



## wwPDB EM Validation Summary Report ⓘ

Nov 12, 2022 – 10:35 PM EST

PDB ID : 6TZ5  
EMDB ID : EMD-20589  
Title : CryoEM reconstruction of membrane-bound ESCRT-III filament composed of CHMP1B+IST1 (left-handed)  
Authors : Nguyen, H.C.; Frost, A.  
Deposited on : 2019-08-10  
Resolution : 3.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

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

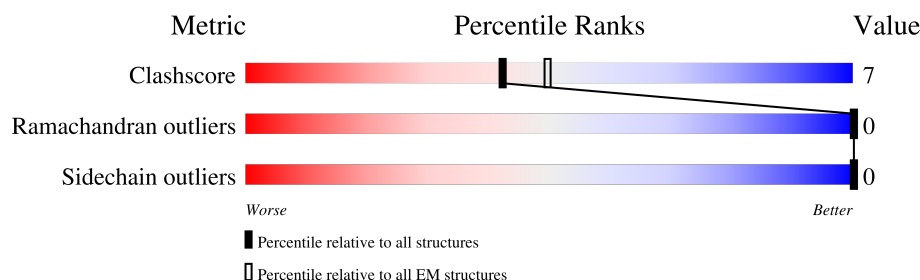
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	AA	199	<div> <div>36%</div> <div>73%</div> <div>15%</div> <div>12%</div> </div>
1	AB	199	<div> <div>31%</div> <div>74%</div> <div>14%</div> <div>12%</div> </div>
1	B	199	<div> <div>39%</div> <div>74%</div> <div>14%</div> <div>12%</div> </div>
1	CA	199	<div> <div>17%</div> <div>70%</div> <div>18%</div> <div>12%</div> </div>
1	CB	199	<div> <div>34%</div> <div>73%</div> <div>15%</div> <div>12%</div> </div>
1	D	199	<div> <div>28%</div> <div>73%</div> <div>15%</div> <div>12%</div> </div>
1	EA	199	<div> <div>32%</div> <div>72%</div> <div>16%</div> <div>12%</div> </div>
1	EB	199	<div> <div>16%</div> <div>73%</div> <div>15%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	199	
1	GA	199	
1	GB	199	
1	H	199	
1	IA	199	
1	IB	199	
1	J	199	
1	KA	199	
1	KB	199	
1	L	199	
1	MA	199	
1	MB	199	
1	N	199	
1	OA	199	
1	OB	199	
1	P	199	
1	QA	199	
1	QB	199	
1	R	199	
1	SA	199	
1	T	199	
1	UA	199	
1	W	199	
1	WA	199	
1	Y	199	

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Mol	Chain	Length	Quality of chain
1	YA	199	
2	A	189	
2	BA	189	
2	BB	189	
2	C	189	
2	DA	189	
2	DB	189	
2	E	189	
2	FA	189	
2	FB	189	
2	G	189	
2	HA	189	
2	HB	189	
2	I	189	
2	JA	189	
2	JB	189	
2	K	189	
2	LA	189	
2	LB	189	
2	M	189	
2	NA	189	
2	NB	189	
2	O	189	
2	PA	189	
2	PB	189	

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Mol	Chain	Length	Quality of chain
2	Q	189	<div> <div>46%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>
2	RA	189	<div> <div>58%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>
2	S	189	<div> <div>28%</div> <div>84%</div> <div>12%</div> <div>.</div> </div>
2	TA	189	<div> <div>53%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>
2	V	189	<div> <div>54%</div> <div>84%</div> <div>12%</div> <div>.</div> </div>
2	VA	189	<div> <div>51%</div> <div>84%</div> <div>12%</div> <div>.</div> </div>
2	X	189	<div> <div>55%</div> <div>84%</div> <div>12%</div> <div>.</div> </div>
2	XA	189	<div> <div>26%</div> <div>83%</div> <div>13%</div> <div>.</div> </div>
2	Z	189	<div> <div>55%</div> <div>84%</div> <div>12%</div> <div>.</div> </div>
2	ZA	189	<div> <div>54%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 93500 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 Charged multivesicular body protein 1b.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	AB	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	CB	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	EB	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	GB	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	IB	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	KB	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	MB	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	OB	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	QB	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	SA	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	UA	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	WA	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	YA	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	CA	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	EA	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	GA	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	IA	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	KA	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	MA	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	OA	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	QA	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	B	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	D	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	F	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	H	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	J	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	L	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	N	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	P	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	R	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	T	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	W	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		
1	Y	175	Total	C	N	O	S	0	0
			1344	828	240	263	13		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
AB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
CB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
EB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
GB	37	GLU	LYS	engineered mutation	UNP Q7LBR1

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Chain	Residue	Modelled	Actual	Comment	Reference
IB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
KB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
MB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
OB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
QB	37	GLU	LYS	engineered mutation	UNP Q7LBR1
SA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
UA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
WA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
YA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
CA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
EA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
GA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
IA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
KA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
MA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
OA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
QA	37	GLU	LYS	engineered mutation	UNP Q7LBR1
B	37	GLU	LYS	engineered mutation	UNP Q7LBR1
D	37	GLU	LYS	engineered mutation	UNP Q7LBR1
F	37	GLU	LYS	engineered mutation	UNP Q7LBR1
H	37	GLU	LYS	engineered mutation	UNP Q7LBR1
J	37	GLU	LYS	engineered mutation	UNP Q7LBR1
L	37	GLU	LYS	engineered mutation	UNP Q7LBR1
N	37	GLU	LYS	engineered mutation	UNP Q7LBR1
P	37	GLU	LYS	engineered mutation	UNP Q7LBR1
R	37	GLU	LYS	engineered mutation	UNP Q7LBR1
T	37	GLU	LYS	engineered mutation	UNP Q7LBR1
W	37	GLU	LYS	engineered mutation	UNP Q7LBR1
Y	37	GLU	LYS	engineered mutation	UNP Q7LBR1

- Molecule 2 is a protein called IST1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BB	181	Total	C	N	O	S	0	0
			1406	895	248	258	5		
2	DB	181	Total	C	N	O	S	0	0
			1406	895	248	258	5		
2	FB	181	Total	C	N	O	S	0	0
			1406	895	248	258	5		
2	HB	181	Total	C	N	O	S	0	0
			1406	895	248	258	5		
2	JB	181	Total	C	N	O	S	0	0
			1406	895	248	258	5		

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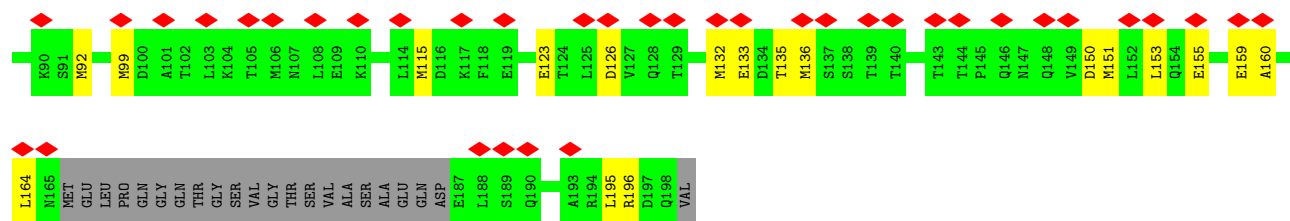
Mol	Chain	Residues	Atoms					AltConf	Trace
2	LB	181	Total 1406	C 895	N 248	O 258	S 5	0	0
2	NB	181	Total 1406	C 895	N 248	O 258	S 5	0	0
2	PB	181	Total 1406	C 895	N 248	O 258	S 5	0	0
2	TA	181	Total 1406	C 895	N 248	O 258	S 5	0	0
2	VA	181	Total 1406	C 895	N 248	O 258	S 5	0	0
2	XA	181	Total 1406	C 895	N 248	O 258	S 5	0	0
2	ZA	181	Total 1406	C 895	N 248	O 258	S 5	0	0
2	BA	181	Total 1406	C 895	N 248	O 258	S 5	0	0
2	A	181	Total 1406	C 895	N 248	O 258	S 5	0	0
2	DA	181	Total 1406	C 895	N 248	O 258	S 5	0	0
2	FA	181	Total 1406	C 895	N 248	O 258	S 5	0	0
2	HA	181	Total 1406	C 895	N 248	O 258	S 5	0	0
2	JA	181	Total 1406	C 895	N 248	O 258	S 5	0	0
2	LA	181	Total 1406	C 895	N 248	O 258	S 5	0	0
2	NA	181	Total 1406	C 895	N 248	O 258	S 5	0	0
2	PA	181	Total 1406	C 895	N 248	O 258	S 5	0	0
2	RA	181	Total 1406	C 895	N 248	O 258	S 5	0	0
2	C	181	Total 1406	C 895	N 248	O 258	S 5	0	0
2	E	181	Total 1406	C 895	N 248	O 258	S 5	0	0
2	G	181	Total 1406	C 895	N 248	O 258	S 5	0	0
2	I	181	Total 1406	C 895	N 248	O 258	S 5	0	0

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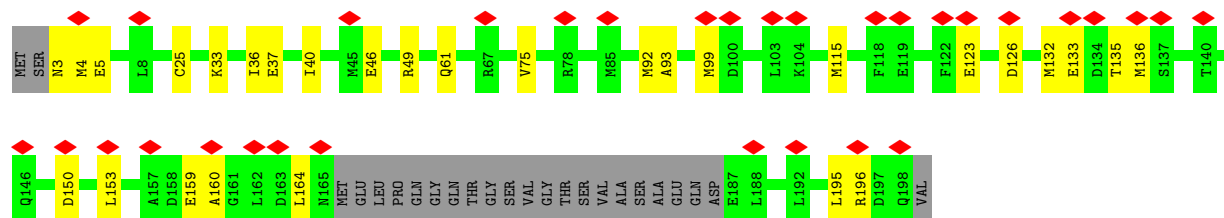
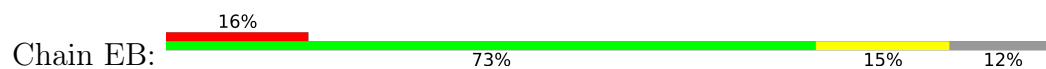
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	181	Total	C	N	O	S	0	0
			1406	895	248	258	5		
2	M	181	Total	C	N	O	S	0	0
			1406	895	248	258	5		
2	O	181	Total	C	N	O	S	0	0
			1406	895	248	258	5		
2	Q	181	Total	C	N	O	S	0	0
			1406	895	248	258	5		
2	S	181	Total	C	N	O	S	0	0
			1406	895	248	258	5		
2	V	181	Total	C	N	O	S	0	0
			1406	895	248	258	5		
2	X	181	Total	C	N	O	S	0	0
			1406	895	248	258	5		
2	Z	181	Total	C	N	O	S	0	0
			1406	895	248	258	5		

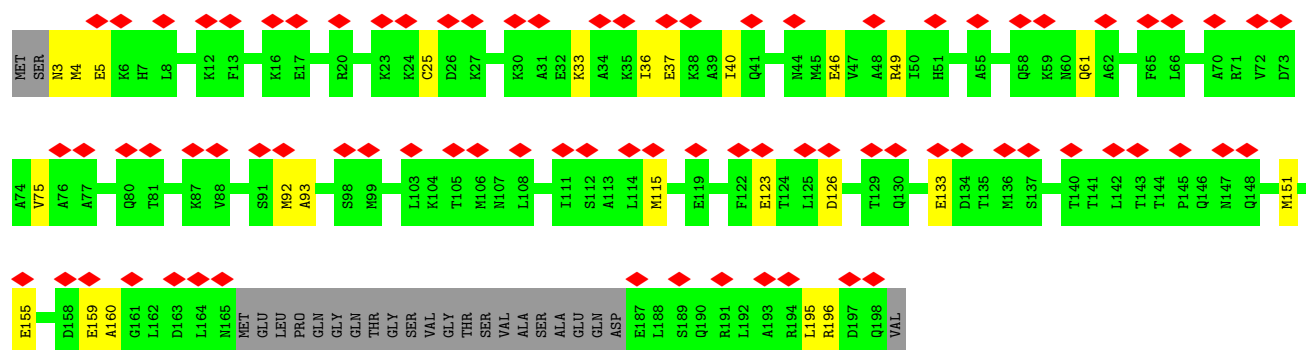
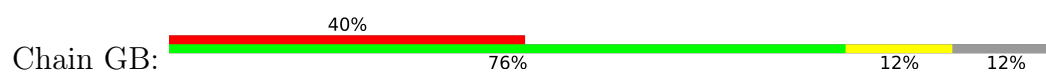




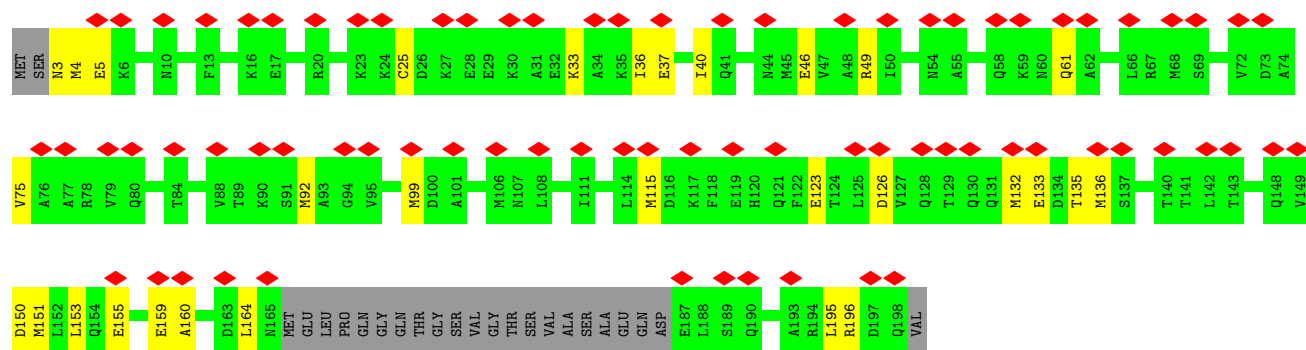
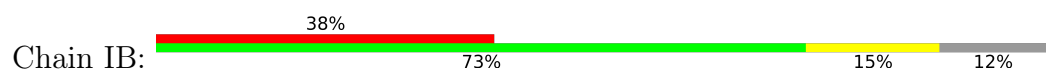
- Molecule 1: Charged multivesicular body protein 1b



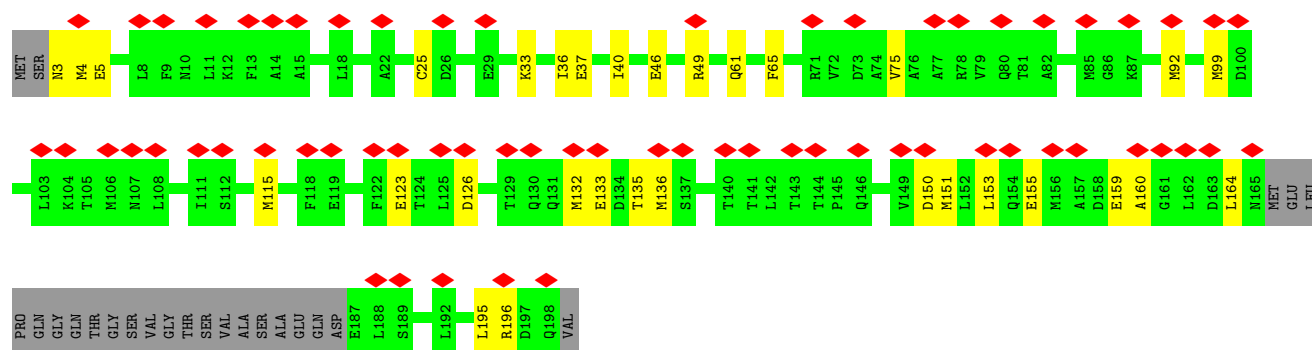
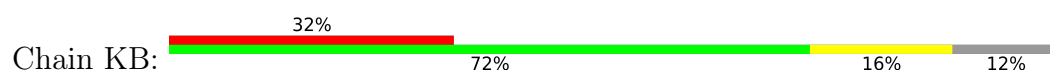
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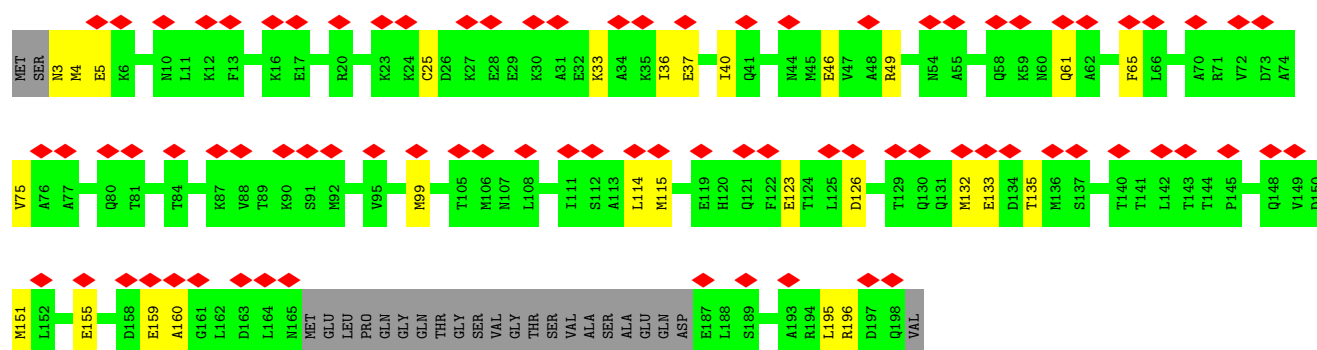
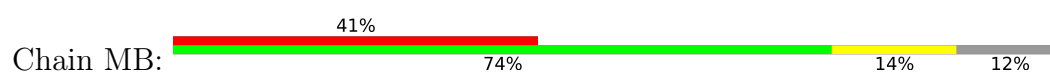
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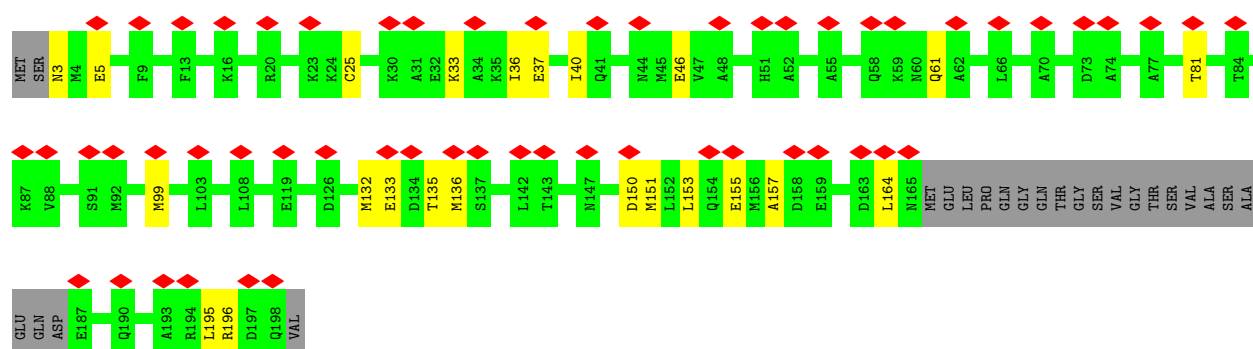
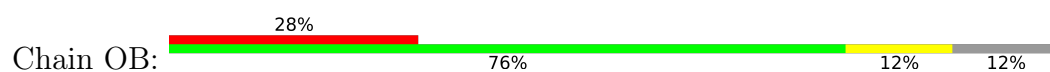
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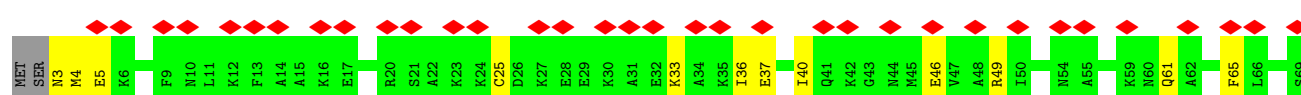
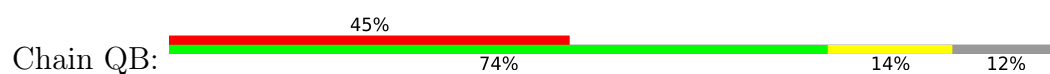
• Molecule 1: Charged multivesicular body protein 1b

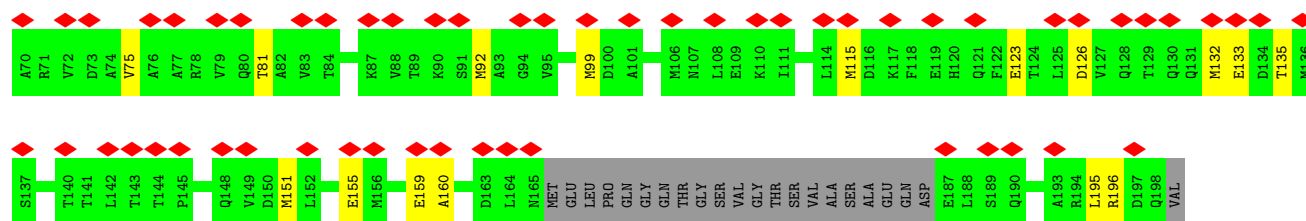


• Molecule 1: Charged multivesicular body protein 1b

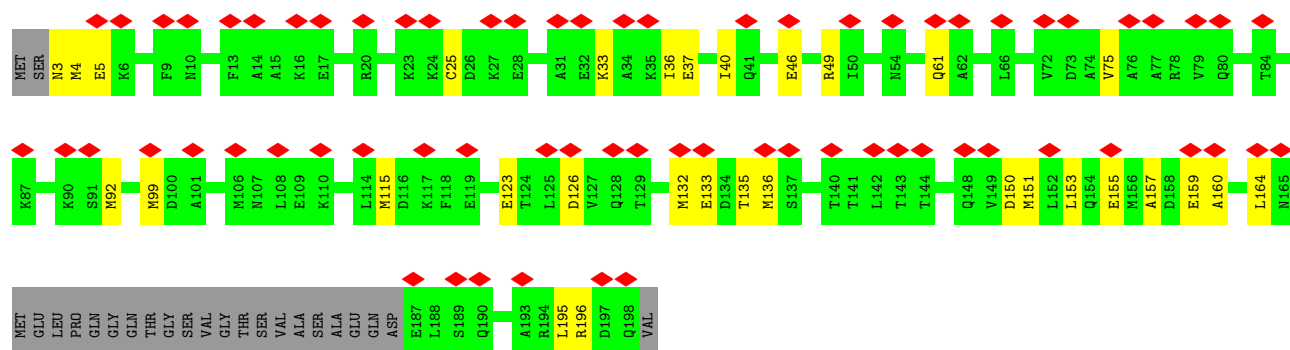
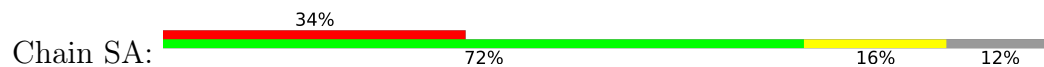


• Molecule 1: Charged multivesicular body protein 1b

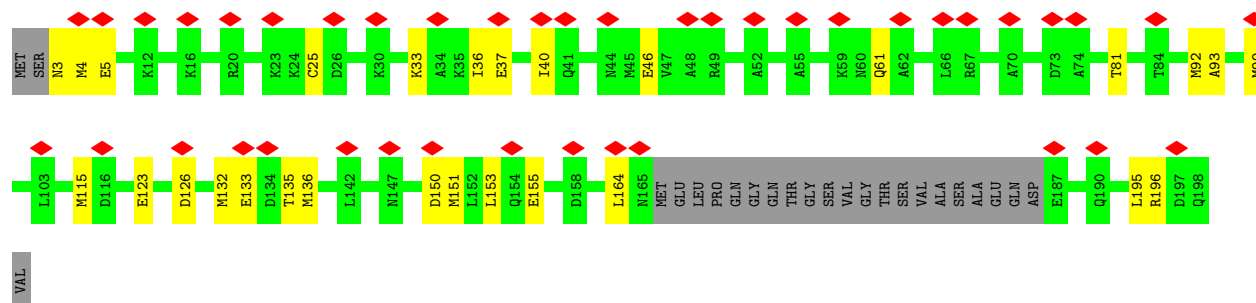
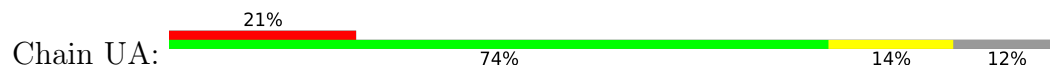




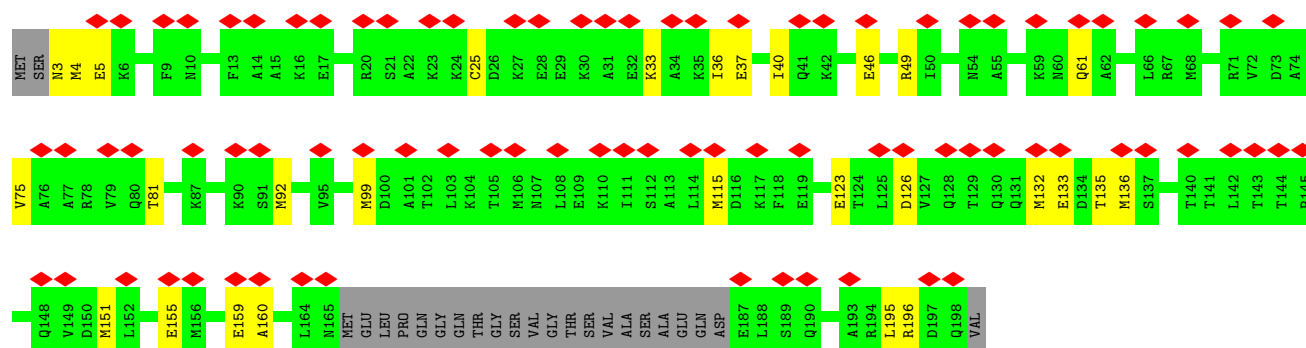
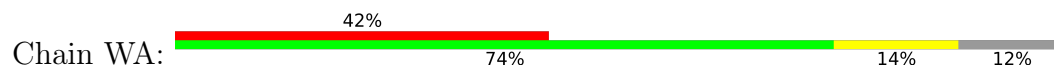
• Molecule 1: Charged multivesicular body protein 1b



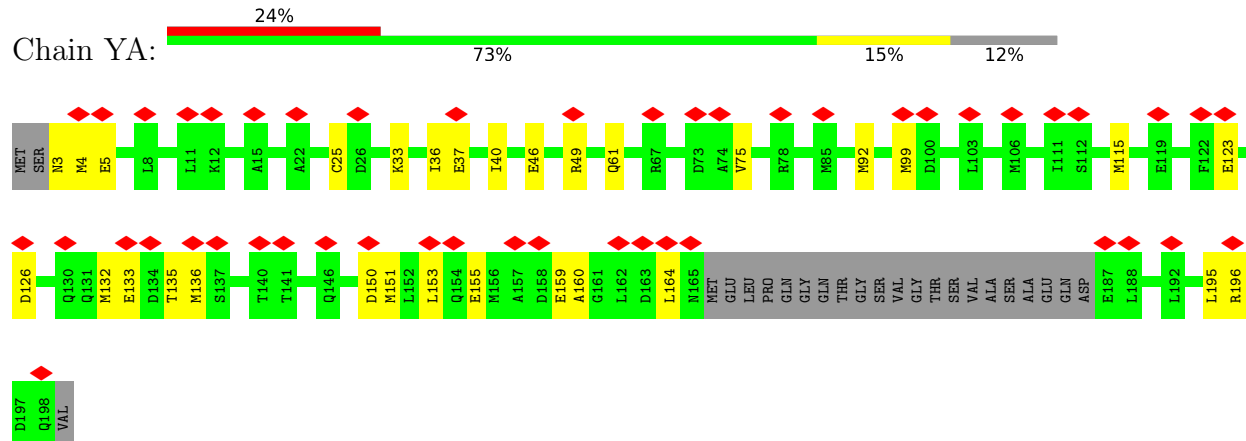
• Molecule 1: Charged multivesicular body protein 1b



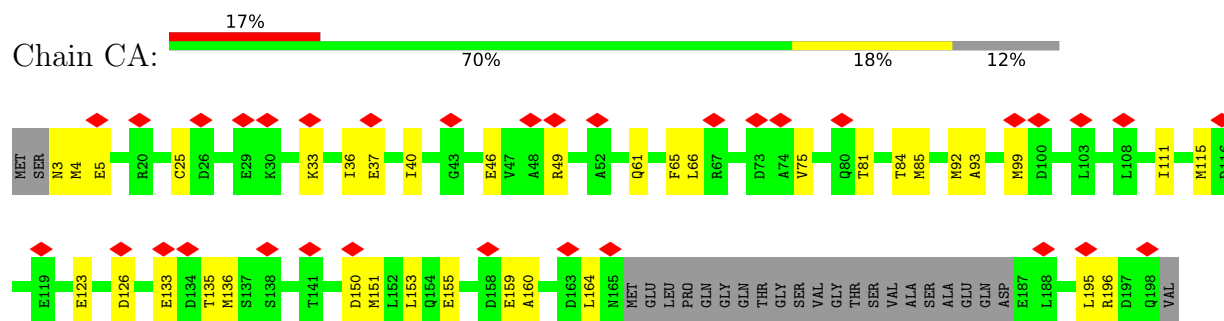
• Molecule 1: Charged multivesicular body protein 1b



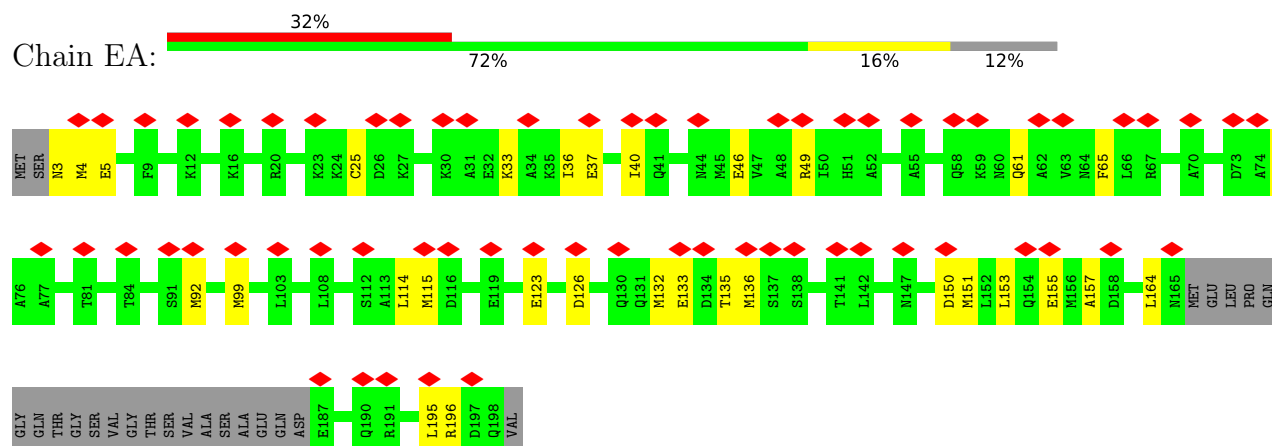
- Molecule 1: Charged multivesicular body protein 1b



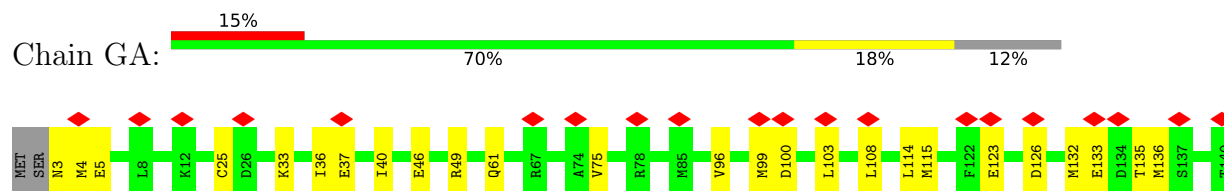
- Molecule 1: Charged multivesicular body protein 1b

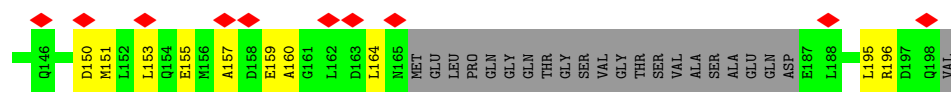


- Molecule 1: Charged multivesicular body protein 1b

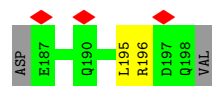
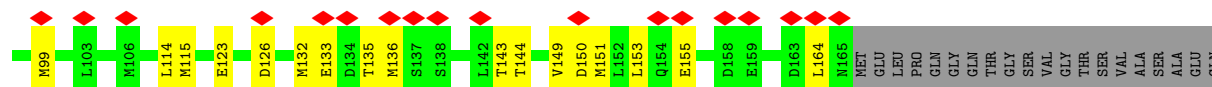
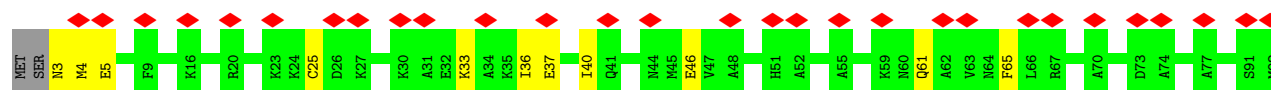
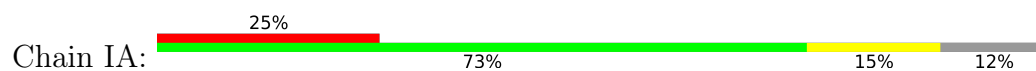


- Molecule 1: Charged multivesicular body protein 1b

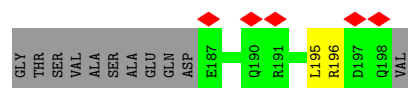
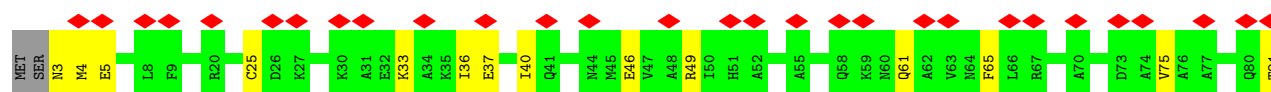
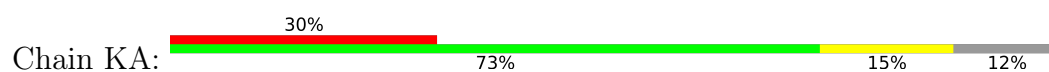




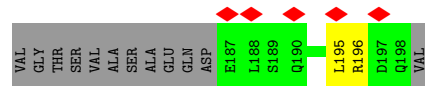
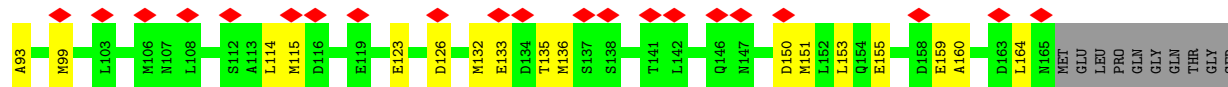
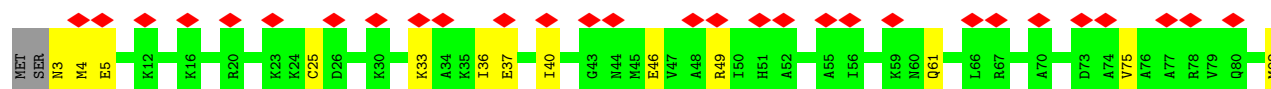
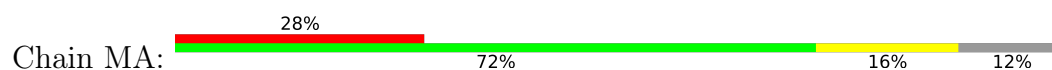
• Molecule 1: Charged multivesicular body protein 1b



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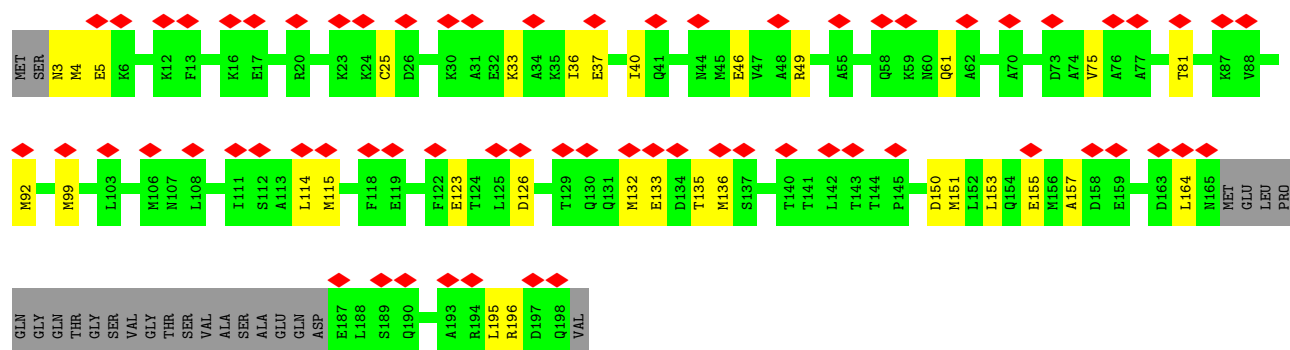
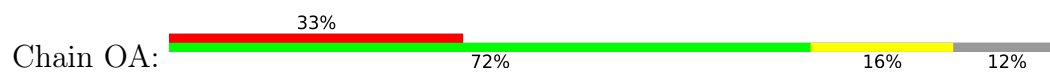


• Molecule 1: Charged multivesicular body protein 1b

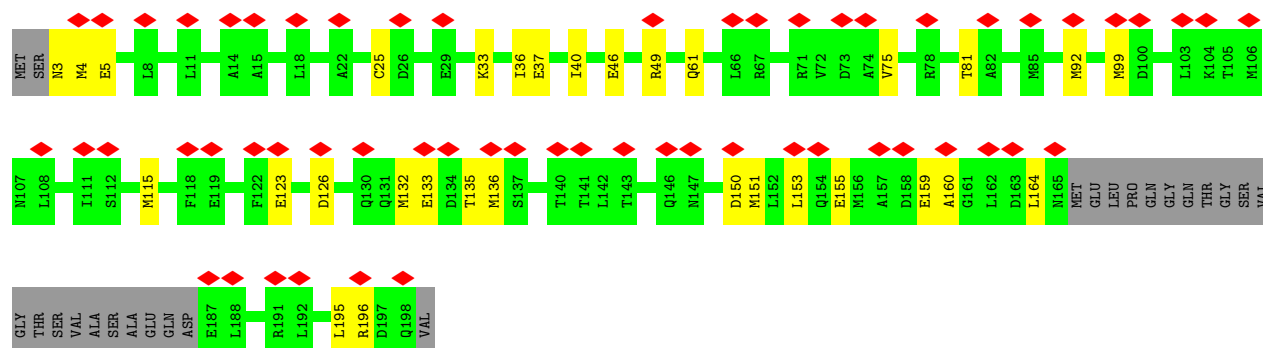
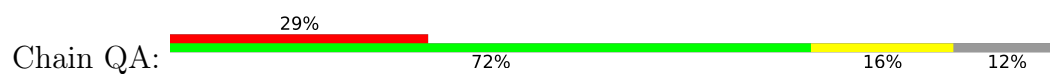


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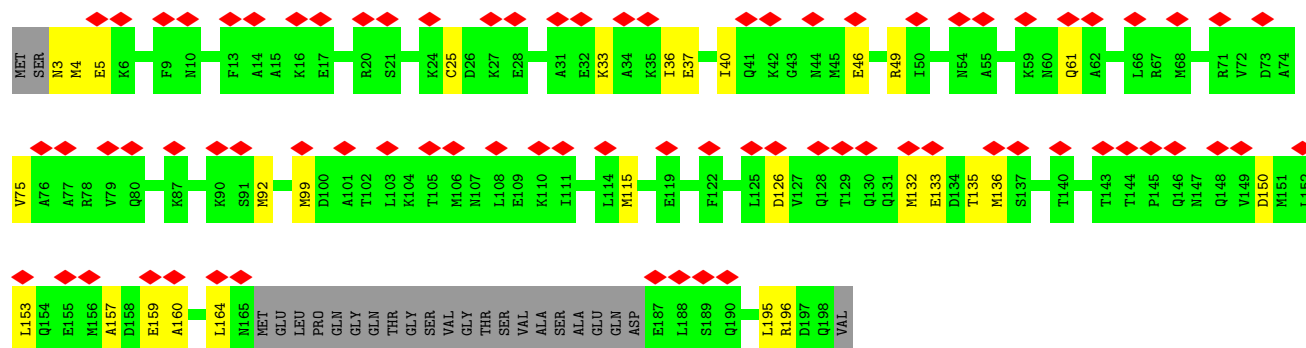
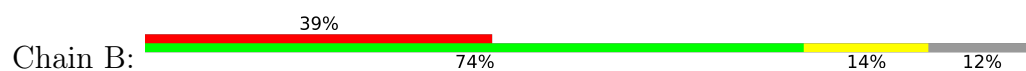




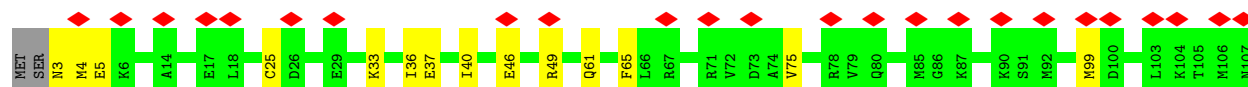
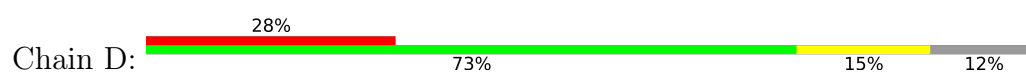
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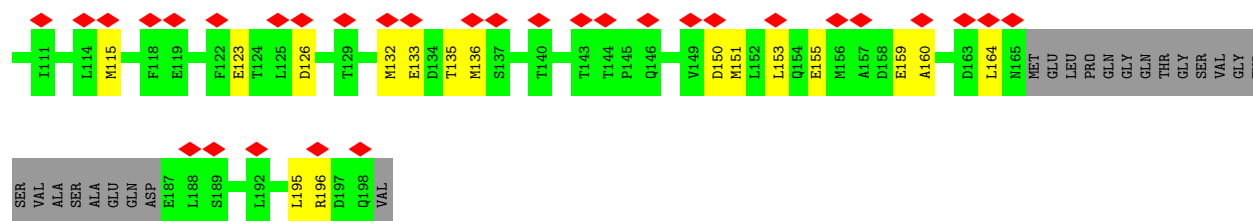


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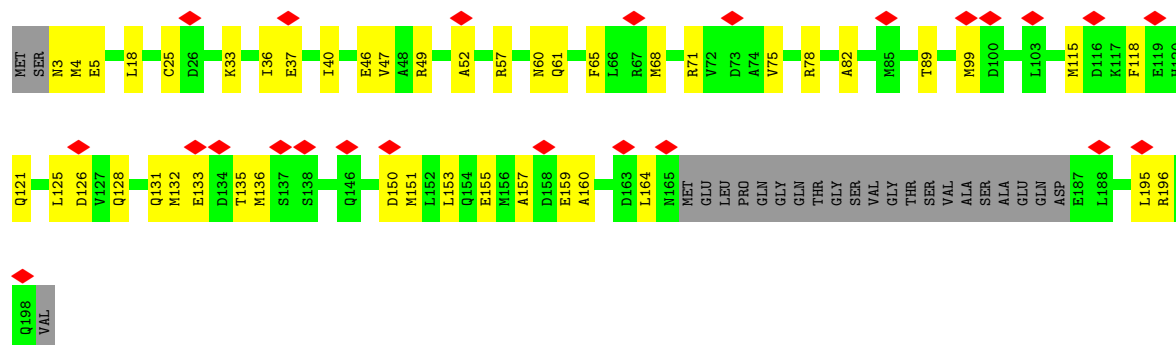


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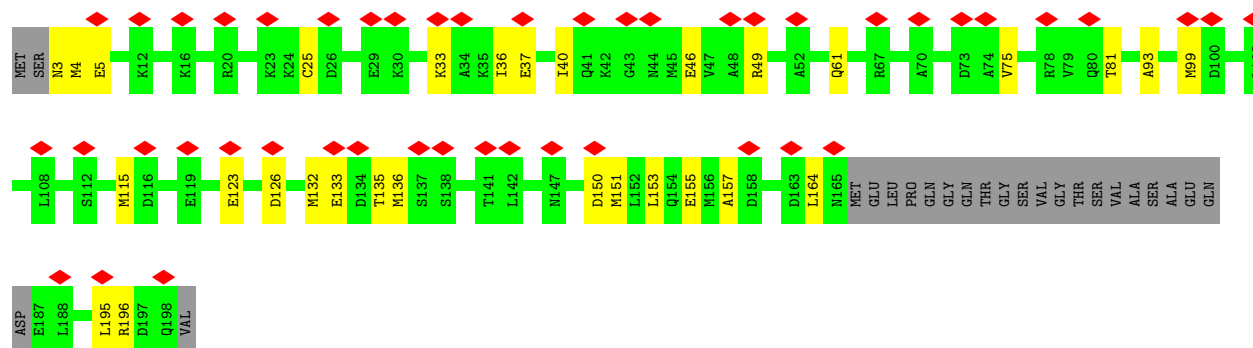
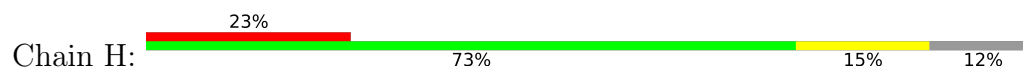




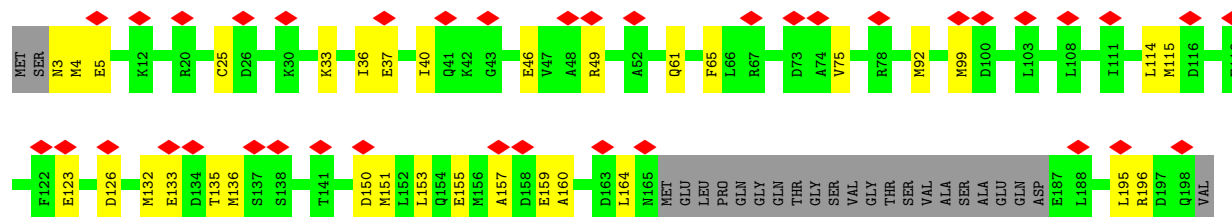
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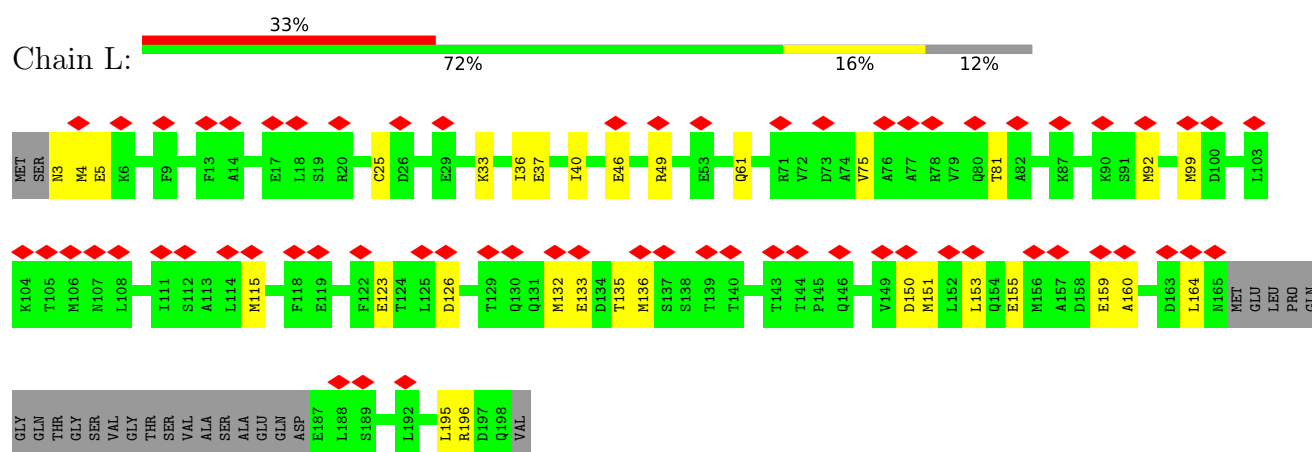
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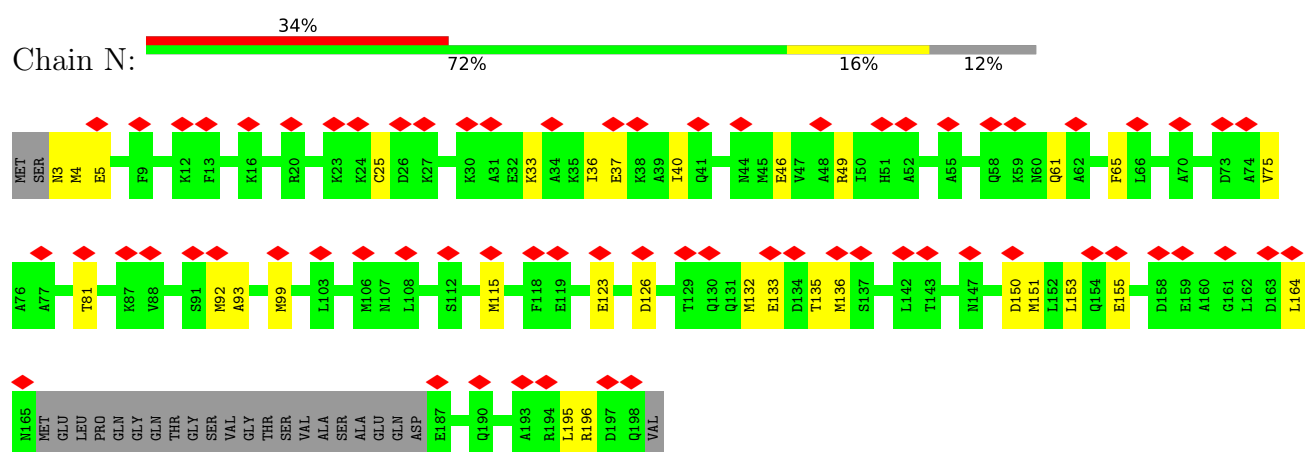
- Molecule 1: Charged multivesicular body protein 1b



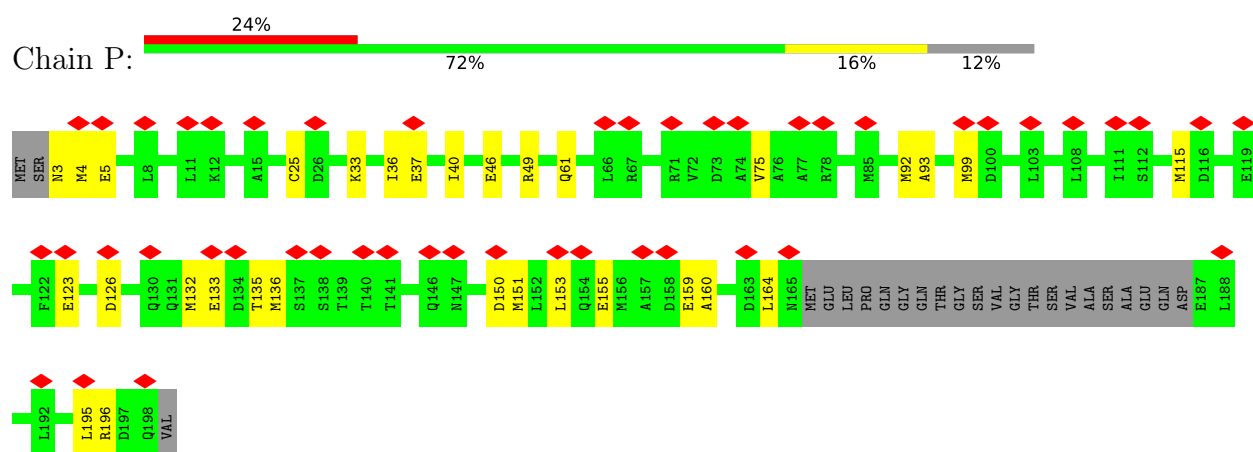
- Molecule 1: Charged multivesicular body protein 1b



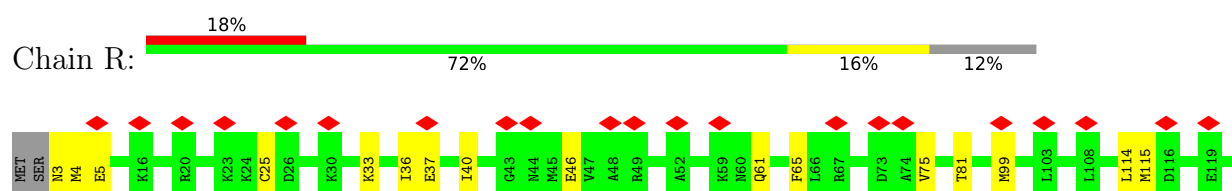
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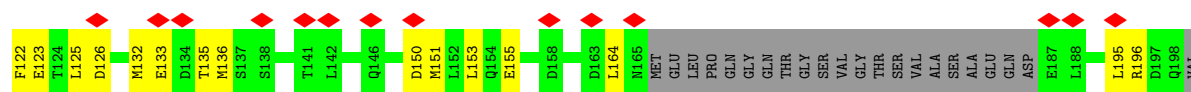


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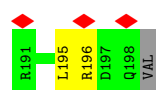
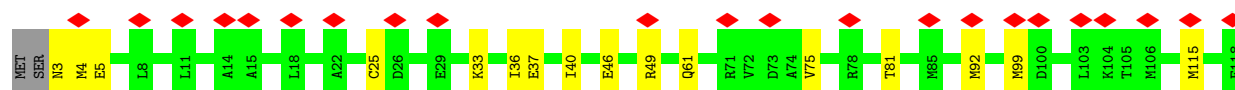
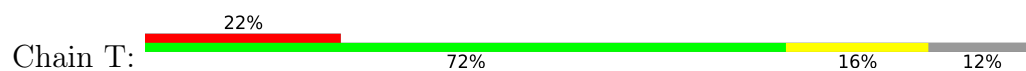


• Molecule 1: Charged multivesicular body protein 1b

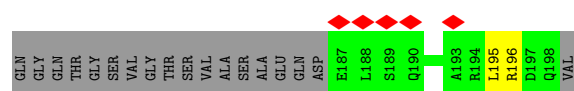
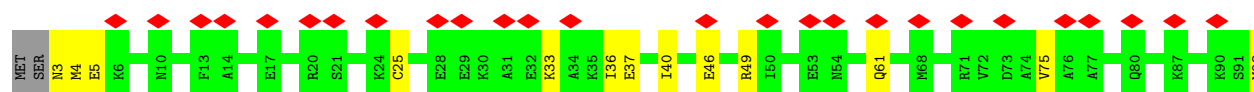
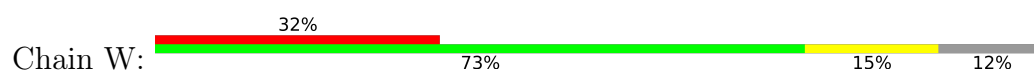




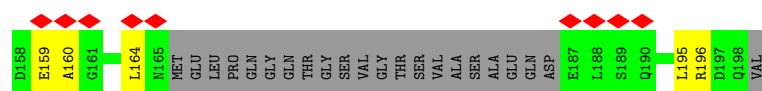
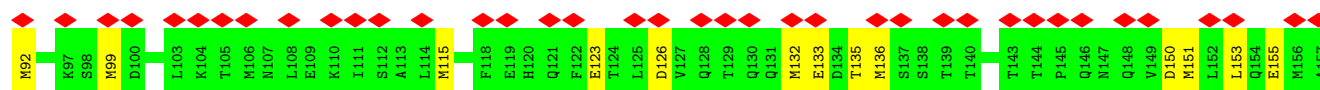
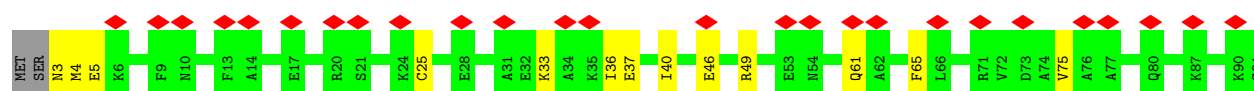
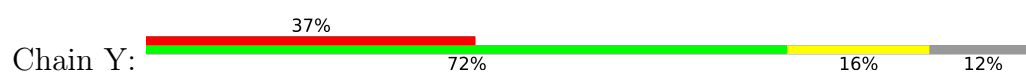
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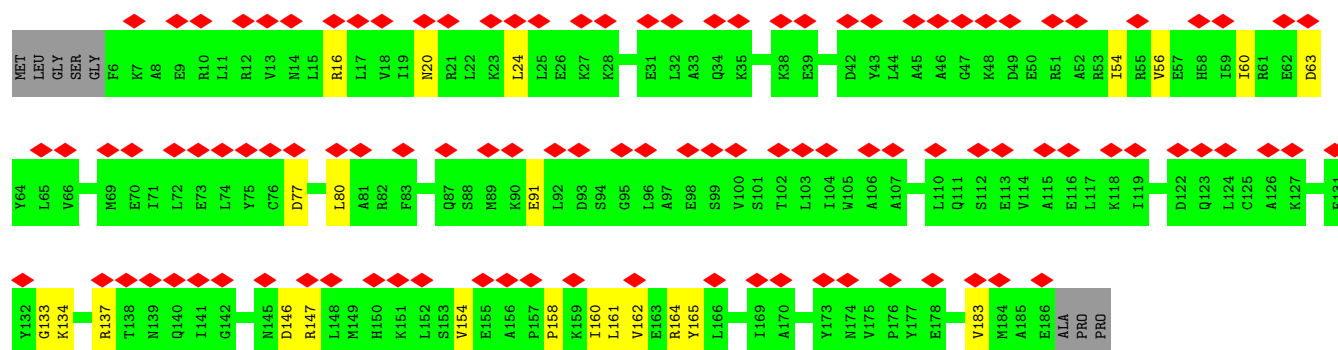
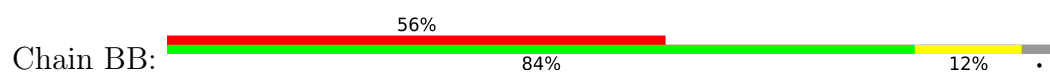
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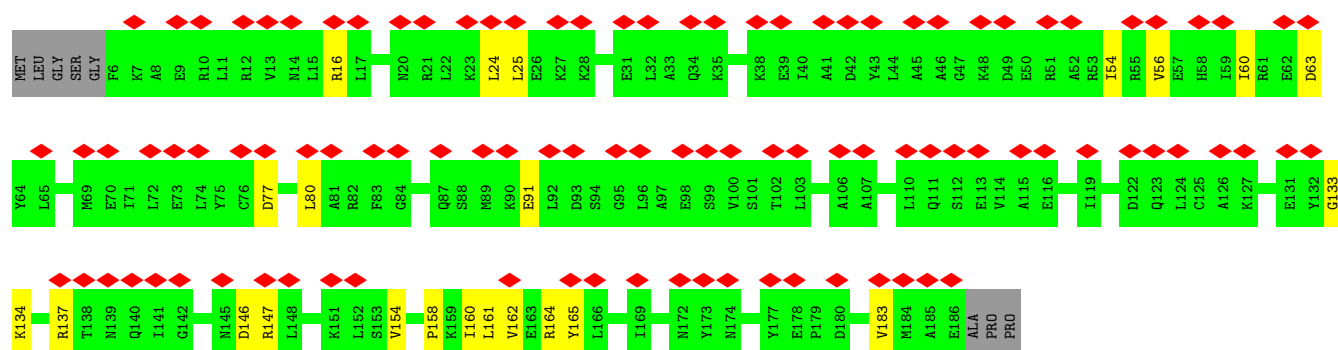
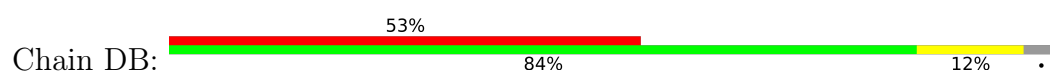
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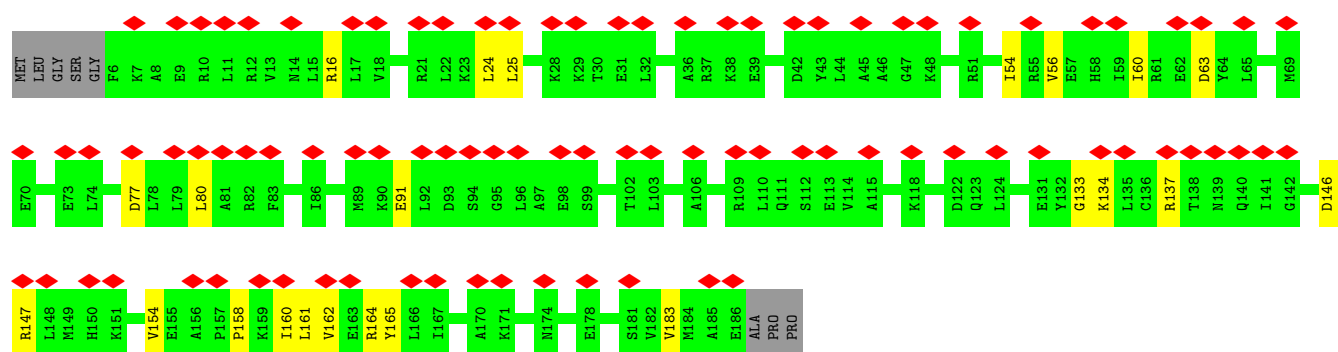
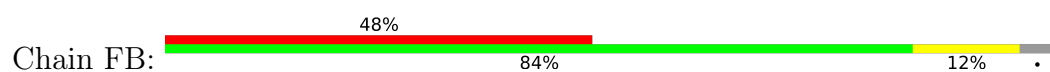
- Molecule 2: IST1 homolog



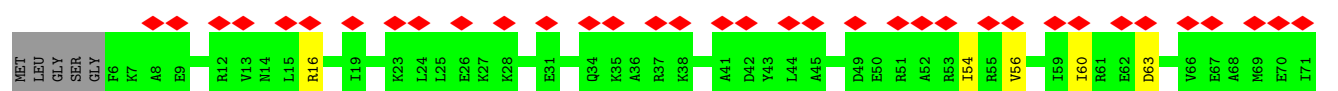
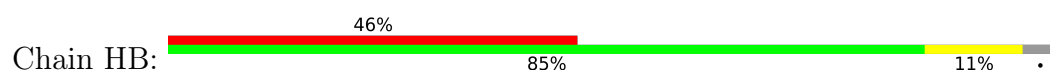
• Molecule 2: IST1 homolog

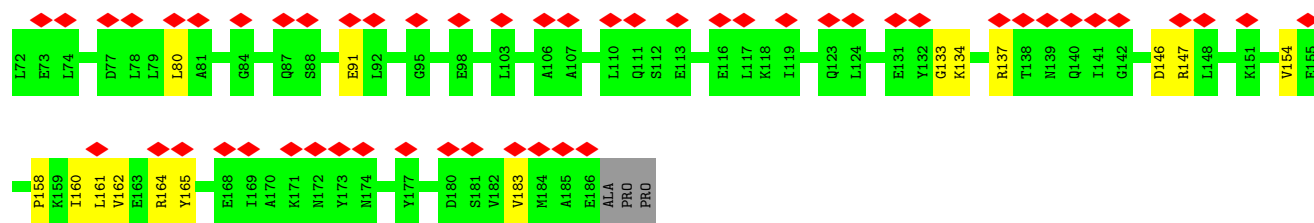


• Molecule 2: IST1 homolog

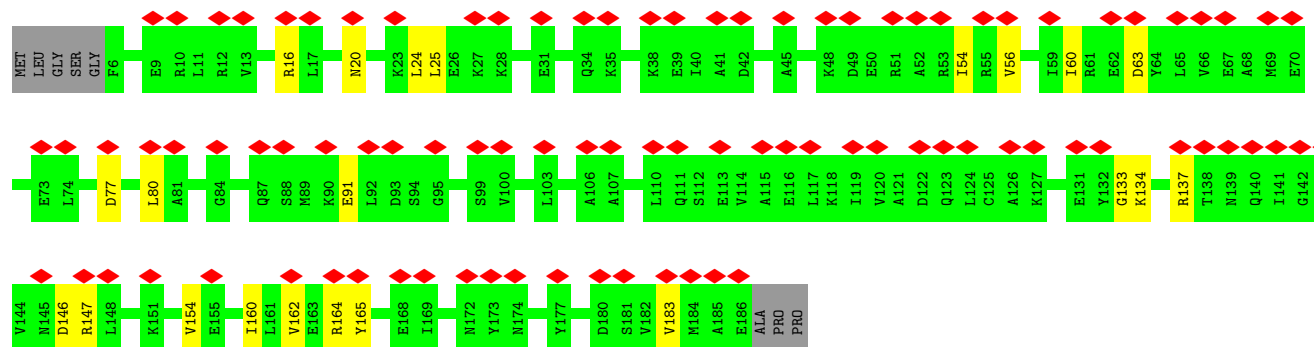
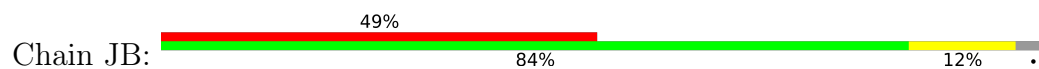


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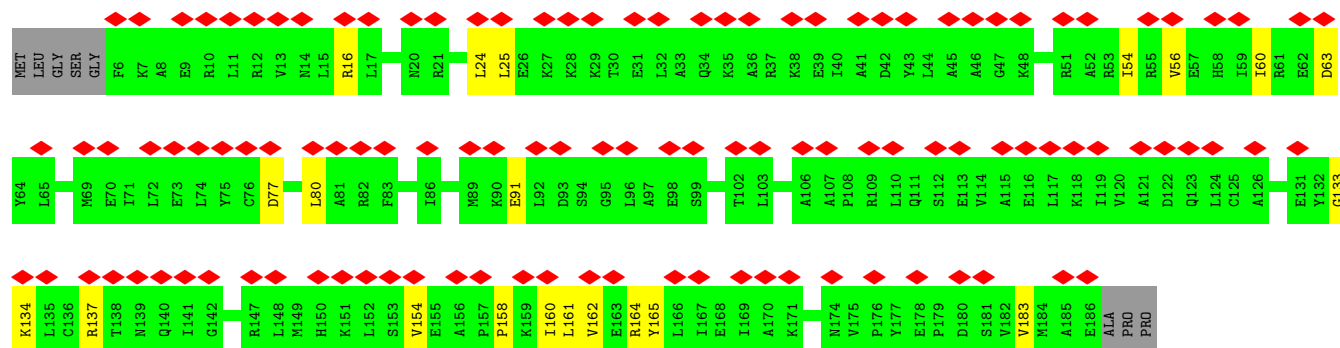
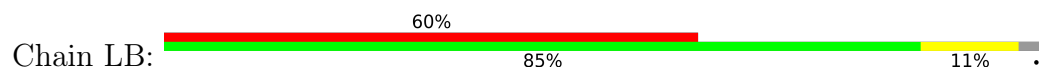




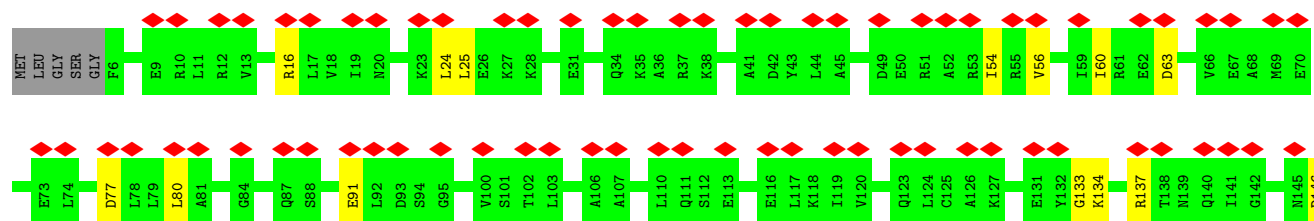
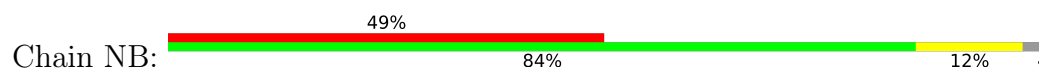
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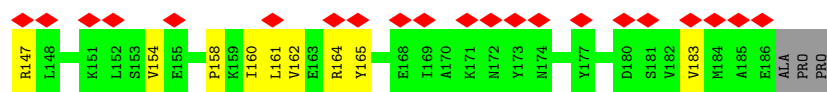


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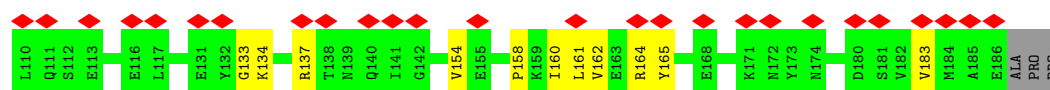
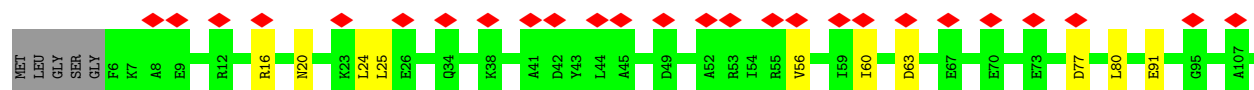
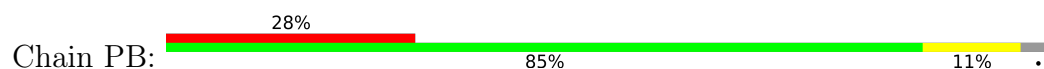


• Molecule 2: IST1 homolog

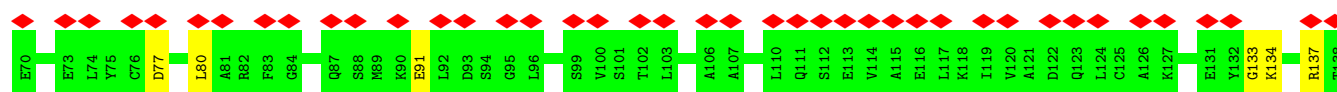
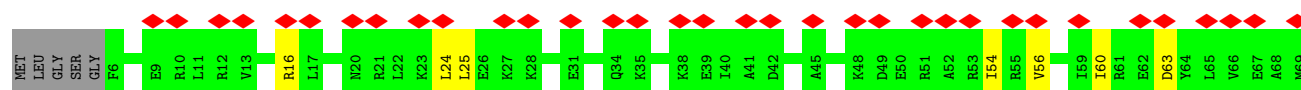
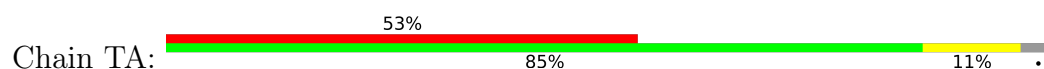




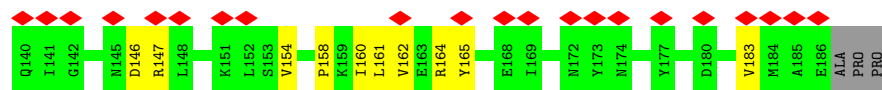
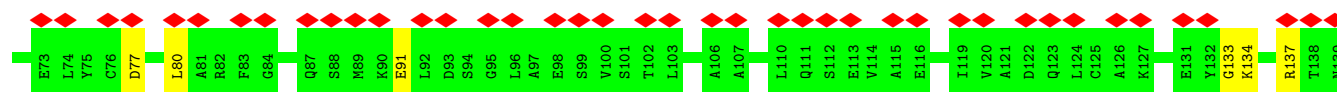
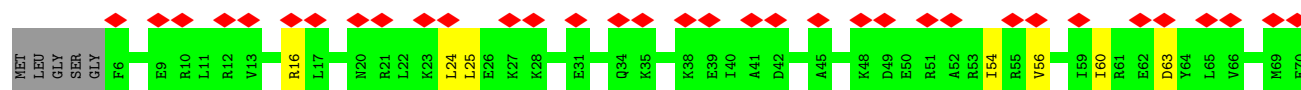
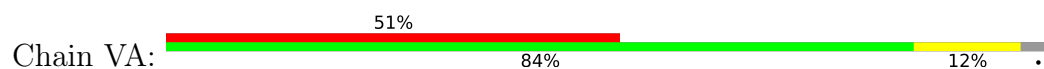
- Molecule 2: IST1 homolog



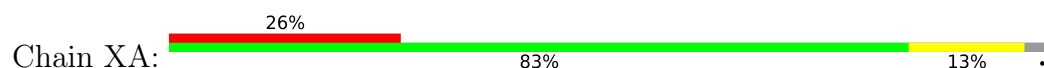
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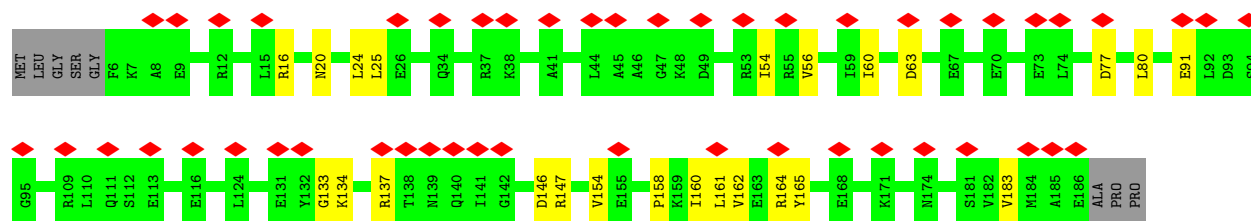


- Molecule 2: IST1 homolog

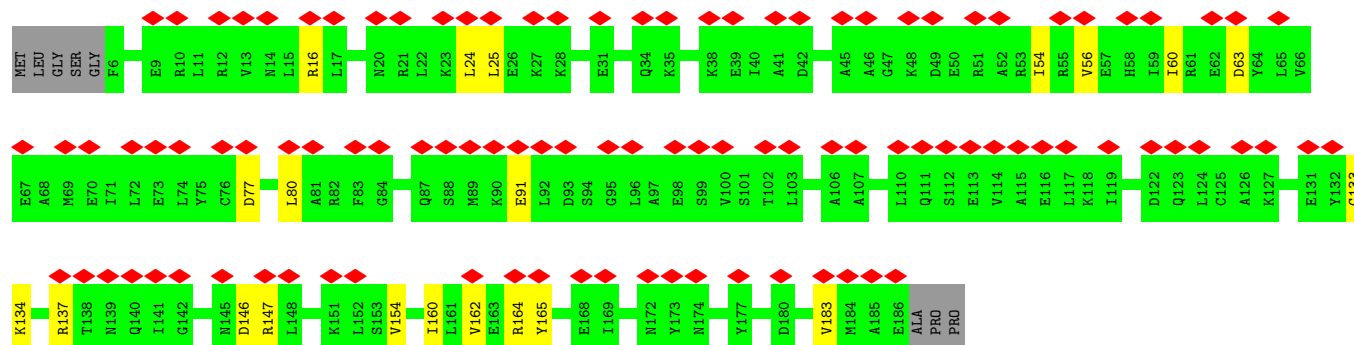
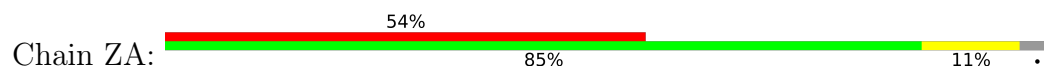


- Molecule 2: IST1 homolog

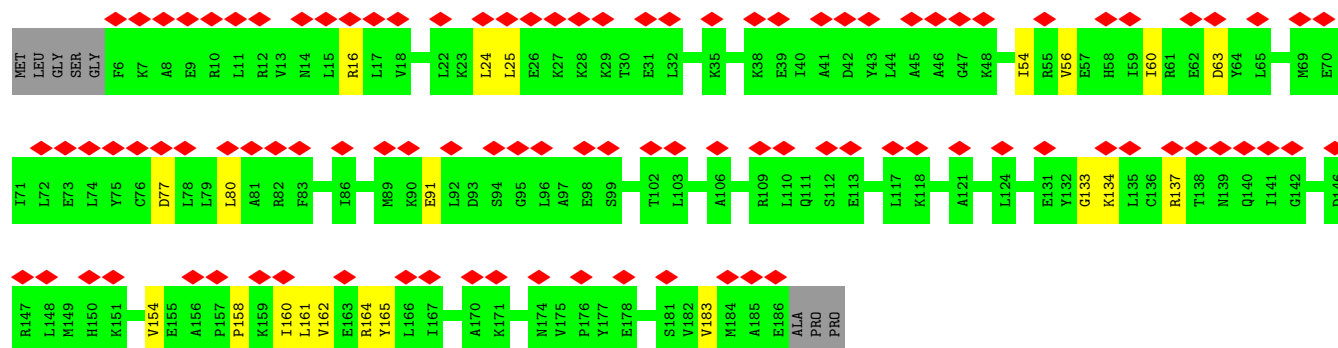
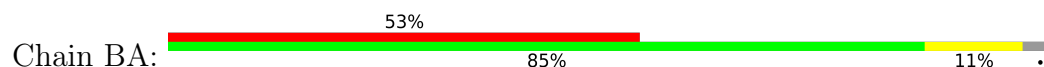




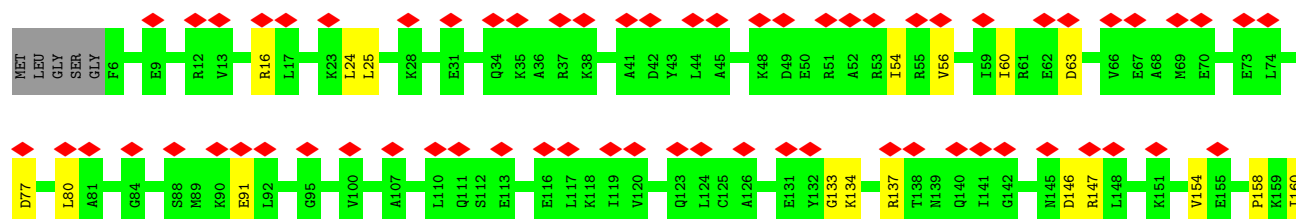
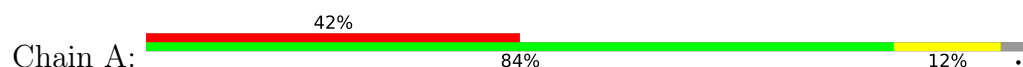
• Molecule 2: IST1 homolog



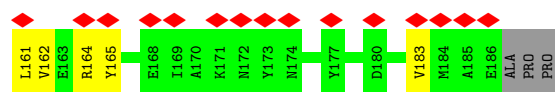
• Molecule 2: IST1 homolog



• Molecule 2: IST1 homolog

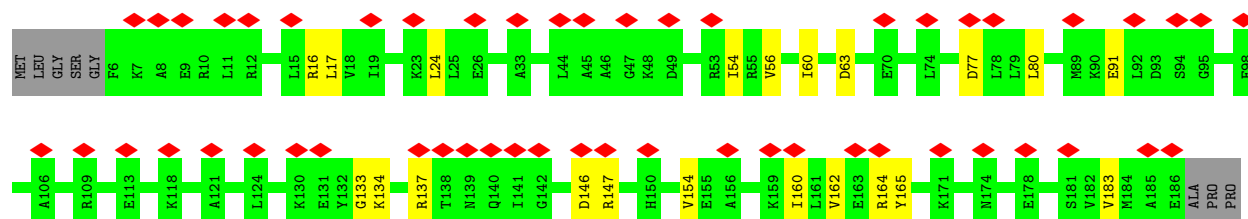






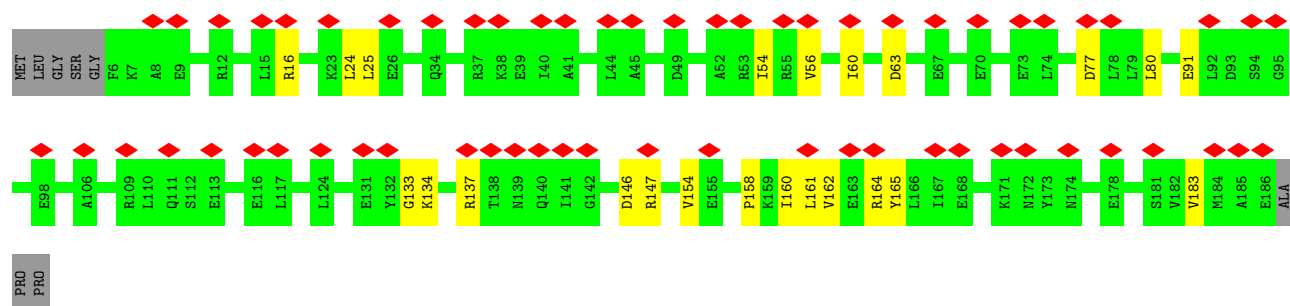
- Molecule 2: IST1 homolog

Chain DA: 28% 85% 11% .



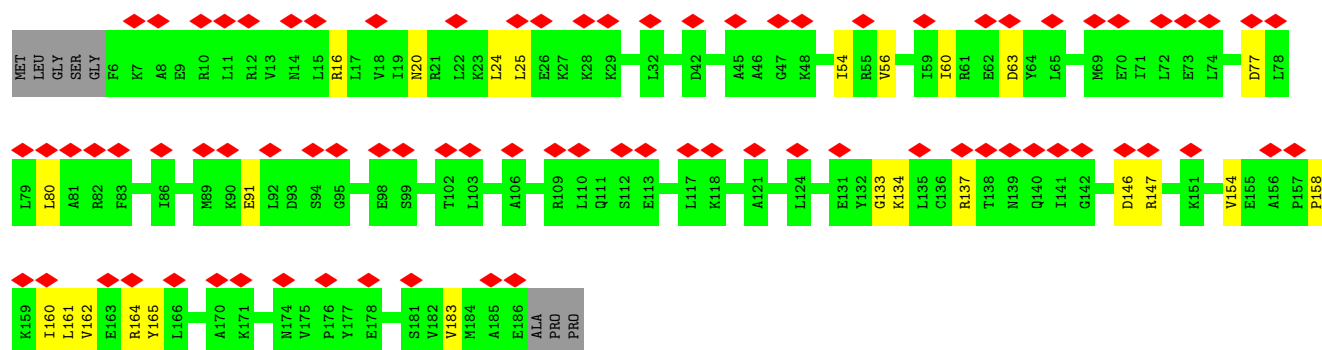
- Molecule 2: IST1 homolog

Chain FA: 32% 84% 12% .



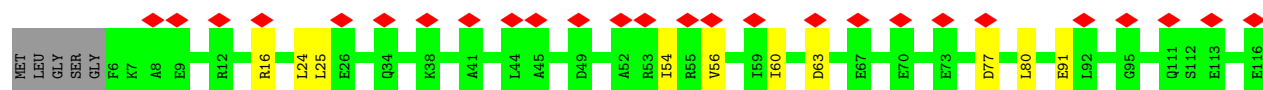
- Molecule 2: IST1 homolog

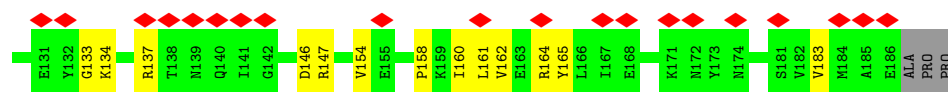
Chain HA: 42% 83% 13% .



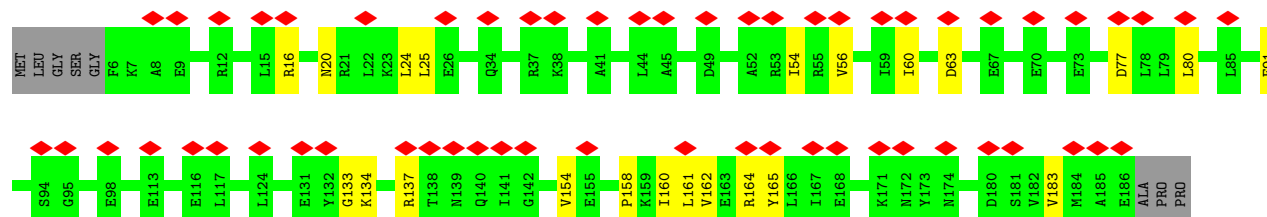
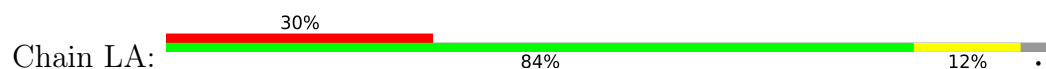
- Molecule 2: IST1 homolog

Chain JA: 24% 84% 12% .

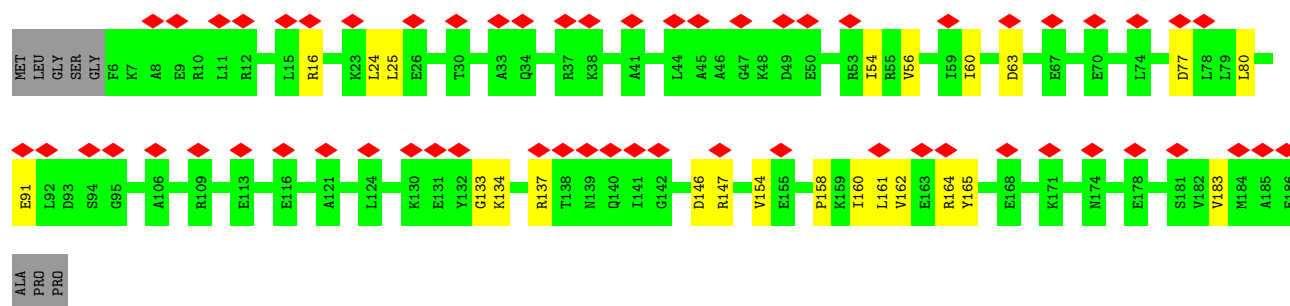
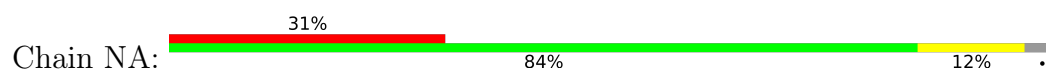




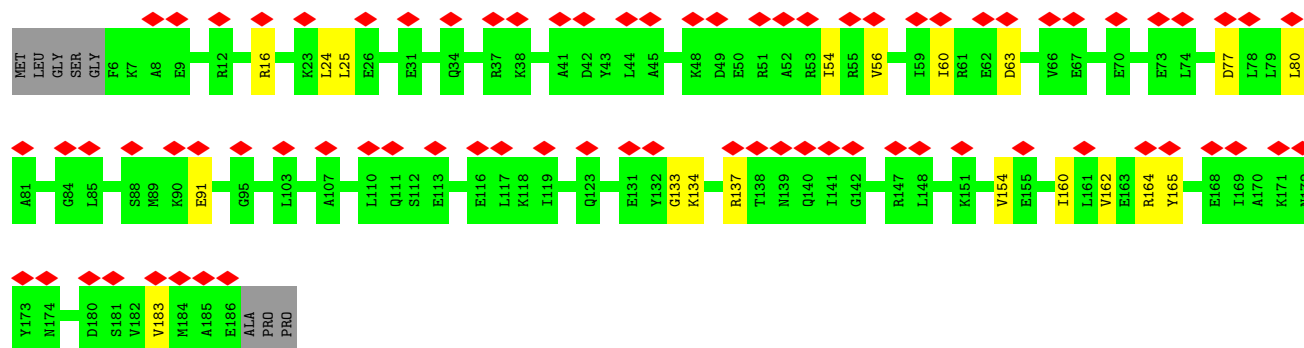
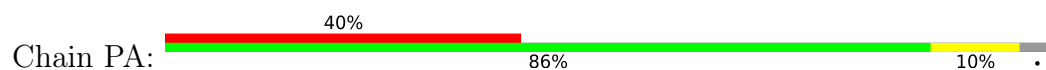
• Molecule 2: IST1 homolog



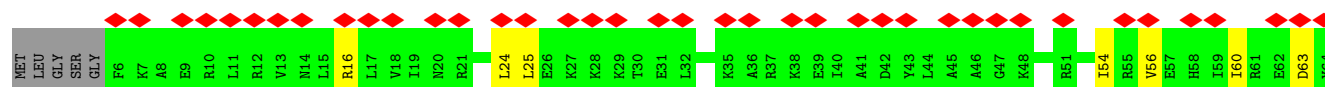
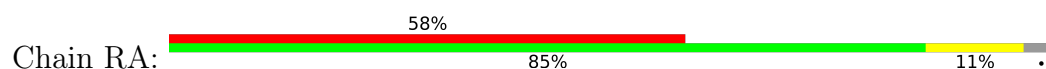
• Molecule 2: IST1 homolog

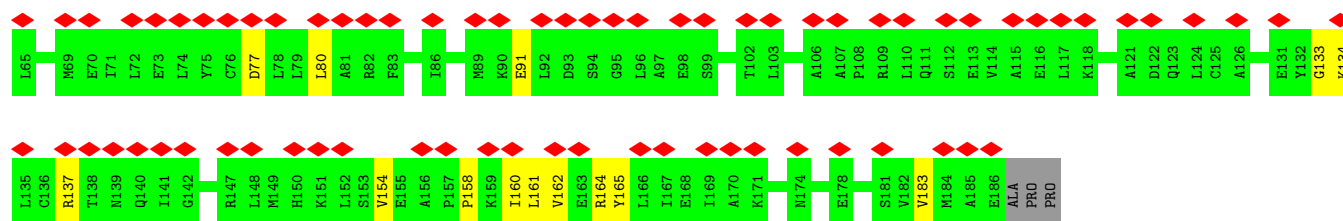


• Molecule 2: IST1 homolog

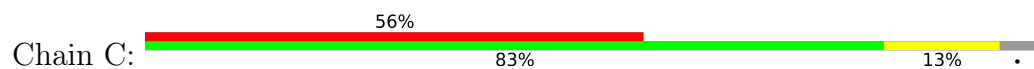


• Molecule 2: IST1 homolog

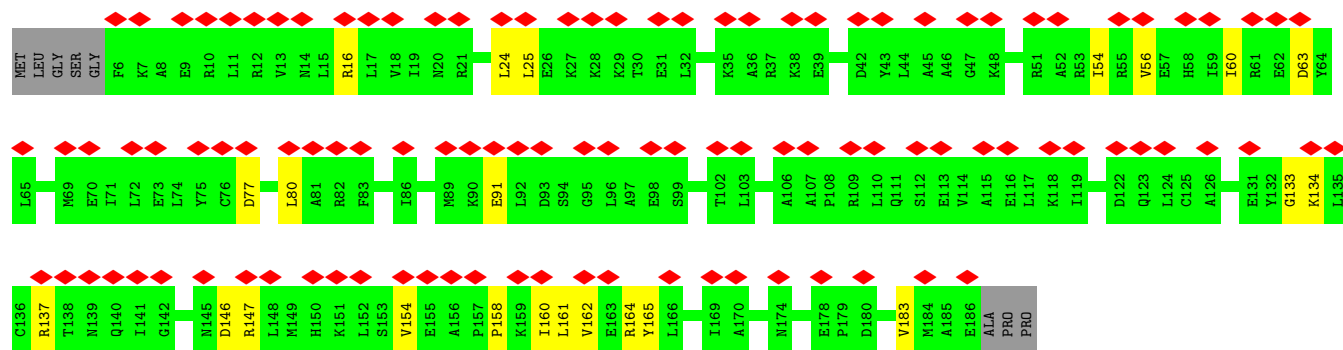
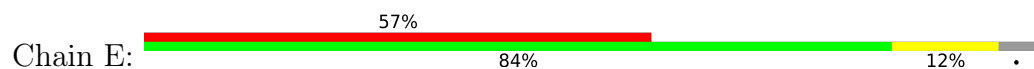




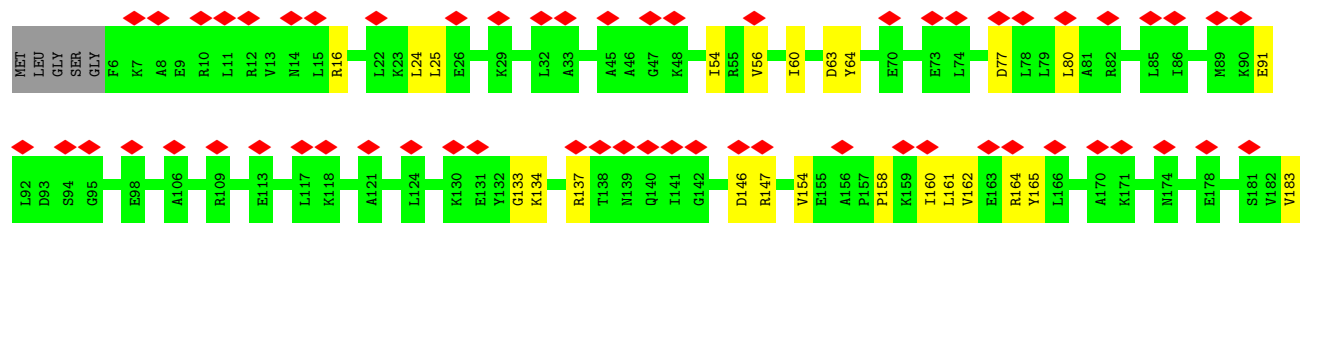
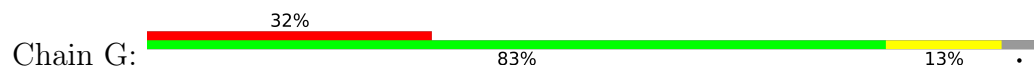
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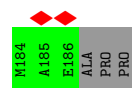


• Molecule 2: IST1 homolog

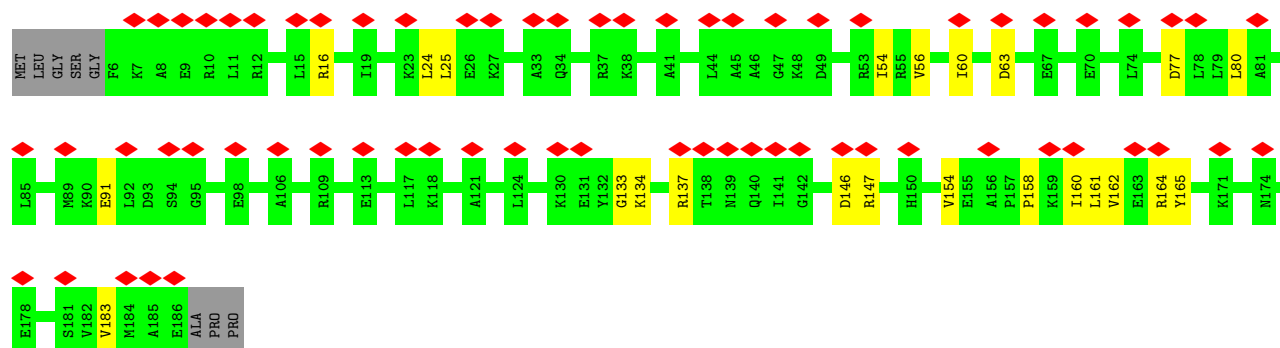
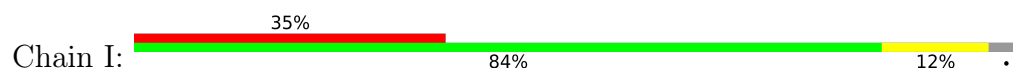


• Molecule 2: IST1 homolog

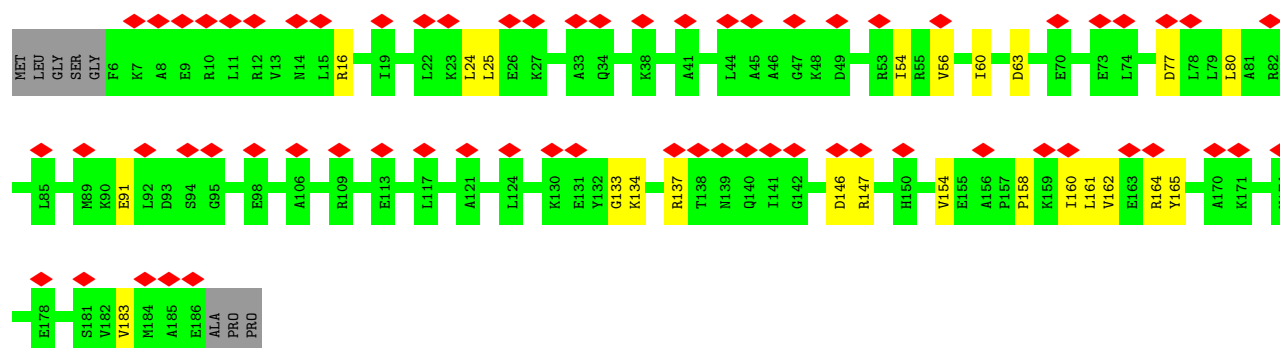
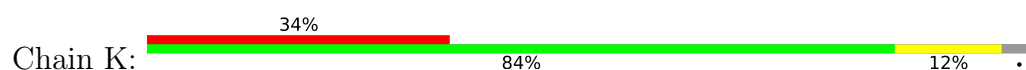




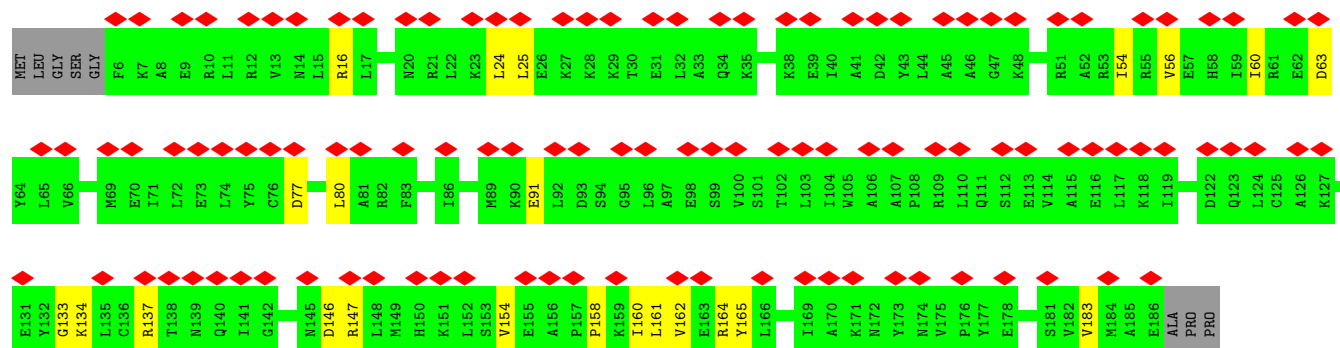
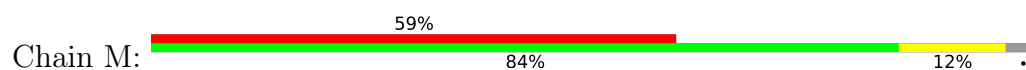
- Molecule 2: IST1 homolog



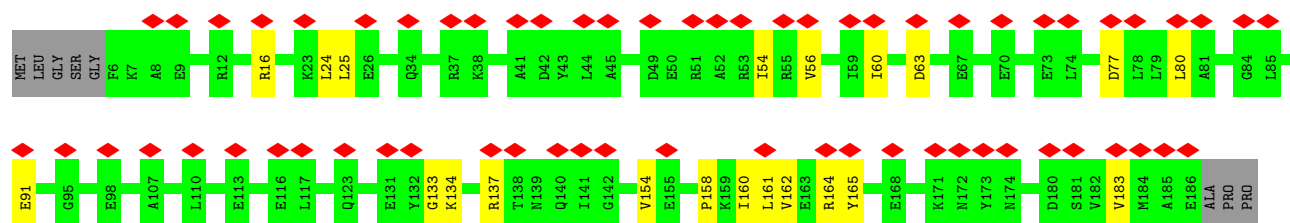
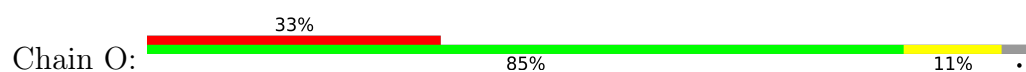
- Molecule 2: IST1 homolog



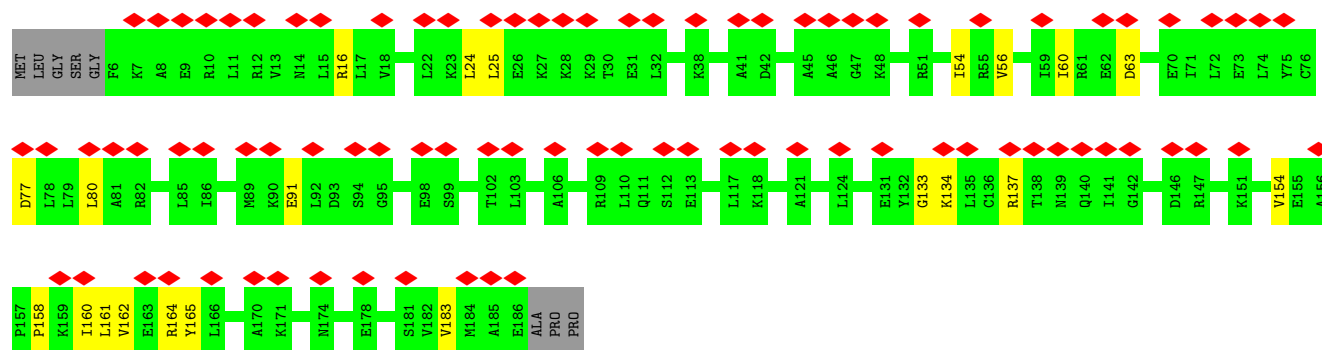
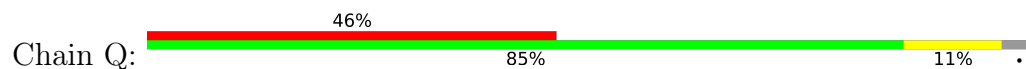
- Molecule 2: IST1 homolog



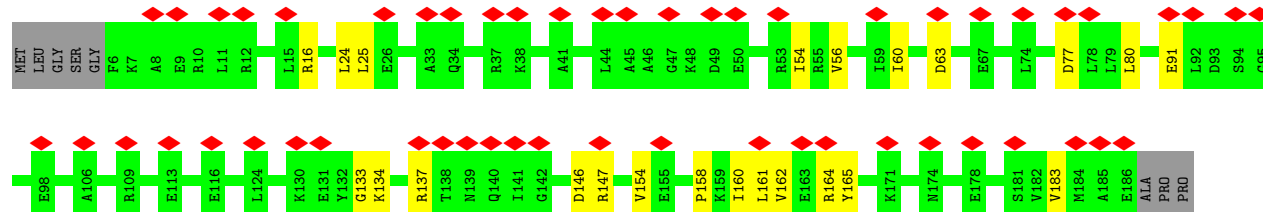
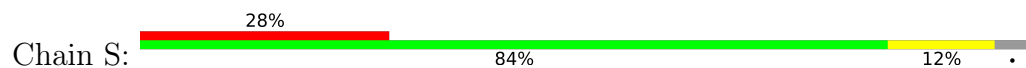
- Molecule 2: IST1 homolog



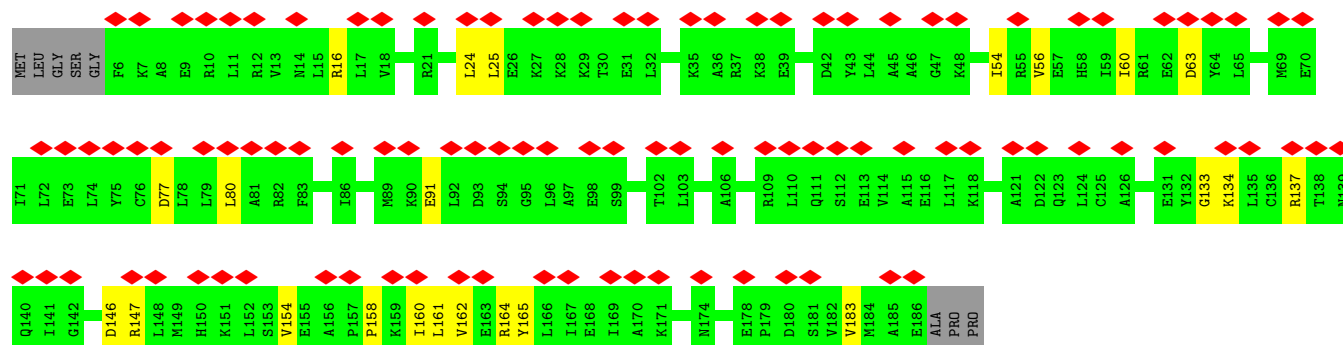
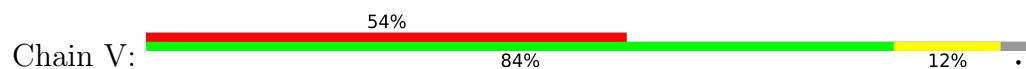
• Molecule 2: IST1 homolog



• Molecule 2: IST1 homolog

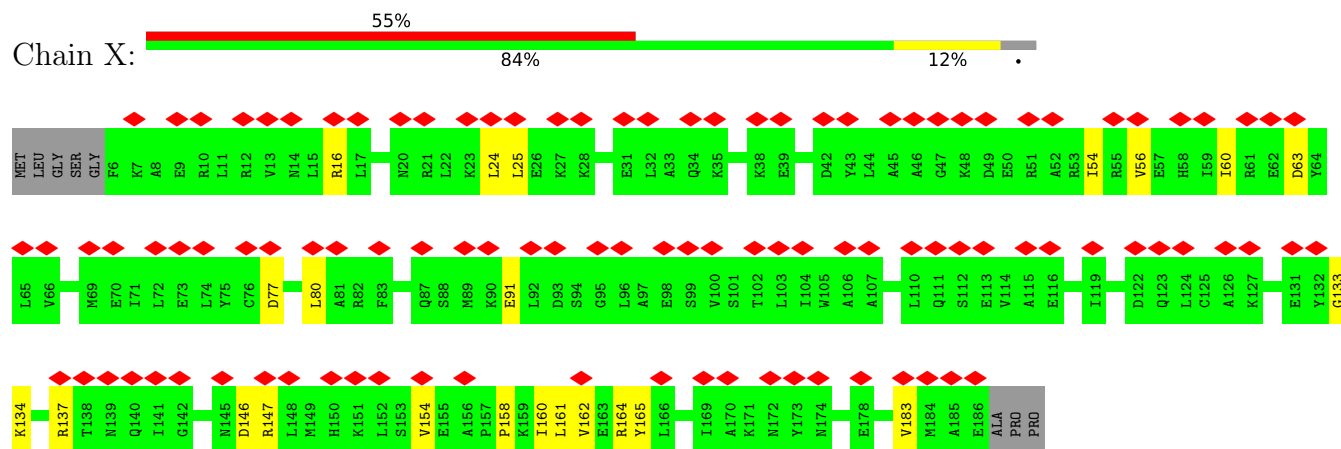


• Molecule 2: IST1 homolog



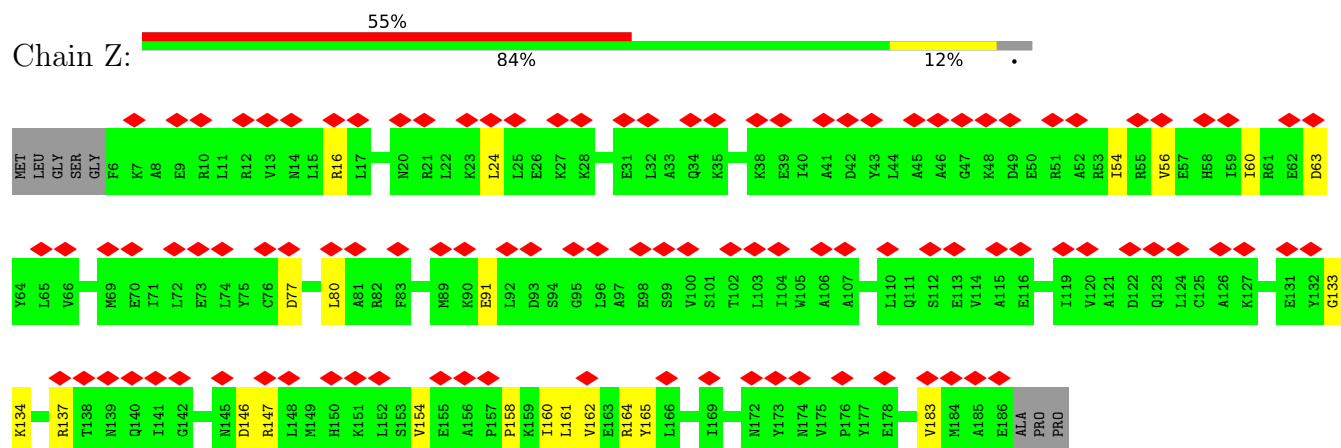
- Molecule 2: IST1 homolog

Chain X:



- Molecule 2: IST1 homolog

Chain Z:



## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-20.77°, rise=3.06 Å, axial sym=C1	Depositor
Number of segments used	73749	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{Å}^2$ )	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	429.44, 429.44, 429.44	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.22, 1.22, 1.22	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	AA	0.26	0/1351	0.40	0/1806
1	AB	0.26	0/1351	0.40	0/1806
1	B	0.26	0/1351	0.40	0/1806
1	CA	0.26	0/1351	0.40	0/1806
1	CB	0.26	0/1351	0.40	0/1806
1	D	0.26	0/1351	0.40	0/1806
1	EA	0.26	0/1351	0.40	0/1806
1	EB	0.26	0/1351	0.40	0/1806
1	F	0.26	0/1351	0.40	0/1806
1	GA	0.26	0/1351	0.40	0/1806
1	GB	0.26	0/1351	0.40	0/1806
1	H	0.26	0/1351	0.40	0/1806
1	IA	0.26	0/1351	0.40	0/1806
1	IB	0.26	0/1351	0.40	0/1806
1	J	0.26	0/1351	0.40	0/1806
1	KA	0.26	0/1351	0.40	0/1806
1	KB	0.26	0/1351	0.40	0/1806
1	L	0.26	0/1351	0.40	0/1806
1	MA	0.26	0/1351	0.40	0/1806
1	MB	0.26	0/1351	0.40	0/1806
1	N	0.26	0/1351	0.40	0/1806
1	OA	0.26	0/1351	0.40	0/1806
1	OB	0.26	0/1351	0.40	0/1806
1	P	0.26	0/1351	0.40	0/1806
1	QA	0.26	0/1351	0.40	0/1806
1	QB	0.26	0/1351	0.40	0/1806
1	R	0.26	0/1351	0.40	0/1806
1	SA	0.26	0/1351	0.40	0/1806
1	T	0.26	0/1351	0.40	0/1806
1	UA	0.26	0/1351	0.40	0/1806
1	W	0.26	0/1351	0.40	0/1806
1	WA	0.26	0/1351	0.40	0/1806
1	Y	0.26	0/1351	0.40	0/1806
1	YA	0.26	0/1351	0.40	0/1806



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	A	0.28	0/1423	0.40	0/1920
2	BA	0.28	0/1423	0.40	0/1920
2	BB	0.28	0/1423	0.40	0/1920
2	C	0.28	0/1423	0.40	0/1920
2	DA	0.28	0/1423	0.40	0/1920
2	DB	0.28	0/1423	0.40	0/1920
2	E	0.28	0/1423	0.40	0/1920
2	FA	0.28	0/1423	0.40	0/1920
2	FB	0.28	0/1423	0.40	0/1920
2	G	0.28	0/1423	0.40	0/1920
2	HA	0.28	0/1423	0.40	0/1920
2	HB	0.28	0/1423	0.40	0/1920
2	I	0.28	0/1423	0.40	0/1920
2	JA	0.28	0/1423	0.40	0/1920
2	JB	0.28	0/1423	0.40	0/1920
2	K	0.28	0/1423	0.40	0/1920
2	LA	0.28	0/1423	0.40	0/1920
2	LB	0.28	0/1423	0.40	0/1920
2	M	0.28	0/1423	0.40	0/1920
2	NA	0.28	0/1423	0.40	0/1920
2	NB	0.28	0/1423	0.40	0/1920
2	O	0.28	0/1423	0.40	0/1920
2	PA	0.28	0/1423	0.40	0/1920
2	PB	0.28	0/1423	0.40	0/1920
2	Q	0.28	0/1423	0.40	0/1920
2	RA	0.28	0/1423	0.40	0/1920
2	S	0.28	0/1423	0.40	0/1920
2	TA	0.28	0/1423	0.40	0/1920
2	V	0.28	0/1423	0.40	0/1920
2	VA	0.28	0/1423	0.40	0/1920
2	X	0.28	0/1423	0.40	0/1920
2	XA	0.28	0/1423	0.40	0/1920
2	Z	0.28	0/1423	0.40	0/1920
2	ZA	0.28	0/1423	0.40	0/1920
All	All	0.27	0/94316	0.40	0/126684

There are no bond length outliers.

There are no bond angle outliers.

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	AA	1344	0	1368	35	0
1	AB	1344	0	1368	33	0
1	B	1344	0	1368	32	0
1	CA	1344	0	1368	44	0
1	CB	1344	0	1368	34	0
1	D	1344	0	1368	34	0
1	EA	1344	0	1368	35	0
1	EB	1344	0	1368	33	0
1	F	1344	0	1368	55	0
1	GA	1344	0	1368	40	0
1	GB	1344	0	1368	27	0
1	H	1344	0	1368	34	0
1	IA	1344	0	1368	31	0
1	IB	1344	0	1368	34	0
1	J	1344	0	1368	37	0
1	KA	1344	0	1368	33	0
1	KB	1344	0	1368	35	0
1	L	1344	0	1368	34	0
1	MA	1344	0	1368	36	0
1	MB	1344	0	1368	29	0
1	N	1344	0	1368	37	0
1	OA	1344	0	1368	36	0
1	OB	1344	0	1368	22	0
1	P	1344	0	1368	36	0
1	QA	1344	0	1368	35	0
1	QB	1344	0	1368	31	0
1	R	1344	0	1368	32	0
1	SA	1344	0	1368	35	0
1	T	1344	0	1368	34	0
1	UA	1344	0	1368	31	0
1	W	1344	0	1368	33	0
1	WA	1344	0	1368	30	0
1	Y	1344	0	1368	34	0
1	YA	1344	0	1368	33	0
2	A	1406	0	1423	26	0
2	BA	1406	0	1423	25	0
2	BB	1406	0	1423	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1406	0	1423	27	0
2	DA	1406	0	1423	26	0
2	DB	1406	0	1423	26	0
2	E	1406	0	1423	27	0
2	FA	1406	0	1423	26	0
2	FB	1406	0	1423	27	0
2	G	1406	0	1423	28	0
2	HA	1406	0	1423	27	0
2	HB	1406	0	1423	20	0
2	I	1406	0	1423	27	0
2	JA	1406	0	1423	27	0
2	JB	1406	0	1423	27	0
2	K	1406	0	1423	27	0
2	LA	1406	0	1423	25	0
2	LB	1406	0	1423	25	0
2	M	1406	0	1423	27	0
2	NA	1406	0	1423	27	0
2	NB	1406	0	1423	27	0
2	O	1406	0	1423	24	0
2	PA	1406	0	1423	24	0
2	PB	1406	0	1423	24	0
2	Q	1406	0	1423	25	0
2	RA	1406	0	1423	25	0
2	S	1406	0	1423	27	0
2	TA	1406	0	1423	26	0
2	V	1406	0	1423	27	0
2	VA	1406	0	1423	27	0
2	X	1406	0	1423	25	0
2	XA	1406	0	1423	28	0
2	Z	1406	0	1423	26	0
2	ZA	1406	0	1423	25	0
All	All	93500	0	94894	1355	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 1355 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:IB:126:ASP:OD2	2:VA:24:LEU:HD12	1.83	0.79
1:CA:126:ASP:OD2	2:S:24:LEU:HD12	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DB:24:LEU:HD12	1:SA:126:ASP:OD2	1.83	0.78
1:AB:126:ASP:OD2	2:E:24:LEU:HD12	1.84	0.78
1:WA:126:ASP:OD2	2:C:24:LEU:HD12	1.83	0.78

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	171/199 (86%)	171 (100%)	0	0	100	100
1	AB	171/199 (86%)	171 (100%)	0	0	100	100
1	B	171/199 (86%)	171 (100%)	0	0	100	100
1	CA	171/199 (86%)	171 (100%)	0	0	100	100
1	CB	171/199 (86%)	171 (100%)	0	0	100	100
1	D	171/199 (86%)	171 (100%)	0	0	100	100
1	EA	171/199 (86%)	171 (100%)	0	0	100	100
1	EB	171/199 (86%)	171 (100%)	0	0	100	100
1	F	171/199 (86%)	171 (100%)	0	0	100	100
1	GA	171/199 (86%)	171 (100%)	0	0	100	100
1	GB	171/199 (86%)	171 (100%)	0	0	100	100
1	H	171/199 (86%)	171 (100%)	0	0	100	100
1	IA	171/199 (86%)	171 (100%)	0	0	100	100
1	IB	171/199 (86%)	171 (100%)	0	0	100	100
1	J	171/199 (86%)	171 (100%)	0	0	100	100
1	KA	171/199 (86%)	171 (100%)	0	0	100	100
1	KB	171/199 (86%)	171 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	171/199 (86%)	171 (100%)	0	0	100	100
1	MA	171/199 (86%)	171 (100%)	0	0	100	100
1	MB	171/199 (86%)	171 (100%)	0	0	100	100
1	N	171/199 (86%)	171 (100%)	0	0	100	100
1	OA	171/199 (86%)	171 (100%)	0	0	100	100
1	OB	171/199 (86%)	171 (100%)	0	0	100	100
1	P	171/199 (86%)	171 (100%)	0	0	100	100
1	QA	171/199 (86%)	171 (100%)	0	0	100	100
1	QB	171/199 (86%)	171 (100%)	0	0	100	100
1	R	171/199 (86%)	171 (100%)	0	0	100	100
1	SA	171/199 (86%)	171 (100%)	0	0	100	100
1	T	171/199 (86%)	171 (100%)	0	0	100	100
1	UA	171/199 (86%)	171 (100%)	0	0	100	100
1	W	171/199 (86%)	171 (100%)	0	0	100	100
1	WA	171/199 (86%)	171 (100%)	0	0	100	100
1	Y	171/199 (86%)	171 (100%)	0	0	100	100
1	YA	171/199 (86%)	171 (100%)	0	0	100	100
2	A	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	BA	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	BB	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	C	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	DA	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	DB	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	E	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	FA	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	FB	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	G	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	HA	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	HB	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	I	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	JA	179/189 (95%)	175 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	JB	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	K	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	LA	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	LB	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	M	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	NA	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	NB	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	O	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	PA	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	PB	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	Q	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	RA	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	S	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	TA	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	V	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	VA	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	X	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	XA	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	Z	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
2	ZA	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
All	All	11900/13192 (90%)	11764 (99%)	136 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	AA	144/169 (85%)	144 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	144/169 (85%)	144 (100%)	0	100	100
1	B	144/169 (85%)	144 (100%)	0	100	100
1	CA	144/169 (85%)	144 (100%)	0	100	100
1	CB	144/169 (85%)	144 (100%)	0	100	100
1	D	144/169 (85%)	144 (100%)	0	100	100
1	EA	144/169 (85%)	144 (100%)	0	100	100
1	EB	144/169 (85%)	144 (100%)	0	100	100
1	F	144/169 (85%)	144 (100%)	0	100	100
1	GA	144/169 (85%)	144 (100%)	0	100	100
1	GB	144/169 (85%)	144 (100%)	0	100	100
1	H	144/169 (85%)	144 (100%)	0	100	100
1	IA	144/169 (85%)	144 (100%)	0	100	100
1	IB	144/169 (85%)	144 (100%)	0	100	100
1	J	144/169 (85%)	144 (100%)	0	100	100
1	KA	144/169 (85%)	144 (100%)	0	100	100
1	KB	144/169 (85%)	144 (100%)	0	100	100
1	L	144/169 (85%)	144 (100%)	0	100	100
1	MA	144/169 (85%)	144 (100%)	0	100	100
1	MB	144/169 (85%)	144 (100%)	0	100	100
1	N	144/169 (85%)	144 (100%)	0	100	100
1	OA	144/169 (85%)	144 (100%)	0	100	100
1	OB	144/169 (85%)	144 (100%)	0	100	100
1	P	144/169 (85%)	144 (100%)	0	100	100
1	QA	144/169 (85%)	144 (100%)	0	100	100
1	QB	144/169 (85%)	144 (100%)	0	100	100
1	R	144/169 (85%)	144 (100%)	0	100	100
1	SA	144/169 (85%)	144 (100%)	0	100	100
1	T	144/169 (85%)	144 (100%)	0	100	100
1	UA	144/169 (85%)	144 (100%)	0	100	100
1	W	144/169 (85%)	144 (100%)	0	100	100
1	WA	144/169 (85%)	144 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Y	144/169 (85%)	144 (100%)	0	100	100
1	YA	144/169 (85%)	144 (100%)	0	100	100
2	A	141/163 (86%)	141 (100%)	0	100	100
2	BA	141/163 (86%)	141 (100%)	0	100	100
2	BB	141/163 (86%)	141 (100%)	0	100	100
2	C	141/163 (86%)	141 (100%)	0	100	100
2	DA	141/163 (86%)	141 (100%)	0	100	100
2	DB	141/163 (86%)	141 (100%)	0	100	100
2	E	141/163 (86%)	141 (100%)	0	100	100
2	FA	141/163 (86%)	141 (100%)	0	100	100
2	FB	141/163 (86%)	141 (100%)	0	100	100
2	G	141/163 (86%)	141 (100%)	0	100	100
2	HA	141/163 (86%)	141 (100%)	0	100	100
2	HB	141/163 (86%)	141 (100%)	0	100	100
2	I	141/163 (86%)	141 (100%)	0	100	100
2	JA	141/163 (86%)	141 (100%)	0	100	100
2	JB	141/163 (86%)	141 (100%)	0	100	100
2	K	141/163 (86%)	141 (100%)	0	100	100
2	LA	141/163 (86%)	141 (100%)	0	100	100
2	LB	141/163 (86%)	141 (100%)	0	100	100
2	M	141/163 (86%)	141 (100%)	0	100	100
2	NA	141/163 (86%)	141 (100%)	0	100	100
2	NB	141/163 (86%)	141 (100%)	0	100	100
2	O	141/163 (86%)	141 (100%)	0	100	100
2	PA	141/163 (86%)	141 (100%)	0	100	100
2	PB	141/163 (86%)	141 (100%)	0	100	100
2	Q	141/163 (86%)	141 (100%)	0	100	100
2	RA	141/163 (86%)	141 (100%)	0	100	100
2	S	141/163 (86%)	141 (100%)	0	100	100
2	TA	141/163 (86%)	141 (100%)	0	100	100
2	V	141/163 (86%)	141 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	VA	141/163 (86%)	141 (100%)	0	100	100
2	X	141/163 (86%)	141 (100%)	0	100	100
2	XA	141/163 (86%)	141 (100%)	0	100	100
2	Z	141/163 (86%)	141 (100%)	0	100	100
2	ZA	141/163 (86%)	141 (100%)	0	100	100
All	All	9690/11288 (86%)	9690 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 136 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	60	ASN
1	R	60	ASN
1	W	165	ASN
1	UA	61	GLN
1	UA	60	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

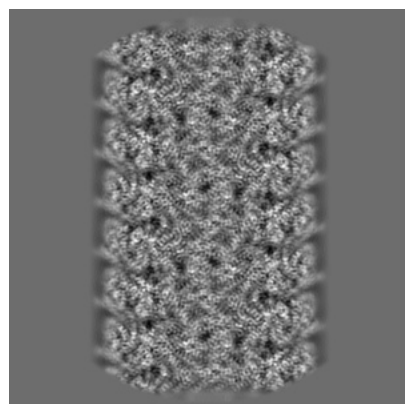
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20589. These allow visual inspection of the internal detail of the map and identification of artifacts.

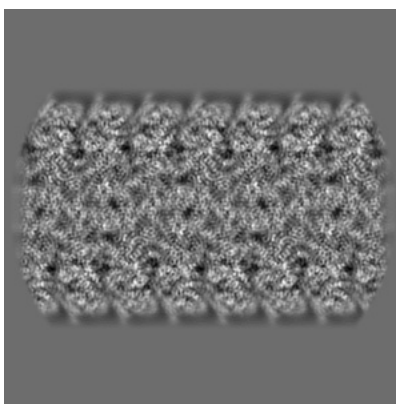
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

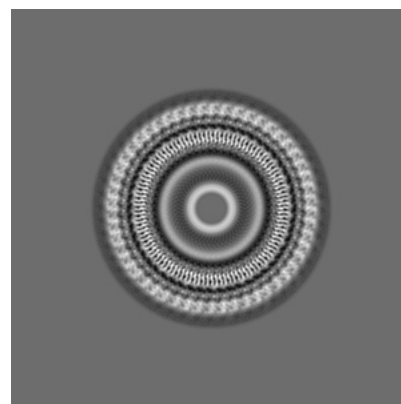
#### 6.1.1 Primary map



X

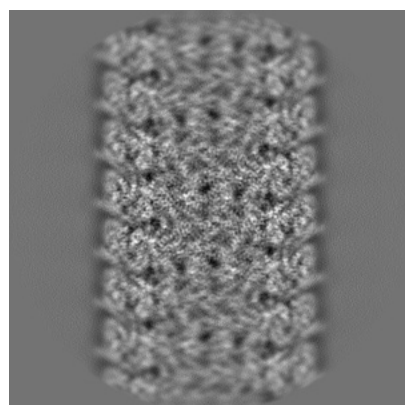


Y

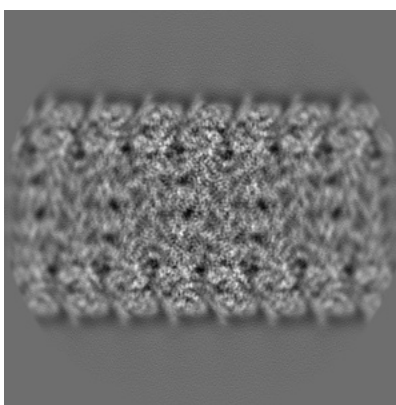


Z

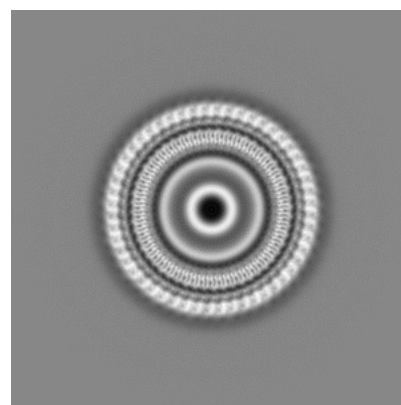
#### 6.1.2 Raw map



X



Y

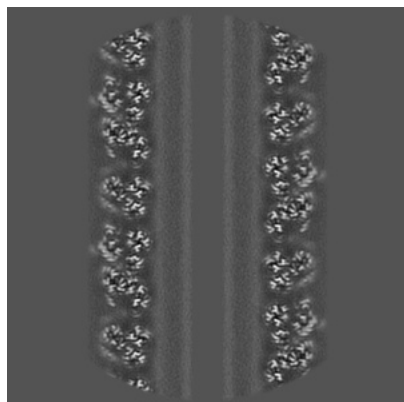


Z

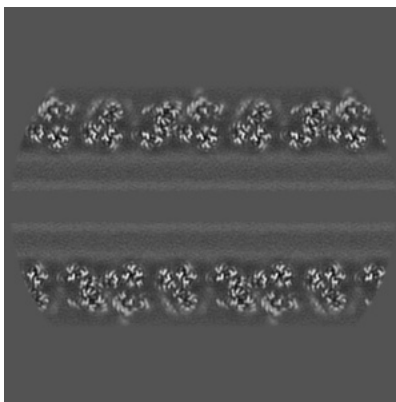
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

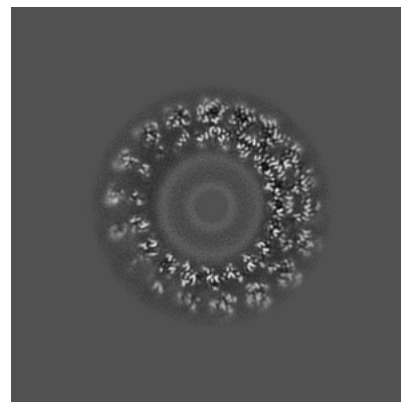
### 6.2.1 Primary map



X Index: 176

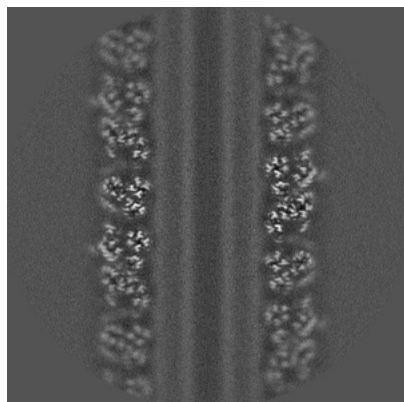


Y Index: 176

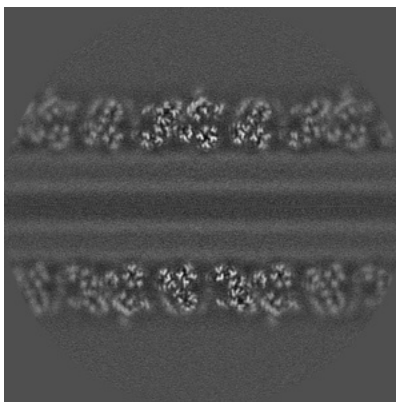


Z Index: 176

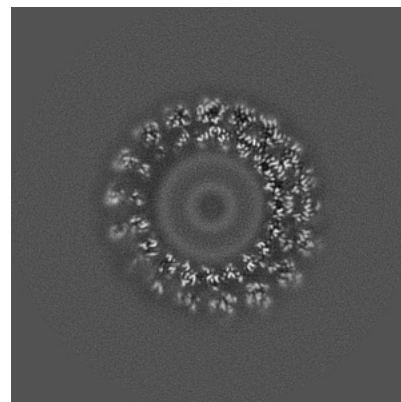
### 6.2.2 Raw map



X Index: 176



Y Index: 176

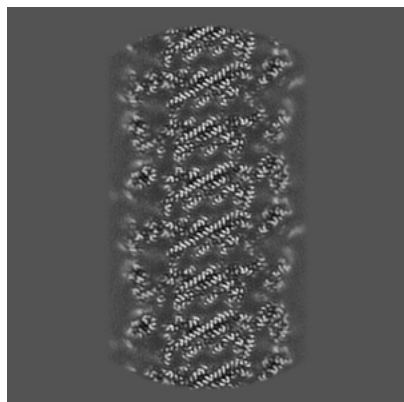


Z Index: 176

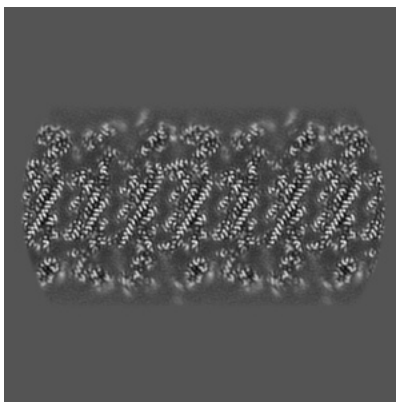
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

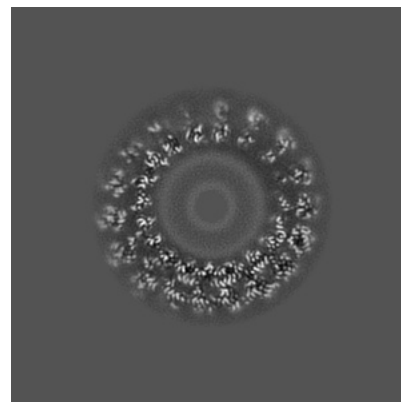
### 6.3.1 Primary map



X Index: 117

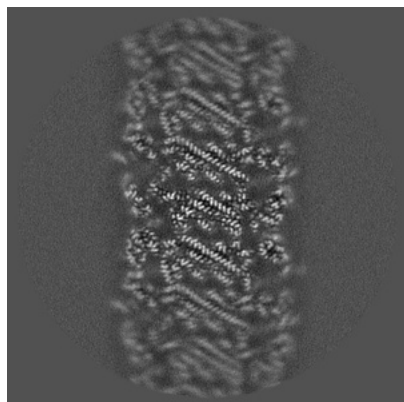


Y Index: 235

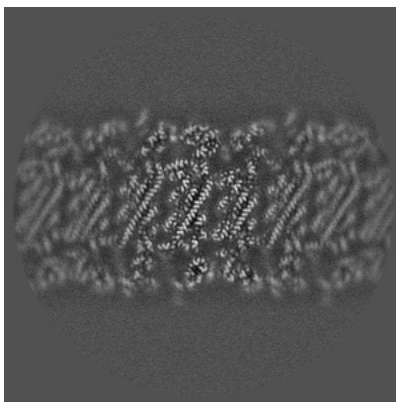


Z Index: 146

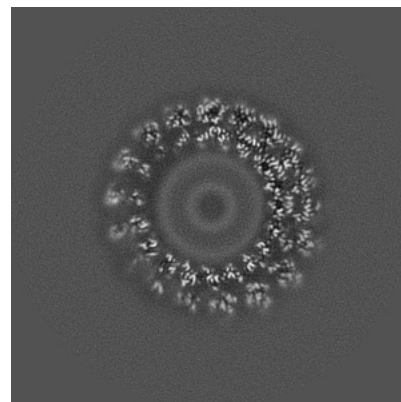
### 6.3.2 Raw map



X Index: 235



Y Index: 235

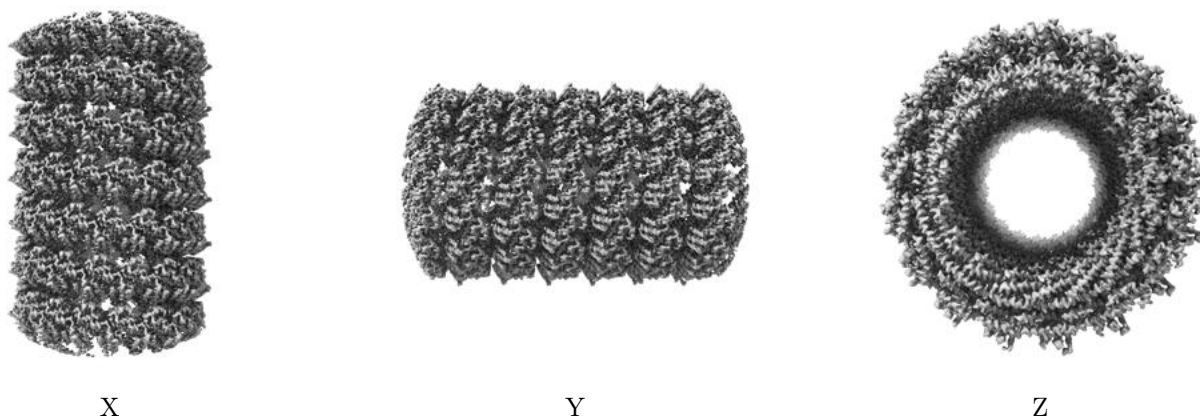


Z Index: 176

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

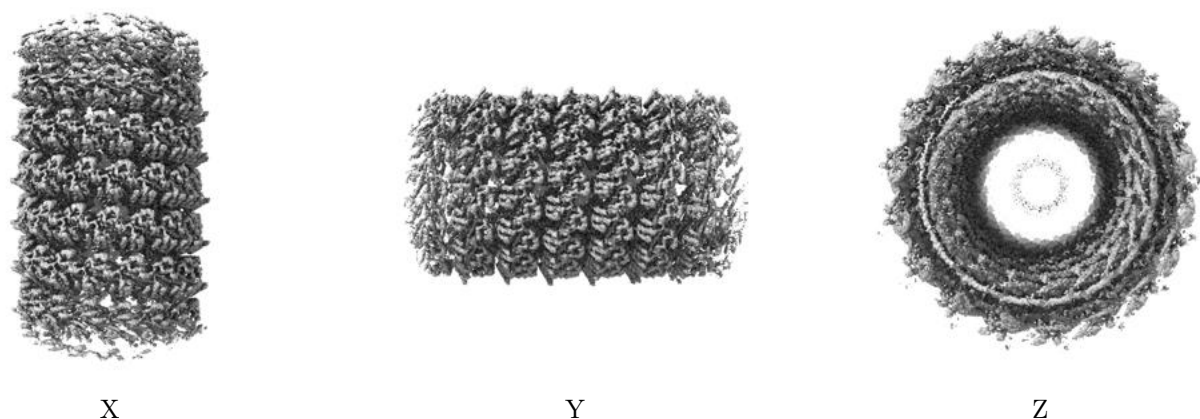
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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.



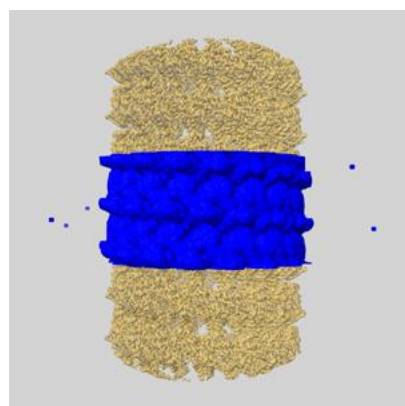
## 6.5 Mask visualisation [i](#)

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

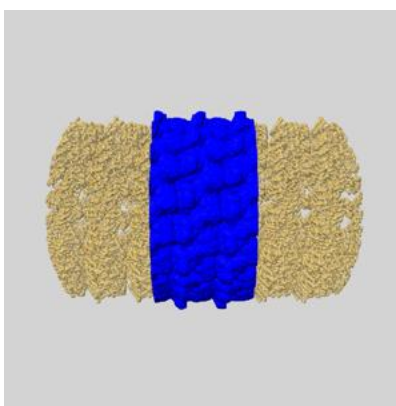
A mask typically either:

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

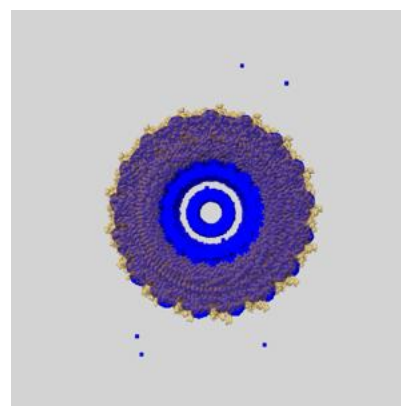
### 6.5.1 emd\_20589\_msk\_1.map [i](#)



X



Y

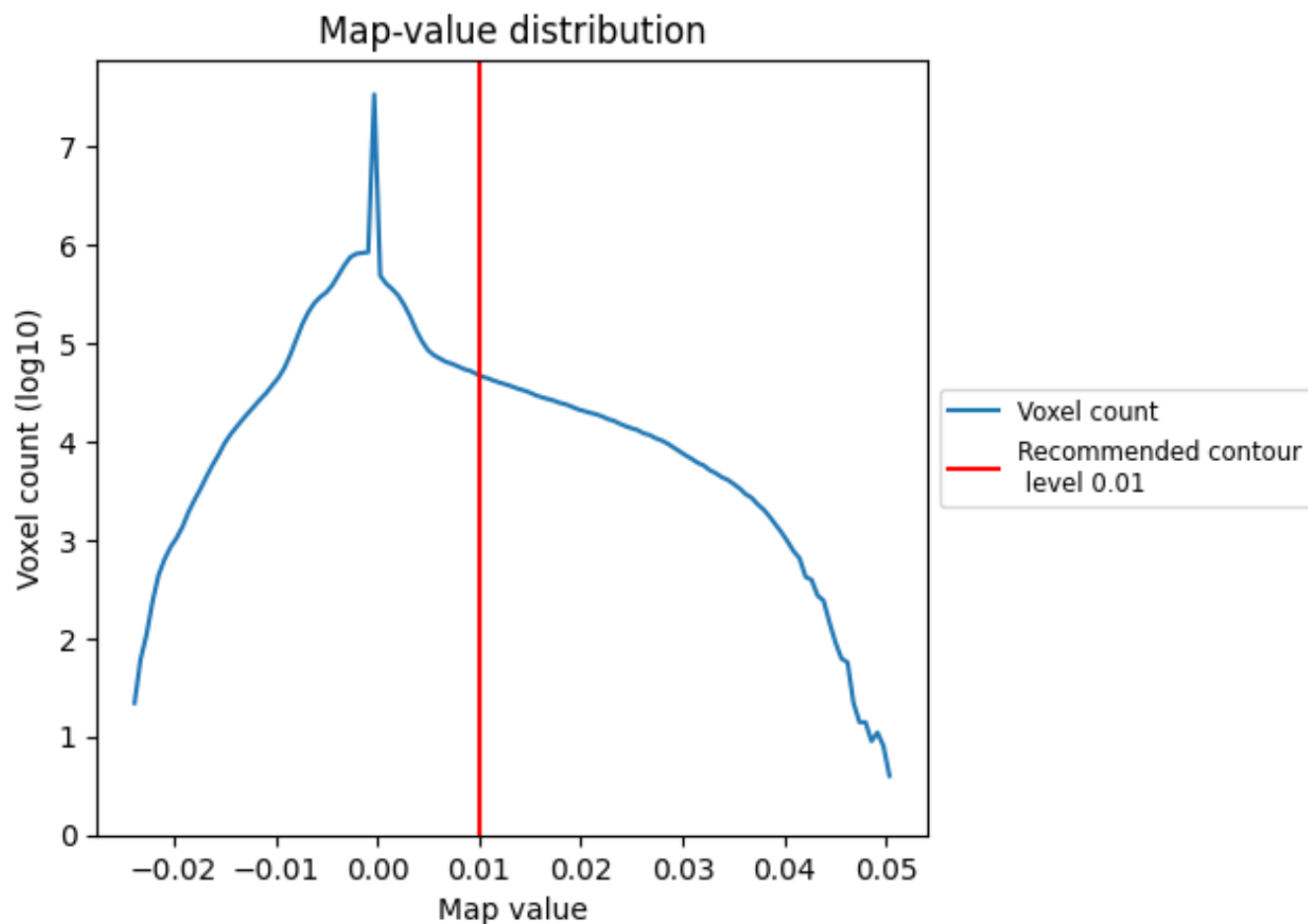


Z

## 7 Map analysis [i](#)

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

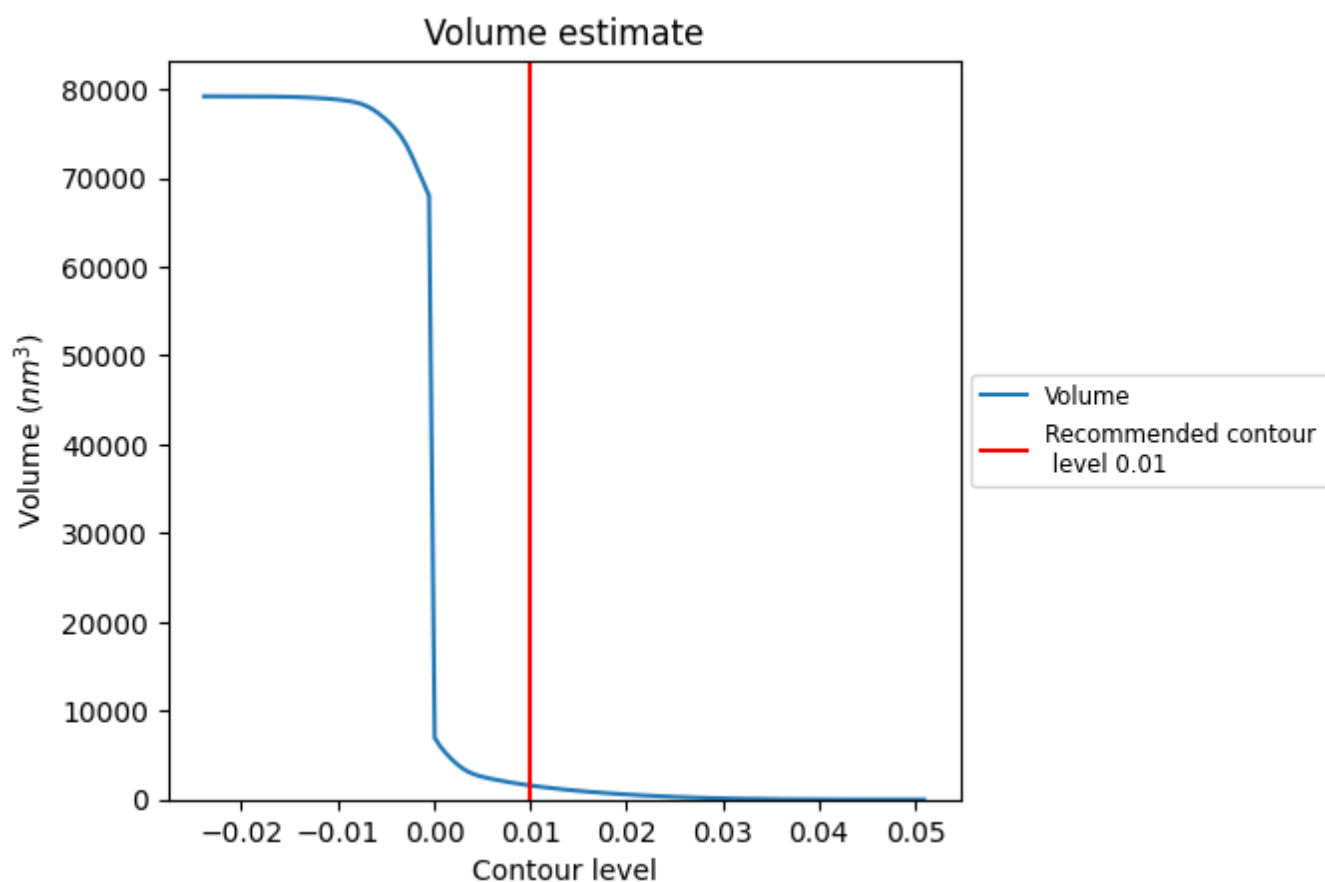
### 7.1 Map-value distribution [i](#)



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.



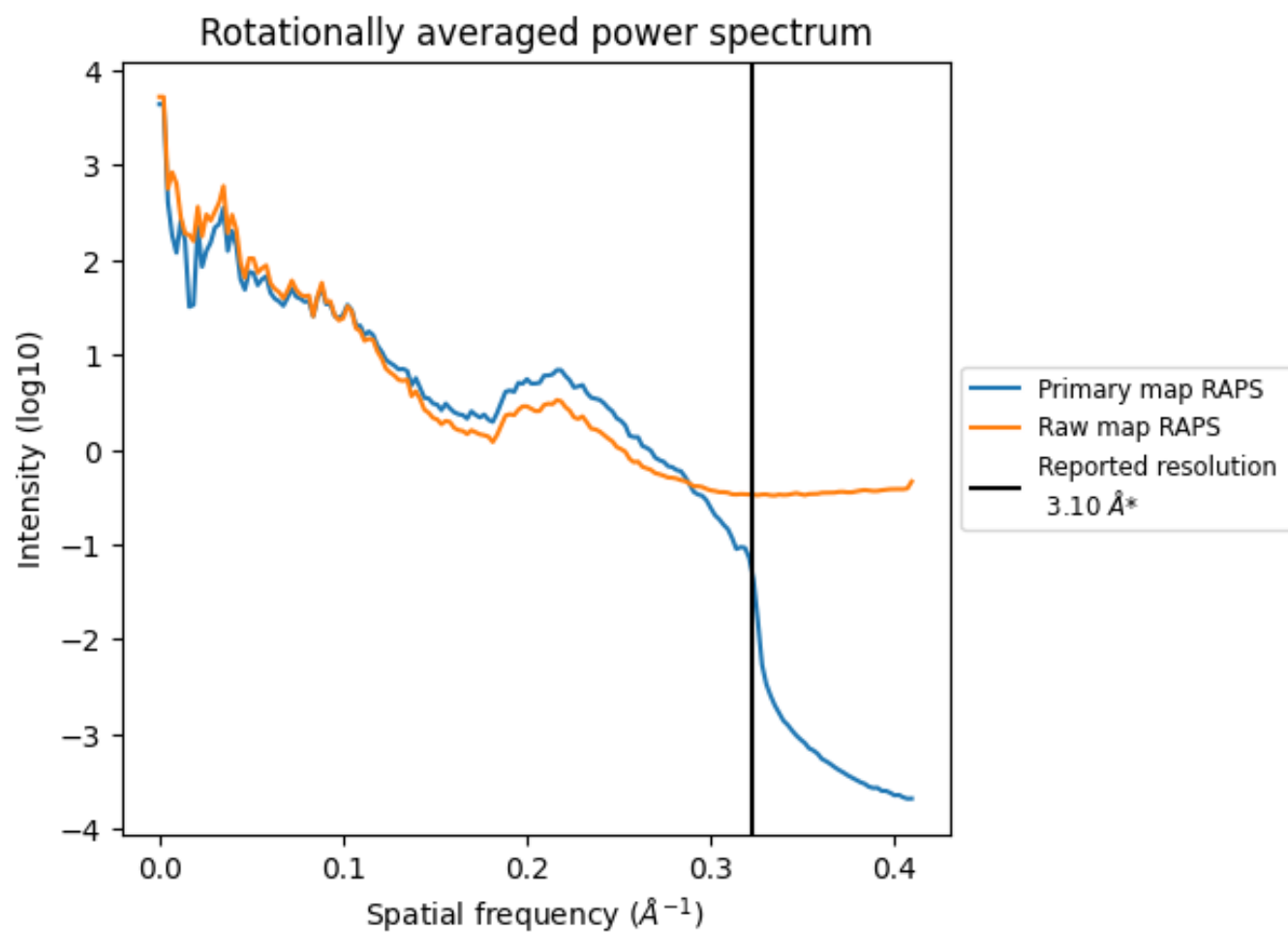
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1587 nm<sup>3</sup>; this corresponds to an approximate mass of 1434 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 ⓘ

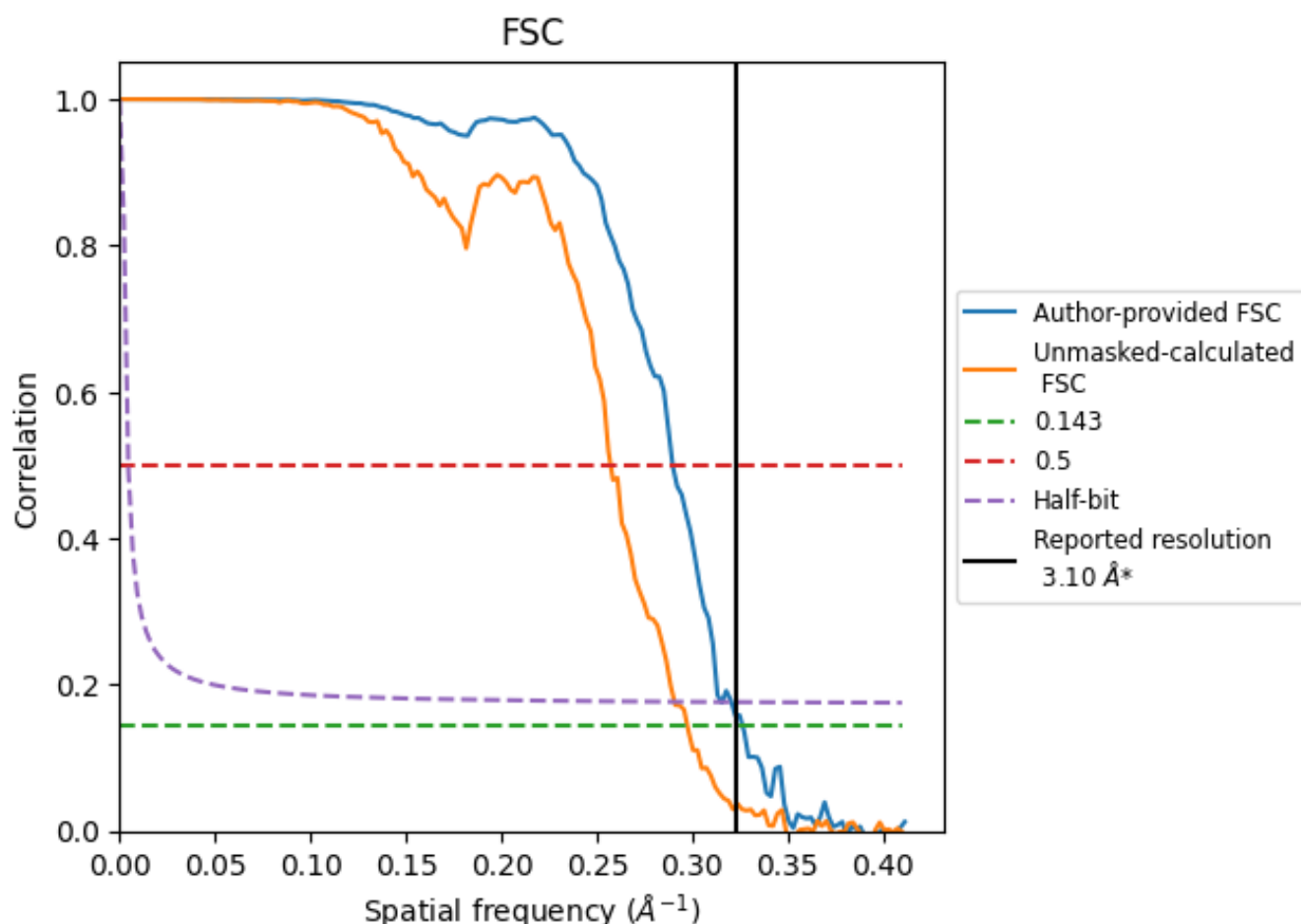


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 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 0.323  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

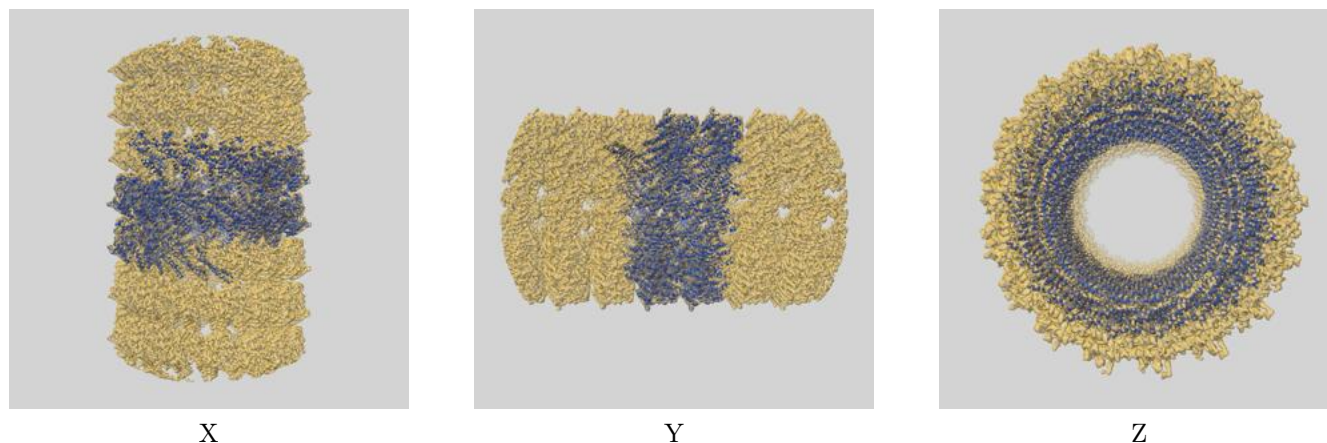
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	3.45	3.17
Unmasked-calculated*	3.36	3.89	3.44

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

## 9 Map-model fit [i](#)

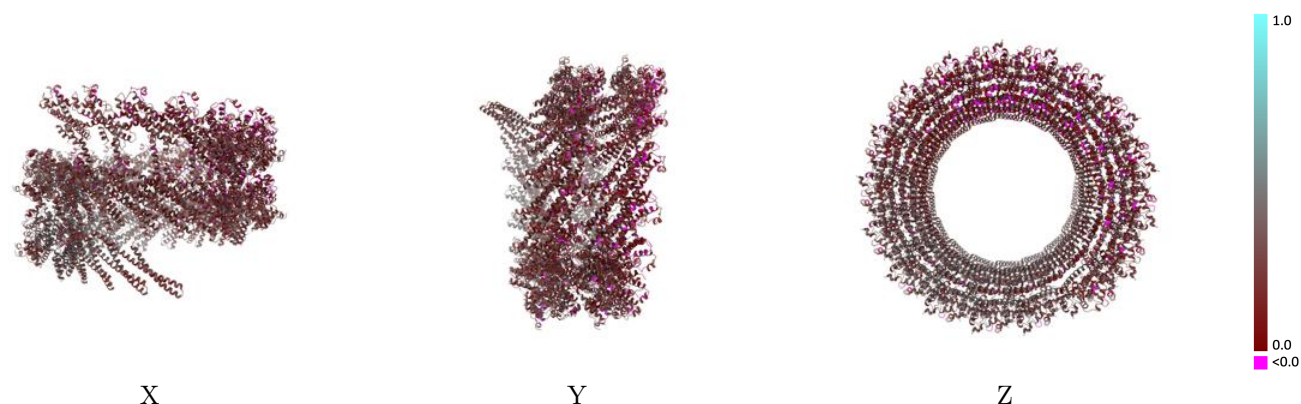
This section contains information regarding the fit between EMDB map EMD-20589 and PDB model 6TZ5. Per-residue inclusion information can be found in section [3](#) on page [11](#).

### 9.1 Map-model overlay [i](#)



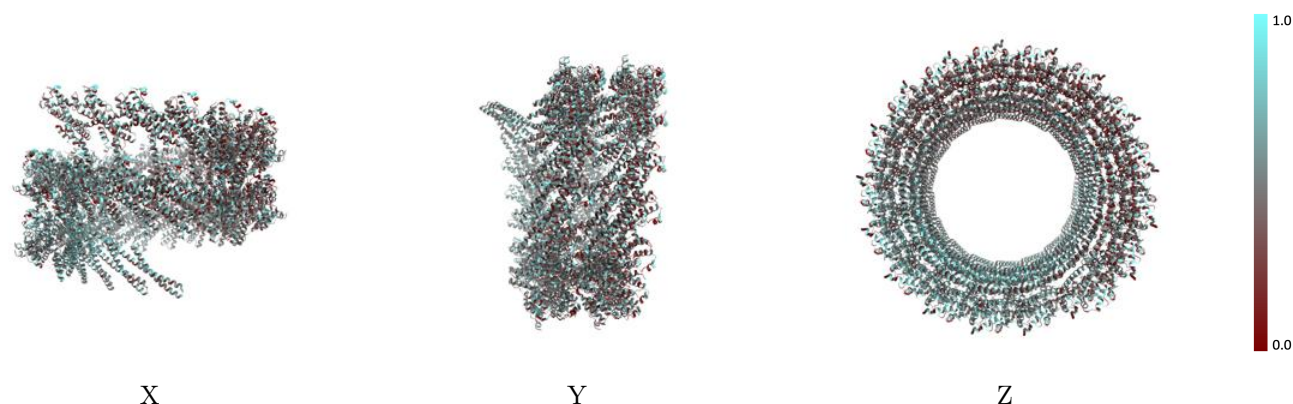
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



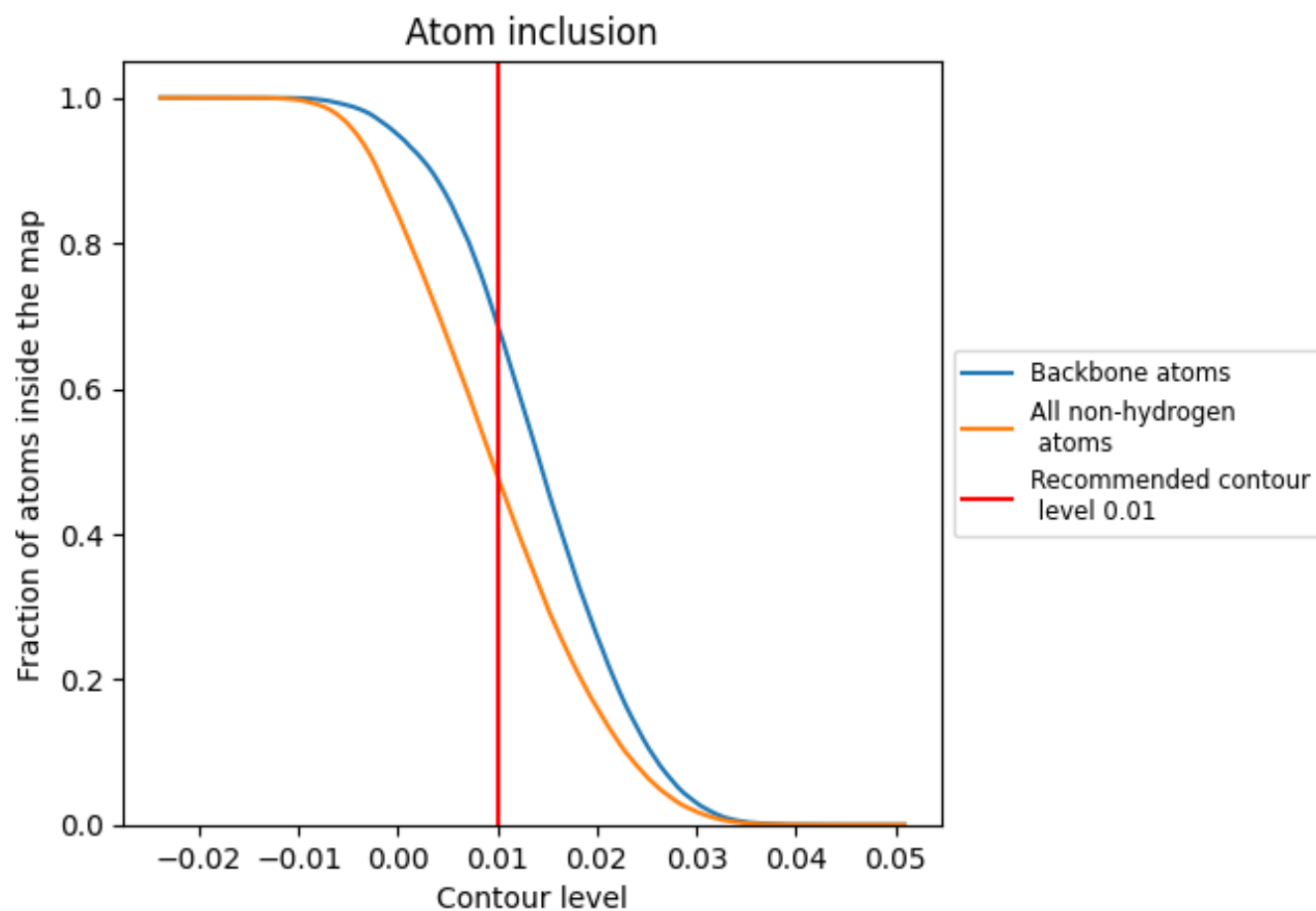
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 48% 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 (0.01) and Q-score for the entire model and for each chain.





































































Chain	Atom inclusion	Q-score
All	 0.4796	 0.2580
A	 0.4643	 0.2760
AA	 0.4835	 0.2300
AB	 0.4602	 0.2270
B	 0.4406	 0.1730
BA	 0.4125	 0.1980
BB	 0.3980	 0.2000
C	 0.3921	 0.1890
CA	 0.5902	 0.3580
CB	 0.4767	 0.2250
D	 0.4752	 0.2510
DA	 0.5394	 0.3320
DB	 0.4140	 0.2290
E	 0.4009	 0.1940
EA	 0.5158	 0.2900
EB	 0.5346	 0.3160
F	 0.5940	 0.3950
FA	 0.5190	 0.3190
FB	 0.4410	 0.2290
G	 0.5066	 0.2980
GA	 0.5729	 0.3450
GB	 0.4534	 0.1960
H	 0.5586	 0.3180
HA	 0.4628	 0.2600
HB	 0.4519	 0.2550
I	 0.5197	 0.2990
IA	 0.5346	 0.3070
IB	 0.4744	 0.2310
J	 0.5684	 0.3270
JA	 0.5394	 0.3470
JB	 0.4439	 0.2670
K	 0.4927	 0.2700
KA	 0.5060	 0.2660
KB	 0.4534	 0.2160
L	 0.4481	 0.1850



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Chain	Atom inclusion	Q-score
LA	 0.5168	 0.3150
LB	 0.3797	 0.1610
M	 0.3739	 0.1590
MA	 0.5414	 0.3100
MB	 0.4489	 0.1920
N	 0.5015	 0.2510
NA	 0.5292	 0.3160
NB	 0.4380	 0.2490
O	 0.5044	 0.3010
OA	 0.4925	 0.2390
OB	 0.5233	 0.2880
P	 0.5406	 0.3070
PA	 0.4789	 0.2920
PB	 0.5313	 0.3310
Q	 0.4417	 0.2270
QA	 0.4812	 0.2470
QB	 0.4383	 0.1880
R	 0.5835	 0.3480
RA	 0.3907	 0.1650
S	 0.5459	 0.3520
SA	 0.4827	 0.2260
T	 0.5075	 0.2830
TA	 0.4162	 0.2290
UA	 0.5526	 0.3260
V	 0.4169	 0.2030
VA	 0.4337	 0.2450
W	 0.4617	 0.2180
WA	 0.4549	 0.1860
X	 0.4052	 0.2100
XA	 0.5452	 0.3530
Y	 0.4353	 0.1750
YA	 0.5218	 0.2860
Z	 0.3812	 0.1740
ZA	 0.4009	 0.2150