wwPDB EM Validation Summary Report

Nov 7, 2022 – 11:52 PM EST

PDB ID	:	6CGR
EMDB ID	:	EMD-7472
Title	:	CryoEM structure of herpes simplex virus 1 capsid with associated tegument protein complexes.
Authors	:	Dai, X.H.; Zhou, Z.H.
Deposited on	:	2018-02-20
Resolution	:	4.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

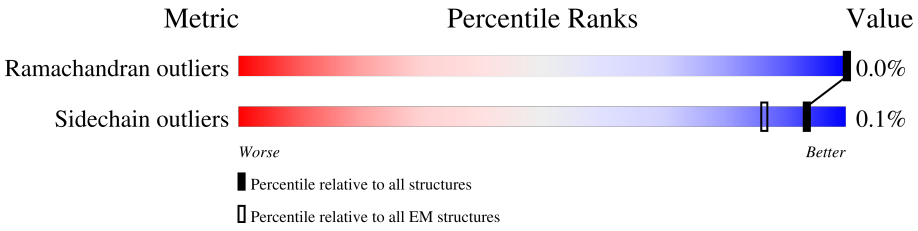
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.20 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)
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	4	1374	49% 91% 8%
1	A	1374	14% 99% .
1	B	1374	12% 99% .
1	C	1374	15% 99% .
1	D	1374	14% 99% .
1	E	1374	16% 99% .
1	F	1374	13% 99% .
1	M	1374	12% 99% .
1	N	1374	12% 99% .

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Mol	Chain	Length	Quality of chain
1	O	1374	13% 99%
1	S	1374	21% 98%
1	T	1374	21% 98%
1	U	1374	17% 99%
1	V	1374	18% 99%
1	W	1374	17% 99%
1	X	1374	21% 98%
2	0	112	55% 90% 10%
2	1	112	48% 90% 10%
2	2	112	54% 90% 10%
2	3	112	53% 90% 10%
2	G	112	47% 90% 10%
2	H	112	40% 90% 10%
2	I	112	46% 90% 10%
2	J	112	38% 90% 10%
2	K	112	48% 90% 10%
2	L	112	41% 90% 10%
2	P	112	36% 90% 10%
2	Q	112	39% 90% 10%
2	R	112	29% 90% 10%
2	Y	112	62% 90% 10%
2	Z	112	61% 90% 10%
3	5	465	21% 76% 24%
3	8	465	11% 77% 22%
3	b	465	17% 78% 22%

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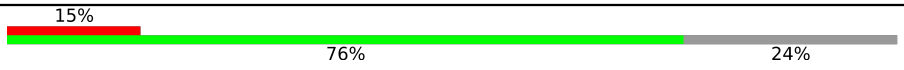
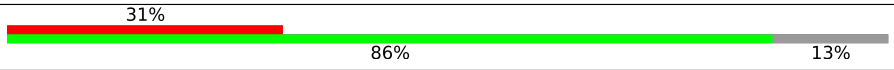
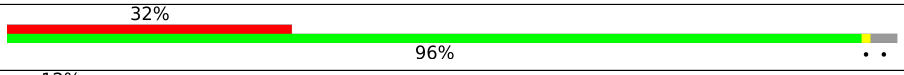
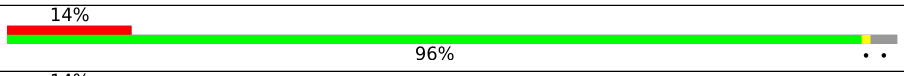
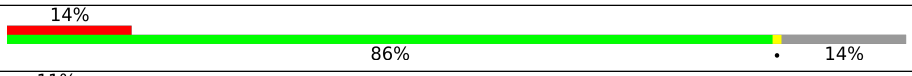
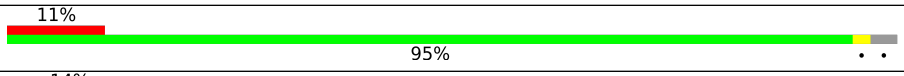
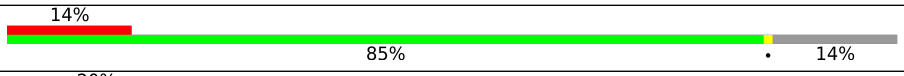
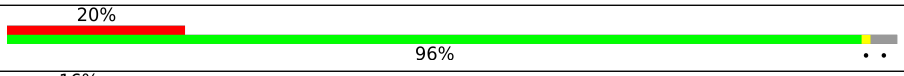
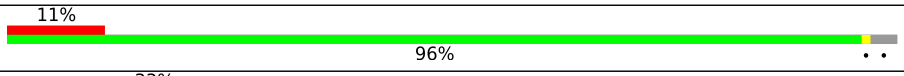
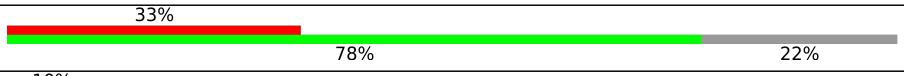
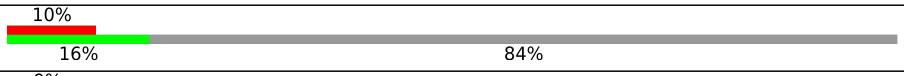
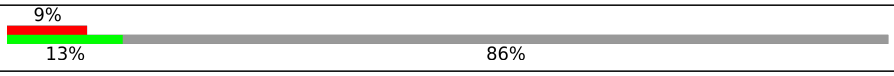
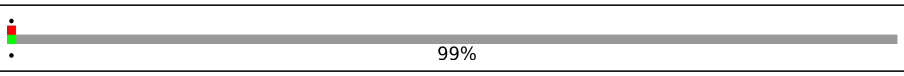
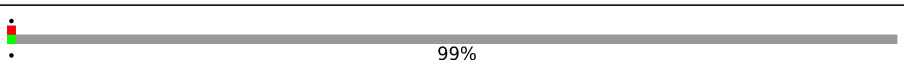
Mol	Chain	Length	Quality of chain
3	e	465	
3	h	465	
4	6	318	
4	7	318	
4	9	318	
4	a	318	
4	c	318	
4	d	318	
4	f	318	
4	g	318	
4	i	318	
4	j	318	
5	k	703	
6	l	580	
6	m	580	
7	n	3139	
7	o	3139	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 219702 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1362	Total	C	N	O	S	0	0
			10409	6575	1871	1909	54		
1	B	1364	Total	C	N	O	S	0	0
			10423	6585	1873	1911	54		
1	C	1364	Total	C	N	O	S	0	0
			10423	6585	1873	1911	54		
1	D	1362	Total	C	N	O	S	0	0
			10409	6575	1871	1909	54		
1	E	1366	Total	C	N	O	S	0	0
			10442	6595	1878	1915	54		
1	F	1362	Total	C	N	O	S	0	0
			10409	6575	1871	1909	54		
1	M	1362	Total	C	N	O	S	0	0
			10409	6575	1871	1909	54		
1	N	1366	Total	C	N	O	S	0	0
			10442	6595	1878	1915	54		
1	O	1364	Total	C	N	O	S	0	0
			10423	6585	1873	1911	54		
1	S	1357	Total	C	N	O	S	0	0
			10365	6547	1864	1900	54		
1	T	1357	Total	C	N	O	S	0	0
			10379	6553	1868	1904	54		
1	U	1364	Total	C	N	O	S	0	0
			10423	6585	1873	1911	54		
1	V	1362	Total	C	N	O	S	0	0
			10409	6575	1871	1909	54		
1	W	1364	Total	C	N	O	S	0	0
			10423	6585	1873	1911	54		
1	X	1348	Total	C	N	O	S	0	0
			10314	6516	1857	1888	53		
1	4	1259	Total	C	N	O	S	0	0
			9648	6103	1726	1769	50		

- Molecule 2 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	H	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	I	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	J	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	K	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	L	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	P	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	Q	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	R	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	Y	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	Z	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	0	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	1	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	2	101	Total	C	N	O	S	0	0
			774	488	146	137	3		
2	3	101	Total	C	N	O	S	0	0
			774	488	146	137	3		

- Molecule 3 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	353	Total	C	N	O	S	0	0
			2724	1708	518	481	17		
3	8	363	Total	C	N	O	S	0	0
			2786	1741	531	496	18		
3	b	363	Total	C	N	O	S	0	0
			2786	1741	531	496	18		
3	e	352	Total	C	N	O	S	0	0
			2720	1706	517	480	17		
3	h	353	Total	C	N	O	S	0	0
			2724	1708	518	481	17		

- Molecule 4 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	276	Total	C	N	O	S	0	0
			2116	1354	375	380	7		
4	7	308	Total	C	N	O	S	0	0
			2341	1487	415	430	9		
4	9	274	Total	C	N	O	S	0	0
			2091	1338	370	376	7		
4	a	308	Total	C	N	O	S	0	0
			2341	1487	415	430	9		
4	c	274	Total	C	N	O	S	0	0
			2091	1338	370	376	7		
4	d	308	Total	C	N	O	S	0	0
			2341	1487	415	430	9		
4	f	272	Total	C	N	O	S	0	0
			2089	1337	371	374	7		
4	g	308	Total	C	N	O	S	0	0
			2341	1487	415	430	9		
4	i	276	Total	C	N	O	S	0	0
			2116	1354	375	380	7		
4	j	308	Total	C	N	O	S	0	0
			2341	1487	415	430	9		

- Molecule 5 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	k	550	Total	C	N	O	S	0	0
			4206	2674	764	747	21		

- Molecule 6 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	l	94	Total	C	N	O	S	0	0
			766	486	138	138	4		
6	m	80	Total	C	N	O	S	0	0
			654	413	124	115	2		

- Molecule 7 is a protein called Large tegument protein deneddylase.

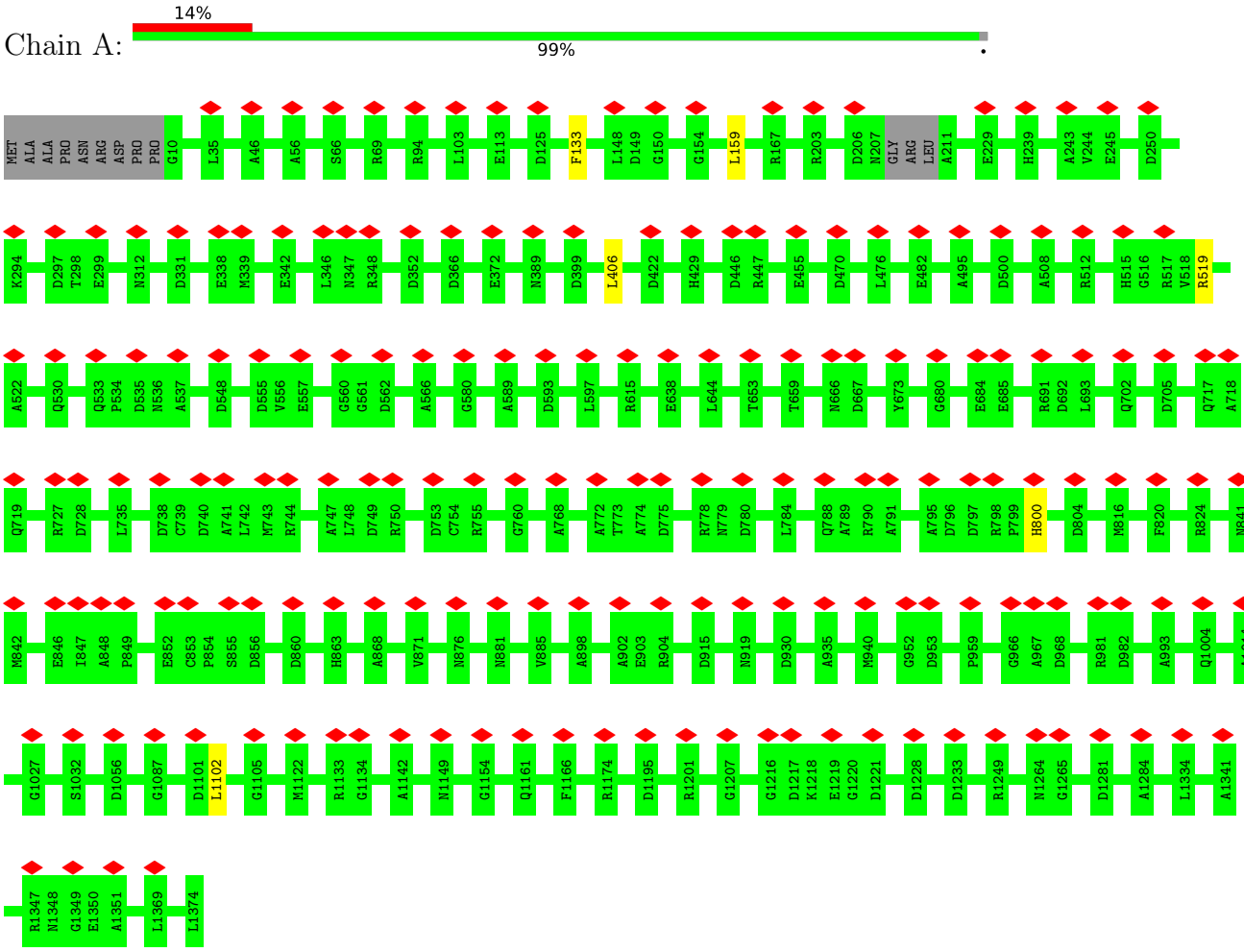
Mol	Chain	Residues	Atoms					AltConf	Trace
7	n	47	Total	C	N	O	S	0	0
			384	237	84	61	2		
7	o	47	Total	C	N	O	S	0	0
			384	237	84	61	2		

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.

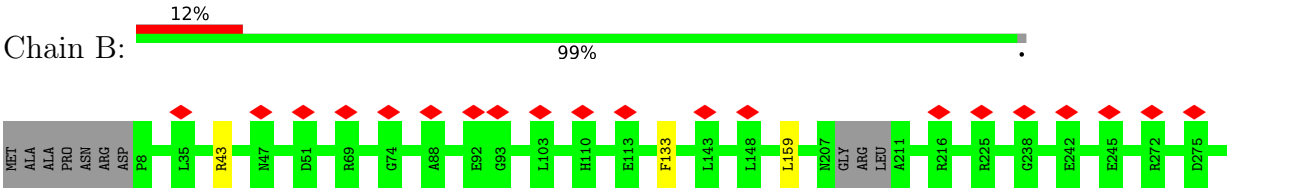
• Molecule 1: Major capsid protein

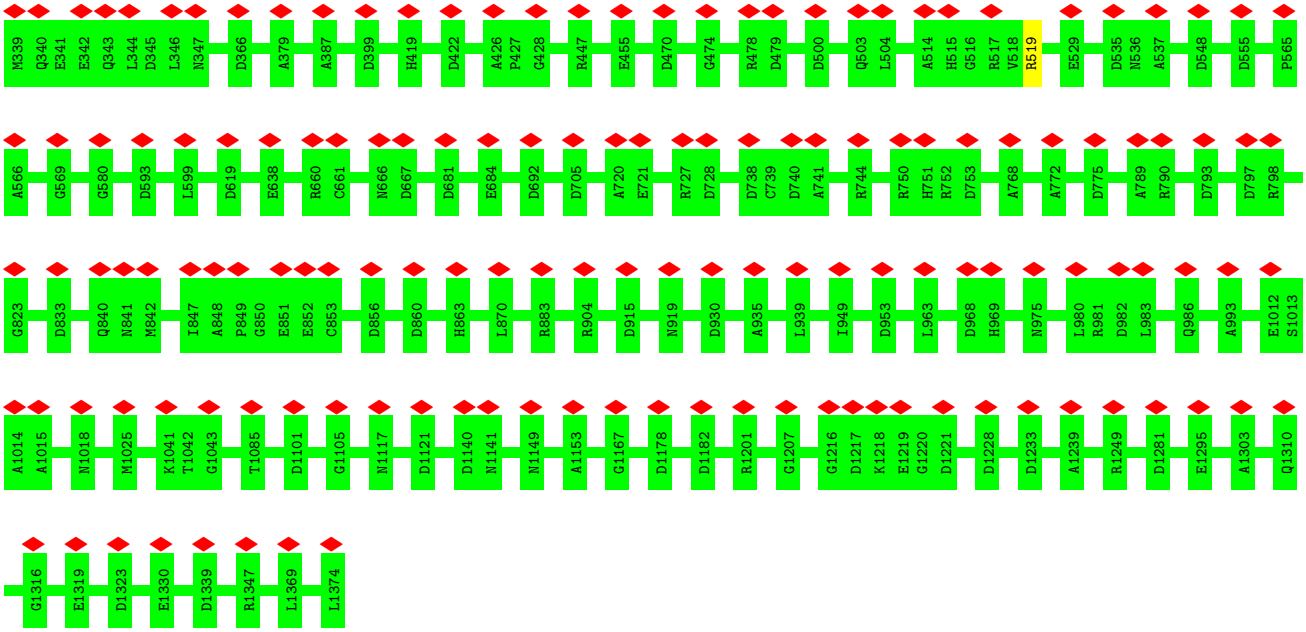
Chain A:



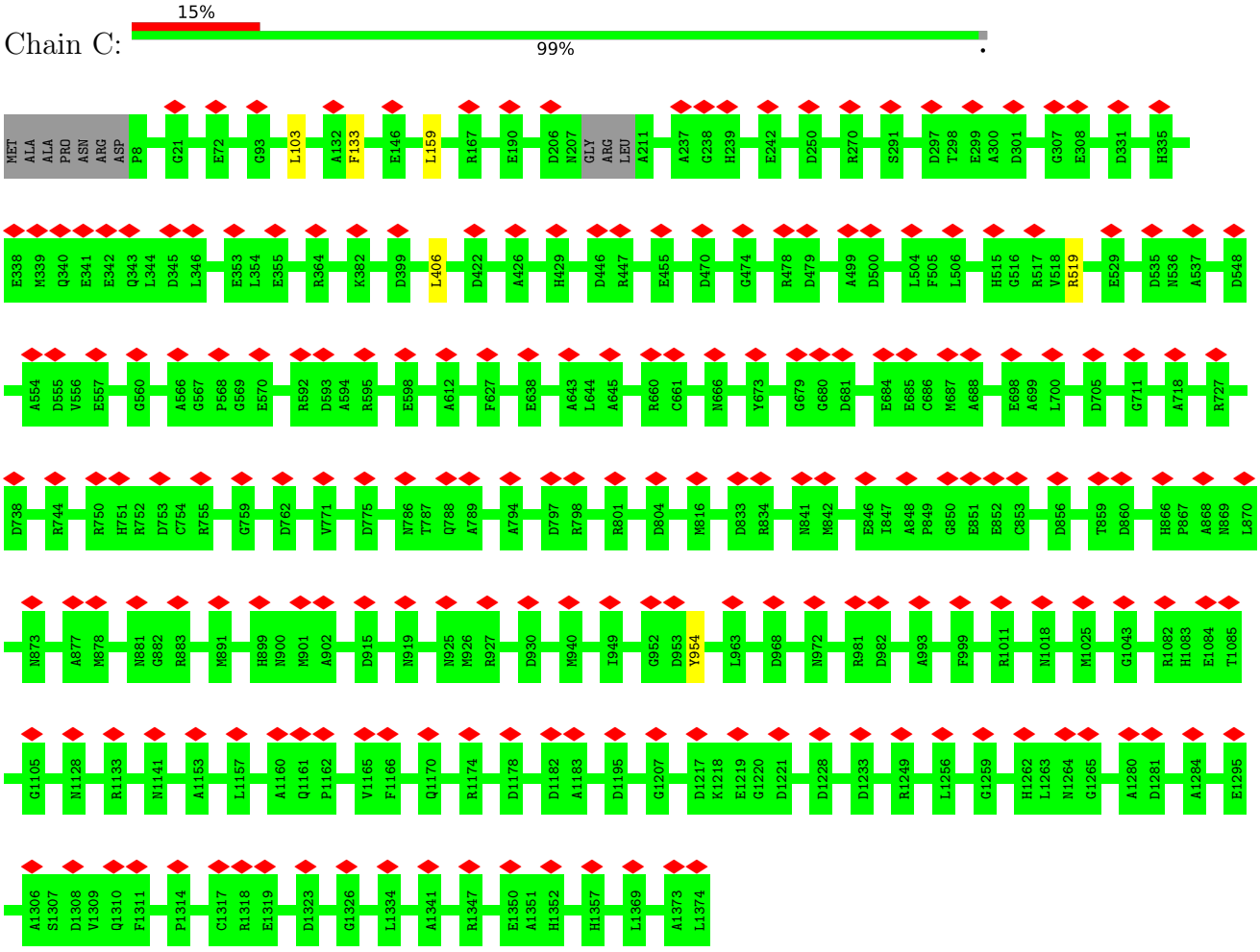
• Molecule 1: Major capsid protein

Chain B:



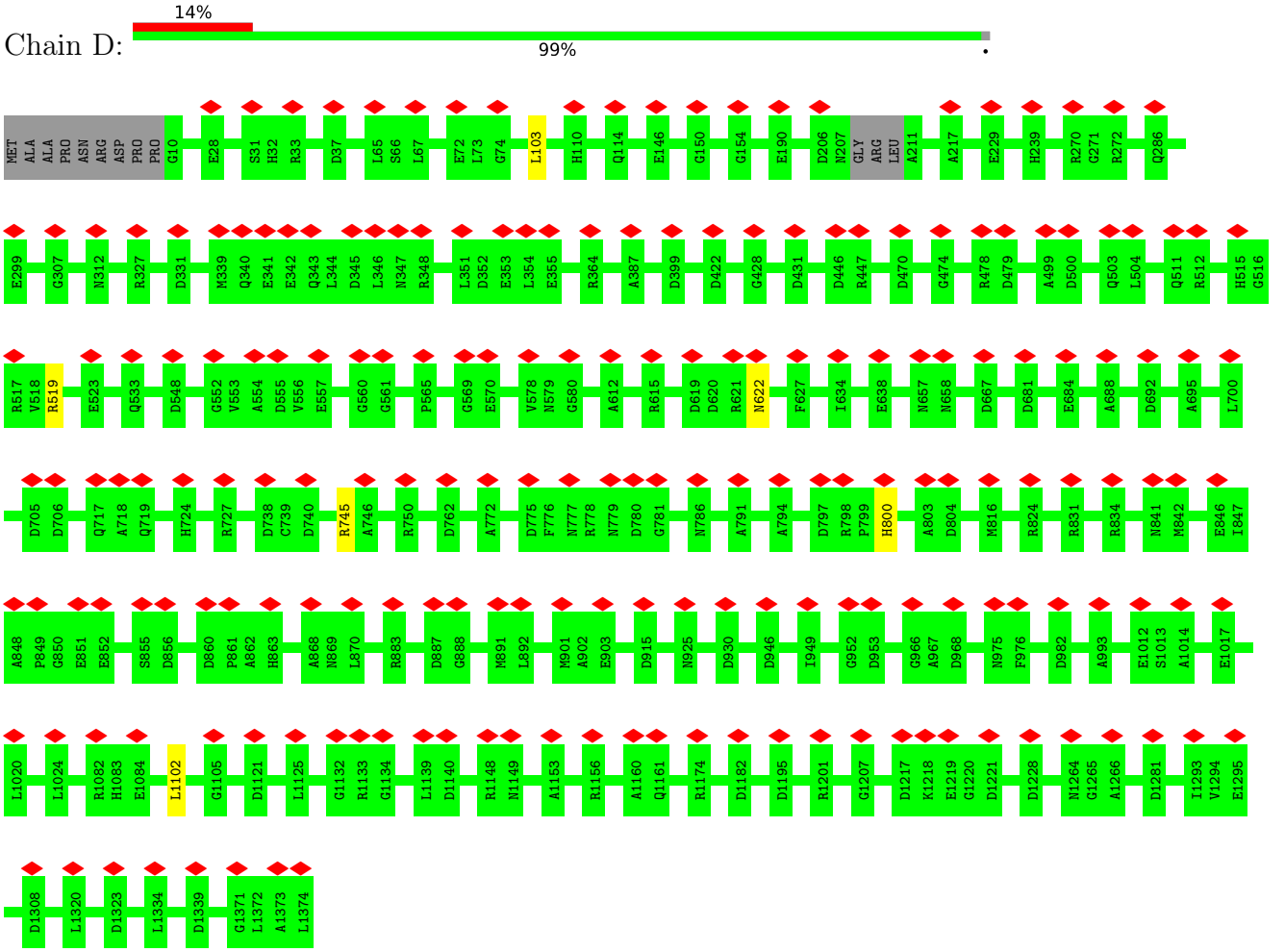


• Molecule 1: Major capsid protein



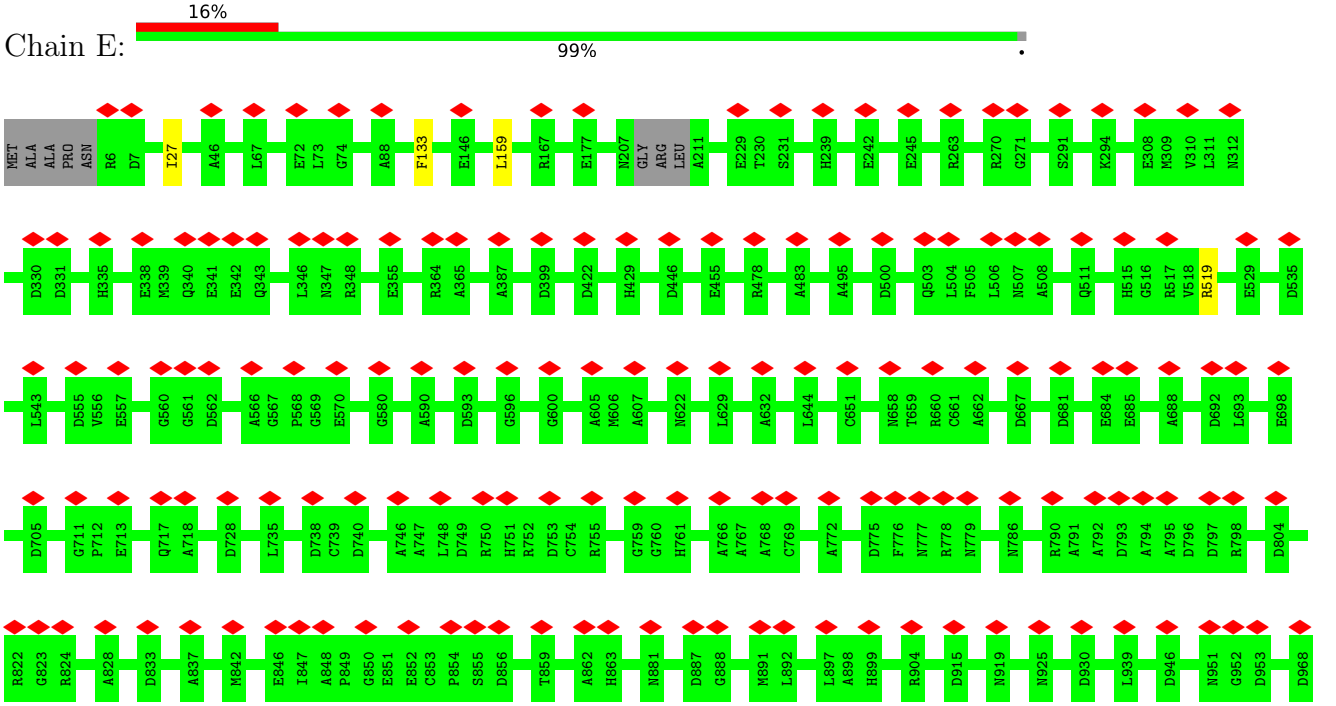
• Molecule 1: Major capsid protein

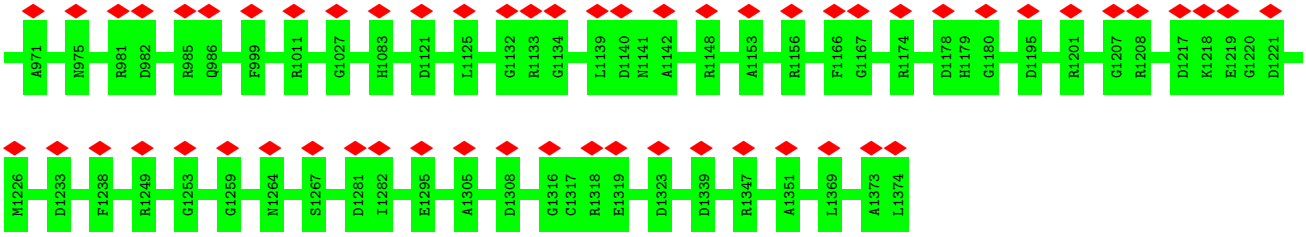
Chain D:



• Molecule 1: Major capsid protein

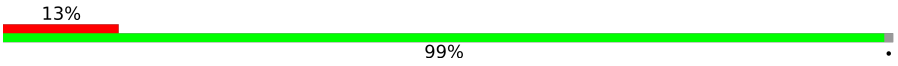
Chain E:

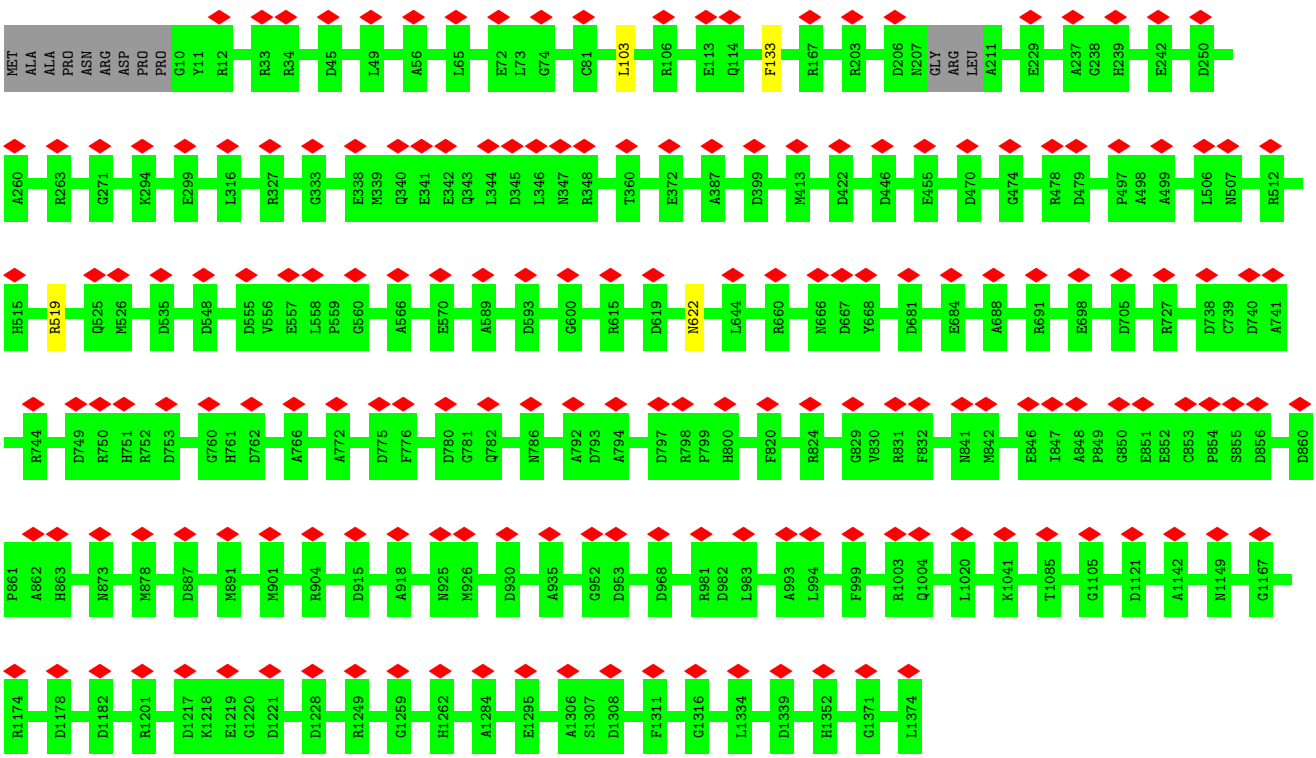




• Molecule 1: Major capsid protein

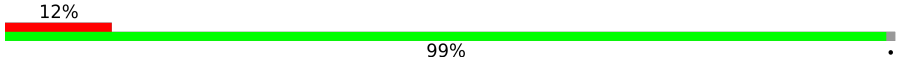
Chain F:

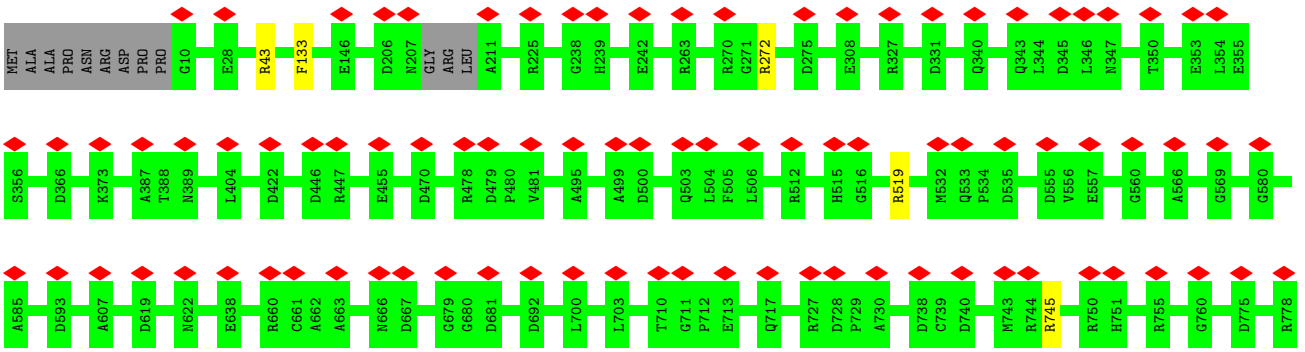


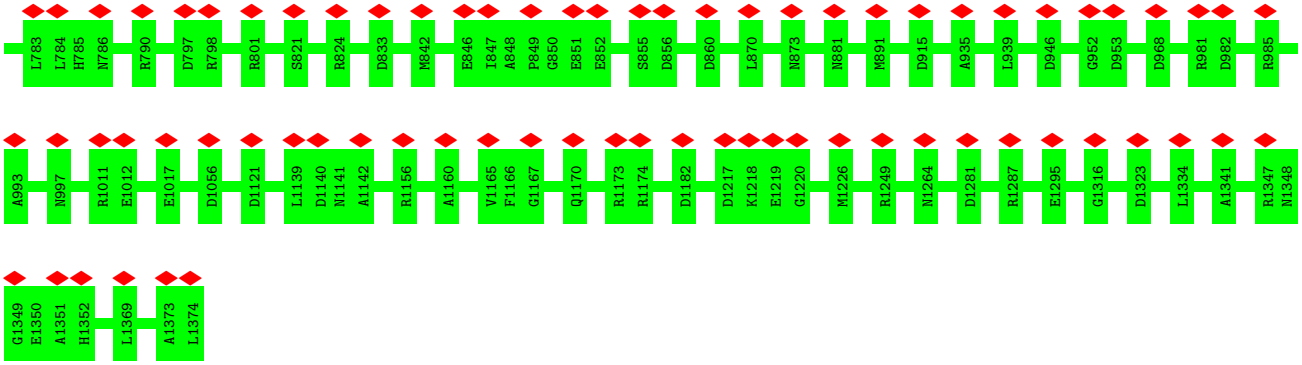


• Molecule 1: Major capsid protein

Chain M:

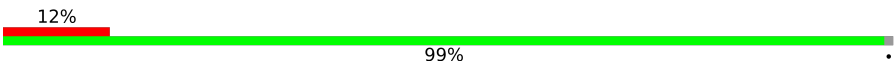






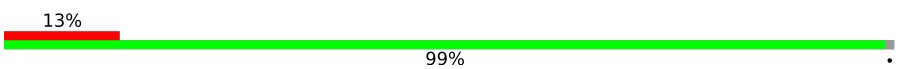
• Molecule 1: Major capsid protein

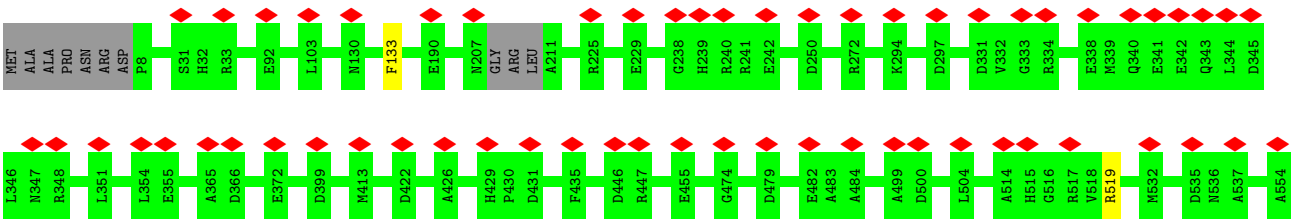
Chain N:

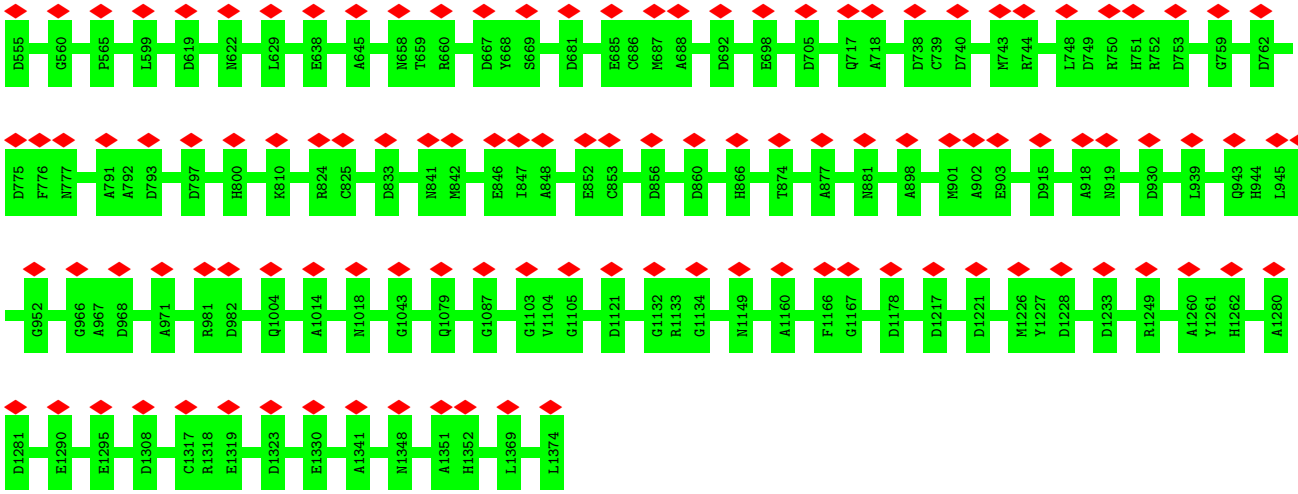


• Molecule 1: Major capsid protein

Chain O:

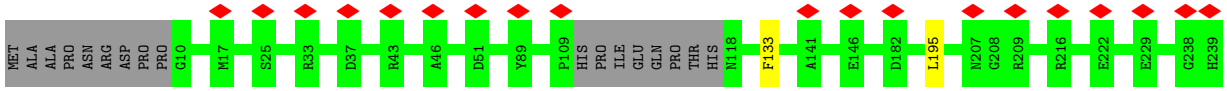


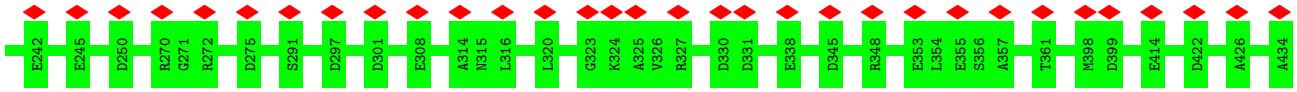


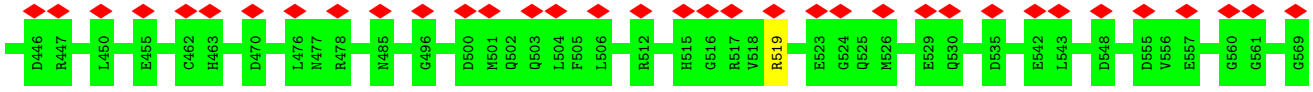


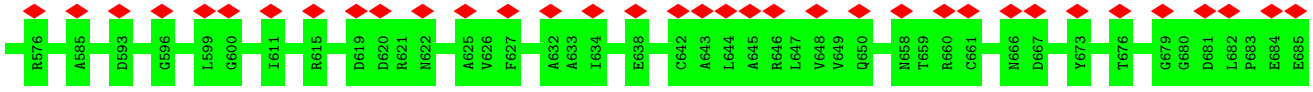
• Molecule 1: Major capsid protein

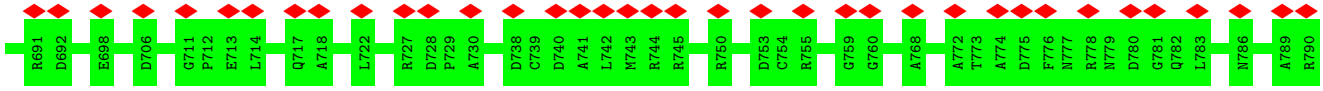
Chain S:

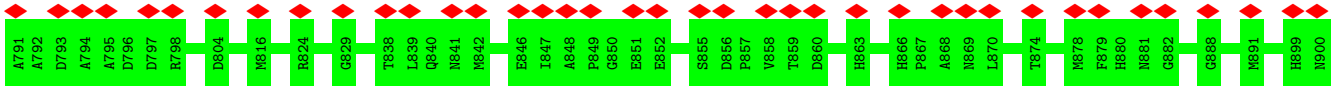


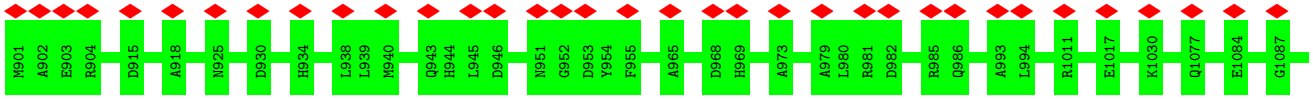


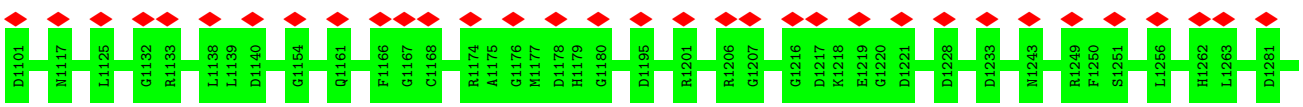


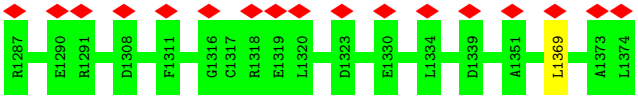






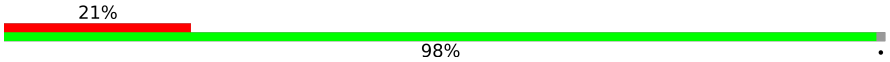


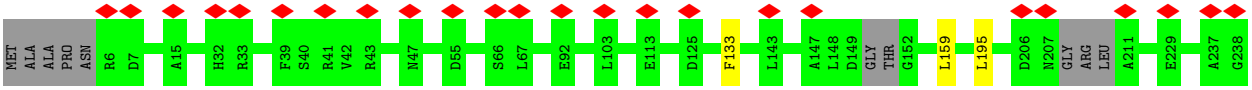


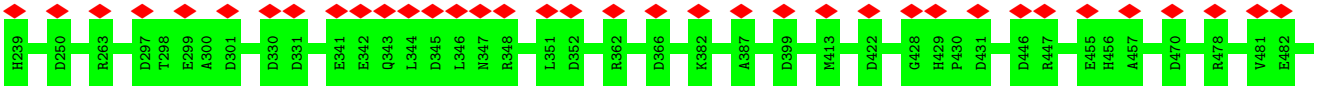


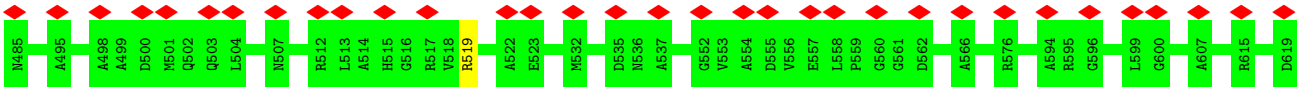
• Molecule 1: Major capsid protein

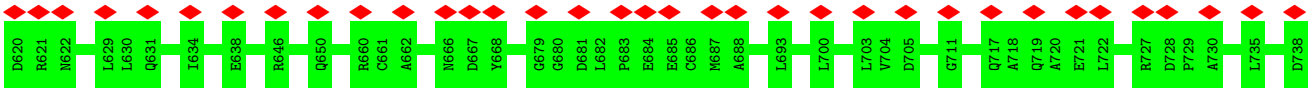
Chain T:

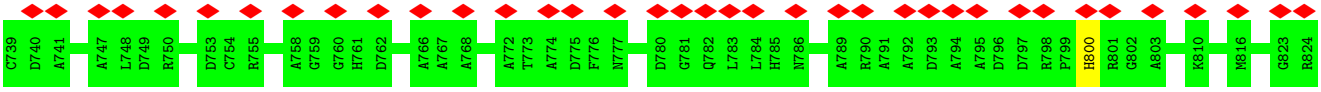


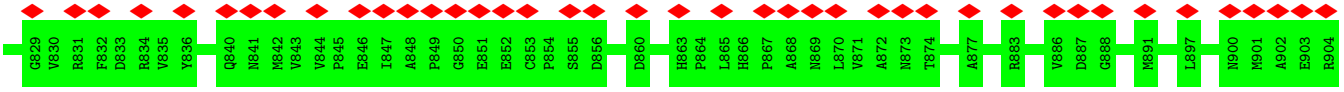


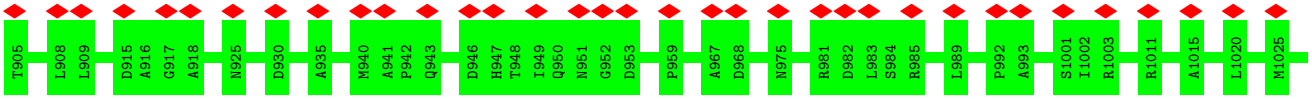


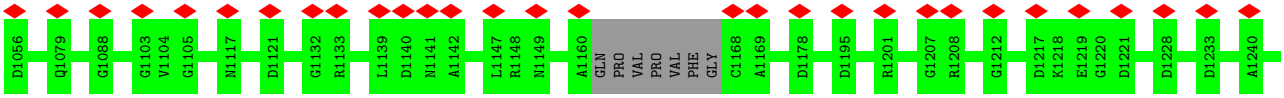


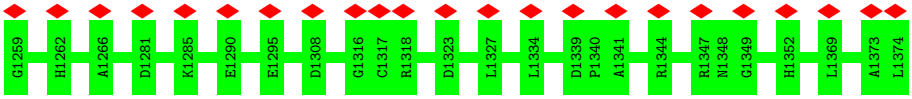






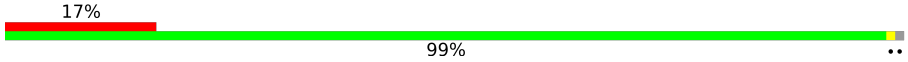


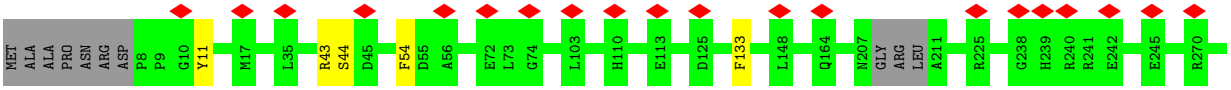


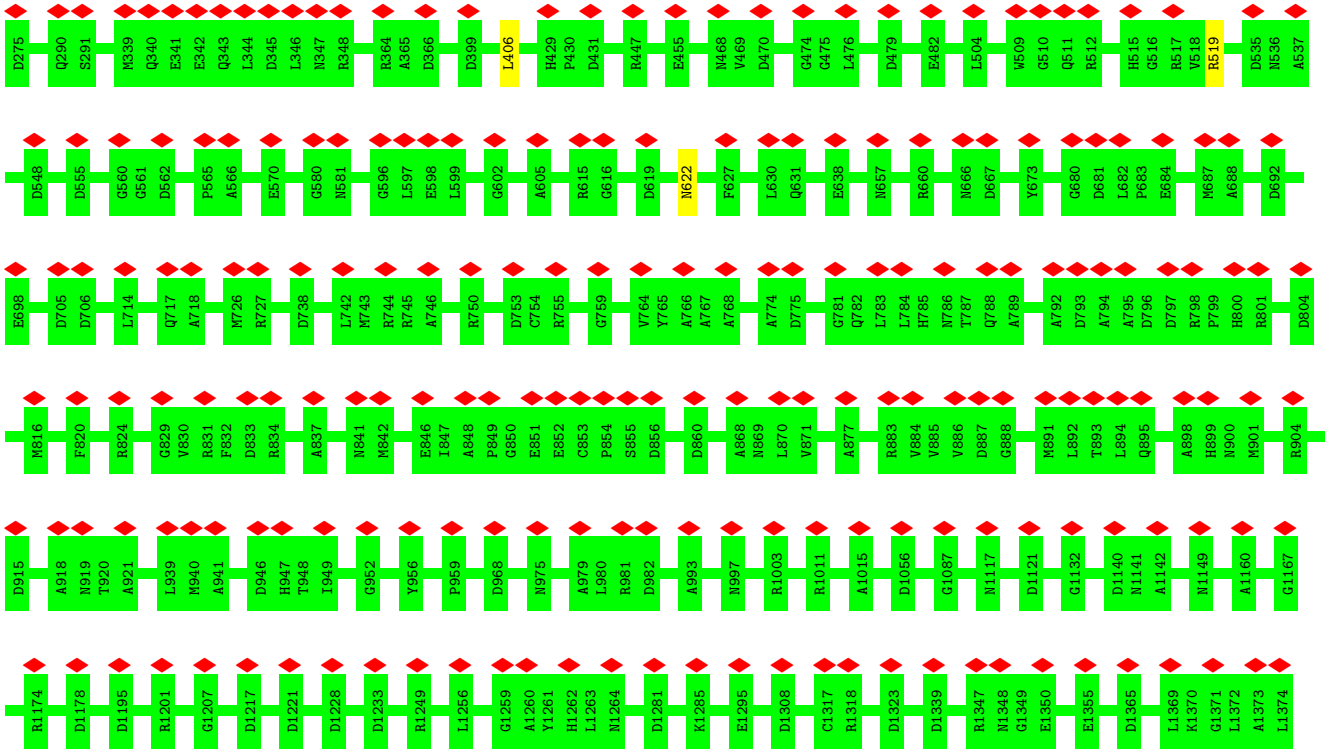


• Molecule 1: Major capsid protein

Chain U:

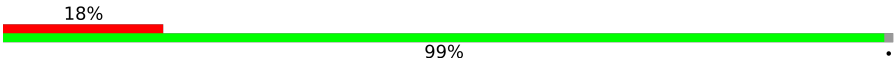


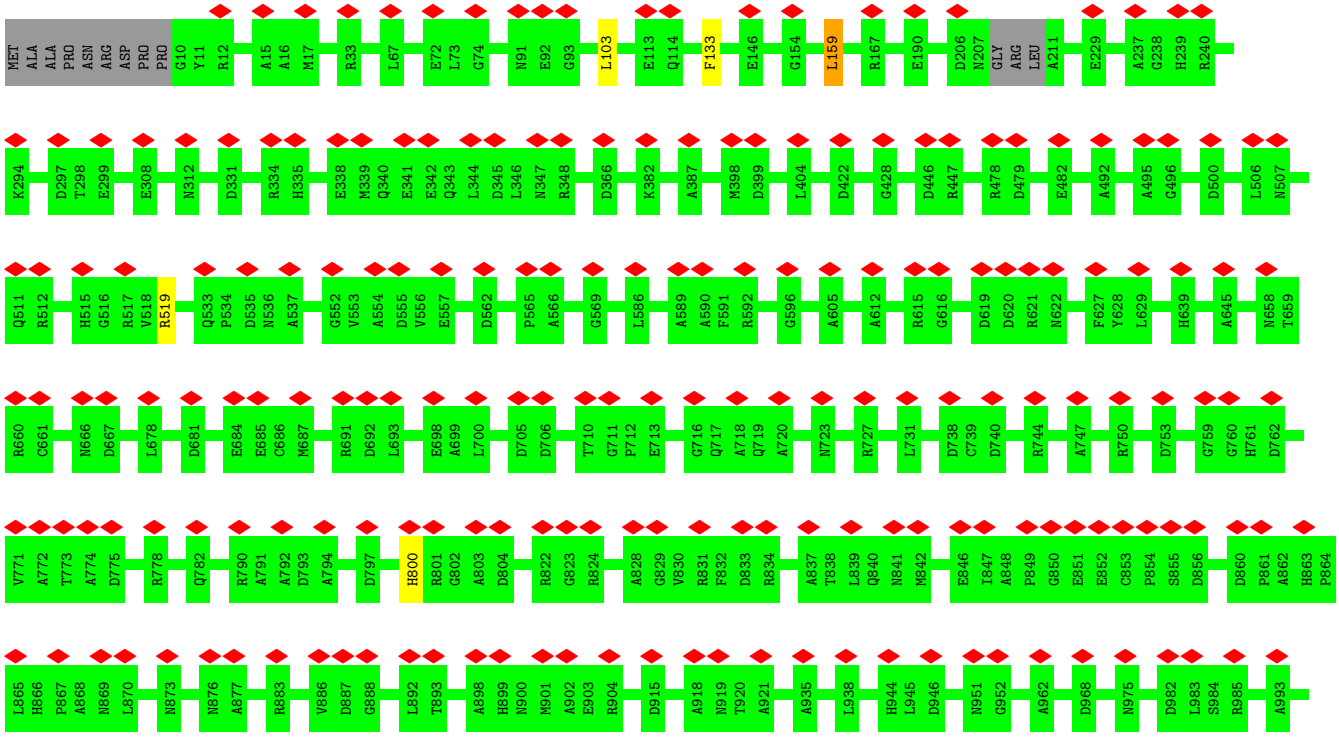


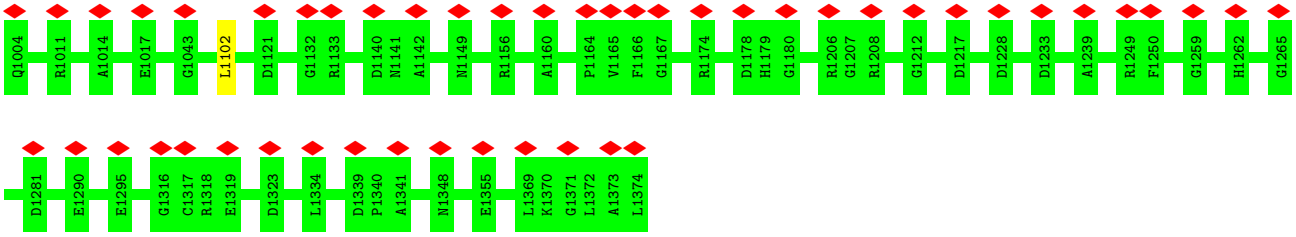


• Molecule 1: Major capsid protein

Chain V:

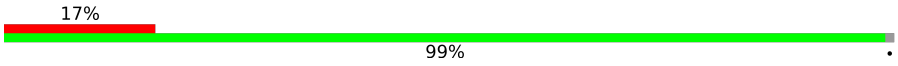


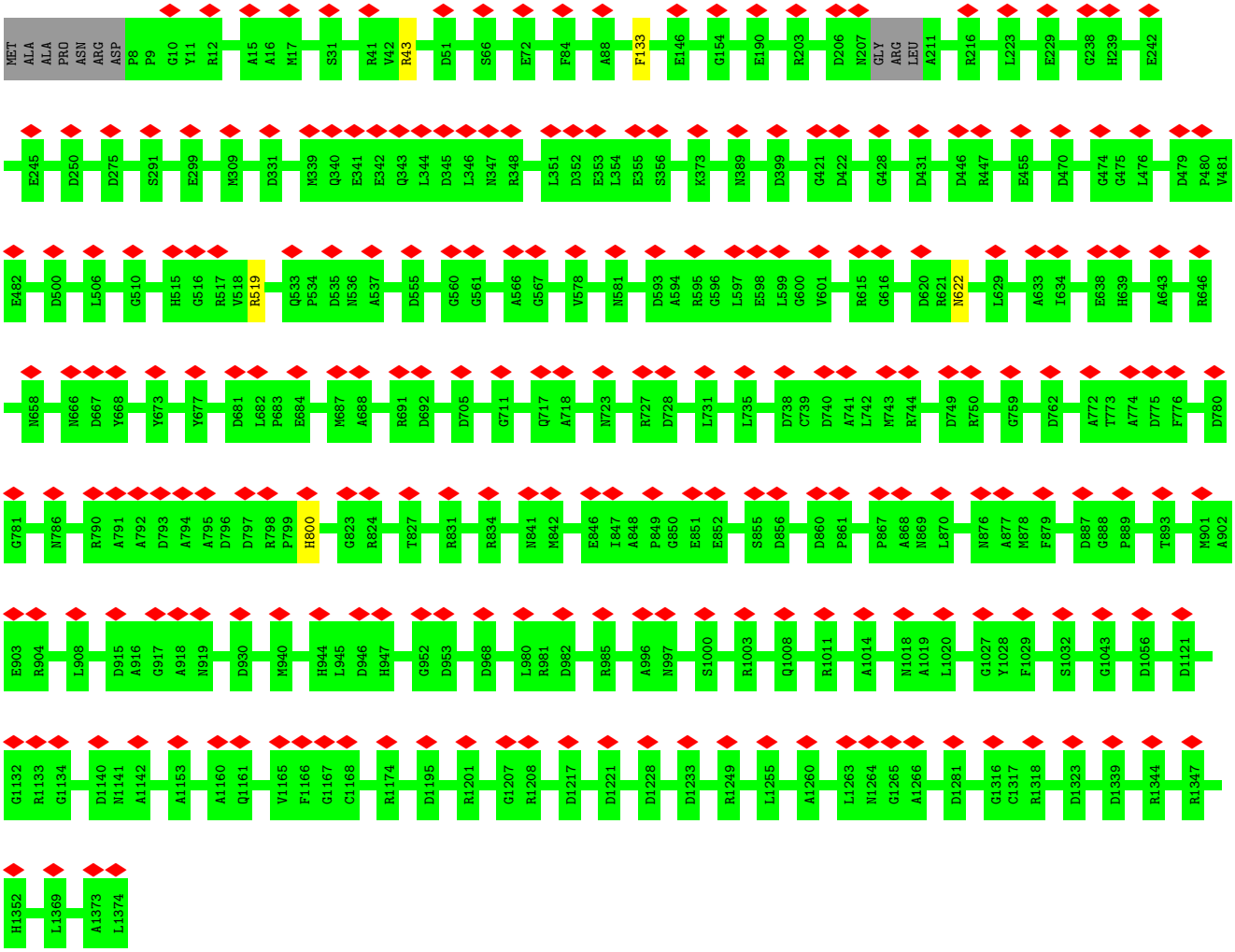




• Molecule 1: Major capsid protein

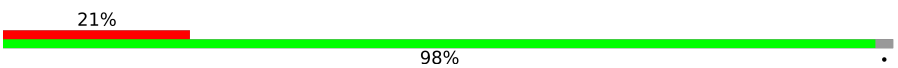
Chain W:

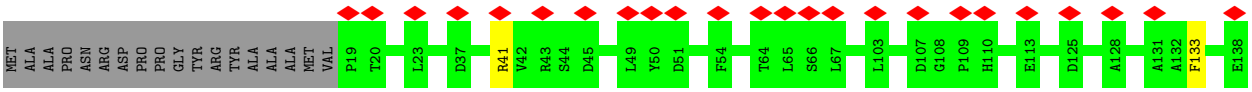


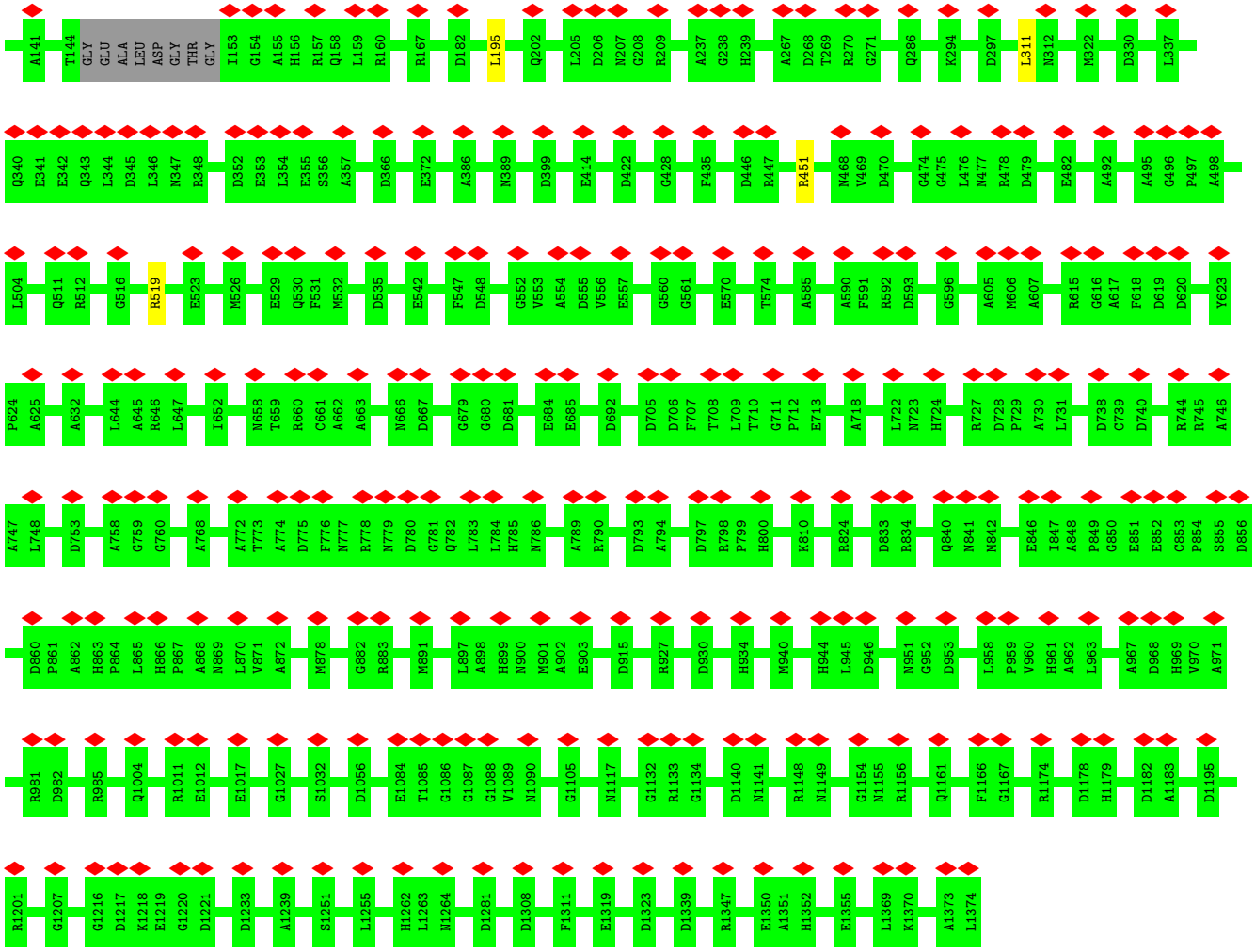


• Molecule 1: Major capsid protein

Chain X:

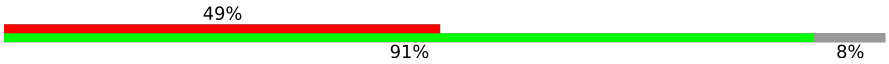


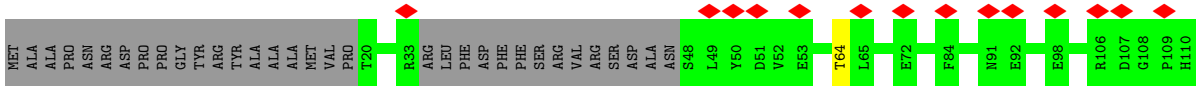


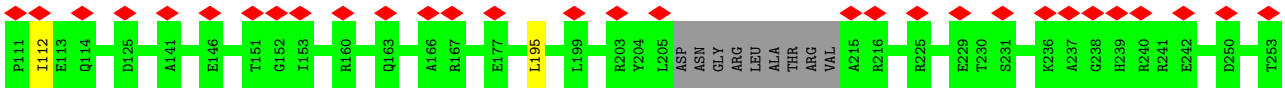


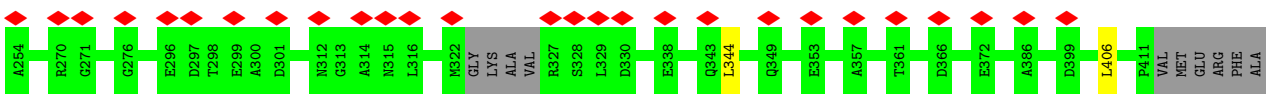
• Molecule 1: Major capsid protein

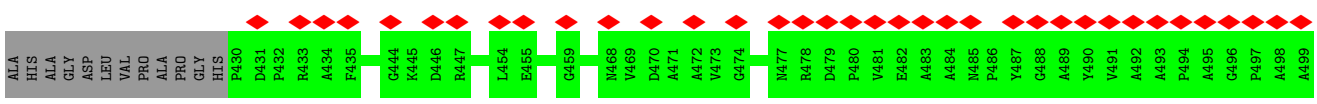
Chain 4:

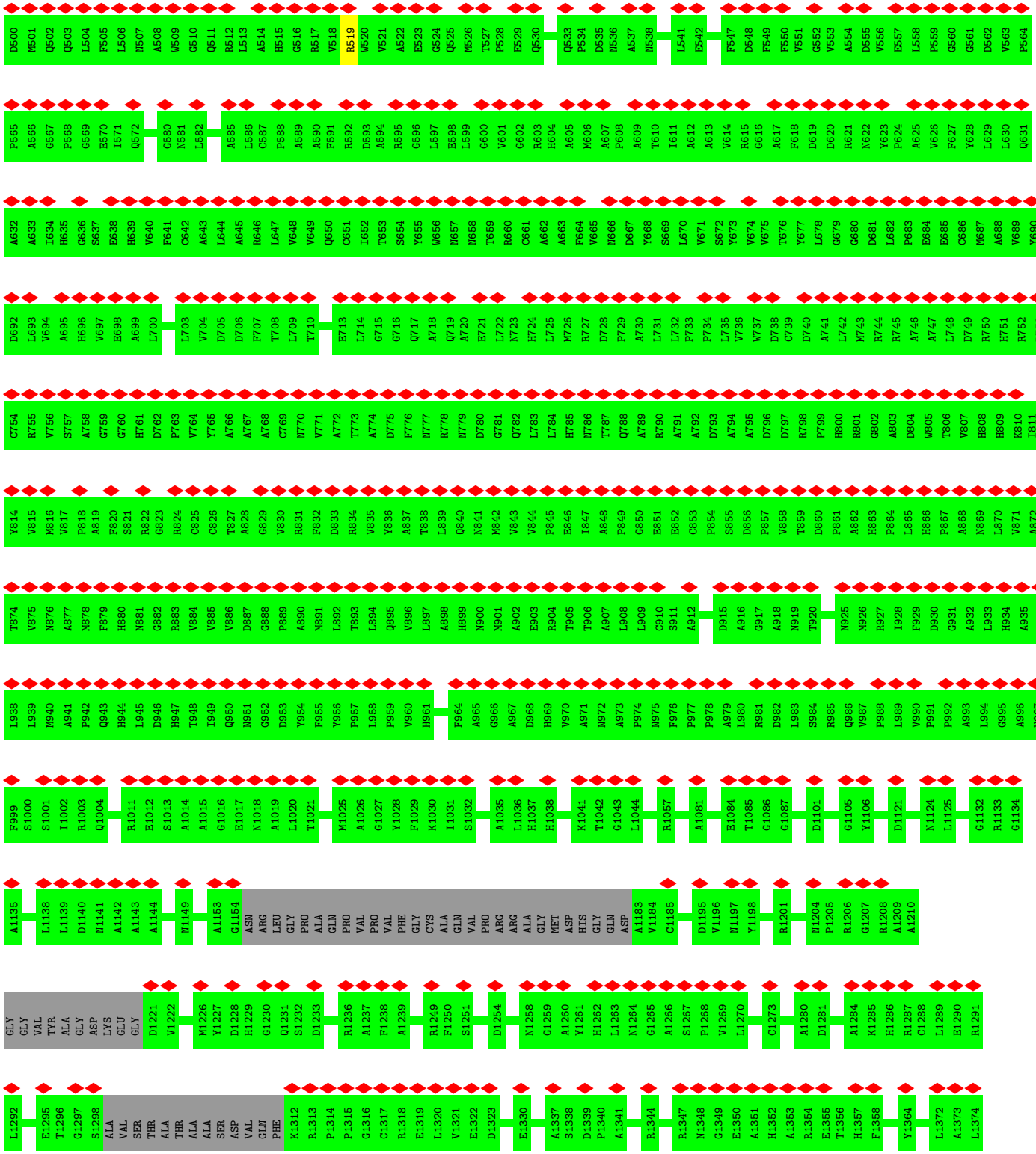






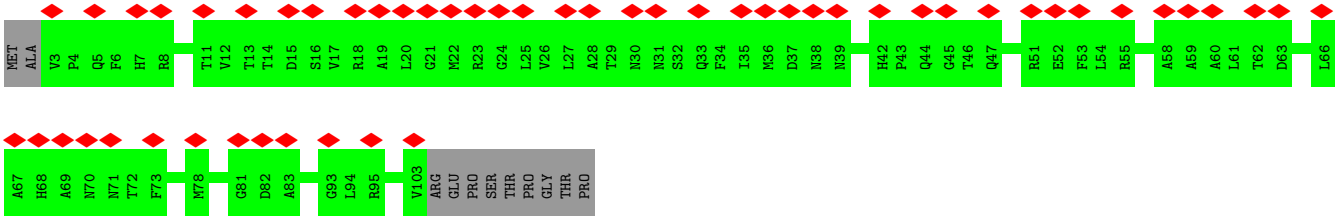






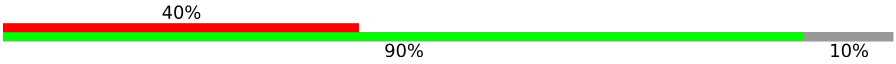
• Molecule 2: Small capsomere-interacting protein

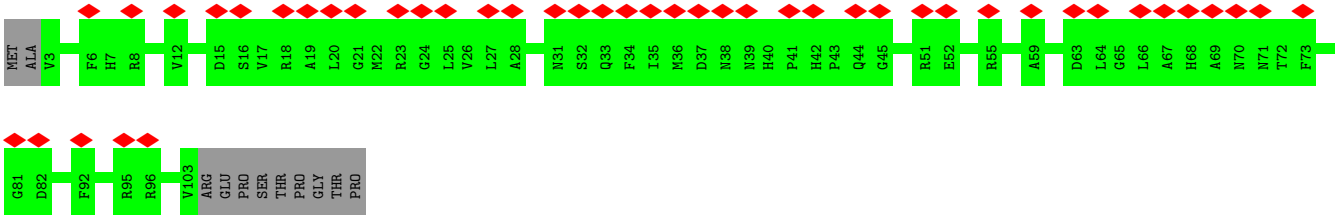
Chain G:



• Molecule 2: Small capsomere-interacting protein

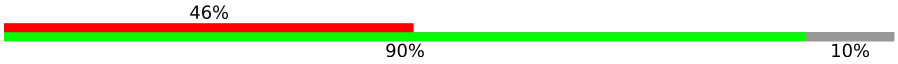
Chain H:

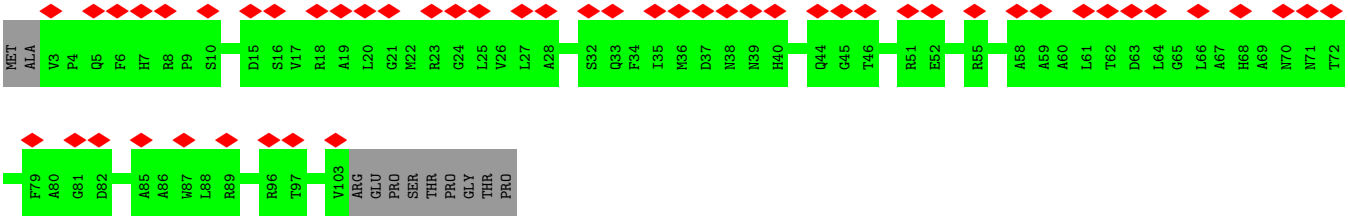




• Molecule 2: Small capsomere-interacting protein

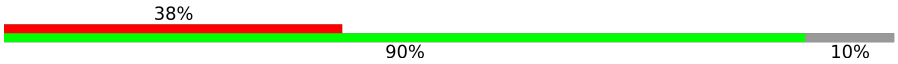
Chain I:

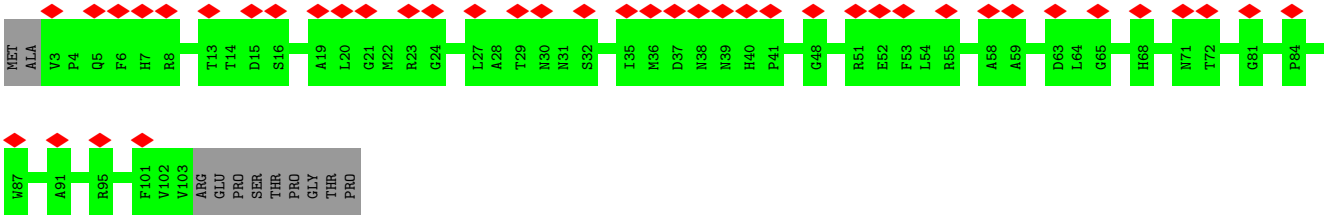




• Molecule 2: Small capsomere-interacting protein

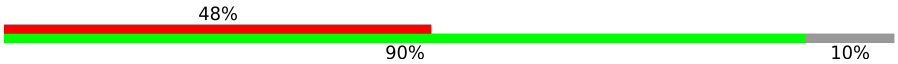
Chain J:

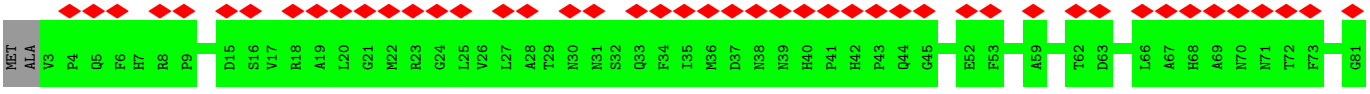


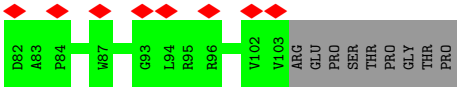


• Molecule 2: Small capsomere-interacting protein

Chain K:

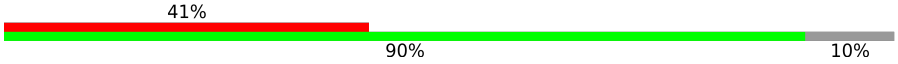


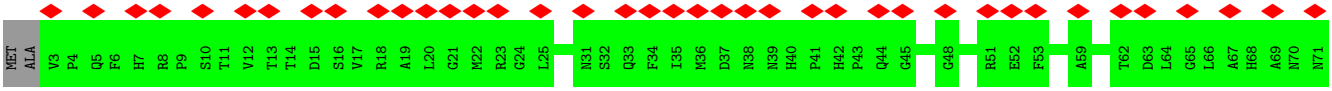


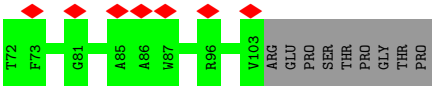


• Molecule 2: Small capsomere-interacting protein

Chain L:

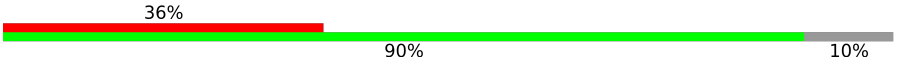


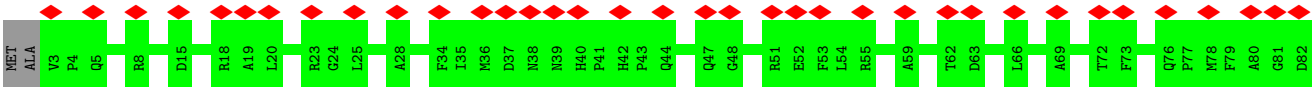


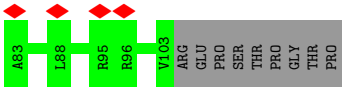


• Molecule 2: Small capsomere-interacting protein

Chain P:

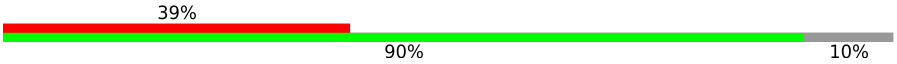


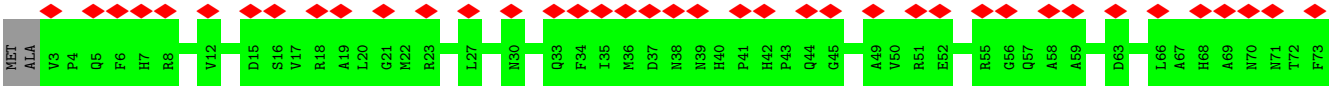


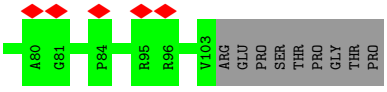


• Molecule 2: Small capsomere-interacting protein

Chain Q:

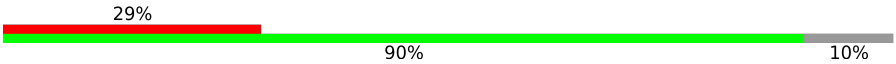


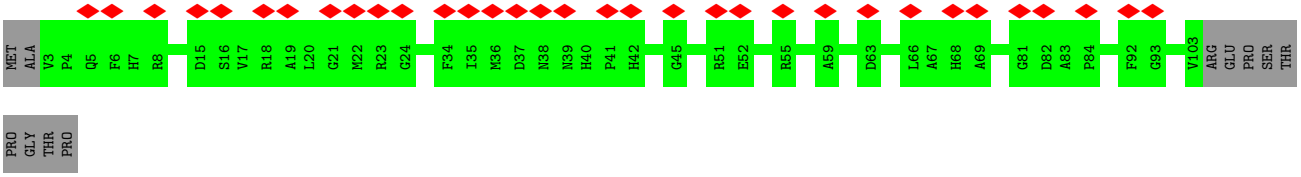




• Molecule 2: Small capsomere-interacting protein

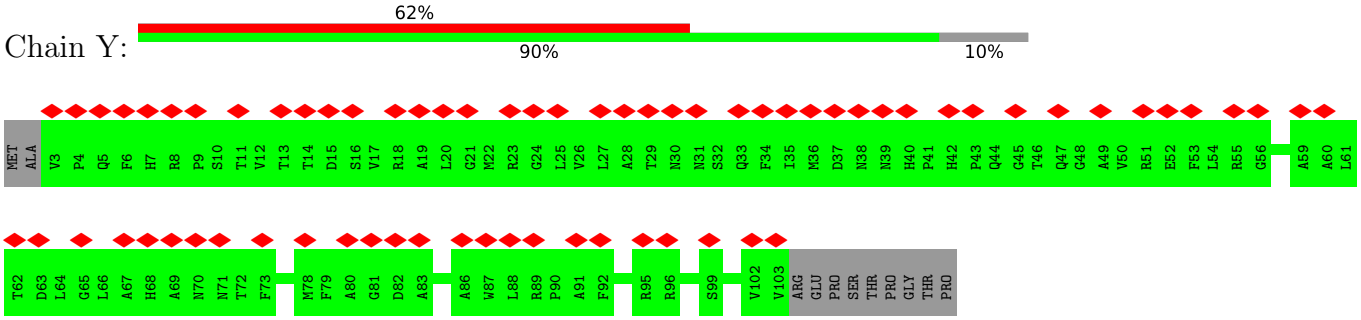
Chain R:





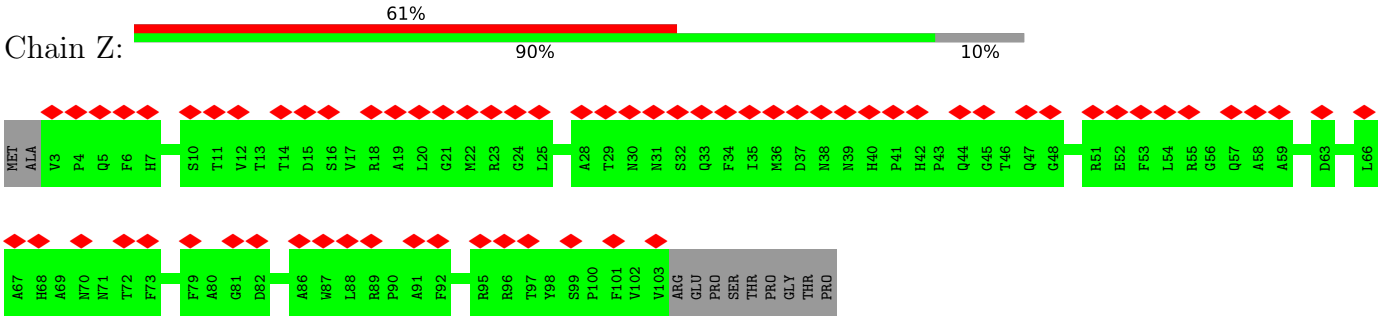
• Molecule 2: Small capsomere-interacting protein

Chain Y:



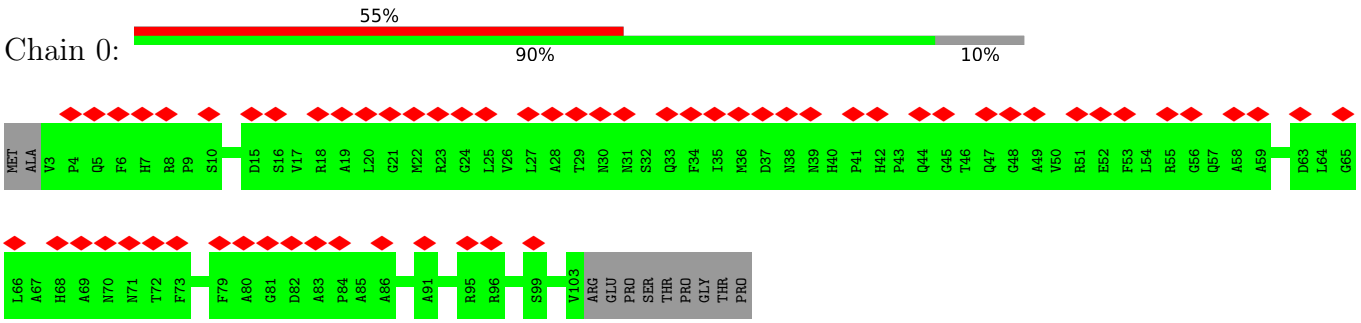
• Molecule 2: Small capsomere-interacting protein

Chain Z:



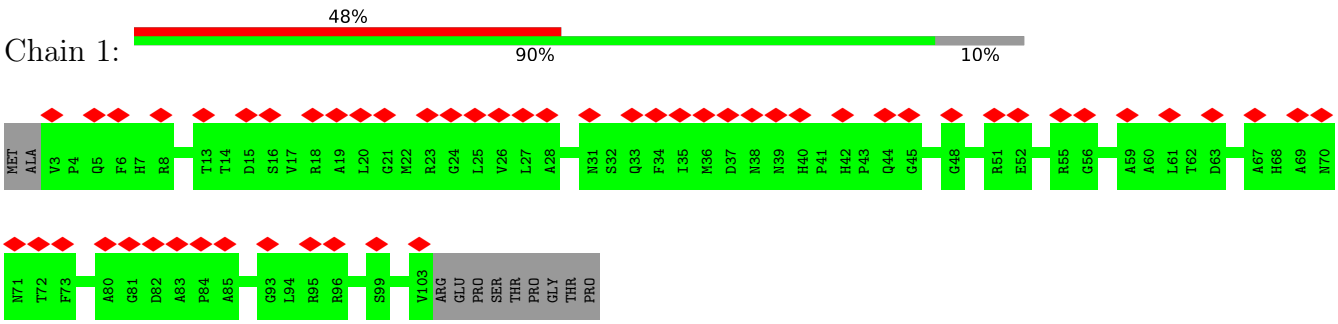
• Molecule 2: Small capsomere-interacting protein

Chain 0:



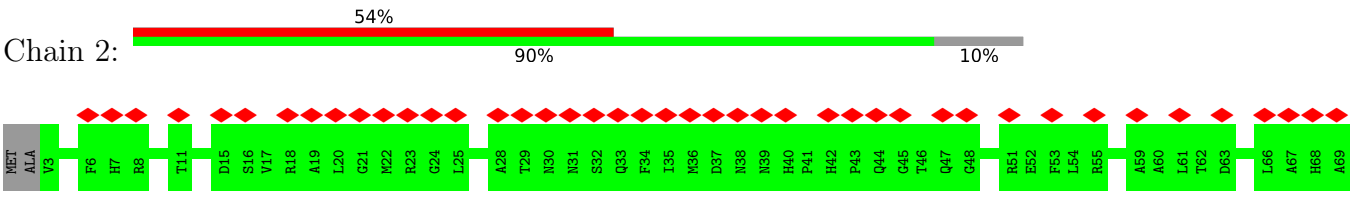
• Molecule 2: Small capsomere-interacting protein

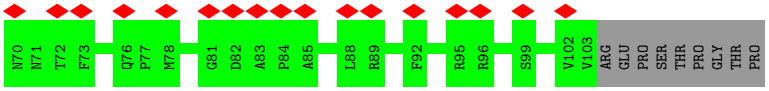
Chain 1:



• Molecule 2: Small capsomere-interacting protein

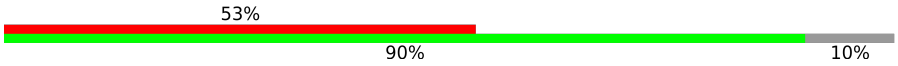
Chain 2:

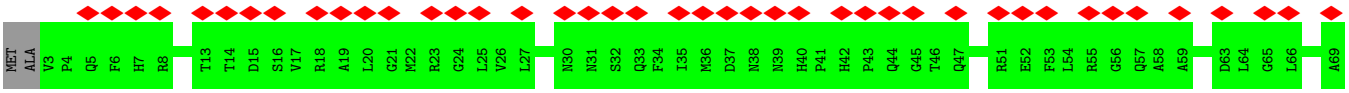


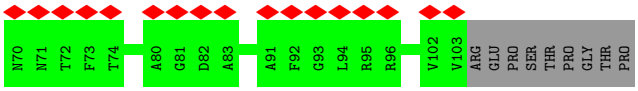


• Molecule 2: Small capsomere-interacting protein

Chain 3:

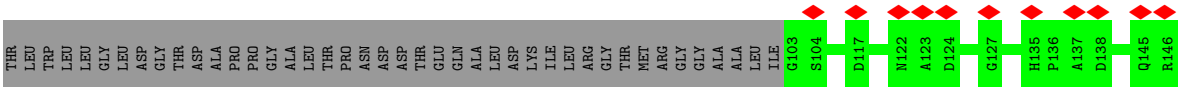


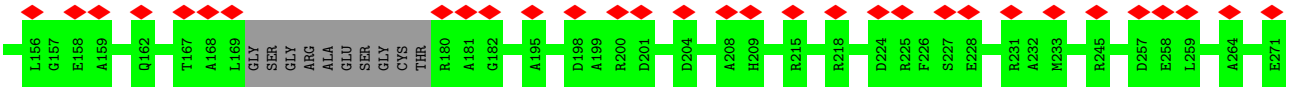


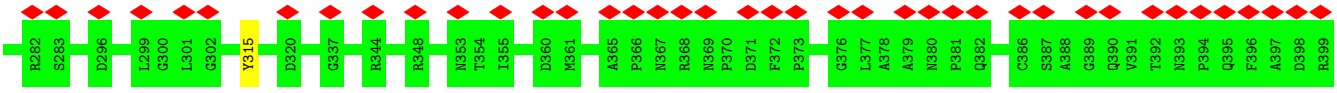


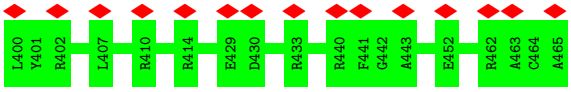
• Molecule 3: Triplex capsid protein 1

Chain 5:



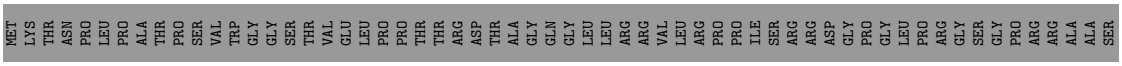


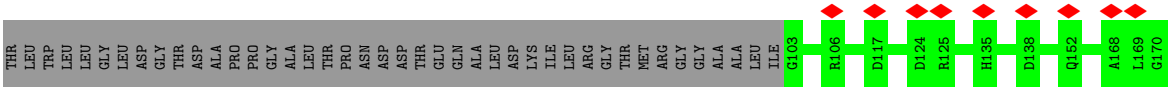


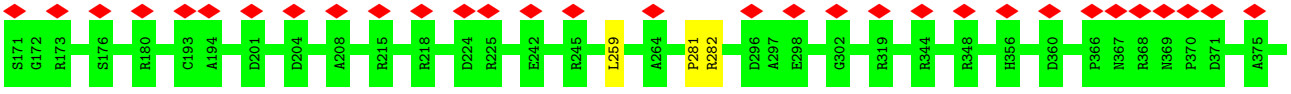


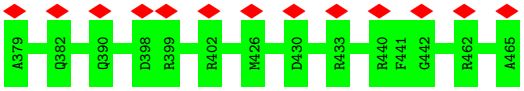
• Molecule 3: Triplex capsid protein 1

Chain 8:



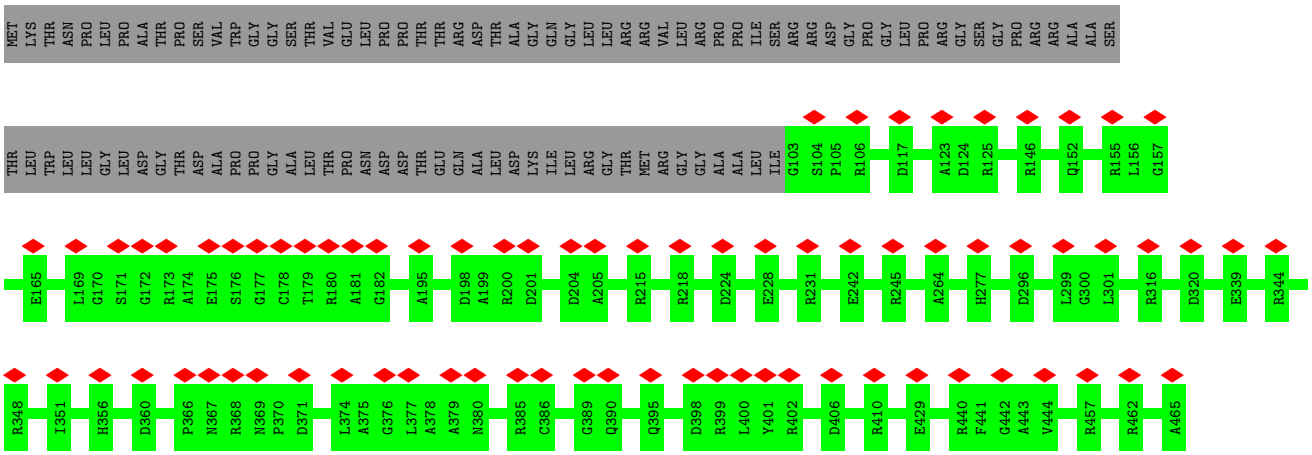






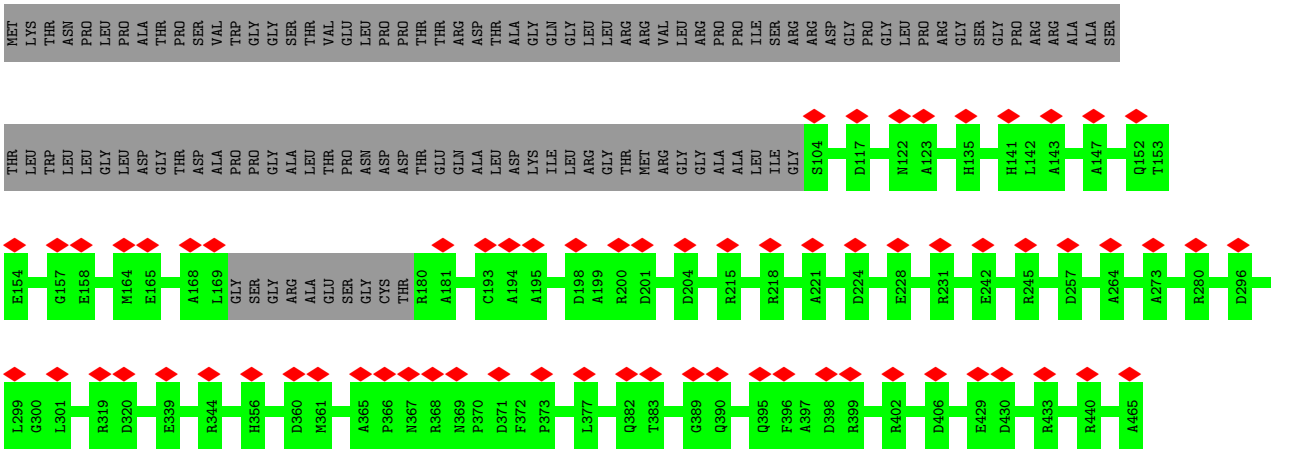
• Molecule 3: Triplex capsid protein 1

Chain b:



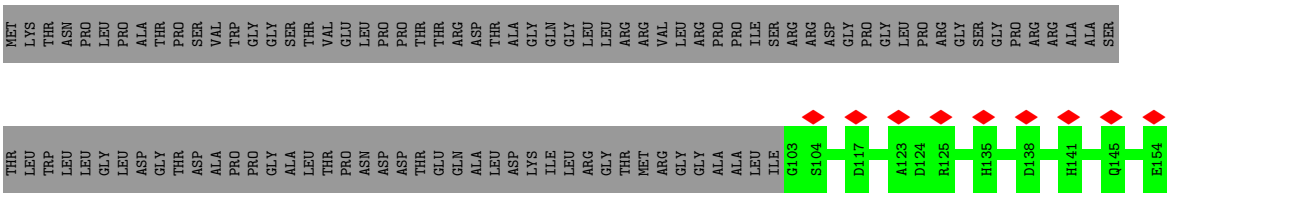
• Molecule 3: Triplex capsid protein 1

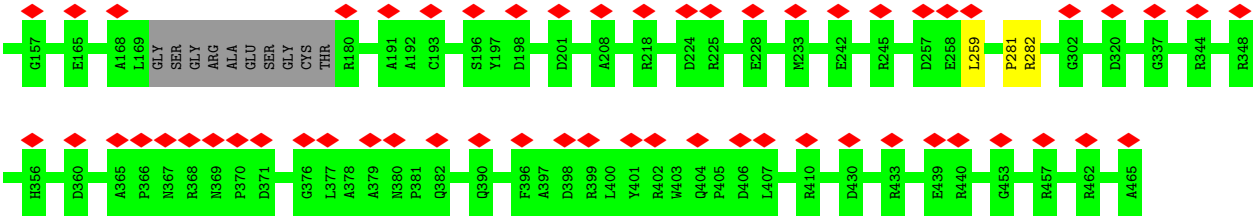
Chain e:



• Molecule 3: Triplex capsid protein 1

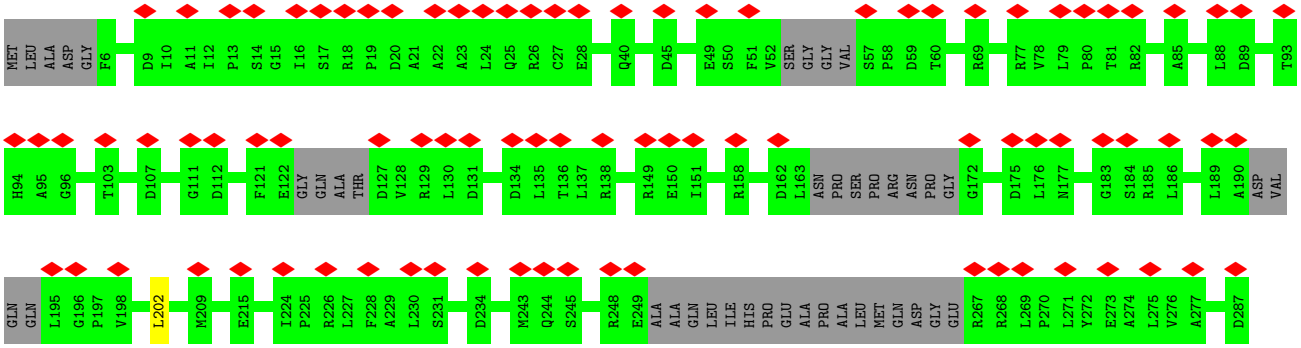
Chain h:





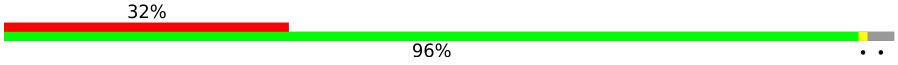
• Molecule 4: Triplex capsid protein 2

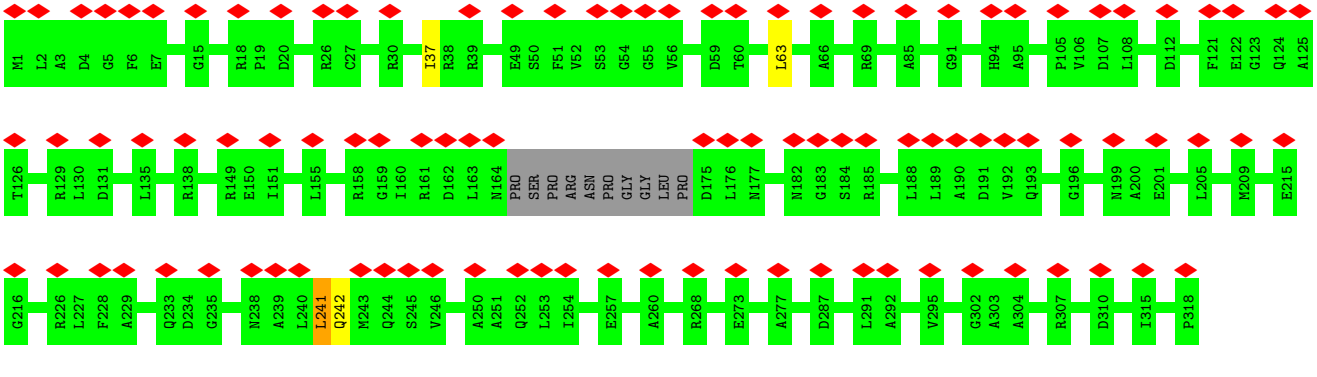
Chain 6:



• Molecule 4: Triplex capsid protein 2

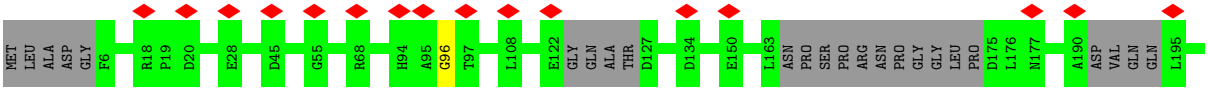
Chain 7:

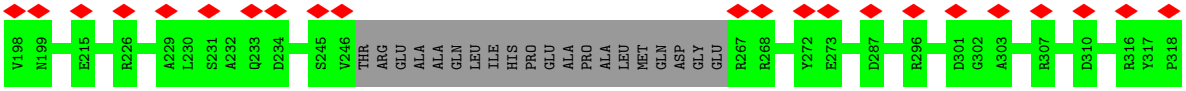




• Molecule 4: Triplex capsid protein 2

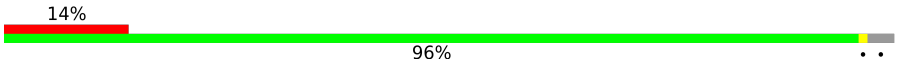
Chain 9:

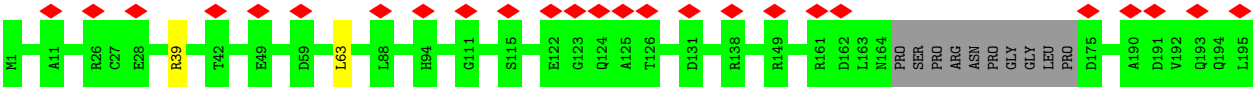


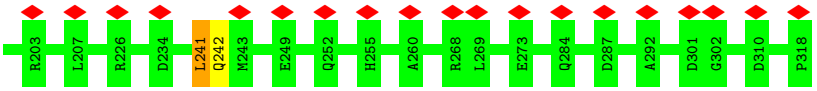


• Molecule 4: Triplex capsid protein 2

Chain a:

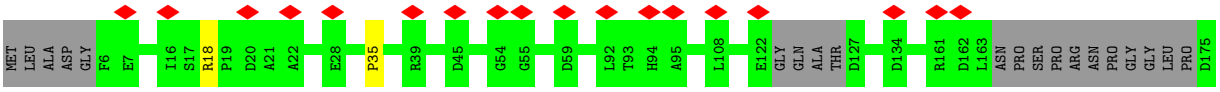


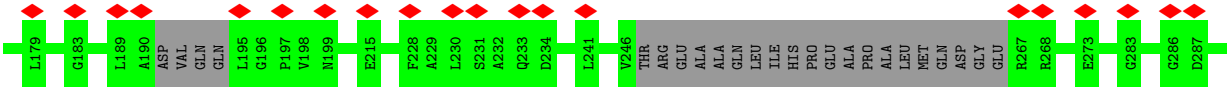


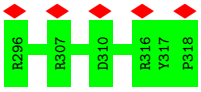


• Molecule 4: Triplex capsid protein 2

Chain c:

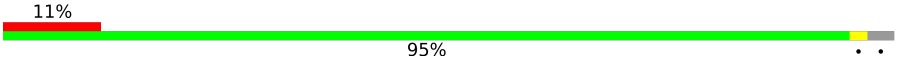


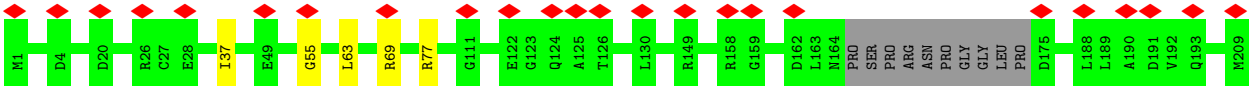


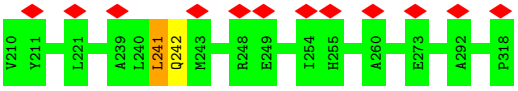


• Molecule 4: Triplex capsid protein 2

Chain d:

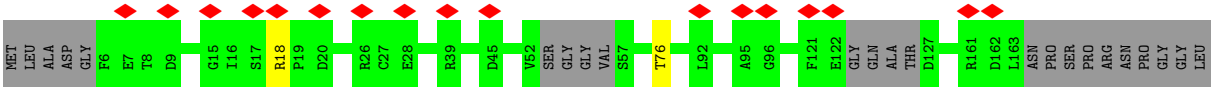


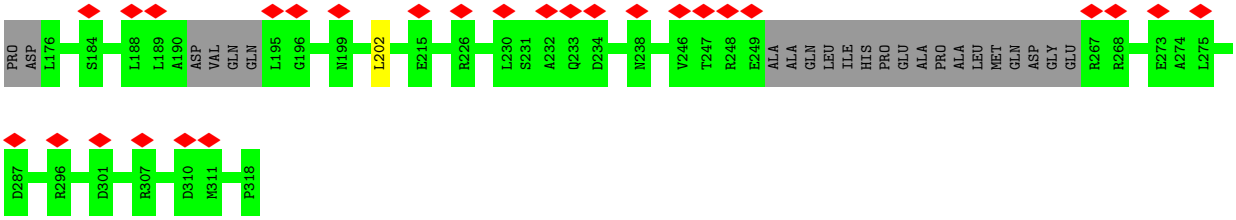




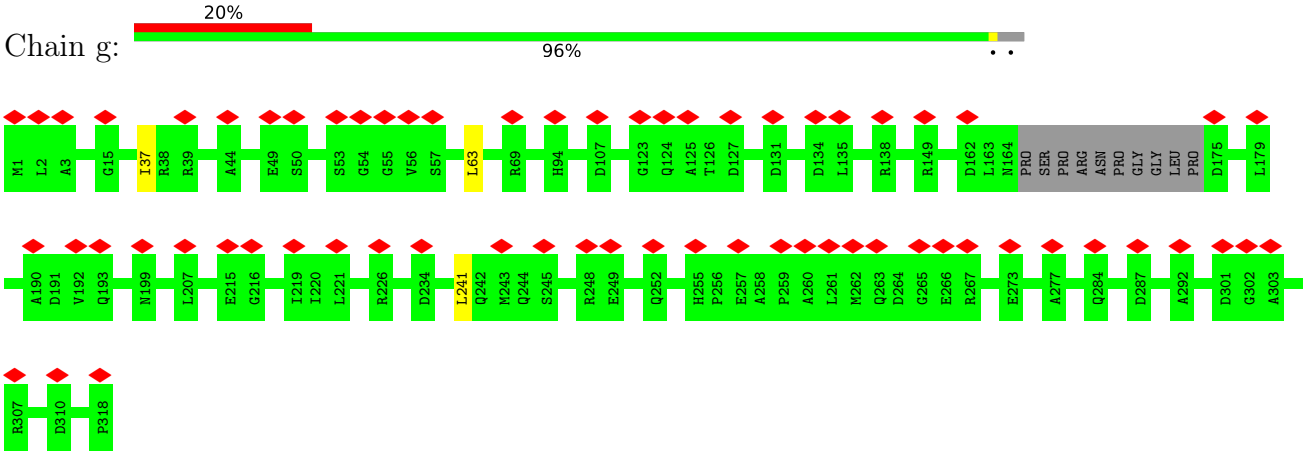
• Molecule 4: Triplex capsid protein 2

Chain f:

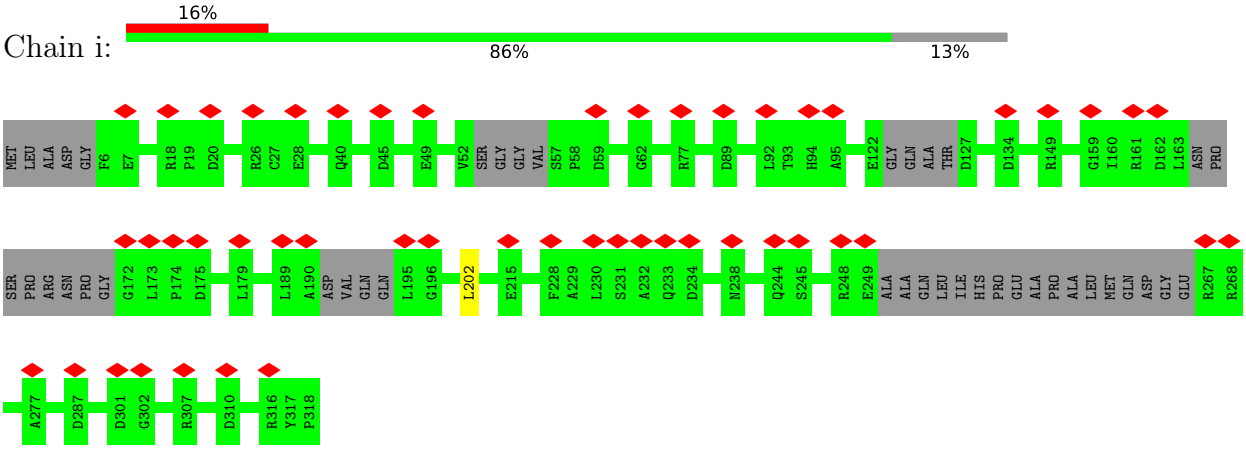




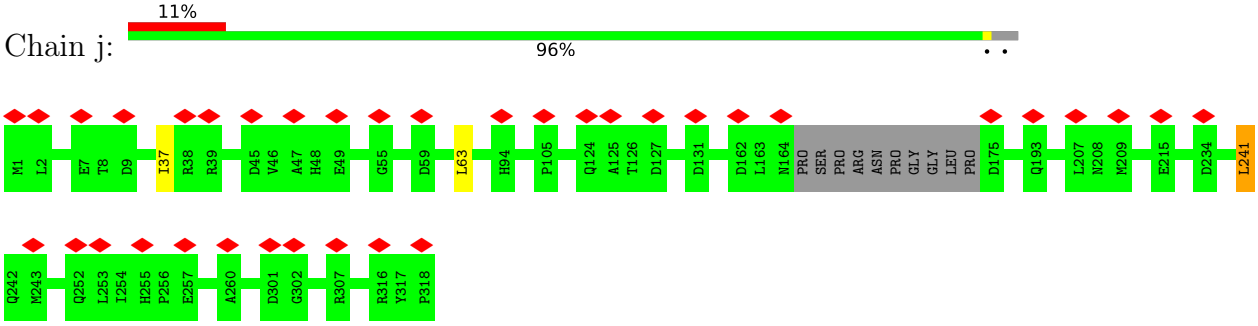
• Molecule 4: Triplex capsid protein 2



• Molecule 4: Triplex capsid protein 2

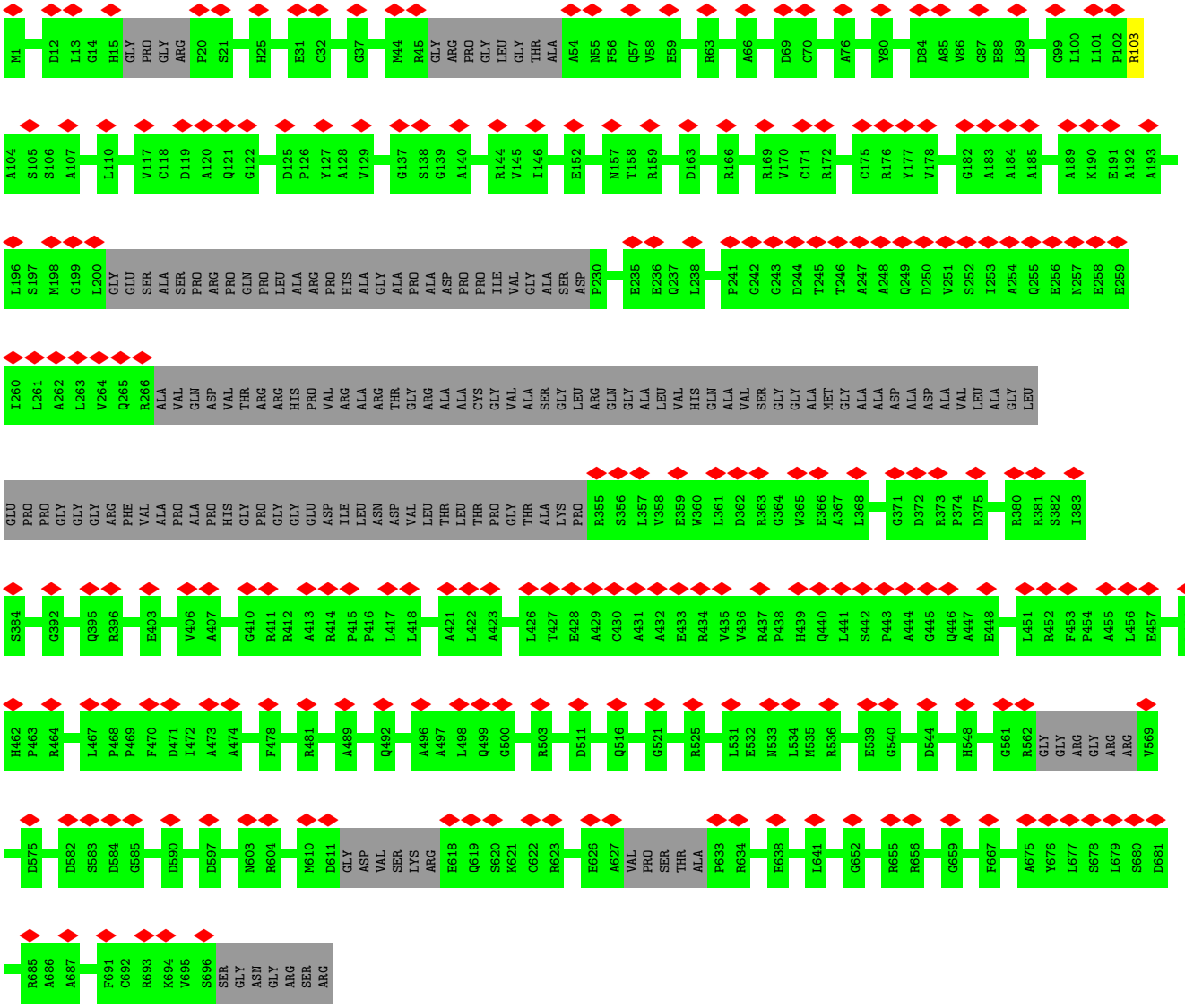


• Molecule 4: Triplex capsid protein 2



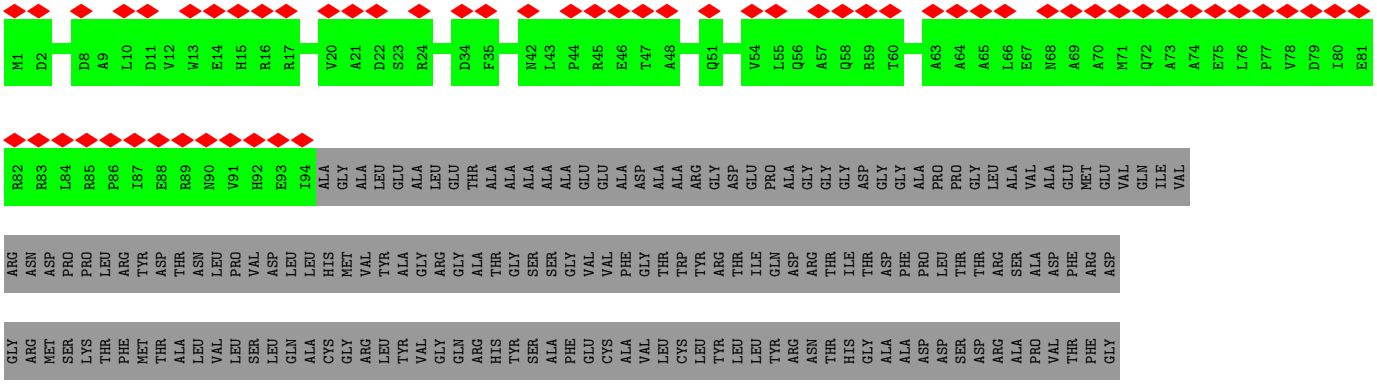
• Molecule 5: Capsid vertex component 1

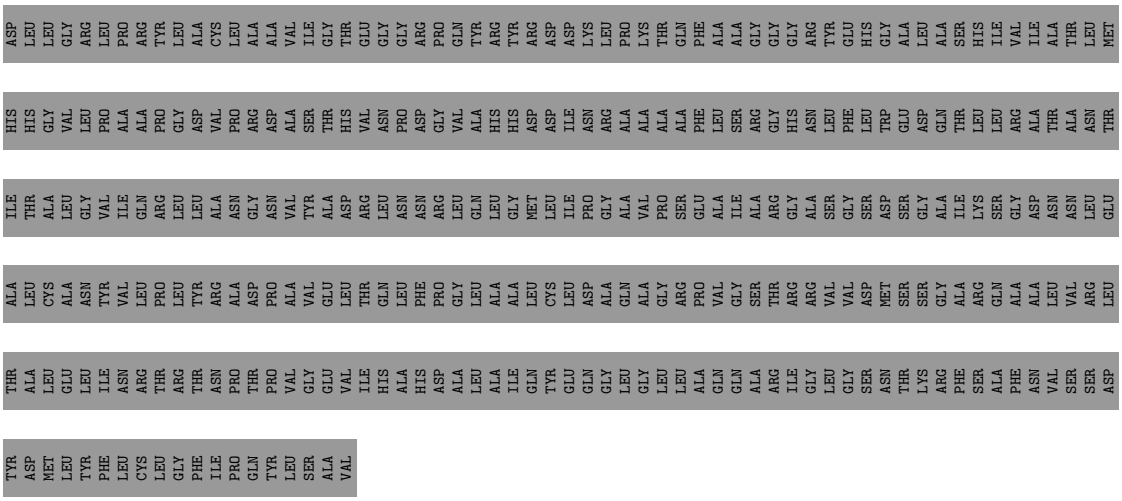
Chain k:



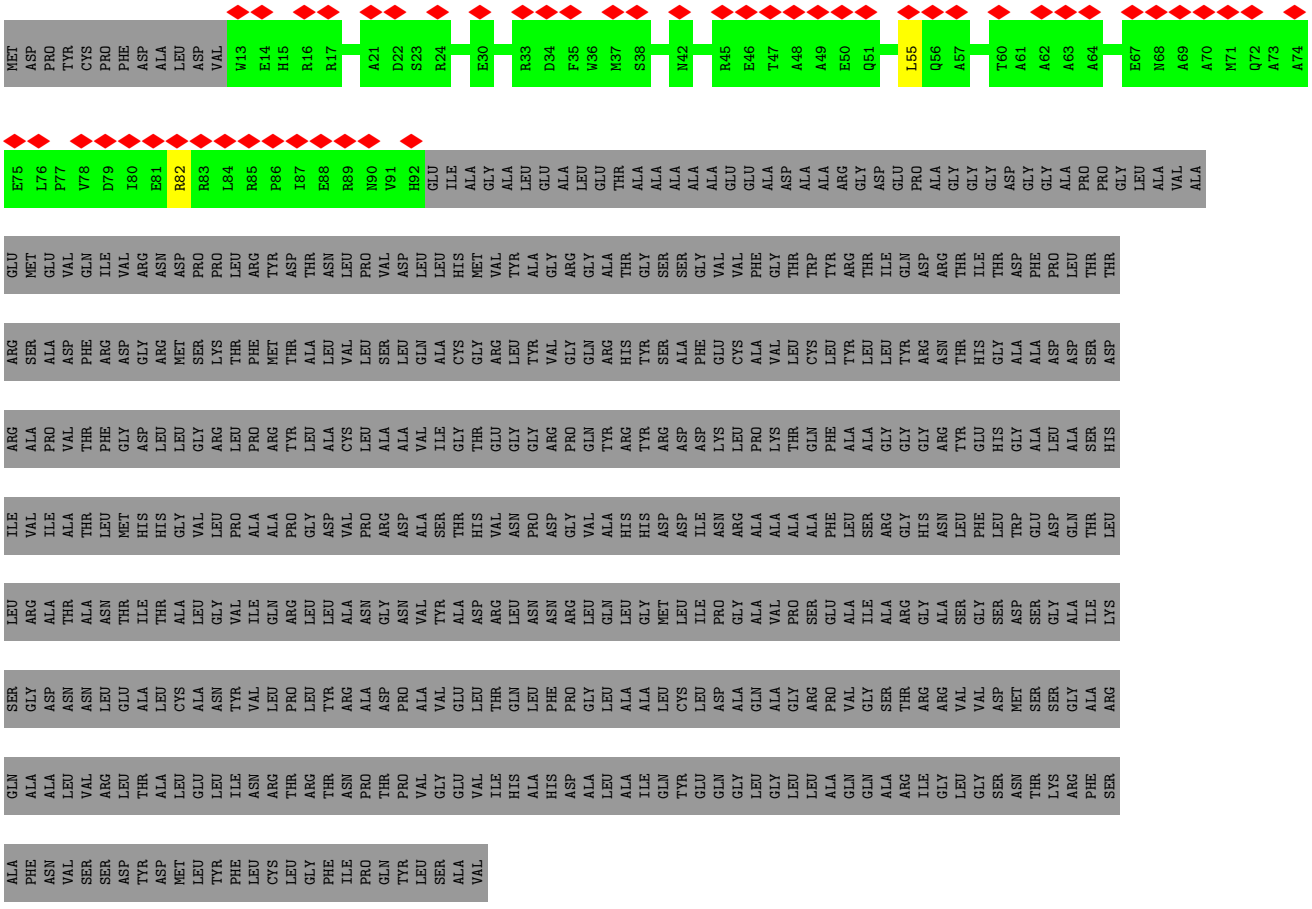
• Molecule 6: Capsid vertex component 2

Chain l:





• Molecule 6: Capsid vertex component 2



• Molecule 7: Large tegument protein deneddylase

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

SER ALA GLU ALA ILE GLU GLY CYS LEU VAL GLU GLY GLY GLU TRP THR ARG ALA THR ALA GLY PRO GLY PRO PRO ARG MET CYS SER ILE VAL GLU LEU PRO ASN PHE LEU GLU TYR PRO GLY ALA ARG GLY GLY LEU ARG CYS VAL PHE SER ARG VAL TYR GLY GLU VAL GLY PHE PHE

GLY GLU PRO ALA ALA GLY LEU LEU GLU THR GLN CYS PRO ALA HIS THR PHE PHE ALA GLY PRO TRP ALA LEU ARG PRO LEU SER TYR THR LEU LEU THR ILE GLY PRO LEU GLY MET GLY LEU PHE ARG ASP GLY ASP THR ALA TYR LEU PHE ASP PRO HIS GLY LEU PRO GLU GLY THR

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

THR TYR LEU GLN ASP GLU ALA PHE SER GLU ARG ARG VAL ALA ILE THR HIS PRO LEU ARG GLY GLU ILE ALA GLY LEU GLY GLU PRO CYS VAL GLY VAL GLY PRO ARG GLU GLY VAL GLY GLY PRO GLY PRO HIS PRO PRO THR ALA ALA GLN SER PRO PRO PRO THR ARG ALA ARG ARG

ASP ASP ARG ALA SER GLU THR SER ARG GLY THR ALA GLY PRO SER ALA LYS PRO GLU ALA LYS ARG PRO ASN ARG ALA PRO ASP ASP VAL TRP ALA VAL ALA LEU LYS GLY THR PRO PRO THR ASP PRO PRO SER ALA ASP PRO PRO SER ALA ASP PRO PRO SER ALA ILE PRO PRO PRO

PRO PRO SER ALA PRO LYS THR PRO ALA ALA GLU ALA ALA GLU GLU ASP ASP ASP MET ARG VAL LEU GLU MET GLY VAL VAL PRO VAL GLY ARG HIS ARG ALA ARG TYR SER ALA GLY LEU PRO LYS ARG ARG ARG PRO THR TRP THR PRO PRO SER SER VAL GLU ASP LEU THR SER

GLY GLU LYS THR LYS ARG SER ALA PRO PRO ALA LYS THR LYS LYS LYS SER THR PRO LYS GLY LYS THR PRO VAL GLY ALA ALA VAL PRO ALA SER VAL PRO GLU PRO VAL LEU ALA SER ALA PRO PRO ASP PRO ALA GLY PRO PRO VAL ALA GLU ALA GLY GLU ASP ASP GLY PRO THR

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

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

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

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

GLU ILE ARG VAL GLU ALA GLU ASP ARG GLN MET ARG GLU ALA LEU ASP ALA LEU ALA ARG GLY VAL ASP ALA VAL SER GLN HIS ALA GLY PRO LEU GLY VAL MET PRO ALA PRO ALA GLY ALA ALA PRO GLN GLY ALA PRO ARG PRO PRO PRO LEU GLY PRO GLU ALA VAL GLN VAL ARG

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

PHE ASP GLN HIS THR ARG ASP ILE ALA GLN ARG ALA ALA ILE PRO ALA PRO PRO ILE ALA THR SER PRO THR ALA ILE LEU LEU ARG ASP LEU ILE GLN ARG GLY GLN THR LEU ASP ALA PRO GLU ASP LEU ALA ALA TRP LEU SER VAL LEU THR ASP ALA ALA ASN GLN GLY LEU

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

ASP ASP GLY GLY LEU SER PRO GLU ALA THR ARG MET ALA GLU GLU ALA LEU ARG GLN ALA ARG ALA MET ASP ALA ALA LYS LEU THR ALA GLU LEU ALA PRO ASP ALA ARG ALA ARG LEU ARG GLU ARG ALA ARG SER LEU GLU ALA MET LEU GLU GLY ALA ARG GLU ARG ALA LYS VAL

ALA ARG ASP ALA ARG GLU LYS PHE LEU HIS LYS LEU GLN GLY VAL LEU ARG PRO LEU PRO ASP PHE VAL GLY LEU LYS ALA CYS PRO ALA VAL LEU ALA THR LEU ARG ALA SER LEU PRO ALA GLY TRP SER ASP LEU PRO GLU ALA VAL ARG GLY ALA PRO PRO GLU VAL THR ALA ALA

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

ILE ILE ALA HIS ALA VAL SER ASN ALA ILE ASN ALA GLY SER ALA ALA VAL ALA THR ALA ASP PRO ALA SER THR VAL ASP ALA ALA VAL ARG ALA HIS ARG VAL LEU VAL ASP ALA VAL THR ALA LEU GLY ALA ALA ALA SER ASP PRO ALA SER PRO LEU ALA PHE LEU ALA ALA MET

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

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

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

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

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

ILE ARG ASP ARG LEU ASP ALA LEU ARG ALA ASP ALA ARG ARG ALA ILE GLY SER VAL ALA LEU ASP LEU ALA ALA ALA GLU GLU ILE SER ALA VAL ARG ASN ASP PRO ALA ALA ALA ALA GLU LEU VAL ARG ALA GLY VAL THR LEU PRO CYS PRO SER GLU ASP ALA LEU VAL ALA

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

ALA ARG GLU ARG ARG ALA GLN LEU GLU ALA GLU GLY LEU ALA ASN LEU LYS THR LEU LEU LYS VAL VAL ALA VAL PRO ALA THR VAL ALA LYS THR LEU ASP GLN ALA ARG SER ALA GLU GLU ILE ALA ASP GLN VAL GLU ILE LEU VAL ASP GLN THR GLU LYS ALA ARG GLU LEU ASP

VAL GLN ALA VAL ALA TRP LEU GLU HIS ALA GLN ARG THR PHE GLU THR HIS PRO LEU SER ALA ALA SER GLY ASP GLY PRO GLY LEU LEU THR ARG GLN GLY ALA ARG LEU GLN ALA LEU PHE ASP THR ARG ARG ARG VAL GLU ALA LEU ARG ARG SER LEU GLU GLU ALA GLU ALA GLU

TRP ASP GLU VAL TRP GLY ARG PHE GLY ARG VAL ARG GLY GLY ALA TRP LYS SER PRO GLU GLY PHE ARG ALA ALA CYS GLU GLN LEU ARG ALA LEU GLN ASP THR THR ASN THR VAL SER GLY LEU ARG ALA GLN ARG ASP TYR GLU ARG LEU PRO ALA LYS TYR GLN GLY VAL LEU GLY

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

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

GLU ALA ASP PRO GLN MET LEU ARG ARG ARG GLY GLU ALA TYR LEU ARG VAL SER GLY GLY PRO GLY PRO LEU VAL LEU ARG GLU ALA THR SER THR LEU ASP ARG PRO PHE ALA PRO SER PHE LEU VAL PRO ASP GLY THR PRO LEU GLN TYR ALA LEU CYS PHE PRO ALA VAL THR ASP

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

ARG HIS ARG GLN ALA ARG TRP GLY ALA SER MET ASP ALA ALA ALA GLU LEU TYR VAL ALA LEU VAL ALA THR THR LEU THR ARG GLU PHE GLY CYS ARG TRP ALA GLN LEU GLU TRP GLY GLY ASP ALA ALA ALA PRO GLY PRO PRO LEU GLY PRO GLN SER SER THR ARG HIS ARG VAL

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

ALA ARG ILE ARG VAL LEU PRO ALA PHE SER ALA GLY GLY PRO PRO THR ARG GLY LEU MET PHE GLY THR ARG LEU ALA ASP TRP ARG ARG GLY LYS LEU SER GLU THR ASP PRO LEU ALA PRO TRP ARG SER VAL PRO GLU LEU GLY THR GLU ARG GLY ALA ALA LEU GLY LYS LEU SER

PRO ALA GLN ALA LEU ALA ALA VAL SER VAL LEU GLY ARG MET CYS LEU PRO SER THR ALA LEU VAL ALA LEU TRP THR THR CYS MET PHE PRO ASP ASP TYR THR GLU TYR ASP SER PHE ASP ALA LEU LEU THR ALA ARG LEU GLU SER GLY GLN THR LEU SER PRO SER GLY GLY ARG GLU

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

ARG GLU SER GLU LEU GLU LEU CYS LEU THR LEU PHE ASP SER ARG ALA ARG GLY PRO ASP ALA ALA LEU ARG ASP ALA VAL SER SER ASP ILE GLU THR TRP ALA VAL ARG LEU LEU HIS ALA ASP LEU ASN PRO ILE GLU ASN ALA CYS LEU ALA ALA GLN LEU PRO ARG LEU SER ALA

LEU ILE ALA GLU ARG PRO LEU ALA ARG GLY PRO PRO CYS LEU VAL LEU VAL ASP ILE SER MET THR PRO VAL ALA VAL LEU TRP GLU ASN PRO ASP PRO PRO GLY PRO PRO ASP VAL ARG PHE VAL GLY SER GLU ALA THR GLU GLU LEU PRO PHE VAL ALA GLY GLY GLU ASP VAL LEU

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

GLU GLY SER LEU GLY PRO GLY SER LEU ALA PRO THR LEU PHE THR ASP ALA THR PRO GLY GLU PRO VAL PRO PRO ARG MET TRP ALA TRP ILE HIS GLY LEU GLU GLU LEU ALA SER ASP ASP SER GLY GLY PRO ALA PRO LEU LEU ALA PRO ASP PRO LEU SER PRO THR ALA ASP GLN

SER VAL PRO THR SER GLN CYS ALA PRO ARG PRO PRO GLY PRO ALA VAL THR ALA ARG GLU ALA ARG PRO GLY VAL PRO ALA GLU SER THR ARG PRO ALA PRO VAL GLY PRO ARG ASP ASP PHE ARG ARG LEU PRO SER PRO GLN SER SER PRO ALA PRO PRO ASP ALA THR ALA PRO ARG

PRO PRO ALA SER SER ARG ALA SER ALA ALA SER SER SER GLY SER ARG ALA ARG ARG HIS ARG ARG ALA ARG SER LEU ALA ARG ALA THR GLN ALA SER ALA THR THR GLN GLY TRP ARG PRO PRO ALA LEU PRO ASP THR VAL ALA PRO VAL THR ASP PHE ALA ARG PRO PRO ALA PRO

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

ALA PRO THR PRO PRO ARG VAL PRO VAL GLY GLY PRO GLN ARG ARG LEU THR ARG PRO ALA VAL ALA SER LEU SER GLU SER ARG GLU SER LEU PRO SER PRO TRP ASP PRO ALA ASP PRO THR ALA PRO VAL LEU GLY ARG ASN PRO ALA GLU PRO THR SER SER SER PRO ALA GLY PRO

SER PRO PRO PRO PRO ALA VAL GLN PRO VAL ALA PRO PRO PRO THR SER GLY PRO PRO PRO THR TYR LEU THR LEU GLU GLY GLY VAL ALA PRO GLY GLY PRO VAL SER ARG ARG PRO THR THR ARG GLN PRO VAL ALA THR PRO THR THR SER ALA ARG PRO ARG GLY HIS LEU THR VAL

SER ARG LEU SER ALA PRO GLN PRO

GLN PRO GLN PRO GLN PRO GLN PRO GLN PRO GLN PRO GLN PRO GLN ASN GLY HIS VAL ALA PRO GLY GLU TYR PRO ALA VAL ARG PHE ARG ALA PRO GLN ASN ARG PRO SER VAL PRO ALA SER ALA SER SER THR ASN PRO ARG THR GLY SER SER LEU SER GLY VAL SER SER TRP ALA

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

ALA LEU SER ALA ASP ASP SER GLN GLU VAL THR ARG LEU GLN PHE GLY PRO PRO VAL SER ALA ASN ALA VAL LEU SER ARG ARG TYR VAL Q3092 R3093 T3094 G3095 R3096 S3097 A3098 L3099 A3100 V3101 L3102 I3103 R3104 A3105 C3106 Y3107 R3108 L3109 Q3110 Q3111 Q3112 L3113 Q3114 R3115 T3116 R3117 R3118 A3119 L3120

L3121 H3122 H3123 S3124 D3125 A3126 V3127 L3128 T3129 S3130 L3131 H3132 H3133 V3134 R3135 M3136 L3137 L3138 GLY

- Molecule 7: Large tegument protein deneddylase

Chain o:

99%

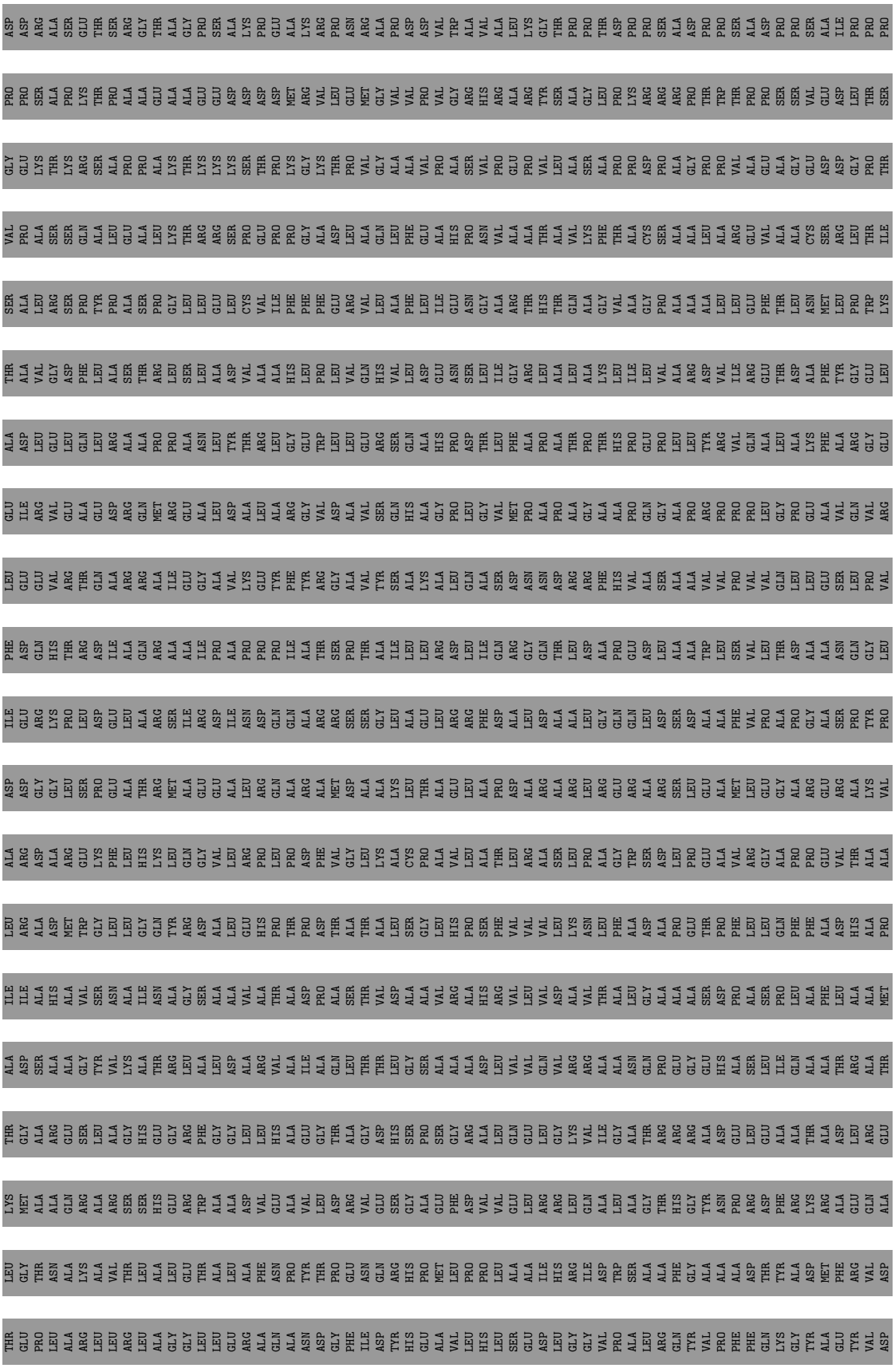
MET ILE ALA GLY THR PRO PRO HIS SER THR MET GLU ARG GLY GLY ASP ARG ASP ILE VAL VAL THR GLY ALA ARG ASN GLN PHE ALA PRO ASP LEU GLU PRO GLY GLY SER VAL SER CYS MET ARG SER SER LEU SER PHE LEU SER LEU ILE PHE ASP VAL GLY PRO ARG ASP VAL LEU

SER ALA GLU ALA ILE GLU GLY CYS LEU VAL GLU GLY GLY GLU TRP THR ARG ALA THR ALA GLY PRO GLY PRO PRO ARG MET CYS SER ILE VAL GLU LEU PRO ASN PHE LEU GLU TYR PRO GLY ALA ARG GLY GLY LEU ARG CYS VAL PHE SER ARG VAL TYR GLY GLU VAL GLY PHE PHE

GLY GLU PRO ALA ALA GLY LEU LEU GLU THR GLN CYS PRO ALA HIS THR PHE PHE ALA GLY PRO TRP ALA LEU ARG PRO LEU SER TYR THR LEU LEU THR ILE GLY PRO LEU GLY MET GLY LEU PHE ARG ASP GLY ASP THR ALA TYR LEU PHE ASP PRO HIS GLY LEU PRO GLU GLY THR

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

THR TYR LEU GLN ASP GLU ALA PHE SER GLU ARG ARG VAL ALA ILE THR HIS PRO LEU ARG GLY GLU ILE ALA GLY LEU GLY GLU PRO CYS VAL GLY VAL GLY PRO ARG GLU GLY VAL GLY GLY PRO GLY PRO HIS PRO PRO THR ALA ALA GLN SER PRO PRO PRO THR ARG ALA ARG ARG



ILE ARG ASP ARG LEU ASP ALA LEU ARG ALA ASP ALA ARG ARG ALA ILE GLY SER VAL ALA LEU ASP LEU ALA ALA ALA ALA GLU GLU ILE SER ALA VAL ARG ASN ASP PRO ALA ALA ALA ALA GLU LEU VAL ARG ALA GLY VAL THR LEU PRO CYS PRO SER GLU ASP ALA LEU VAL ALA

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

ALA ARG GLU ARG ARG ALA GLN LEU GLU ALA GLY GLY LEU ALA ASN LEU LYS THR LEU LEU LYS VAL VAL ALA VAL PRO ALA THR VAL ALA LYS THR LEU ASP GLN ALA ARG SER ALA GLU GLU ILE ALA ASP GLN VAL GLU ILE LEU VAL ASP GLN THR GLU LYS ALA ARG GLU LEU ASP

VAL GLN ALA VAL ALA TRP LEU GLU HIS ALA GLN ARG THR PHE GLU THR HIS PRO LEU SER ALA ALA SER GLY ASP GLY PRO GLY LEU LEU THR ARG GLN GLY ALA ARG LEU GLN ALA LEU PHE ASP THR ARG ARG ARG VAL GLU ALA LEU ARG ARG SER LEU GLU GLU ALA GLU ALA GLU

TRP ASP GLU VAL TRP GLY ARG PHE GLY ARG VAL ARG GLY GLY ALA TRP LYS SER PRO GLU GLY PHE ARG ALA ALA CYS GLU GLN LEU ARG ALA LEU GLN ASP THR THR ASN THR VAL SER GLY LEU ARG ALA GLN ARG ASP TYR GLU ARG LEU PRO ALA LYS TYR GLN GLY VAL LEU GLY

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

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

GLU ALA ASP PRO GLN MET LEU ARG ARG ARG GLY GLU ALA TYR LEU ARG VAL SER GLY GLY PRO GLY PRO LEU VAL LEU ARG GLU ALA THR SER THR LEU ASP ARG PRO PHE ALA PRO SER PHE LEU VAL PRO ASP GLY THR PRO LEU GLN TYR ALA LEU CYS PHE PRO ALA VAL THR ASP

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

ARG HIS ARG GLN ALA ARG TRP GLY ALA SER MET ASP ALA ALA ALA GLU LEU TYR VAL ALA LEU VAL ALA THR THR LEU THR ARG GLU PHE GLY CYS ARG TRP ALA GLN LEU GLU TRP GLY GLY ASP ALA ALA ALA PRO GLY PRO PRO LEU GLY PRO GLN SER SER THR ARG HIS ARG VAL

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

ALA ARG ILE ARG VAL LEU PRO ALA PHE SER ALA GLY GLY PRO PRO THR ARG GLY LEU MET PHE GLY THR ARG LEU ALA ASP TRP ARG ARG GLY LYS LEU SER GLU THR ASP PRO LEU ALA PRO TRP ARG SER VAL PRO GLU LEU GLY THR GLU ARG GLY ALA ALA LEU GLY LYS LEU SER

PRO ALA GLN ALA LEU ALA ALA VAL SER VAL LEU GLY ARG MET CYS LEU PRO SER THR ALA LEU VAL ALA LEU TRP THR CYS MET PHE PRO ASP ASP TYR THR GLU TYR ASP SER PHE ASP ALA LEU LEU THR ALA ARG LEU GLU SER GLY GLN THR LEU SER PRO SER GLY GLY ARG GLU

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

ARG GLU SER GLU LEU GLU LEU CYS LEU THR LEU PHE ASP SER ARG ALA ARG GLY PRO ASP ALA ALA LEU ARG ASP ALA VAL SER SER ASP ILE GLU THR TRP ALA VAL ARG LEU LEU HIS ALA ASP LEU ASN PRO ILE GLU ASN ALA CYS LEU ALA ALA GLN LEU PRO ARG LEU SER ALA

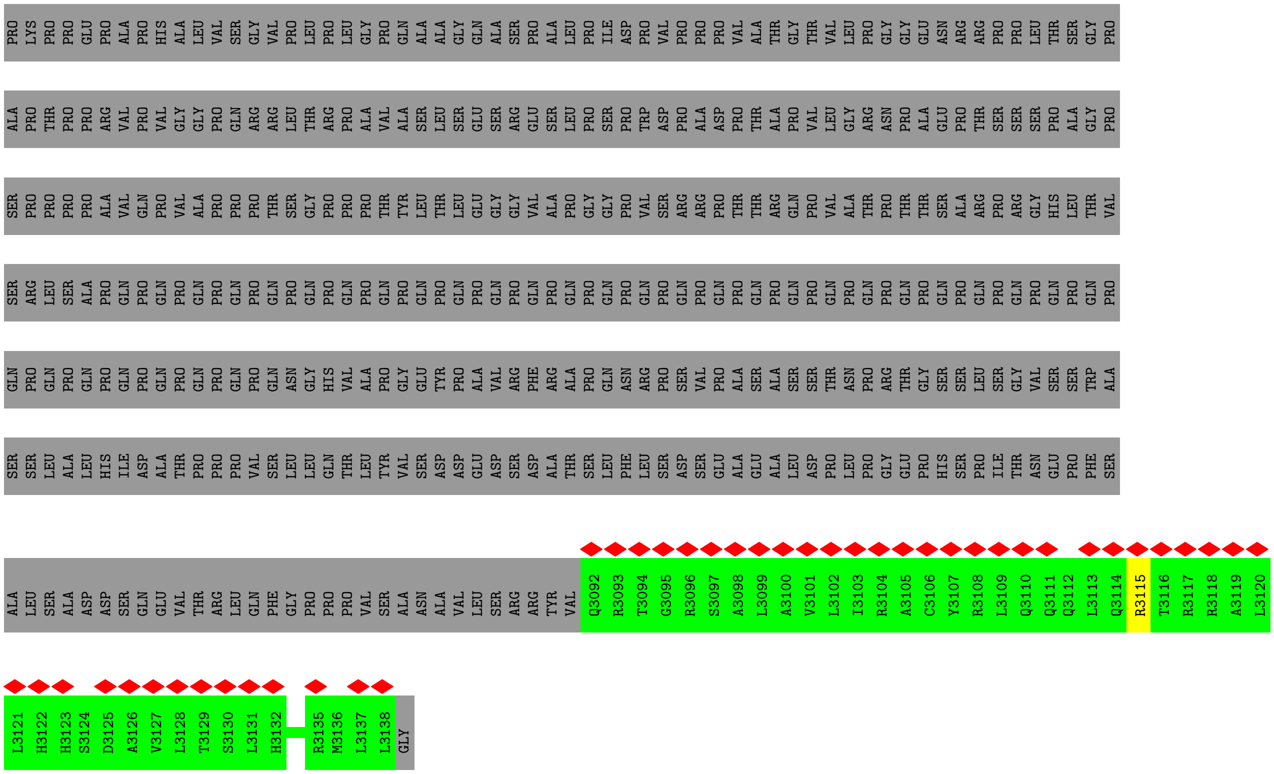
LEU ILE ALA GLU ARG PRO LEU ALA ARG GLY PRO PRO CYS LEU VAL LEU VAL ASP ILE SER MET THR PRO VAL ALA VAL LEU TRP GLU ASN PRO ASP PRO PRO GLY PRO PRO ASP VAL ARG PHE VAL GLY SER GLU ALA THR GLU GLU LEU PRO PHE VAL ALA GLY GLY GLU ASP VAL LEU

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

GLU GLY SER LEU GLY PRO GLY SER LEU ALA PRO THR LEU PHE THR ASP ALA THR PRO GLY GLU PRO VAL PRO PRO ARG MET TRP ALA TRP ILE HIS GLY LEU GLU GLU LEU ALA SER ASP ASP SER GLY GLY PRO ALA PRO LEU LEU ALA PRO ASP PRO LEU SER PRO THR ALA ASP GLN

SER VAL PRO THR SER GLN CYS ALA PRO ARG PRO PRO GLY PRO ALA VAL THR ALA ARG GLU ALA ARG PRO GLY VAL PRO ALA GLU SER THR ARG PRO ALA PRO VAL GLY PRO ARG ASP ASP PHE ARG ARG LEU PRO SER PRO GLN SER SER PRO ALA PRO PRO ASP ALA THR ALA PRO ARG

PRO PRO ALA SER SER ARG ALA SER ALA ALA SER SER SER GLY SER ARG ALA ARG ARG HIS ARG ARG ALA ARG SER LEU ALA ARG ALA THR GLN ALA SER ALA THR THR GLN GLY TRP ARG PRO PRO ALA LEU PRO ASP THR VAL ALA PRO VAL THR ASP PHE ALA ARG PRO PRO ALA PRO


PRO LYS PRO PRO GLU PRO ALA PRO HIS ALA LEU VAL SER GLY VAL PRO LEU PRO LEU GLY PRO GLN ALA ALA GLY GLN ALA SER PRO ALA LEU PRO ILE ASP PRO VAL PRO PRO PRO VAL ALA THR GLY THR VAL LEU PRO GLY GLY GLU ASN ARG ARG PRO PRO LEU THR SER GLY PRO
ALA PRO THR PRO PRO ARG VAL PRO VAL GLY GLY PRO GLN ARG ARG LEU THR ARG PRO ALA VAL ALA SER LEU SER GLU SER ARG GLU SER LEU PRO SER PRO TRP ASP PRO ALA ASP PRO THR ALA PRO VAL LEU GLY ARG ASN PRO ALA GLU PRO THR SER SER SER PRO ALA GLY PRO
SER PRO PRO PRO PRO ALA VAL GLN PRO VAL ALA PRO PRO PRO THR SER GLY PRO PRO PRO THR TYR LEU THR LEU GLU GLY GLY VAL ALA PRO GLY GLY PRO VAL SER ARG ARG PRO THR THR ARG GLN PRO VAL ALA THR PRO THR THR SER ALA ARG PRO ARG GLY HIS LEU THR VAL
SER ARG LEU SER ALA PRO GLN PRO
GLN PRO GLN PRO GLN PRO GLN PRO GLN PRO GLN PRO GLN PRO GLN ASN GLY HIS VAL ALA PRO GLY GLU TYR PRO ALA VAL ARG PHE ARG ALA PRO GLN ASN ARG PRO SER VAL PRO ALA SER ALA SER SER THR ASN PRO ARG THR GLY SER SER LEU SER GLY VAL SER SER TRP ALA
SER SER LEU ALA LEU HIS ILE ASP ALA THR PRO PRO PRO VAL SER LEU LEU GLN THR LEU TYR VAL SER ASP ASP GLU ASP SER ASP ALA THR SER LEU PHE LEU SER ASP SER GLU ALA GLU ALA LEU ASP PRO LEU PRO GLY GLU PRO HIS SER PRO ILE THR ASN GLU PRO PHE SER
ALA LEU SER ALA ASP ASP SER GLN GLU VAL THR ARG LEU GLN PHE GLY PRO PRO PRO VAL SER ALA ASN ALA VAL LEU SER ARG ARG TYR VAL Q3092 R3093 T3094 G3095 R3096 S3097 A3098 L3099 A3100 V3101 L3102 I3103 R3104 A3105 C3106 Y3107 R3108 L3109 Q3110 Q3111 Q3112 L3113 Q3114 R3115 T3116 R3117 R3118 A3119 L3120
L3121 H3122 H3123 S3124 D3125 A3126 V3127 L3128 T3129 S3130 L3131 H3132 R3135 M3136 L3137 L3138 GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	28042	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 ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	24271	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	14.209	Depositor
Minimum map value	-10.389	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.999	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	1318.3999, 1318.3999, 1318.3999	wwPDB
Map dimensions	1280, 1280, 1280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	4	0.34	0/9878	0.57	3/13478 (0.0%)
1	A	0.36	0/10664	0.58	3/14556 (0.0%)
1	B	0.37	0/10680	0.59	1/14579 (0.0%)
1	C	0.37	1/10680 (0.0%)	0.58	3/14579 (0.0%)
1	D	0.39	0/10664	0.60	3/14556 (0.0%)
1	E	0.39	0/10699	0.60	2/14605 (0.0%)
1	F	0.38	0/10664	0.59	1/14556 (0.0%)
1	M	0.38	0/10664	0.60	1/14556 (0.0%)
1	N	0.39	0/10699	0.59	0/14605
1	O	0.37	0/10680	0.58	0/14579
1	S	0.36	0/10616	0.58	2/14487 (0.0%)
1	T	0.38	0/10631	0.60	2/14507 (0.0%)
1	U	0.39	1/10680 (0.0%)	0.60	1/14579 (0.0%)
1	V	0.37	0/10664	0.59	3/14556 (0.0%)
1	W	0.37	0/10680	0.58	0/14579
1	X	0.37	0/10567	0.59	3/14423 (0.0%)
2	0	0.31	0/796	0.48	0/1087
2	1	0.31	0/796	0.48	0/1087
2	2	0.31	0/796	0.48	0/1087
2	3	0.31	0/796	0.48	0/1087
2	G	0.31	0/796	0.48	0/1087
2	H	0.31	0/796	0.48	0/1087
2	I	0.31	0/796	0.48	0/1087
2	J	0.31	0/796	0.48	0/1087
2	K	0.31	0/796	0.48	0/1087
2	L	0.31	0/796	0.48	0/1087
2	P	0.31	0/796	0.48	0/1087
2	Q	0.31	0/796	0.48	0/1087
2	R	0.31	0/796	0.48	0/1087
2	Y	0.31	0/796	0.48	0/1087
2	Z	0.31	0/796	0.48	0/1087
3	5	0.38	1/2795 (0.0%)	0.57	0/3810
3	8	0.37	0/2858	0.59	1/3895 (0.0%)
3	b	0.37	0/2858	0.58	0/3895

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	e	0.35	0/2791	0.57	0/3805
3	h	0.35	0/2795	0.59	1/3810 (0.0%)
4	6	0.36	0/2152	0.62	1/2939 (0.0%)
4	7	0.36	0/2383	0.66	2/3259 (0.1%)
4	9	0.36	0/2127	0.62	0/2906
4	a	0.38	0/2383	0.68	3/3259 (0.1%)
4	c	0.36	0/2127	0.64	1/2906 (0.0%)
4	d	0.38	0/2383	0.67	3/3259 (0.1%)
4	f	0.36	0/2124	0.63	2/2900 (0.1%)
4	g	0.37	0/2383	0.63	2/3259 (0.1%)
4	i	0.35	0/2152	0.60	1/2939 (0.0%)
4	j	0.36	0/2383	0.65	2/3259 (0.1%)
5	k	0.33	0/4307	0.54	0/5866
6	l	0.33	0/786	0.52	0/1072
6	m	0.34	0/670	0.57	1/912 (0.1%)
7	n	0.22	0/388	0.40	0/521
7	o	0.22	0/388	0.40	0/521
All	All	0.37	3/224983 (0.0%)	0.59	48/307077 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	4	0	2
1	A	0	2
1	B	0	2
1	C	0	1
1	D	0	2
1	E	0	1
1	F	0	2
1	M	0	2
1	N	0	2
1	O	0	1
1	S	0	1
1	T	0	2
1	U	0	5
1	V	0	3
1	W	0	4
1	X	0	1
3	8	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	h	0	1
4	7	0	1
4	9	0	1
4	a	0	1
4	d	0	1
4	g	0	1
4	j	0	1
All	All	0	41

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	315	TYR	CD1-CE1	-6.41	1.29	1.39
1	C	954	TYR	CD1-CE1	-6.12	1.30	1.39
1	U	11	TYR	CD2-CE2	-5.88	1.30	1.39

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	159	LEU	CB-CG-CD1	-8.25	96.97	111.00
4	j	63	LEU	CA-CB-CG	7.91	133.48	115.30
4	a	63	LEU	CA-CB-CG	7.26	132.00	115.30
6	m	55	LEU	CA-CB-CG	7.17	131.79	115.30
4	7	63	LEU	CA-CB-CG	7.08	131.58	115.30

There are no chirality outliers.

5 of 41 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	PHE	Peptide
1	A	800	HIS	Peptide
1	B	133	PHE	Peptide
1	B	43	ARG	Peptide
1	C	133	PHE	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	4	1243/1374 (90%)	1169 (94%)	74 (6%)	0	100	100
1	A	1358/1374 (99%)	1262 (93%)	96 (7%)	0	100	100
1	B	1360/1374 (99%)	1258 (92%)	102 (8%)	0	100	100
1	C	1360/1374 (99%)	1265 (93%)	95 (7%)	0	100	100
1	D	1358/1374 (99%)	1246 (92%)	112 (8%)	0	100	100
1	E	1362/1374 (99%)	1254 (92%)	108 (8%)	0	100	100
1	F	1358/1374 (99%)	1244 (92%)	114 (8%)	0	100	100
1	M	1358/1374 (99%)	1244 (92%)	114 (8%)	0	100	100
1	N	1362/1374 (99%)	1253 (92%)	108 (8%)	1 (0%)	51	85
1	O	1360/1374 (99%)	1260 (93%)	100 (7%)	0	100	100
1	S	1353/1374 (98%)	1272 (94%)	81 (6%)	0	100	100
1	T	1349/1374 (98%)	1272 (94%)	77 (6%)	0	100	100
1	U	1360/1374 (99%)	1244 (92%)	116 (8%)	0	100	100
1	V	1358/1374 (99%)	1247 (92%)	111 (8%)	0	100	100
1	W	1360/1374 (99%)	1252 (92%)	108 (8%)	0	100	100
1	X	1344/1374 (98%)	1260 (94%)	84 (6%)	0	100	100
2	0	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	1	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	2	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	3	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	G	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	H	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	I	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	J	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	K	99/112 (88%)	94 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	P	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	Q	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	R	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	Y	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
2	Z	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
3	5	349/465 (75%)	332 (95%)	17 (5%)	0	100	100
3	8	361/465 (78%)	340 (94%)	20 (6%)	1 (0%)	41	76
3	b	361/465 (78%)	341 (94%)	20 (6%)	0	100	100
3	e	348/465 (75%)	324 (93%)	24 (7%)	0	100	100
3	h	349/465 (75%)	326 (93%)	22 (6%)	1 (0%)	41	76
4	6	264/318 (83%)	249 (94%)	15 (6%)	0	100	100
4	7	304/318 (96%)	283 (93%)	19 (6%)	2 (1%)	22	62
4	9	264/318 (83%)	244 (92%)	20 (8%)	0	100	100
4	a	304/318 (96%)	277 (91%)	25 (8%)	2 (1%)	22	62
4	c	264/318 (83%)	246 (93%)	17 (6%)	1 (0%)	34	72
4	d	304/318 (96%)	274 (90%)	27 (9%)	3 (1%)	15	54
4	f	260/318 (82%)	238 (92%)	21 (8%)	1 (0%)	34	72
4	g	304/318 (96%)	276 (91%)	28 (9%)	0	100	100
4	i	264/318 (83%)	246 (93%)	18 (7%)	0	100	100
4	j	304/318 (96%)	273 (90%)	30 (10%)	1 (0%)	41	76
5	k	534/703 (76%)	514 (96%)	20 (4%)	0	100	100
6	l	92/580 (16%)	87 (95%)	5 (5%)	0	100	100
6	m	78/580 (13%)	77 (99%)	1 (1%)	0	100	100
7	n	45/3139 (1%)	45 (100%)	0	0	100	100
7	o	45/3139 (1%)	45 (100%)	0	0	100	100
All	All	28486/37310 (76%)	26449 (93%)	2024 (7%)	13 (0%)	100	100

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	8	282	ARG
4	7	241	LEU

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Mol	Chain	Res	Type
4	d	241	LEU
4	d	242	GLN
3	h	282	ARG

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	4	1003/1085 (92%)	1002 (100%)	1 (0%)	93	97
1	A	1076/1085 (99%)	1075 (100%)	1 (0%)	93	97
1	B	1078/1085 (99%)	1077 (100%)	1 (0%)	93	97
1	C	1078/1085 (99%)	1077 (100%)	1 (0%)	93	97
1	D	1076/1085 (99%)	1075 (100%)	1 (0%)	93	97
1	E	1080/1085 (100%)	1079 (100%)	1 (0%)	93	97
1	F	1076/1085 (99%)	1075 (100%)	1 (0%)	93	97
1	M	1076/1085 (99%)	1074 (100%)	2 (0%)	93	96
1	N	1080/1085 (100%)	1078 (100%)	2 (0%)	93	96
1	O	1078/1085 (99%)	1077 (100%)	1 (0%)	93	97
1	S	1070/1085 (99%)	1069 (100%)	1 (0%)	93	97
1	T	1073/1085 (99%)	1072 (100%)	1 (0%)	93	97
1	U	1078/1085 (99%)	1077 (100%)	1 (0%)	93	97
1	V	1076/1085 (99%)	1075 (100%)	1 (0%)	93	97
1	W	1078/1085 (99%)	1077 (100%)	1 (0%)	93	97
1	X	1069/1085 (98%)	1067 (100%)	2 (0%)	93	96
2	0	80/89 (90%)	80 (100%)	0	100	100
2	1	80/89 (90%)	80 (100%)	0	100	100
2	2	80/89 (90%)	80 (100%)	0	100	100
2	3	80/89 (90%)	80 (100%)	0	100	100
2	G	80/89 (90%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	80/89 (90%)	80 (100%)	0	100	100
2	I	80/89 (90%)	80 (100%)	0	100	100
2	J	80/89 (90%)	80 (100%)	0	100	100
2	K	80/89 (90%)	80 (100%)	0	100	100
2	L	80/89 (90%)	80 (100%)	0	100	100
2	P	80/89 (90%)	80 (100%)	0	100	100
2	Q	80/89 (90%)	80 (100%)	0	100	100
2	R	80/89 (90%)	80 (100%)	0	100	100
2	Y	80/89 (90%)	80 (100%)	0	100	100
2	Z	80/89 (90%)	80 (100%)	0	100	100
3	5	279/364 (77%)	279 (100%)	0	100	100
3	8	285/364 (78%)	285 (100%)	0	100	100
3	b	285/364 (78%)	285 (100%)	0	100	100
3	e	279/364 (77%)	279 (100%)	0	100	100
3	h	279/364 (77%)	279 (100%)	0	100	100
4	6	234/264 (89%)	234 (100%)	0	100	100
4	7	256/264 (97%)	256 (100%)	0	100	100
4	9	231/264 (88%)	231 (100%)	0	100	100
4	a	256/264 (97%)	256 (100%)	0	100	100
4	c	231/264 (88%)	231 (100%)	0	100	100
4	d	256/264 (97%)	255 (100%)	1 (0%)	91	94
4	f	231/264 (88%)	231 (100%)	0	100	100
4	g	256/264 (97%)	256 (100%)	0	100	100
4	i	234/264 (89%)	234 (100%)	0	100	100
4	j	256/264 (97%)	256 (100%)	0	100	100
5	k	429/529 (81%)	428 (100%)	1 (0%)	93	96
6	l	80/448 (18%)	80 (100%)	0	100	100
6	m	67/448 (15%)	66 (98%)	1 (2%)	65	80
7	n	41/2430 (2%)	40 (98%)	1 (2%)	49	69
7	o	41/2430 (2%)	40 (98%)	1 (2%)	49	69
All	All	22851/29440 (78%)	22827 (100%)	24 (0%)	93	97

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	519	ARG
1	X	519	ARG
1	X	451	ARG
1	4	519	ARG
1	M	272	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 345 such sidechains are listed below:

Mol	Chain	Res	Type
1	U	1039	GLN
2	Z	68	HIS
1	V	502	GLN
1	W	866	HIS
1	4	969	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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

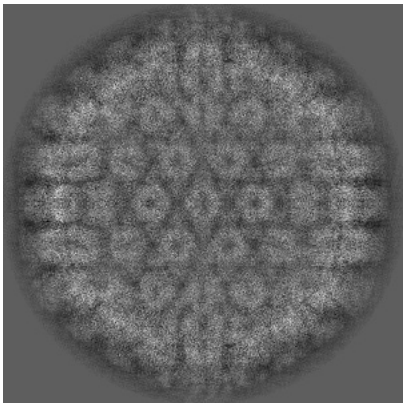
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7472. These allow visual inspection of the internal detail of the map and identification of artifacts.

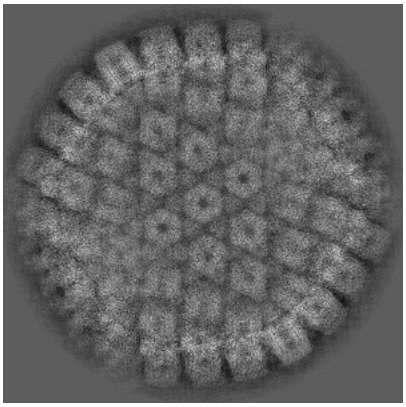
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

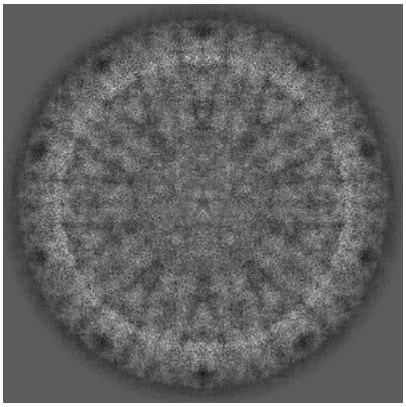
6.1.1 Primary map



X



Y

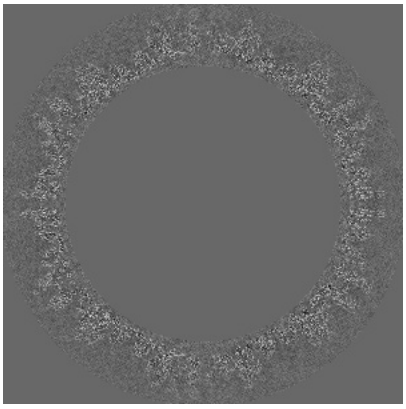


Z

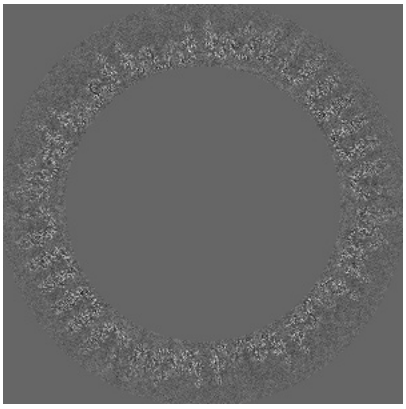
The images above show the map projected in three orthogonal directions.

6.2 Central slices

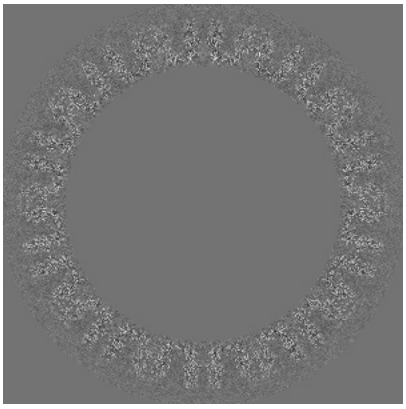
6.2.1 Primary map



X Index: 640



Y Index: 640

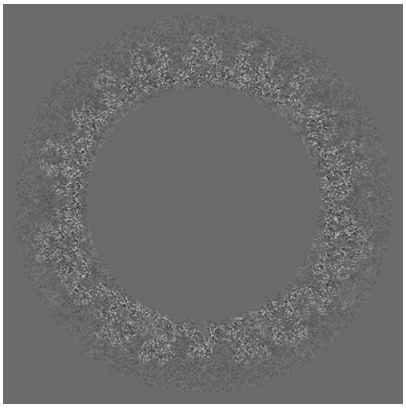


Z Index: 640

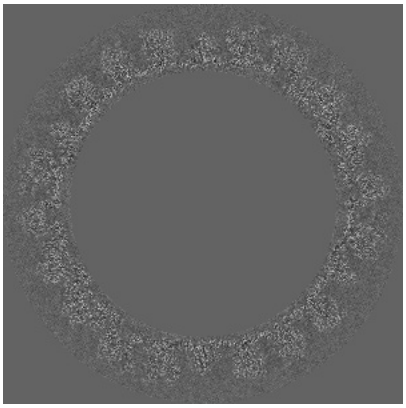
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

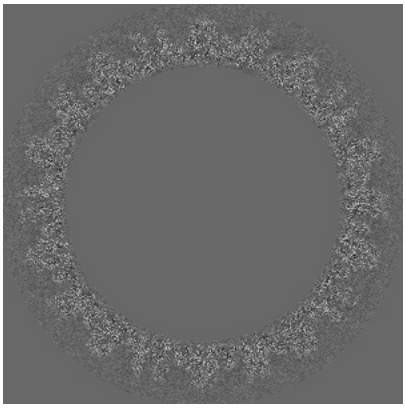
6.3.1 Primary map



X Index: 405



Y Index: 753

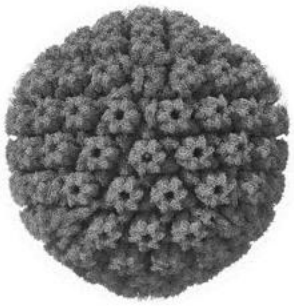


Z Index: 668

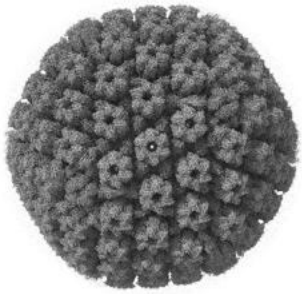
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

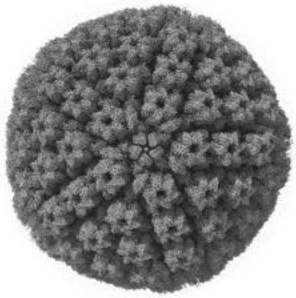
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

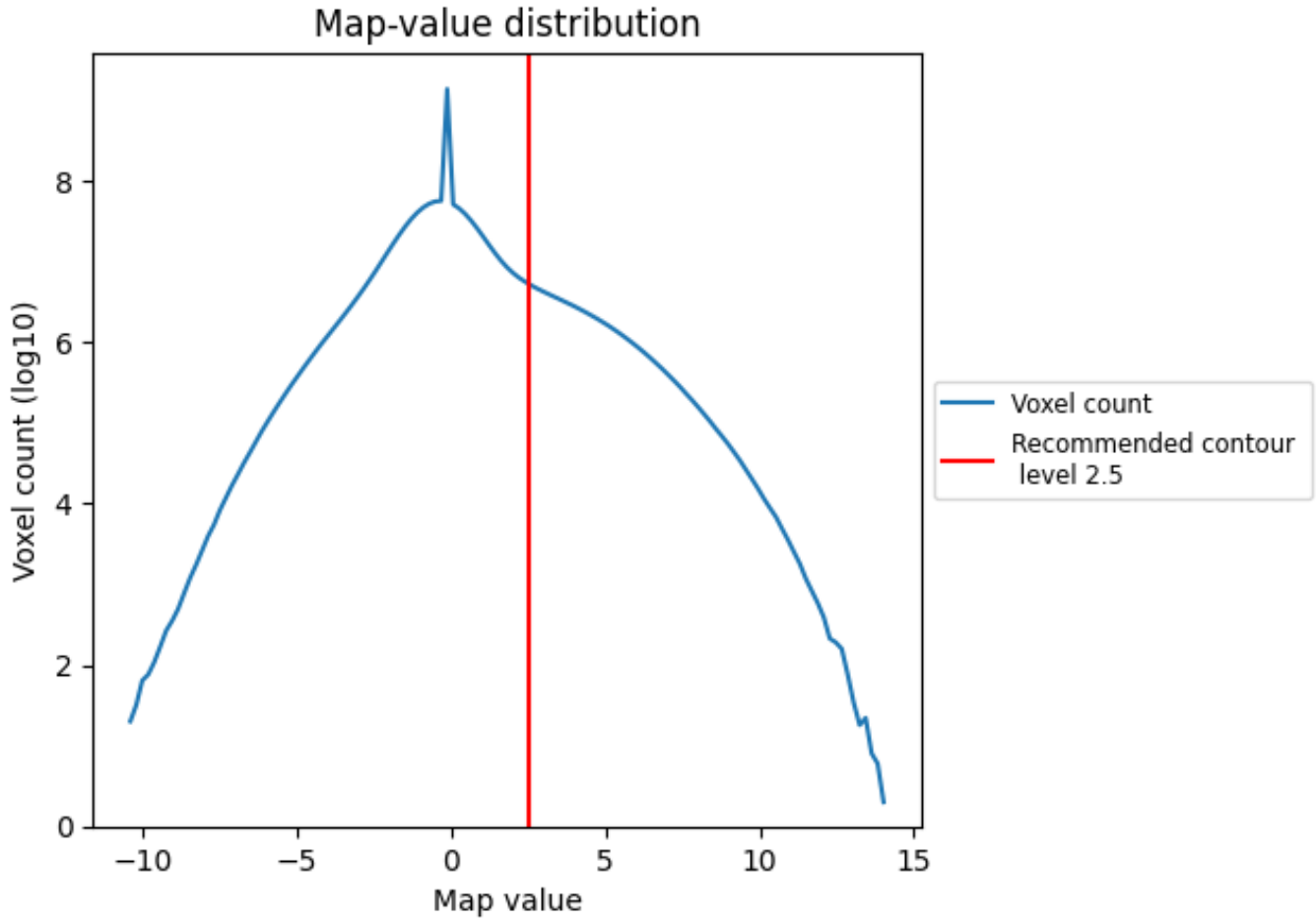
6.5 Mask visualisation (i)

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

7 Map analysis

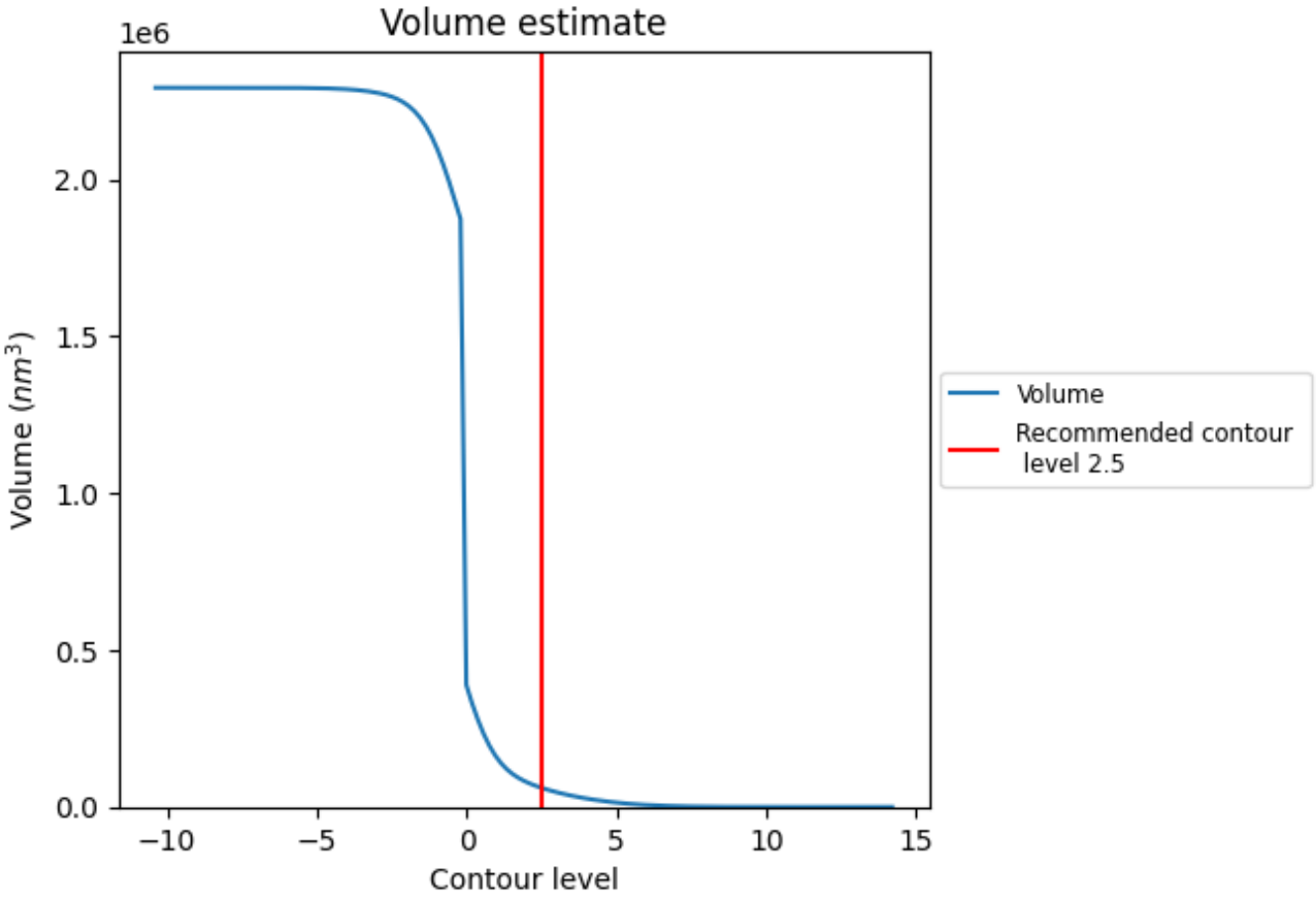
This section contains the results of statistical analysis of the map.

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.

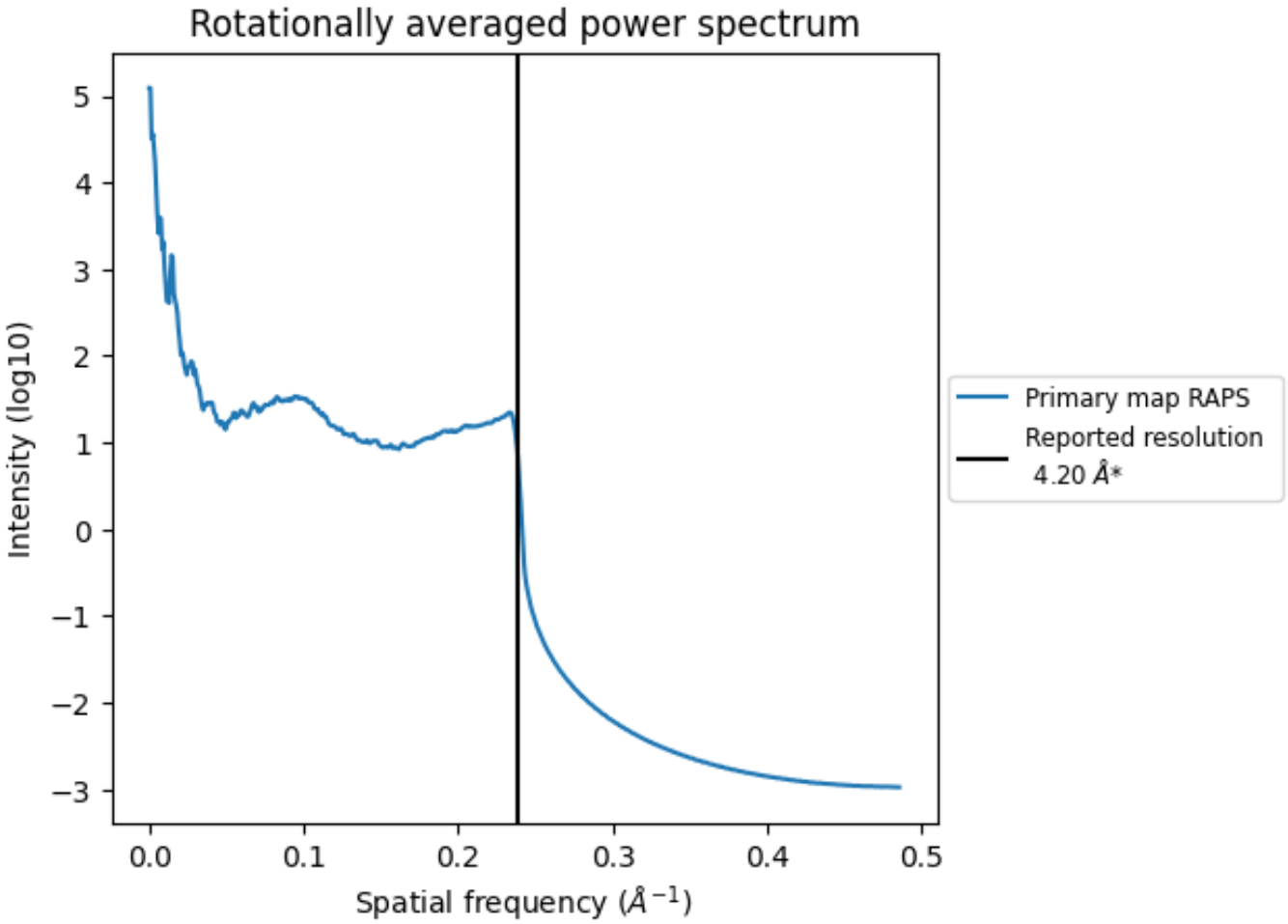
7.2 Volume estimate (i)



The volume at the recommended contour level is 60862 nm^3; this corresponds to an approximate mass of 54978 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 0.238 Å^{-1}

8 Fourier-Shell correlation (i)

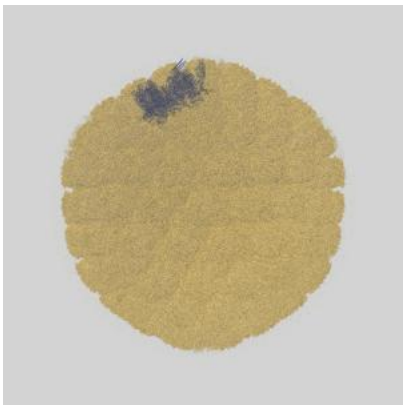
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

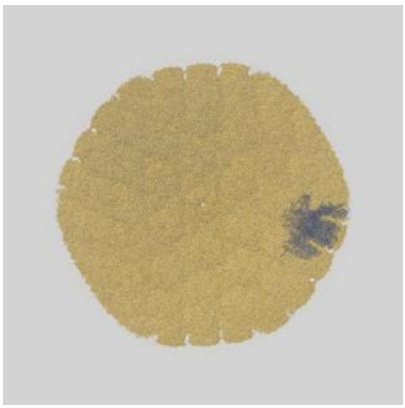
This section contains information regarding the fit between EMDB map EMD-7472 and PDB model 6CGR. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlays

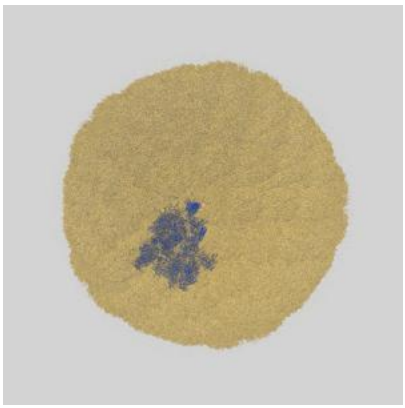
9.1.1 Map-model overlay



X

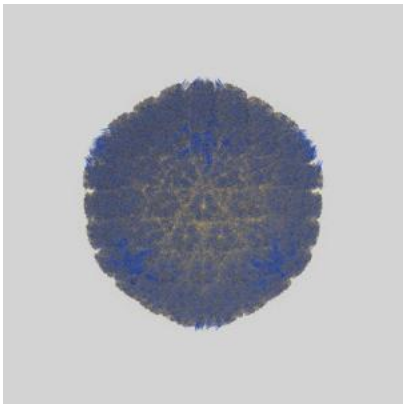


Y

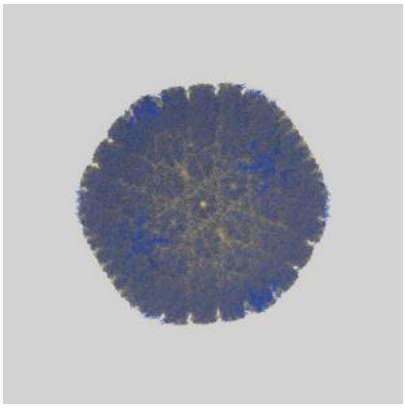


Z

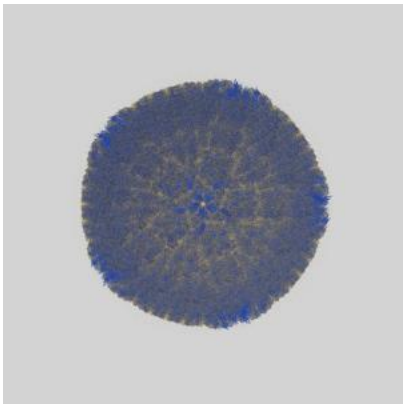
9.1.2 Map-model assembly overlay



X



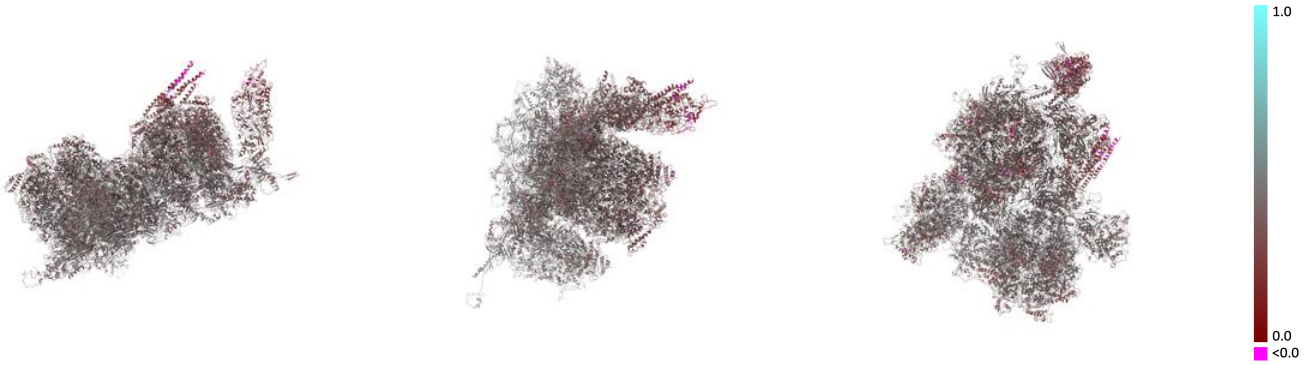
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5 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.

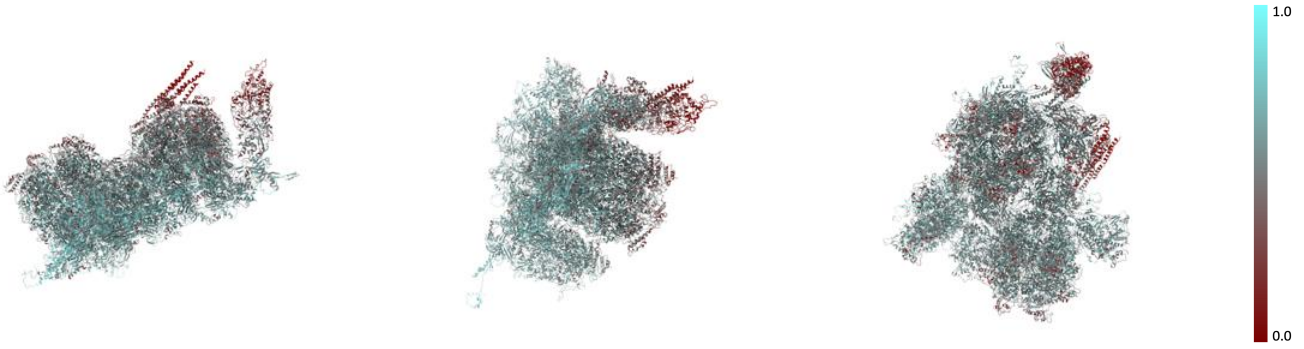
9.2 Q-score mapped to coordinate model (i)



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.

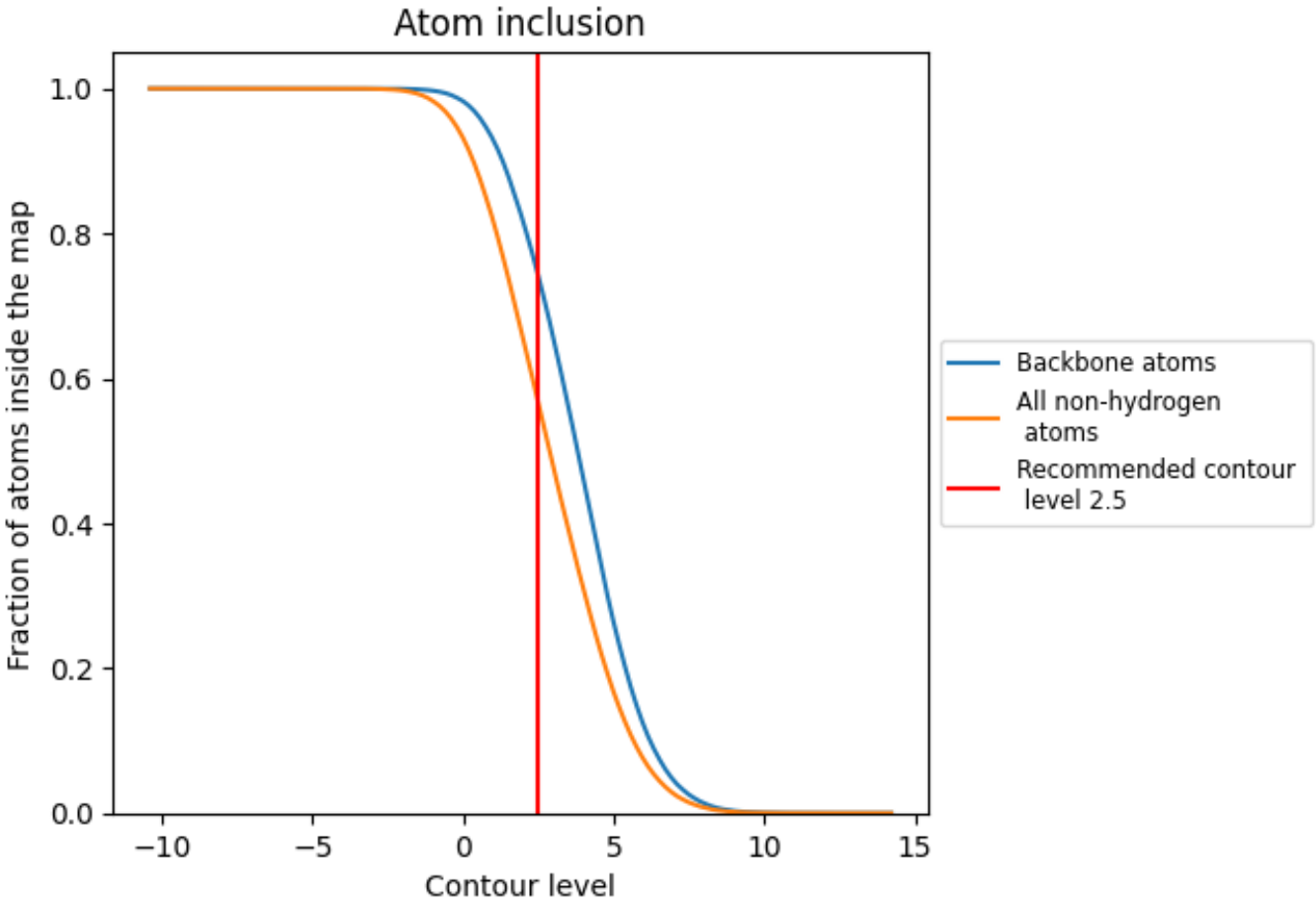
9.3 Atom inclusion mapped to coordinate model (i)



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 (2.5).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 57% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5656	0.3920
0	0.3439	0.3060
1	0.3955	0.3050
2	0.3664	0.2980
3	0.3611	0.3360
4	0.3638	0.3180
5	0.5292	0.3910
6	0.4635	0.3550
7	0.4840	0.3510
8	0.6060	0.4140
9	0.6134	0.4020
A	0.6090	0.4070
B	0.6191	0.4130
C	0.6008	0.4070
D	0.6100	0.4090
E	0.5999	0.4020
F	0.6034	0.4090
G	0.4193	0.3370
H	0.4272	0.3240
I	0.4140	0.3400
J	0.4140	0.3330
K	0.3902	0.2940
L	0.3968	0.3340
M	0.6239	0.4150
N	0.6233	0.4120
O	0.6211	0.4140
P	0.4630	0.3390
Q	0.4550	0.3590
R	0.4907	0.3630
S	0.5516	0.3880
T	0.5605	0.3780
U	0.5929	0.4070
V	0.5955	0.4050
W	0.5802	0.4020
X	0.5511	0.3820

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Chain	Atom inclusion	Q-score
Y	0.3108	0.3090
Z	0.3267	0.3010
a	0.6107	0.4070
b	0.5830	0.4050
c	0.5903	0.4000
d	0.6168	0.4090
e	0.5695	0.4090
f	0.5806	0.4000
g	0.5712	0.4010
h	0.5925	0.4080
i	0.5880	0.3950
j	0.5949	0.4030
k	0.4474	0.3600
l	0.3136	0.3060
m	0.3386	0.3010
n	0.0899	0.1410
o	0.1526	0.1920