



wwPDB EM Validation Summary Report ⓘ

Aug 25, 2026 – 10:42 pm BST

PDB ID : 9SQR / pdb_00009sqr
EMDB ID : EMD-55116
Title : Symmetry relaxed reconstruction of Rhodospirillum rubrum encapsulin:encapsulated ferritin nanocompartment
Authors : McIver, Z.; McCorvie, T.J.; Basle, A.; Marles-Wright, J.
Deposited on : 2025-09-23
Resolution : 3.73 Å(reported)
Based on initial model : .

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

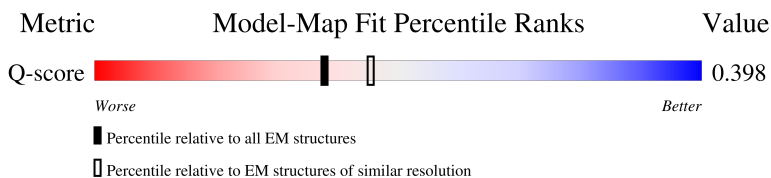
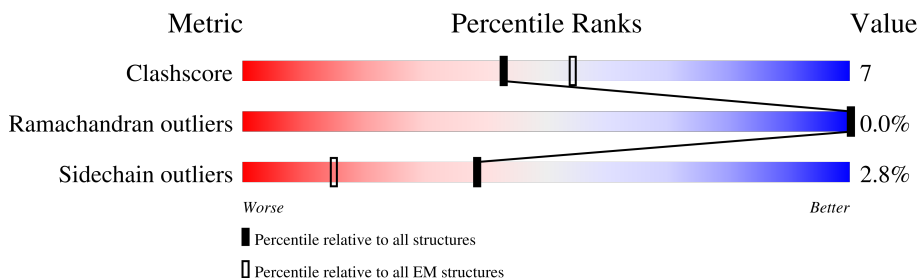
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 3.73 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10415 (3.23 - 4.23)

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

Mol	Chain	Length	Quality of chain
1	A	280	7% 78% 15% • 6%
1	A0	280	6% 76% 17% • 6%
1	AA	280	8% 78% 14% • 6%
1	AB	280	8% 77% 17% 6%

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Mol	Chain	Length	Quality of chain
1	B	280	
1	BA	280	
1	BB	280	
1	C	280	
1	CA	280	
1	CB	280	
1	D	280	
1	DA	280	
1	DB	280	
1	E	280	
1	EA	280	
1	EB	280	
1	F	280	
1	FA	280	
1	FB	280	
1	G	280	
1	GA	280	
1	GB	280	
1	H	280	
1	HA	280	
1	HB	280	
1	I	280	
1	IA	280	
1	J	280	
1	JA	280	

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Mol	Chain	Length	Quality of chain
1	K	280	
1	KA	280	
1	L	280	
1	LA	280	
1	M	280	
1	MA	280	
1	N	280	
1	NA	280	
1	O	280	
1	OA	280	
1	P	280	
1	PA	280	
1	Q	280	
1	QA	280	
1	R	280	
1	RA	280	
1	S	280	
1	SA	280	
1	T	280	
1	TA	280	
1	UA	280	
1	V	280	
1	VA	280	
1	W	280	
1	WA	280	

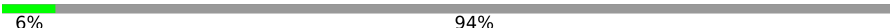
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Mol	Chain	Length	Quality of chain
1	X	280	
1	XA	280	
1	Y	280	
1	YA	280	
1	Z	280	
1	ZA	280	
2	1	140	
2	10	140	
2	11	140	
2	12	140	
2	13	140	
2	14	140	
2	15	140	
2	16	140	
2	17	140	
2	18	140	
2	19	140	
2	2	140	
2	20	140	
2	3	140	
2	4	140	
2	5	140	
2	6	140	
2	7	140	
2	8	140	

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Mol	Chain	Length	Quality of chain
2	9	140	 6% 94%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 119496 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 Type 1 encapsulin shell protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A0	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	A	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	B	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	C	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	D	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	E	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	F	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	G	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	H	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	I	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	J	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	K	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	L	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	M	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	N	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	O	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	P	262	Total 1975	C 1251	N 350	O 367	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	R	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	S	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	T	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	V	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	W	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	X	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	Y	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	Z	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	AA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	BA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	CA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	DA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	EA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	FA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	GA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	HA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	IA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	JA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	KA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	LA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	MA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	NA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	OA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	PA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	QA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	RA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	SA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	TA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	UA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	VA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	WA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	XA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	YA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	ZA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	AB	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	BB	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	CB	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	DB	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	EB	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	FB	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	GB	262	Total 1975	C 1251	N 350	O 367	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	HB	262	Total	C	N	O	S	0	0
			1975	1251	350	367	7		

- Molecule 2 is a protein called Encapsulated ferritin-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	8	Total	C	N	O		0	0
			48	30	8	10			
2	2	8	Total	C	N	O		0	0
			48	30	8	10			
2	3	8	Total	C	N	O		0	0
			48	30	8	10			
2	4	9	Total	C	N	O		0	0
			57	36	10	11			
2	5	8	Total	C	N	O		0	0
			48	30	8	10			
2	6	8	Total	C	N	O		0	0
			48	30	8	10			
2	7	9	Total	C	N	O		0	0
			57	36	10	11			
2	8	9	Total	C	N	O		0	0
			57	36	10	11			
2	9	8	Total	C	N	O		0	0
			48	30	8	10			
2	10	9	Total	C	N	O		0	0
			57	36	10	11			
2	11	8	Total	C	N	O		0	0
			48	30	8	10			
2	12	8	Total	C	N	O		0	0
			48	30	8	10			
2	13	8	Total	C	N	O		0	0
			48	30	8	10			
2	14	8	Total	C	N	O		0	0
			48	30	8	10			
2	15	8	Total	C	N	O		0	0
			48	30	8	10			
2	16	8	Total	C	N	O		0	0
			48	30	8	10			
2	17	8	Total	C	N	O		0	0
			48	30	8	10			
2	18	8	Total	C	N	O		0	0
			48	30	8	10			

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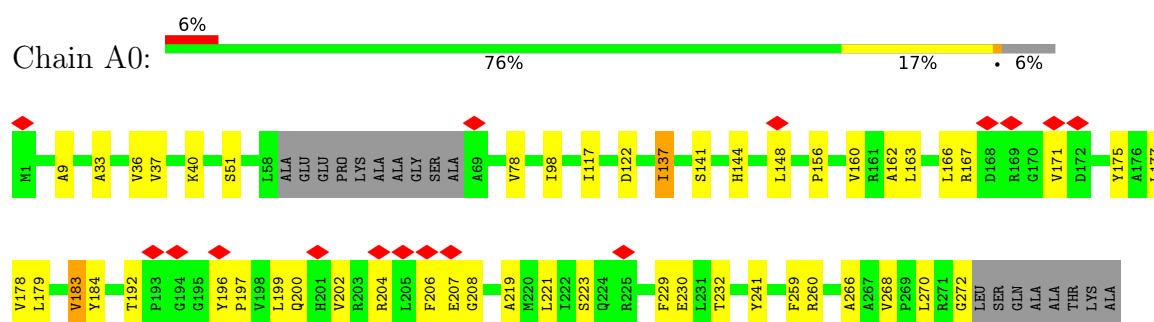
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Mol	Chain	Residues	Atoms				AltConf	Trace
2	19	8	Total	C	N	O	0	0
			48	30	8	10		
2	20	8	Total	C	N	O	0	0
			48	30	8	10		

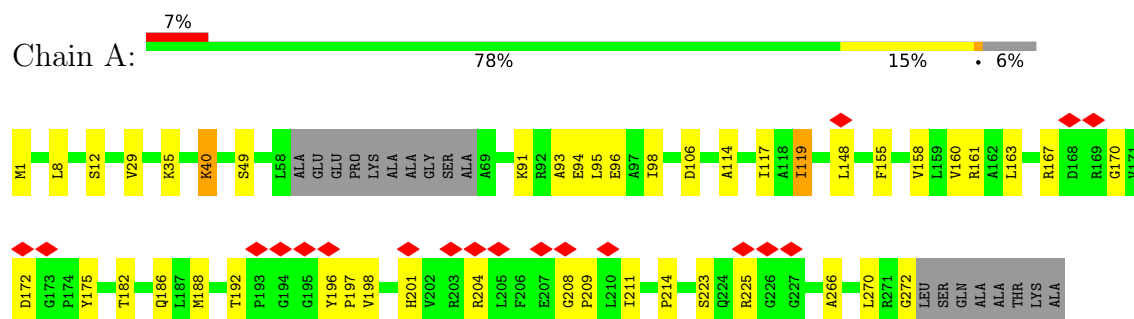
3 Residue-property plots [i](#)

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.

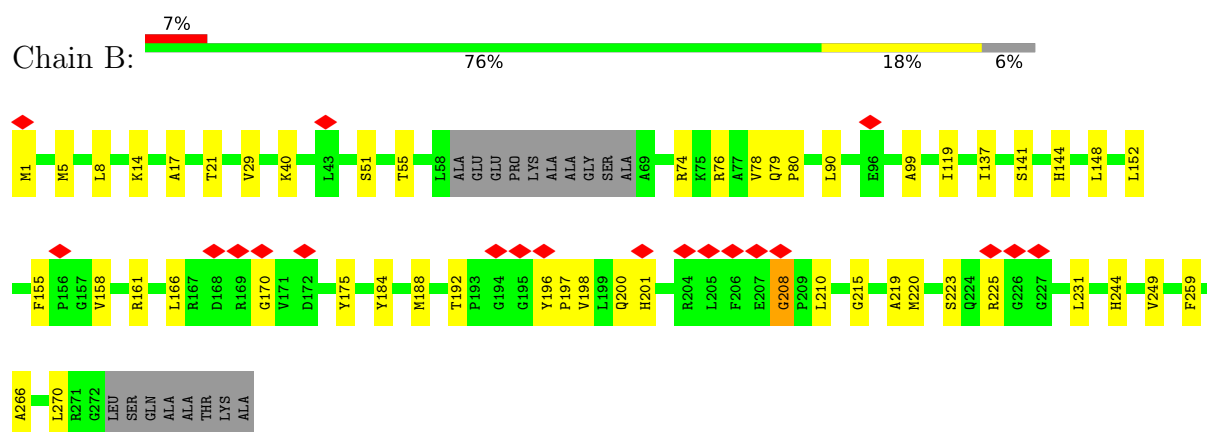
- Molecule 1: Type 1 encapsulin shell protein



- Molecule 1: Type 1 encapsulin shell protein

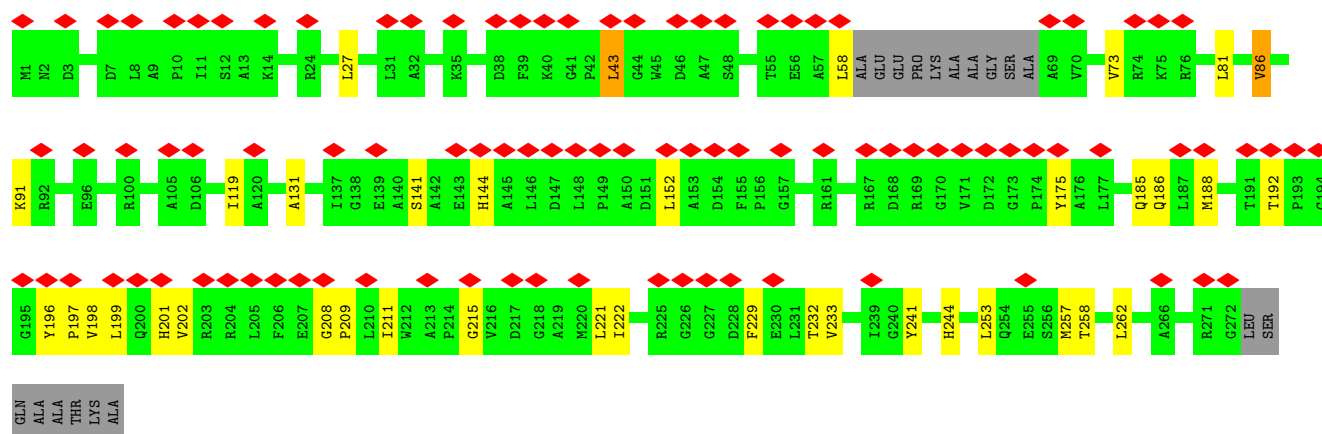


- Molecule 1: Type 1 encapsulin shell protein



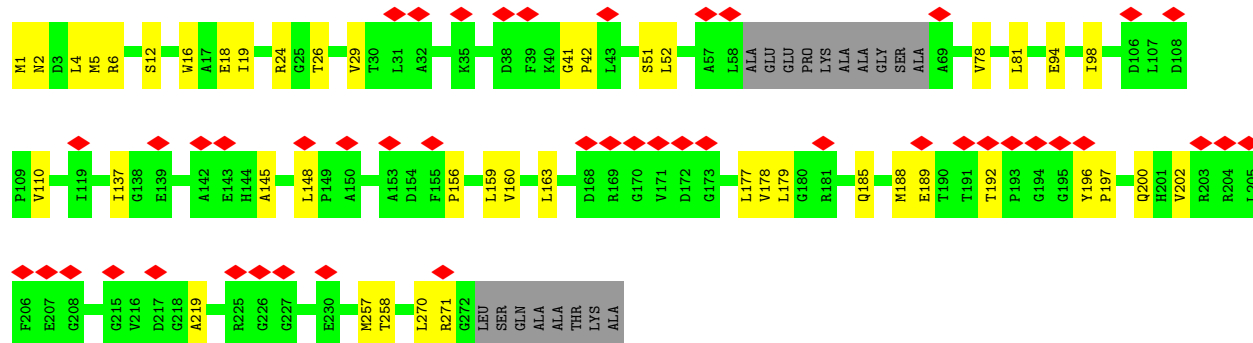
- Molecule 1: Type 1 encapsulin shell protein

Chain C: 



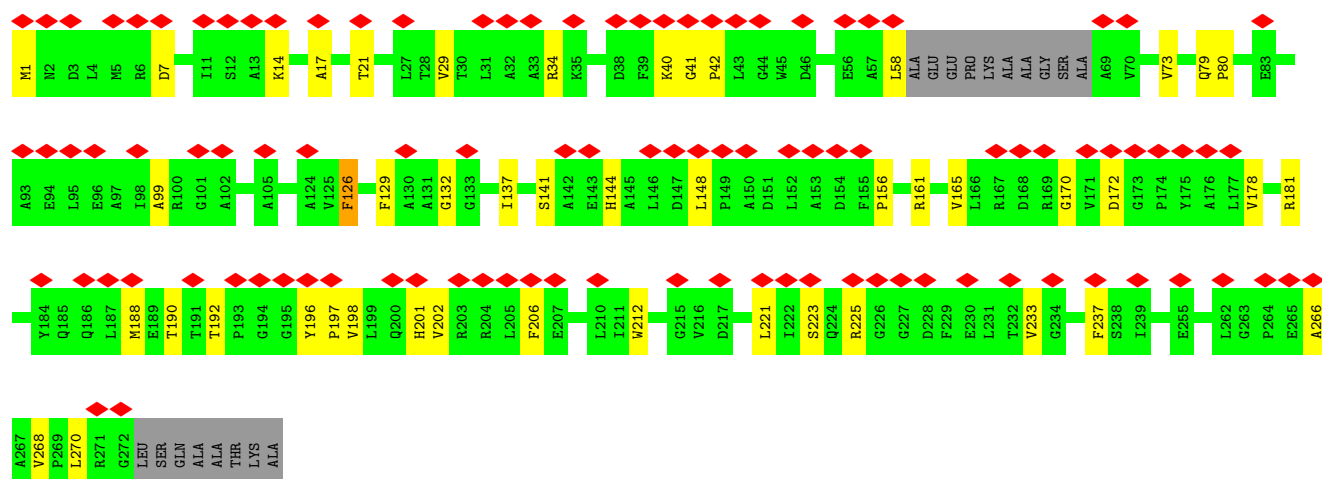
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Chain D: 

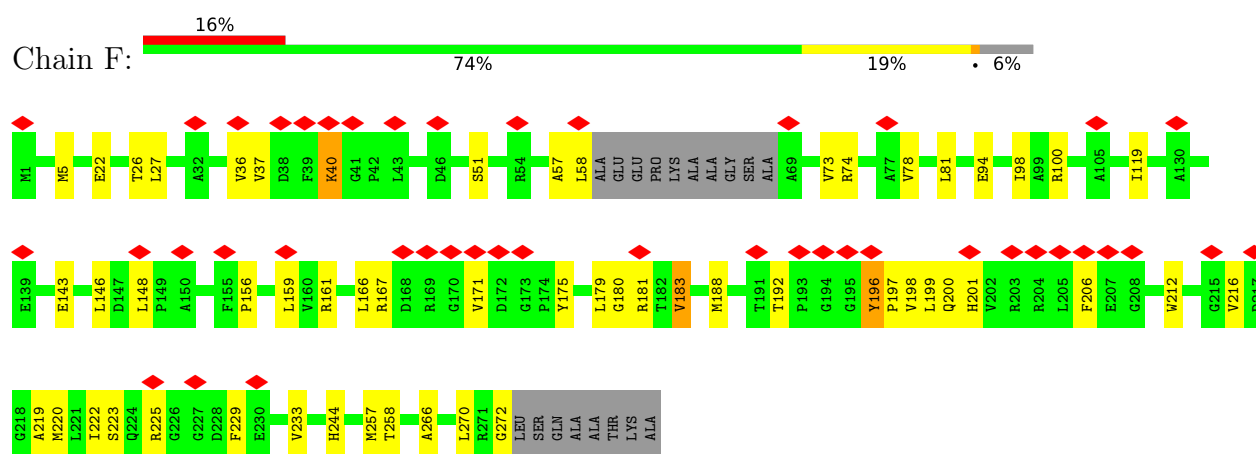


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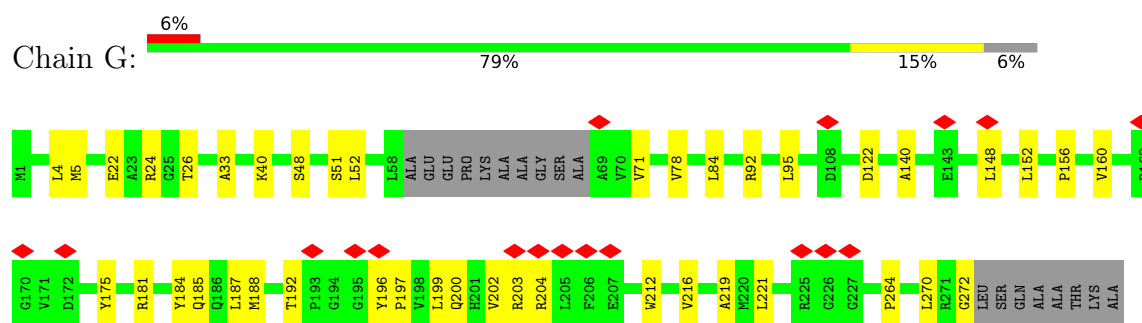
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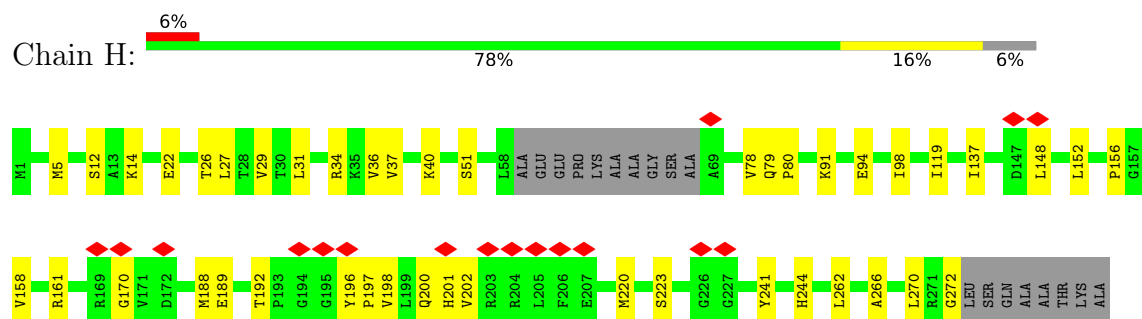
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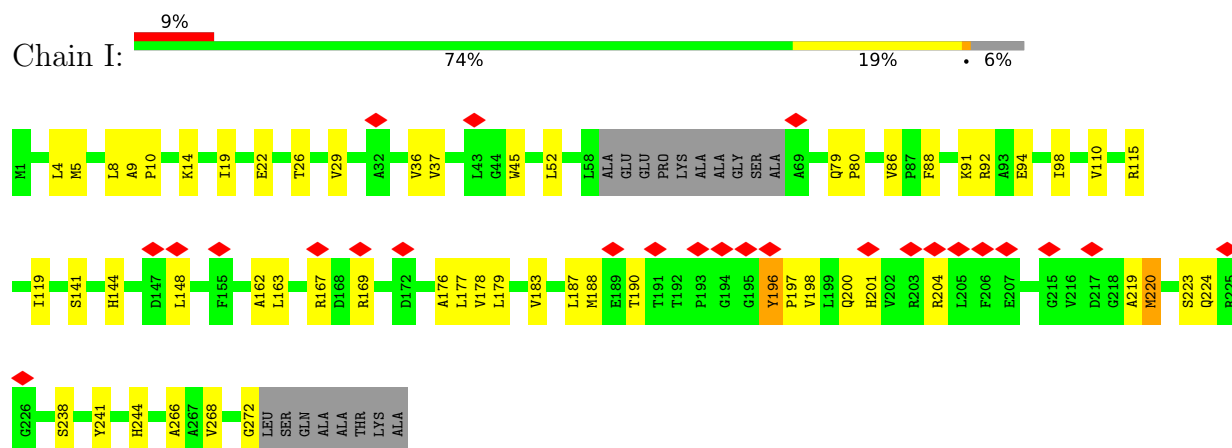
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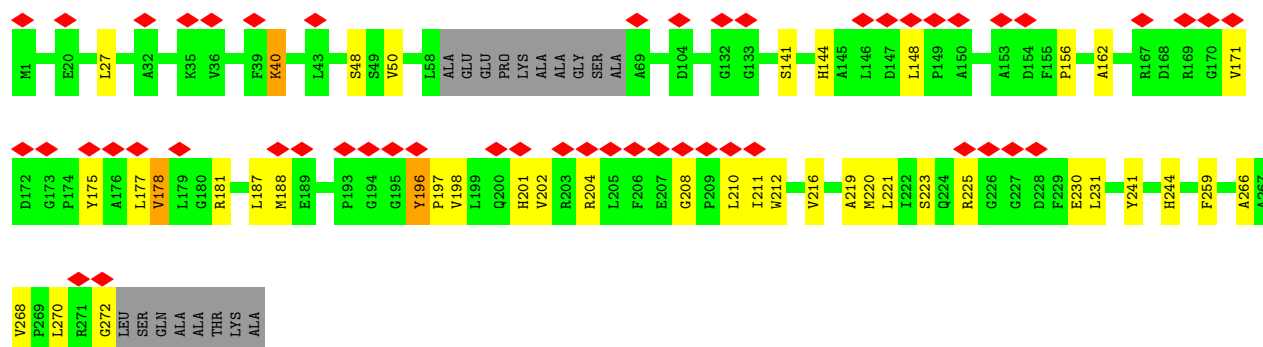


- Molecule 1: Type 1 encapsulin shell protein



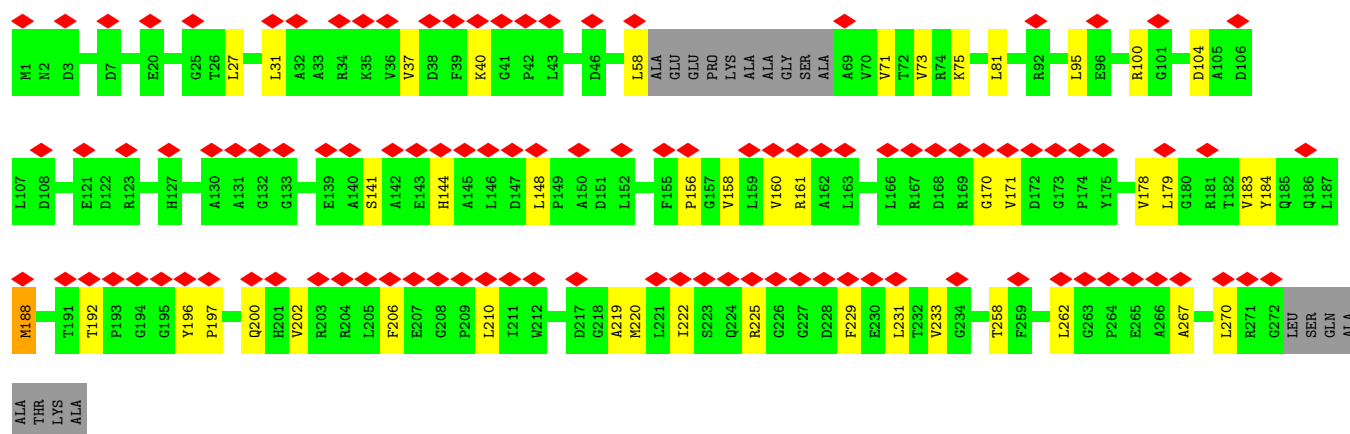
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Chain J: 



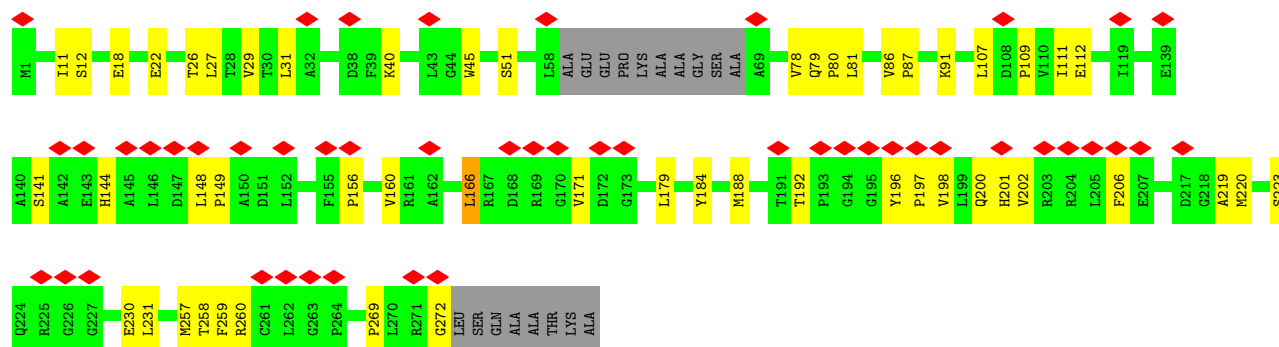
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Chain K: 



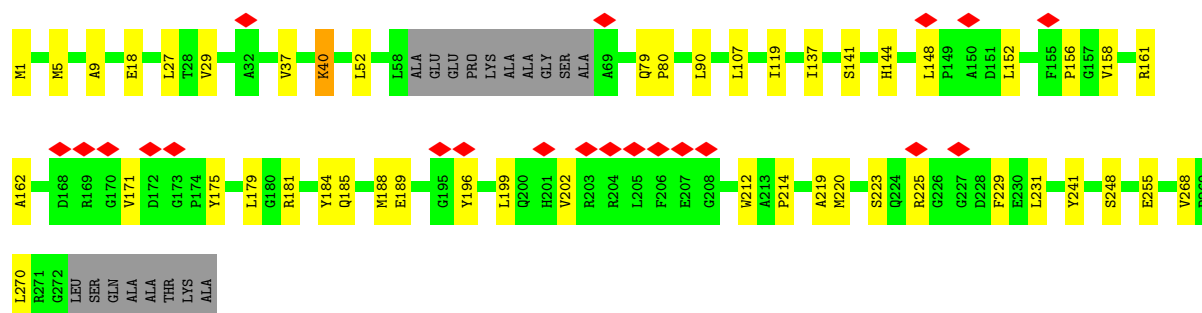
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Chain L: 

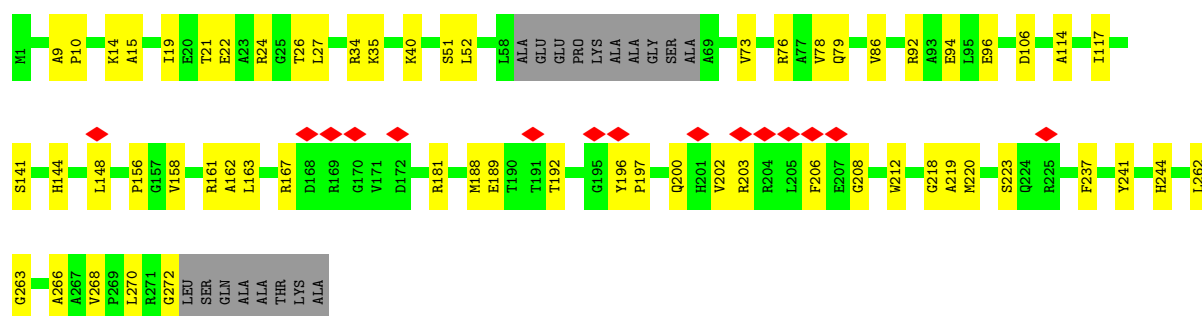
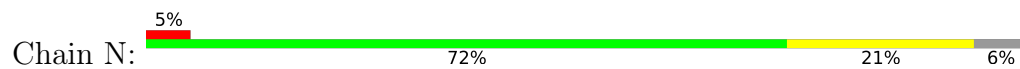


- Molecule 1: Type 1 encapsulin shell protein

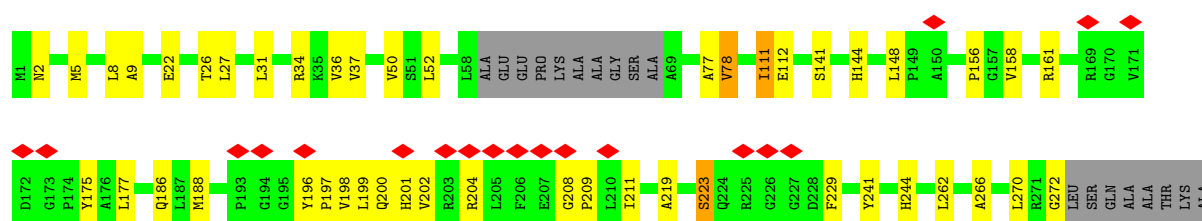
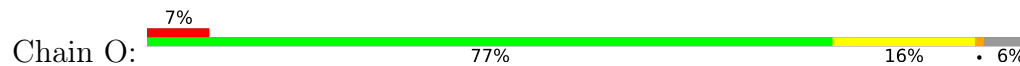
Chain M: 



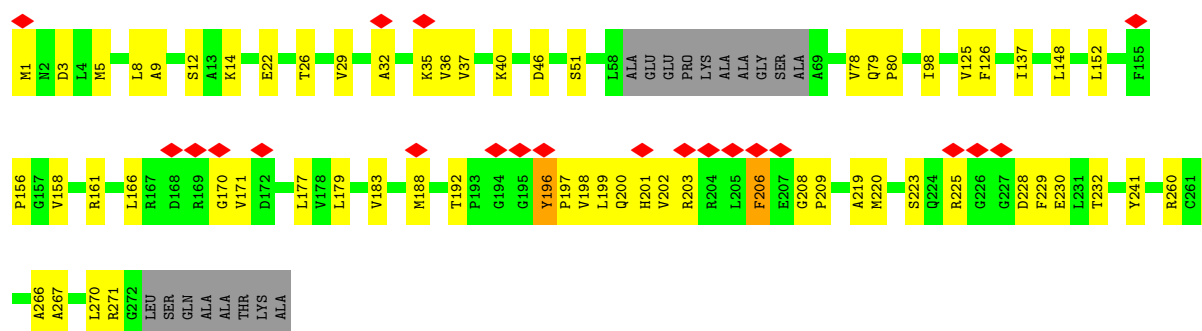
- Molecule 1: Type 1 encapsulin shell protein



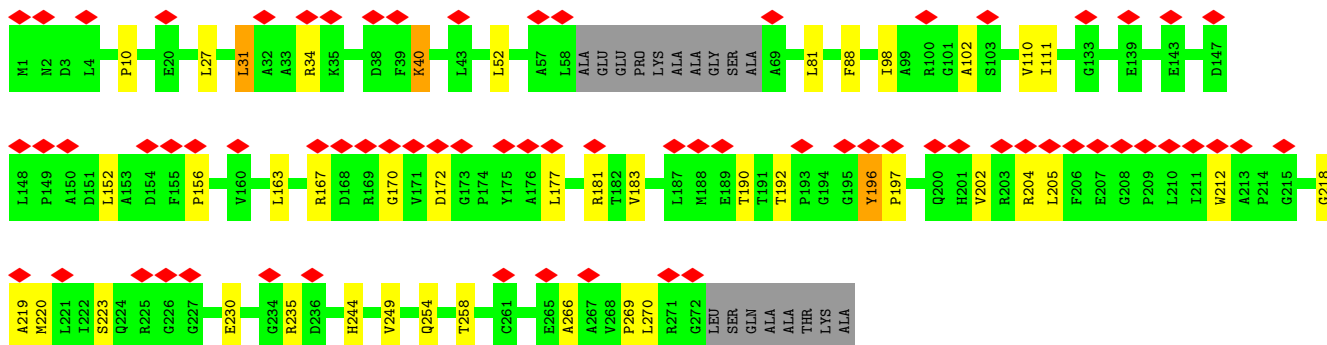
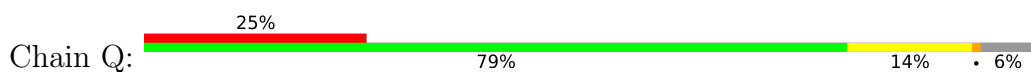
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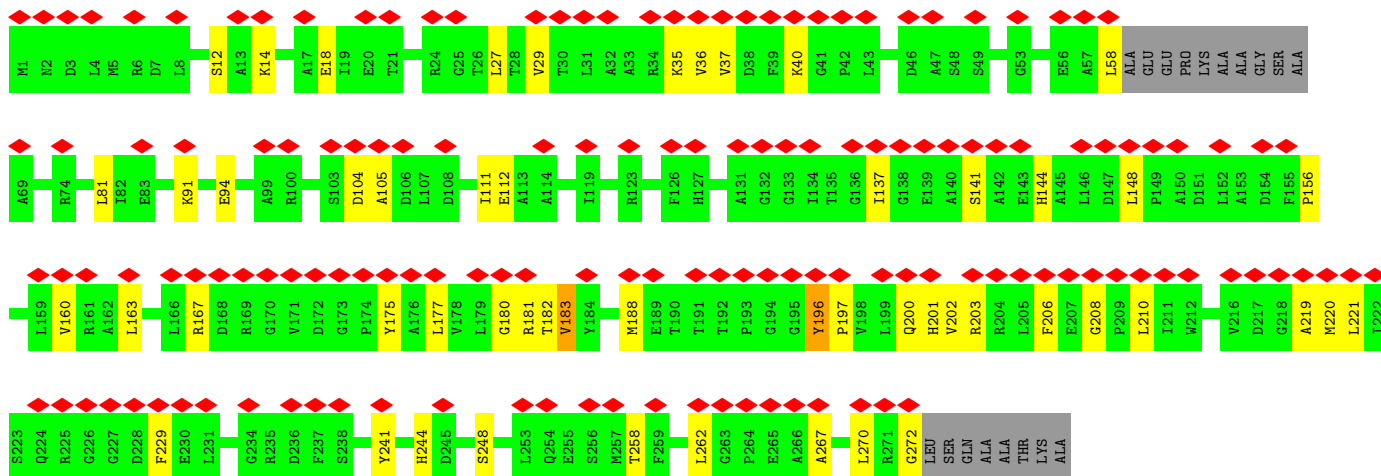
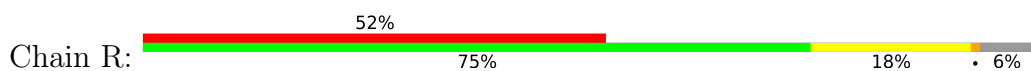
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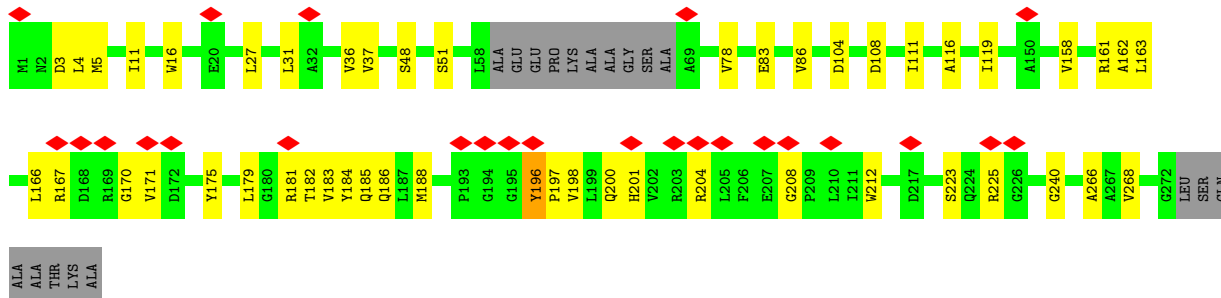
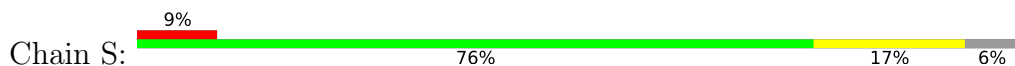
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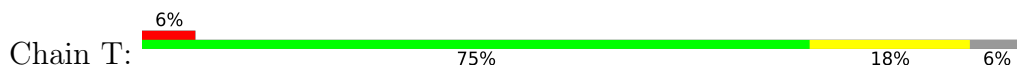
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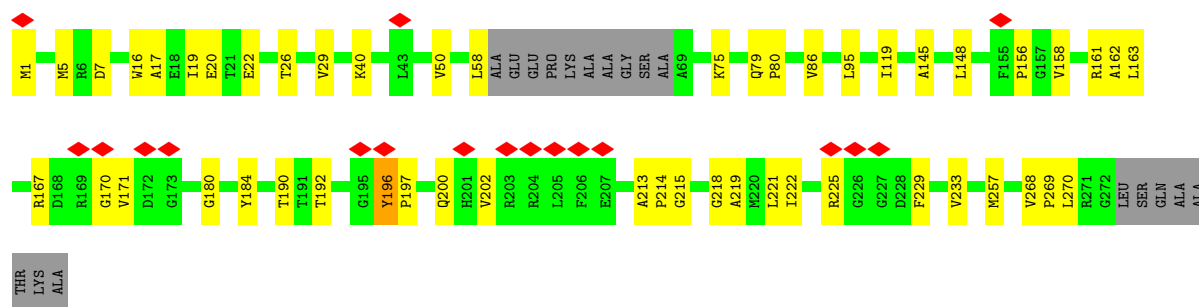


- Molecule 1: Type 1 encapsulin shell protein

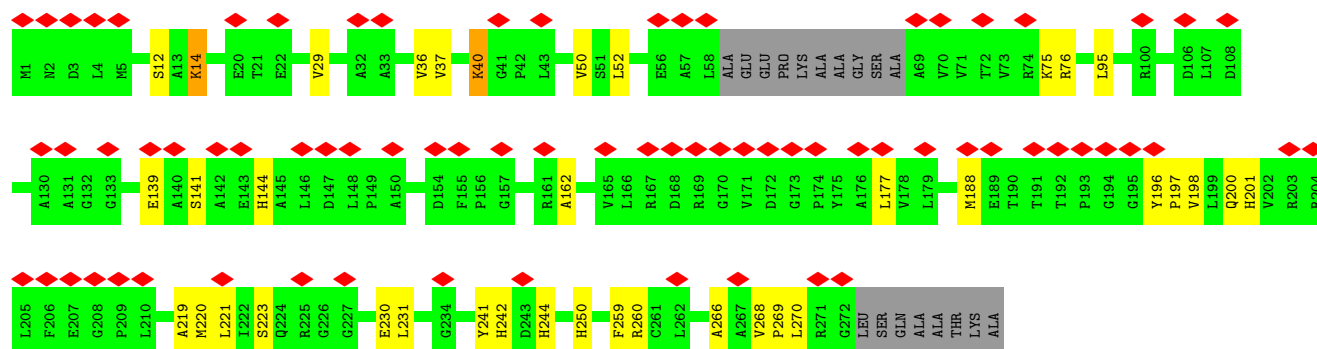
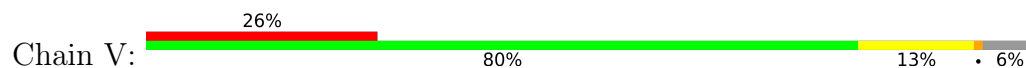


- Molecule 1: Type 1 encapsulin shell protein

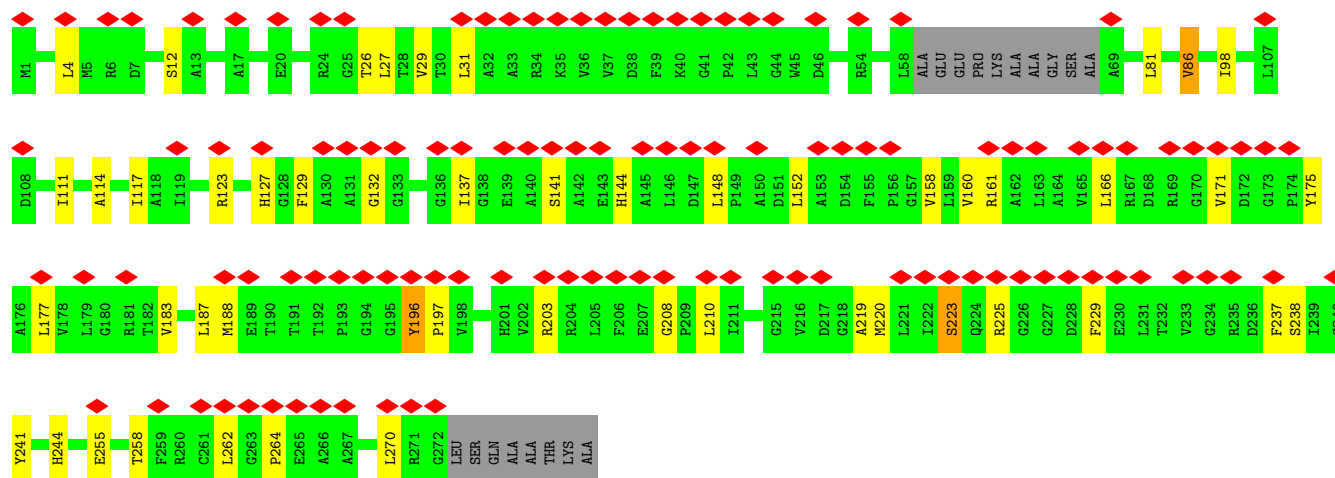
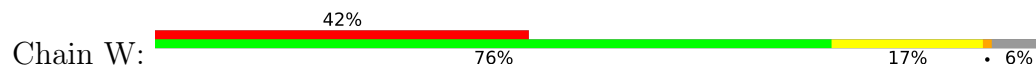




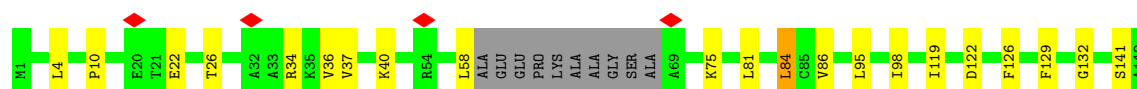
- Molecule 1: Type 1 encapsulin shell protein

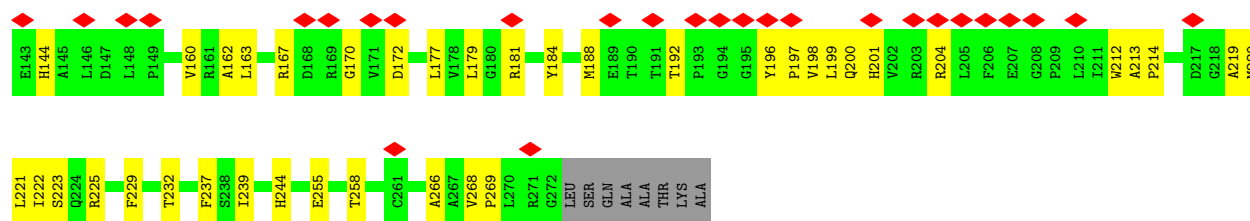


- Molecule 1: Type 1 encapsulin shell protein

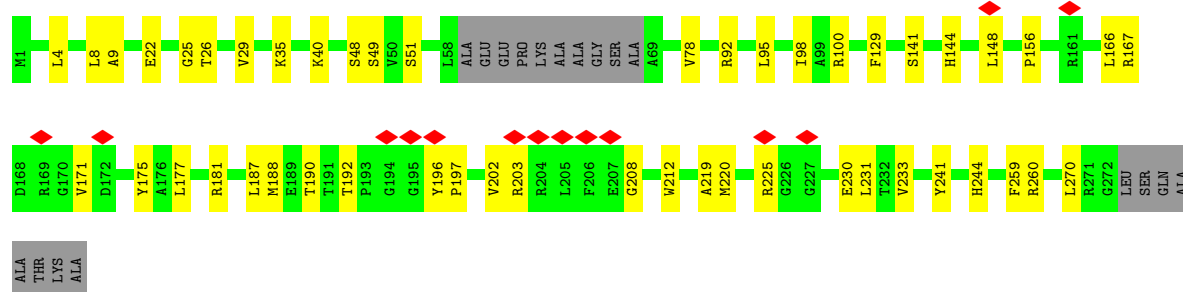
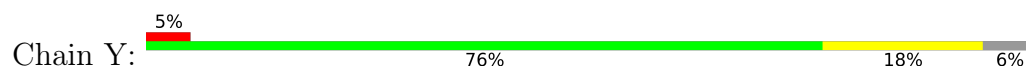


- Molecule 1: Type 1 encapsulin shell protein

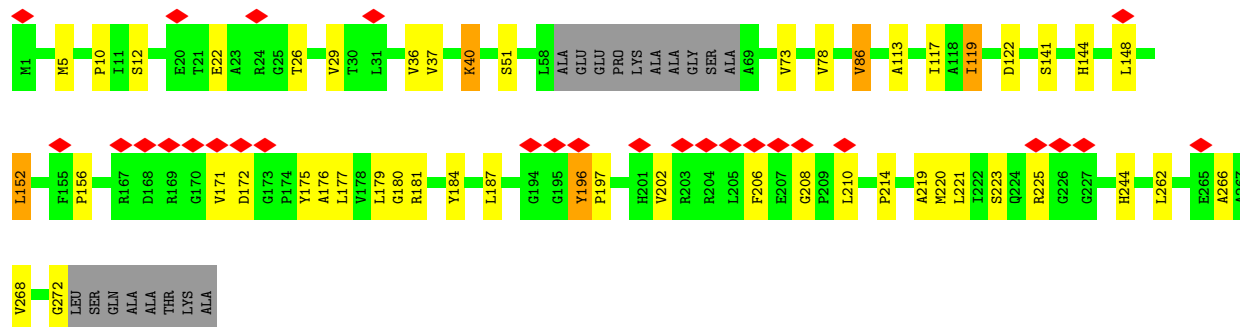
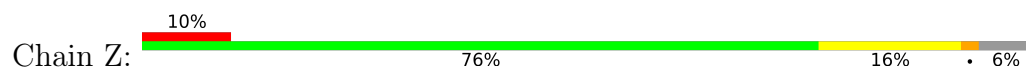




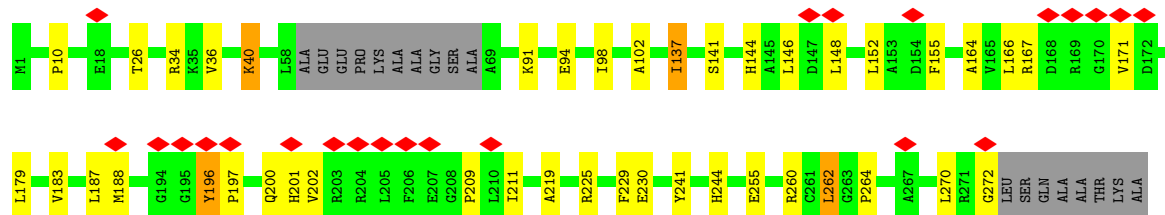
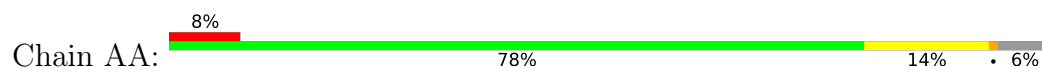
- Molecule 1: Type 1 encapsulin shell protein



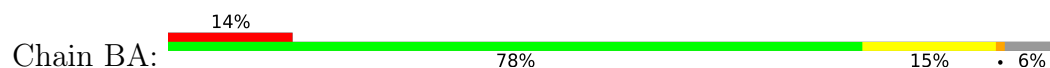
- Molecule 1: Type 1 encapsulin shell protein

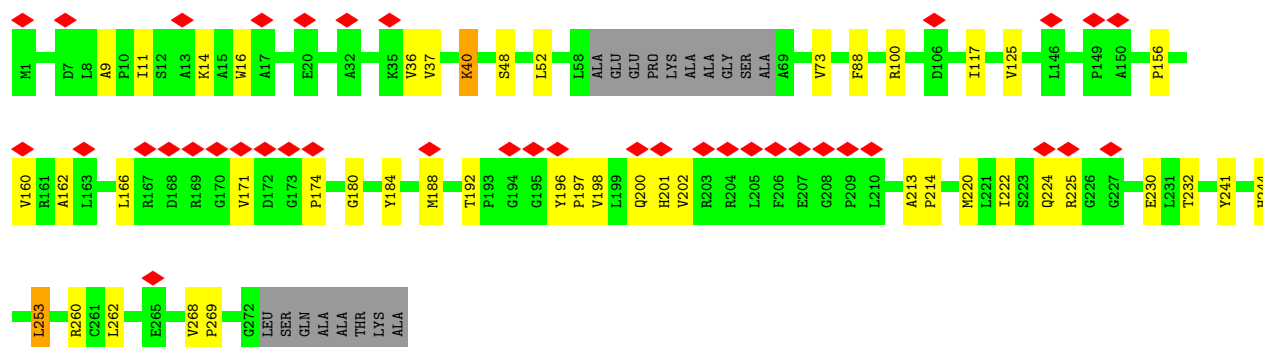


- Molecule 1: Type 1 encapsulin shell protein



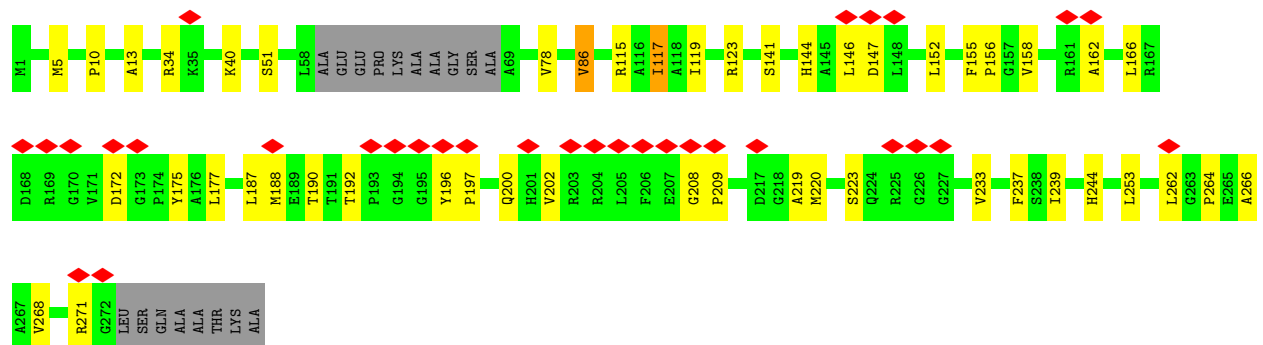
- Molecule 1: Type 1 encapsulin shell protein





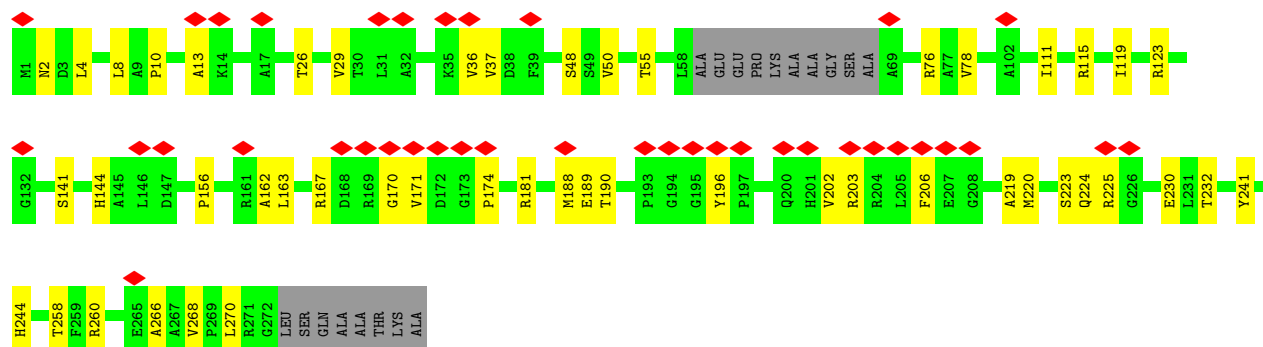
• Molecule 1: Type 1 encapsulin shell protein

Chain CA: 11% 76% 16% 6%



• Molecule 1: Type 1 encapsulin shell protein

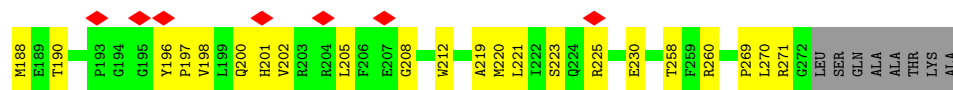
Chain DA: 14% 76% 18% 6%



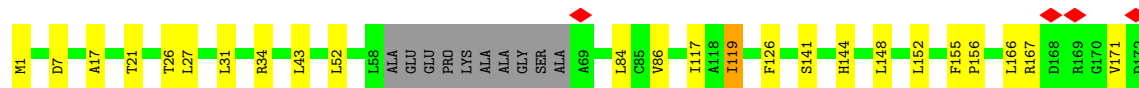
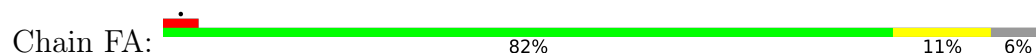
• Molecule 1: Type 1 encapsulin shell protein

Chain EA: 78% 16% 6%

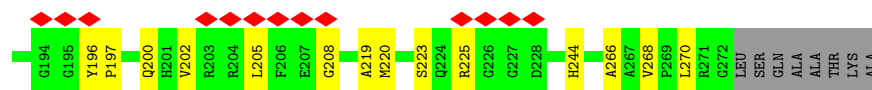
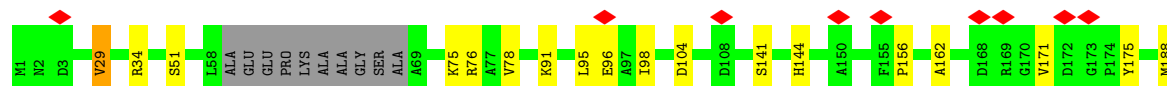
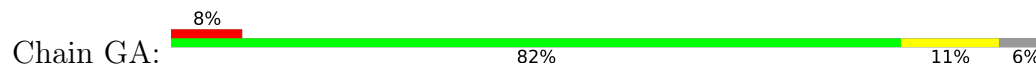




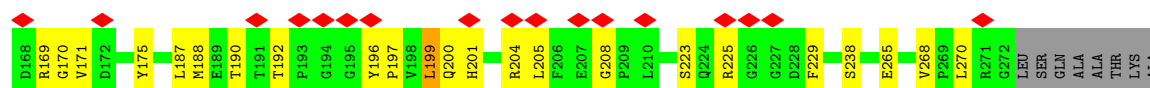
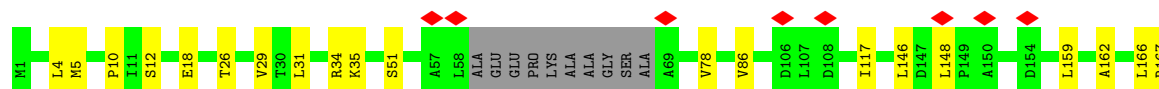
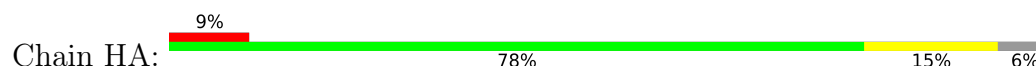
- Molecule 1: Type 1 encapsulin shell protein



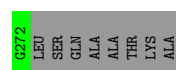
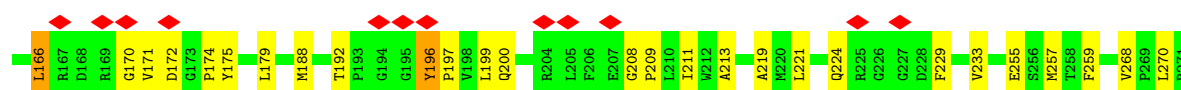
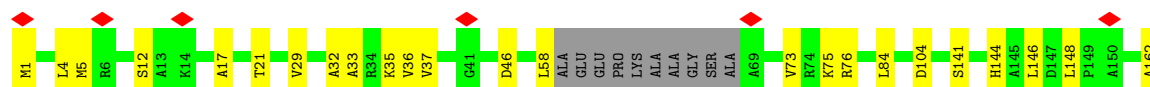
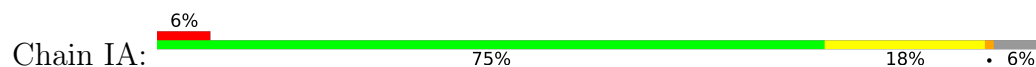
- Molecule 1: Type 1 encapsulin shell protein



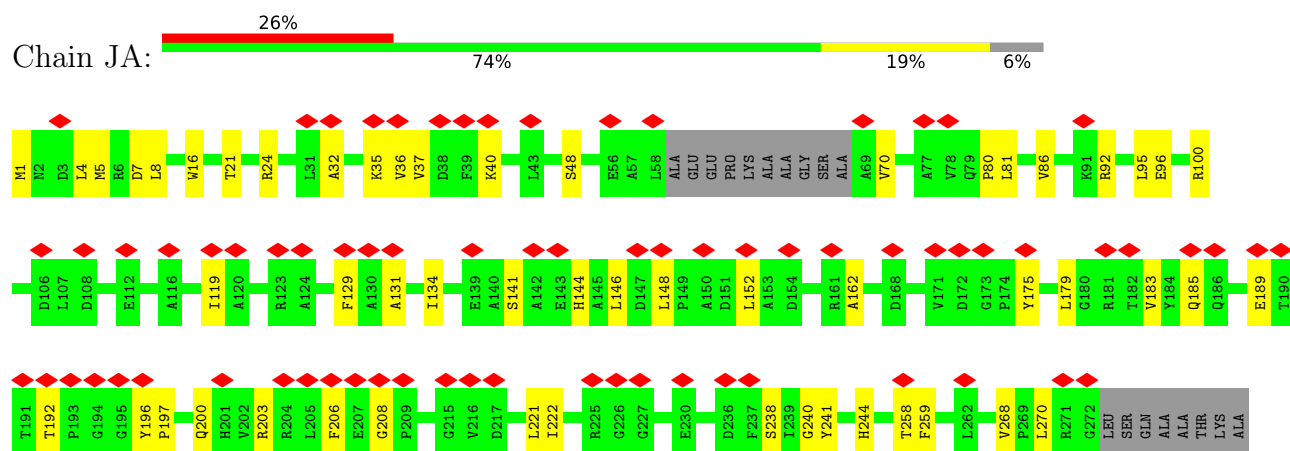
- Molecule 1: Type 1 encapsulin shell protein



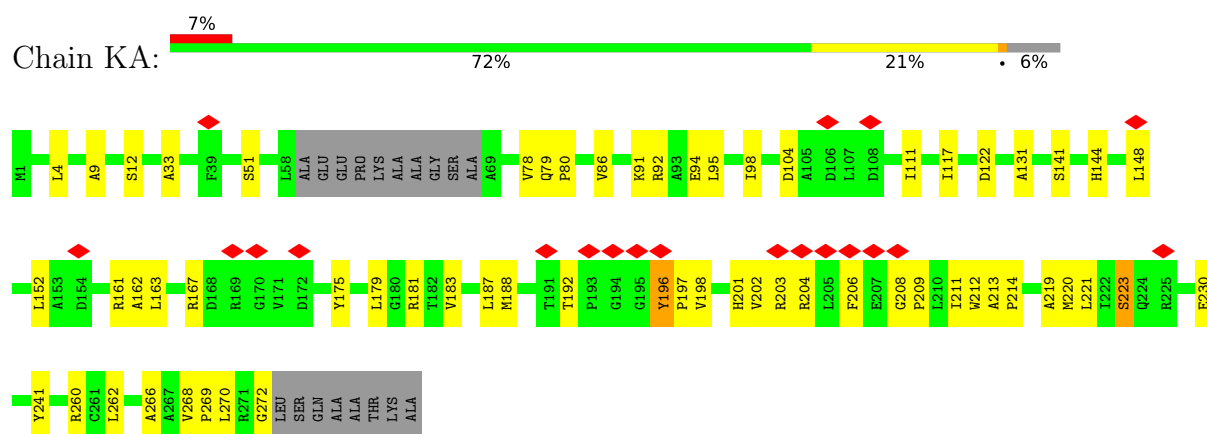
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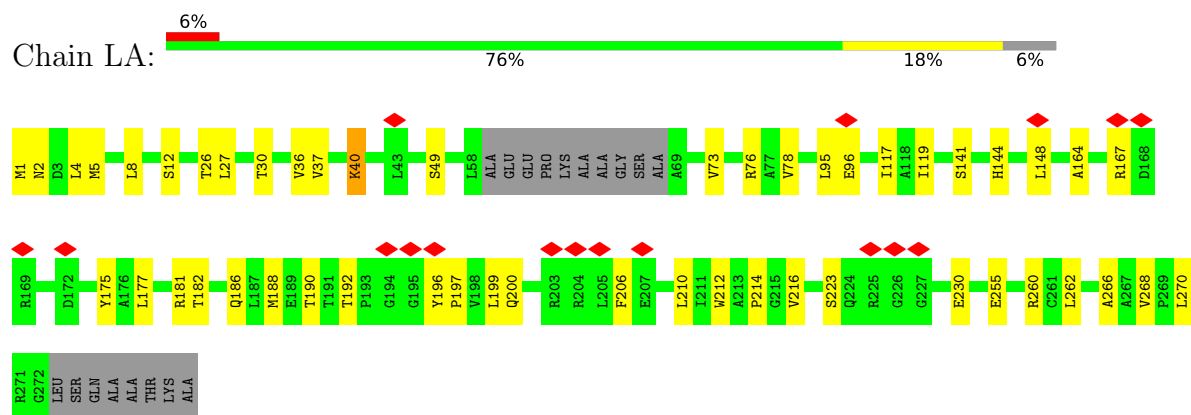
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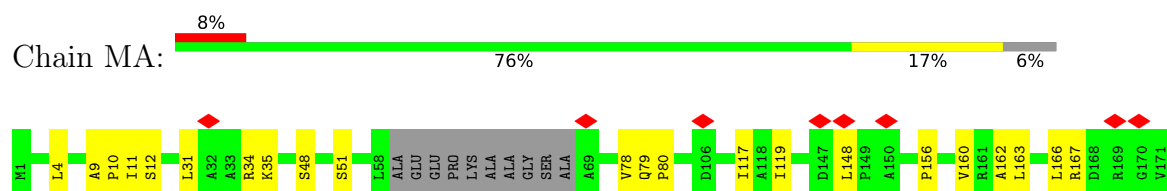
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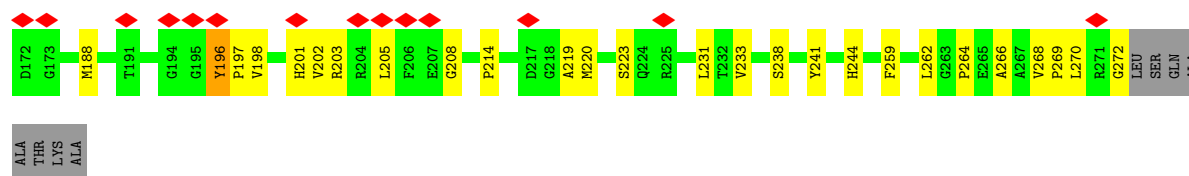


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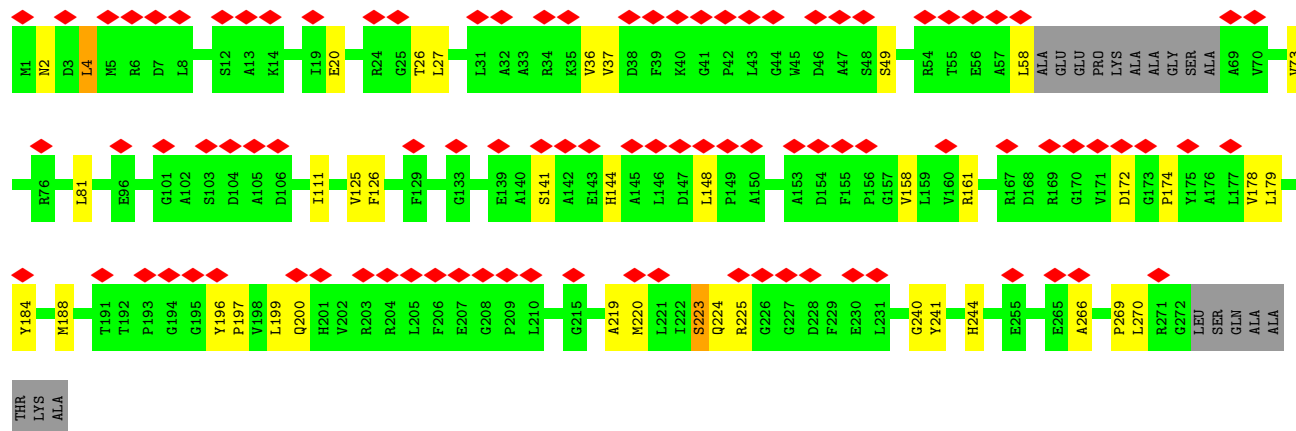
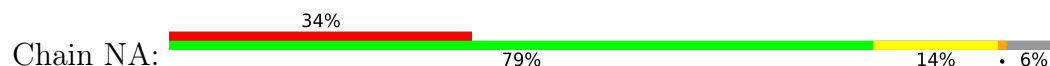


- Molecule 1: Type 1 encapsulin shell protein

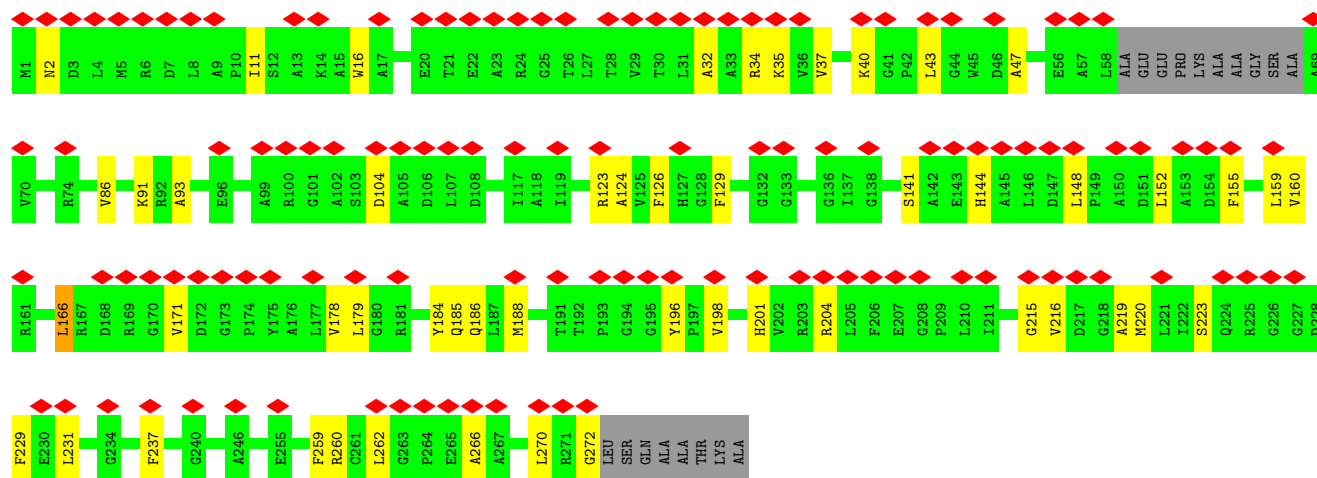


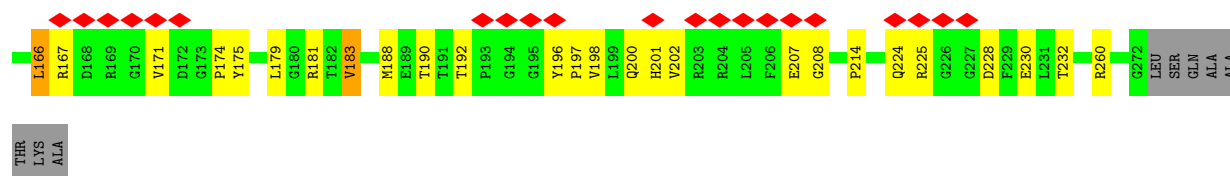


- Molecule 1: Type 1 encapsulin shell protein

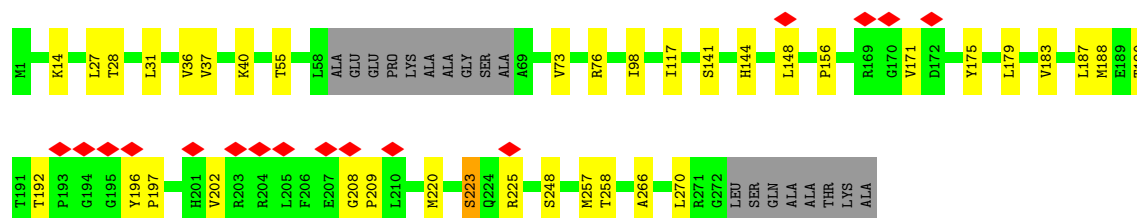
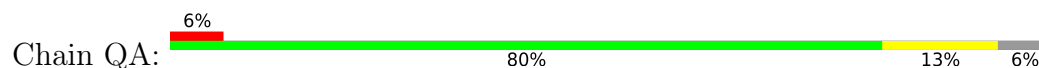


- Molecule 1: Type 1 encapsulin shell protein

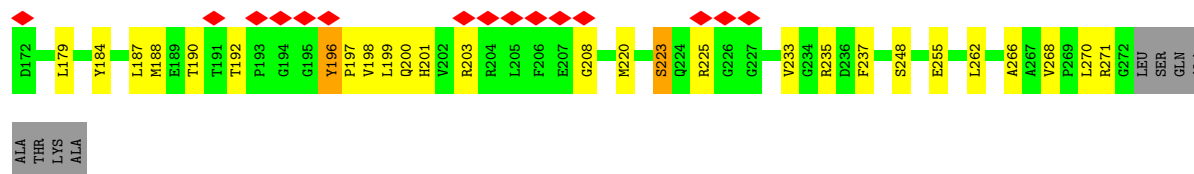
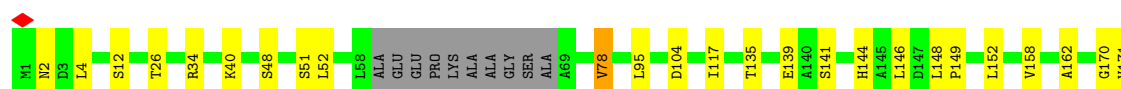
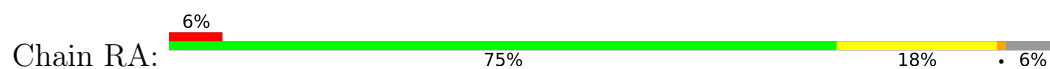




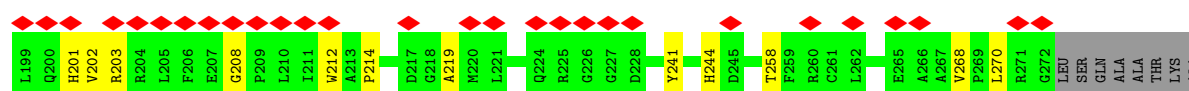
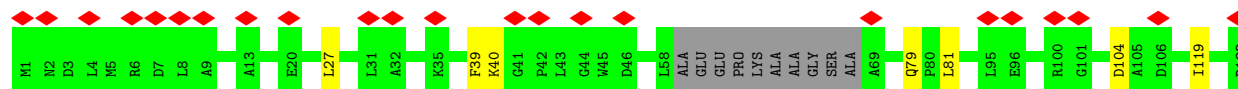
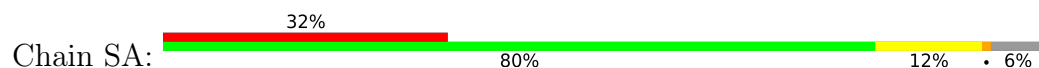
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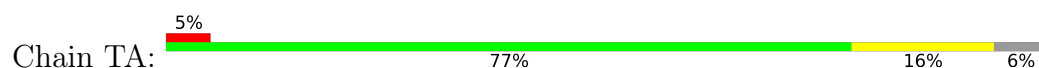
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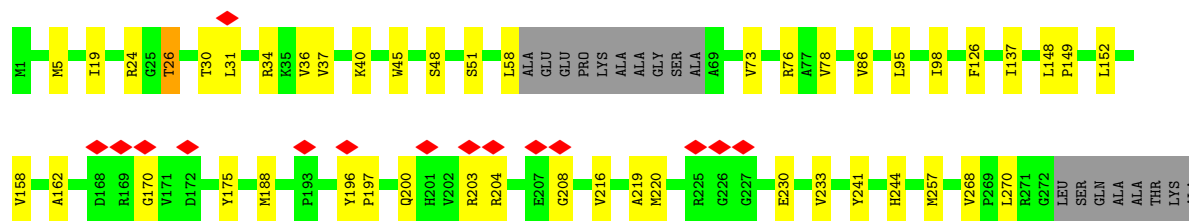


- Molecule 1: Type 1 encapsulin shell protein

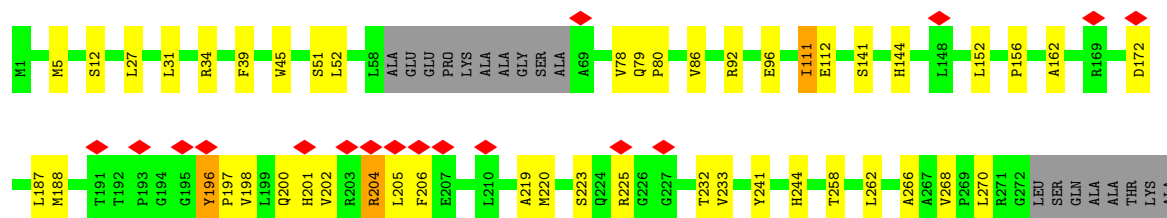
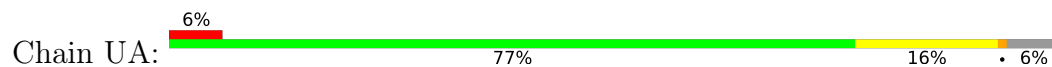


- Molecule 1: Type 1 encapsulin shell protein

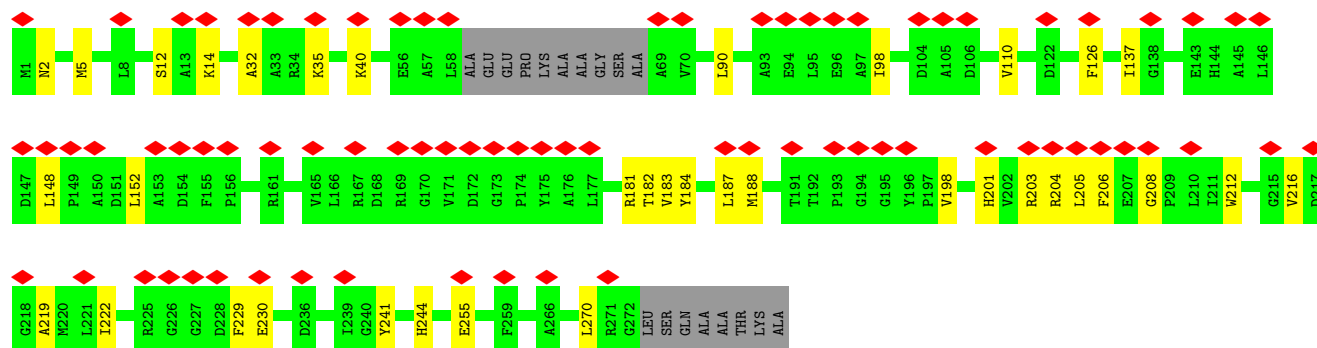
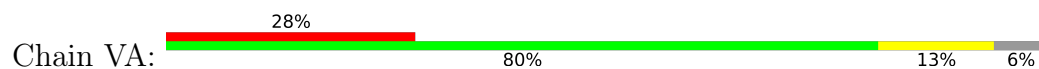


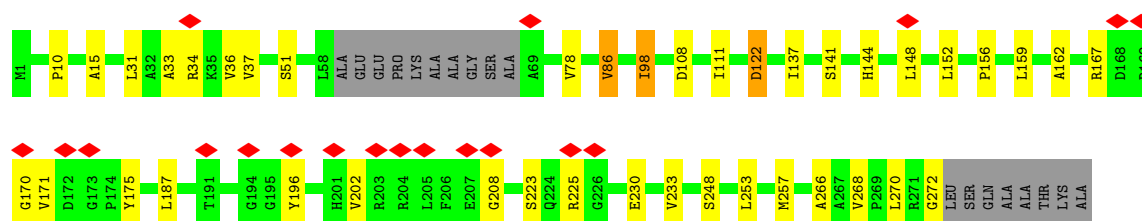
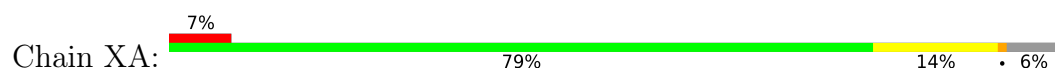


- Molecule 1: Type 1 encapsulin shell protein

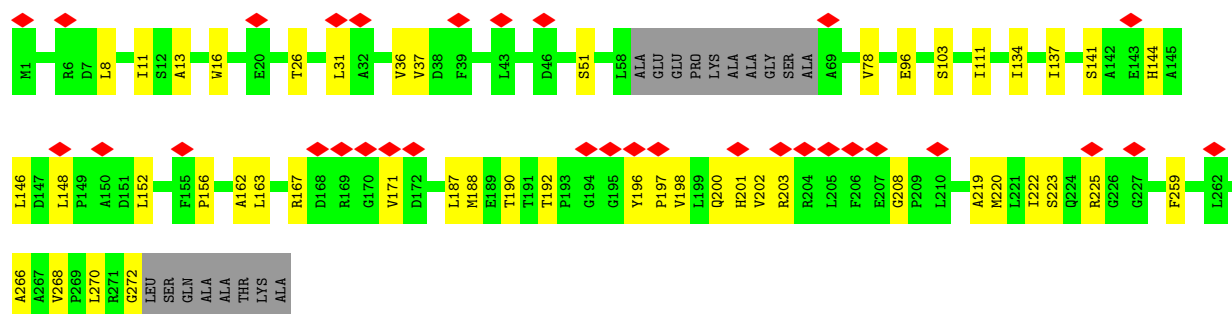
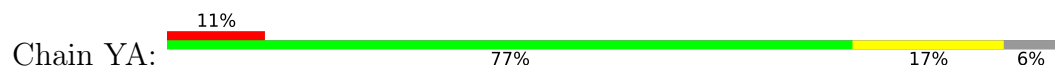


- Molecule 1: Type 1 encapsulin shell protein

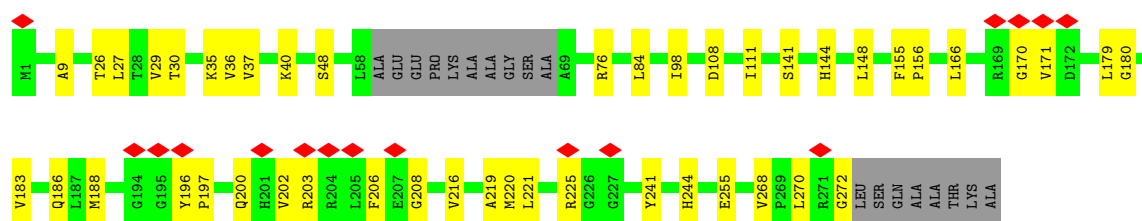
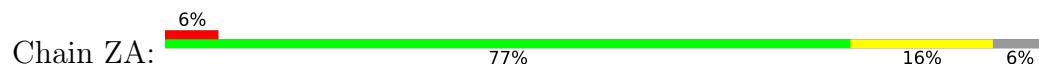




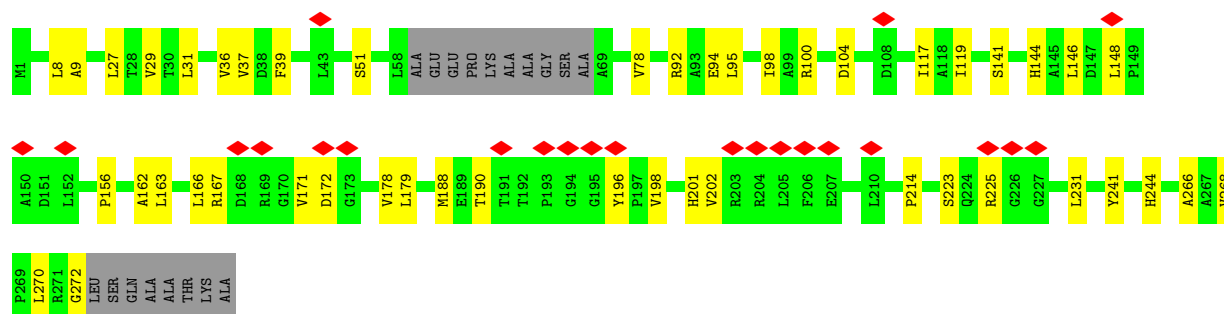
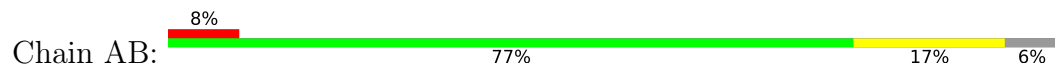
- Molecule 1: Type 1 encapsulin shell protein



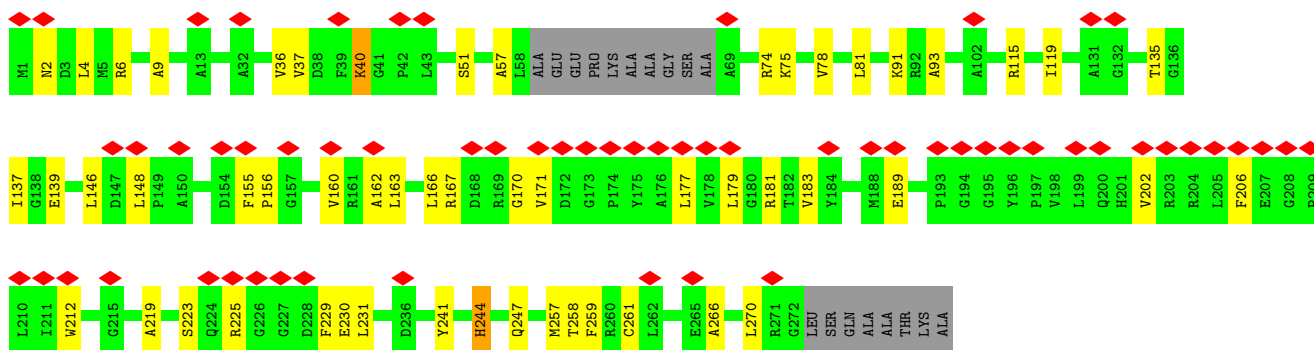
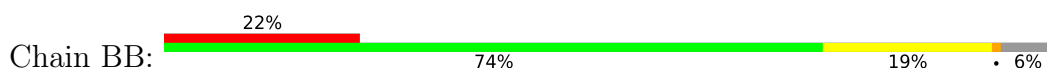
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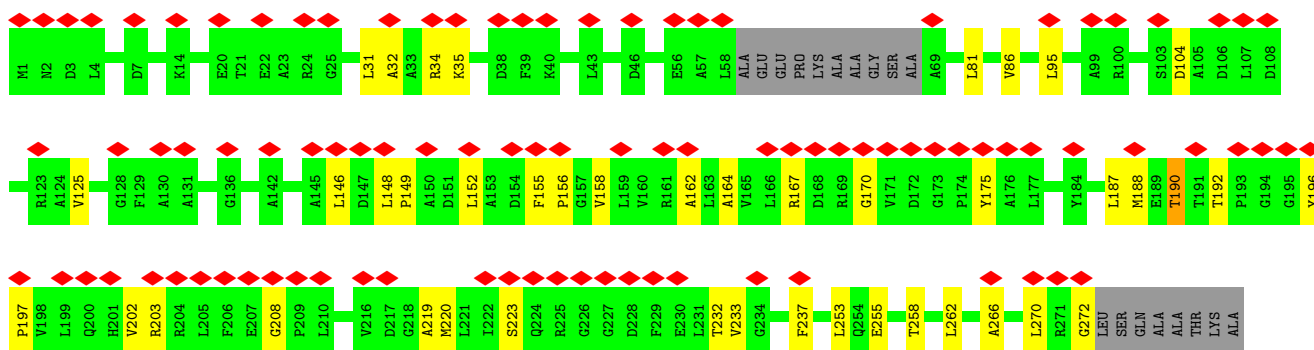
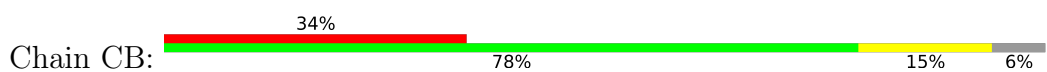
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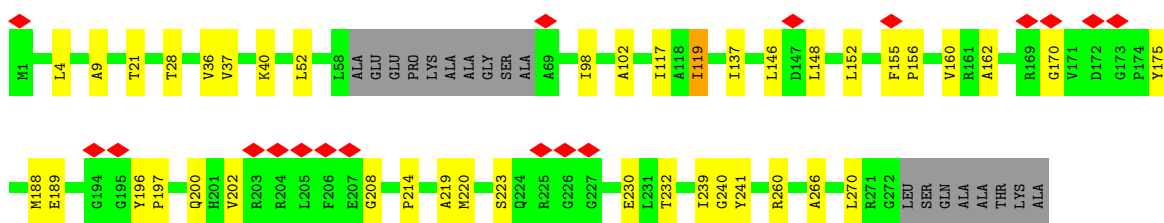
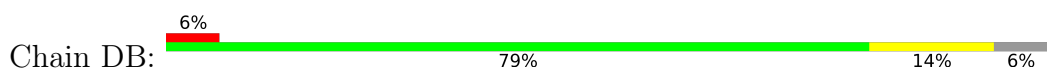
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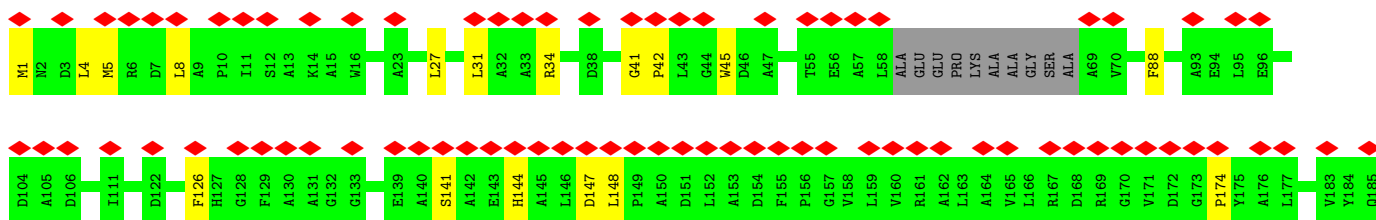
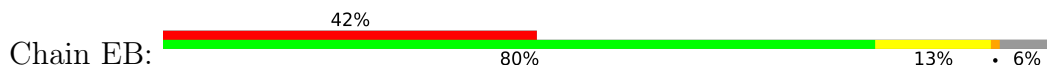
- Molecule 1: Type 1 encapsulin shell protein



- Molecule 1: Type 1 encapsulin shell protein



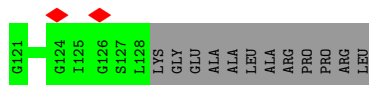
- Molecule 1: Type 1 encapsulin shell protein



Chain 1:  6% 94%

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

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

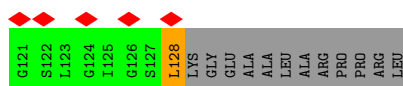
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- Molecule 2: Encapsulated ferritin-like protein

Chain 2:  5% 94%

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

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

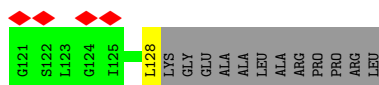
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- Molecule 2: Encapsulated ferritin-like protein

Chain 3:  5% 94%

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

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

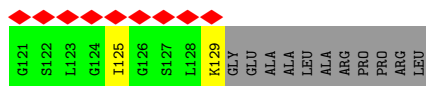
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- Molecule 2: Encapsulated ferritin-like protein

Chain 4:  6% 94%

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

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

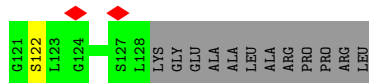
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- Molecule 2: Encapsulated ferritin-like protein

Chain 5:  5% . 94%

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

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

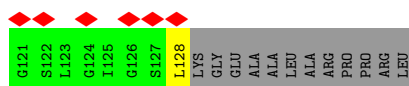


- Molecule 2: Encapsulated ferritin-like protein

Chain 6:  5% . 94%

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

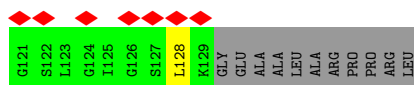


- Molecule 2: Encapsulated ferritin-like protein

Chain 7:  5% 6% . 94%

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



- Molecule 2: Encapsulated ferritin-like protein

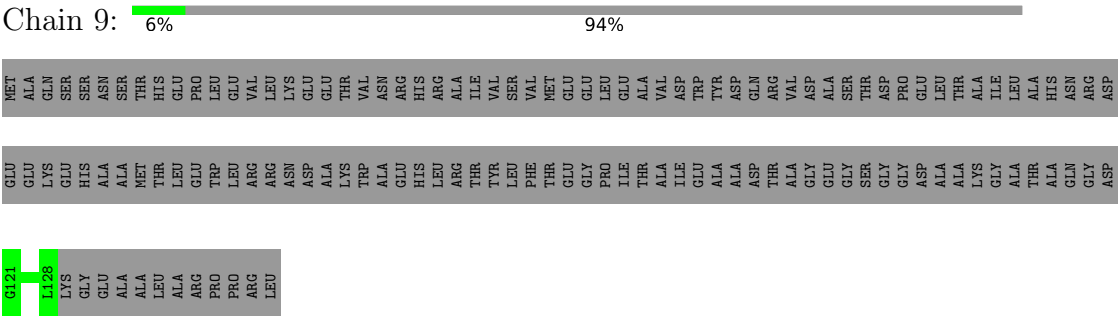
Chain 8:  5% 5% . 94%

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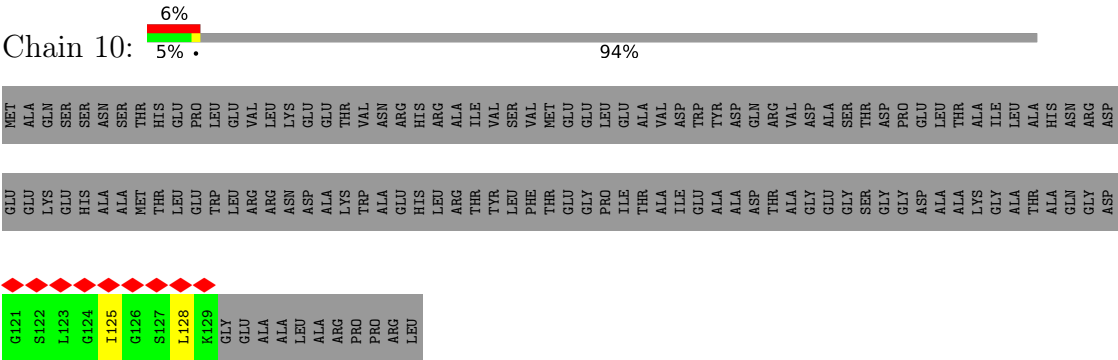
GLU GLU LYS HIS ALA ALA THR MET THR LEU LEU TRP LEU ARG ARG LYS ASN ASP ASP GLU THR LYS TRP ALA ALA ASP ASP GLN ARG VAL ASP ASP THR SER THR ASP GLY PRO GLU LEU THR ALA HIS ASN ASP



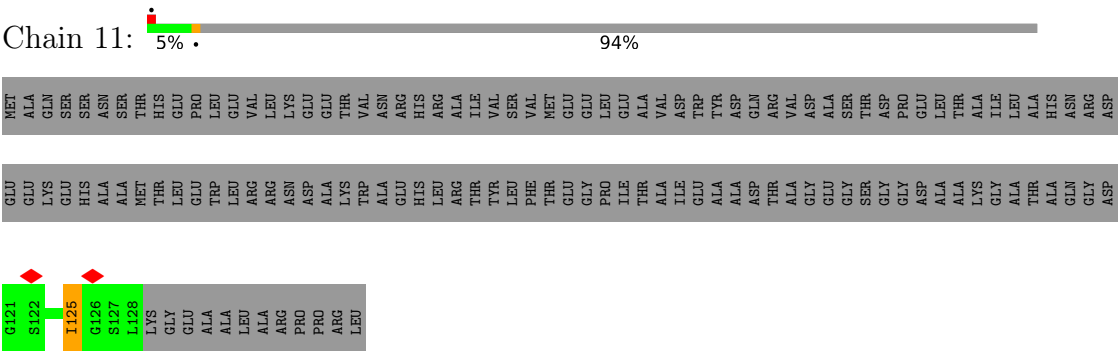
- Molecule 2: Encapsulated ferritin-like protein



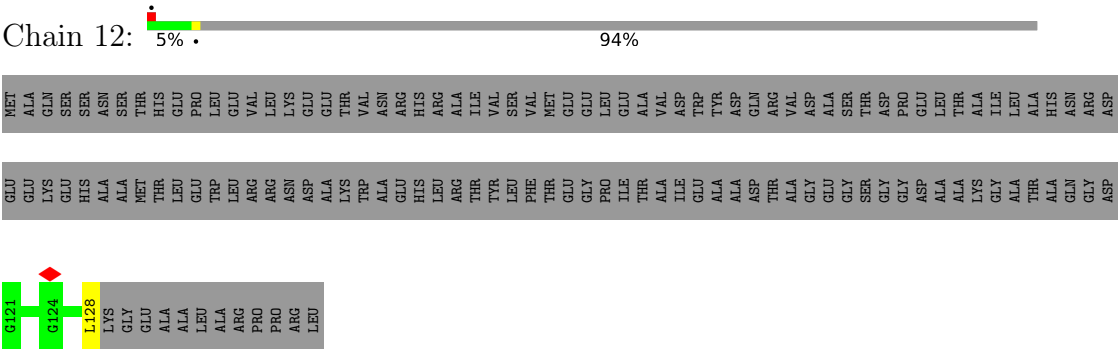
• Molecule 2: Encapsulated ferritin-like protein



• Molecule 2: Encapsulated ferritin-like protein

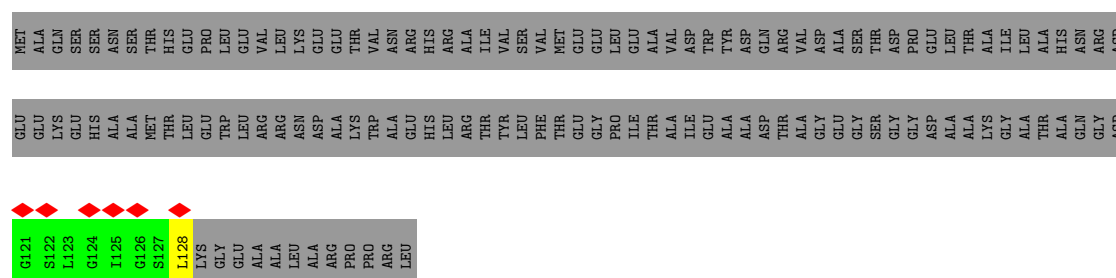


• Molecule 2: Encapsulated ferritin-like protein

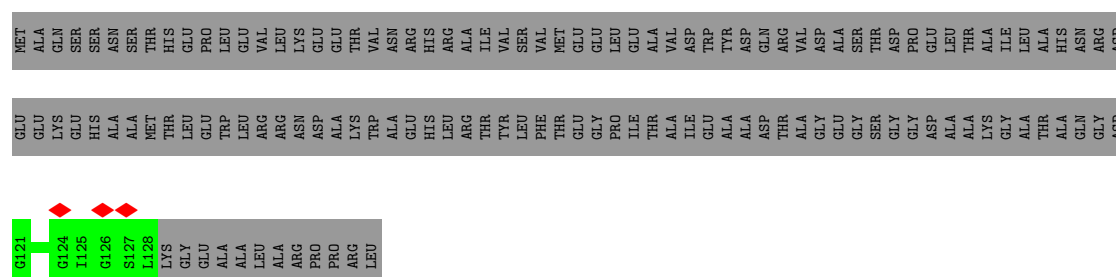


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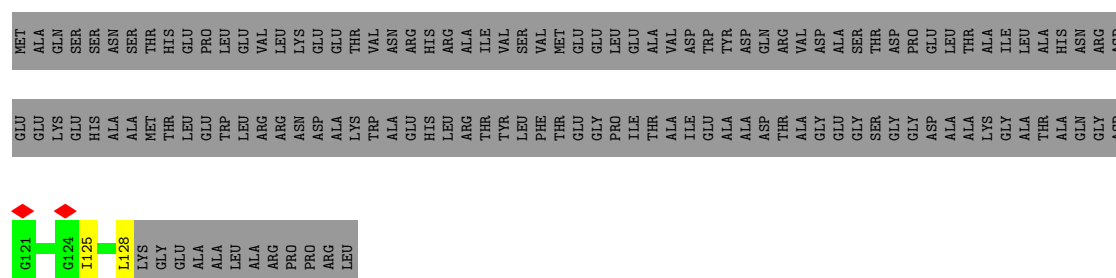
- Molecule 2: Encapsulated ferritin-like protein



- Molecule 2: Encapsulated ferritin-like protein



- Molecule 2: Encapsulated ferritin-like protein



- Molecule 2: Encapsulated ferritin-like protein

G121	G124	S127	L128	L129	L130	L131	L132	L133	L134	L135	L136	L137	L138	L139	L140	L141	L142	L143	L144	L145	L146	L147	L148	L149	L150	L151	L152	L153	L154	L155	L156	L157	L158	L159	L160	L161	L162	L163	L164	L165	L166	L167	L168	L169	L170	L171	L172	L173	L174	L175	L176	L177	L178	L179	L180	L181	L182	L183	L184	L185	L186	L187	L188	L189	L190	L191	L192	L193	L194	L195	L196	L197	L198	L199	L200	L201	L202	L203	L204	L205	L206	L207	L208	L209	L210	L211	L212	L213	L214	L215	L216	L217	L218	L219	L220	L221	L222	L223	L224	L225	L226	L227	L228	L229	L230	L231	L232	L233	L234	L235	L236	L237	L238	L239	L240	L241	L242	L243	L244	L245	L246	L247	L248	L249	L250	L251	L252	L253	L254	L255	L256	L257	L258	L259	L260	L261	L262	L263	L264	L265	L266	L267	L268	L269	L270	L271	L272	L273	L274	L275	L276	L277	L278	L279	L280	L281	L282	L283	L284	L285	L286	L287	L288	L289	L290	L291	L292	L293	L294	L295	L296	L297	L298	L299	L300	L301	L302	L303	L304	L305	L306	L307	L308	L309	L310	L311	L312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L63
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	G121	L128	L129	L130	L131	L132	L133	L134	L135	L136	L137	L138	L139	L140	L141	L142	L143	L144	L145	L146	L147	L148	L149	L150	L151	L152	L153	L154	L155	L156	L157	L158	L159	L160	L161	L162	L163	L164	L165	L166	L167	L168	L169	L170	L171	L172	L173	L174	L175	L176	L177	L178	L179	L180	L181	L182	L183	L184	L185	L186	L187	L188	L189	L190	L191	L192	L193	L194	L195	L196	L197	L198	L199	L200	L201	L202	L203	L204	L205	L206	L207	L208	L209	L210	L211	L212	L213	L214	L215	L216	L217	L218	L219	L220	L221	L222	L223	L224	L225	L226	L227	L228	L229	L230	L231	L232	L233	L234	L235	L236	L237	L238	L239	L240	L241	L242	L243	L244	L245	L246	L247	L248	L249	L250	L251	L252	L253	L254	L255	L256	L257	L258	L259	L260	L261	L262	L263	L264	L265	L266	L267	L268	L269	L270	L271	L272	L273	L274	L275	L276	L277	L278	L279	L280	L281	L282	L283	L284	L285	L286	L287	L288	L289	L290	L291	L292	L293	L294	L295	L296	L297	L298	L299	L300	L301	L302	L303	L304	L305	L306	L307	L308	L309	L310	L311	L312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637
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G121	S122	G124	I125	G126	S127	L128	LYS	GLY	ALA	ALA	LEU	ARG	PRO	PRO	ARG	LEU
◆	◆	◆	◆	◆	◆	◆										
GLU	LYS	HIS	ALA	ALA	THR	LEU	GLU	TRP	LEU	ARG	ASN	ASP	ALA	LYS	HIS	LEU
GLU	LYS	HIS	ALA	ALA	THR	LEU	GLU	TRP	LEU	ARG	ASN	ASP	ALA	LYS	HIS	LEU
GLN	SER	SER	ASN	SER	HIS	PRO	LEU	LEU	VAL	VAL	GLY	GLU	THR	VAL	ARG	ARG
MET	ALA	THR	ASN	THR	GLU	LYS	GLY	TRP	GLU	VAL	GLU	THR	VAL	VAL	SER	MET

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	41954	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.425	Depositor
Minimum map value	-0.176	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	432.576, 432.576, 432.576	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1265, 1.1265, 1.1265	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	A	0.31	0/2013	0.71	2/2737 (0.1%)
1	A0	0.30	0/2013	0.71	2/2737 (0.1%)
1	AA	0.30	0/2013	0.72	2/2737 (0.1%)
1	AB	0.29	0/2013	0.69	2/2737 (0.1%)
1	B	0.30	0/2013	0.71	4/2737 (0.1%)
1	BA	0.30	0/2013	0.73	2/2737 (0.1%)
1	BB	0.28	0/2013	0.69	0/2737
1	C	0.29	0/2013	0.69	2/2737 (0.1%)
1	CA	0.29	0/2013	0.70	2/2737 (0.1%)
1	CB	0.28	0/2013	0.72	2/2737 (0.1%)
1	D	0.29	0/2013	0.70	2/2737 (0.1%)
1	DA	0.29	0/2013	0.71	2/2737 (0.1%)
1	DB	0.30	0/2013	0.70	2/2737 (0.1%)
1	E	0.29	0/2013	0.70	2/2737 (0.1%)
1	EA	0.29	0/2013	0.69	2/2737 (0.1%)
1	EB	0.28	0/2013	0.70	2/2737 (0.1%)
1	F	0.29	0/2013	0.70	2/2737 (0.1%)
1	FA	0.29	0/2013	0.69	2/2737 (0.1%)
1	FB	0.29	0/2013	0.70	2/2737 (0.1%)
1	G	0.30	0/2013	0.70	2/2737 (0.1%)
1	GA	0.29	0/2013	0.68	2/2737 (0.1%)
1	GB	0.30	0/2013	0.70	2/2737 (0.1%)
1	H	0.30	0/2013	0.70	2/2737 (0.1%)
1	HA	0.29	0/2013	0.72	2/2737 (0.1%)
1	HB	0.30	0/2013	0.70	2/2737 (0.1%)
1	I	0.31	0/2013	0.74	2/2737 (0.1%)
1	IA	0.30	0/2013	0.71	2/2737 (0.1%)
1	J	0.29	0/2013	0.69	2/2737 (0.1%)
1	JA	0.28	0/2013	0.69	2/2737 (0.1%)
1	K	0.29	0/2013	0.68	2/2737 (0.1%)
1	KA	0.29	0/2013	0.70	2/2737 (0.1%)
1	L	0.30	0/2013	0.69	2/2737 (0.1%)
1	LA	0.31	0/2013	0.71	2/2737 (0.1%)
1	M	0.30	0/2013	0.69	2/2737 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	MA	0.29	0/2013	0.69	2/2737 (0.1%)
1	N	0.30	0/2013	0.69	2/2737 (0.1%)
1	NA	0.29	0/2013	0.70	2/2737 (0.1%)
1	O	0.30	0/2013	0.70	2/2737 (0.1%)
1	OA	0.29	0/2013	0.70	2/2737 (0.1%)
1	P	0.29	0/2013	0.70	2/2737 (0.1%)
1	PA	0.29	0/2013	0.69	2/2737 (0.1%)
1	Q	0.29	0/2013	0.68	2/2737 (0.1%)
1	QA	0.30	0/2013	0.71	2/2737 (0.1%)
1	R	0.29	0/2013	0.70	2/2737 (0.1%)
1	RA	0.29	0/2013	0.70	2/2737 (0.1%)
1	S	0.30	0/2013	0.69	2/2737 (0.1%)
1	SA	0.29	0/2013	0.72	4/2737 (0.1%)
1	T	0.29	0/2013	0.70	2/2737 (0.1%)
1	TA	0.29	0/2013	0.71	2/2737 (0.1%)
1	UA	0.29	0/2013	0.71	2/2737 (0.1%)
1	V	0.29	0/2013	0.70	2/2737 (0.1%)
1	VA	0.29	0/2013	0.69	0/2737
1	W	0.28	0/2013	0.69	2/2737 (0.1%)
1	WA	0.28	0/2013	0.68	0/2737
1	X	0.30	0/2013	0.69	2/2737 (0.1%)
1	XA	0.29	0/2013	0.70	2/2737 (0.1%)
1	Y	0.30	0/2013	0.71	2/2737 (0.1%)
1	YA	0.30	0/2013	0.71	2/2737 (0.1%)
1	Z	0.29	0/2013	0.68	2/2737 (0.1%)
1	ZA	0.30	0/2013	0.71	2/2737 (0.1%)
2	1	0.26	0/47	0.59	0/61
2	10	0.33	0/56	0.70	0/72
2	11	0.18	0/47	0.54	0/61
2	12	0.24	0/47	0.56	0/61
2	13	0.24	0/47	0.57	0/61
2	14	0.29	0/47	0.78	0/61
2	15	0.21	0/47	0.59	0/61
2	16	0.28	0/47	0.71	0/61
2	17	0.26	0/47	0.55	0/61
2	18	0.24	0/47	0.49	0/61
2	19	0.37	0/47	0.57	0/61
2	2	0.22	0/47	0.54	0/61
2	20	0.28	0/47	0.63	0/61
2	3	0.24	0/47	0.60	0/61
2	4	0.22	0/56	0.58	0/72
2	5	0.24	0/47	0.69	0/61
2	6	0.26	0/47	0.54	0/61

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	7	0.29	0/56	0.66	0/72
2	8	0.21	0/56	0.53	0/72
2	9	0.23	0/47	0.48	0/61
All	All	0.29	0/121756	0.70	118/165484 (0.1%)

There are no bond length outliers.

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	196	TYR	CA-C-N	7.02	128.61	119.84
1	P	196	TYR	C-N-CA	7.02	128.61	119.84
1	J	196	TYR	CA-C-N	6.78	128.31	119.84
1	J	196	TYR	C-N-CA	6.78	128.31	119.84
1	L	196	TYR	CA-C-N	6.62	128.12	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1975	0	1984	30	0
1	A0	1975	0	1984	30	0
1	AA	1975	0	1984	28	0
1	AB	1975	0	1984	27	0
1	B	1975	0	1984	29	0
1	BA	1975	0	1984	28	0
1	BB	1975	0	1984	35	0
1	C	1975	0	1984	24	0
1	CA	1975	0	1984	30	0
1	CB	1975	0	1984	27	0
1	D	1975	0	1984	24	0
1	DA	1975	0	1984	26	0
1	DB	1975	0	1984	23	0
1	E	1975	0	1984	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	EA	1975	0	1984	22	0
1	EB	1975	0	1984	24	0
1	F	1975	0	1984	33	0
1	FA	1975	0	1984	17	0
1	FB	1975	0	1984	21	0
1	G	1975	0	1984	24	0
1	GA	1975	0	1984	17	0
1	GB	1975	0	1984	30	0
1	H	1975	0	1984	25	0
1	HA	1975	0	1984	23	0
1	HB	1975	0	1984	27	0
1	I	1975	0	1984	40	0
1	IA	1975	0	1984	35	0
1	J	1975	0	1984	23	0
1	JA	1975	0	1984	33	0
1	K	1975	0	1984	33	0
1	KA	1975	0	1984	34	0
1	L	1975	0	1984	32	0
1	LA	1975	0	1984	28	0
1	M	1975	0	1984	26	0
1	MA	1975	0	1984	28	0
1	N	1975	0	1984	38	0
1	NA	1975	0	1984	23	0
1	O	1975	0	1984	28	0
1	OA	1975	0	1984	29	0
1	P	1975	0	1984	40	0
1	PA	1975	0	1984	22	0
1	Q	1975	0	1984	22	0
1	QA	1975	0	1984	18	0
1	R	1975	0	1984	37	0
1	RA	1975	0	1984	30	0
1	S	1975	0	1984	30	0
1	SA	1975	0	1984	21	0
1	T	1975	0	1984	31	0
1	TA	1975	0	1984	26	0
1	UA	1975	0	1984	31	0
1	V	1975	0	1984	26	0
1	VA	1975	0	1984	24	0
1	W	1975	0	1984	31	0
1	WA	1975	0	1984	23	0
1	X	1975	0	1984	36	0
1	XA	1975	0	1984	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	1975	0	1984	30	0
1	YA	1975	0	1984	32	0
1	Z	1975	0	1984	30	0
1	ZA	1975	0	1984	30	0
2	1	48	0	51	0	0
2	10	57	0	64	1	0
2	11	48	0	51	1	0
2	12	48	0	51	1	0
2	13	48	0	51	0	0
2	14	48	0	51	1	0
2	15	48	0	51	0	0
2	16	48	0	51	2	0
2	17	48	0	51	1	0
2	18	48	0	51	2	0
2	19	48	0	51	1	0
2	2	48	0	51	1	0
2	20	48	0	51	0	0
2	3	48	0	51	1	0
2	4	57	0	64	1	0
2	5	48	0	51	0	0
2	6	48	0	51	1	0
2	7	57	0	64	1	0
2	8	57	0	64	2	0
2	9	48	0	51	0	0
All	All	119496	0	120112	1581	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 7.

The worst 5 of 1581 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:91:LYS:HZ2	1:I:92:ARG:H	1.24	0.81
1:HA:199:LEU:HB2	1:KA:204:ARG:HH12	1.49	0.78
1:AB:171:VAL:HG22	1:AB:225:ARG:HE	1.50	0.77
1:B:119:ILE:HD11	1:B:215:GLY:HA3	1.68	0.75
1:R:91:LYS:HE3	1:R:91:LYS:HA	1.67	0.75

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	A0	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	AA	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	AB	258/280 (92%)	248 (96%)	10 (4%)	0	100	100
1	B	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	BA	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
1	BB	258/280 (92%)	248 (96%)	10 (4%)	0	100	100
1	C	258/280 (92%)	248 (96%)	10 (4%)	0	100	100
1	CA	258/280 (92%)	249 (96%)	9 (4%)	0	100	100
1	CB	258/280 (92%)	250 (97%)	8 (3%)	0	100	100
1	D	258/280 (92%)	249 (96%)	9 (4%)	0	100	100
1	DA	258/280 (92%)	250 (97%)	8 (3%)	0	100	100
1	DB	258/280 (92%)	249 (96%)	9 (4%)	0	100	100
1	E	258/280 (92%)	243 (94%)	15 (6%)	0	100	100
1	EA	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	EB	258/280 (92%)	251 (97%)	7 (3%)	0	100	100
1	F	258/280 (92%)	249 (96%)	9 (4%)	0	100	100
1	FA	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
1	FB	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	G	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	GA	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	GB	258/280 (92%)	248 (96%)	10 (4%)	0	100	100
1	H	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	HA	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
1	HB	258/280 (92%)	246 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	258/280 (92%)	243 (94%)	15 (6%)	0	100	100
1	IA	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
1	J	258/280 (92%)	248 (96%)	10 (4%)	0	100	100
1	JA	258/280 (92%)	249 (96%)	9 (4%)	0	100	100
1	K	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	KA	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
1	L	258/280 (92%)	245 (95%)	13 (5%)	0	100	100
1	LA	258/280 (92%)	248 (96%)	10 (4%)	0	100	100
1	M	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	MA	258/280 (92%)	249 (96%)	9 (4%)	0	100	100
1	N	258/280 (92%)	244 (95%)	14 (5%)	0	100	100
1	NA	258/280 (92%)	250 (97%)	8 (3%)	0	100	100
1	O	258/280 (92%)	248 (96%)	10 (4%)	0	100	100
1	OA	258/280 (92%)	248 (96%)	10 (4%)	0	100	100
1	P	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	PA	258/280 (92%)	244 (95%)	14 (5%)	0	100	100
1	Q	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	QA	258/280 (92%)	245 (95%)	13 (5%)	0	100	100
1	R	258/280 (92%)	248 (96%)	10 (4%)	0	100	100
1	RA	258/280 (92%)	244 (95%)	14 (5%)	0	100	100
1	S	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
1	SA	258/280 (92%)	249 (96%)	9 (4%)	0	100	100
1	T	258/280 (92%)	244 (95%)	14 (5%)	0	100	100
1	TA	258/280 (92%)	249 (96%)	9 (4%)	0	100	100
1	UA	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	V	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	VA	258/280 (92%)	251 (97%)	7 (3%)	0	100	100
1	W	258/280 (92%)	251 (97%)	7 (3%)	0	100	100
1	WA	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
1	X	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
1	XA	258/280 (92%)	245 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	258/280 (92%)	248 (96%)	10 (4%)	0	100	100
1	YA	258/280 (92%)	248 (96%)	10 (4%)	0	100	100
1	Z	258/280 (92%)	244 (95%)	14 (5%)	0	100	100
1	ZA	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
2	1	6/140 (4%)	6 (100%)	0	0	100	100
2	10	7/140 (5%)	6 (86%)	1 (14%)	0	100	100
2	11	6/140 (4%)	5 (83%)	0	1 (17%)	0	2
2	12	6/140 (4%)	6 (100%)	0	0	100	100
2	13	6/140 (4%)	6 (100%)	0	0	100	100
2	14	6/140 (4%)	5 (83%)	1 (17%)	0	100	100
2	15	6/140 (4%)	6 (100%)	0	0	100	100
2	16	6/140 (4%)	5 (83%)	1 (17%)	0	100	100
2	17	6/140 (4%)	6 (100%)	0	0	100	100
2	18	6/140 (4%)	5 (83%)	1 (17%)	0	100	100
2	19	6/140 (4%)	6 (100%)	0	0	100	100
2	2	6/140 (4%)	6 (100%)	0	0	100	100
2	20	6/140 (4%)	2 (33%)	3 (50%)	1 (17%)	0	2
2	3	6/140 (4%)	5 (83%)	1 (17%)	0	100	100
2	4	7/140 (5%)	7 (100%)	0	0	100	100
2	5	6/140 (4%)	5 (83%)	1 (17%)	0	100	100
2	6	6/140 (4%)	6 (100%)	0	0	100	100
2	7	7/140 (5%)	6 (86%)	1 (14%)	0	100	100
2	8	7/140 (5%)	7 (100%)	0	0	100	100
2	9	6/140 (4%)	6 (100%)	0	0	100	100
All	All	15604/19600 (80%)	14935 (96%)	667 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	20	125	ILE
2	11	125	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	200/210 (95%)	197 (98%)	3 (2%)	57	68
1	A0	200/210 (95%)	195 (98%)	5 (2%)	42	61
1	AA	200/210 (95%)	192 (96%)	8 (4%)	28	52
1	AB	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	B	200/210 (95%)	195 (98%)	5 (2%)	42	61
1	BA	200/210 (95%)	195 (98%)	5 (2%)	42	61
1	BB	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	C	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	CA	200/210 (95%)	194 (97%)	6 (3%)	36	57
1	CB	200/210 (95%)	194 (97%)	6 (3%)	36	57
1	D	200/210 (95%)	194 (97%)	6 (3%)	36	57
1	DA	200/210 (95%)	192 (96%)	8 (4%)	28	52
1	DB	200/210 (95%)	194 (97%)	6 (3%)	36	57
1	E	200/210 (95%)	197 (98%)	3 (2%)	57	68
1	EA	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	EB	200/210 (95%)	197 (98%)	3 (2%)	57	68
1	F	200/210 (95%)	194 (97%)	6 (3%)	36	57
1	FA	200/210 (95%)	195 (98%)	5 (2%)	42	61
1	FB	200/210 (95%)	193 (96%)	7 (4%)	32	54
1	G	200/210 (95%)	195 (98%)	5 (2%)	42	61
1	GA	200/210 (95%)	194 (97%)	6 (3%)	36	57
1	GB	200/210 (95%)	191 (96%)	9 (4%)	24	49
1	H	200/210 (95%)	194 (97%)	6 (3%)	36	57
1	HA	200/210 (95%)	191 (96%)	9 (4%)	24	49
1	HB	200/210 (95%)	192 (96%)	8 (4%)	28	52
1	I	200/210 (95%)	197 (98%)	3 (2%)	57	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	IA	200/210 (95%)	194 (97%)	6 (3%)	36	57
1	J	200/210 (95%)	192 (96%)	8 (4%)	28	52
1	JA	200/210 (95%)	193 (96%)	7 (4%)	32	54
1	K	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	KA	200/210 (95%)	193 (96%)	7 (4%)	32	54
1	L	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	LA	200/210 (95%)	193 (96%)	7 (4%)	32	54
1	M	200/210 (95%)	195 (98%)	5 (2%)	42	61
1	MA	200/210 (95%)	195 (98%)	5 (2%)	42	61
1	N	200/210 (95%)	198 (99%)	2 (1%)	68	74
1	NA	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	O	200/210 (95%)	193 (96%)	7 (4%)	32	54
1	OA	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	P	200/210 (95%)	195 (98%)	5 (2%)	42	61
1	PA	200/210 (95%)	192 (96%)	8 (4%)	28	52
1	Q	200/210 (95%)	191 (96%)	9 (4%)	24	49
1	QA	200/210 (95%)	194 (97%)	6 (3%)	36	57
1	R	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	RA	200/210 (95%)	190 (95%)	10 (5%)	22	47
1	S	200/210 (95%)	199 (100%)	1 (0%)	81	80
1	SA	200/210 (95%)	197 (98%)	3 (2%)	57	68
1	T	200/210 (95%)	197 (98%)	3 (2%)	57	68
1	TA	200/210 (95%)	193 (96%)	7 (4%)	32	54
1	UA	200/210 (95%)	195 (98%)	5 (2%)	42	61
1	V	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	VA	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	W	200/210 (95%)	192 (96%)	8 (4%)	28	52
1	WA	200/210 (95%)	195 (98%)	5 (2%)	42	61
1	X	200/210 (95%)	194 (97%)	6 (3%)	36	57
1	XA	200/210 (95%)	193 (96%)	7 (4%)	32	54
1	Y	200/210 (95%)	194 (97%)	6 (3%)	36	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	YA	200/210 (95%)	195 (98%)	5 (2%)	42	61
1	Z	200/210 (95%)	192 (96%)	8 (4%)	28	52
1	ZA	200/210 (95%)	196 (98%)	4 (2%)	48	64
2	1	5/108 (5%)	5 (100%)	0	100	100
2	10	6/108 (6%)	5 (83%)	1 (17%)	2	14
2	11	5/108 (5%)	5 (100%)	0	100	100
2	12	5/108 (5%)	5 (100%)	0	100	100
2	13	5/108 (5%)	3 (60%)	2 (40%)	0	0
2	14	5/108 (5%)	5 (100%)	0	100	100
2	15	5/108 (5%)	5 (100%)	0	100	100
2	16	5/108 (5%)	5 (100%)	0	100	100
2	17	5/108 (5%)	5 (100%)	0	100	100
2	18	5/108 (5%)	4 (80%)	1 (20%)	1	9
2	19	5/108 (5%)	4 (80%)	1 (20%)	1	9
2	2	5/108 (5%)	4 (80%)	1 (20%)	1	9
2	20	5/108 (5%)	4 (80%)	1 (20%)	1	9
2	3	5/108 (5%)	5 (100%)	0	100	100
2	4	6/108 (6%)	5 (83%)	1 (17%)	2	14
2	5	5/108 (5%)	4 (80%)	1 (20%)	1	9
2	6	5/108 (5%)	5 (100%)	0	100	100
2	7	6/108 (6%)	6 (100%)	0	100	100
2	8	6/108 (6%)	5 (83%)	1 (17%)	2	14
2	9	5/108 (5%)	5 (100%)	0	100	100
All	All	12104/14760 (82%)	11762 (97%)	342 (3%)	38	58

5 of 342 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	QA	40	LYS
1	AB	104	ASP
1	RA	48	SER
1	VA	12	SER
1	DB	28	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
1	SA	224	GLN
1	BB	254	GLN
1	TA	254	GLN
1	XA	144	HIS
1	DB	200	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

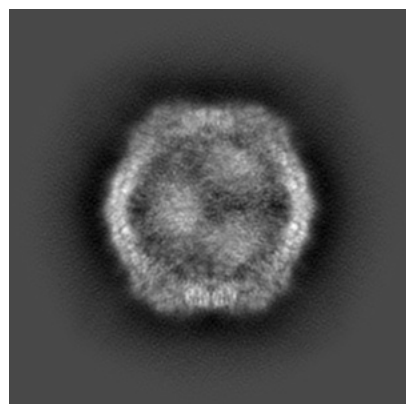
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55116. These allow visual inspection of the internal detail of the map and identification of artifacts.

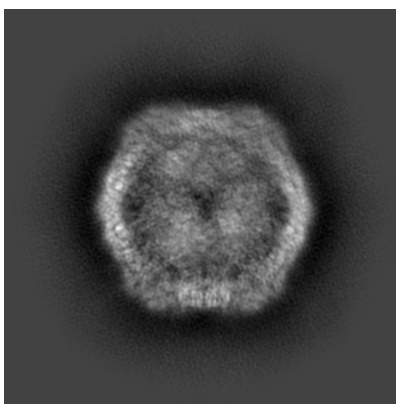
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

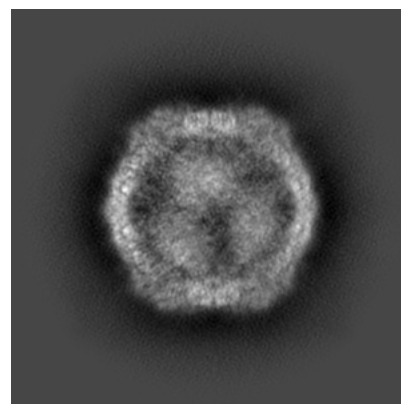
6.1.1 Primary map



X

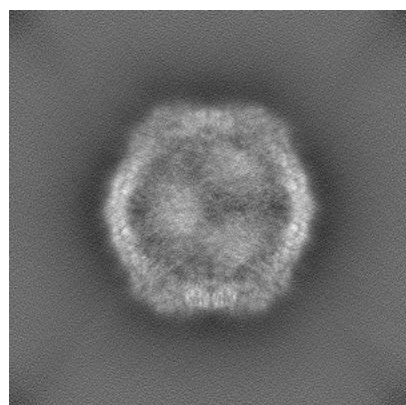


Y

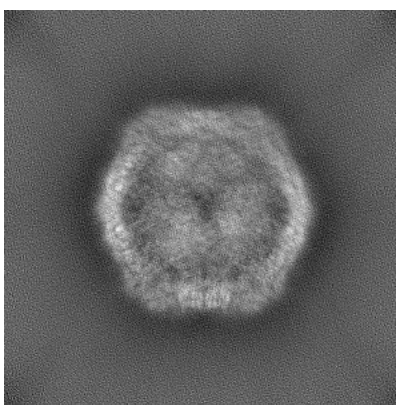


Z

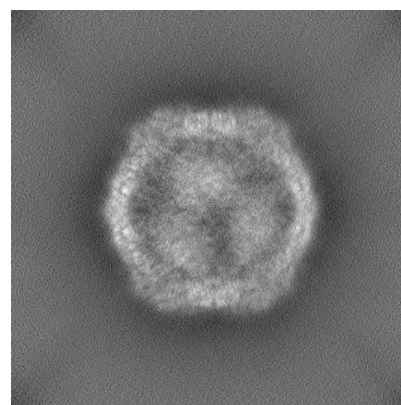
6.1.2 Raw map



X



Y

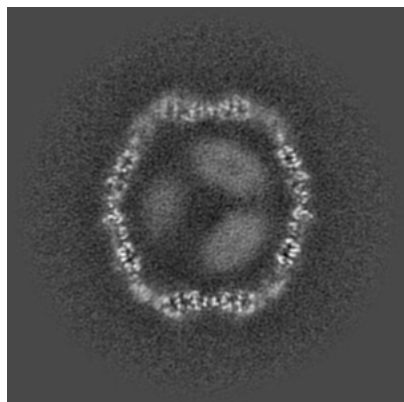


Z

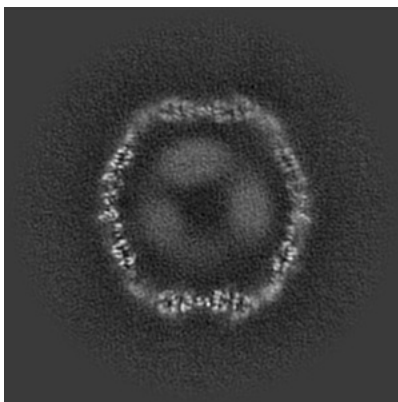
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

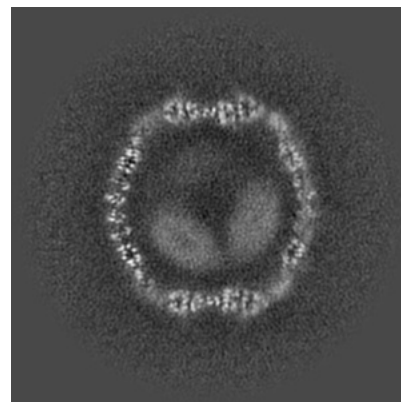
6.2.1 Primary map



X Index: 192

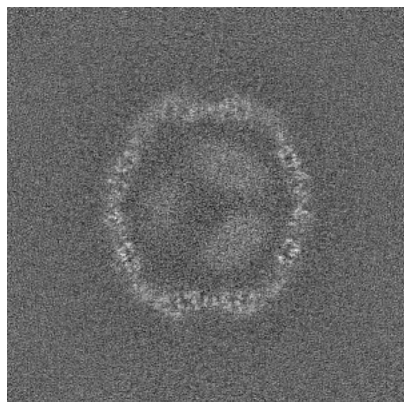


Y Index: 192

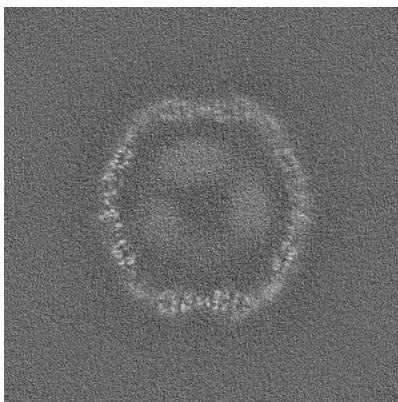


Z Index: 192

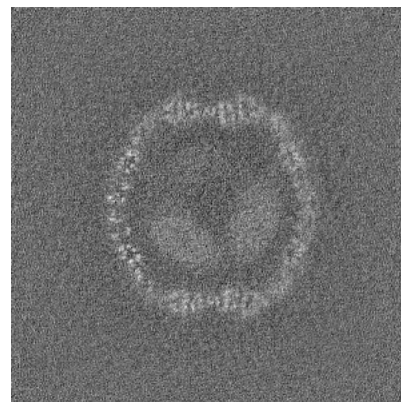
6.2.2 Raw map



X Index: 192



Y Index: 192

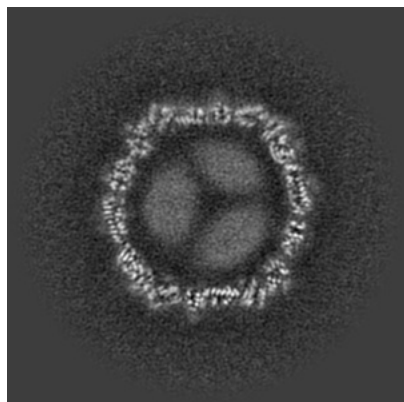


Z Index: 192

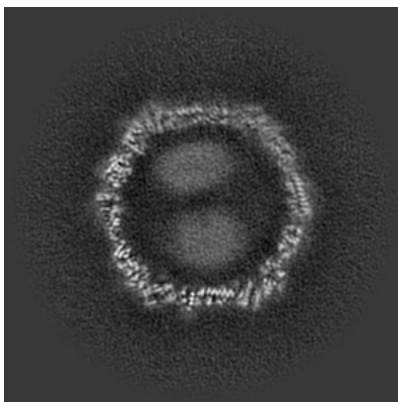
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

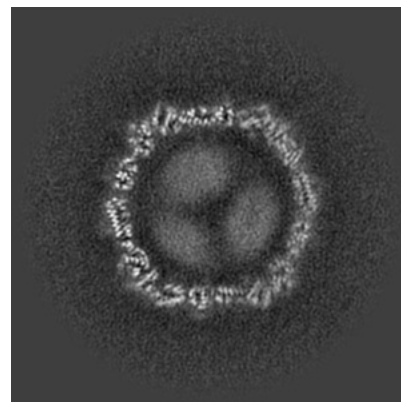
6.3.1 Primary map



X Index: 173

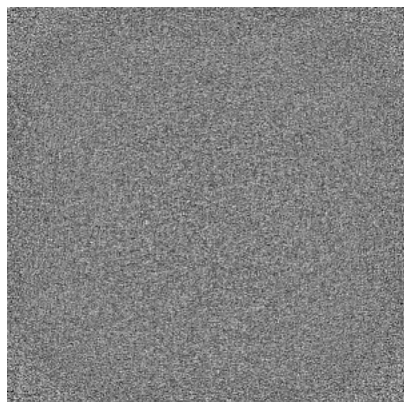


Y Index: 171

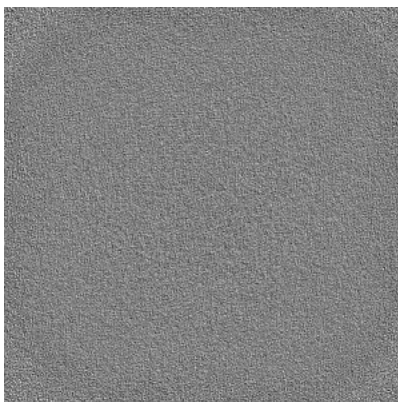


Z Index: 173

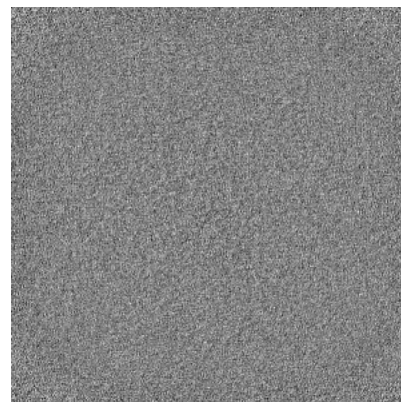
6.3.2 Raw map



X Index: 0



Y Index: 0

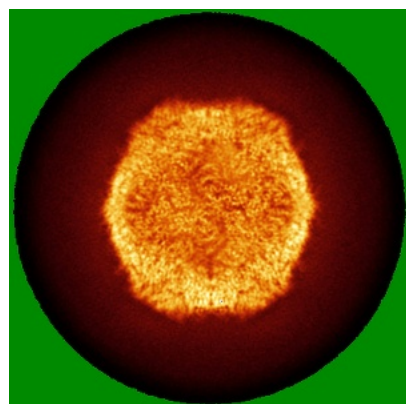


Z Index: 0

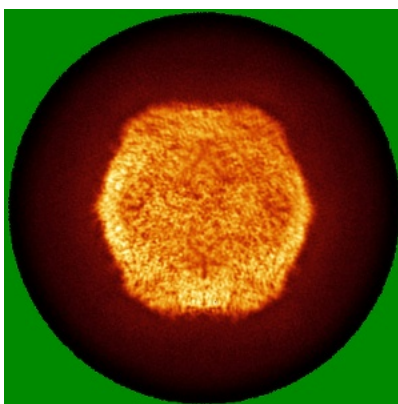
The images above show the largest variance slices of the map in three orthogonal directions.

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

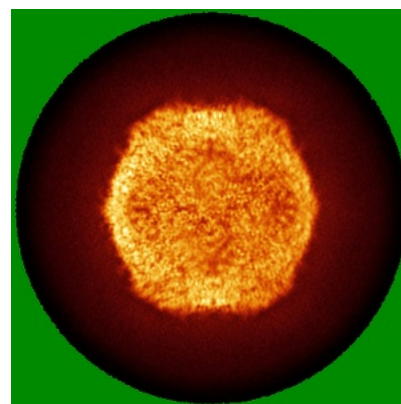
6.4.1 Primary map



X

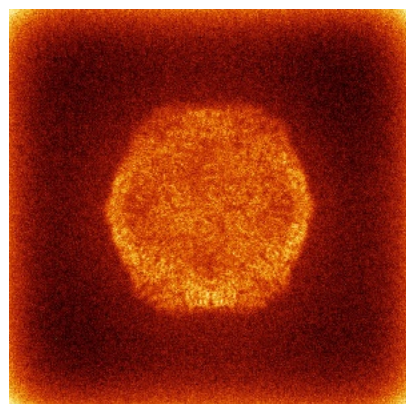


Y

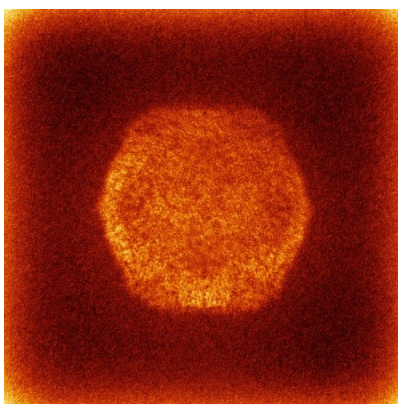


Z

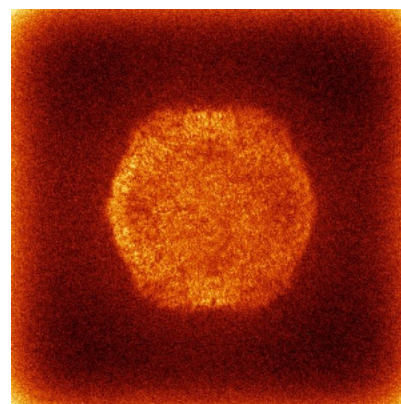
6.4.2 Raw map



X



Y

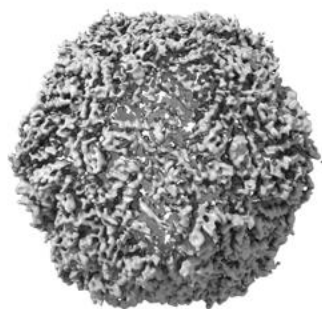


Z

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

6.5 Orthogonal surface views [i](#)

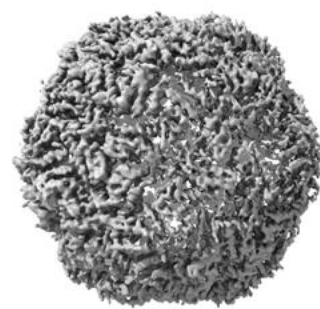
6.5.1 Primary map



X



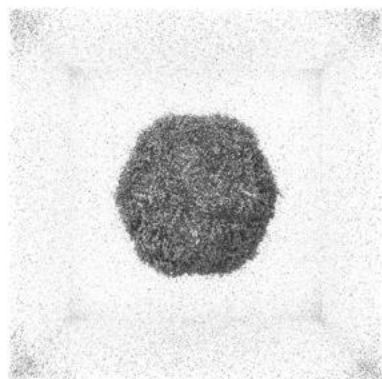
Y



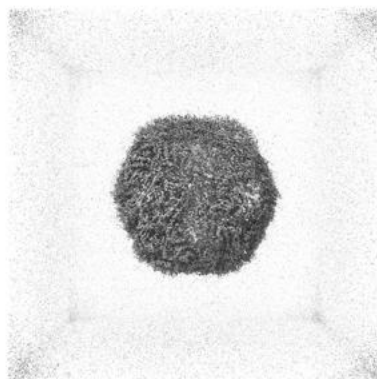
Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

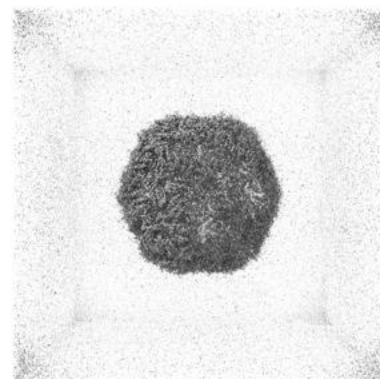
6.5.2 Raw map



X



Y



Z

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

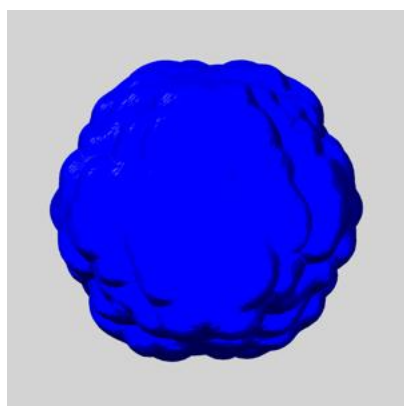
6.6 Mask visualisation [i](#)

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

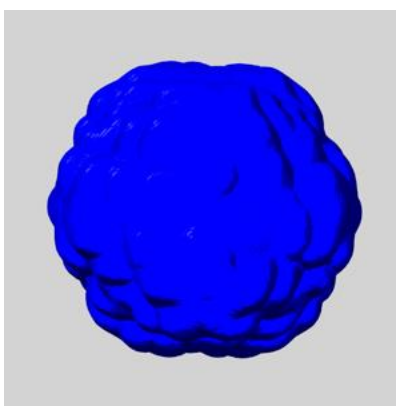
A mask typically either:

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

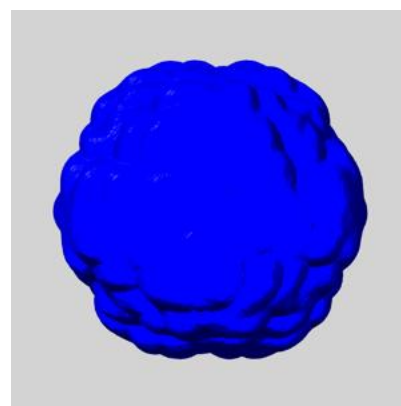
6.6.1 emd_55116_msk_1.map [i](#)



X



Y

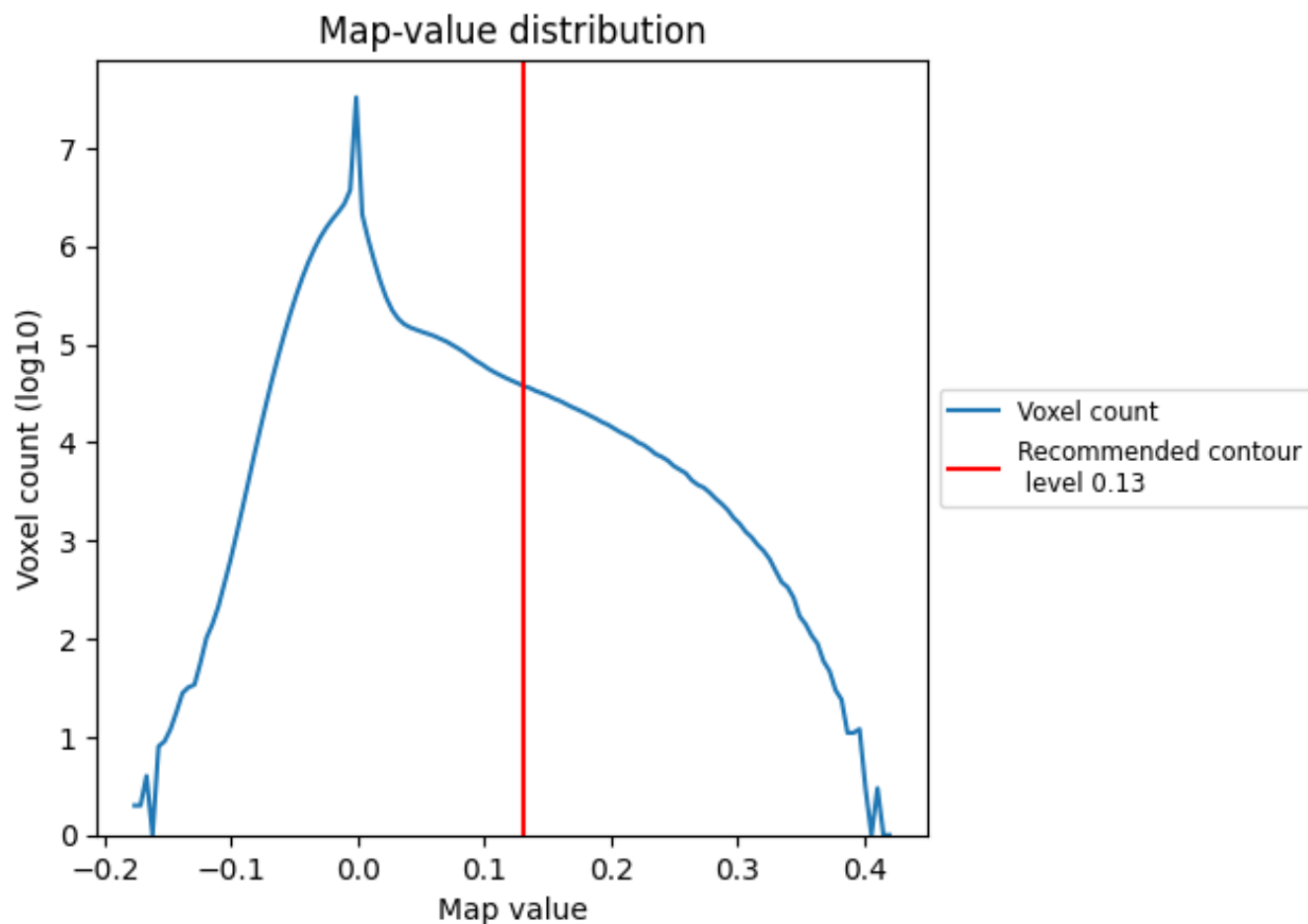


Z

7 Map analysis [i](#)

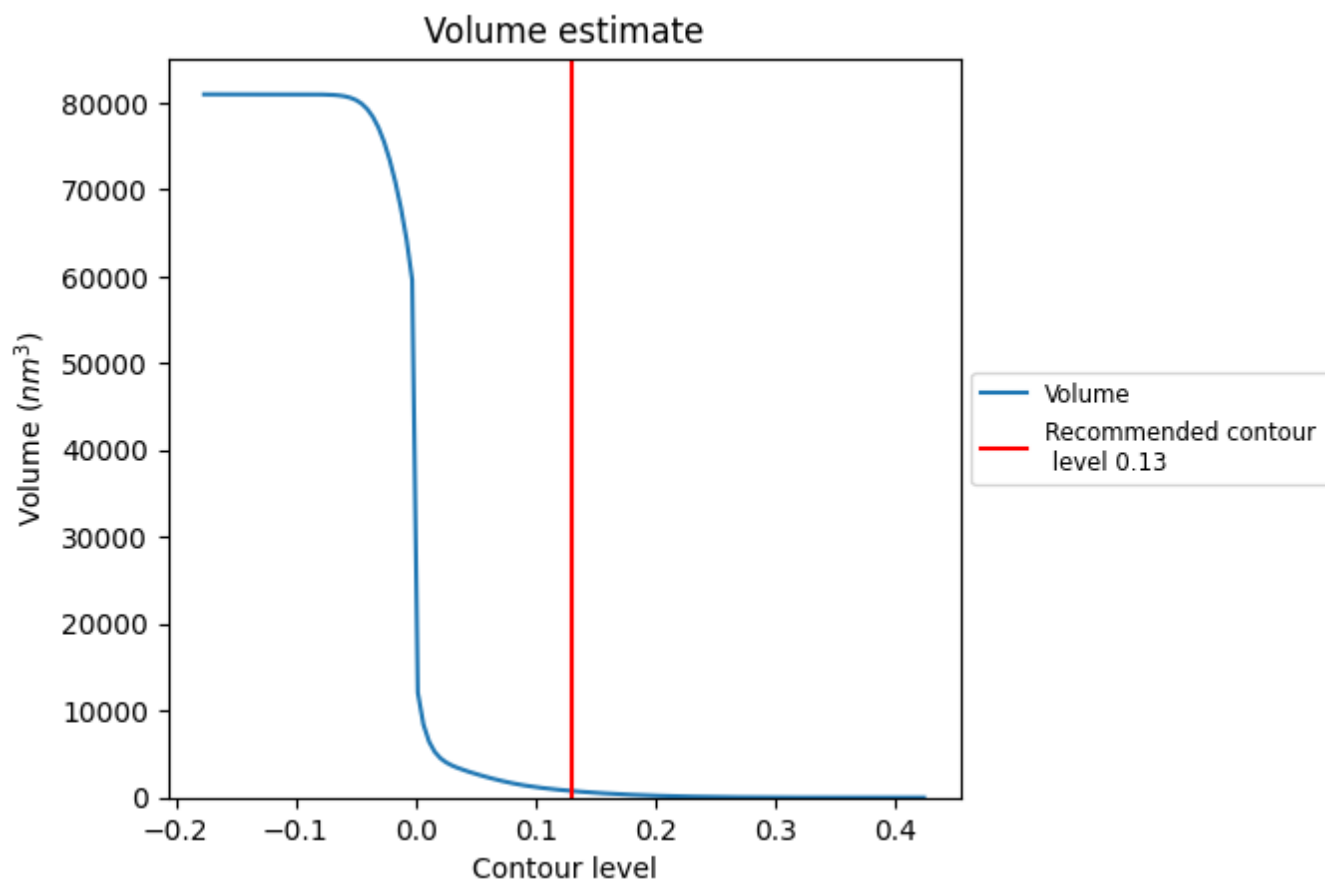
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

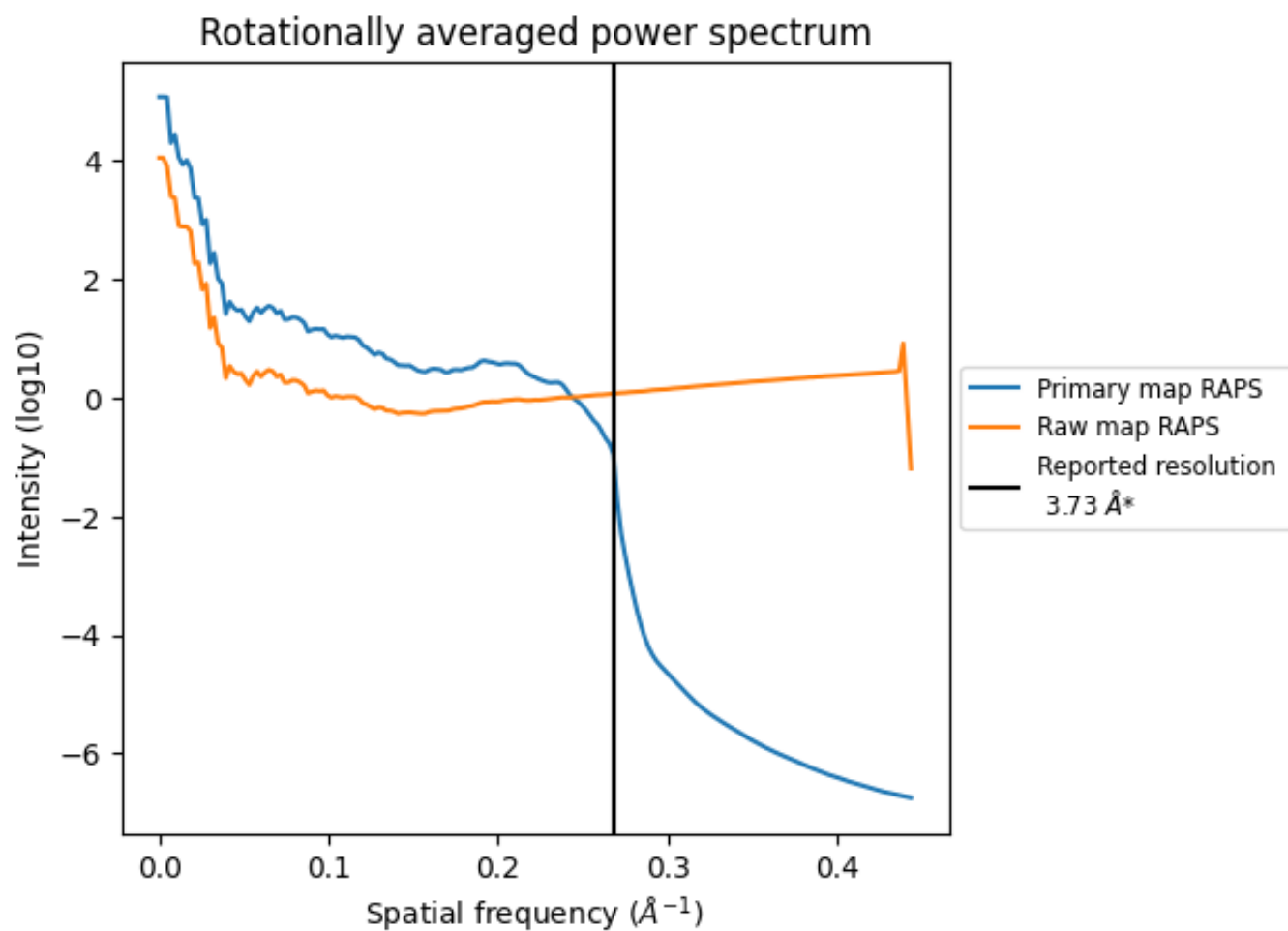
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 768 nm³; this corresponds to an approximate mass of 694 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

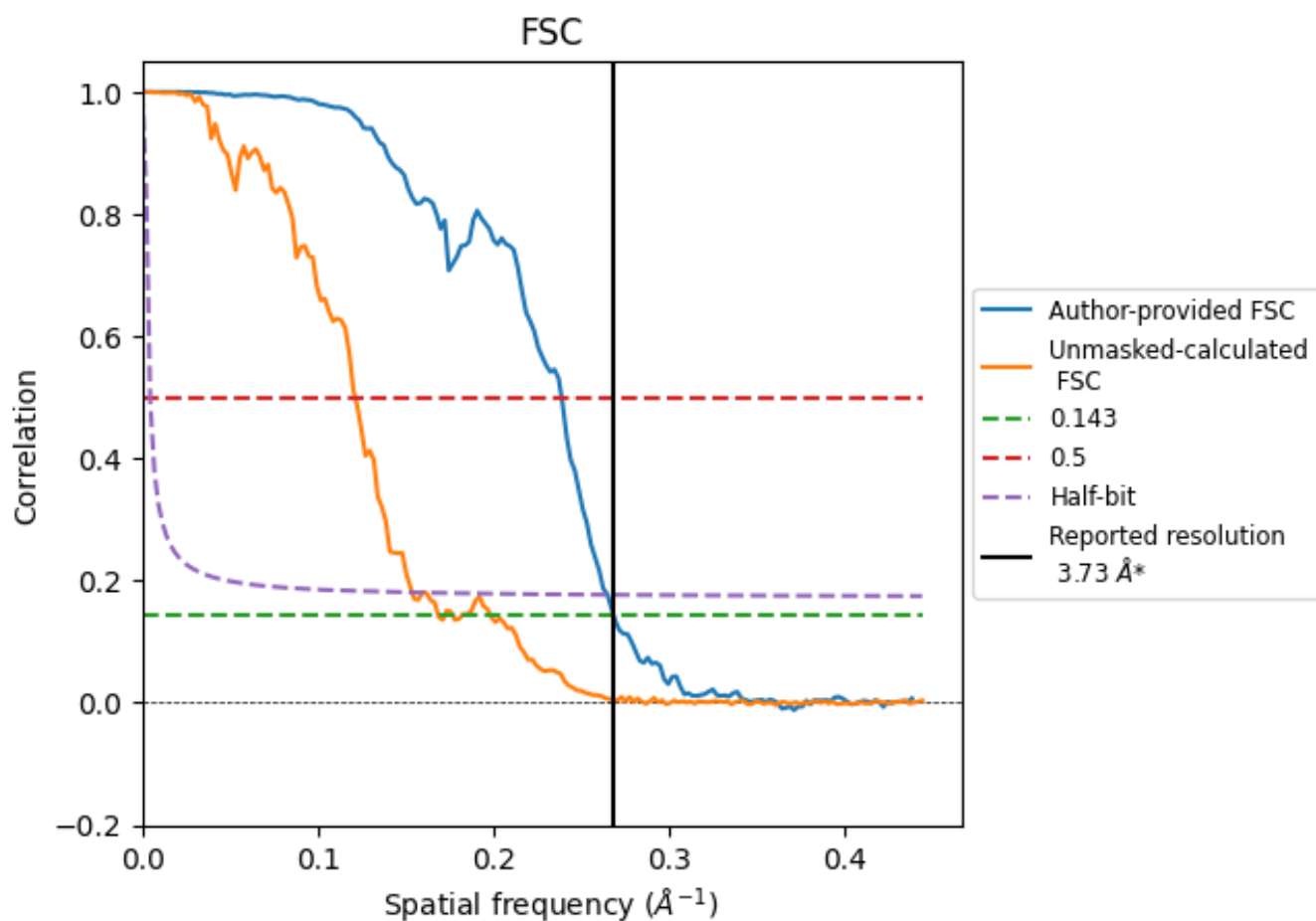


*Reported resolution corresponds to spatial frequency of 0.268 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.268 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

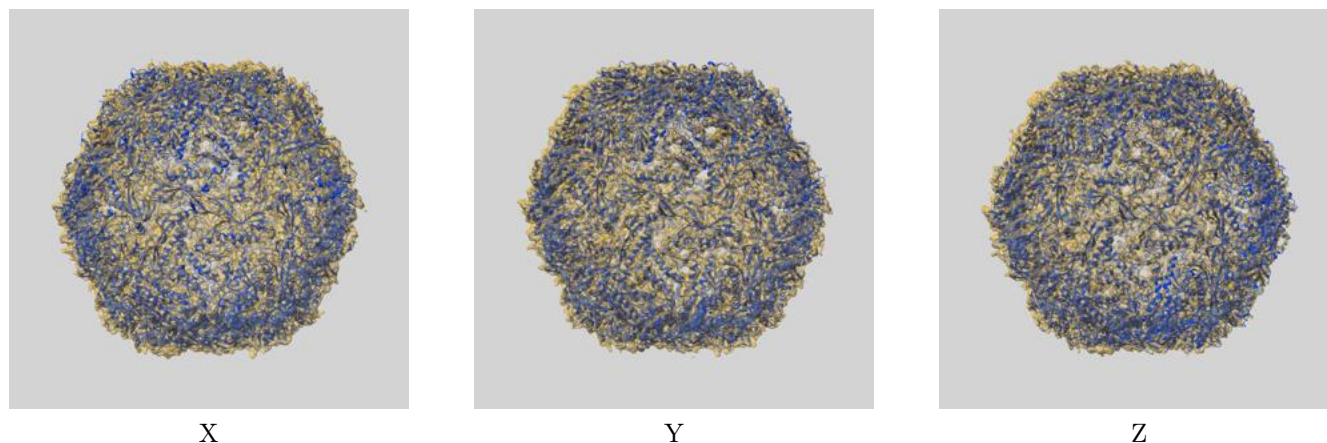
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.73	-	-
Author-provided FSC curve	3.73	4.19	3.78
Unmasked-calculated*	5.93	8.25	6.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.93 differs from the reported value 3.73 by more than 10 %

9 Map-model fit [i](#)

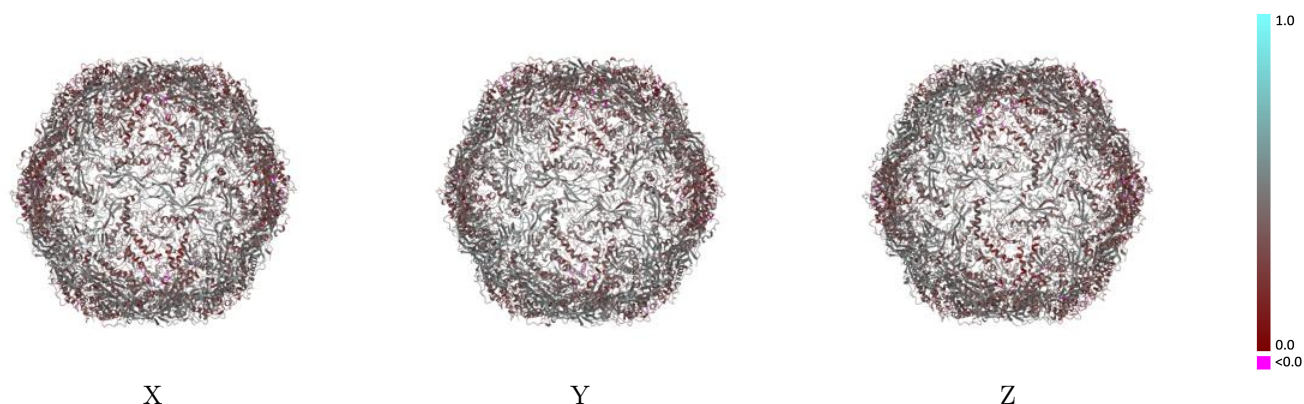
This section contains information regarding the fit between EMDB map EMD-55116 and PDB model 9SQR. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



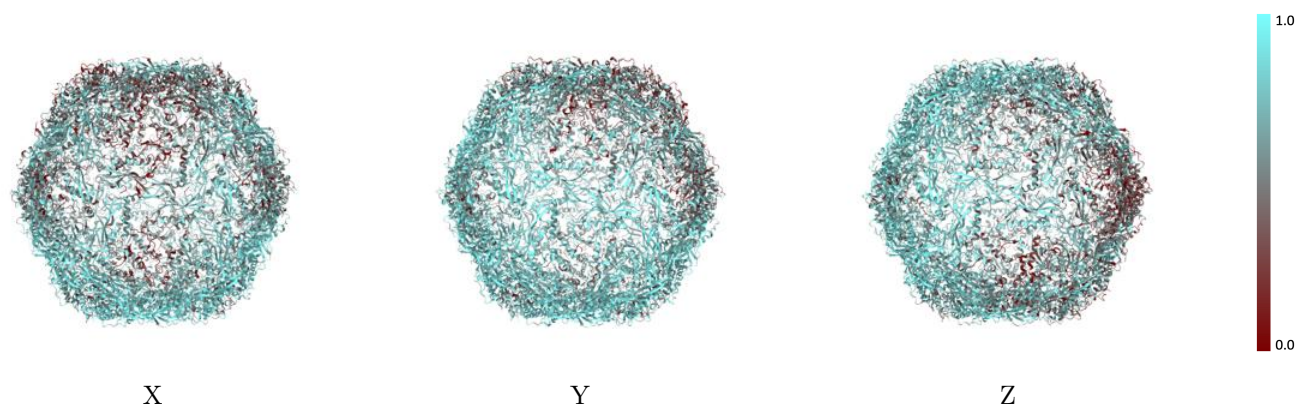
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



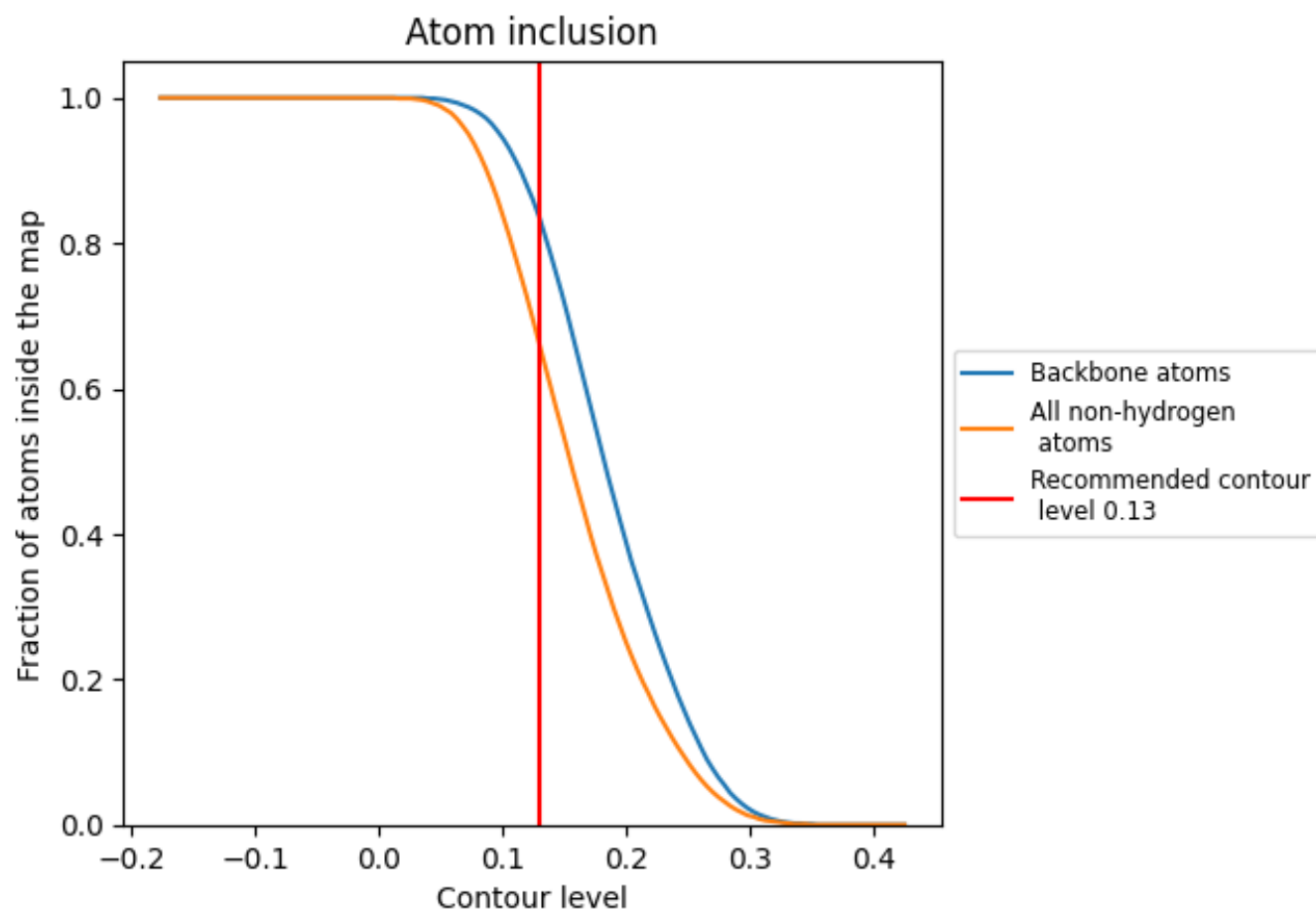
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6600	 0.3980
1	 0.5210	 0.4900
10	 0.1750	 0.4070
11	 0.5210	 0.4750
12	 0.5620	 0.4990
13	 0.3960	 0.4520
14	 0.3120	 0.4410
15	 0.4580	 0.4370
16	 0.5000	 0.4670
17	 0.4790	 0.4570
18	 0.5000	 0.4350
19	 0.2710	 0.4120
2	 0.3750	 0.4640
20	 0.5620	 0.4960
3	 0.4380	 0.4490
4	 0.1930	 0.3730
5	 0.4580	 0.4460
6	 0.3330	 0.4550
7	 0.3680	 0.4280
8	 0.2810	 0.4420
9	 0.5830	 0.4710
A	 0.7420	 0.4210
A0	 0.7610	 0.4270
AA	 0.7180	 0.3960
AB	 0.7250	 0.4250
B	 0.7360	 0.3940
BA	 0.6880	 0.3770
BB	 0.5670	 0.3620
C	 0.4910	 0.3760
CA	 0.6910	 0.3940
CB	 0.4850	 0.3690
D	 0.6320	 0.3890
DA	 0.6790	 0.3850
DB	 0.7420	 0.4070
E	 0.4930	 0.3750



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Chain	Atom inclusion	Q-score
EA	 0.7620	 0.4170
EB	 0.4340	 0.3730
F	 0.6320	 0.3770
FA	 0.7690	 0.4200
FB	 0.6050	 0.3940
G	 0.7340	 0.4220
GA	 0.7410	 0.4100
GB	 0.7560	 0.4150
H	 0.7490	 0.4220
HA	 0.7240	 0.4130
HB	 0.7370	 0.4280
I	 0.6980	 0.3980
IA	 0.7720	 0.4070
J	 0.6130	 0.3600
JA	 0.5750	 0.3820
K	 0.4660	 0.3580
KA	 0.7490	 0.4250
L	 0.6410	 0.3870
LA	 0.7540	 0.4290
M	 0.7360	 0.4160
MA	 0.7240	 0.4050
N	 0.7520	 0.4110
NA	 0.4840	 0.3780
O	 0.7320	 0.4260
OA	 0.4240	 0.3620
P	 0.7470	 0.4070
PA	 0.6850	 0.4020
Q	 0.5780	 0.3660
QA	 0.7570	 0.4270
R	 0.3730	 0.3700
RA	 0.7660	 0.4220
S	 0.6860	 0.3980
SA	 0.5120	 0.3660
T	 0.7560	 0.4080
TA	 0.7630	 0.4280
UA	 0.7430	 0.4130
V	 0.5720	 0.3530
VA	 0.5300	 0.3730
W	 0.4100	 0.3730
WA	 0.6170	 0.3840
X	 0.6880	 0.3990
XA	 0.7220	 0.4140

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Chain	Atom inclusion	Q-score
Y	 0.7540	 0.4220
YA	 0.7030	 0.3970
Z	 0.6960	 0.3850
ZA	 0.7640	 0.4190