



Full wwPDB EM Validation Report ⓘ

Mar 3, 2024 – 04:05 PM EST

PDB ID : 5W7G
EMDB ID : EMD-8780
Title : An envelope of a filamentous hyperthermophilic virus carries lipids in a horse-shoe conformation
Authors : Kasson, P.; DiMaio, F.; Yu, X.; Lucas-Staat, S.; Krupovic, M.; Schouten, S.; Prangishvili, D.; Egelman, E.
Deposited on : 2017-06-19
Resolution : 4.50 Å(reported)

This is a Full wwPDB EM Validation 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:

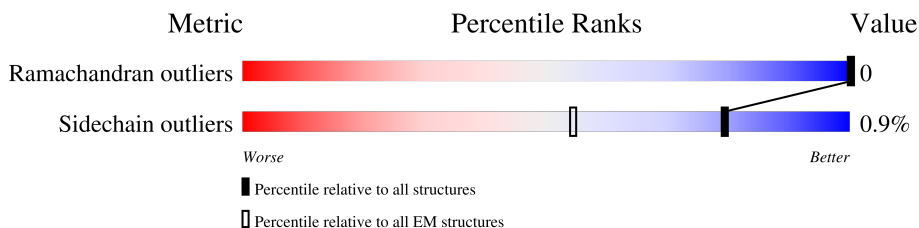
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 4.50 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 $\leq 5\%$. 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	140	69% 92% • 6%
1	C	140	66% 92% • 6%
1	E	140	67% 92% • 6%
1	G	140	64% 92% • 6%
1	I	140	69% 92% • 6%
1	K	140	66% 92% • 6%
1	M	140	69% 92% • 6%
1	O	140	65% 92% • 6%
1	Q	140	67% 92% • 6%

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Mol	Chain	Length	Quality of chain
1	S	140	67% 92% • 6%
1	U	140	66% 92% • 6%
1	W	140	67% 92% • 6%
1	Y	140	66% 92% • 6%
1	a	140	67% 92% • 6%
1	c	140	66% 92% • 6%
1	e	140	69% 92% • 6%
1	g	140	67% 92% • 6%
1	i	140	69% 92% • 6%
1	k	140	69% 92% • 6%
1	m	140	68% 92% • 6%
1	o	140	70% 92% • 6%
2	B	132	72% 95% • 5%
2	D	132	69% 95% • 5%
2	F	132	71% 95% • 5%
2	H	132	73% 95% • 5%
2	J	132	72% 95% • 5%
2	L	132	72% 95% • 5%
2	N	132	67% 95% • 5%
2	P	132	71% 95% • 5%
2	R	132	70% 95% • 5%
2	T	132	69% 95% • 5%
2	V	132	73% 95% • 5%
2	X	132	70% 95% • 5%
2	Z	132	70% 95% • 5%

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Mol	Chain	Length	Quality of chain
2	b	132	<p>71% 95% • 5%</p>
2	d	132	<p>70% 95% • 5%</p>
2	f	132	<p>70% 95% • 5%</p>
2	h	132	<p>72% 95% • 5%</p>
2	j	132	<p>69% 95% • 5%</p>
2	l	132	<p>70% 95% • 5%</p>
2	n	132	<p>73% 95% • 5%</p>
2	p	132	<p>72% 95% • 5%</p>
3	q	252	<p>5% 97% •</p>
3	r	252	<p>6% 92% 8%</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 53508 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 ORF140.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	131	1054	666	174	210	4	0	0
1	C	131	1054	666	174	210	4	0	0
1	E	131	1054	666	174	210	4	0	0
1	G	131	1054	666	174	210	4	0	0
1	I	131	1054	666	174	210	4	0	0
1	K	131	1054	666	174	210	4	0	0
1	M	131	1054	666	174	210	4	0	0
1	O	131	1054	666	174	210	4	0	0
1	Q	131	1054	666	174	210	4	0	0
1	S	131	1054	666	174	210	4	0	0
1	U	131	1054	666	174	210	4	0	0
1	W	131	1054	666	174	210	4	0	0
1	Y	131	1054	666	174	210	4	0	0
1	a	131	1054	666	174	210	4	0	0
1	c	131	1054	666	174	210	4	0	0
1	e	131	1054	666	174	210	4	0	0
1	g	131	1054	666	174	210	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	i	131	Total	C	N	O	S	0	0
			1054	666	174	210	4		
1	k	131	Total	C	N	O	S	0	0
			1054	666	174	210	4		
1	m	131	Total	C	N	O	S	0	0
			1054	666	174	210	4		
1	o	131	Total	C	N	O	S	0	0
			1054	666	174	210	4		

- Molecule 2 is a protein called ORF132.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	126	Total	C	N	O	S	0	0
			1002	638	168	191	5		
2	D	126	Total	C	N	O	S	0	0
			1002	638	168	191	5		
2	F	126	Total	C	N	O	S	0	0
			1002	638	168	191	5		
2	H	126	Total	C	N	O	S	0	0
			1002	638	168	191	5		
2	J	126	Total	C	N	O	S	0	0
			1002	638	168	191	5		
2	L	126	Total	C	N	O	S	0	0
			1002	638	168	191	5		
2	N	126	Total	C	N	O	S	0	0
			1002	638	168	191	5		
2	P	126	Total	C	N	O	S	0	0
			1002	638	168	191	5		
2	R	126	Total	C	N	O	S	0	0
			1002	638	168	191	5		
2	T	126	Total	C	N	O	S	0	0
			1002	638	168	191	5		
2	V	126	Total	C	N	O	S	0	0
			1002	638	168	191	5		
2	X	126	Total	C	N	O	S	0	0
			1002	638	168	191	5		
2	Z	126	Total	C	N	O	S	0	0
			1002	638	168	191	5		
2	b	126	Total	C	N	O	S	0	0
			1002	638	168	191	5		
2	d	126	Total	C	N	O	S	0	0
			1002	638	168	191	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	f	126	Total	C	N	O	S	0	0
			1002	638	168	191	5		
2	h	126	Total	C	N	O	S	0	0
			1002	638	168	191	5		
2	j	126	Total	C	N	O	S	0	0
			1002	638	168	191	5		
2	l	126	Total	C	N	O	S	0	0
			1002	638	168	191	5		
2	n	126	Total	C	N	O	S	0	0
			1002	638	168	191	5		
2	p	126	Total	C	N	O	S	0	0
			1002	638	168	191	5		

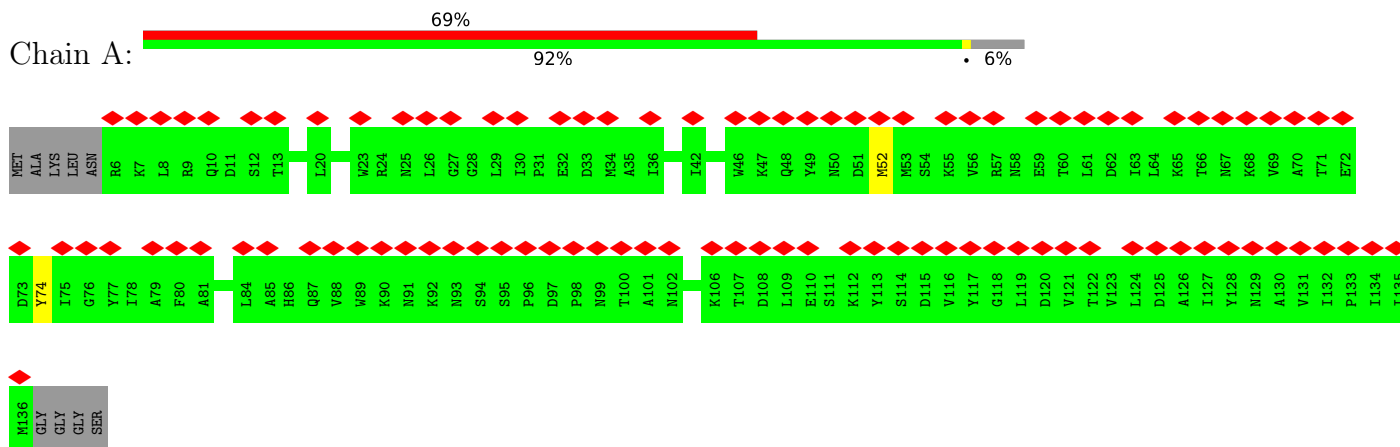
- Molecule 3 is a DNA chain called DNA (253-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	q	252	Total	C	N	O	P	0	0
			5166	2520	882	1512	252		
3	r	252	Total	C	N	O	P	0	0
			5166	2520	882	1512	252		

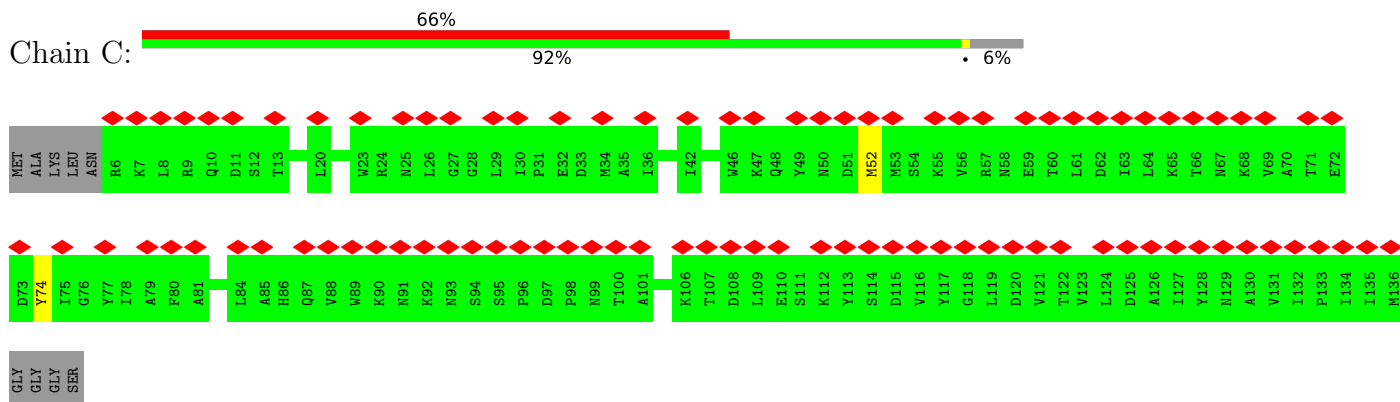
3 Residue-property plots [i](#)

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.

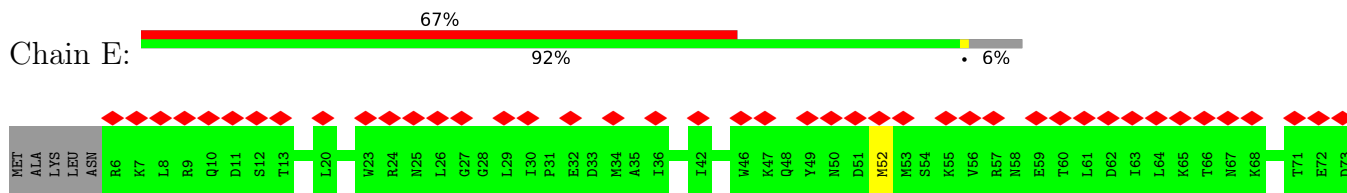
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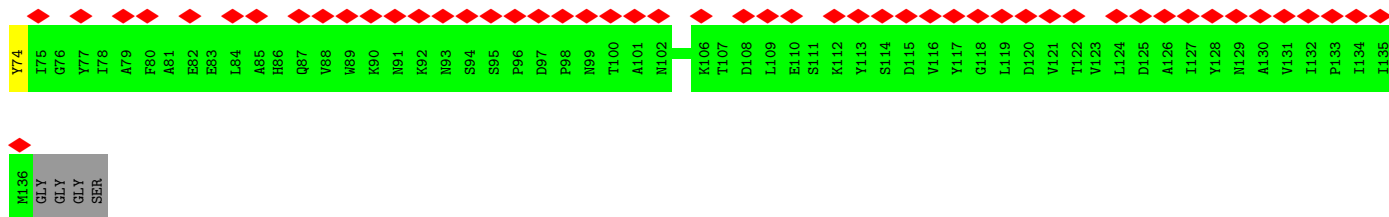


- Molecule 1: ORF140

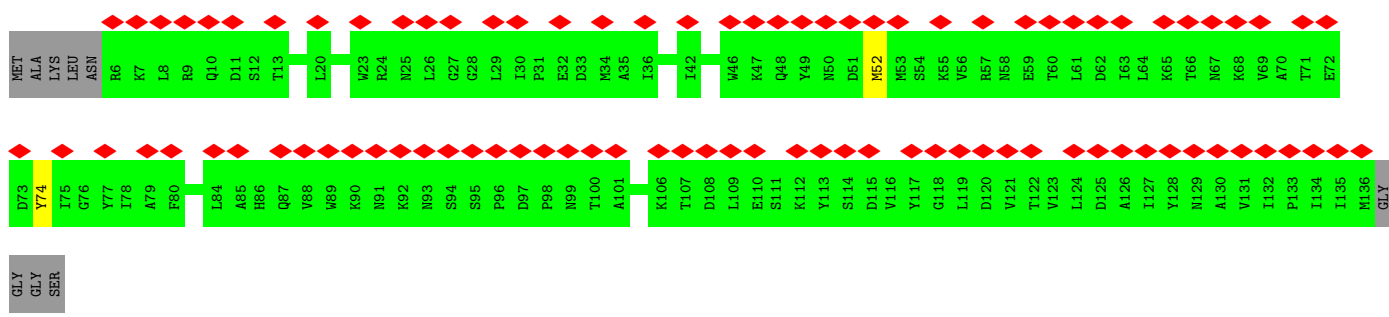
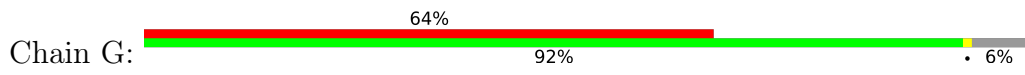


- Molecule 1: ORF140

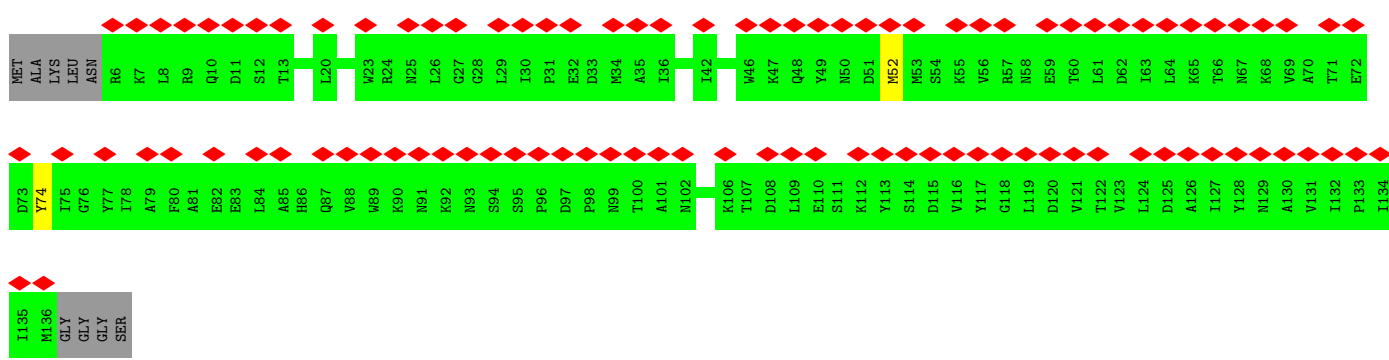
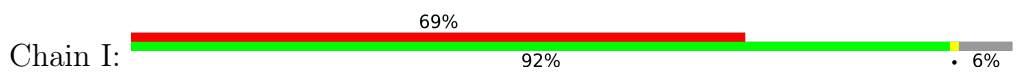




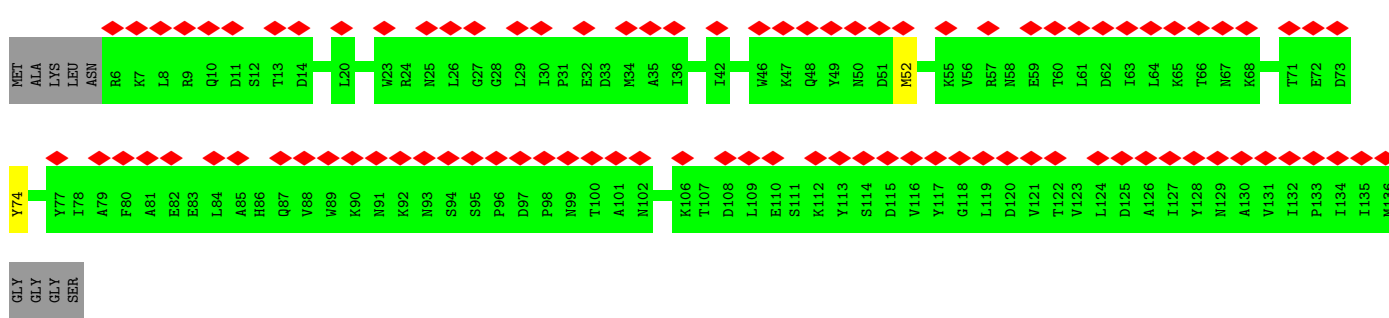
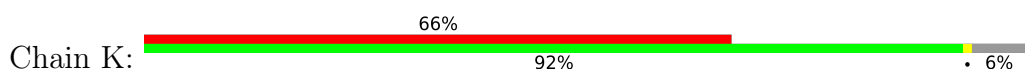
• Molecule 1: ORF140



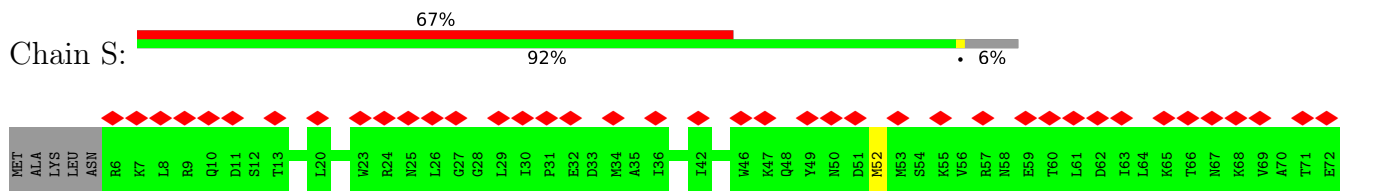
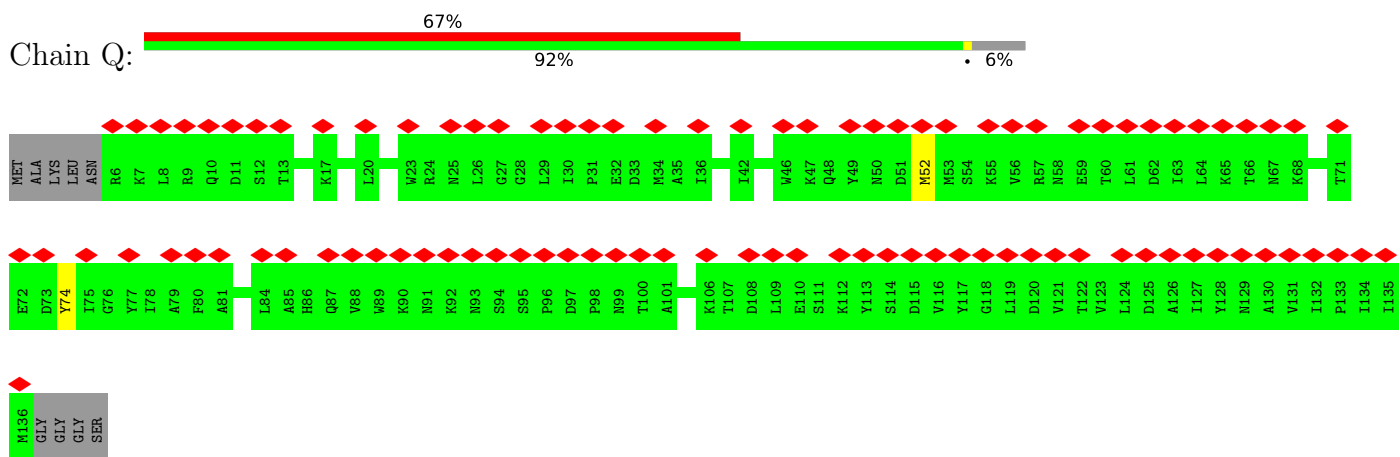
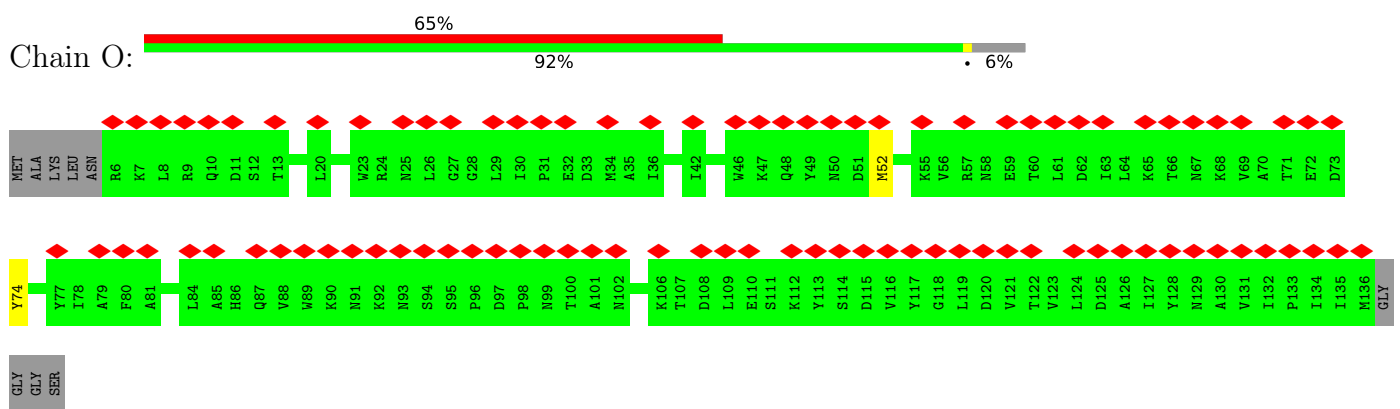
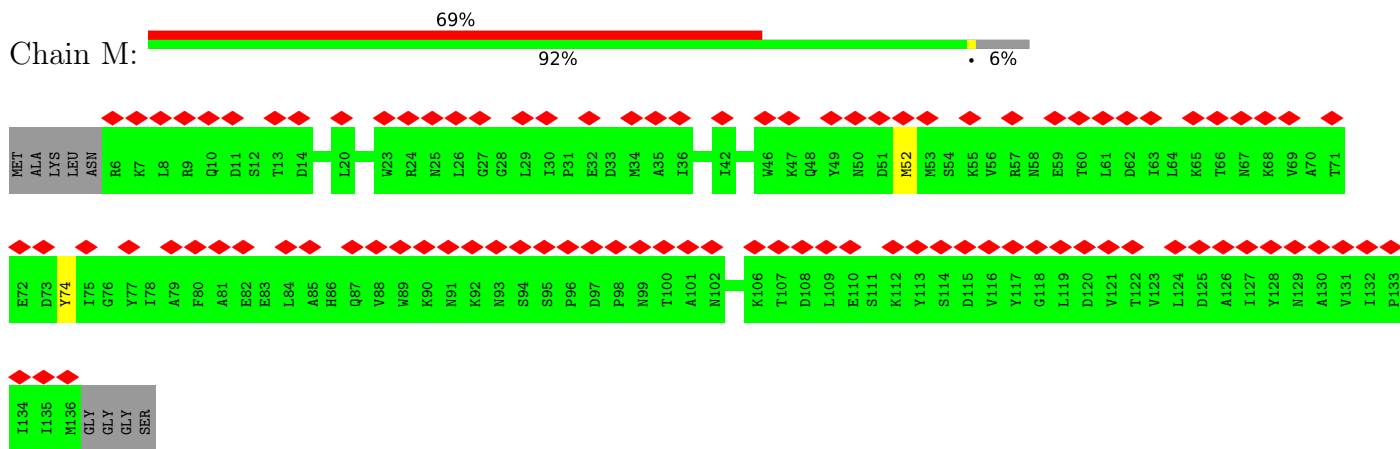
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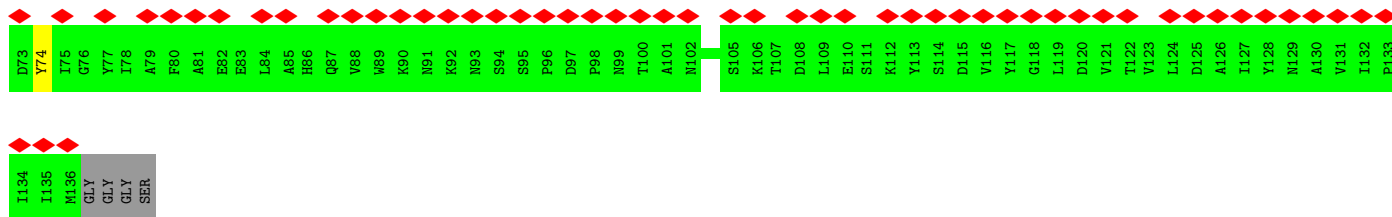


• Molecule 1: ORF140

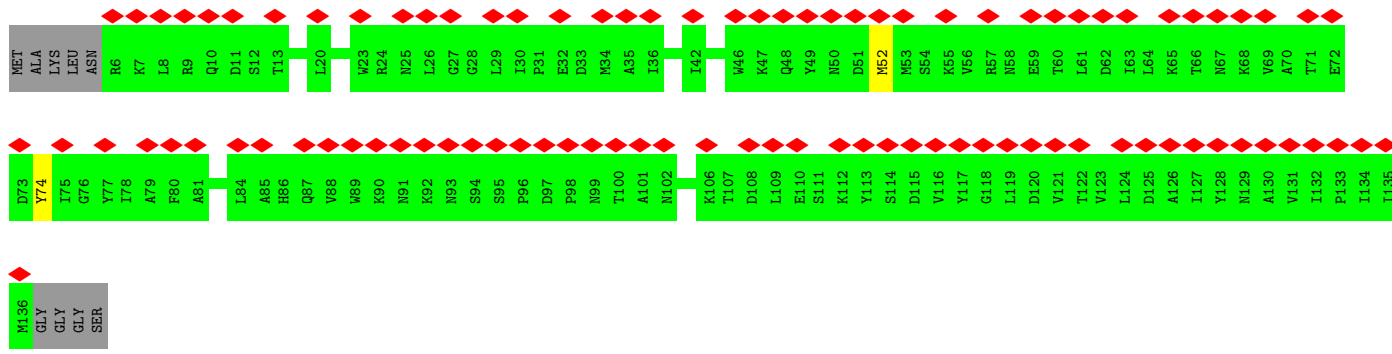


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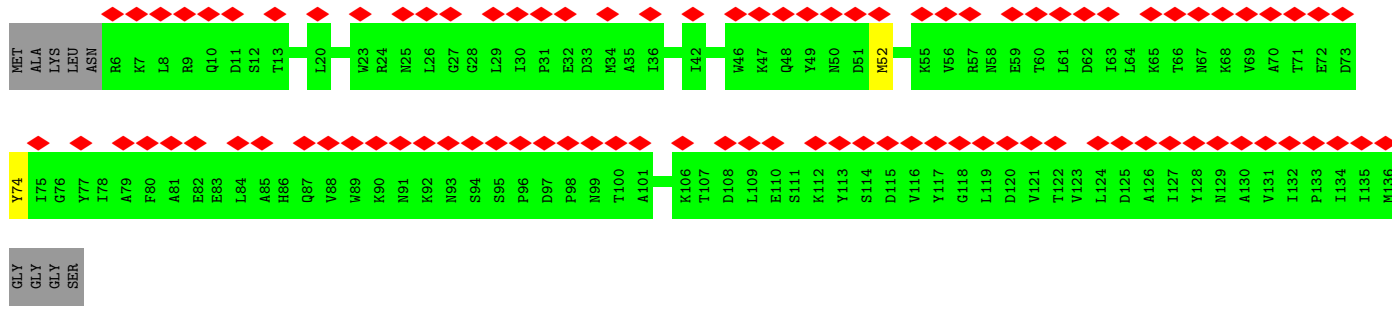
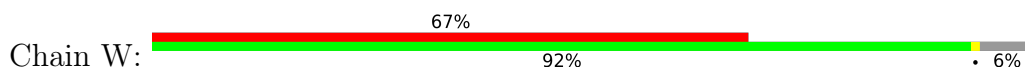




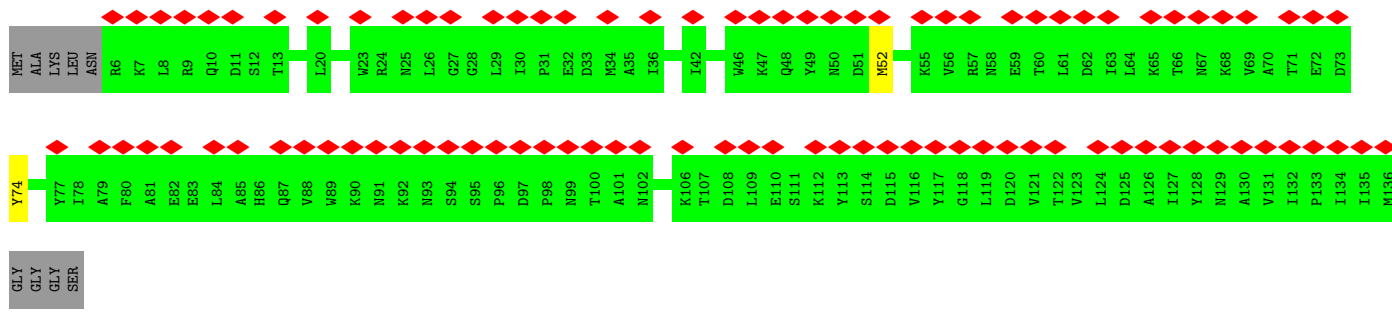
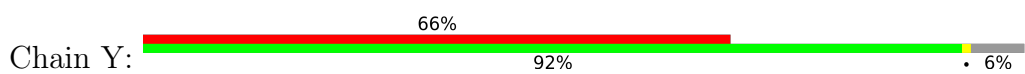
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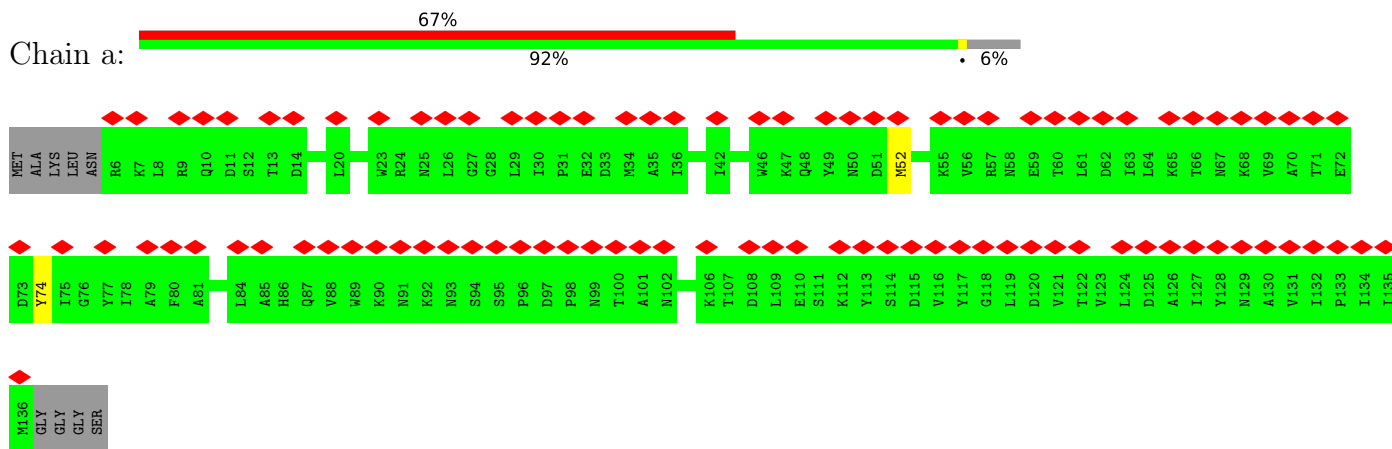
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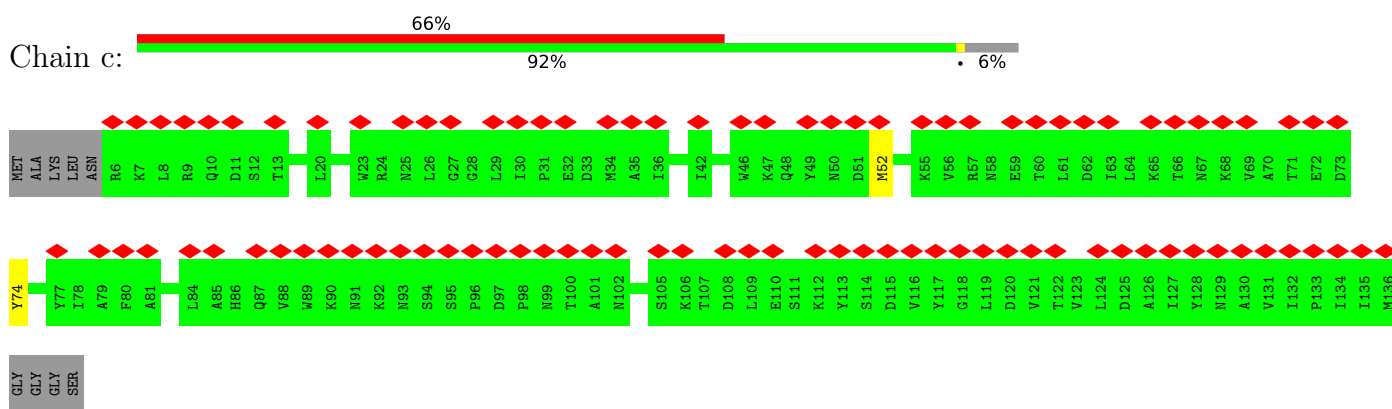
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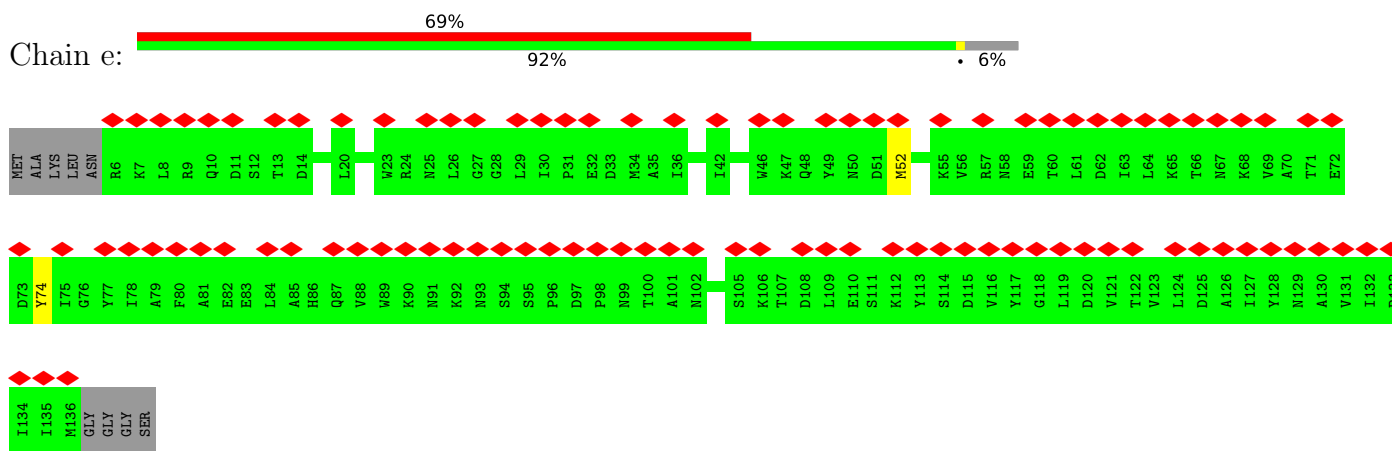
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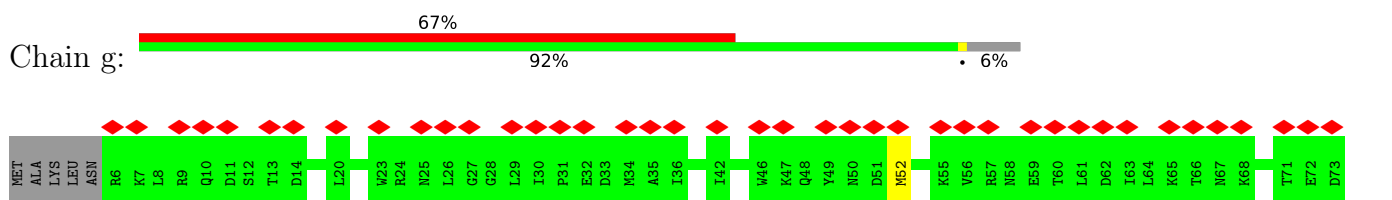
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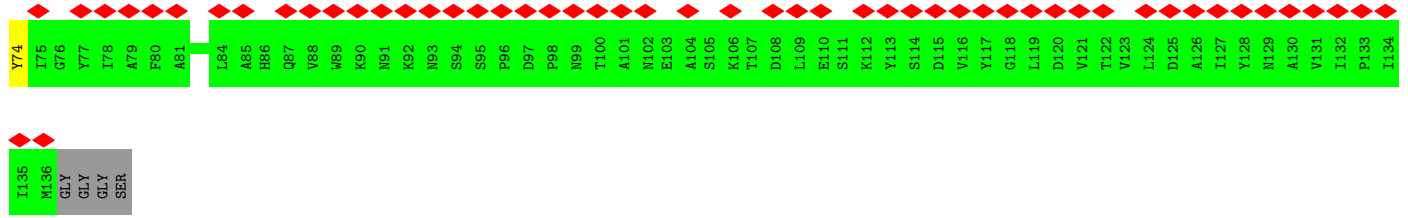


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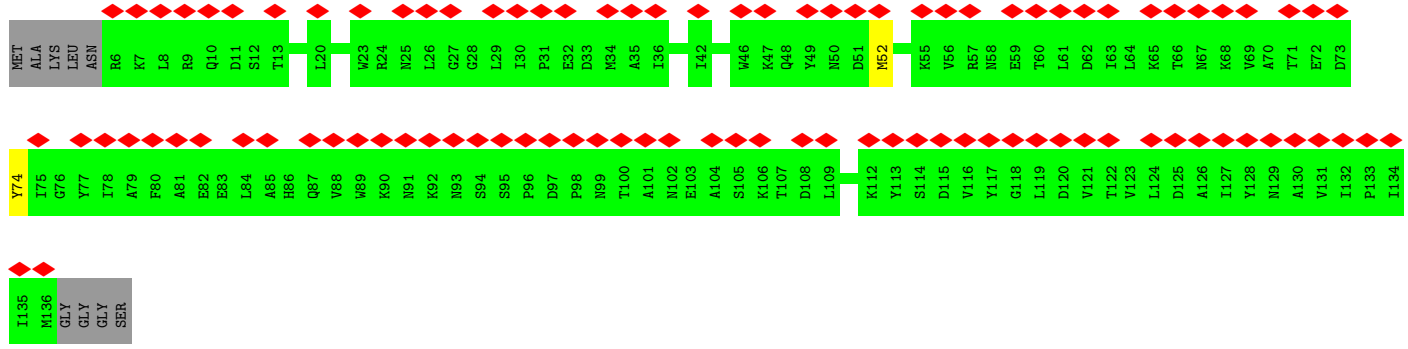


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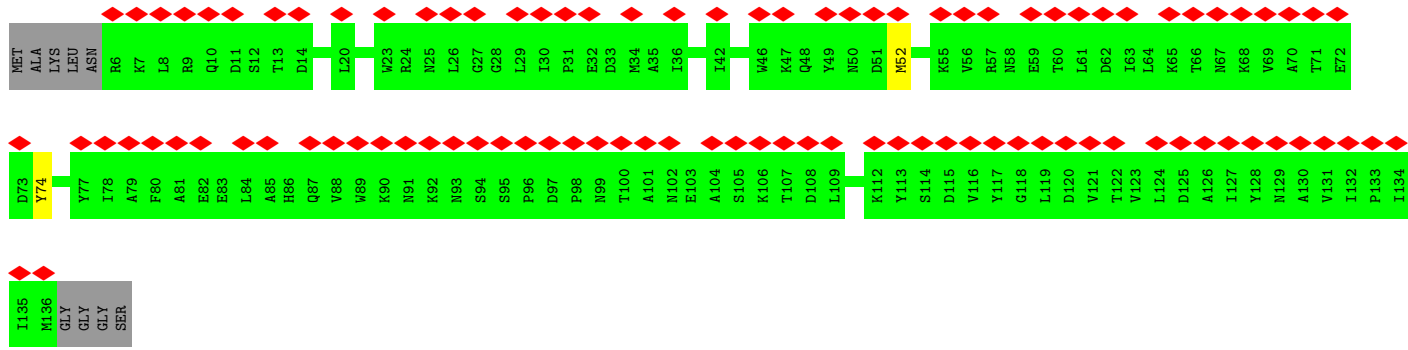
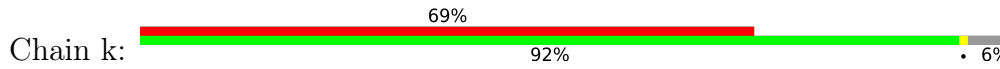




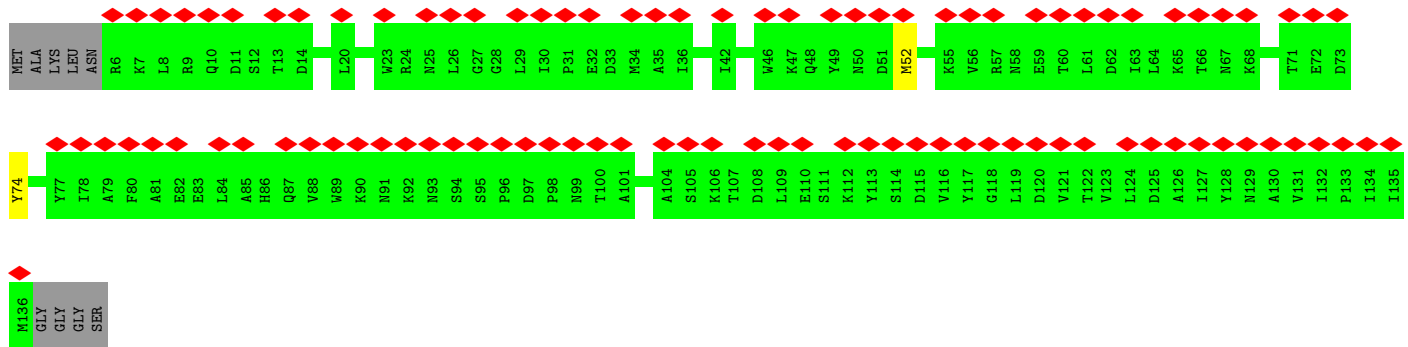
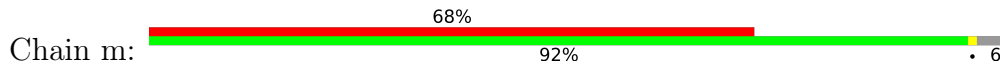
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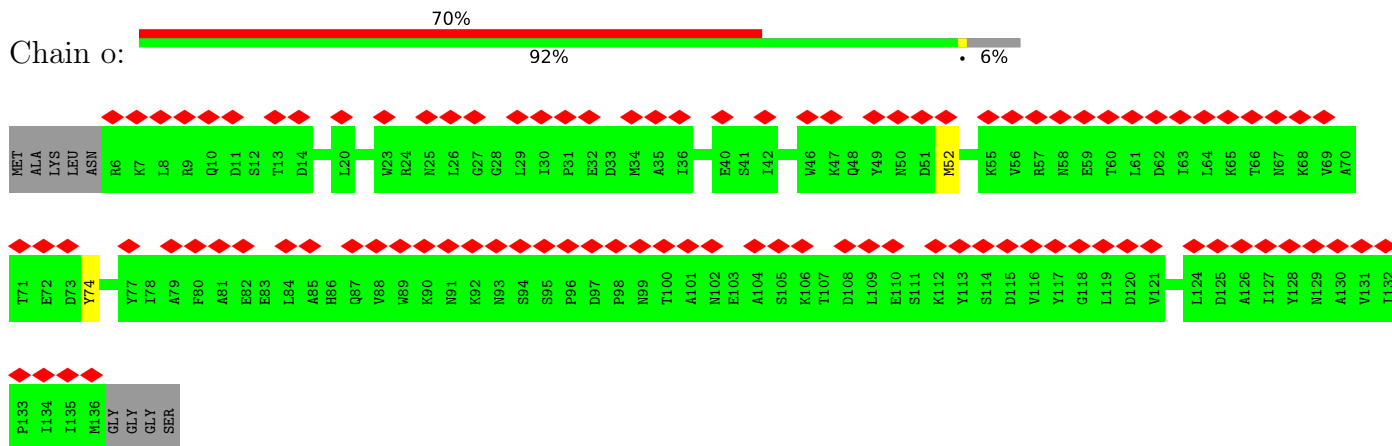
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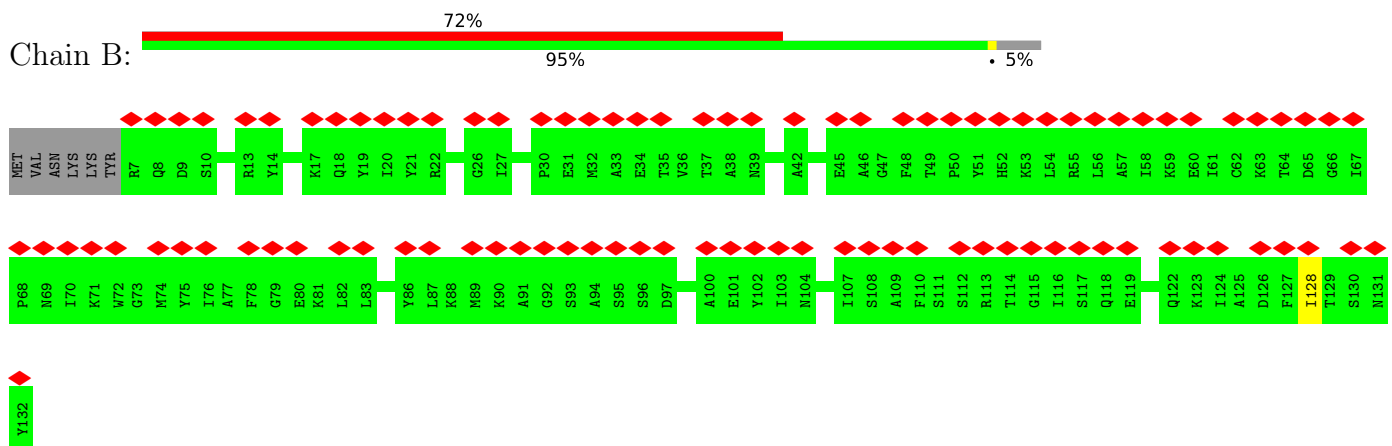
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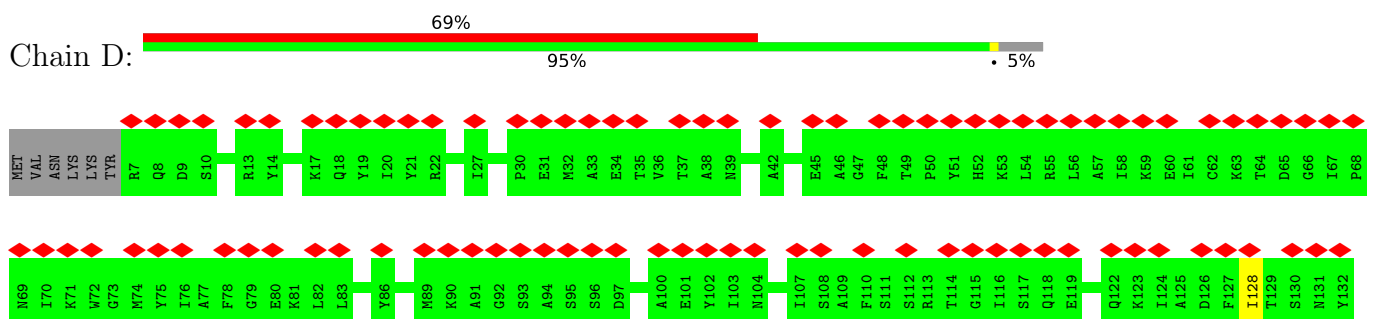
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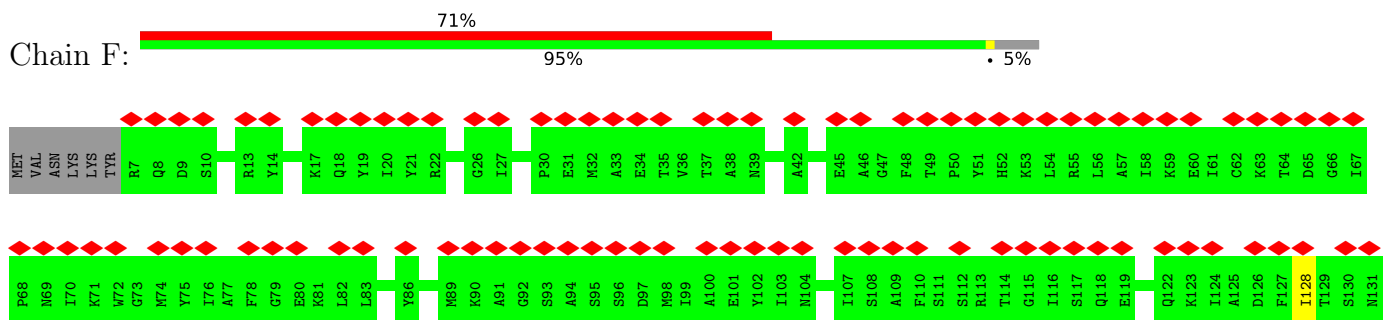
• Molecule 2: ORF132



• Molecule 2: ORF132

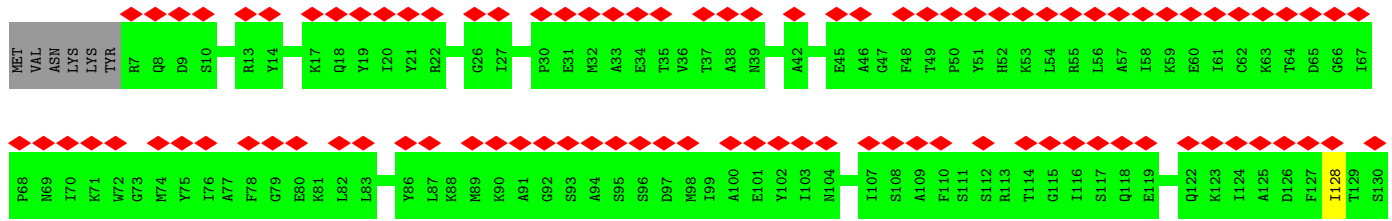
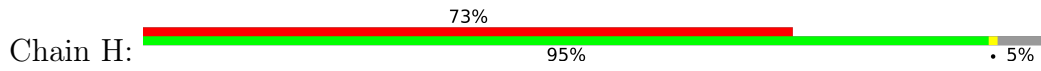


• Molecule 2: ORF132



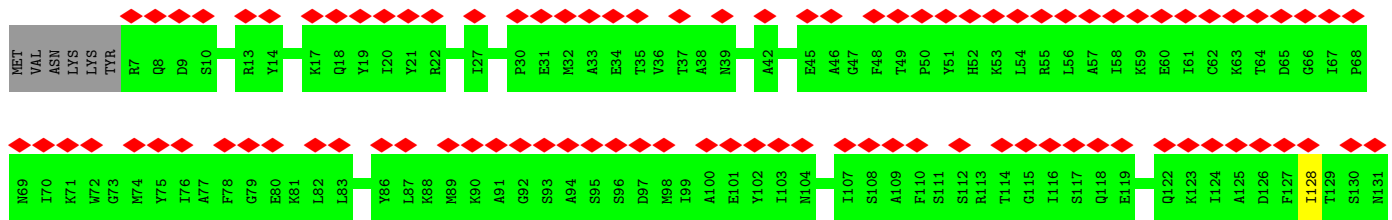
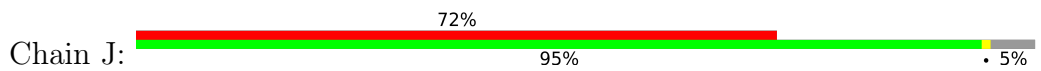
Y132

• Molecule 2: ORF132



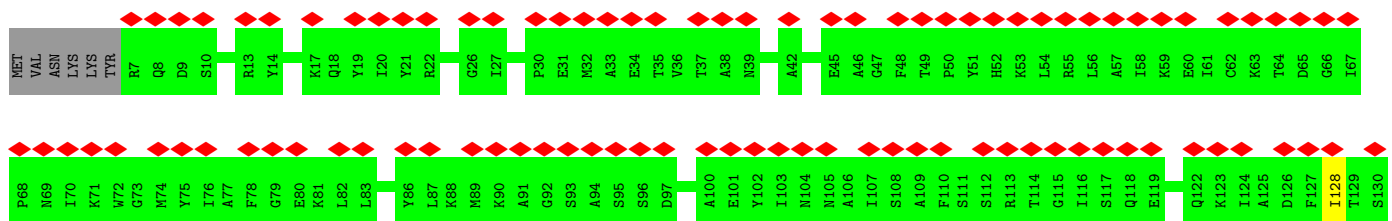
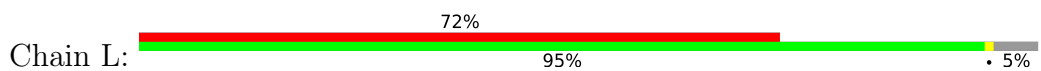
M131
Y132

• Molecule 2: ORF132



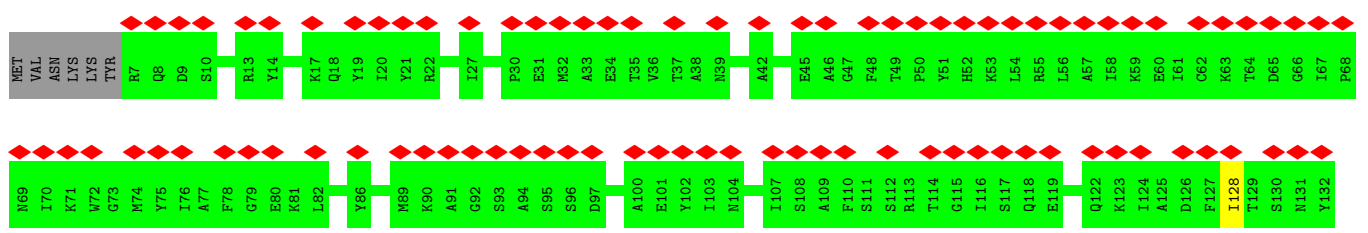
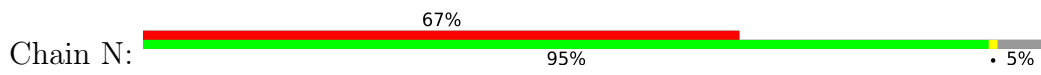
Y132

• Molecule 2: ORF132

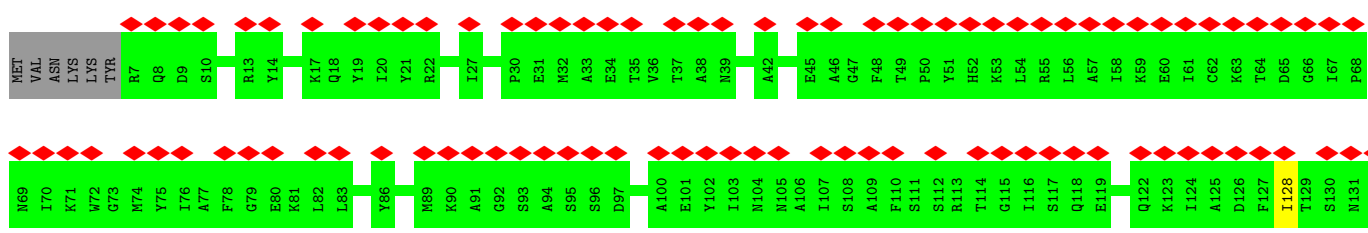
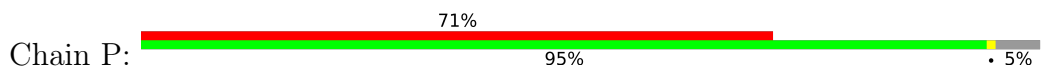


M131
Y132

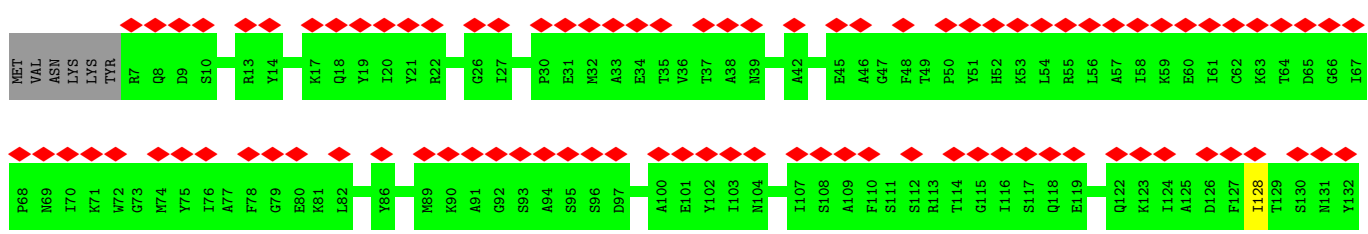
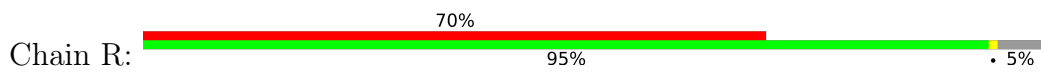
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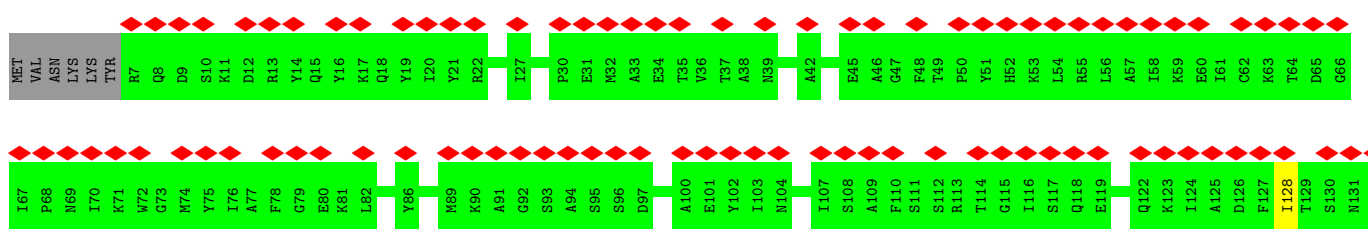
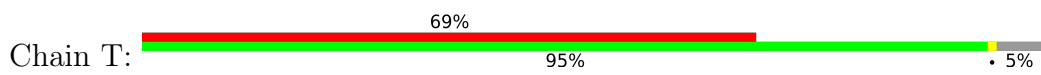
• Molecule 2: ORF132



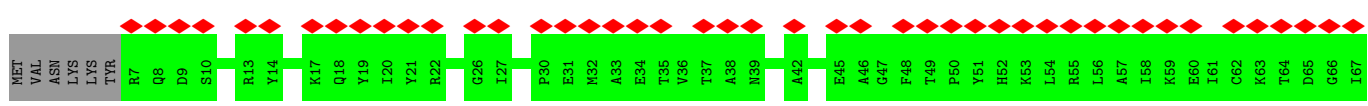
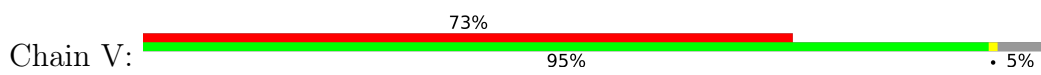
• Molecule 2: ORF132

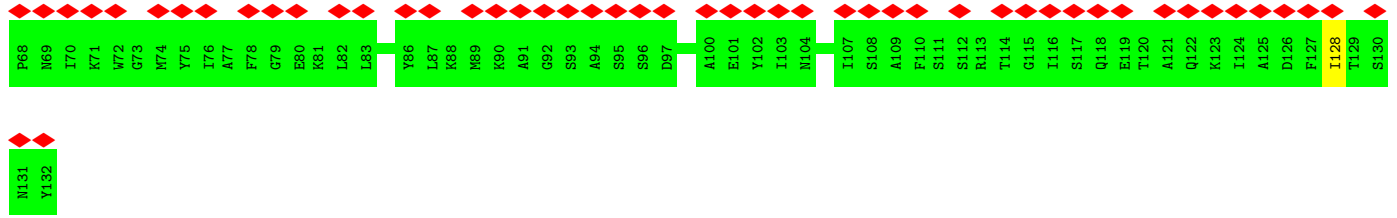


• Molecule 2: ORF132

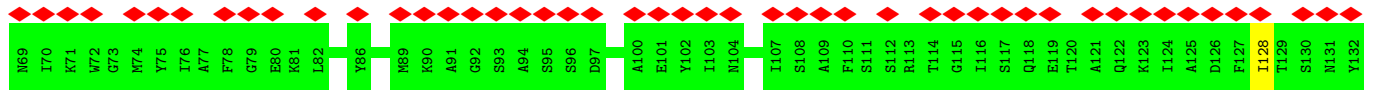
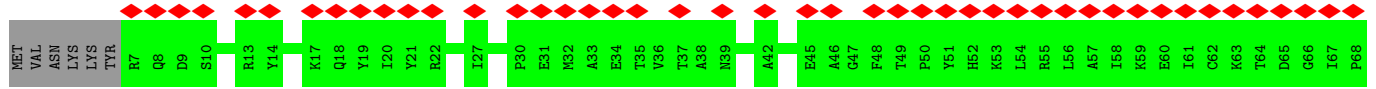


• Molecule 2: ORF132

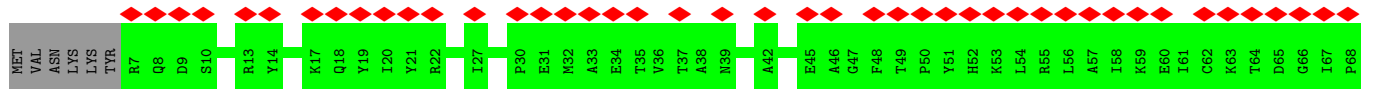
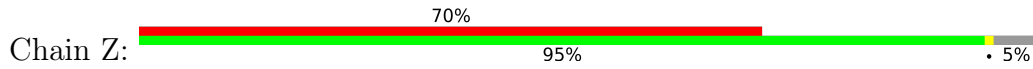




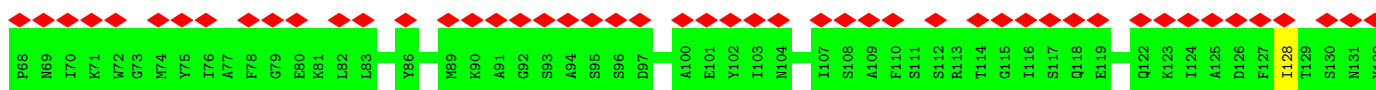
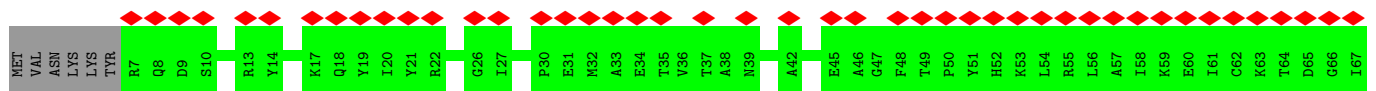
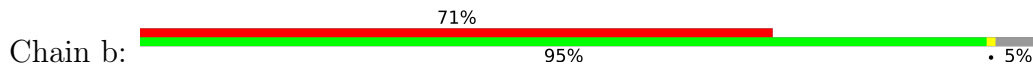
• Molecule 2: ORF132



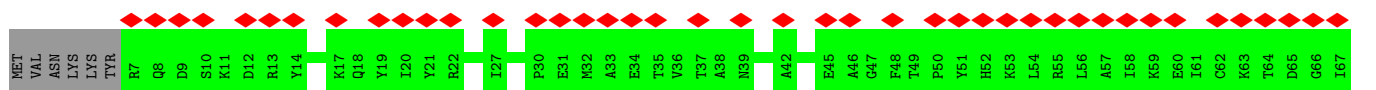
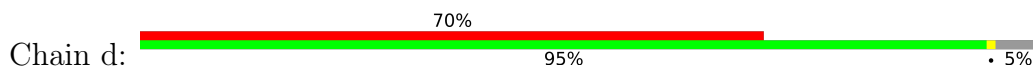
• Molecule 2: ORF132

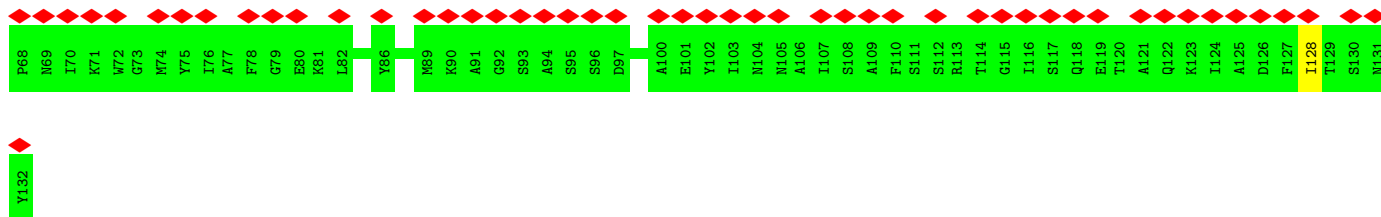


• Molecule 2: ORF132

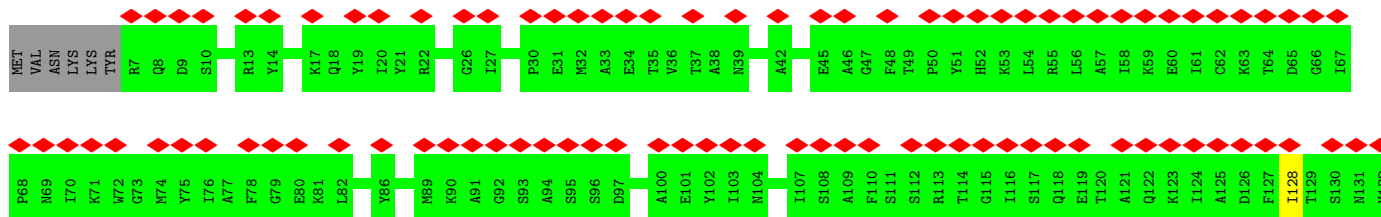
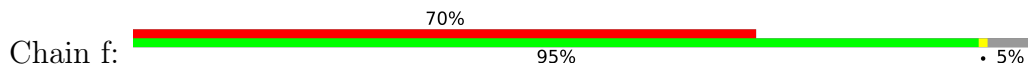


• Molecule 2: ORF132

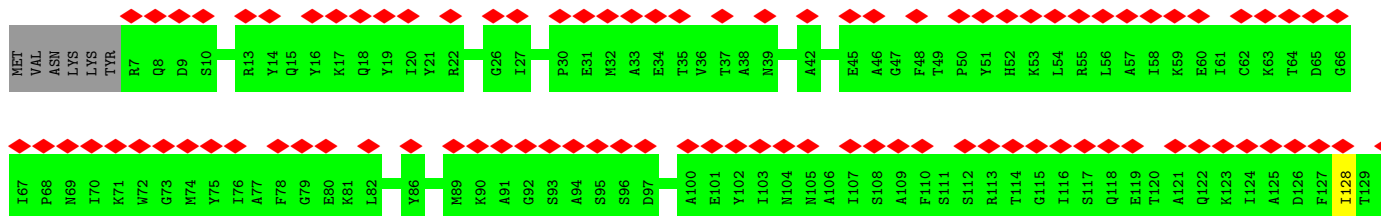




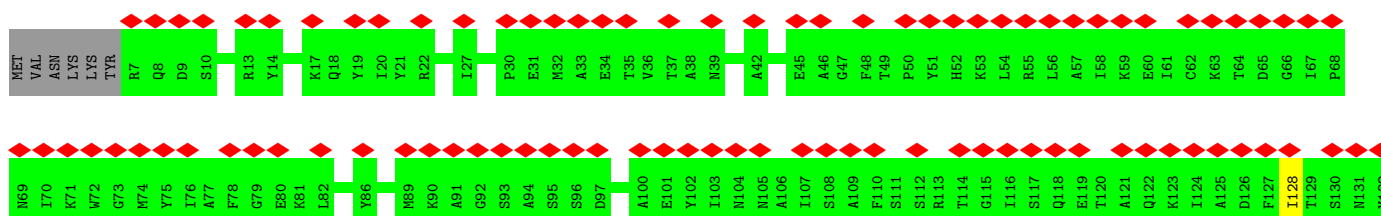
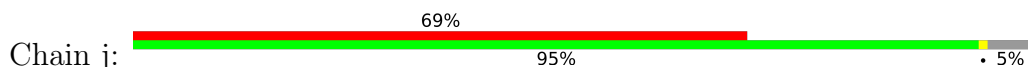
• Molecule 2: ORF132



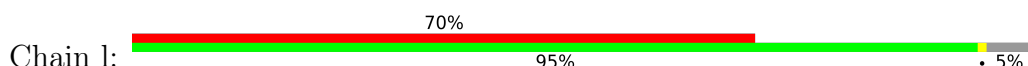
• Molecule 2: ORF132

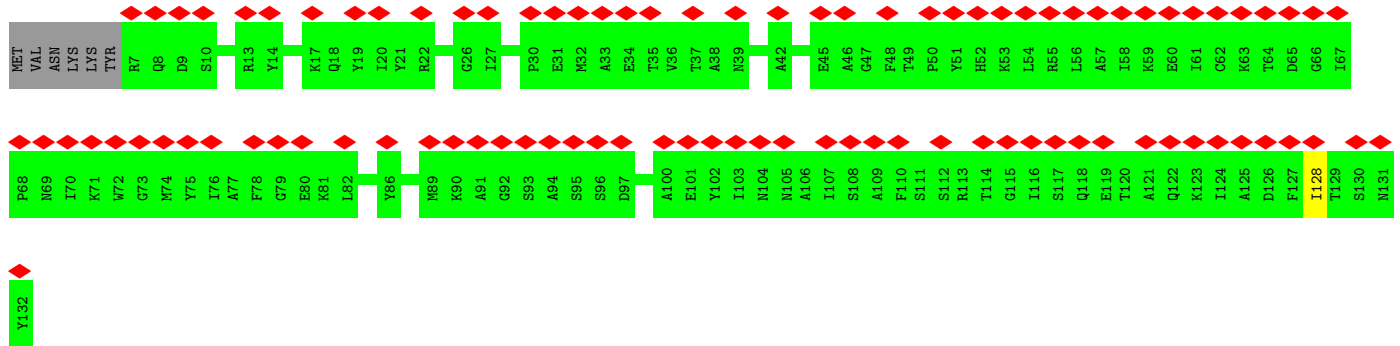


• Molecule 2: ORF132

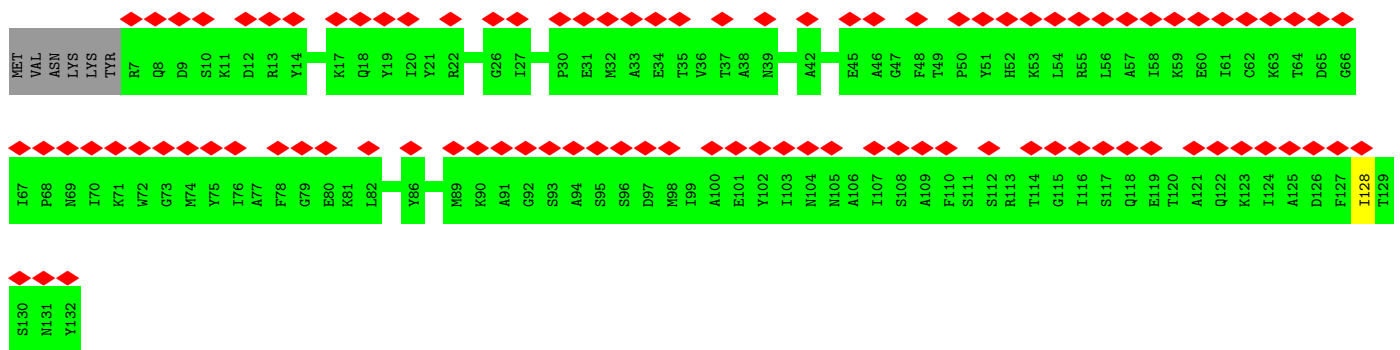
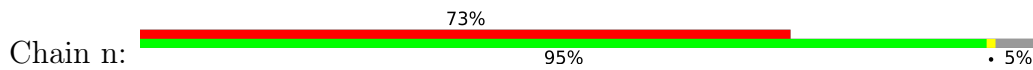


• Molecule 2: ORF132

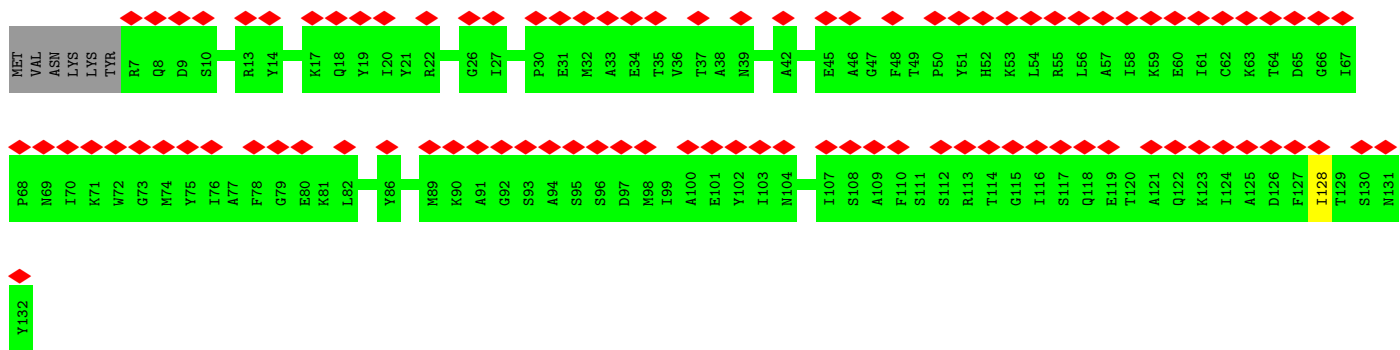
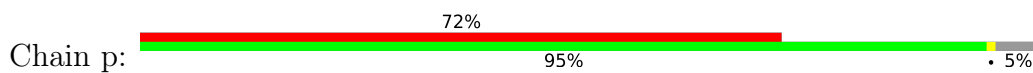




• Molecule 2: ORF132



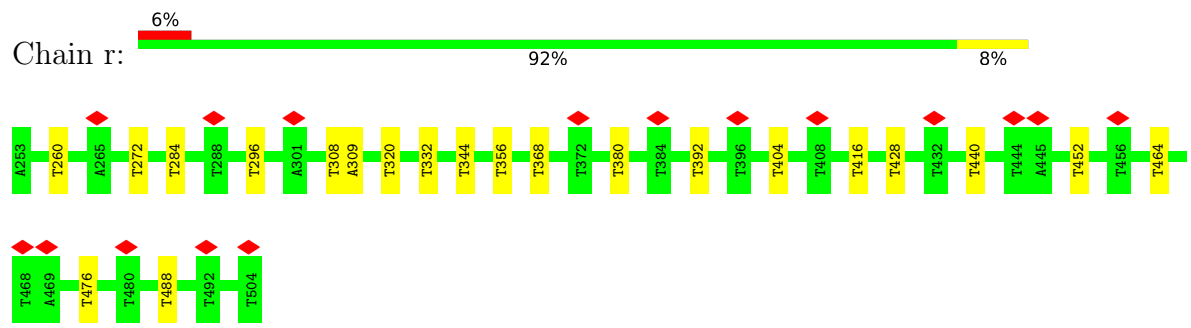
• Molecule 2: ORF132



• Molecule 3: DNA (253-MER)



• Molecule 3: DNA (253-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=38.7°, rise=4.6 Å, axial sym=C1	Depositor
Number of segments used	119495	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.957	Depositor
Minimum map value	-0.447	Depositor
Average map value	0.059	Depositor
Map value standard deviation	0.149	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	201.59999, 201.59999, 209.99998	wwPDB
Map dimensions	192, 192, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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	0.94	2/1073 (0.2%)	0.65	1/1456 (0.1%)
1	C	0.95	2/1073 (0.2%)	0.65	1/1456 (0.1%)
1	E	0.94	2/1073 (0.2%)	0.65	1/1456 (0.1%)
1	G	0.94	2/1073 (0.2%)	0.65	1/1456 (0.1%)
1	I	0.95	2/1073 (0.2%)	0.65	1/1456 (0.1%)
1	K	0.95	2/1073 (0.2%)	0.65	1/1456 (0.1%)
1	M	0.94	2/1073 (0.2%)	0.65	1/1456 (0.1%)
1	O	0.94	2/1073 (0.2%)	0.65	1/1456 (0.1%)
1	Q	0.94	2/1073 (0.2%)	0.65	1/1456 (0.1%)
1	S	0.94	2/1073 (0.2%)	0.65	1/1456 (0.1%)
1	U	0.94	2/1073 (0.2%)	0.65	1/1456 (0.1%)
1	W	0.95	2/1073 (0.2%)	0.65	1/1456 (0.1%)
1	Y	0.95	2/1073 (0.2%)	0.65	1/1456 (0.1%)
1	a	0.94	2/1073 (0.2%)	0.65	1/1456 (0.1%)
1	c	0.95	2/1073 (0.2%)	0.65	1/1456 (0.1%)
1	e	0.95	2/1073 (0.2%)	0.65	1/1456 (0.1%)
1	g	0.95	2/1073 (0.2%)	0.65	1/1456 (0.1%)
1	i	0.94	2/1073 (0.2%)	0.65	1/1456 (0.1%)
1	k	0.95	2/1073 (0.2%)	0.65	1/1456 (0.1%)
1	m	0.95	2/1073 (0.2%)	0.65	1/1456 (0.1%)
1	o	0.95	2/1073 (0.2%)	0.65	1/1456 (0.1%)
2	B	0.89	0/1023	0.60	0/1377
2	D	0.89	0/1023	0.60	0/1377
2	F	0.89	0/1023	0.60	0/1377
2	H	0.89	0/1023	0.60	0/1377
2	J	0.89	0/1023	0.60	0/1377
2	L	0.89	0/1023	0.60	0/1377
2	N	0.88	0/1023	0.60	0/1377
2	P	0.88	0/1023	0.60	0/1377
2	R	0.89	0/1023	0.60	0/1377
2	T	0.89	0/1023	0.60	0/1377
2	V	0.89	0/1023	0.60	0/1377
2	X	0.89	0/1023	0.60	0/1377
2	Z	0.89	0/1023	0.60	0/1377

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	b	0.88	0/1023	0.60	0/1377
2	d	0.89	0/1023	0.60	0/1377
2	f	0.89	0/1023	0.60	0/1377
2	h	0.89	0/1023	0.60	0/1377
2	j	0.88	0/1023	0.60	0/1377
2	l	0.89	0/1023	0.60	0/1377
2	n	0.89	0/1023	0.60	0/1377
2	p	0.89	0/1023	0.60	0/1377
3	q	0.55	0/5795	0.95	8/8942 (0.1%)
3	r	0.54	0/5795	0.93	21/8942 (0.2%)
All	All	0.85	42/55606 (0.1%)	0.71	50/77377 (0.1%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	c	74	TYR	CG-CD1	-6.05	1.31	1.39
1	Y	74	TYR	CG-CD1	-6.01	1.31	1.39
1	C	74	TYR	CG-CD1	-6.00	1.31	1.39
1	e	74	TYR	CG-CD1	-6.00	1.31	1.39
1	O	74	TYR	CG-CD1	-5.99	1.31	1.39
1	S	74	TYR	CG-CD1	-5.99	1.31	1.39
1	a	74	TYR	CG-CD1	-5.99	1.31	1.39
1	M	74	TYR	CG-CD1	-5.99	1.31	1.39
1	K	74	TYR	CG-CD1	-5.98	1.31	1.39
1	A	74	TYR	CG-CD1	-5.97	1.31	1.39
1	G	74	TYR	CG-CD1	-5.97	1.31	1.39
1	Q	74	TYR	CG-CD1	-5.97	1.31	1.39
1	U	74	TYR	CG-CD1	-5.97	1.31	1.39
1	o	74	TYR	CG-CD1	-5.97	1.31	1.39
1	I	74	TYR	CG-CD1	-5.97	1.31	1.39
1	E	74	TYR	CG-CD1	-5.96	1.31	1.39
1	m	74	TYR	CG-CD1	-5.96	1.31	1.39
1	k	74	TYR	CG-CD1	-5.95	1.31	1.39
1	i	74	TYR	CG-CD1	-5.93	1.31	1.39
1	W	74	TYR	CG-CD1	-5.92	1.31	1.39
1	g	74	TYR	CG-CD1	-5.91	1.31	1.39
1	I	74	TYR	CE1-CZ	-5.29	1.31	1.38
1	i	74	TYR	CE1-CZ	-5.29	1.31	1.38
1	W	74	TYR	CE1-CZ	-5.29	1.31	1.38
1	e	74	TYR	CE1-CZ	-5.28	1.31	1.38
1	g	74	TYR	CE1-CZ	-5.27	1.31	1.38
1	m	74	TYR	CE1-CZ	-5.27	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	74	TYR	CE1-CZ	-5.26	1.31	1.38
1	E	74	TYR	CE1-CZ	-5.26	1.31	1.38
1	a	74	TYR	CE1-CZ	-5.26	1.31	1.38
1	K	74	TYR	CE1-CZ	-5.26	1.31	1.38
1	A	74	TYR	CE1-CZ	-5.25	1.31	1.38
1	c	74	TYR	CE1-CZ	-5.25	1.31	1.38
1	k	74	TYR	CE1-CZ	-5.24	1.31	1.38
1	U	74	TYR	CE1-CZ	-5.24	1.31	1.38
1	o	74	TYR	CE1-CZ	-5.24	1.31	1.38
1	G	74	TYR	CE1-CZ	-5.23	1.31	1.38
1	O	74	TYR	CE1-CZ	-5.23	1.31	1.38
1	Q	74	TYR	CE1-CZ	-5.23	1.31	1.38
1	Y	74	TYR	CE1-CZ	-5.23	1.31	1.38
1	C	74	TYR	CE1-CZ	-5.22	1.31	1.38
1	S	74	TYR	CE1-CZ	-5.21	1.31	1.38

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	q	181	DA	O4'-C4'-C3'	-6.88	101.75	104.50
3	r	309	DA	O4'-C4'-C3'	-6.07	102.07	104.50
3	q	182	DT	O4'-C4'-C3'	-6.00	102.10	104.50
1	g	74	TYR	CB-CG-CD1	-5.93	117.44	121.00
1	A	74	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	C	74	TYR	CB-CG-CD1	-5.87	117.48	121.00
1	a	74	TYR	CB-CG-CD1	-5.87	117.48	121.00
1	m	74	TYR	CB-CG-CD1	-5.86	117.48	121.00
1	U	74	TYR	CB-CG-CD1	-5.84	117.49	121.00
1	o	74	TYR	CB-CG-CD1	-5.84	117.49	121.00
1	G	74	TYR	CB-CG-CD1	-5.84	117.50	121.00
1	Q	74	TYR	CB-CG-CD1	-5.84	117.50	121.00
1	c	74	TYR	CB-CG-CD1	-5.83	117.50	121.00
1	i	74	TYR	CB-CG-CD1	-5.83	117.50	121.00
1	E	74	TYR	CB-CG-CD1	-5.83	117.50	121.00
1	k	74	TYR	CB-CG-CD1	-5.83	117.50	121.00
1	K	74	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	W	74	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	I	74	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	e	74	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	M	74	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	O	74	TYR	CB-CG-CD1	-5.79	117.52	121.00
1	Y	74	TYR	CB-CG-CD1	-5.73	117.56	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	74	TYR	CB-CG-CD1	-5.72	117.57	121.00
3	r	344	DT	O4'-C4'-C3'	-5.40	102.34	104.50
3	r	440	DT	O4'-C4'-C3'	-5.40	102.34	104.50
3	r	488	DT	O4'-C4'-C3'	-5.39	102.34	104.50
3	r	308	DT	O4'-C4'-C3'	-5.39	102.34	104.50
3	r	368	DT	O4'-C4'-C3'	-5.37	102.35	104.50
3	r	272	DT	O4'-C4'-C3'	-5.35	102.36	104.50
3	r	428	DT	O4'-C4'-C3'	-5.35	102.36	104.50
3	r	296	DT	O4'-C4'-C3'	-5.34	102.36	104.50
3	r	464	DT	O4'-C4'-C3'	-5.33	102.37	104.50
3	r	452	DT	O4'-C4'-C3'	-5.30	102.38	104.50
3	r	260	DT	O4'-C4'-C3'	-5.29	102.38	104.50
3	r	404	DT	O4'-C4'-C3'	-5.29	102.38	104.50
3	r	476	DT	O4'-C4'-C3'	-5.28	102.39	104.50
3	r	284	DT	O4'-C4'-C3'	-5.28	102.39	104.50
3	r	416	DT	O4'-C4'-C3'	-5.28	102.39	104.50
3	r	356	DT	O4'-C4'-C3'	-5.27	102.39	104.50
3	r	380	DT	O4'-C4'-C3'	-5.26	102.39	104.50
3	r	332	DT	O4'-C4'-C3'	-5.24	102.40	104.50
3	r	320	DT	O4'-C4'-C3'	-5.23	102.41	104.50
3	r	392	DT	O4'-C4'-C3'	-5.23	102.41	104.50
3	q	121	DA	O4'-C4'-C3'	-5.10	102.46	104.50
3	q	98	DT	O4'-C4'-C3'	-5.09	102.47	104.50
3	q	73	DA	O4'-C4'-C3'	-5.06	102.48	104.50
3	q	38	DT	O4'-C4'-C3'	-5.05	102.48	104.50
3	q	158	DT	O4'-C4'-C3'	-5.03	102.49	104.50
3	q	205	DA	O4'-C4'-C3'	-5.00	102.50	104.50

There are no chirality outliers.

There are no planarity outliers.

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	A	129/140 (92%)	129 (100%)	0	0	100	100
1	C	129/140 (92%)	129 (100%)	0	0	100	100
1	E	129/140 (92%)	129 (100%)	0	0	100	100
1	G	129/140 (92%)	129 (100%)	0	0	100	100
1	I	129/140 (92%)	129 (100%)	0	0	100	100
1	K	129/140 (92%)	129 (100%)	0	0	100	100
1	M	129/140 (92%)	129 (100%)	0	0	100	100
1	O	129/140 (92%)	129 (100%)	0	0	100	100
1	Q	129/140 (92%)	129 (100%)	0	0	100	100
1	S	129/140 (92%)	129 (100%)	0	0	100	100
1	U	129/140 (92%)	129 (100%)	0	0	100	100
1	W	129/140 (92%)	129 (100%)	0	0	100	100
1	Y	129/140 (92%)	129 (100%)	0	0	100	100
1	a	129/140 (92%)	129 (100%)	0	0	100	100
1	c	129/140 (92%)	129 (100%)	0	0	100	100
1	e	129/140 (92%)	129 (100%)	0	0	100	100
1	g	129/140 (92%)	129 (100%)	0	0	100	100
1	i	129/140 (92%)	129 (100%)	0	0	100	100
1	k	129/140 (92%)	129 (100%)	0	0	100	100
1	m	129/140 (92%)	129 (100%)	0	0	100	100
1	o	129/140 (92%)	129 (100%)	0	0	100	100
2	B	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
2	D	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
2	F	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
2	H	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
2	J	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
2	L	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
2	N	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
2	P	124/132 (94%)	121 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	R	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
2	T	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
2	V	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
2	X	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
2	Z	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
2	b	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
2	d	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
2	f	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
2	h	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
2	j	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
2	l	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
2	n	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
2	p	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
All	All	5313/5712 (93%)	5250 (99%)	63 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	A	117/122 (96%)	116 (99%)	1 (1%)	78	87
1	C	117/122 (96%)	116 (99%)	1 (1%)	78	87
1	E	117/122 (96%)	116 (99%)	1 (1%)	78	87
1	G	117/122 (96%)	116 (99%)	1 (1%)	78	87
1	I	117/122 (96%)	116 (99%)	1 (1%)	78	87
1	K	117/122 (96%)	116 (99%)	1 (1%)	78	87
1	M	117/122 (96%)	116 (99%)	1 (1%)	78	87
1	O	117/122 (96%)	116 (99%)	1 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	117/122 (96%)	116 (99%)	1 (1%)	78	87
1	S	117/122 (96%)	116 (99%)	1 (1%)	78	87
1	U	117/122 (96%)	116 (99%)	1 (1%)	78	87
1	W	117/122 (96%)	116 (99%)	1 (1%)	78	87
1	Y	117/122 (96%)	116 (99%)	1 (1%)	78	87
1	a	117/122 (96%)	116 (99%)	1 (1%)	78	87
1	c	117/122 (96%)	116 (99%)	1 (1%)	78	87
1	e	117/122 (96%)	116 (99%)	1 (1%)	78	87
1	g	117/122 (96%)	116 (99%)	1 (1%)	78	87
1	i	117/122 (96%)	116 (99%)	1 (1%)	78	87
1	k	117/122 (96%)	116 (99%)	1 (1%)	78	87
1	m	117/122 (96%)	116 (99%)	1 (1%)	78	87
1	o	117/122 (96%)	116 (99%)	1 (1%)	78	87
2	B	105/111 (95%)	104 (99%)	1 (1%)	76	86
2	D	105/111 (95%)	104 (99%)	1 (1%)	76	86
2	F	105/111 (95%)	104 (99%)	1 (1%)	76	86
2	H	105/111 (95%)	104 (99%)	1 (1%)	76	86
2	J	105/111 (95%)	104 (99%)	1 (1%)	76	86
2	L	105/111 (95%)	104 (99%)	1 (1%)	76	86
2	N	105/111 (95%)	104 (99%)	1 (1%)	76	86
2	P	105/111 (95%)	104 (99%)	1 (1%)	76	86
2	R	105/111 (95%)	104 (99%)	1 (1%)	76	86
2	T	105/111 (95%)	104 (99%)	1 (1%)	76	86
2	V	105/111 (95%)	104 (99%)	1 (1%)	76	86
2	X	105/111 (95%)	104 (99%)	1 (1%)	76	86
2	Z	105/111 (95%)	104 (99%)	1 (1%)	76	86
2	b	105/111 (95%)	104 (99%)	1 (1%)	76	86
2	d	105/111 (95%)	104 (99%)	1 (1%)	76	86
2	f	105/111 (95%)	104 (99%)	1 (1%)	76	86
2	h	105/111 (95%)	104 (99%)	1 (1%)	76	86
2	j	105/111 (95%)	104 (99%)	1 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	l	105/111 (95%)	104 (99%)	1 (1%)	76	86
2	n	105/111 (95%)	104 (99%)	1 (1%)	76	86
2	p	105/111 (95%)	104 (99%)	1 (1%)	76	86
All	All	4662/4893 (95%)	4620 (99%)	42 (1%)	79	87

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	MET
2	B	128	ILE
1	C	52	MET
2	D	128	ILE
1	E	52	MET
2	F	128	ILE
1	G	52	MET
2	H	128	ILE
1	I	52	MET
2	J	128	ILE
1	K	52	MET
2	L	128	ILE
1	M	52	MET
2	N	128	ILE
1	O	52	MET
2	P	128	ILE
1	Q	52	MET
2	R	128	ILE
1	S	52	MET
2	T	128	ILE
1	U	52	MET
2	V	128	ILE
1	W	52	MET
2	X	128	ILE
1	Y	52	MET
2	Z	128	ILE
1	a	52	MET
2	b	128	ILE
1	c	52	MET
2	d	128	ILE
1	e	52	MET
2	f	128	ILE
1	g	52	MET

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Mol	Chain	Res	Type
2	h	128	ILE
1	i	52	MET
2	j	128	ILE
1	k	52	MET
2	l	128	ILE
1	m	52	MET
2	n	128	ILE
1	o	52	MET
2	p	128	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	15	GLN
2	B	105	ASN
2	D	105	ASN
2	F	105	ASN
2	H	105	ASN
2	J	105	ASN
2	L	105	ASN
2	P	105	ASN
2	R	105	ASN
2	T	105	ASN
2	V	105	ASN
2	X	105	ASN
2	Z	105	ASN
2	b	105	ASN
2	d	105	ASN
2	f	105	ASN
2	h	105	ASN
2	j	105	ASN
2	l	105	ASN
2	n	105	ASN
2	p	105	ASN

5.3.3 RNA

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 [i](#)

This section contains visualisations of the EMDB entry EMD-8780. These allow visual inspection of the internal detail of the map and identification of artifacts.

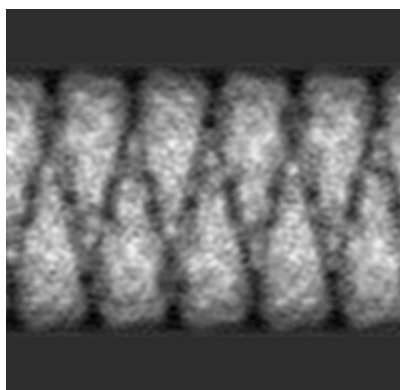
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

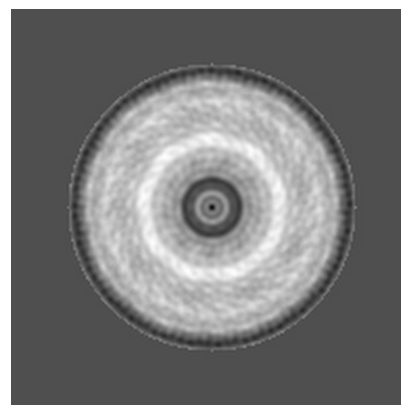
6.1.1 Primary map



X



Y

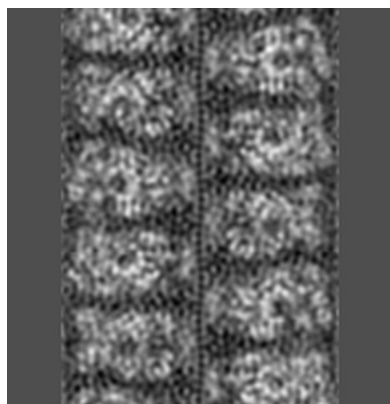


Z

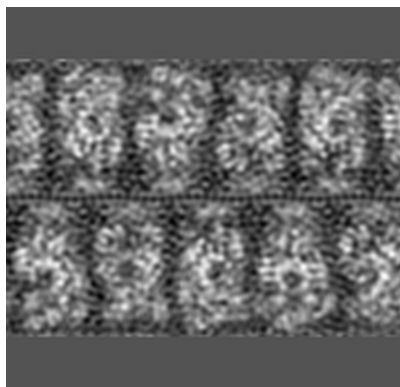
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

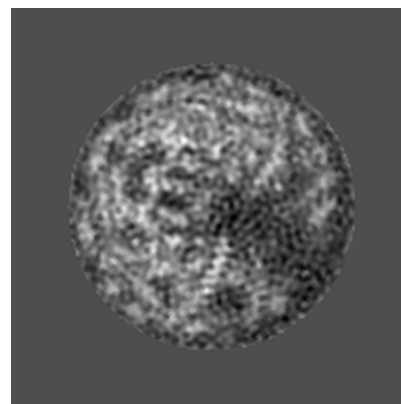
6.2.1 Primary map



X Index: 96



Y Index: 96

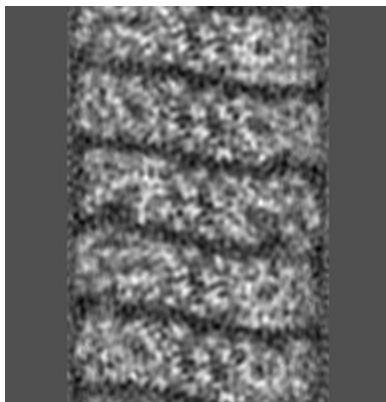


Z Index: 100

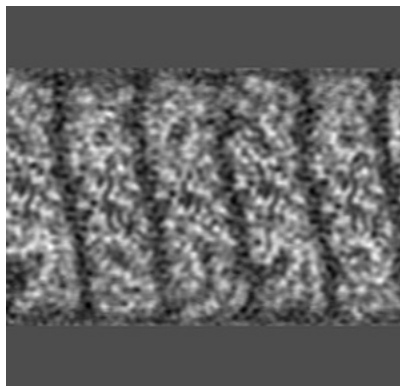
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

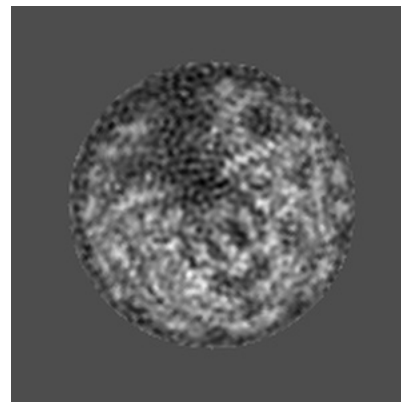
6.3.1 Primary map



X Index: 74



Y Index: 120

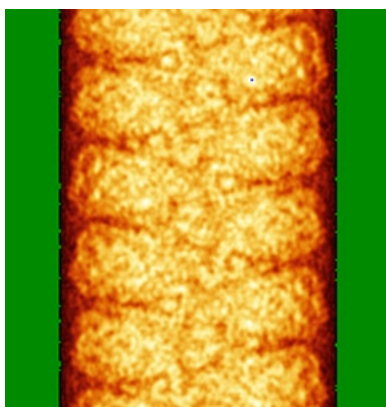


Z Index: 35

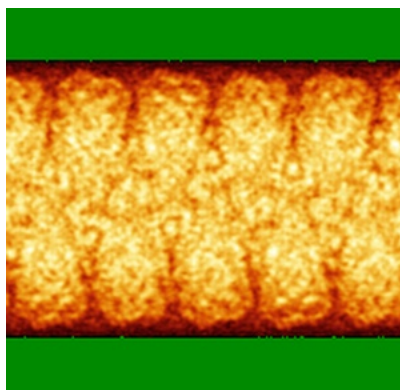
The images above show the largest variance slices of the map in three orthogonal directions.

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

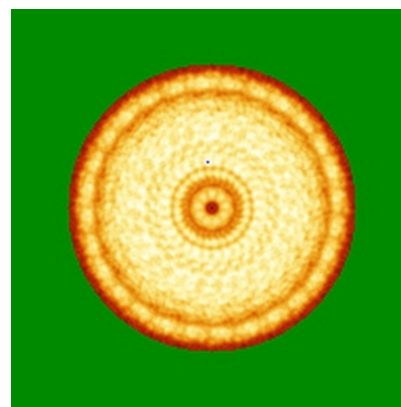
6.4.1 Primary map



X



Y

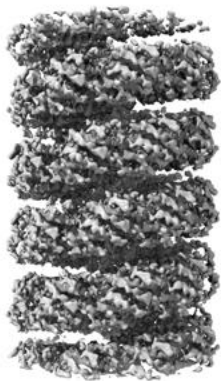


Z

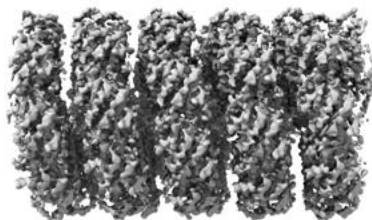
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

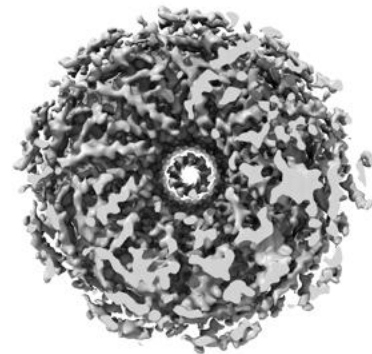
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

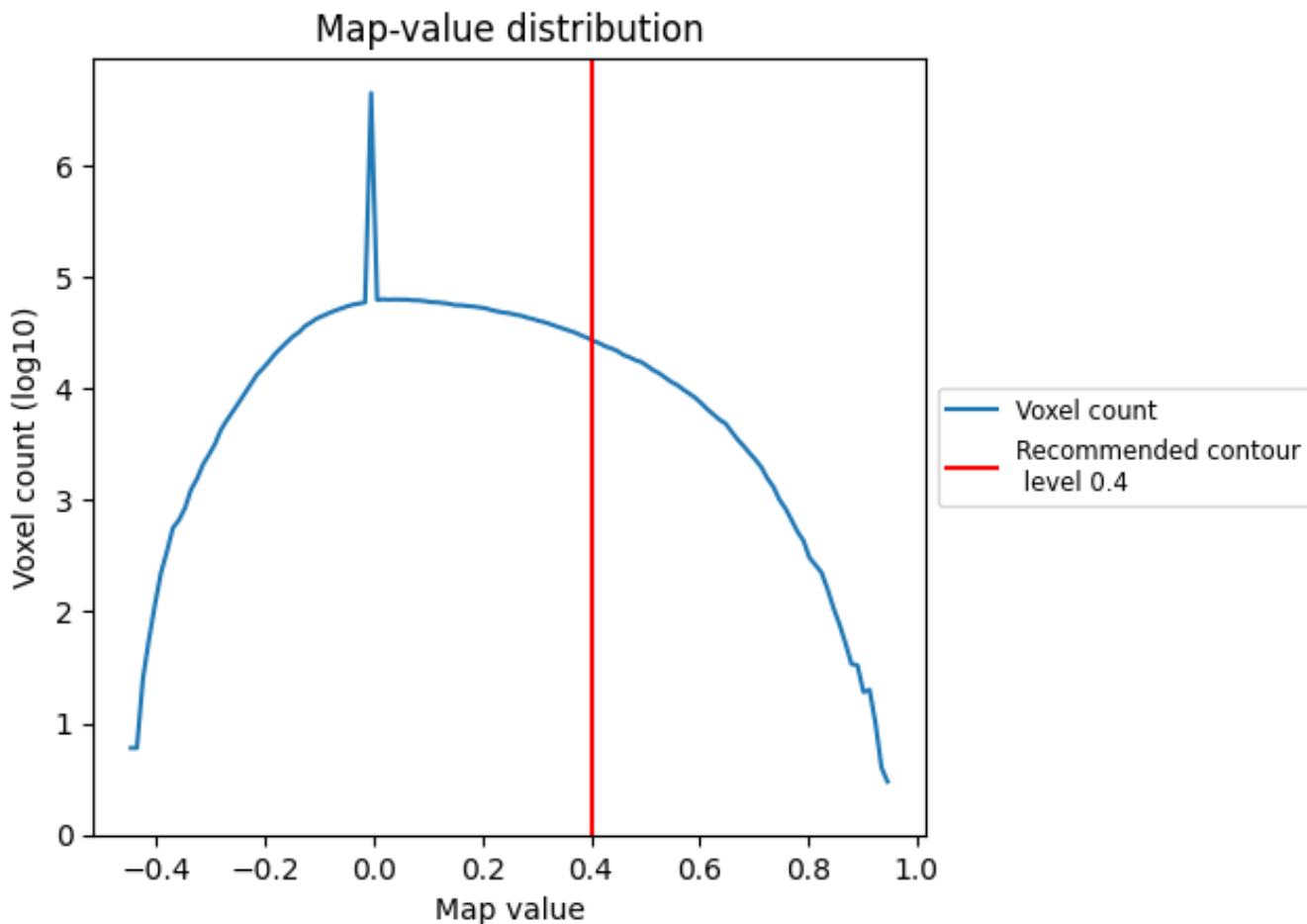
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

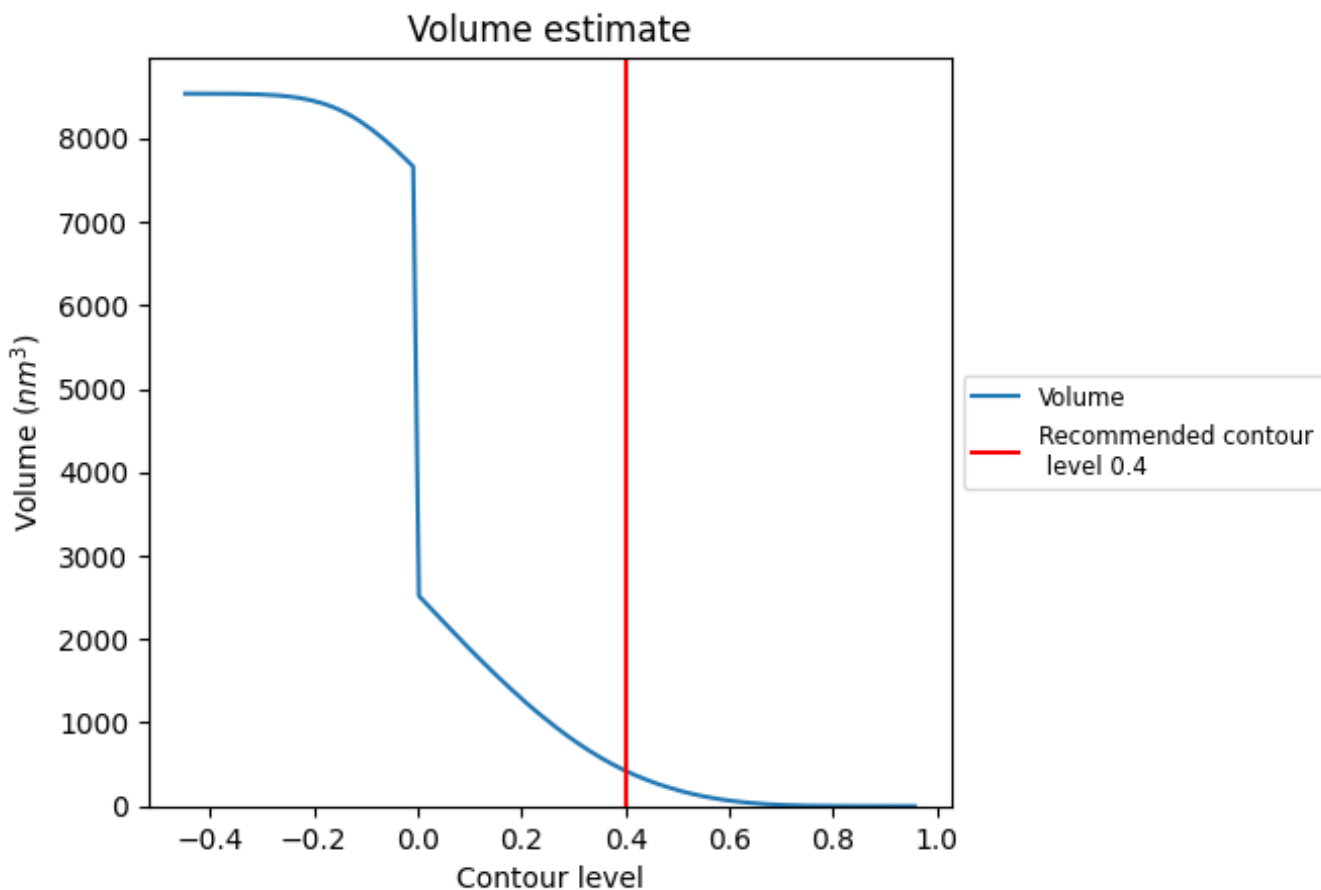
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 425 nm^3 ; this corresponds to an approximate mass of 384 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

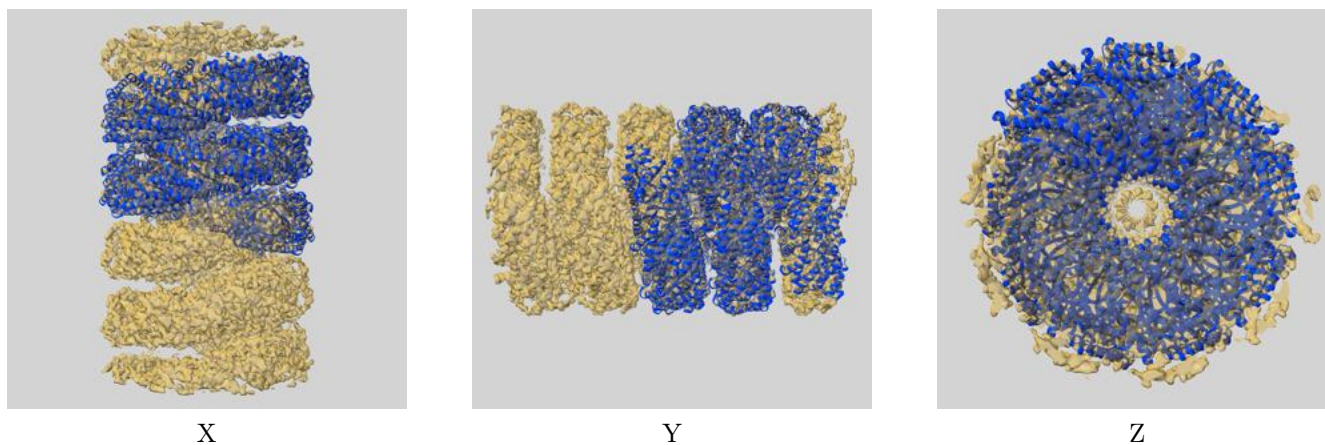
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

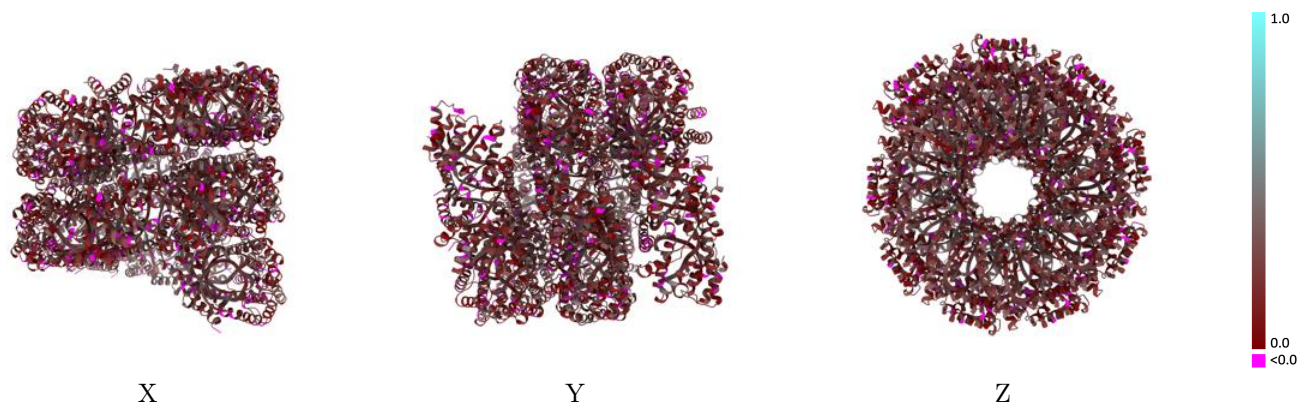
This section contains information regarding the fit between EMDB map EMD-8780 and PDB model 5W7G. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



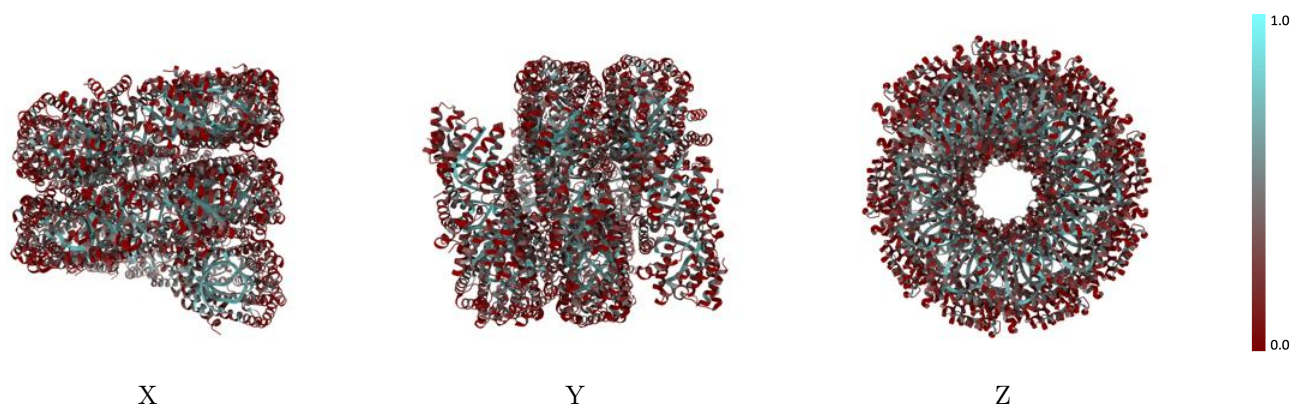
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



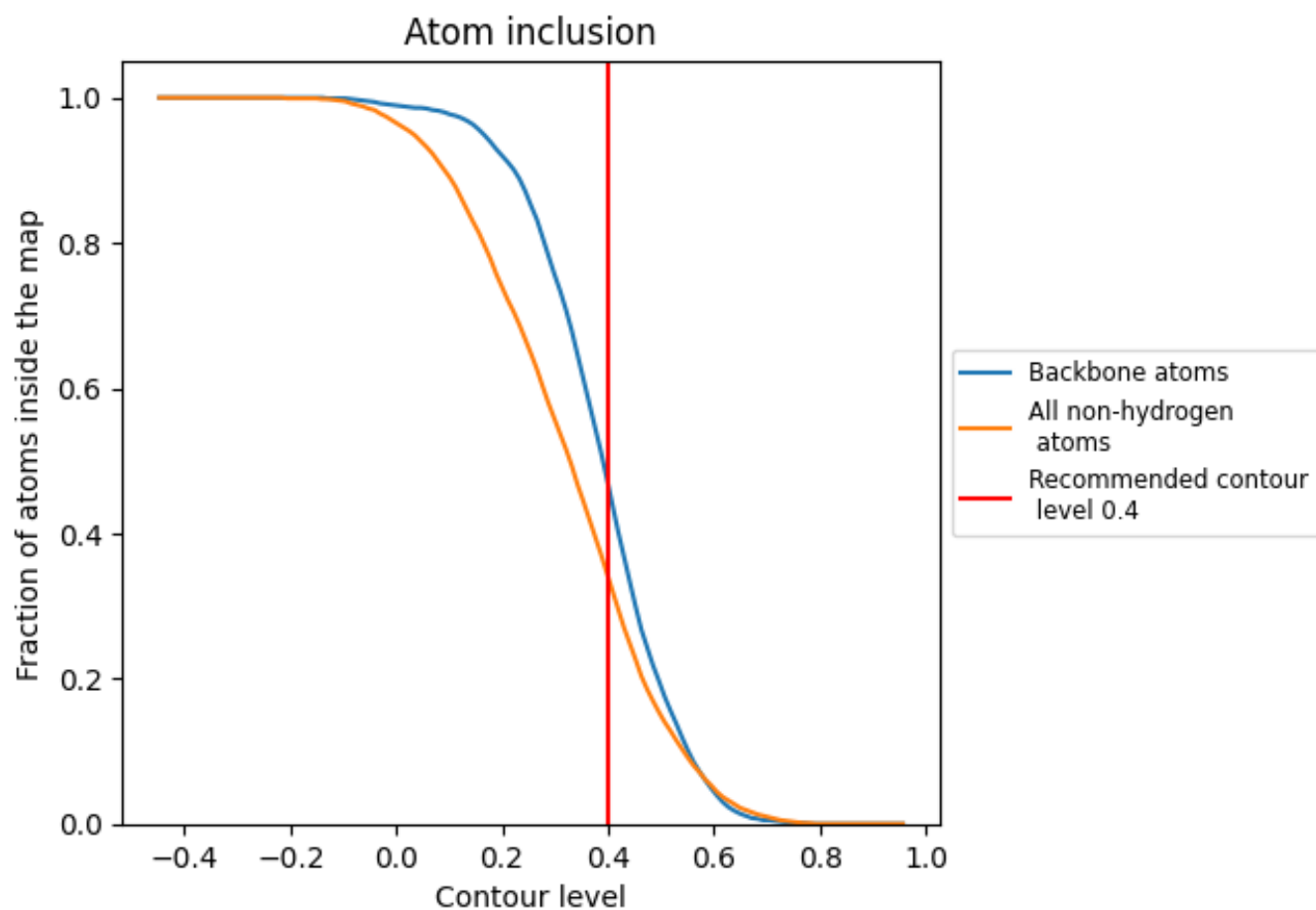
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 47% of all backbone atoms, 34% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3410	0.1980
A	0.2580	0.1660
B	0.2470	0.1940
C	0.2700	0.1630
D	0.2530	0.2040
E	0.2680	0.1630
F	0.2490	0.2050
G	0.2680	0.1630
H	0.2450	0.2070
I	0.2550	0.1620
J	0.2520	0.2110
K	0.2640	0.1620
L	0.2520	0.2080
M	0.2750	0.1660
N	0.2550	0.2050
O	0.2620	0.1660
P	0.2490	0.2060
Q	0.2720	0.1650
R	0.2520	0.2060
S	0.2700	0.1640
T	0.2520	0.2040
U	0.2630	0.1640
V	0.2520	0.2040
W	0.2710	0.1640
X	0.2540	0.2070
Y	0.2700	0.1640
Z	0.2500	0.2090
a	0.2700	0.1640
b	0.2520	0.2060
c	0.2730	0.1610
d	0.2520	0.2070
e	0.2690	0.1640
f	0.2560	0.2100
g	0.2740	0.1650
h	0.2470	0.2060



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Chain	Atom inclusion	Q-score
i	 0.2650	 0.1630
j	 0.2540	 0.2050
k	 0.2740	 0.1650
l	 0.2490	 0.2020
m	 0.2650	 0.1650
n	 0.2480	 0.2050
o	 0.2680	 0.1630
p	 0.2510	 0.2040
q	 0.6800	 0.2470
r	 0.6660	 0.2700