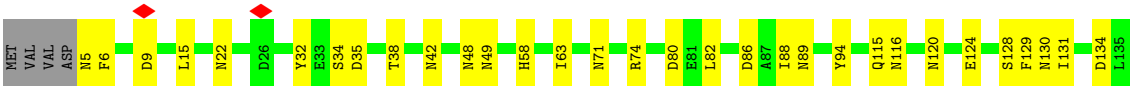
• Molecule 4: Fiber Lower, gp62

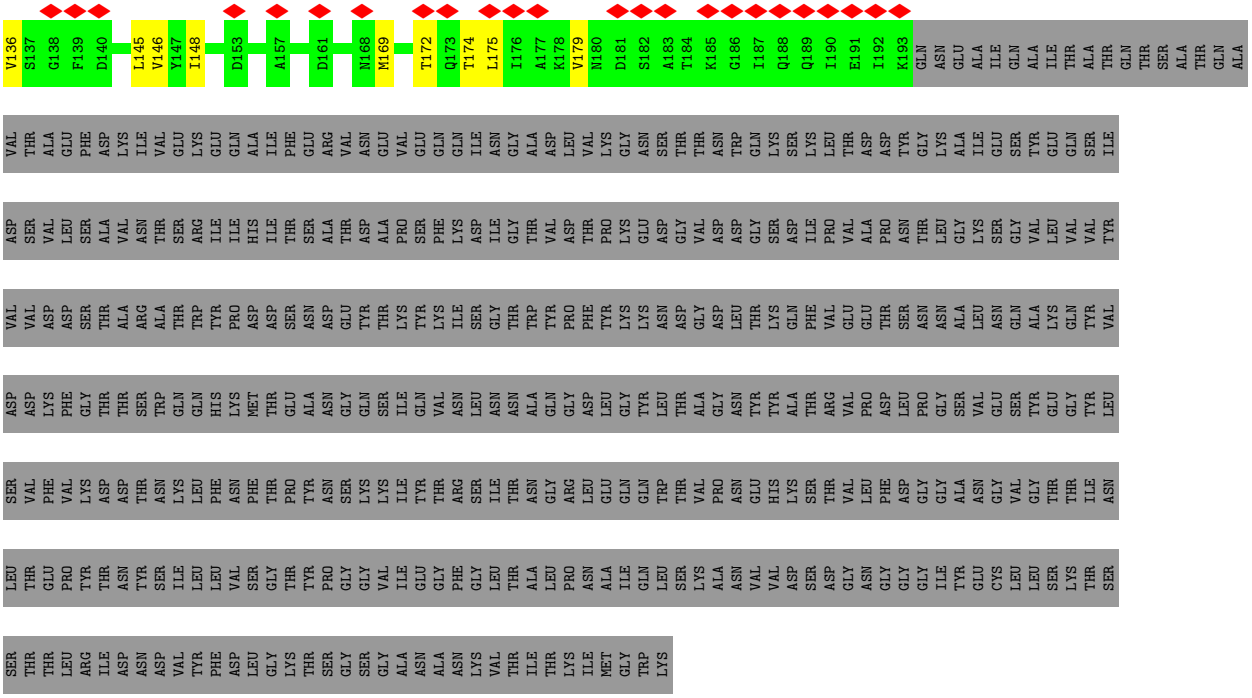
Chain FJ:



• Molecule 4: Fiber Lower, gp62

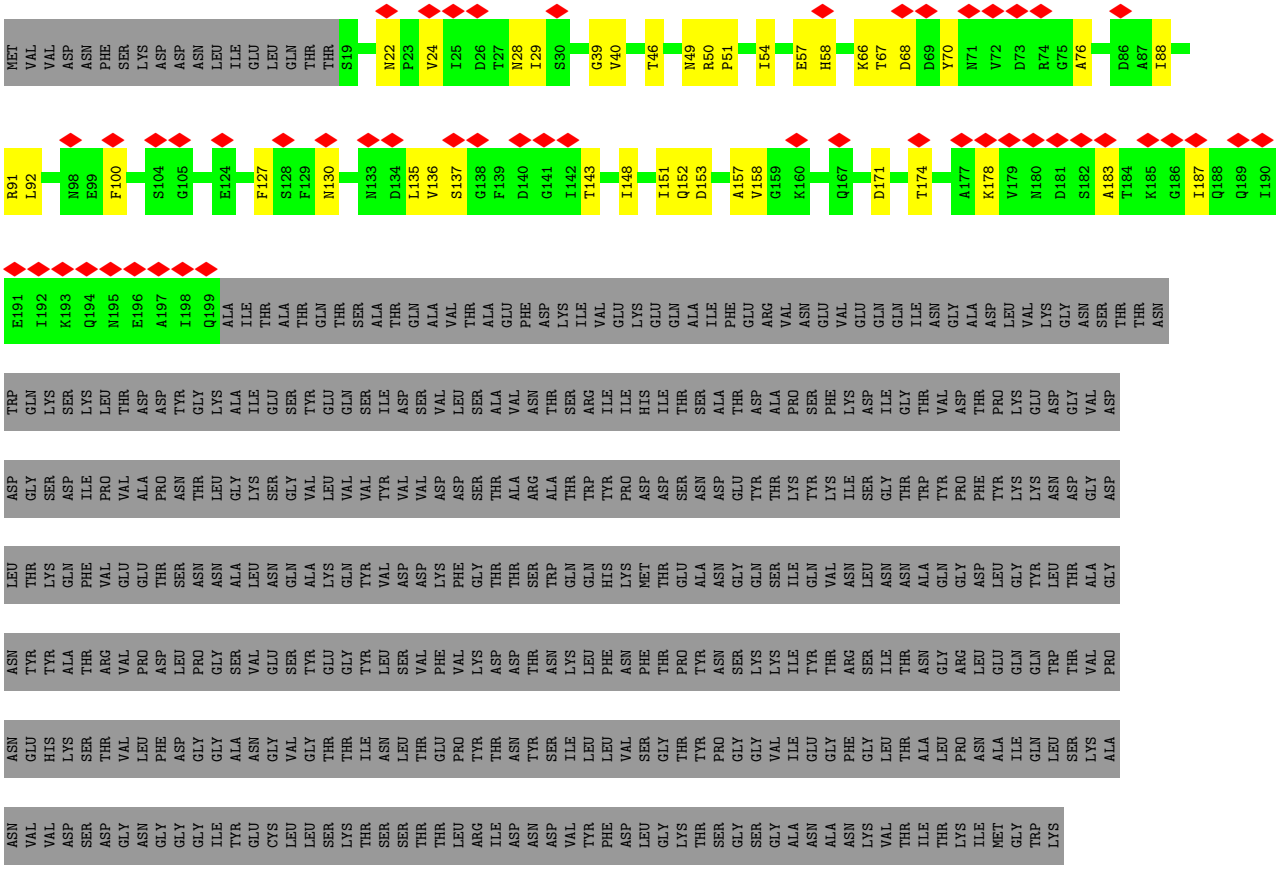
Chain FK:





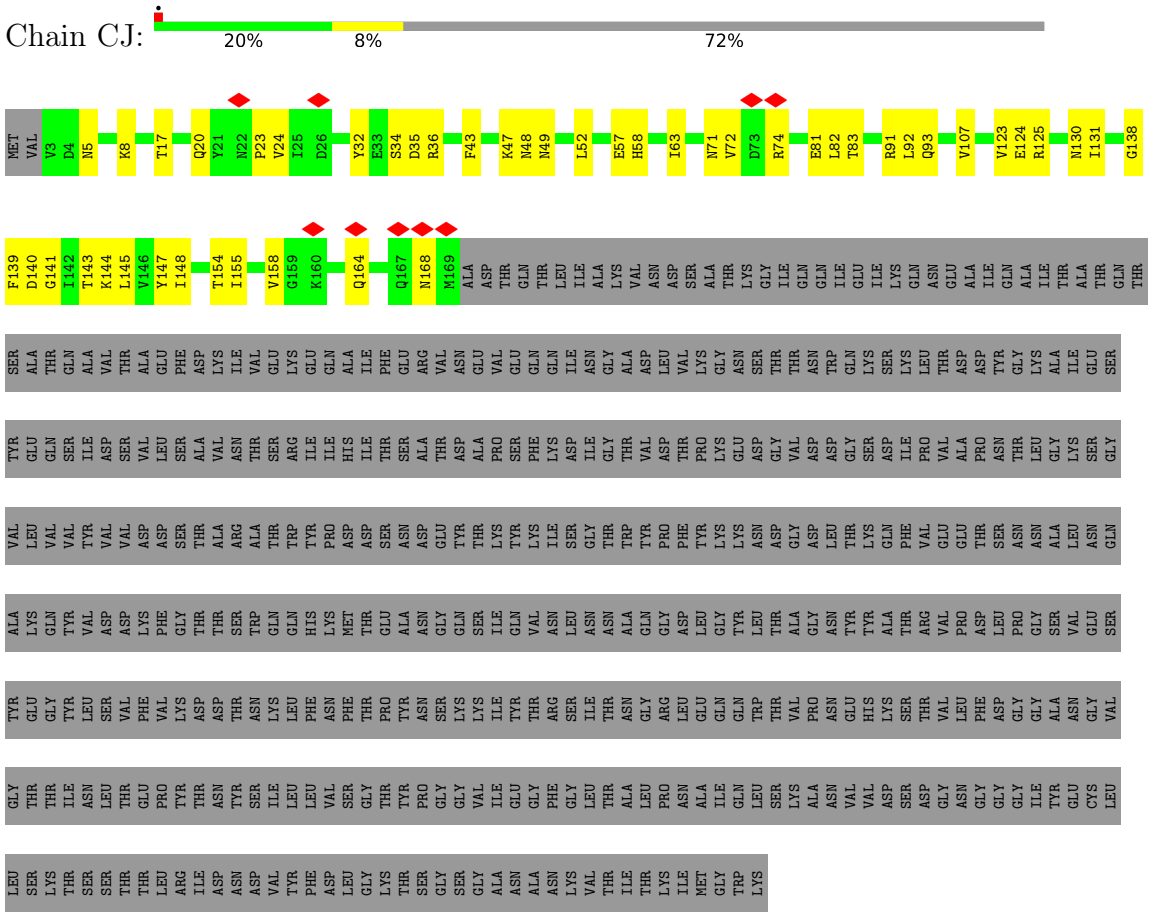
• Molecule 4: Fiber Lower, gp62

Chain FL:



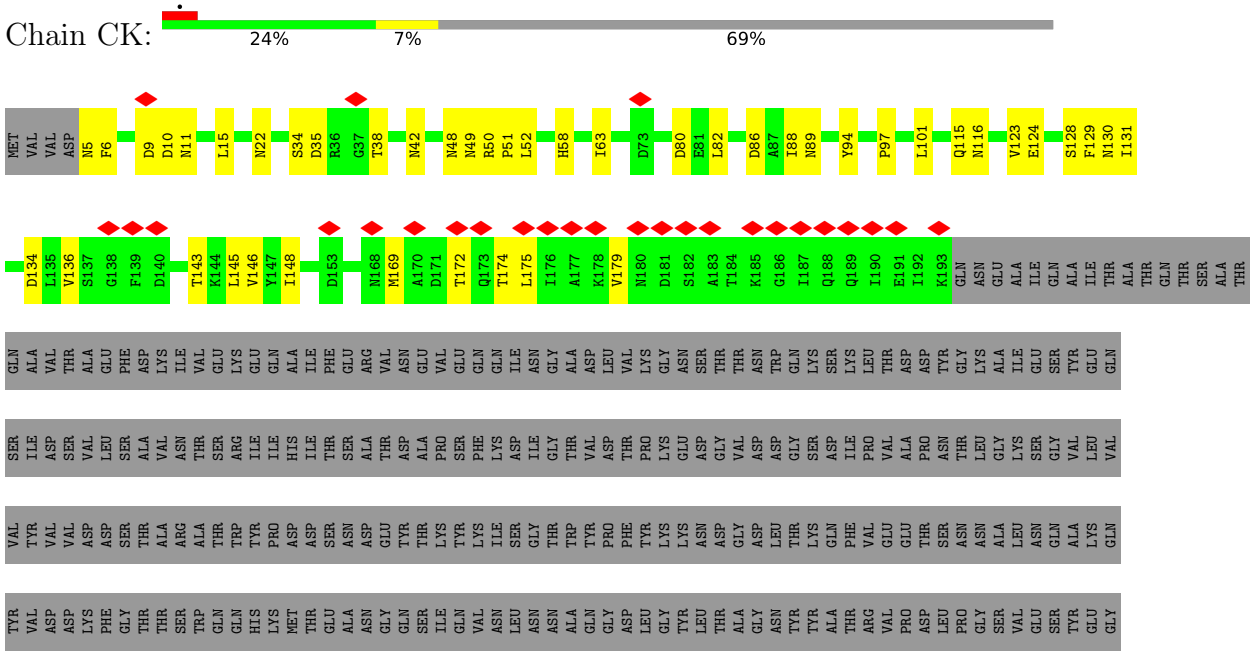
• Molecule 4: Fiber Lower, gp62

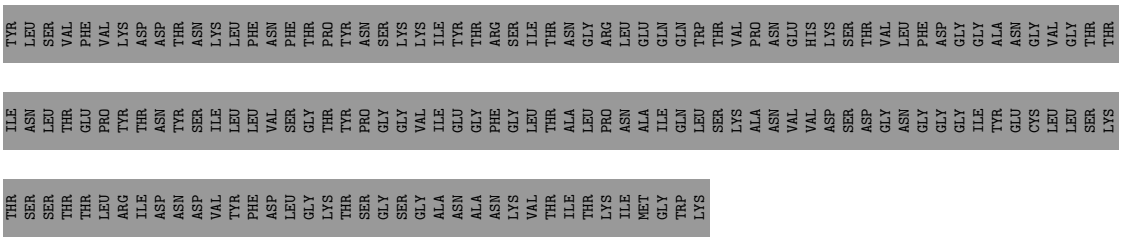
Chain CJ:



• Molecule 4: Fiber Lower, gp62

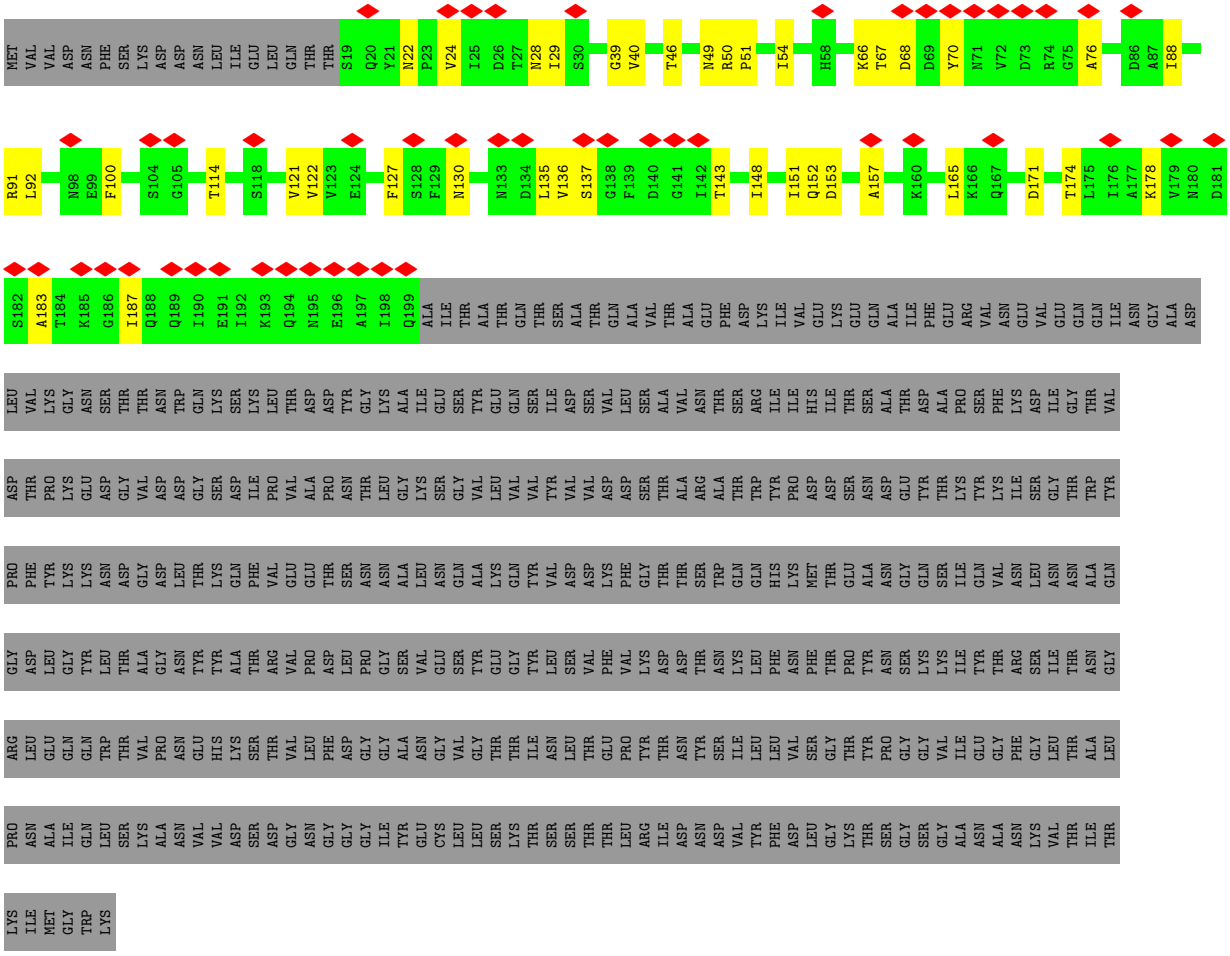
Chain CK:





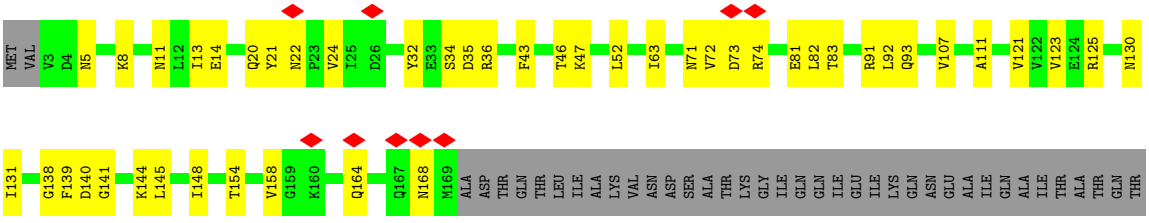
• Molecule 4: Fiber Lower, gp62

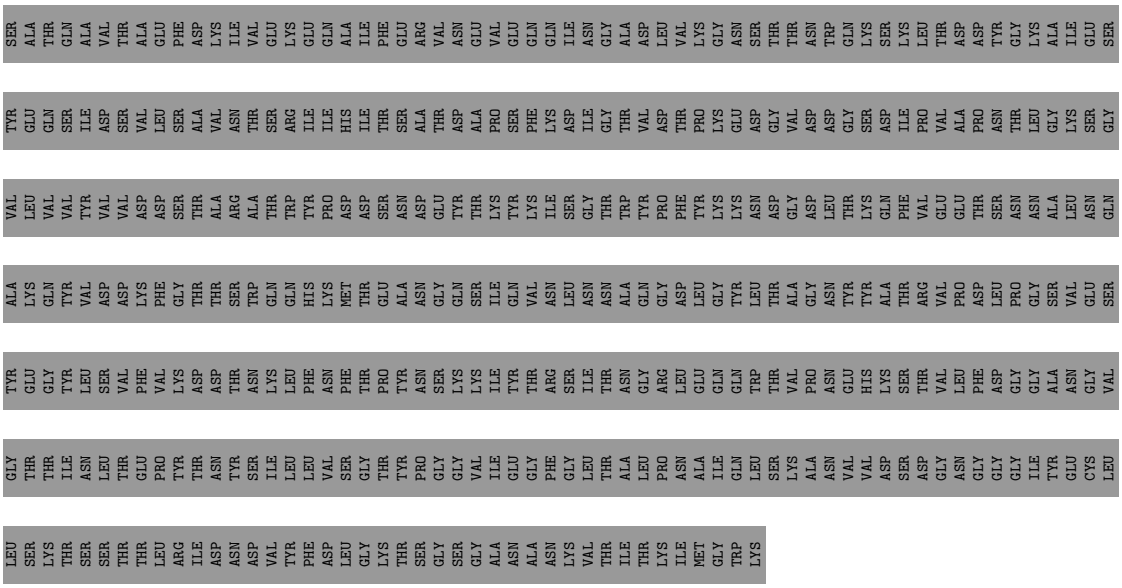
Chain CL:



• Molecule 4: Fiber Lower, gp62

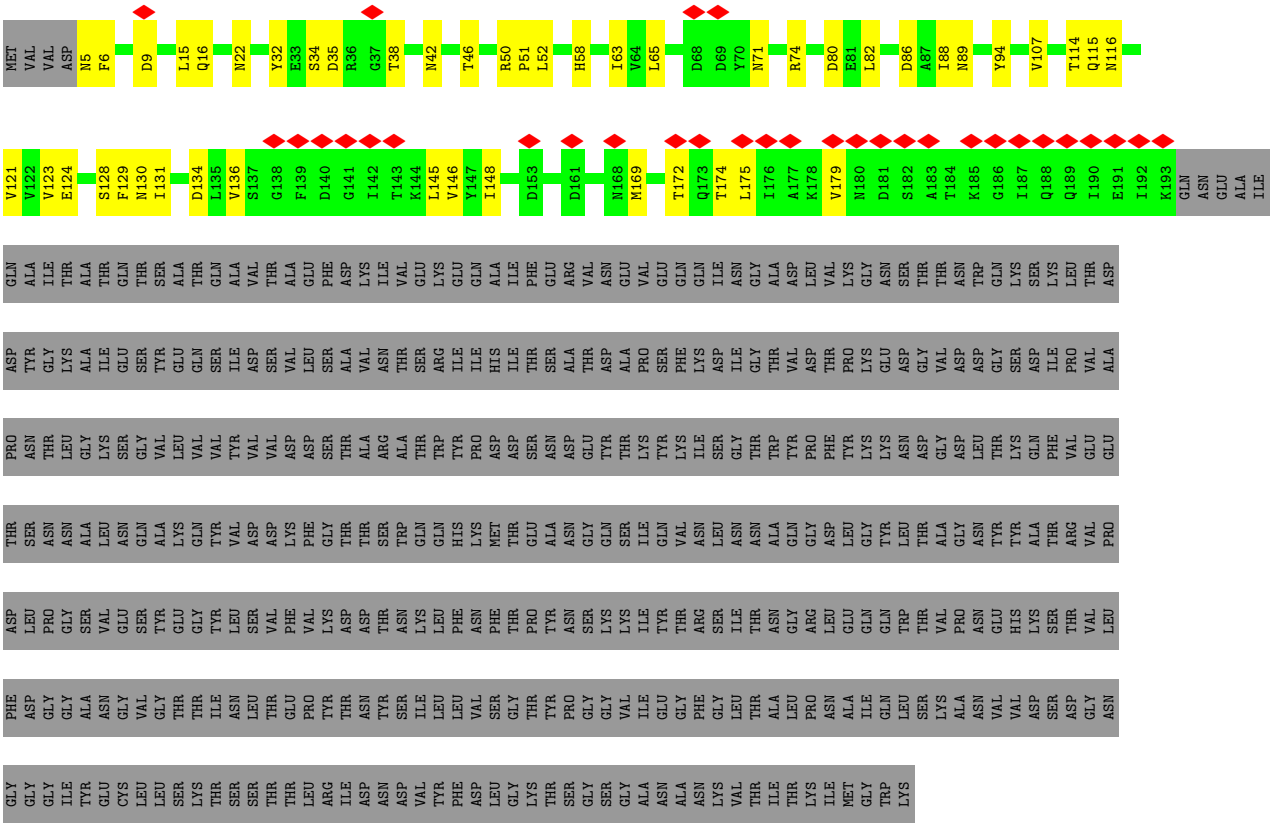
Chain EJ:





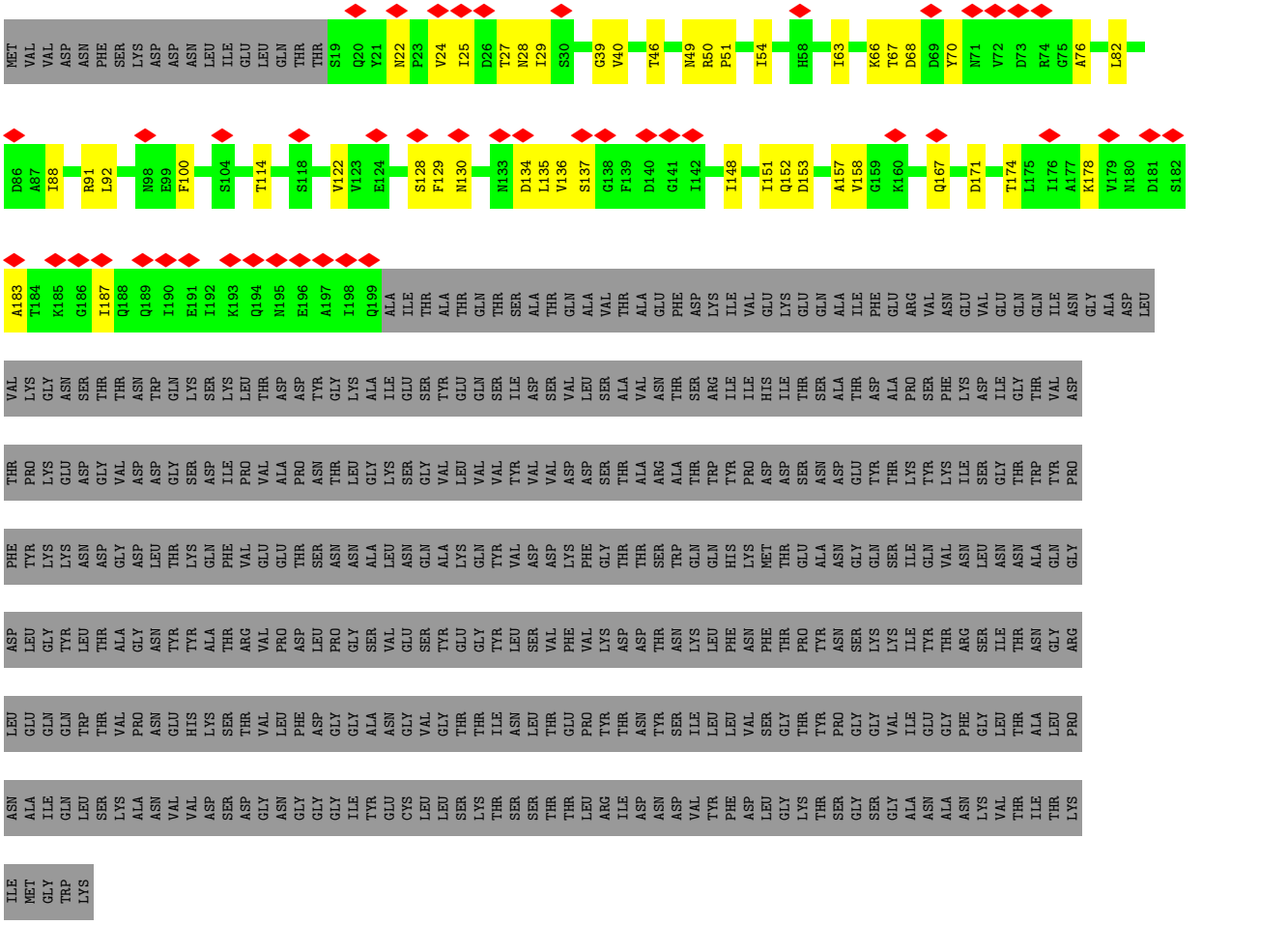
• Molecule 4: Fiber Lower, gp62

Chain EK:



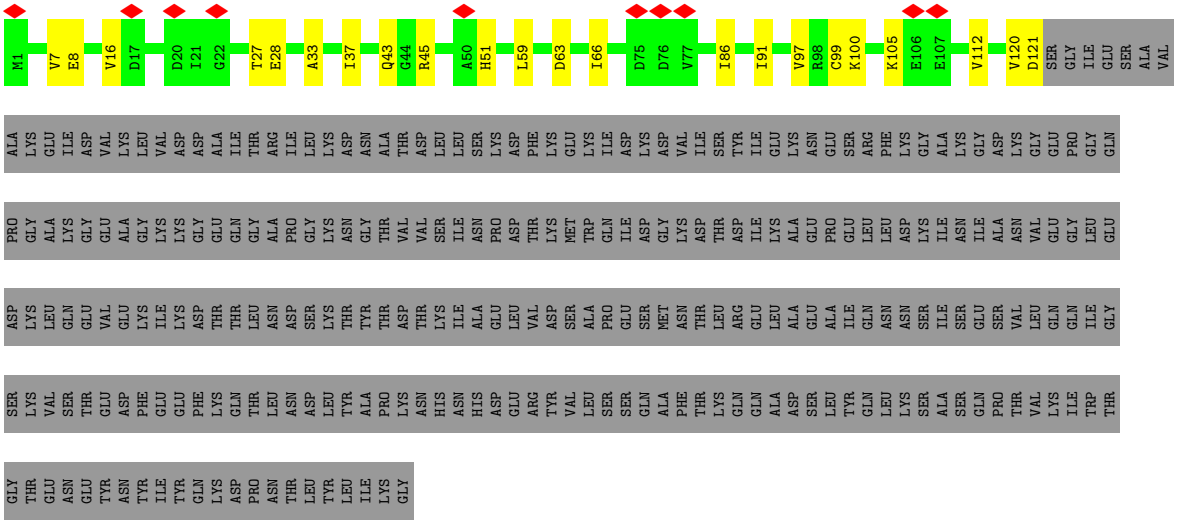
• Molecule 4: Fiber Lower, gp62

Chain EL:



• Molecule 5: Fiber Upper, gp68

Chain BN:



• Molecule 5: Fiber Upper, gp68

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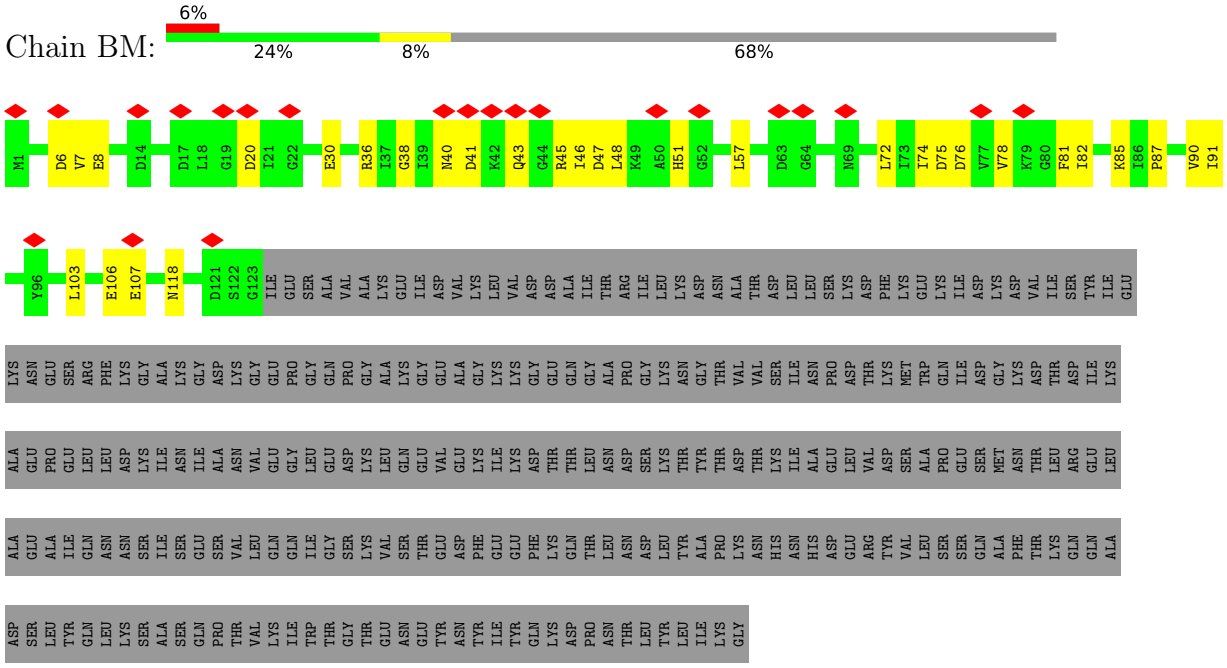
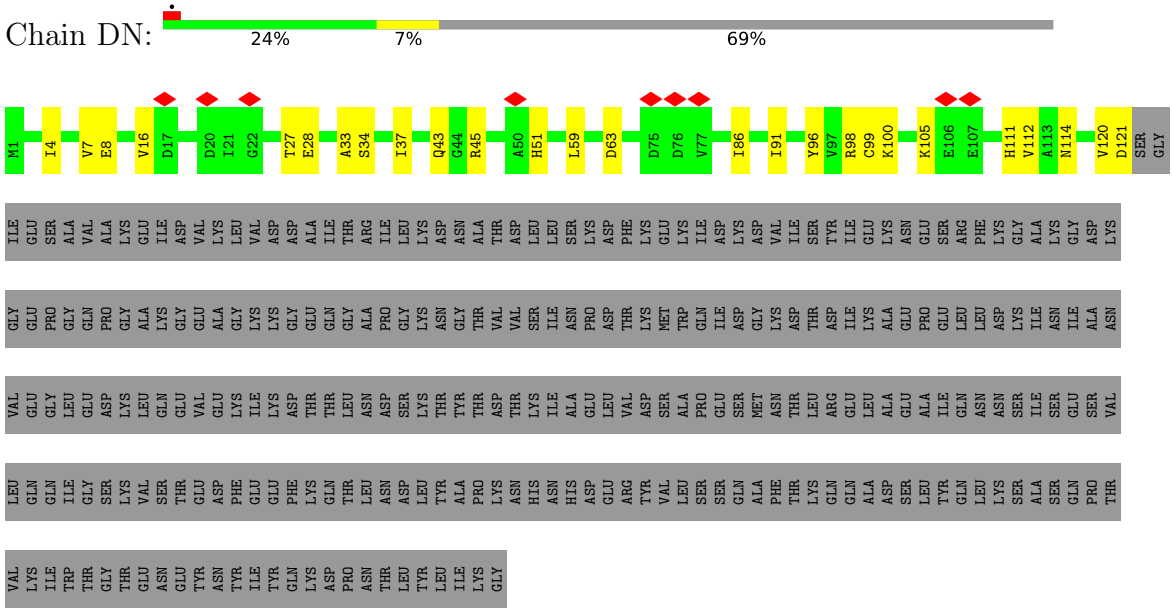


• Molecule 5: Fiber Upper, gp68

Chain DN:



• Molecule 5: Fiber Upper, gp68

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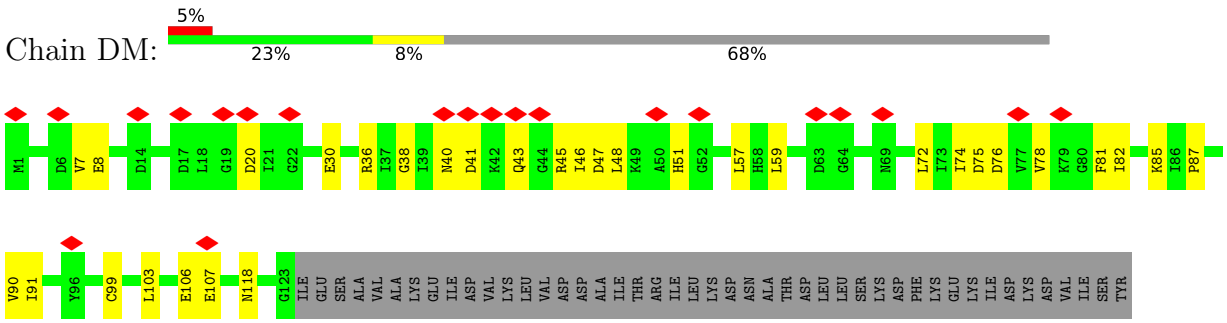
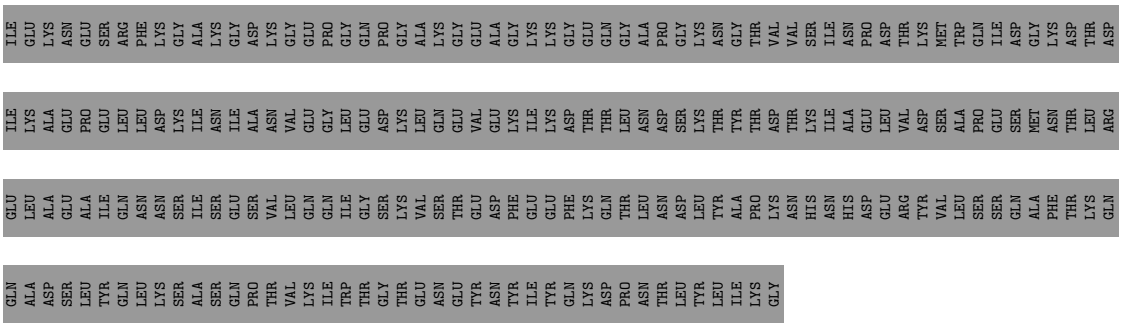
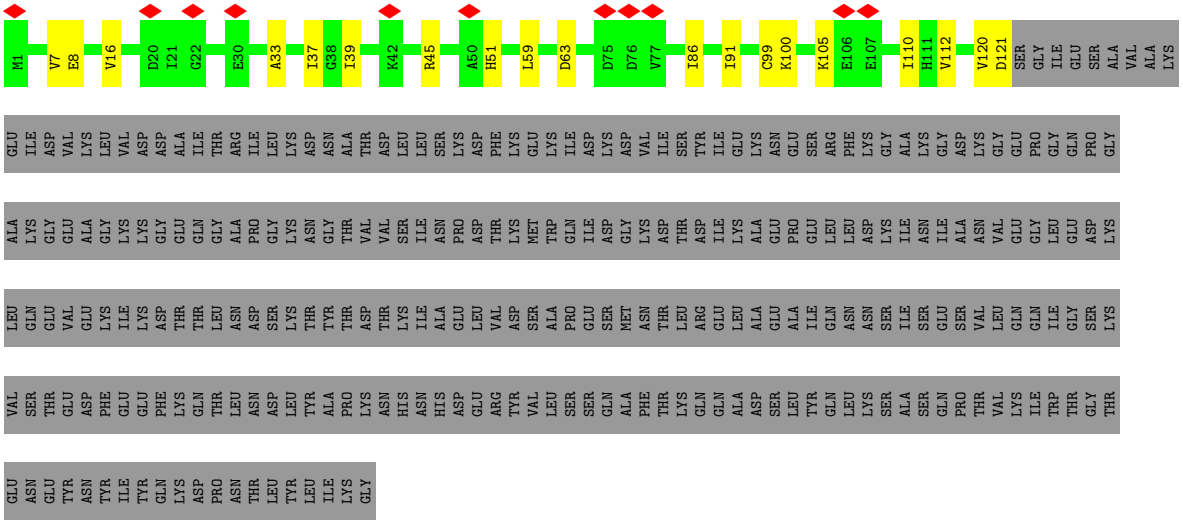




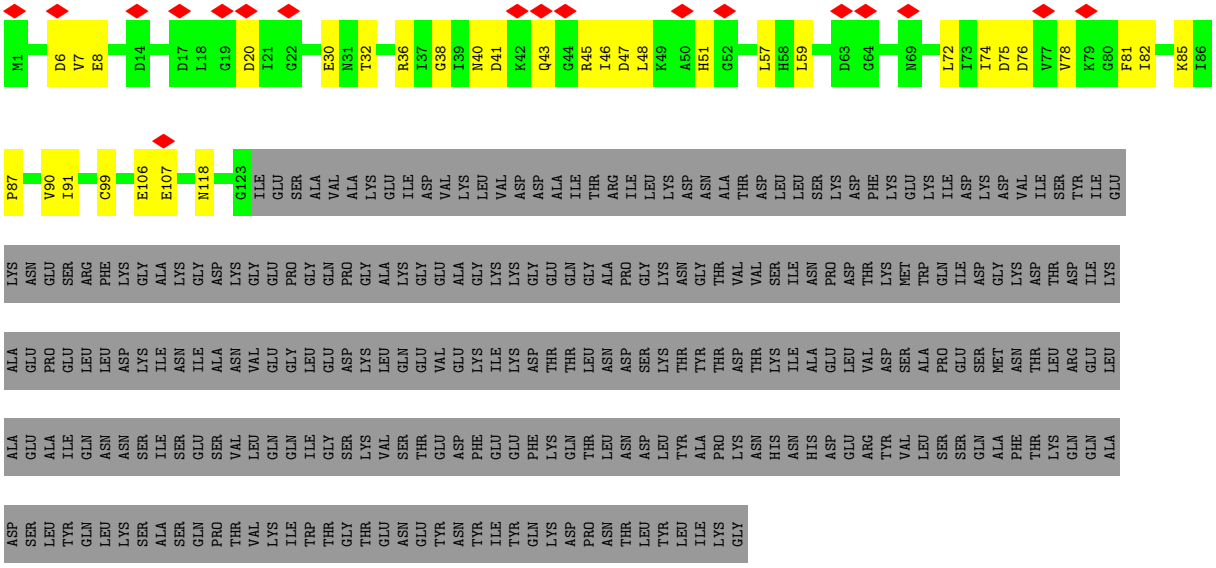
• Molecule 5: Fiber Upper, gp68

Chain AN:



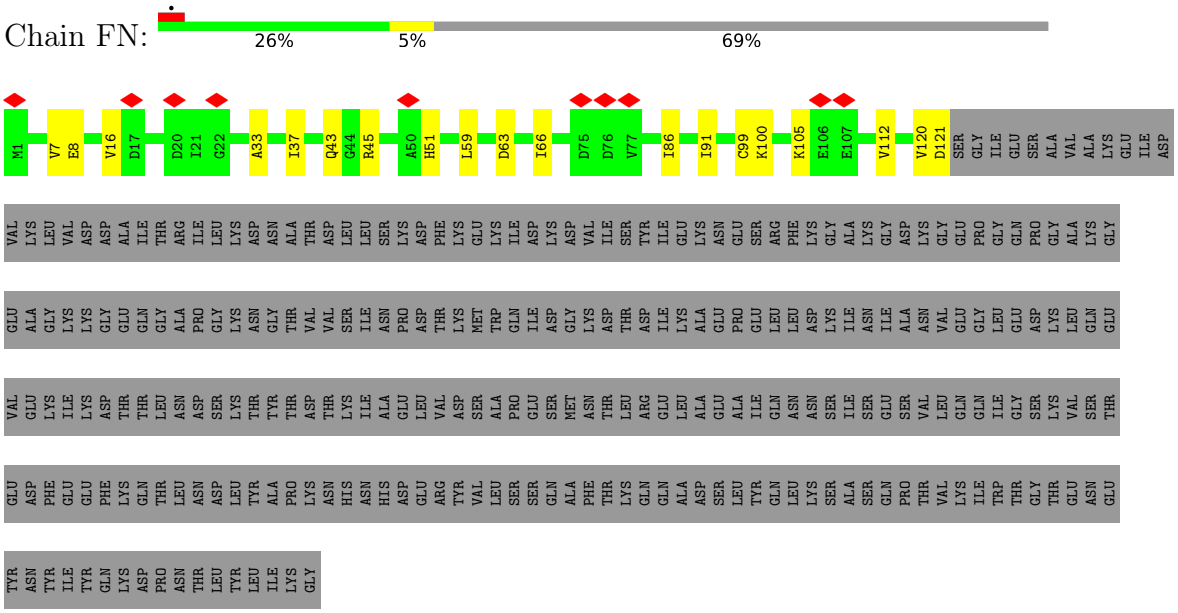
• Molecule 5: Fiber Upper, gp68

Chain AM:



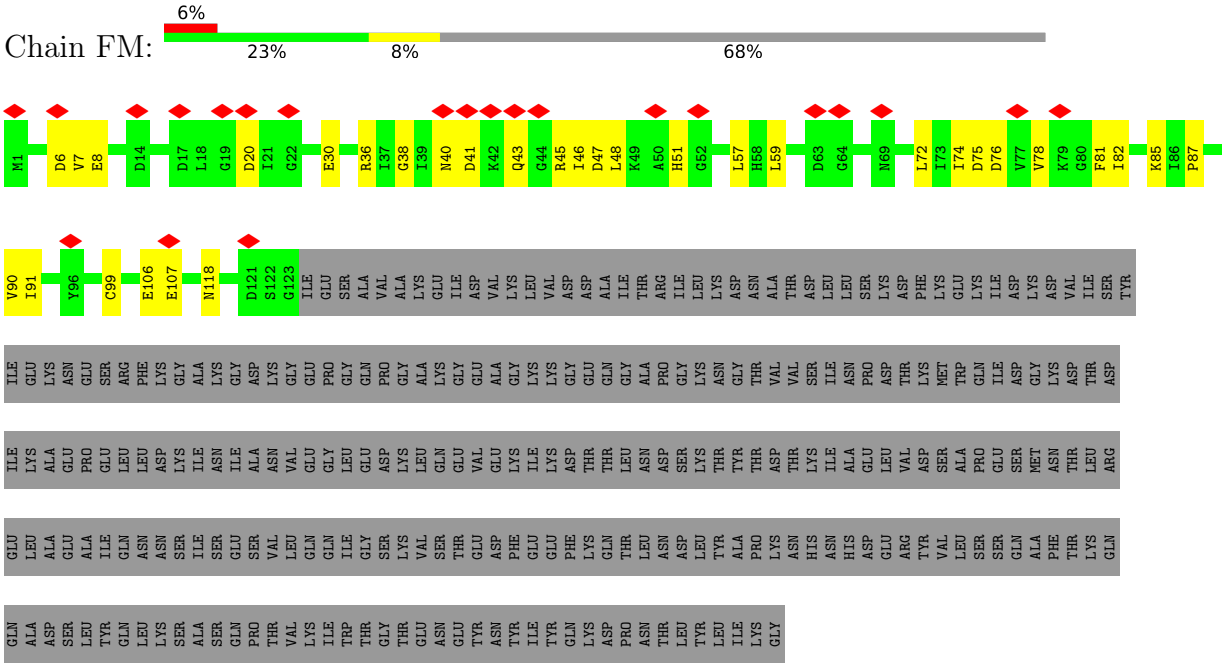
• Molecule 5: Fiber Upper, gp68

Chain FN:



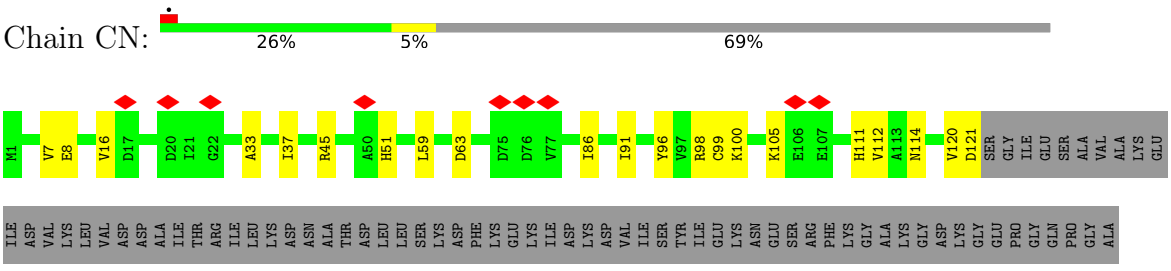
• Molecule 5: Fiber Upper, gp68

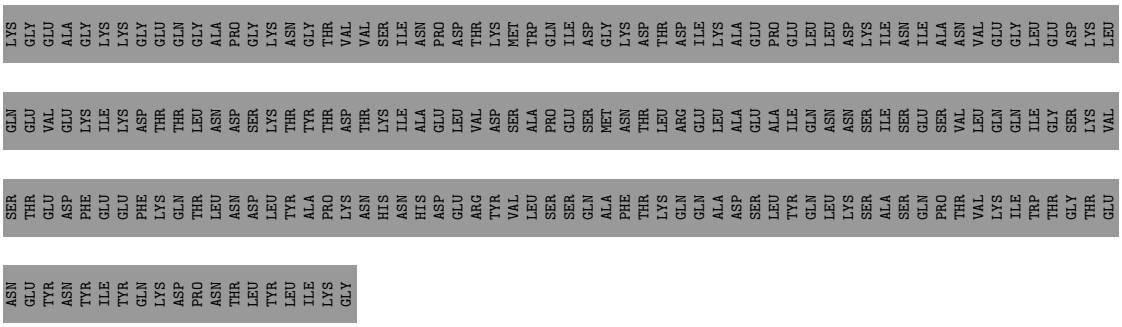
Chain FM:



• Molecule 5: Fiber Upper, gp68

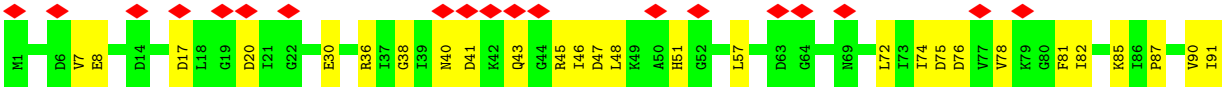
Chain CN:

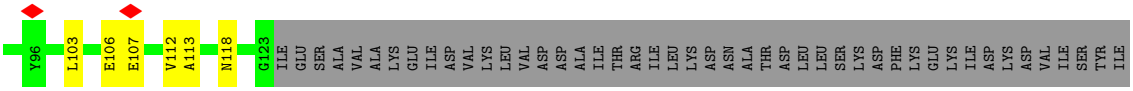




• Molecule 5: Fiber Upper, gp68

Chain CM:





• Molecule 5: Fiber Upper, gp68

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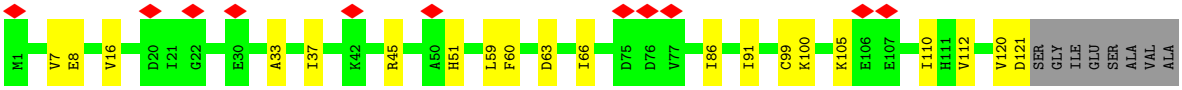
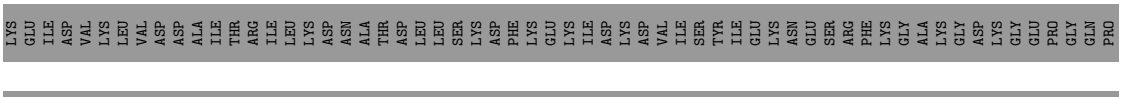
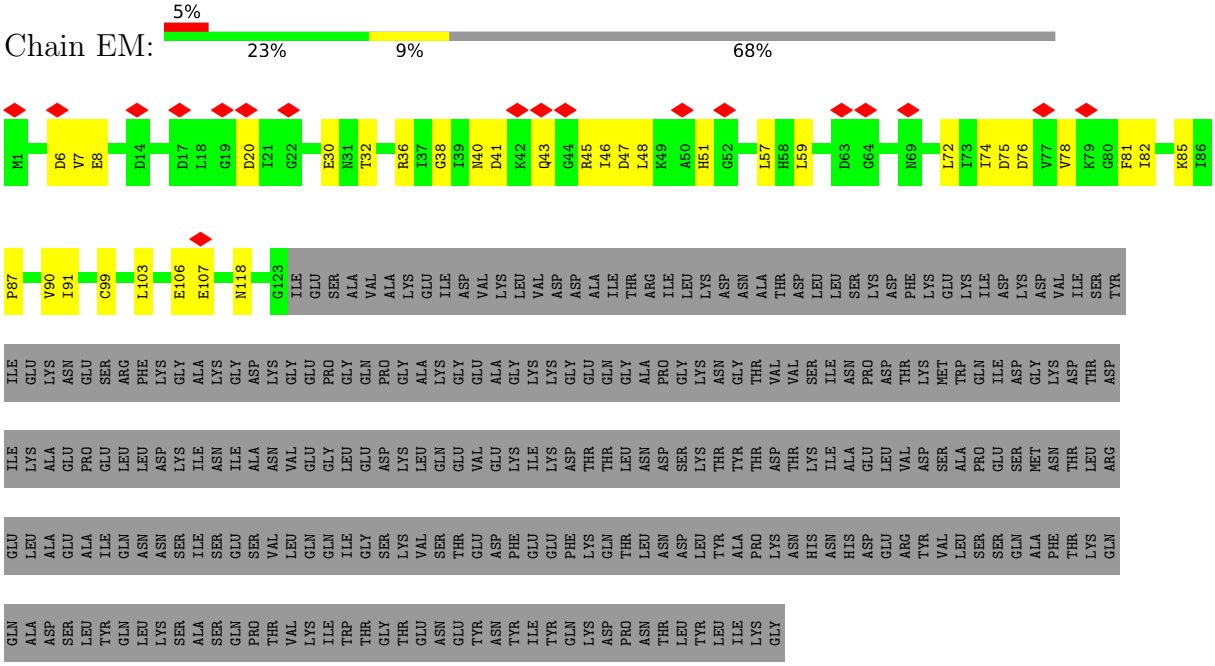




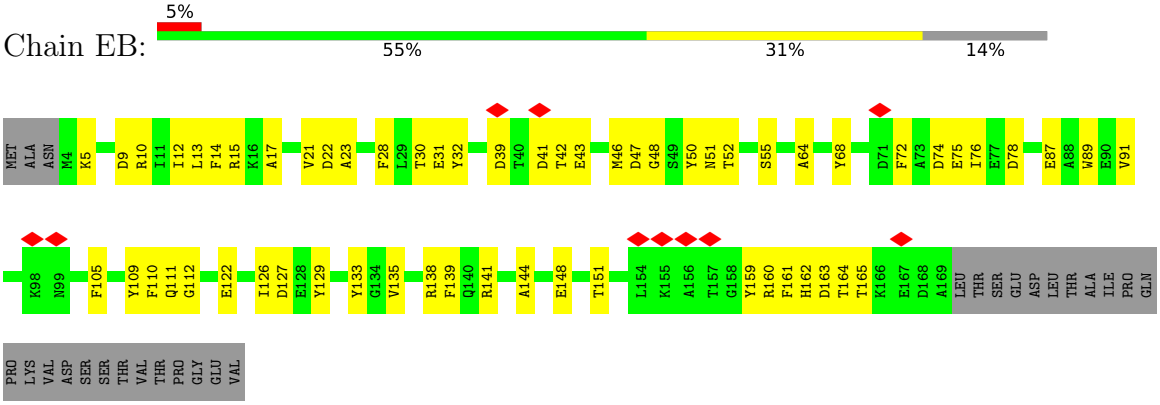
• Molecule 5: Fiber Upper, gp68

Chain EM:



• Molecule 6: Major Tail Protein, gp53

Chain EB:



• Molecule 6: Major Tail Protein, gp53

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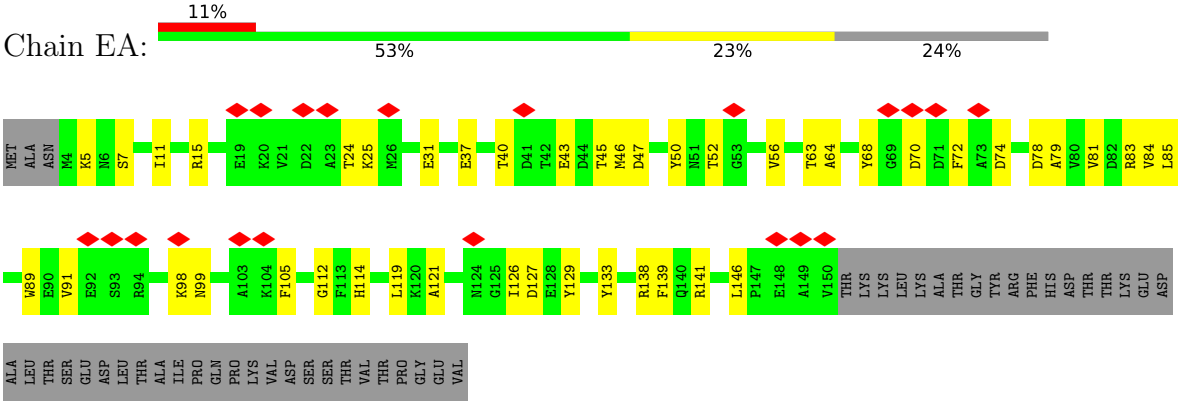
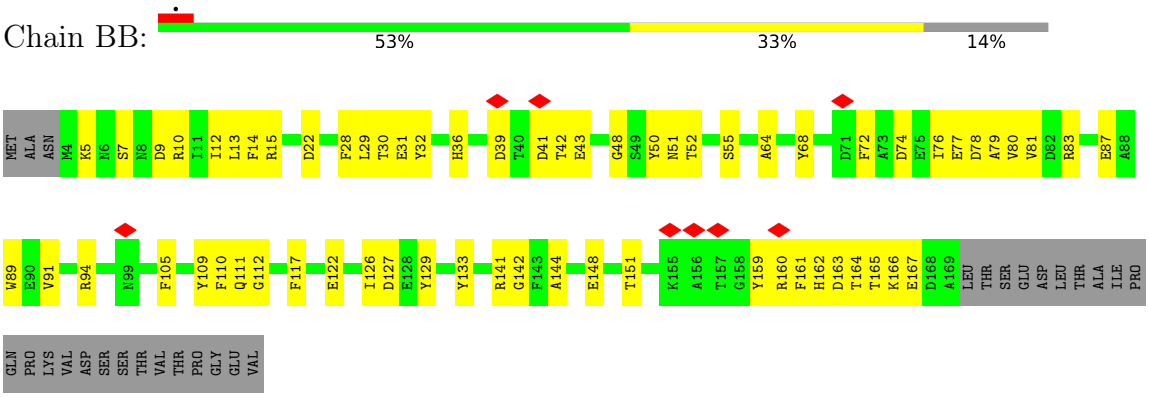


• Molecule 6: Major Tail Protein, gp53

Chain BB:



• Molecule 6: Major Tail Protein, gp53

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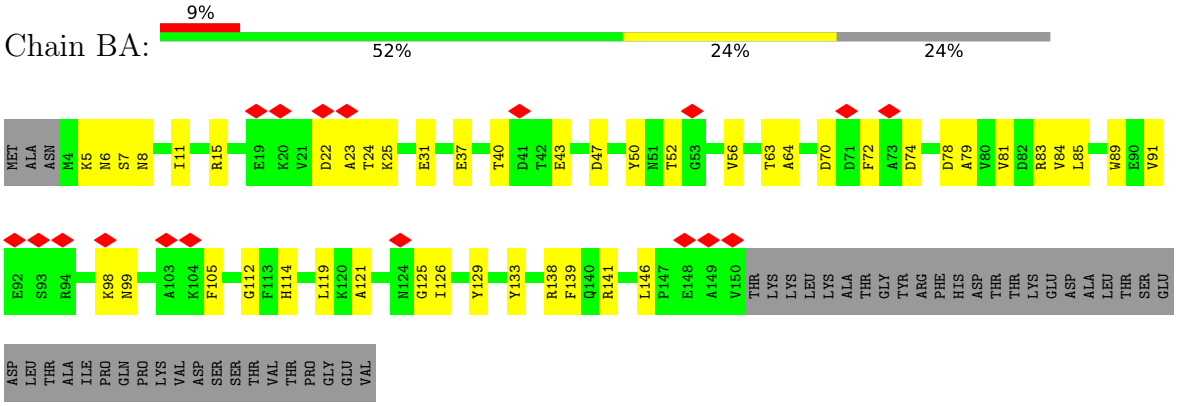
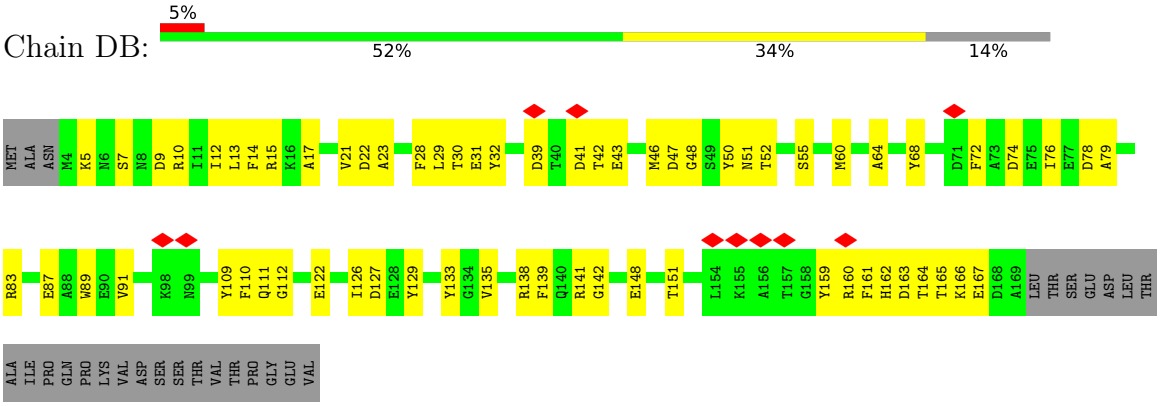


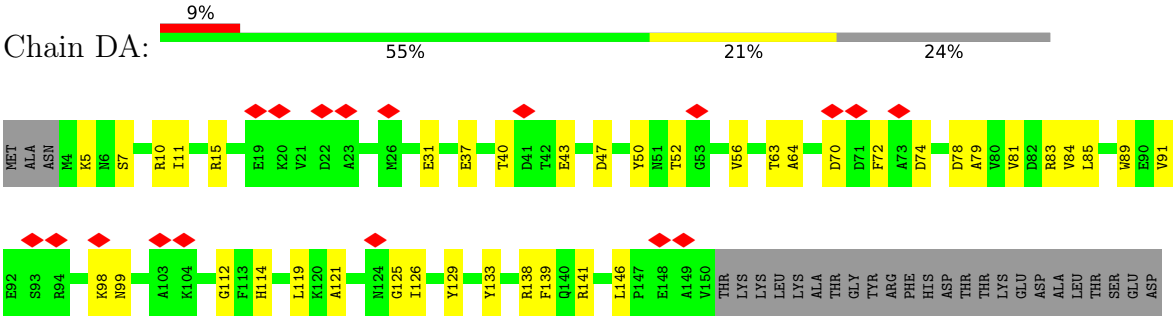
• Molecule 6: Major Tail Protein, gp53

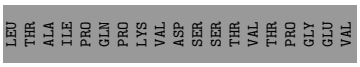
Chain DB:



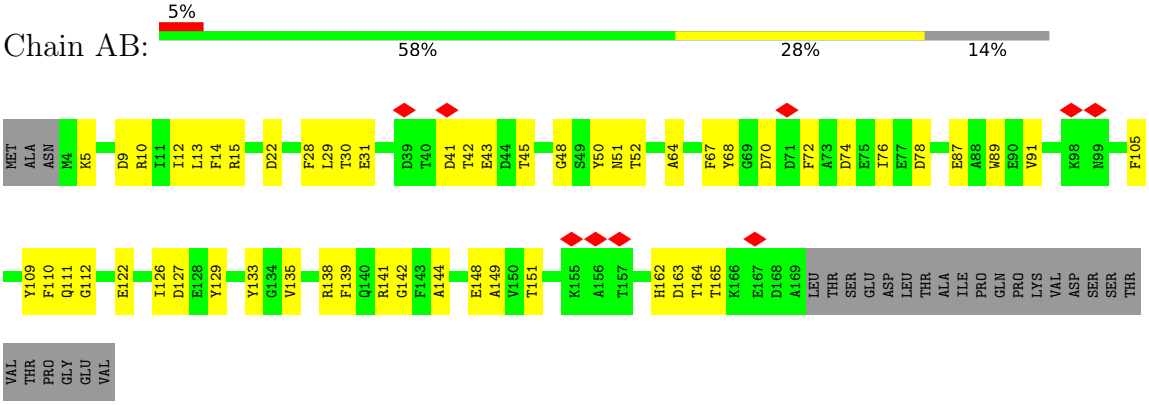
• Molecule 6: Major Tail Protein, gp53

Chain DA:

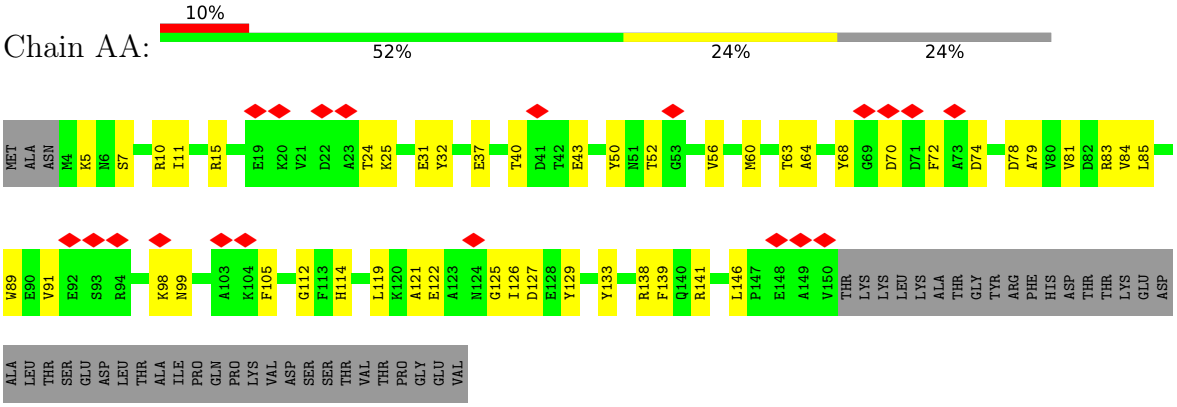




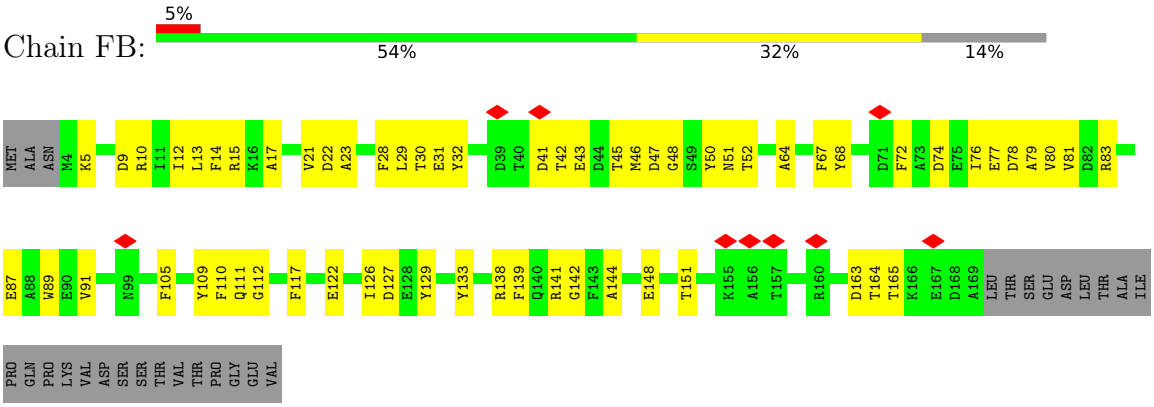
• Molecule 6: Major Tail Protein, gp53



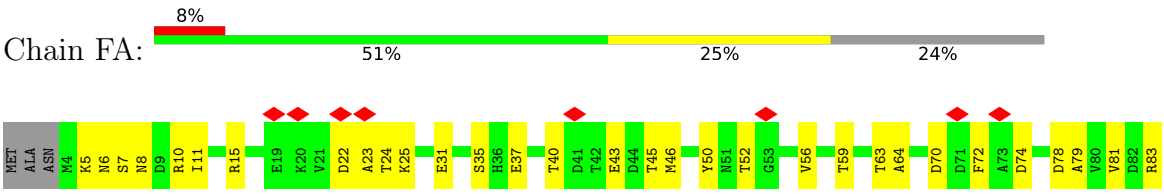
• Molecule 6: Major Tail Protein, gp53

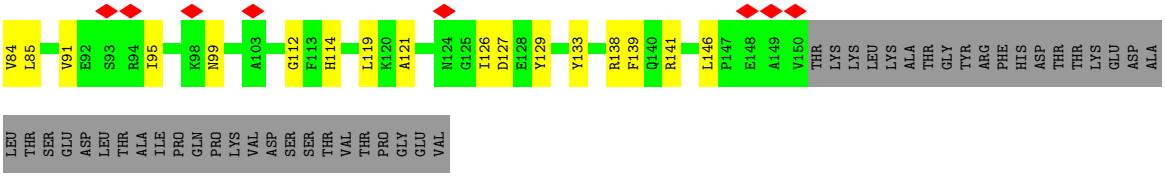


• Molecule 6: Major Tail Protein, gp53

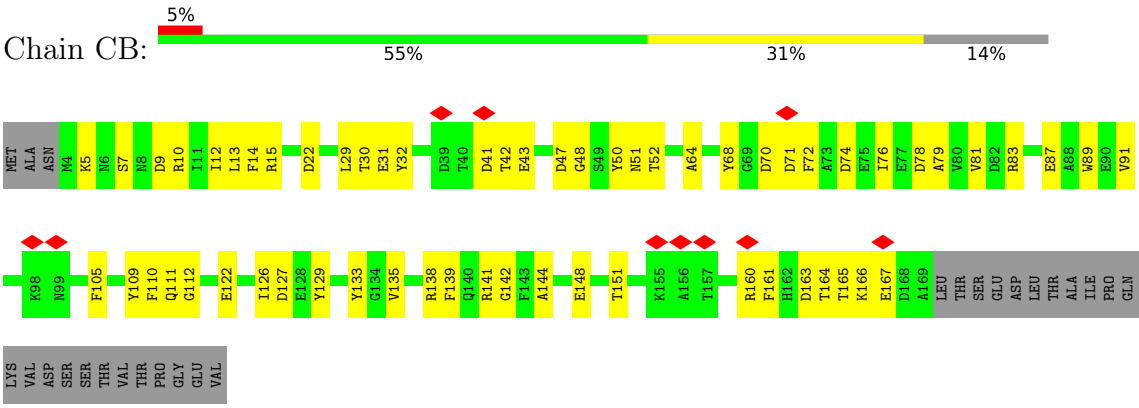


• Molecule 6: Major Tail Protein, gp53

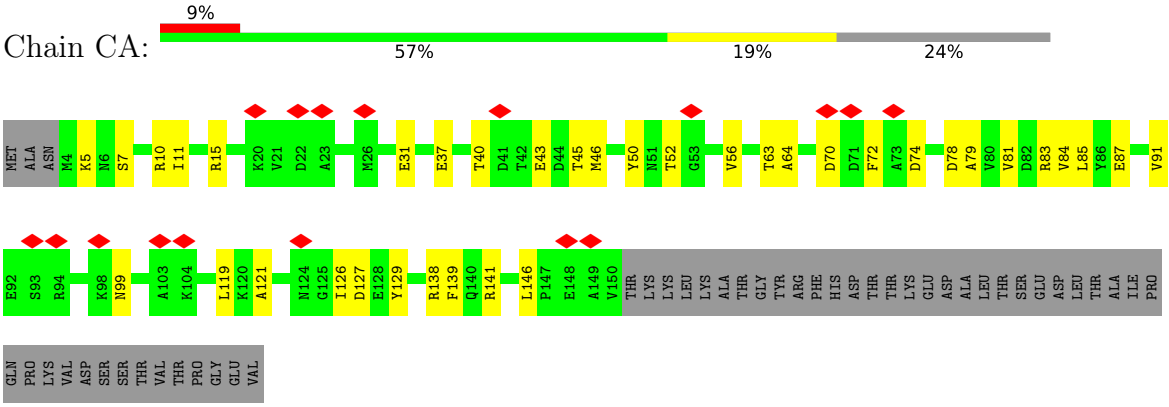




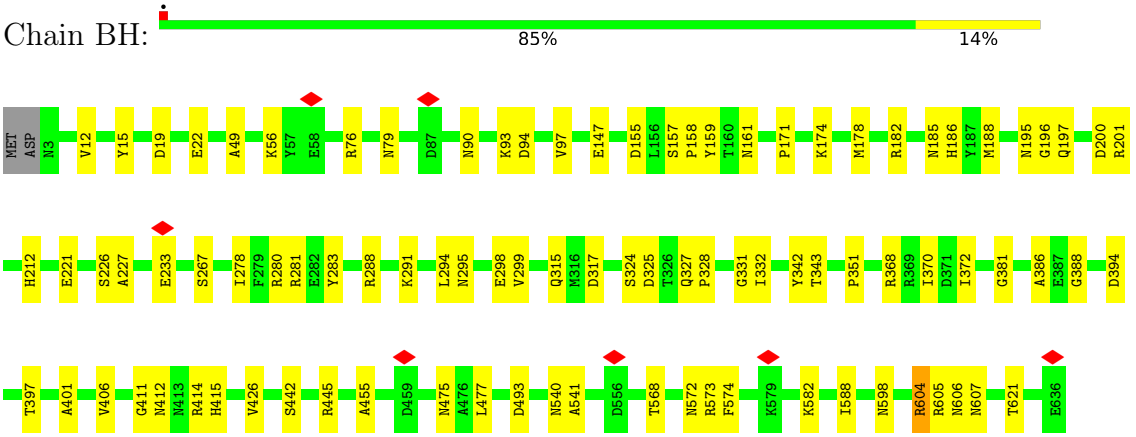
• Molecule 6: Major Tail Protein, gp53



• Molecule 6: Major Tail Protein, gp53

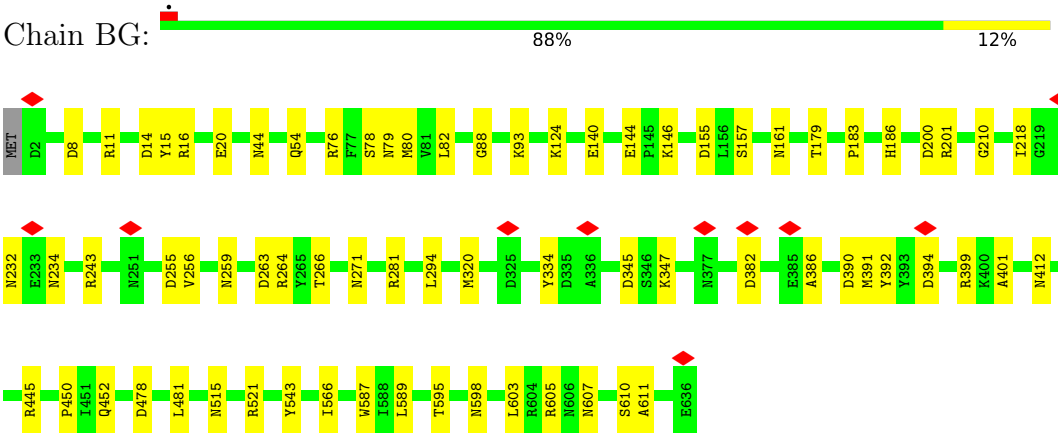


• Molecule 7: Receptor Binding Protein, gp61



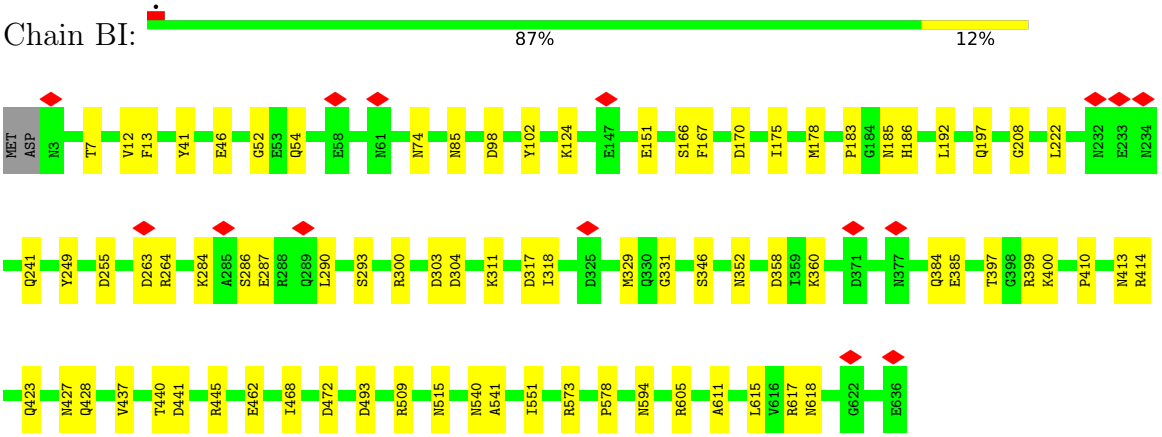
• Molecule 7: Receptor Binding Protein, gp61

Chain BG:



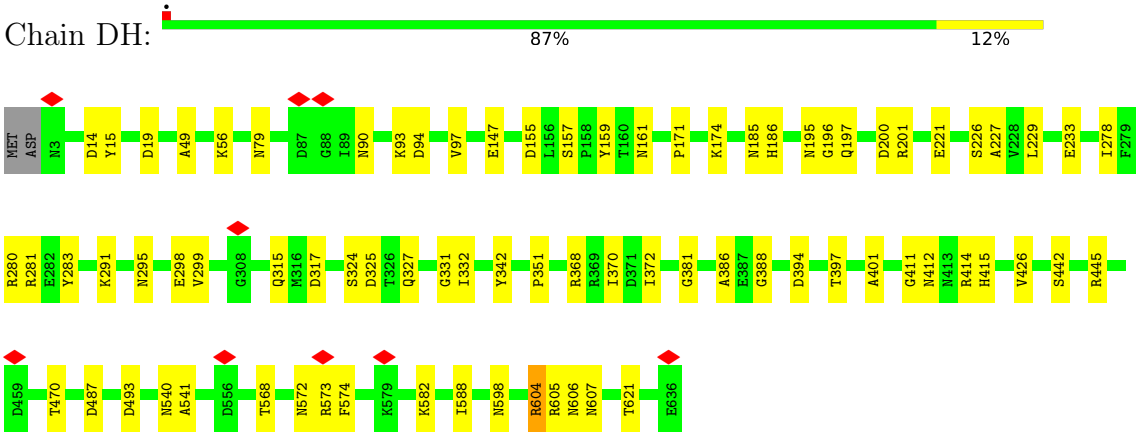
• Molecule 7: Receptor Binding Protein, gp61

Chain BI:



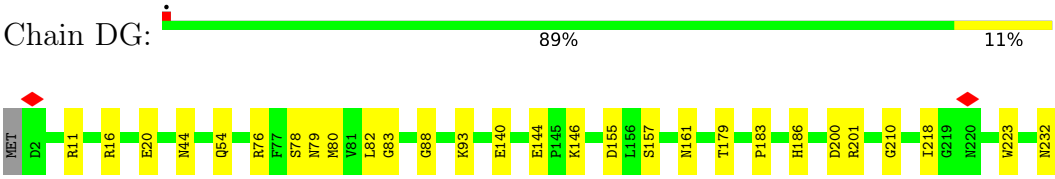
• Molecule 7: Receptor Binding Protein, gp61

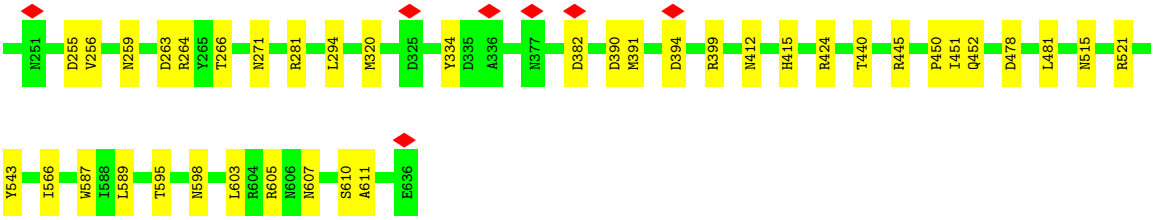
Chain DH:



• Molecule 7: Receptor Binding Protein, gp61

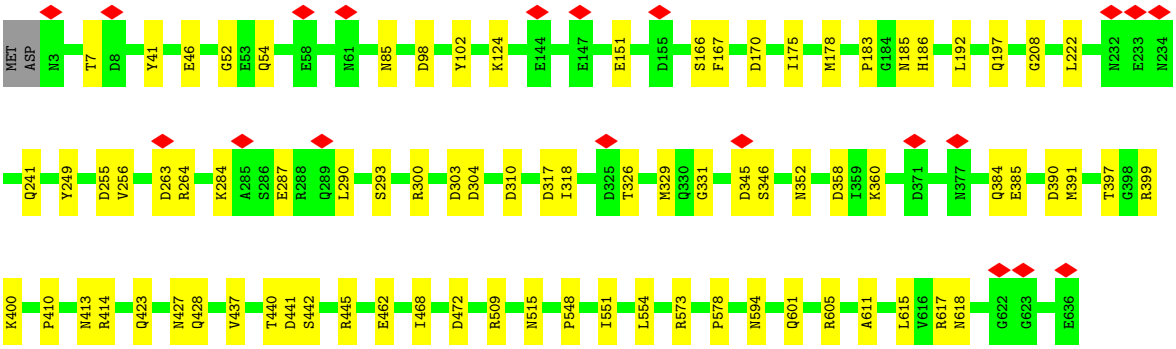
Chain DG:





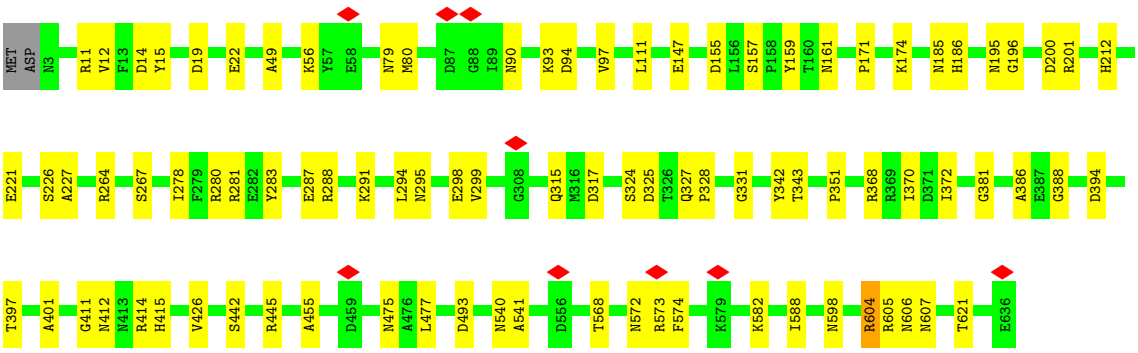
• Molecule 7: Receptor Binding Protein, gp61

Chain DI:



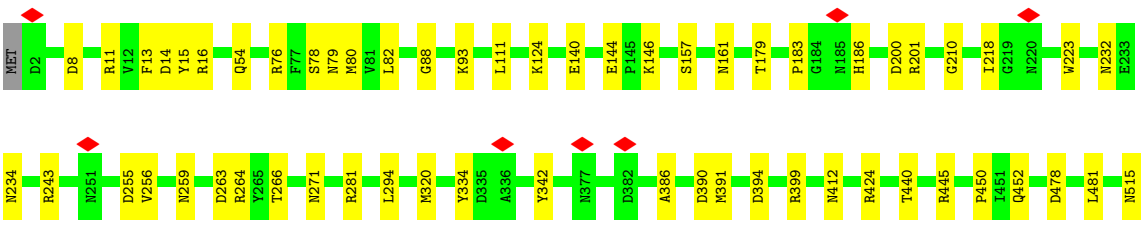
• Molecule 7: Receptor Binding Protein, gp61

Chain AH:



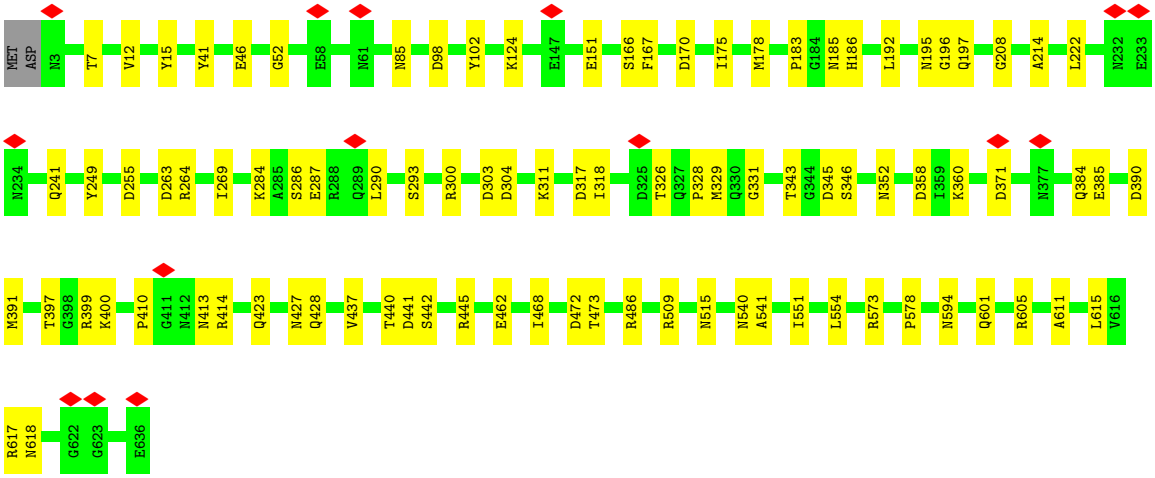
• Molecule 7: Receptor Binding Protein, gp61

Chain AG:



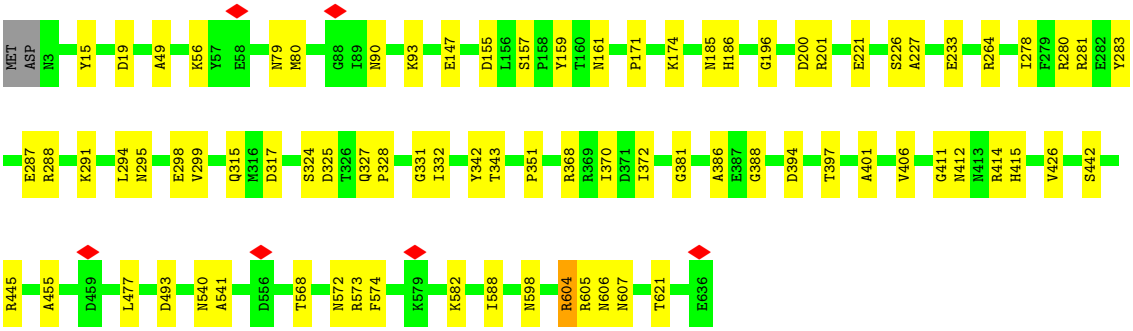
• Molecule 7: Receptor Binding Protein, gp61

Chain AI:



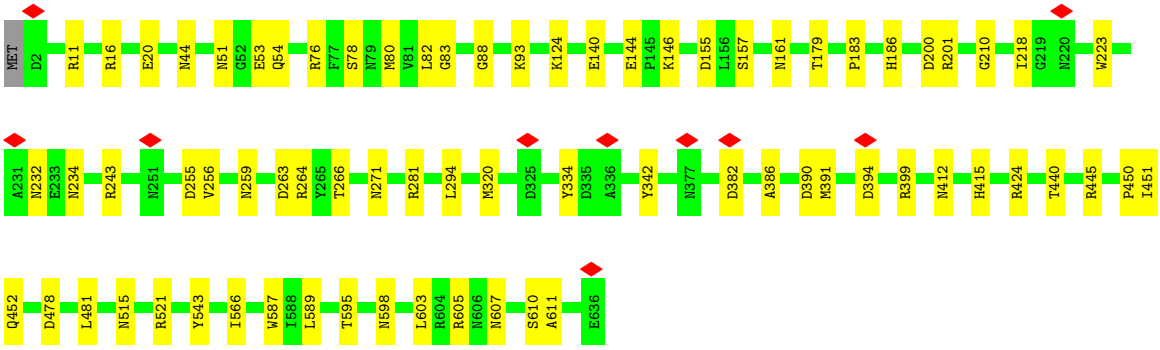
• Molecule 7: Receptor Binding Protein, gp61

Chain FH:



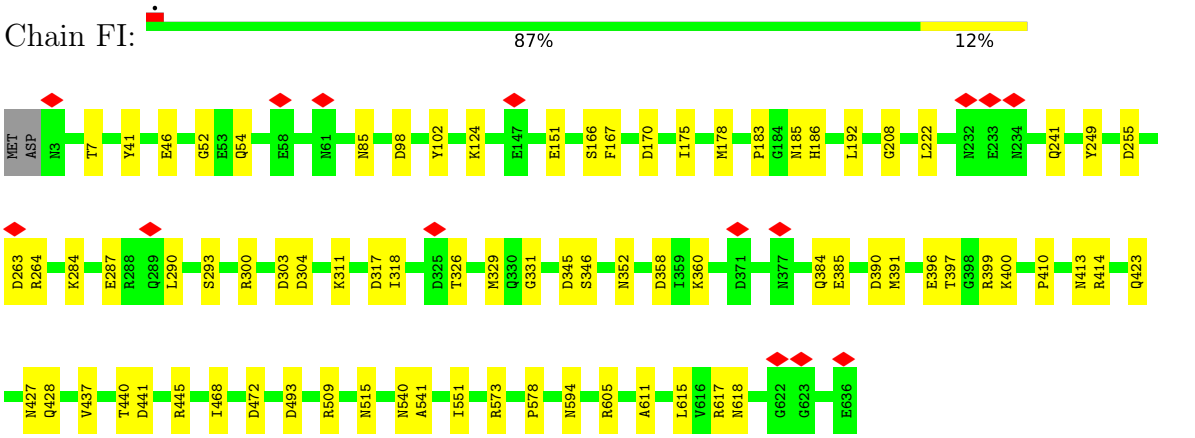
• Molecule 7: Receptor Binding Protein, gp61

Chain FG:



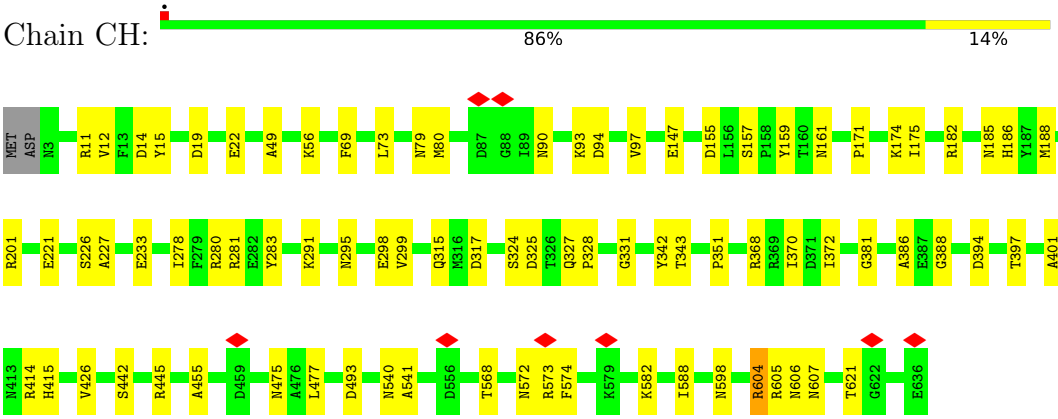
• Molecule 7: Receptor Binding Protein, gp61

Chain FI:



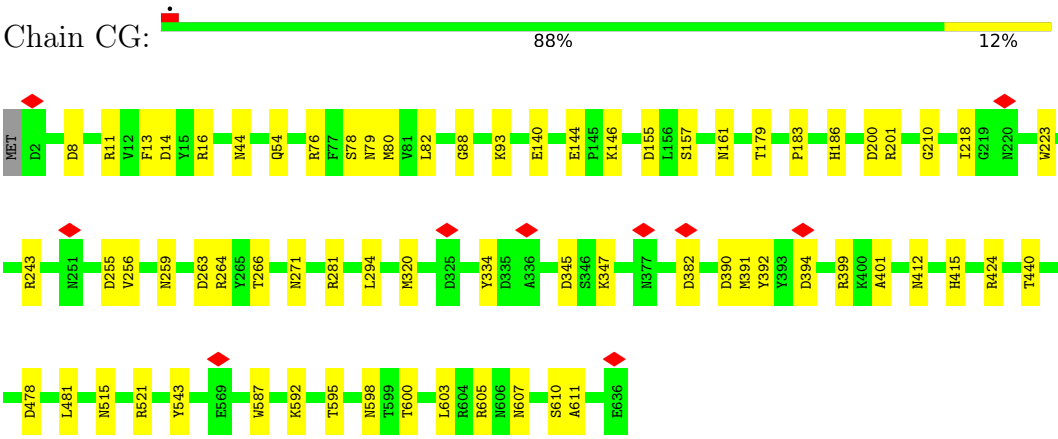
• Molecule 7: Receptor Binding Protein, gp61

Chain CH:



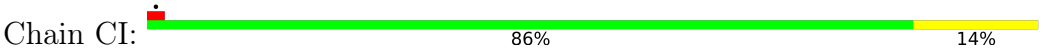
• Molecule 7: Receptor Binding Protein, gp61

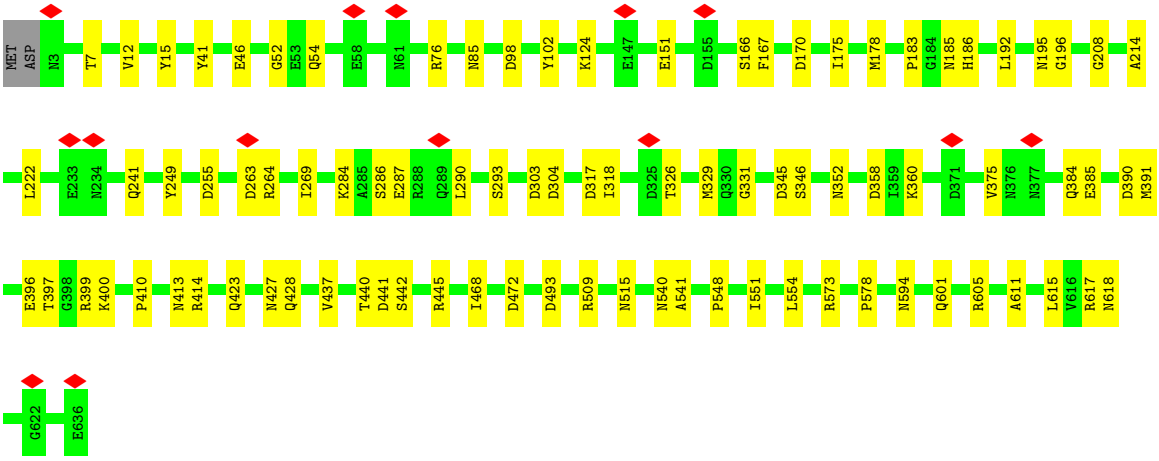
Chain CG:



• Molecule 7: Receptor Binding Protein, gp61

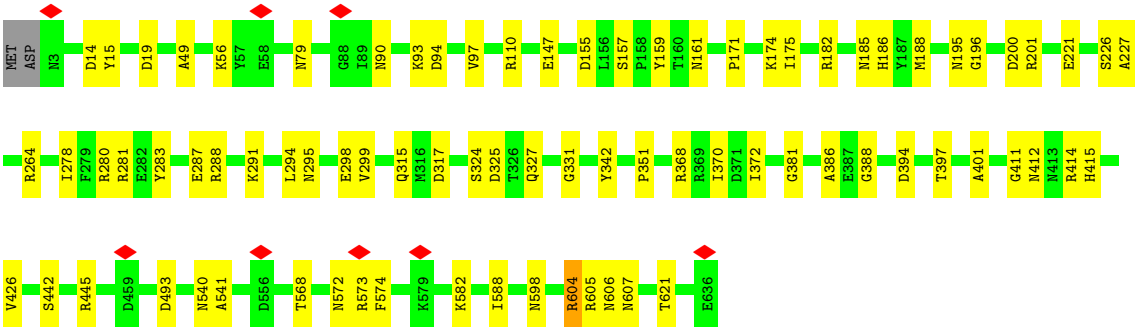
Chain CI:





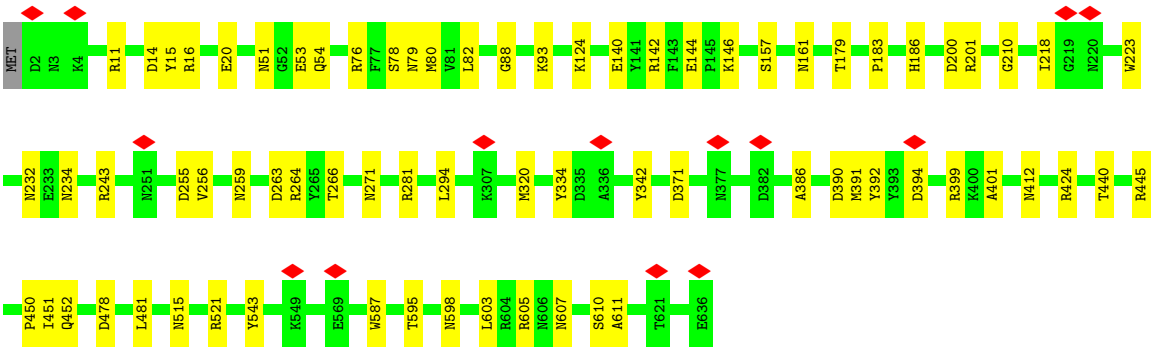
• Molecule 7: Receptor Binding Protein, gp61

Chain EH:



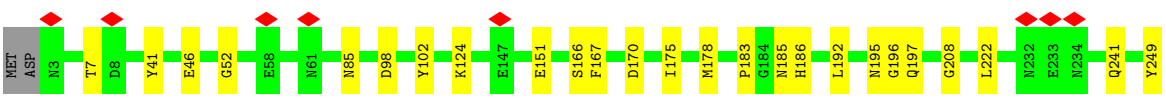
• Molecule 7: Receptor Binding Protein, gp61

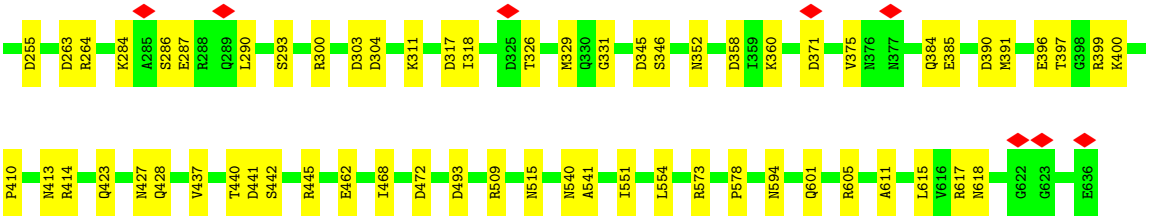
Chain EG:



• Molecule 7: Receptor Binding Protein, gp61

Chain EI:




D255
D263
R264
K284
A285
S286
E287
R288
Q289
L290
S293
R300
D303
D304
K311
D317
I318
D325
T326
M329
Q330
G331
D345
S346
N352
D358
I359
K360
D371
V375
N376
N377
Q384
E385
D390
M391
E396
T397
G398
R399
K400
P410
N413
R414
Q423
N427
Q428
V437
T440
D441
S442
R445
E462
I468
D472
D493
R509
N515
N540
A541
I551
L554
R573
P578
N594
Q601
R605
A611
L615
V616
R617
N618
G622
G623
E636

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	43601	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	104.33	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	3700	Depositor
Magnification	29000	Depositor
Image detector	DIRECT ELECTRON DE-20 (5k x 3k)	Depositor
Maximum map value	30.060	Depositor
Minimum map value	-18.991	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.967	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	619.52, 619.52, 619.52	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.21, 1.21, 1.21	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: FE

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	AC	0.54	0/2658	0.64	0/3579
1	AD	0.54	0/2658	0.64	0/3579
1	BC	0.54	0/2658	0.64	0/3579
1	BD	0.54	0/2658	0.64	0/3579
1	CC	0.54	0/2658	0.64	0/3579
1	CD	0.54	0/2658	0.64	0/3579
2	AE	0.49	0/3116	0.63	0/4198
2	BE	0.49	0/3116	0.64	0/4198
2	CE	0.49	0/3116	0.63	0/4198
3	AF	0.45	0/161	0.68	0/216
3	BF	0.45	0/161	0.67	0/216
3	CF	0.45	0/161	0.68	0/216
4	AJ	0.28	0/1353	0.46	0/1833
4	AK	0.28	0/1518	0.45	0/2055
4	AL	0.26	0/1451	0.44	0/1964
4	BJ	0.29	0/1353	0.45	0/1833
4	BK	0.28	0/1518	0.45	0/2055
4	BL	0.26	0/1451	0.43	0/1964
4	CJ	0.28	0/1353	0.46	0/1833
4	CK	0.28	0/1518	0.45	0/2055
4	CL	0.26	0/1451	0.43	0/1964
4	DJ	0.28	0/1353	0.45	0/1833
4	DK	0.28	0/1518	0.45	0/2055
4	DL	0.26	0/1451	0.43	0/1964
4	EJ	0.28	0/1353	0.45	0/1833
4	EK	0.28	0/1518	0.45	0/2055
4	EL	0.26	0/1451	0.43	0/1964
4	FJ	0.29	0/1353	0.45	0/1833
4	FK	0.28	0/1518	0.45	0/2055
4	FL	0.26	0/1451	0.43	0/1964
5	AM	0.26	0/1008	0.46	0/1351
5	AN	0.25	0/998	0.46	0/1338

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
5	BM	0.26	0/1008	0.45	0/1351
5	BN	0.26	0/998	0.46	0/1338
5	CM	0.25	0/1008	0.46	0/1351
5	CN	0.25	0/998	0.45	0/1338
5	DM	0.26	0/1008	0.47	0/1351
5	DN	0.25	0/998	0.45	0/1338
5	EM	0.26	0/1008	0.45	0/1351
5	EN	0.25	0/998	0.46	0/1338
5	FM	0.26	0/1008	0.45	0/1351
5	FN	0.26	0/998	0.46	0/1338
6	AA	0.43	0/1188	0.49	0/1596
6	AB	0.63	0/1346	0.54	0/1807
6	BA	0.43	0/1188	0.49	0/1596
6	BB	0.62	1/1346 (0.1%)	0.54	0/1807
6	CA	0.43	0/1188	0.49	0/1596
6	CB	0.62	0/1346	0.54	0/1807
6	DA	0.43	0/1188	0.49	0/1596
6	DB	0.62	0/1346	0.54	0/1807
6	EA	0.43	0/1188	0.49	0/1596
6	EB	0.63	0/1346	0.54	0/1807
6	FA	0.44	0/1188	0.49	0/1596
6	FB	0.62	0/1346	0.54	0/1807
7	AG	0.42	0/5332	0.56	0/7216
7	AH	0.44	0/5324	0.58	1/7205 (0.0%)
7	AI	0.44	0/5324	0.58	1/7205 (0.0%)
7	BG	0.44	0/5332	0.58	1/7216 (0.0%)
7	BH	0.45	0/5324	0.58	1/7205 (0.0%)
7	BI	0.45	0/5324	0.59	1/7205 (0.0%)
7	CG	0.43	0/5332	0.57	0/7216
7	CH	0.45	0/5324	0.58	1/7205 (0.0%)
7	CI	0.45	0/5324	0.59	2/7205 (0.0%)
7	DG	0.43	0/5332	0.57	0/7216
7	DH	0.45	0/5324	0.58	1/7205 (0.0%)
7	DI	0.45	0/5324	0.59	1/7205 (0.0%)
7	EG	0.43	0/5332	0.57	0/7216
7	EH	0.44	0/5324	0.58	2/7205 (0.0%)
7	EI	0.44	0/5324	0.59	1/7205 (0.0%)
7	FG	0.43	0/5332	0.57	0/7216
7	FH	0.45	0/5324	0.58	1/7205 (0.0%)
7	FI	0.44	0/5324	0.58	1/7205 (0.0%)
All	All	0.43	1/174831 (0.0%)	0.56	15/236136 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	BB	36	HIS	CA-CB	-5.21	1.42	1.53

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	CI	76	ARG	NE-CZ-NH2	-6.13	117.23	120.30
7	EH	110	ARG	NE-CZ-NH2	-5.77	117.41	120.30
7	BG	386	ALA	CB-CA-C	5.25	117.98	110.10
7	BI	617	ARG	NE-CZ-NH2	5.20	122.90	120.30
7	FH	604	ARG	NE-CZ-NH2	5.16	122.88	120.30

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	AC	2601	0	2549	88	0
1	AD	2601	0	2550	121	0
1	BC	2601	0	2549	92	0
1	BD	2601	0	2550	118	0
1	CC	2601	0	2549	91	0
1	CD	2601	0	2550	120	0
2	AE	3068	0	3098	30	0
2	BE	3068	0	3098	32	0
2	CE	3068	0	3098	33	0
3	AF	160	0	156	3	0
3	BF	160	0	156	6	0
3	CF	160	0	156	8	0
4	AJ	1331	0	1292	32	0
4	AK	1496	0	1470	35	0
4	AL	1430	0	1406	58	0
4	BJ	1331	0	1292	39	0
4	BK	1496	0	1470	34	0
4	BL	1430	0	1406	69	0
4	CJ	1331	0	1292	33	0
4	CK	1496	0	1470	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CL	1430	0	1406	63	0
4	DJ	1331	0	1292	36	0
4	DK	1496	0	1470	31	0
4	DL	1430	0	1406	63	0
4	EJ	1331	0	1292	35	0
4	EK	1496	0	1470	37	0
4	EL	1430	0	1406	63	0
4	FJ	1331	0	1292	34	0
4	FK	1496	0	1470	33	0
4	FL	1430	0	1406	62	0
5	AM	991	0	1010	40	0
5	AN	981	0	1002	14	0
5	BM	991	0	1010	41	0
5	BN	981	0	1002	24	0
5	CM	991	0	1010	47	0
5	CN	981	0	1002	14	0
5	DM	991	0	1010	44	0
5	DN	981	0	1002	17	0
5	EM	991	0	1010	44	0
5	EN	981	0	1002	15	0
5	FM	991	0	1010	43	0
5	FN	981	0	1002	15	0
6	AA	1165	0	1085	39	0
6	AB	1320	0	1241	86	0
6	BA	1165	0	1085	40	0
6	BB	1320	0	1241	90	0
6	CA	1165	0	1085	29	0
6	CB	1320	0	1241	85	0
6	DA	1165	0	1085	38	0
6	DB	1320	0	1241	102	0
6	EA	1165	0	1085	38	0
6	EB	1320	0	1241	104	0
6	FA	1165	0	1085	37	0
6	FB	1320	0	1241	107	0
7	AG	5201	0	5001	51	0
7	AH	5193	0	4997	84	0
7	AI	5193	0	4997	60	0
7	BG	5201	0	5001	51	0
7	BH	5193	0	4997	80	0
7	BI	5193	0	4997	50	0
7	CG	5201	0	5001	52	0
7	CH	5193	0	4997	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	CI	5193	0	4997	57	0
7	DG	5201	0	5001	50	0
7	DH	5193	0	4997	59	0
7	DI	5193	0	4997	52	0
7	EG	5201	0	5001	50	0
7	EH	5193	0	4997	58	0
7	EI	5193	0	4997	58	0
7	FG	5201	0	5001	49	0
7	FH	5193	0	4997	62	0
7	FI	5193	0	4997	50	0
8	AH	1	0	0	0	0
8	BH	1	0	0	0	0
8	CH	1	0	0	0	0
8	DH	1	0	0	0	0
8	EH	1	0	0	0	0
8	FH	1	0	0	0	0
All	All	171102	0	166065	2715	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 8.

The worst 5 of 2715 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)
4:BL:58:HIS:CE1	5:BN:43:GLN:HG2	1.29	1.66
4:BL:58:HIS:ND1	5:BN:43:GLN:HG2	1.41	1.35
4:FL:174:THR:OG1	7:FH:90:ASN:ND2	1.63	1.31
1:CD:149:GLN:NE2	6:AB:41:ASP:OD1	1.64	1.28
1:AD:149:GLN:NE2	6:BB:41:ASP:OD1	1.63	1.28

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	AC	312/315 (99%)	278 (89%)	34 (11%)	0	100	100
1	AD	312/315 (99%)	278 (89%)	34 (11%)	0	100	100
1	BC	312/315 (99%)	278 (89%)	34 (11%)	0	100	100
1	BD	312/315 (99%)	278 (89%)	34 (11%)	0	100	100
1	CC	312/315 (99%)	278 (89%)	34 (11%)	0	100	100
1	CD	312/315 (99%)	278 (89%)	34 (11%)	0	100	100
2	AE	385/633 (61%)	339 (88%)	46 (12%)	0	100	100
2	BE	385/633 (61%)	339 (88%)	46 (12%)	0	100	100
2	CE	385/633 (61%)	339 (88%)	46 (12%)	0	100	100
3	AF	18/1154 (2%)	17 (94%)	1 (6%)	0	100	100
3	BF	18/1154 (2%)	17 (94%)	1 (6%)	0	100	100
3	CF	18/1154 (2%)	17 (94%)	1 (6%)	0	100	100
4	AJ	165/607 (27%)	137 (83%)	28 (17%)	0	100	100
4	AK	187/607 (31%)	169 (90%)	18 (10%)	0	100	100
4	AL	179/607 (30%)	158 (88%)	21 (12%)	0	100	100
4	BJ	165/607 (27%)	133 (81%)	32 (19%)	0	100	100
4	BK	187/607 (31%)	166 (89%)	21 (11%)	0	100	100
4	BL	179/607 (30%)	157 (88%)	22 (12%)	0	100	100
4	CJ	165/607 (27%)	136 (82%)	28 (17%)	1 (1%)	25	62
4	CK	187/607 (31%)	169 (90%)	18 (10%)	0	100	100
4	CL	179/607 (30%)	159 (89%)	20 (11%)	0	100	100
4	DJ	165/607 (27%)	136 (82%)	29 (18%)	0	100	100
4	DK	187/607 (31%)	168 (90%)	19 (10%)	0	100	100
4	DL	179/607 (30%)	160 (89%)	19 (11%)	0	100	100
4	EJ	165/607 (27%)	137 (83%)	28 (17%)	0	100	100
4	EK	187/607 (31%)	166 (89%)	21 (11%)	0	100	100
4	EL	179/607 (30%)	158 (88%)	21 (12%)	0	100	100
4	FJ	165/607 (27%)	133 (81%)	32 (19%)	0	100	100
4	FK	187/607 (31%)	166 (89%)	21 (11%)	0	100	100
4	FL	179/607 (30%)	158 (88%)	21 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AM	121/390 (31%)	102 (84%)	19 (16%)	0	100	100
5	AN	119/390 (30%)	103 (87%)	16 (13%)	0	100	100
5	BM	121/390 (31%)	101 (84%)	20 (16%)	0	100	100
5	BN	119/390 (30%)	106 (89%)	13 (11%)	0	100	100
5	CM	121/390 (31%)	101 (84%)	20 (16%)	0	100	100
5	CN	119/390 (30%)	104 (87%)	15 (13%)	0	100	100
5	DM	121/390 (31%)	100 (83%)	21 (17%)	0	100	100
5	DN	119/390 (30%)	104 (87%)	15 (13%)	0	100	100
5	EM	121/390 (31%)	102 (84%)	19 (16%)	0	100	100
5	EN	119/390 (30%)	103 (87%)	16 (13%)	0	100	100
5	FM	121/390 (31%)	102 (84%)	19 (16%)	0	100	100
5	FN	119/390 (30%)	106 (89%)	13 (11%)	0	100	100
6	AA	145/193 (75%)	139 (96%)	6 (4%)	0	100	100
6	AB	164/193 (85%)	152 (93%)	12 (7%)	0	100	100
6	BA	145/193 (75%)	140 (97%)	5 (3%)	0	100	100
6	BB	164/193 (85%)	147 (90%)	17 (10%)	0	100	100
6	CA	145/193 (75%)	142 (98%)	3 (2%)	0	100	100
6	CB	164/193 (85%)	146 (89%)	18 (11%)	0	100	100
6	DA	145/193 (75%)	142 (98%)	3 (2%)	0	100	100
6	DB	164/193 (85%)	149 (91%)	15 (9%)	0	100	100
6	EA	145/193 (75%)	139 (96%)	6 (4%)	0	100	100
6	EB	164/193 (85%)	150 (92%)	14 (8%)	0	100	100
6	FA	145/193 (75%)	141 (97%)	4 (3%)	0	100	100
6	FB	164/193 (85%)	148 (90%)	16 (10%)	0	100	100
7	AG	633/636 (100%)	567 (90%)	65 (10%)	1 (0%)	47	78
7	AH	632/636 (99%)	576 (91%)	56 (9%)	0	100	100
7	AI	632/636 (99%)	579 (92%)	53 (8%)	0	100	100
7	BG	633/636 (100%)	570 (90%)	62 (10%)	1 (0%)	47	78
7	BH	632/636 (99%)	576 (91%)	56 (9%)	0	100	100
7	BI	632/636 (99%)	581 (92%)	51 (8%)	0	100	100
7	CG	633/636 (100%)	567 (90%)	65 (10%)	1 (0%)	47	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	CH	632/636 (99%)	577 (91%)	55 (9%)	0	100	100
7	CI	632/636 (99%)	582 (92%)	50 (8%)	0	100	100
7	DG	633/636 (100%)	567 (90%)	65 (10%)	1 (0%)	47	78
7	DH	632/636 (99%)	576 (91%)	56 (9%)	0	100	100
7	DI	632/636 (99%)	582 (92%)	50 (8%)	0	100	100
7	EG	633/636 (100%)	570 (90%)	62 (10%)	1 (0%)	47	78
7	EH	632/636 (99%)	576 (91%)	56 (9%)	0	100	100
7	EI	632/636 (99%)	580 (92%)	52 (8%)	0	100	100
7	FG	633/636 (100%)	569 (90%)	63 (10%)	1 (0%)	47	78
7	FH	632/636 (99%)	571 (90%)	61 (10%)	0	100	100
7	FI	632/636 (99%)	578 (92%)	54 (8%)	0	100	100
All	All	20943/36621 (57%)	18815 (90%)	2121 (10%)	7 (0%)	100	100

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	DG	481	LEU
7	CG	481	LEU
7	BG	481	LEU
7	AG	481	LEU
7	FG	481	LEU

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	AC	288/290 (99%)	285 (99%)	3 (1%)	76	86
1	AD	288/290 (99%)	285 (99%)	3 (1%)	76	86
1	BC	288/290 (99%)	285 (99%)	3 (1%)	76	86
1	BD	288/290 (99%)	285 (99%)	3 (1%)	76	86
1	CC	288/290 (99%)	285 (99%)	3 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CD	288/290 (99%)	285 (99%)	3 (1%)	76	86
2	AE	339/549 (62%)	335 (99%)	4 (1%)	71	84
2	BE	339/549 (62%)	335 (99%)	4 (1%)	71	84
2	CE	339/549 (62%)	335 (99%)	4 (1%)	71	84
3	AF	17/965 (2%)	17 (100%)	0	100	100
3	BF	17/965 (2%)	17 (100%)	0	100	100
3	CF	17/965 (2%)	17 (100%)	0	100	100
4	AJ	152/526 (29%)	152 (100%)	0	100	100
4	AK	170/526 (32%)	170 (100%)	0	100	100
4	AL	161/526 (31%)	160 (99%)	1 (1%)	86	93
4	BJ	152/526 (29%)	152 (100%)	0	100	100
4	BK	170/526 (32%)	170 (100%)	0	100	100
4	BL	161/526 (31%)	160 (99%)	1 (1%)	86	93
4	CJ	152/526 (29%)	152 (100%)	0	100	100
4	CK	170/526 (32%)	170 (100%)	0	100	100
4	CL	161/526 (31%)	160 (99%)	1 (1%)	86	93
4	DJ	152/526 (29%)	152 (100%)	0	100	100
4	DK	170/526 (32%)	170 (100%)	0	100	100
4	DL	161/526 (31%)	160 (99%)	1 (1%)	86	93
4	EJ	152/526 (29%)	152 (100%)	0	100	100
4	EK	170/526 (32%)	170 (100%)	0	100	100
4	EL	161/526 (31%)	160 (99%)	1 (1%)	86	93
4	FJ	152/526 (29%)	152 (100%)	0	100	100
4	FK	170/526 (32%)	170 (100%)	0	100	100
4	FL	161/526 (31%)	160 (99%)	1 (1%)	86	93
5	AM	109/342 (32%)	109 (100%)	0	100	100
5	AN	108/342 (32%)	108 (100%)	0	100	100
5	BM	109/342 (32%)	109 (100%)	0	100	100
5	BN	108/342 (32%)	108 (100%)	0	100	100
5	CM	109/342 (32%)	109 (100%)	0	100	100
5	CN	108/342 (32%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	DM	109/342 (32%)	109 (100%)	0	100	100
5	DN	108/342 (32%)	108 (100%)	0	100	100
5	EM	109/342 (32%)	109 (100%)	0	100	100
5	EN	108/342 (32%)	108 (100%)	0	100	100
5	FM	109/342 (32%)	109 (100%)	0	100	100
5	FN	108/342 (32%)	108 (100%)	0	100	100
6	AA	120/160 (75%)	120 (100%)	0	100	100
6	AB	136/160 (85%)	136 (100%)	0	100	100
6	BA	120/160 (75%)	120 (100%)	0	100	100
6	BB	136/160 (85%)	136 (100%)	0	100	100
6	CA	120/160 (75%)	120 (100%)	0	100	100
6	CB	136/160 (85%)	136 (100%)	0	100	100
6	DA	120/160 (75%)	120 (100%)	0	100	100
6	DB	136/160 (85%)	136 (100%)	0	100	100
6	EA	120/160 (75%)	120 (100%)	0	100	100
6	EB	136/160 (85%)	136 (100%)	0	100	100
6	FA	120/160 (75%)	120 (100%)	0	100	100
6	FB	136/160 (85%)	136 (100%)	0	100	100
7	AG	561/562 (100%)	559 (100%)	2 (0%)	91	95
7	AH	560/562 (100%)	559 (100%)	1 (0%)	93	97
7	AI	560/562 (100%)	559 (100%)	1 (0%)	93	97
7	BG	561/562 (100%)	559 (100%)	2 (0%)	91	95
7	BH	560/562 (100%)	559 (100%)	1 (0%)	93	97
7	BI	560/562 (100%)	559 (100%)	1 (0%)	93	97
7	CG	561/562 (100%)	560 (100%)	1 (0%)	93	97
7	CH	560/562 (100%)	559 (100%)	1 (0%)	93	97
7	CI	560/562 (100%)	559 (100%)	1 (0%)	93	97
7	DG	561/562 (100%)	560 (100%)	1 (0%)	93	97
7	DH	560/562 (100%)	559 (100%)	1 (0%)	93	97
7	DI	560/562 (100%)	559 (100%)	1 (0%)	93	97
7	EG	561/562 (100%)	559 (100%)	2 (0%)	91	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	EH	560/562 (100%)	559 (100%)	1 (0%)	93 97
7	EI	560/562 (100%)	559 (100%)	1 (0%)	93 97
7	FG	561/562 (100%)	559 (100%)	2 (0%)	91 95
7	FH	560/562 (100%)	559 (100%)	1 (0%)	93 97
7	FI	560/562 (100%)	559 (100%)	1 (0%)	93 97
All	All	18618/31890 (58%)	18560 (100%)	58 (0%)	92 96

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	BE	165	LYS
7	EG	124	LYS
4	EL	66	LYS
7	EH	573	ARG
7	FG	243	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
7	AH	90	ASN
7	CI	613	GLN
7	AG	61	ASN
7	FI	241	GLN
7	EI	241	GLN

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)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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.

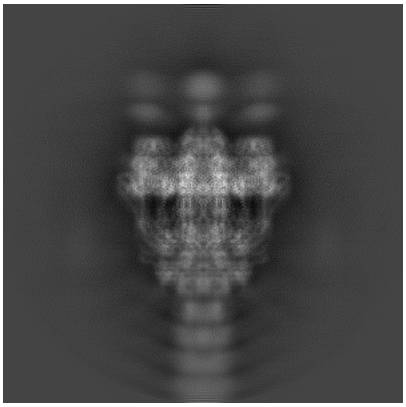
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20872. These allow visual inspection of the internal detail of the map and identification of artifacts.

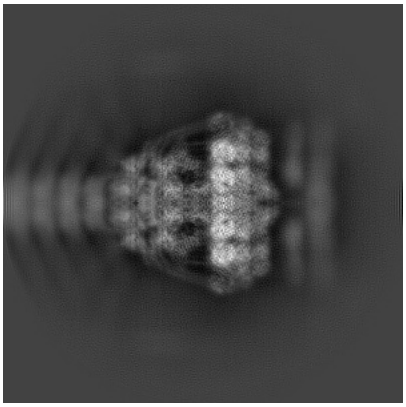
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

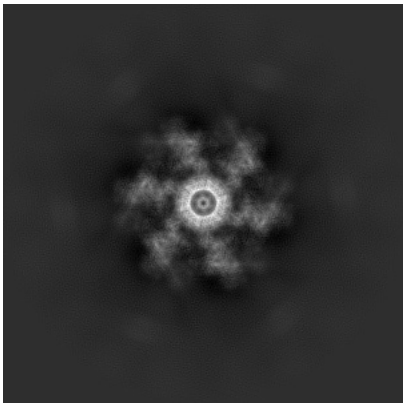
6.1.1 Primary map



X



Y

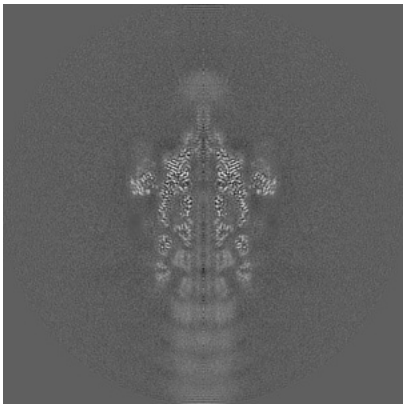


Z

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

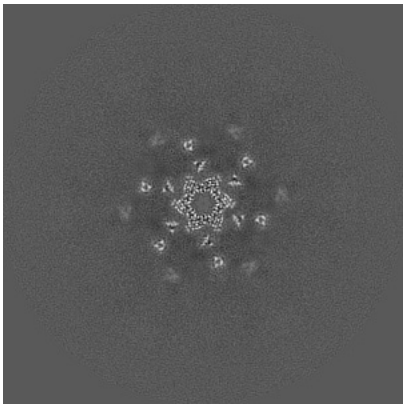
6.2 Central slices

6.2.1 Primary map



X Index: 256

Y Index: 256

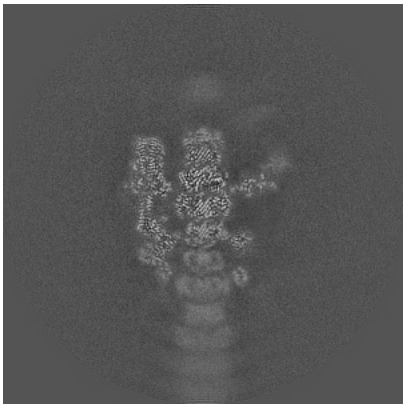


Z Index: 256

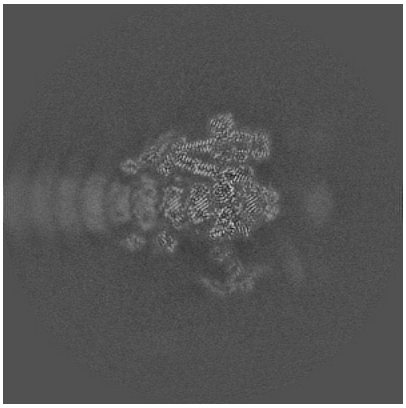
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

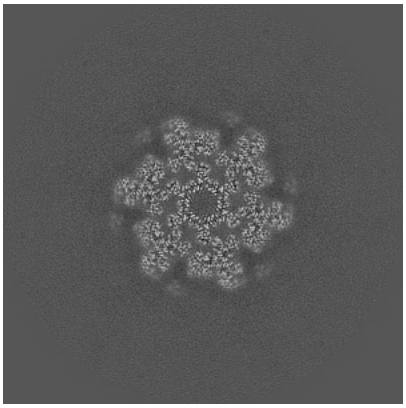
6.3.1 Primary map



X Index: 274



Y Index: 238



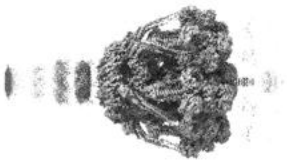
Z Index: 281

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

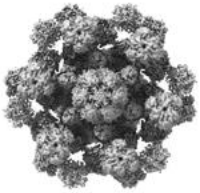
6.4 Orthogonal surface views (i)

6.4.1 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.

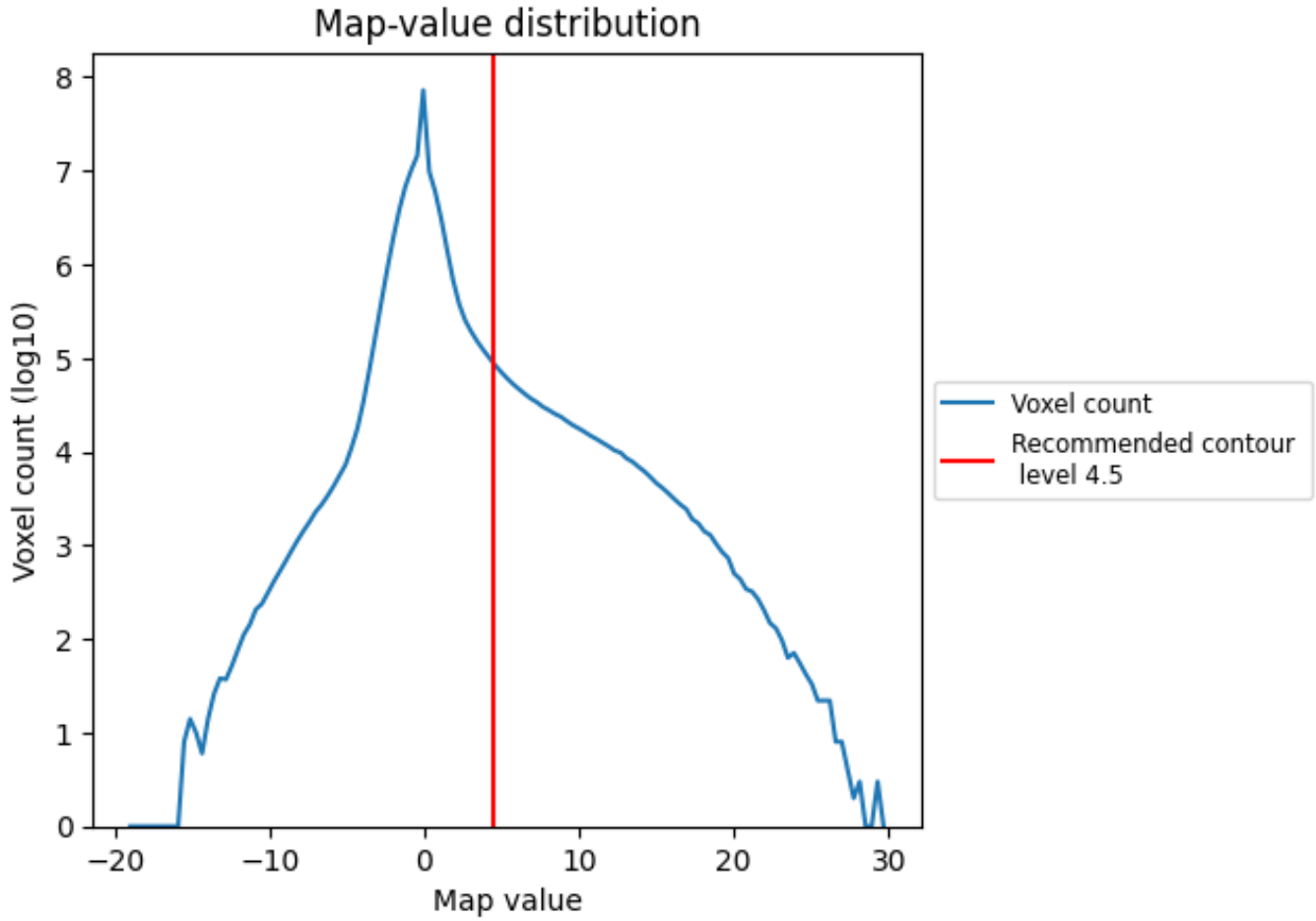
6.5 Mask visualisation (i)

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

7 Map analysis

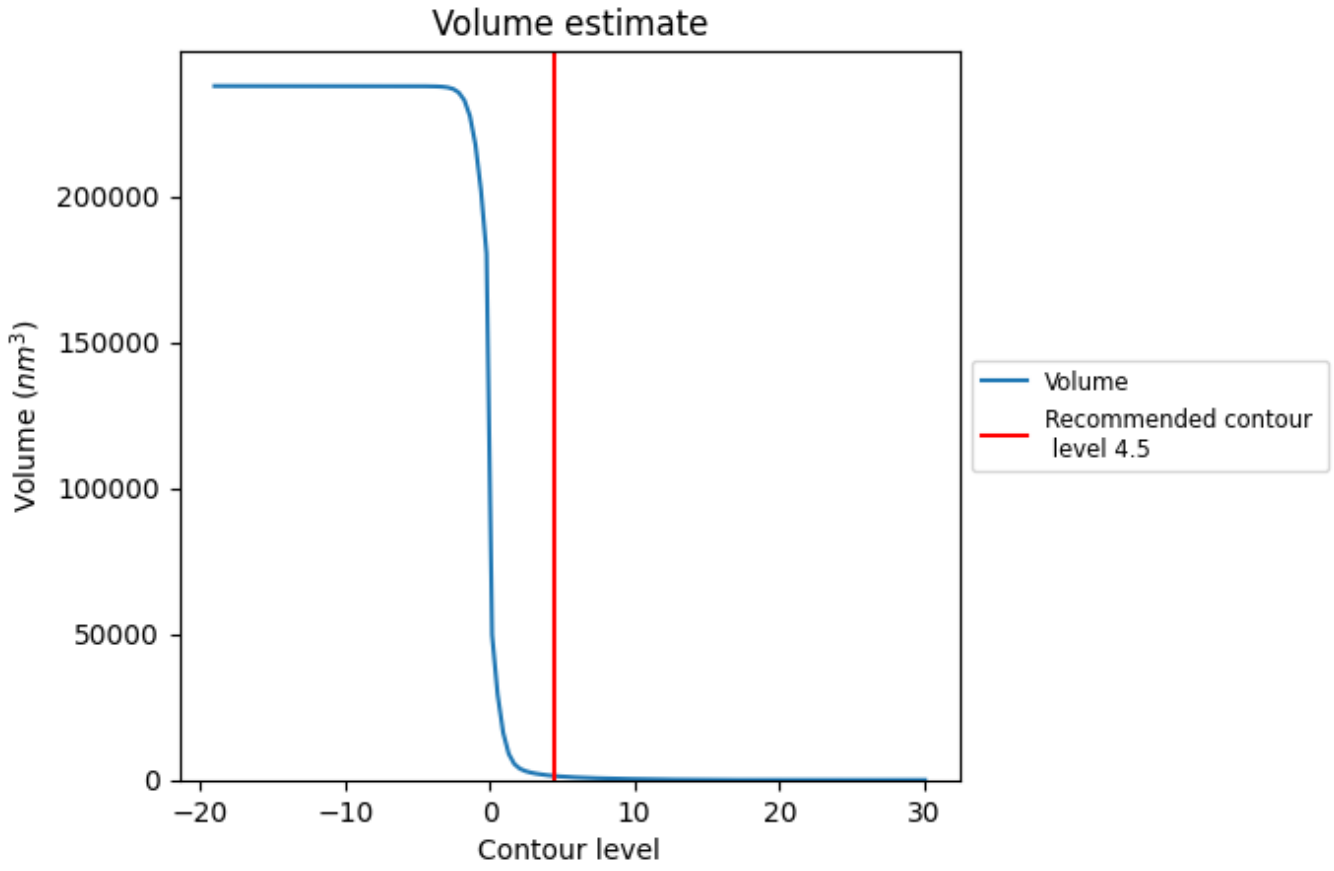
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

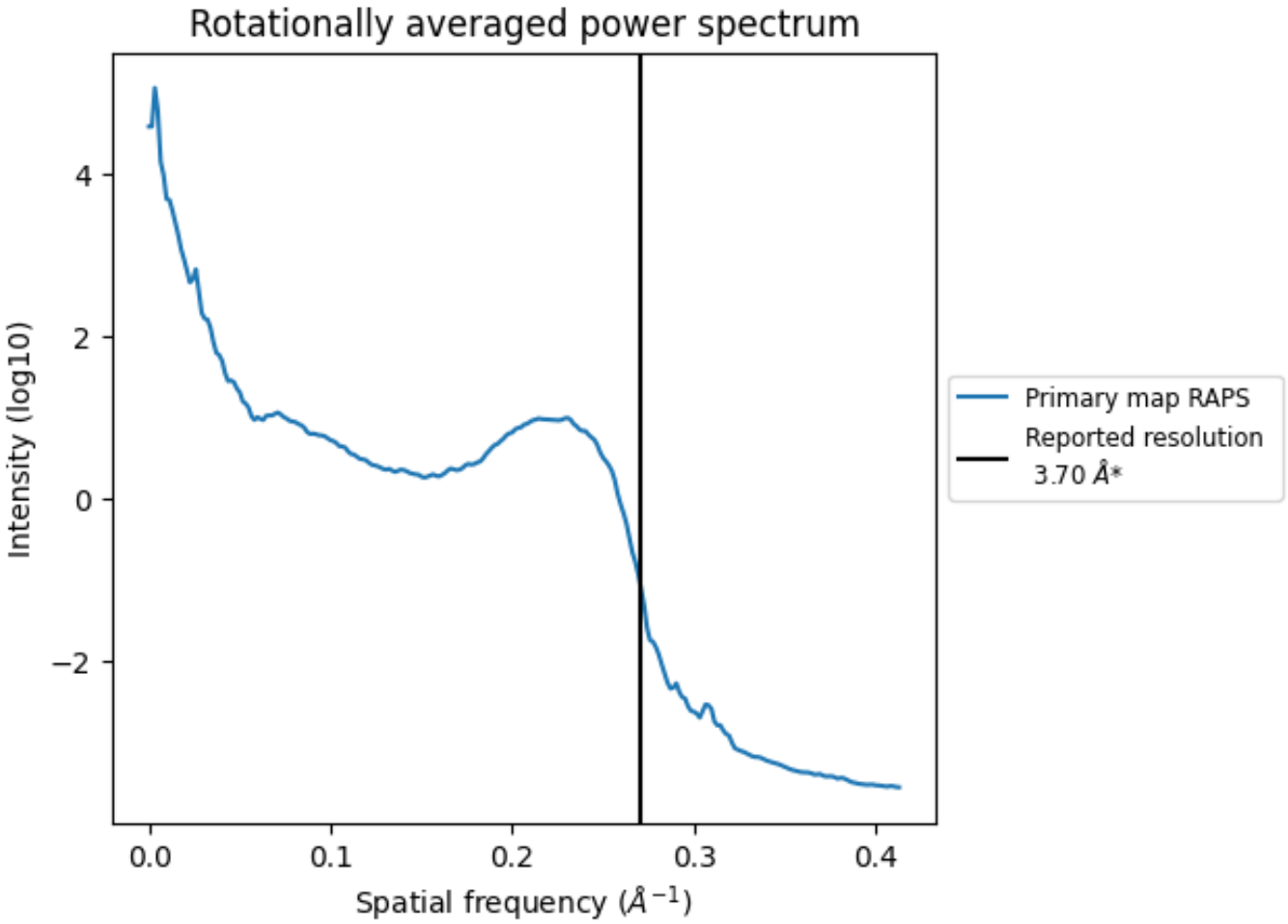
7.2 Volume estimate (i)



The volume at the recommended contour level is 1359 nm^3; this corresponds to an approximate mass of 1228 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)

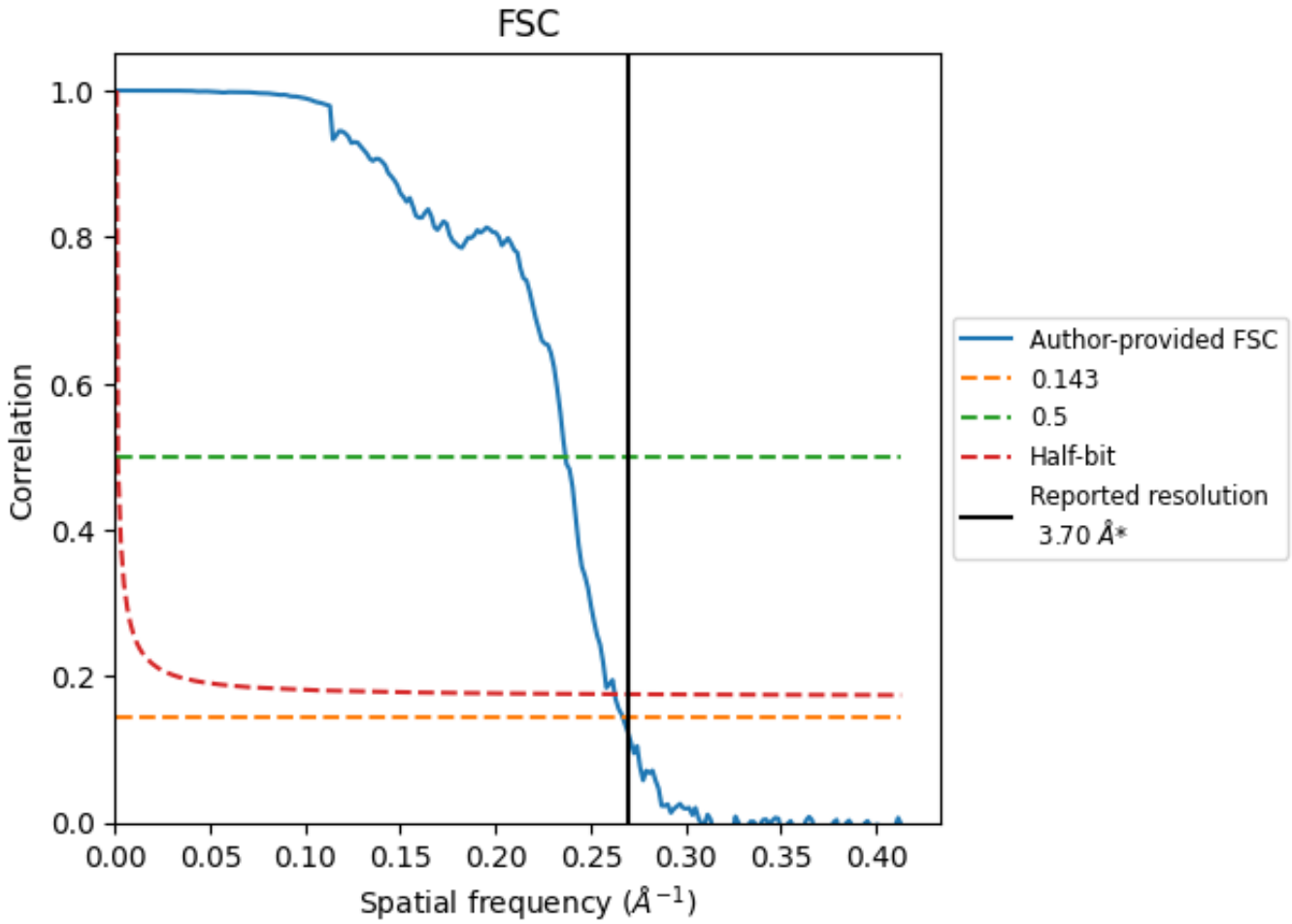


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

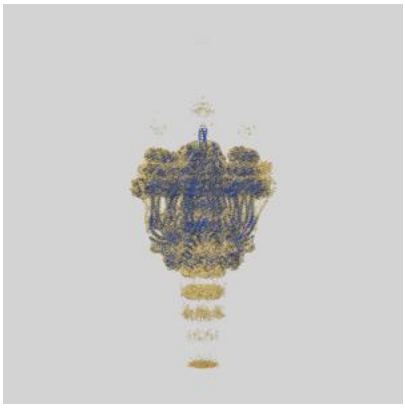
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.75	4.22	3.81
Unmasked-calculated*	-	-	-

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

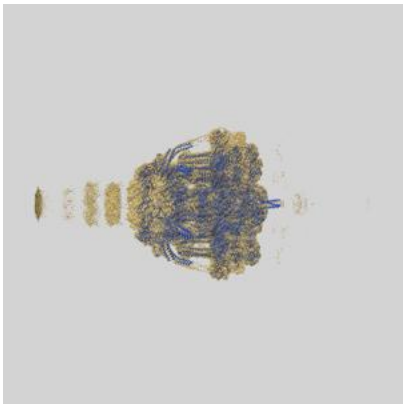
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20872 and PDB model 6V8I. Per-residue inclusion information can be found in section 3 on page 11.

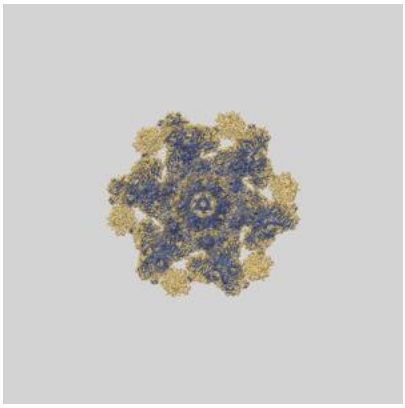
9.1 Map-model overlay



X



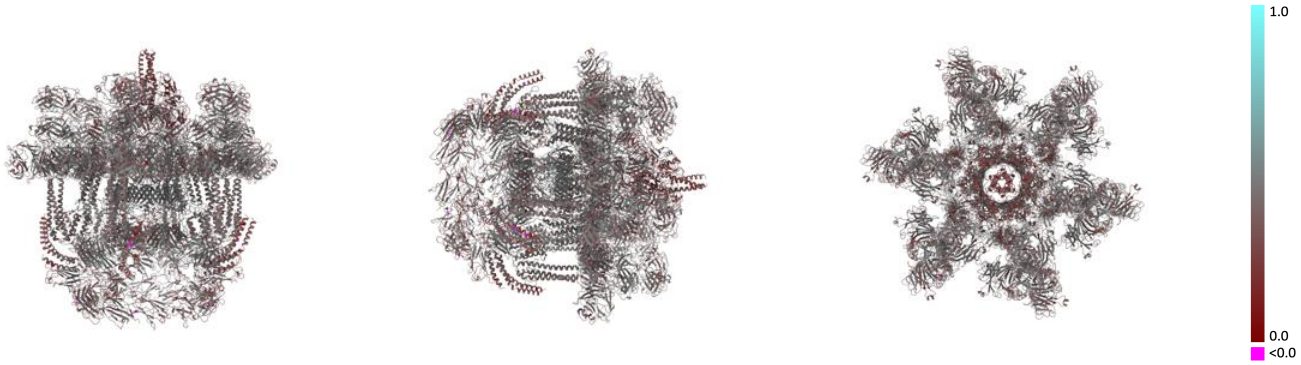
Y



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.

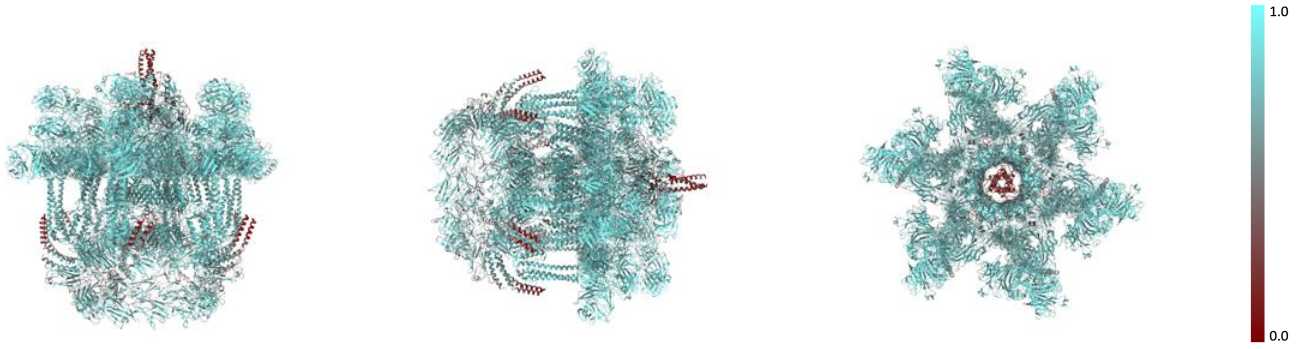
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

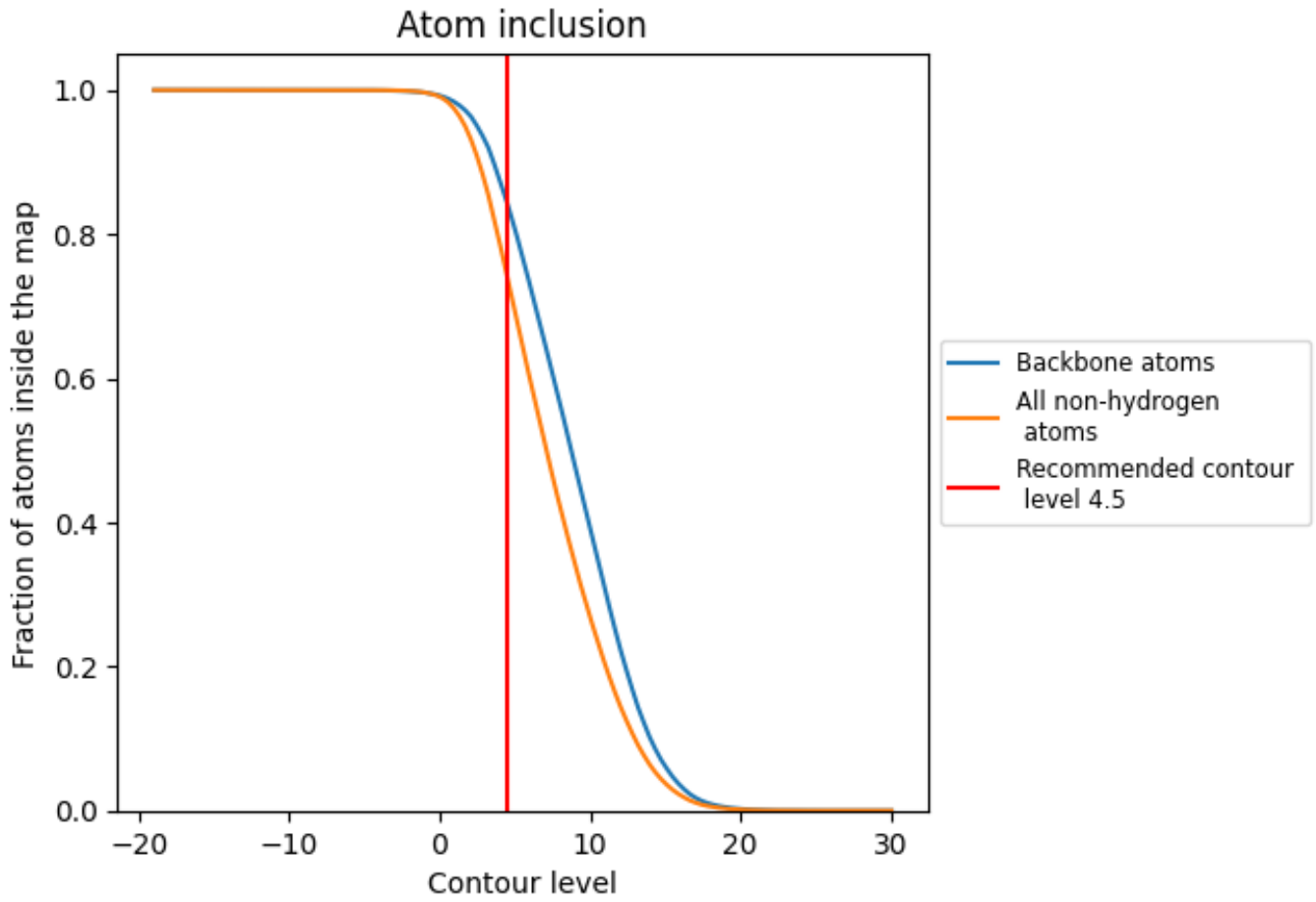
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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, 84% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7408	0.4140
AA	0.6862	0.4320
AB	0.7647	0.4670
AC	0.7582	0.3920
AD	0.7680	0.4140
AE	0.5600	0.3230
AF	0.2273	0.2350
AG	0.8055	0.4240
AH	0.7938	0.4270
AI	0.7797	0.4280
AJ	0.7354	0.4220
AK	0.6878	0.4210
AL	0.5530	0.3610
AM	0.6687	0.3710
AN	0.6725	0.3850
BA	0.6914	0.4320
BB	0.7855	0.4650
BC	0.7535	0.3890
BD	0.7696	0.4150
BE	0.5626	0.3250
BF	0.1948	0.2340
BG	0.8108	0.4240
BH	0.7920	0.4300
BI	0.7841	0.4300
BJ	0.7255	0.4260
BK	0.6892	0.4220
BL	0.5233	0.3600
BM	0.6544	0.3700
BN	0.6694	0.3840
CA	0.6757	0.4330
CB	0.7647	0.4680
CC	0.7500	0.3920
CD	0.7719	0.4130
CE	0.5567	0.3200
CF	0.1818	0.1940

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Chain	Atom inclusion	Q-score
CG	0.8023	0.4240
CH	0.7887	0.4280
CI	0.7859	0.4300
CJ	0.7506	0.4220
CK	0.6899	0.4170
CL	0.5297	0.3620
CM	0.6667	0.3720
CN	0.6767	0.3840
DA	0.6897	0.4320
DB	0.7701	0.4660
DG	0.8021	0.4240
DH	0.7853	0.4280
DI	0.7764	0.4290
DJ	0.7437	0.4230
DK	0.6845	0.4190
DL	0.5262	0.3610
DM	0.6626	0.3700
DN	0.6746	0.3840
EA	0.6879	0.4330
EB	0.7500	0.4690
EG	0.8088	0.4240
EH	0.7946	0.4290
EI	0.7766	0.4280
EJ	0.7346	0.4260
EK	0.6676	0.4220
EL	0.5509	0.3640
EM	0.6687	0.3720
EN	0.6736	0.3840
FA	0.7002	0.4360
FB	0.7832	0.4680
FG	0.8133	0.4240
FH	0.7881	0.4270
FI	0.7839	0.4280
FJ	0.7483	0.4250
FK	0.7054	0.4200
FL	0.5396	0.3630
FM	0.6544	0.3720
FN	0.6705	0.3850