Full wwPDB EM Validation Report

Dec 11, 2022 – 09:34 am GMT

PDB ID	:	6S6B
EMDB ID	:	EMD-10102
Title	:	Type III-B Cmr-beta Cryo-EM structure of the Apo state
Authors	:	Sofos, N.; Montoya, G.; Stella, S.
Deposited on	:	2019-07-02
Resolution	:	2.75 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 (i) symbol.

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

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

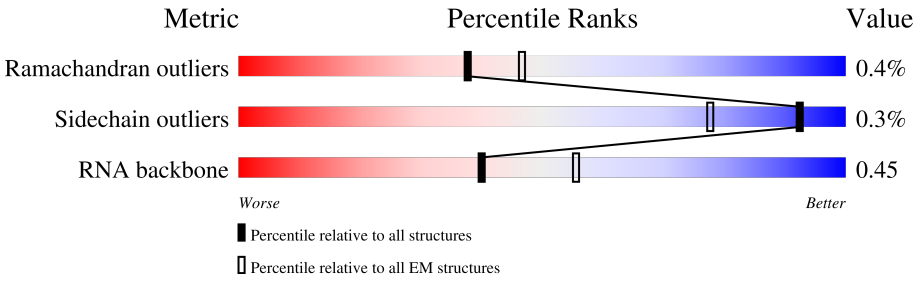
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.75 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.



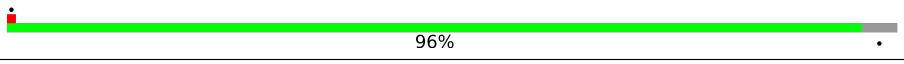
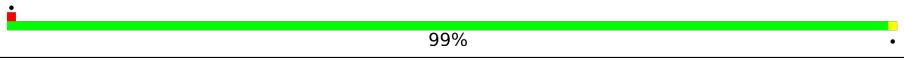
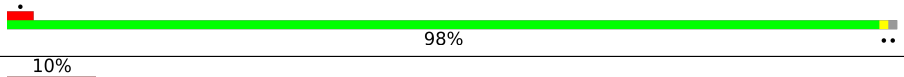
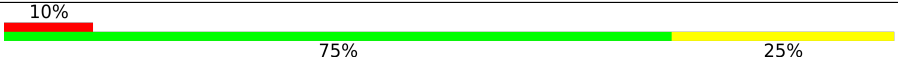
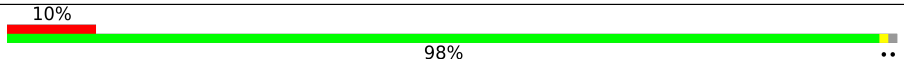
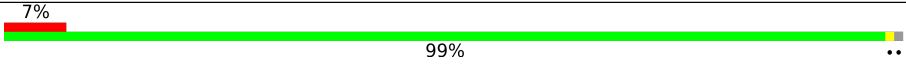
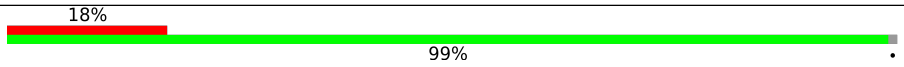
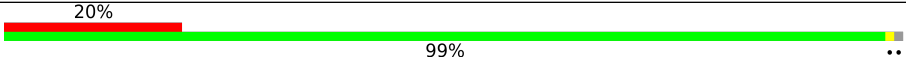
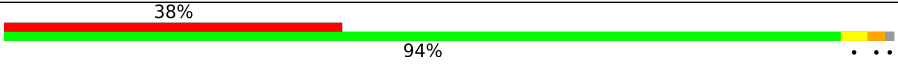
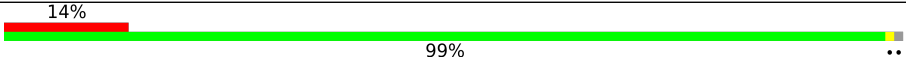
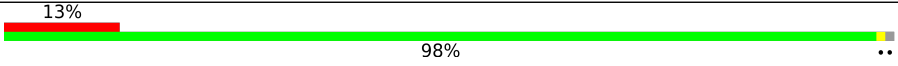
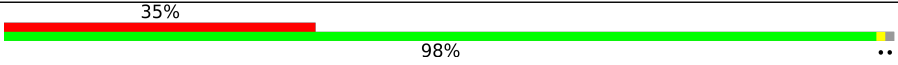
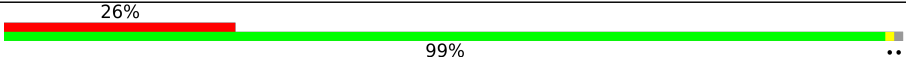
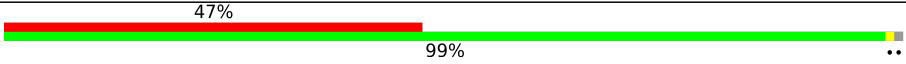
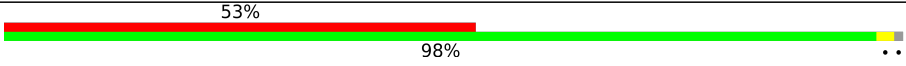
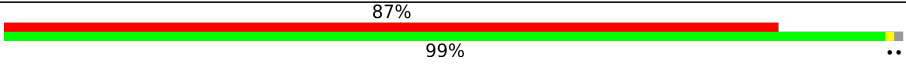
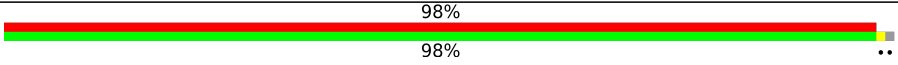
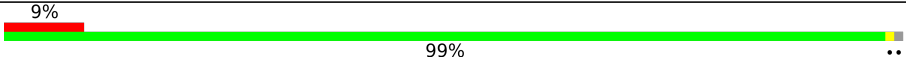
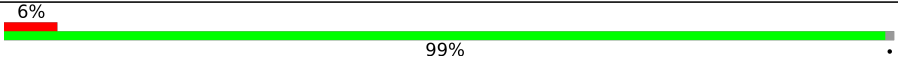
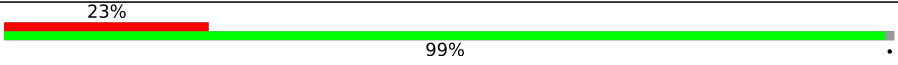
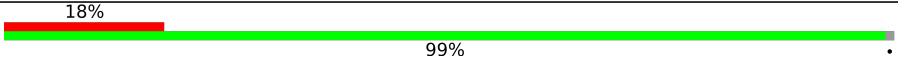
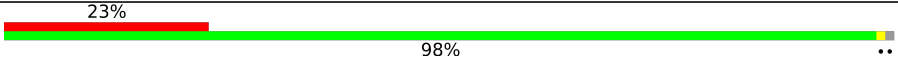
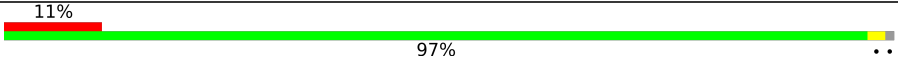
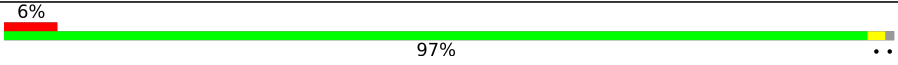
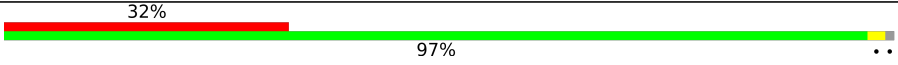
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	155	98%
1	B	155	99%
1	C	155	99%
2	D	286	99%
2	E	286	100%
2	F	286	100%
2	G	286	98%
3	H	313	99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	I	296	
5	J	476	
6	K	1037	
7	V	51	
8	L	174	
8	M	174	
8	N	174	
8	O	174	
8	P	174	
8	Q	174	
8	R	174	
8	S	174	
8	T	174	
8	W	174	
8	X	174	
8	Y	174	
8	Z	174	
8	l	174	
8	m	174	
8	n	174	
8	o	174	
8	p	174	
8	q	174	
8	r	174	
8	s	174	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	t	174	41% 98%
8	w	174	37% 99%
8	x	174	65% 99%
8	y	174	89% 98%
8	z	174	97% 99%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 66914 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 CRISPR-associated protein, Cmr5 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	153	Total	C	N	O	S	0	0
			1253	817	205	230	1		
1	B	154	Total	C	N	O	S	0	0
			1261	823	206	231	1		
1	C	154	Total	C	N	O	S	0	0
			1261	823	206	231	1		

- Molecule 2 is a protein called CRISPR-associated RAMP protein, Cmr4 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	285	Total	C	N	O	S	0	0
			2276	1479	369	426	2		
2	E	285	Total	C	N	O	S	0	0
			2276	1479	369	426	2		
2	F	285	Total	C	N	O	S	0	0
			2277	1479	369	427	2		
2	G	285	Total	C	N	O	S	0	0
			2276	1479	369	426	2		

- Molecule 3 is a protein called CRISPR-associated protein, Cmr3 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	312	Total	C	N	O	S	0	0
			2528	1630	418	473	7		

- Molecule 4 is a protein called CRISPR-associated RAMP protein, Cmr6 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	284	Total	C	N	O	S	0	0
			2282	1470	381	427	4		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	284	ALA	-	expression tag	UNP F0NDX3
I	285	ALA	-	expression tag	UNP F0NDX3
I	286	ALA	-	expression tag	UNP F0NDX3
I	287	HIS	-	expression tag	UNP F0NDX3
I	288	HIS	-	expression tag	UNP F0NDX3
I	289	HIS	-	expression tag	UNP F0NDX3
I	290	HIS	-	expression tag	UNP F0NDX3
I	291	HIS	-	expression tag	UNP F0NDX3
I	292	HIS	-	expression tag	UNP F0NDX3
I	293	HIS	-	expression tag	UNP F0NDX3
I	294	HIS	-	expression tag	UNP F0NDX3
I	295	HIS	-	expression tag	UNP F0NDX3
I	296	HIS	-	expression tag	UNP F0NDX3

- Molecule 5 is a protein called Cmr1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	475	Total	C	N	O	S	0	0
			3890	2517	632	728	13		

- Molecule 6 is a protein called CRISPR-associated protein, Cmr2 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	1024	Total	C	N	O	S	0	0
			8418	5444	1394	1556	24		

- Molecule 7 is a RNA chain called crRNA (51-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	V	51	Total	C	N	O	P	0	0
			1087	489	203	345	50		

- Molecule 8 is a protein called CRISPR-associated protein Cmrx.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	R	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	S	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	Q	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	W	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	T	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	Z	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	Y	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	r	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	s	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	q	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	p	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	w	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	t	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	z	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	y	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	m	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	L	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	l	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	O	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	o	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	N	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	n	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		
8	x	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	173	Total	C	N	O	S	0	0
			1378	880	227	269	2		

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

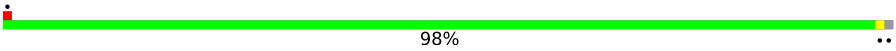
Mol	Chain	Residues	Atoms		AltConf
9	K	1	Total	Zn	0
			1	1	

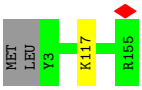
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CRISPR-associated protein, Cmr5 family

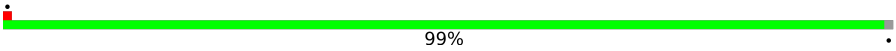
Chain A:

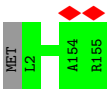




• Molecule 1: CRISPR-associated protein, Cmr5 family

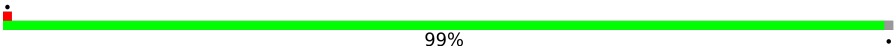
Chain B:





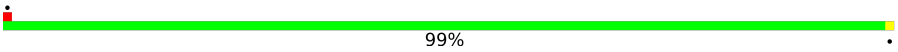
• Molecule 1: CRISPR-associated protein, Cmr5 family

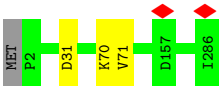
Chain C:



• Molecule 2: CRISPR-associated RAMP protein, Cmr4 family

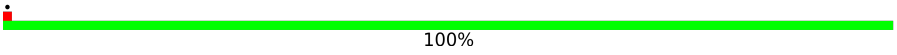
Chain D:

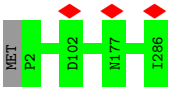




• Molecule 2: CRISPR-associated RAMP protein, Cmr4 family

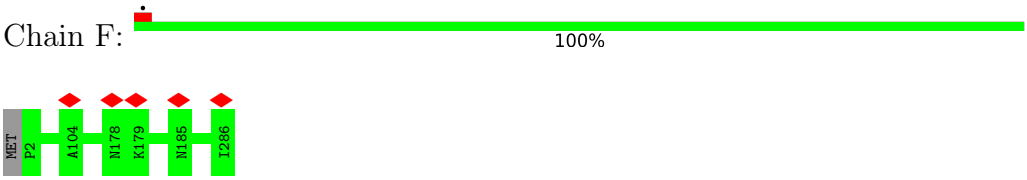
Chain E:





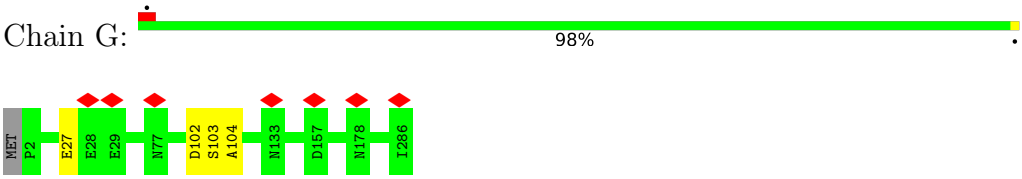
• Molecule 2: CRISPR-associated RAMP protein, Cmr4 family

Chain F:



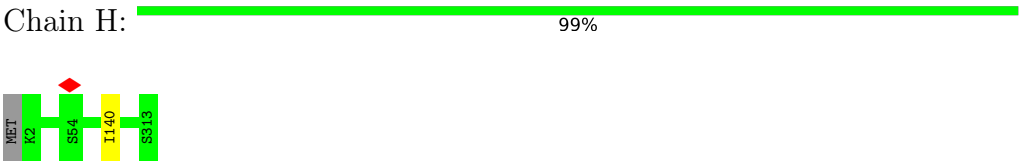
• Molecule 2: CRISPR-associated RAMP protein, Cmr4 family

Chain G:



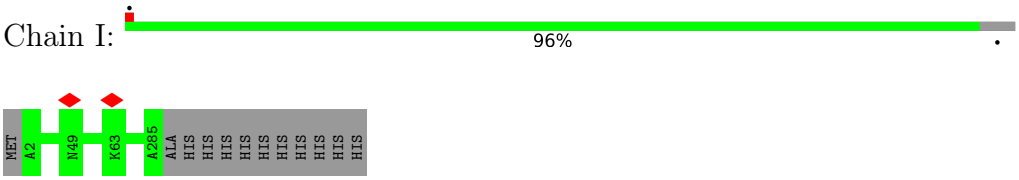
• Molecule 3: CRISPR-associated protein, Cmr3 family

Chain H:



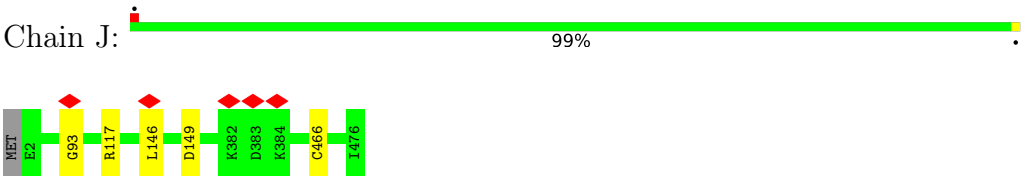
• Molecule 4: CRISPR-associated RAMP protein, Cmr6 family

Chain I:



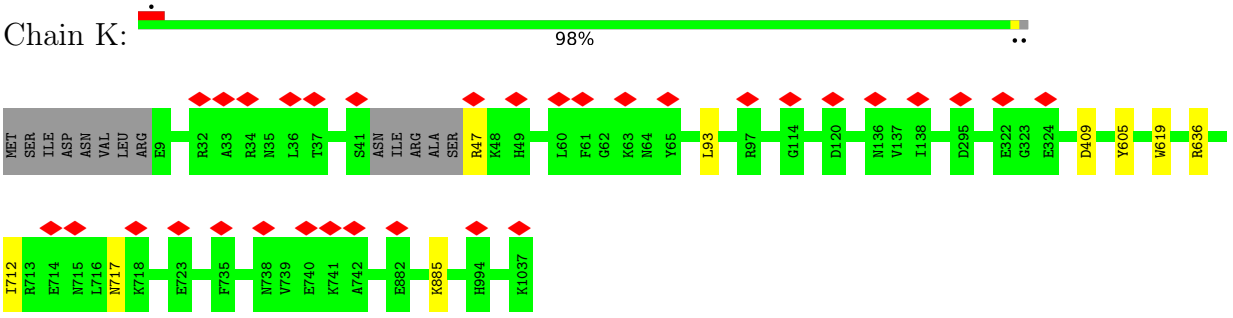
• Molecule 5: Cmr1

Chain J:



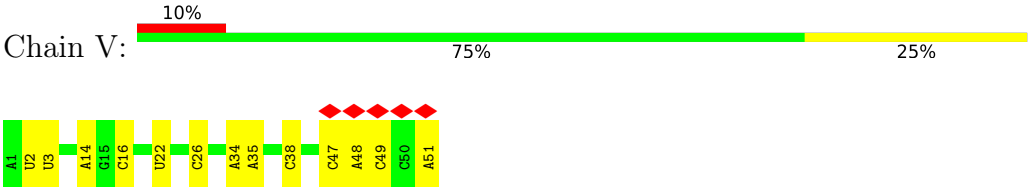
• Molecule 6: CRISPR-associated protein, Cmr2 family

Chain K:



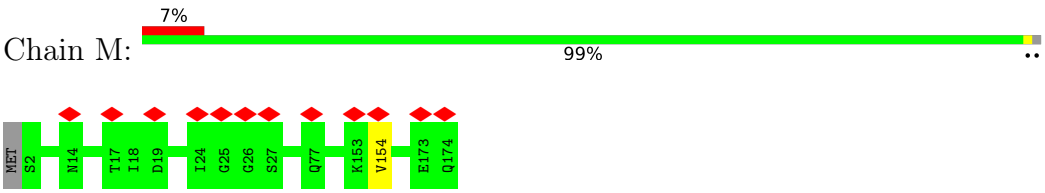
• Molecule 7: crRNA (51-mer)

Chain V:



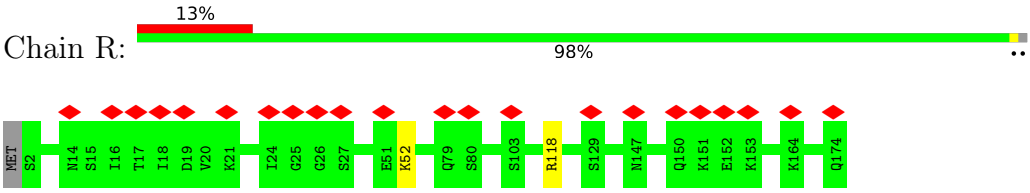
• Molecule 8: CRISPR-associated protein Cmrx

Chain M:



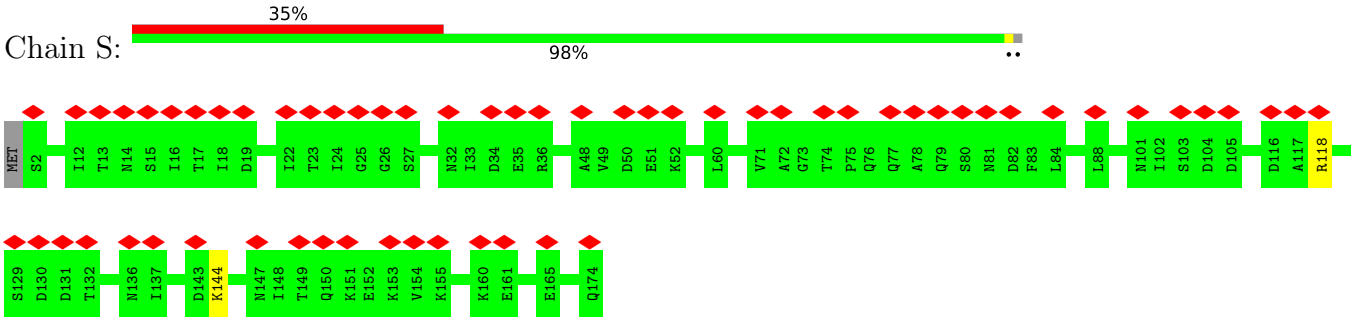
• Molecule 8: CRISPR-associated protein Cmrx

Chain R:



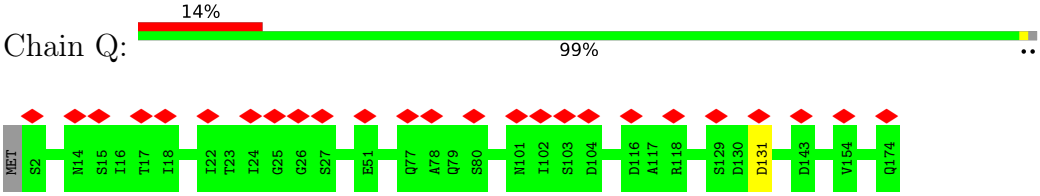
• Molecule 8: CRISPR-associated protein Cmrx

Chain S:



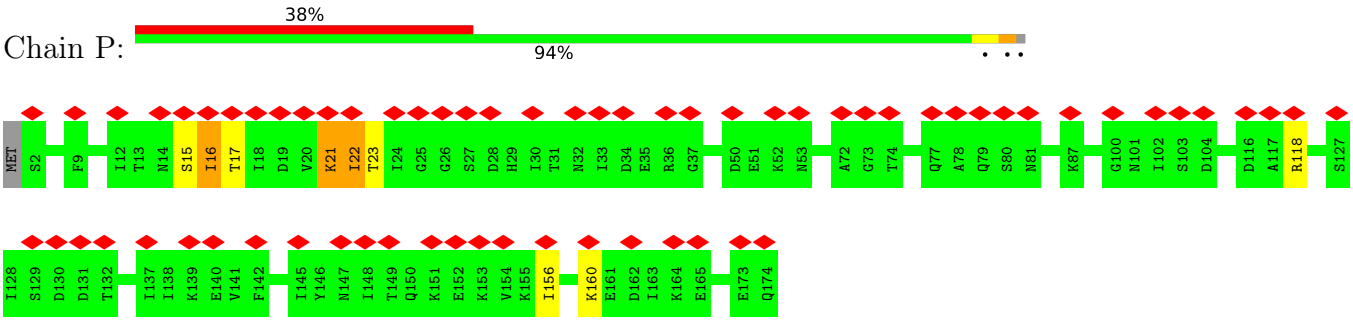
• Molecule 8: CRISPR-associated protein Cmrx

Chain Q:



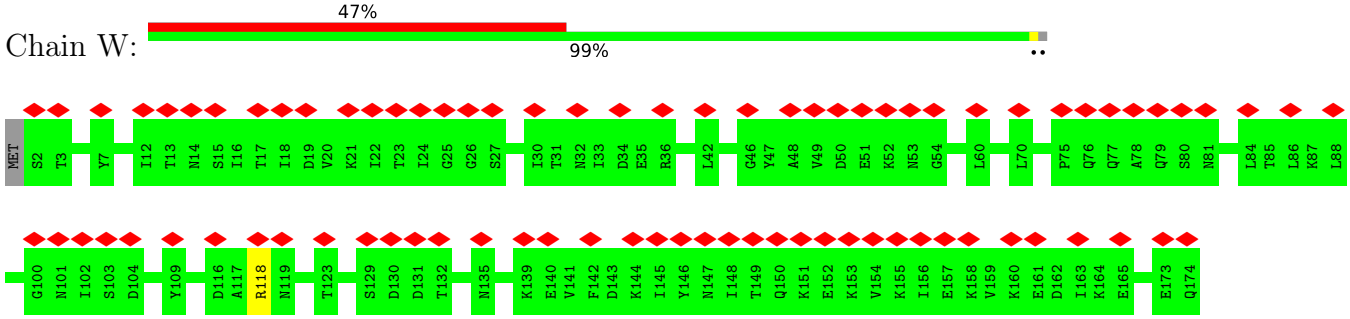
• Molecule 8: CRISPR-associated protein Cmrx

Chain P:



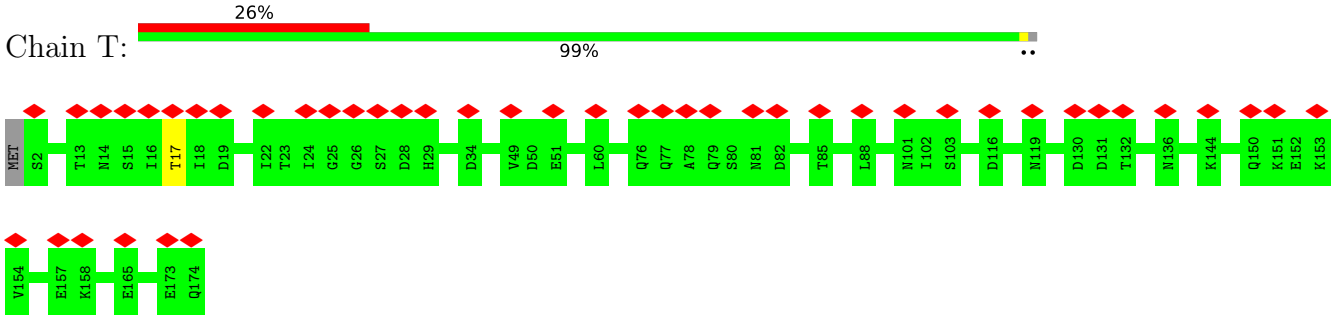
• Molecule 8: CRISPR-associated protein Cmrx

Chain W:



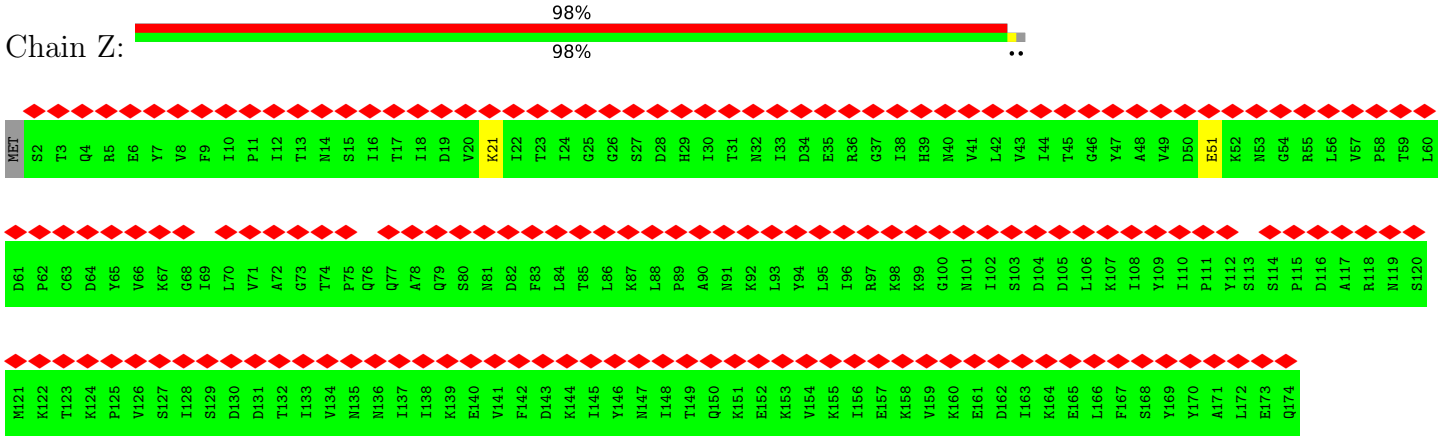
• Molecule 8: CRISPR-associated protein Cmrx

Chain T:



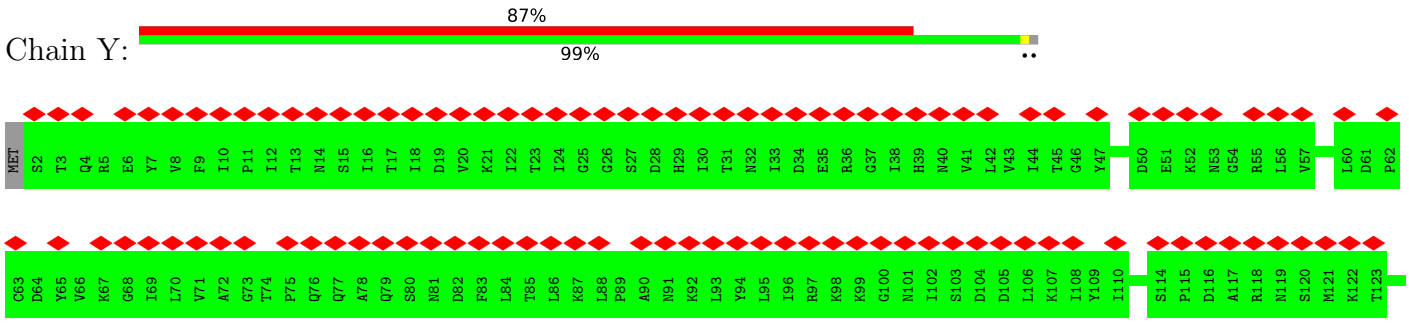
• Molecule 8: CRISPR-associated protein Cmrx

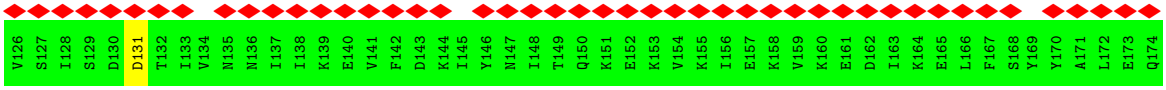
Chain Z:



• Molecule 8: CRISPR-associated protein Cmrx

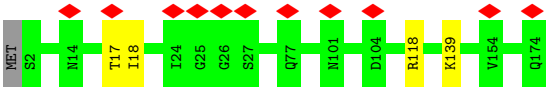
Chain Y:





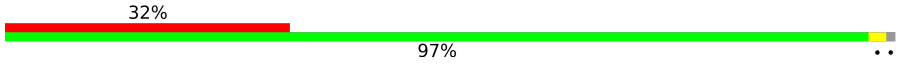
• Molecule 8: CRISPR-associated protein Cmrx

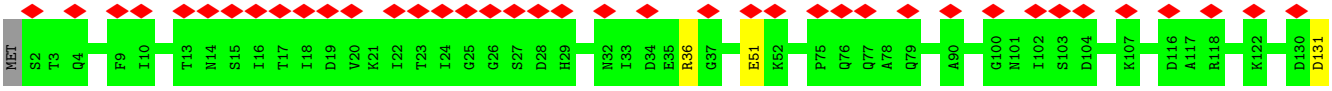
Chain r:

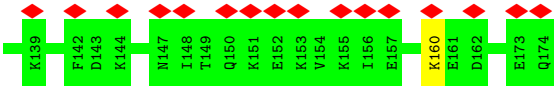


• Molecule 8: CRISPR-associated protein Cmrx

Chain s:

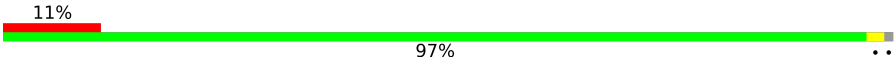


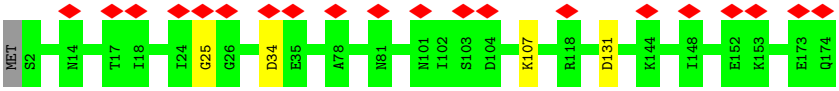




• Molecule 8: CRISPR-associated protein Cmrx

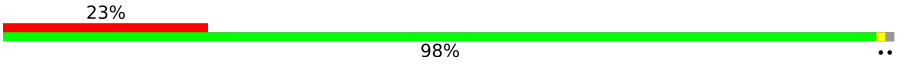
Chain q:

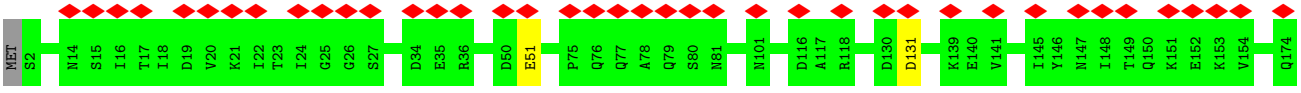




• Molecule 8: CRISPR-associated protein Cmrx

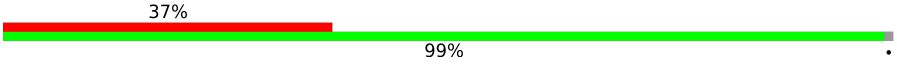
Chain p:

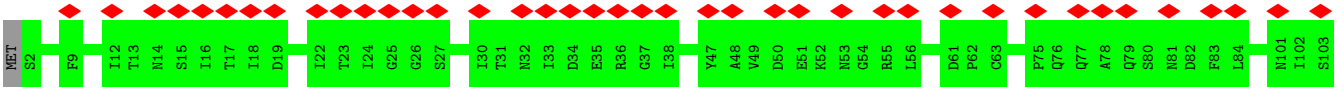


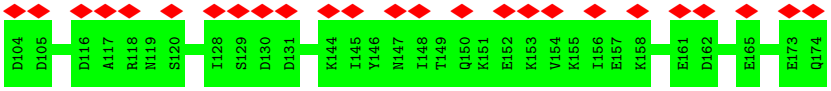


• Molecule 8: CRISPR-associated protein Cmrx

Chain w:

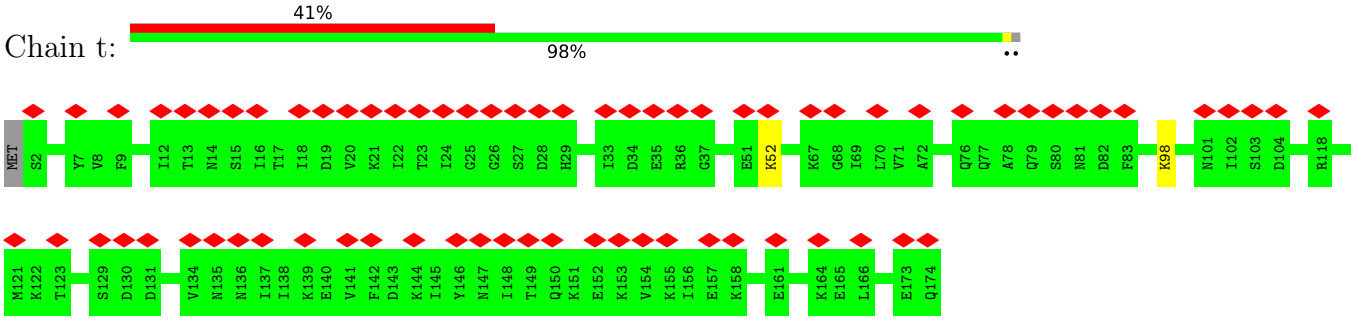






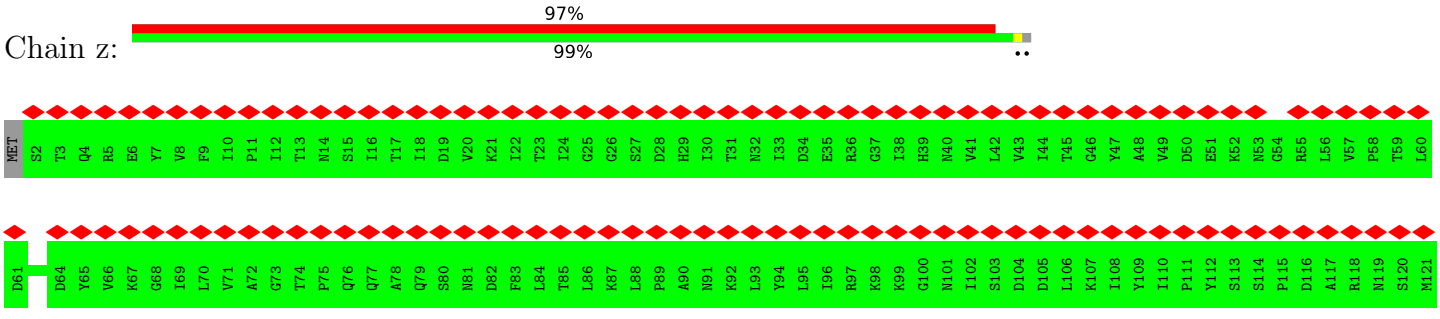
• Molecule 8: CRISPR-associated protein Cmrx

Chain t:



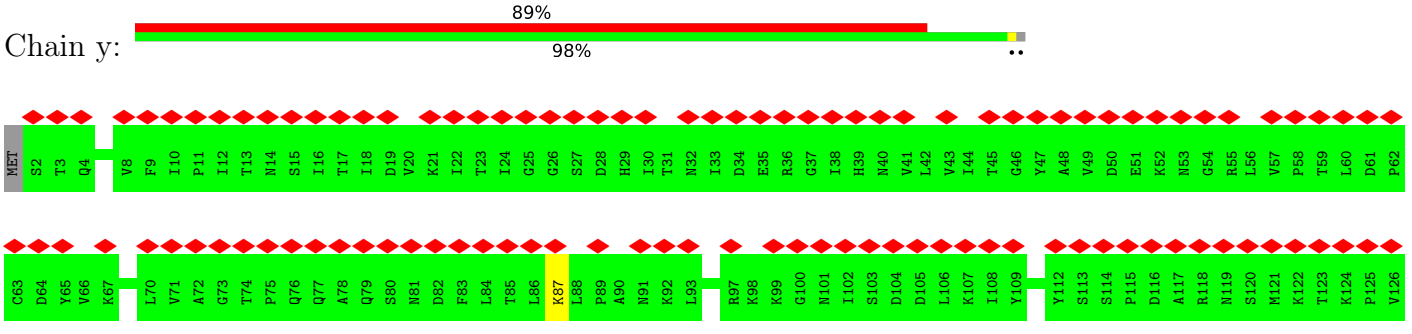
• Molecule 8: CRISPR-associated protein Cmrx

Chain z:



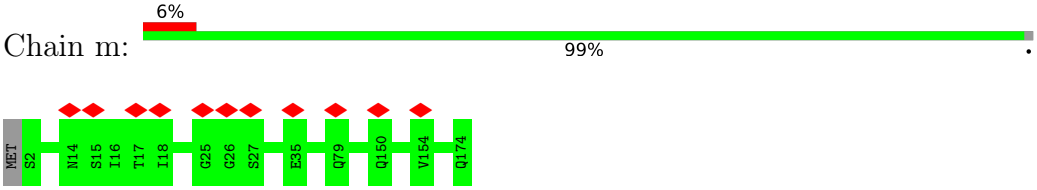
• Molecule 8: CRISPR-associated protein Cmrx

Chain y:



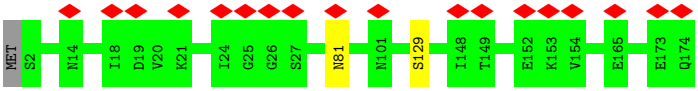
• Molecule 8: CRISPR-associated protein Cmrx

Chain m:



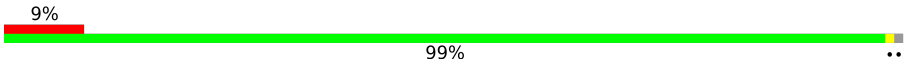
• Molecule 8: CRISPR-associated protein Cmrx

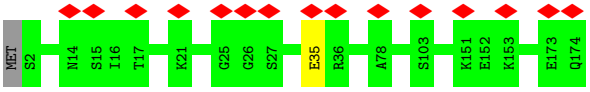
Chain L:



• Molecule 8: CRISPR-associated protein Cmrx

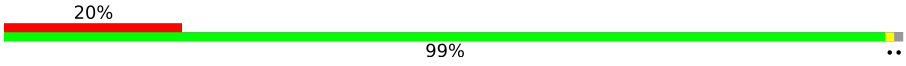
Chain l:

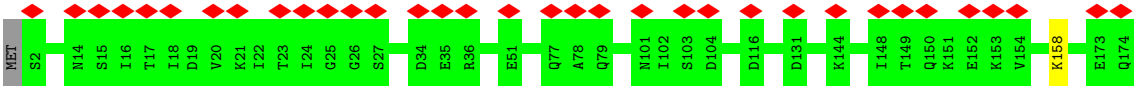




• Molecule 8: CRISPR-associated protein Cmrx

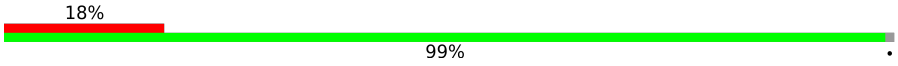
Chain O:

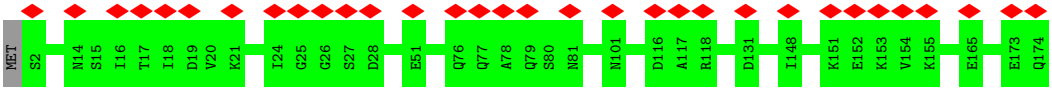




• Molecule 8: CRISPR-associated protein Cmrx

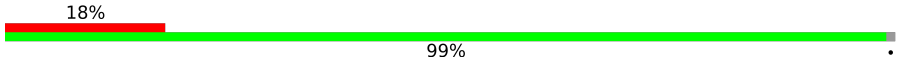
Chain o:

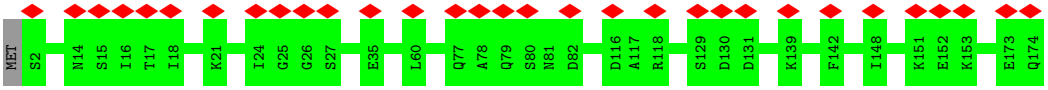




• Molecule 8: CRISPR-associated protein Cmrx

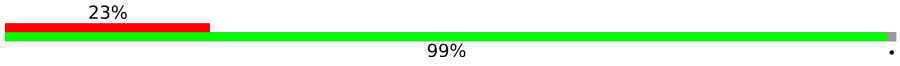
Chain N:

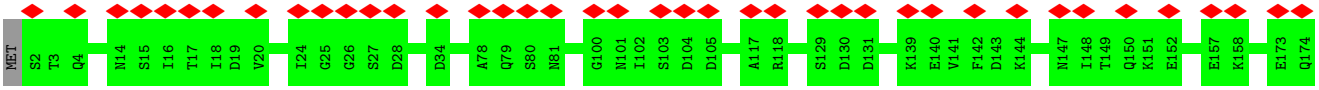




• Molecule 8: CRISPR-associated protein Cmrx

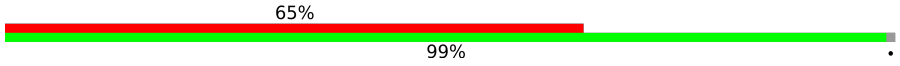
Chain n:

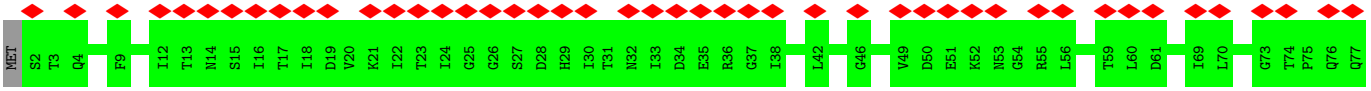


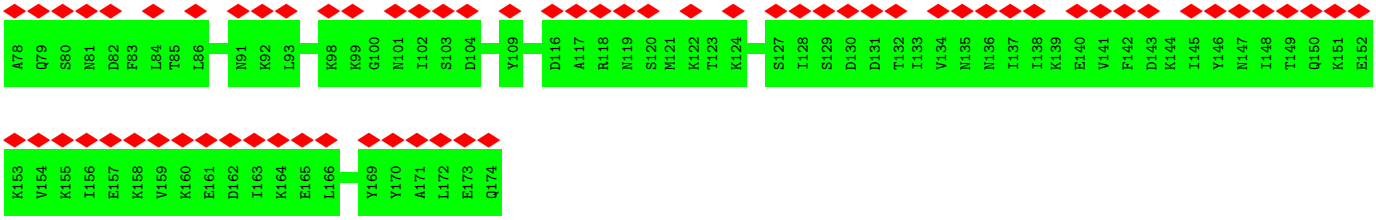


• Molecule 8: CRISPR-associated protein Cmrx

Chain x:

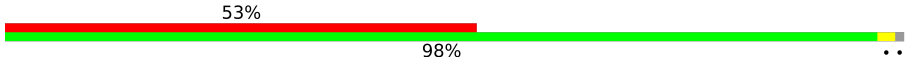


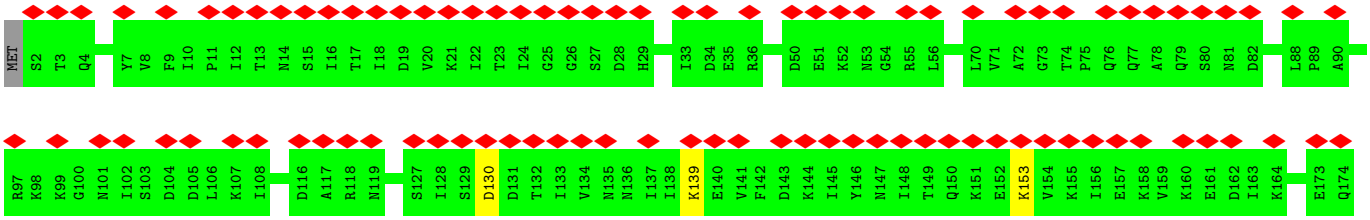




• Molecule 8: CRISPR-associated protein Cmrx

Chain X:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	69043	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	23.336	Depositor
Minimum map value	-11.328	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.609	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	416.00003, 415.99997, 416.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8320001, 0.83199996, 0.832	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.36	0/1275	0.44	0/1716
1	B	0.37	0/1283	0.41	0/1727
1	C	0.37	0/1283	0.40	0/1727
2	D	0.40	0/2320	0.48	0/3137
2	E	0.40	0/2320	0.47	0/3137
2	F	0.41	0/2321	0.48	0/3138
2	G	0.38	0/2320	0.50	0/3137
3	H	0.35	0/2574	0.48	0/3469
4	I	0.37	0/2325	0.45	0/3138
5	J	0.32	0/3957	0.47	1/5320 (0.0%)
6	K	0.33	0/8590	0.46	1/11599 (0.0%)
7	V	0.68	0/1218	0.83	3/1896 (0.2%)
8	L	0.30	0/1400	0.48	0/1895
8	M	0.30	0/1400	0.47	0/1895
8	N	0.28	0/1400	0.49	0/1895
8	O	0.29	0/1400	0.49	0/1895
8	P	0.29	0/1400	0.55	0/1895
8	Q	0.29	0/1400	0.50	0/1895
8	R	0.29	0/1400	0.51	0/1895
8	S	0.27	0/1400	0.49	0/1895
8	T	0.26	0/1400	0.51	0/1895
8	W	0.26	0/1400	0.50	0/1895
8	X	0.27	0/1400	0.51	0/1895
8	Y	0.26	0/1400	0.54	0/1895
8	Z	0.27	0/1400	0.53	0/1895
8	l	0.30	0/1400	0.50	0/1895
8	m	0.33	0/1400	0.50	0/1895
8	n	0.27	0/1400	0.48	0/1895
8	o	0.28	0/1400	0.48	0/1895
8	p	0.27	0/1400	0.51	0/1895
8	q	0.29	0/1400	0.55	0/1895
8	r	0.29	0/1400	0.50	0/1895

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
8	s	0.27	0/1400	0.51	0/1895
8	t	0.26	0/1400	0.50	0/1895
8	w	0.26	0/1400	0.48	0/1895
8	x	0.27	0/1400	0.48	0/1895
8	y	0.26	0/1400	0.53	0/1895
8	z	0.25	0/1400	0.56	0/1895
All	All	0.33	0/68186	0.50	5/92411 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	3
6	K	0	1
8	L	0	1
8	P	0	4
8	T	0	1
8	r	0	1
All	All	0	11

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	146	LEU	CA-CB-CG	6.34	129.87	115.30
6	K	409	ASP	CB-CG-OD1	6.17	123.85	118.30
7	V	38	C	C2-N1-C1'	5.12	124.43	118.80
7	V	38	C	N1-C2-O2	5.08	121.95	118.90
7	V	38	C	N3-C2-O2	-5.02	118.39	121.90

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	102	ASP	Peptide
2	G	104	ALA	Peptide
2	G	27	GLU	Peptide
6	K	712	ILE	Peptide
8	L	129	SER	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
8	P	15	SER	Peptide
8	P	16	ILE	Peptide
8	P	21	LYS	Peptide
8	P	22	ILE	Peptide
8	T	17	THR	Peptide
8	r	17	THR	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	151/155 (97%)	143 (95%)	8 (5%)	0	100	100
1	B	152/155 (98%)	146 (96%)	6 (4%)	0	100	100
1	C	152/155 (98%)	150 (99%)	2 (1%)	0	100	100
2	D	283/286 (99%)	258 (91%)	22 (8%)	3 (1%)	14	25
2	E	283/286 (99%)	264 (93%)	19 (7%)	0	100	100
2	F	283/286 (99%)	263 (93%)	20 (7%)	0	100	100
2	G	283/286 (99%)	250 (88%)	32 (11%)	1 (0%)	34	53
3	H	310/313 (99%)	276 (89%)	34 (11%)	0	100	100
4	I	282/296 (95%)	265 (94%)	17 (6%)	0	100	100
5	J	473/476 (99%)	422 (89%)	49 (10%)	2 (0%)	34	53
6	K	1020/1037 (98%)	892 (88%)	124 (12%)	4 (0%)	34	53
8	L	171/174 (98%)	133 (78%)	38 (22%)	0	100	100
8	M	171/174 (98%)	140 (82%)	30 (18%)	1 (1%)	25	42
8	N	171/174 (98%)	136 (80%)	35 (20%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	O	171/174 (98%)	142 (83%)	29 (17%)	0	100 100
8	P	171/174 (98%)	134 (78%)	31 (18%)	6 (4%)	3 5
8	Q	171/174 (98%)	128 (75%)	42 (25%)	1 (1%)	25 42
8	R	171/174 (98%)	137 (80%)	34 (20%)	0	100 100
8	S	171/174 (98%)	136 (80%)	35 (20%)	0	100 100
8	T	171/174 (98%)	129 (75%)	42 (25%)	0	100 100
8	W	171/174 (98%)	138 (81%)	33 (19%)	0	100 100
8	X	171/174 (98%)	136 (80%)	34 (20%)	1 (1%)	25 42
8	Y	171/174 (98%)	134 (78%)	36 (21%)	1 (1%)	25 42
8	Z	171/174 (98%)	128 (75%)	42 (25%)	1 (1%)	25 42
8	l	171/174 (98%)	137 (80%)	33 (19%)	1 (1%)	25 42
8	m	171/174 (98%)	144 (84%)	27 (16%)	0	100 100
8	n	171/174 (98%)	142 (83%)	29 (17%)	0	100 100
8	o	171/174 (98%)	136 (80%)	35 (20%)	0	100 100
8	p	171/174 (98%)	134 (78%)	35 (20%)	2 (1%)	13 23
8	q	171/174 (98%)	129 (75%)	38 (22%)	4 (2%)	6 10
8	r	171/174 (98%)	135 (79%)	35 (20%)	1 (1%)	25 42
8	s	171/174 (98%)	127 (74%)	42 (25%)	2 (1%)	13 23
8	t	171/174 (98%)	134 (78%)	37 (22%)	0	100 100
8	w	171/174 (98%)	134 (78%)	37 (22%)	0	100 100
8	x	171/174 (98%)	139 (81%)	32 (19%)	0	100 100
8	y	171/174 (98%)	143 (84%)	27 (16%)	1 (1%)	25 42
8	z	171/174 (98%)	130 (76%)	40 (23%)	1 (1%)	25 42
All	All	8118/8255 (98%)	6844 (84%)	1241 (15%)	33 (0%)	38 53

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	71	VAL
2	G	103	SER
6	K	605	TYR
8	P	16	ILE
8	P	17	THR
8	P	22	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	P	23	THR
8	Z	51	GLU
2	D	31	ASP
2	D	70	LYS
6	K	93	LEU
6	K	717	ASN
8	q	131	ASP
5	J	149	ASP
8	M	154	VAL
8	Q	131	ASP
8	P	21	LYS
8	s	51	GLU
8	z	131	ASP
6	K	619	TRP
8	Y	131	ASP
8	r	18	ILE
8	q	107	LYS
8	p	131	ASP
8	l	35	GLU
8	s	131	ASP
8	q	34	ASP
8	p	51	GLU
8	y	131	ASP
8	q	25	GLY
8	X	130	ASP
5	J	93	GLY
8	P	156	ILE

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	134/136 (98%)	133 (99%)	1 (1%)	84 89
1	B	135/136 (99%)	135 (100%)	0	100 100
1	C	135/136 (99%)	135 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	252/254 (99%)	252 (100%)	0	100	100
2	E	252/254 (99%)	252 (100%)	0	100	100
2	F	253/254 (100%)	253 (100%)	0	100	100
2	G	252/254 (99%)	252 (100%)	0	100	100
3	H	279/280 (100%)	278 (100%)	1 (0%)	91	93
4	I	255/266 (96%)	255 (100%)	0	100	100
5	J	443/445 (100%)	441 (100%)	2 (0%)	88	92
6	K	937/949 (99%)	934 (100%)	3 (0%)	92	95
8	L	159/160 (99%)	158 (99%)	1 (1%)	86	90
8	M	159/160 (99%)	159 (100%)	0	100	100
8	N	159/160 (99%)	159 (100%)	0	100	100
8	O	159/160 (99%)	158 (99%)	1 (1%)	86	90
8	P	159/160 (99%)	157 (99%)	2 (1%)	69	81
8	Q	159/160 (99%)	159 (100%)	0	100	100
8	R	159/160 (99%)	157 (99%)	2 (1%)	69	81
8	S	159/160 (99%)	157 (99%)	2 (1%)	69	81
8	T	159/160 (99%)	159 (100%)	0	100	100
8	W	159/160 (99%)	158 (99%)	1 (1%)	86	90
8	X	159/160 (99%)	157 (99%)	2 (1%)	69	81
8	Y	159/160 (99%)	159 (100%)	0	100	100
8	Z	159/160 (99%)	158 (99%)	1 (1%)	86	90
8	l	159/160 (99%)	159 (100%)	0	100	100
8	m	159/160 (99%)	159 (100%)	0	100	100
8	n	159/160 (99%)	159 (100%)	0	100	100
8	o	159/160 (99%)	159 (100%)	0	100	100
8	p	159/160 (99%)	159 (100%)	0	100	100
8	q	159/160 (99%)	159 (100%)	0	100	100
8	r	159/160 (99%)	157 (99%)	2 (1%)	69	81
8	s	159/160 (99%)	157 (99%)	2 (1%)	69	81
8	t	159/160 (99%)	157 (99%)	2 (1%)	69	81
8	w	159/160 (99%)	159 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	x	159/160 (99%)	159 (100%)	0	100 100
8	y	159/160 (99%)	158 (99%)	1 (1%)	86 90
8	z	159/160 (99%)	159 (100%)	0	100 100
All	All	7461/7524 (99%)	7435 (100%)	26 (0%)	92 95

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	LYS
3	H	140	ILE
5	J	117	ARG
5	J	466	CYS
6	K	47	ARG
6	K	636	ARG
6	K	885	LYS
8	R	52	LYS
8	R	118	ARG
8	S	118	ARG
8	S	144	LYS
8	P	118	ARG
8	P	160	LYS
8	W	118	ARG
8	Z	21	LYS
8	r	118	ARG
8	r	139	LYS
8	s	36	ARG
8	s	160	LYS
8	t	52	LYS
8	t	98	LYS
8	y	87	LYS
8	L	81	ASN
8	O	158	LYS
8	X	139	LYS
8	X	153	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	28	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	28	GLN
1	B	60	ASN
1	C	23	HIS
2	D	17	HIS
2	D	138	ASN
2	E	19	HIS
2	E	130	GLN
2	E	133	ASN
2	E	153	ASN
2	E	260	ASN
2	F	13	HIS
2	F	17	HIS
2	F	133	ASN
2	F	141	ASN
2	F	153	ASN
2	F	203	ASN
2	F	260	ASN
2	G	13	HIS
2	G	19	HIS
2	G	77	ASN
3	H	28	HIS
3	H	253	ASN
4	I	8	ASN
4	I	21	ASN
4	I	172	GLN
4	I	210	HIS
5	J	220	HIS
5	J	223	ASN
5	J	265	ASN
5	J	310	ASN
5	J	424	GLN
5	J	440	ASN
5	J	443	ASN
6	K	24	ASN
6	K	39	GLN
6	K	49	HIS
6	K	64	ASN
6	K	175	HIS
6	K	292	ASN
6	K	344	ASN
6	K	392	GLN
6	K	635	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	K	695	ASN
6	K	728	ASN
6	K	779	ASN
6	K	845	ASN
6	K	1024	ASN
8	M	29	HIS
8	M	32	ASN
8	M	53	ASN
8	M	79	GLN
8	M	101	ASN
8	M	119	ASN
8	M	174	GLN
8	R	39	HIS
8	R	136	ASN
8	S	91	ASN
8	Q	40	ASN
8	Q	76	GLN
8	Q	119	ASN
8	Q	150	GLN
8	P	14	ASN
8	P	40	ASN
8	P	53	ASN
8	P	136	ASN
8	T	77	GLN
8	Z	77	GLN
8	Z	135	ASN
8	Y	53	ASN
8	Y	77	GLN
8	Y	79	GLN
8	Y	174	GLN
8	r	39	HIS
8	s	150	GLN
8	q	77	GLN
8	p	40	ASN
8	p	135	ASN
8	p	136	ASN
8	w	29	HIS
8	w	119	ASN
8	w	150	GLN
8	t	4	GLN
8	t	76	GLN
8	t	79	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	t	101	ASN
8	z	77	GLN
8	y	40	ASN
8	y	101	ASN
8	y	150	GLN
8	m	14	ASN
8	m	32	ASN
8	m	40	ASN
8	m	76	GLN
8	L	39	HIS
8	L	101	ASN
8	l	32	ASN
8	l	39	HIS
8	l	53	ASN
8	l	76	GLN
8	l	101	ASN
8	l	150	GLN
8	O	40	ASN
8	O	53	ASN
8	O	76	GLN
8	O	79	GLN
8	O	81	ASN
8	O	119	ASN
8	O	135	ASN
8	O	174	GLN
8	o	40	ASN
8	o	174	GLN
8	N	29	HIS
8	N	32	ASN
8	N	40	ASN
8	N	53	ASN
8	N	77	GLN
8	N	79	GLN
8	n	39	HIS
8	n	135	ASN
8	x	29	HIS
8	x	32	ASN
8	x	76	GLN
8	x	174	GLN
8	X	4	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	V	50/51 (98%)	11 (22%)	1 (2%)

All (11) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	V	2	U
7	V	3	U
7	V	14	A
7	V	16	C
7	V	22	U
7	V	26	C
7	V	34	A
7	V	35	A
7	V	48	A
7	V	49	C
7	V	51	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	V	47	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

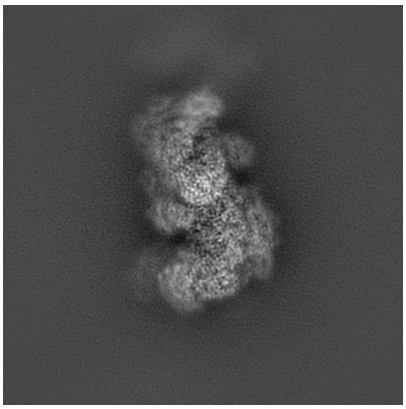
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10102. These allow visual inspection of the internal detail of the map and identification of artifacts.

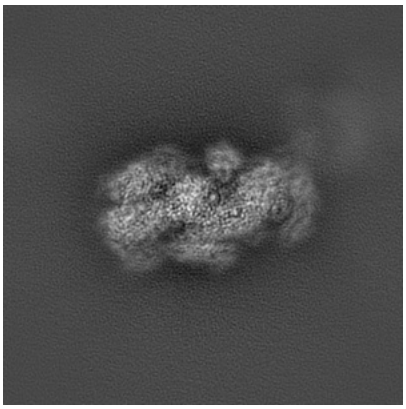
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

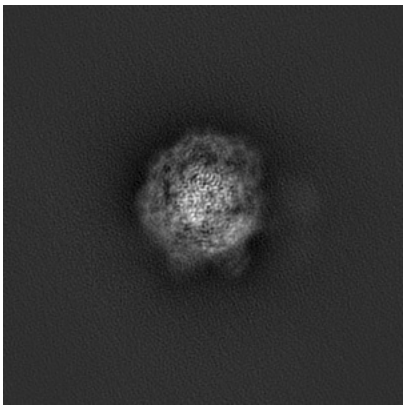
6.1.1 Primary map



X

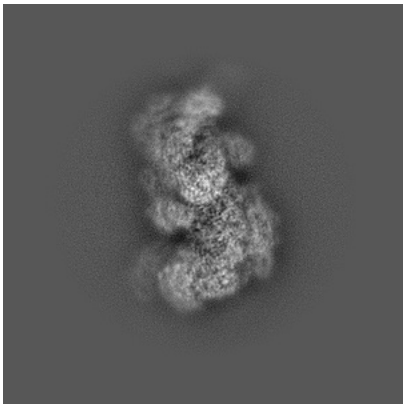


Y

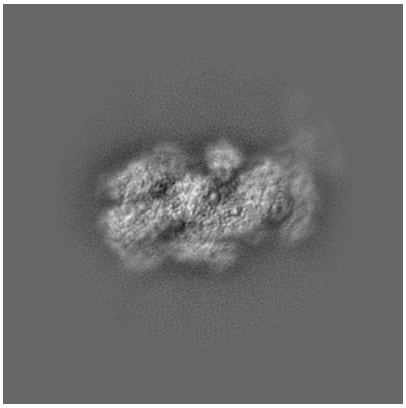


Z

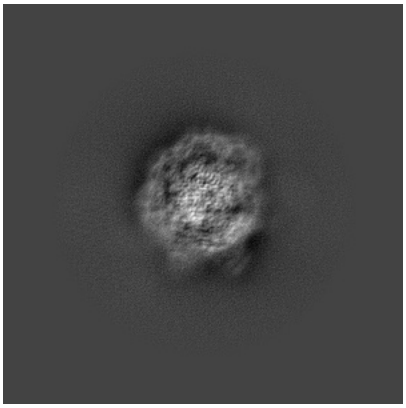
6.1.2 Raw map



X



Y

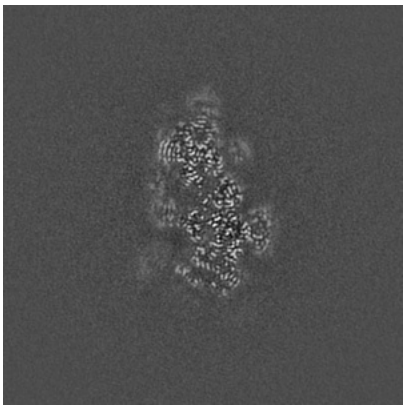


Z

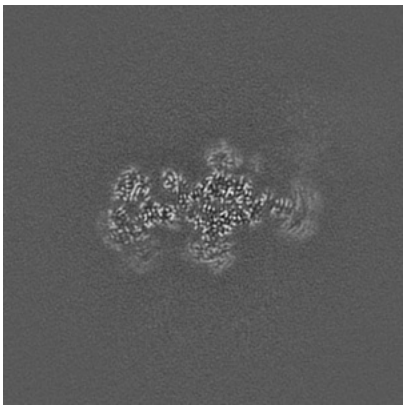
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

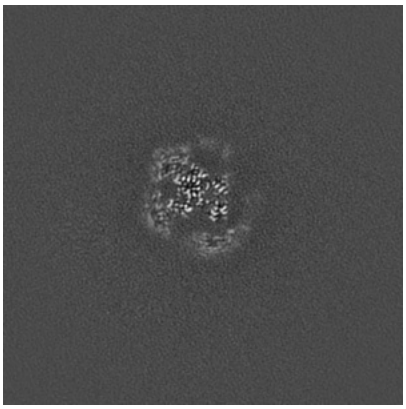
6.2.1 Primary map



X Index: 250

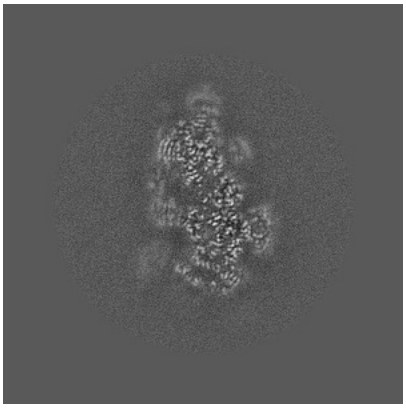


Y Index: 250

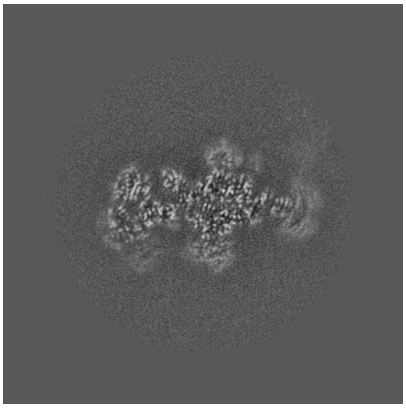


Z Index: 250

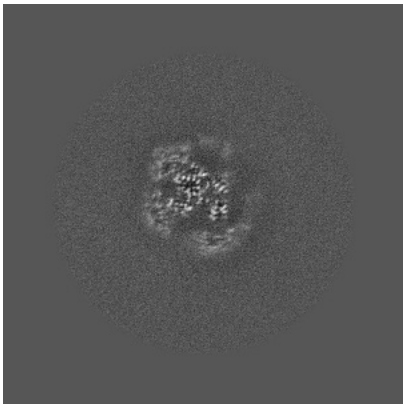
6.2.2 Raw map



X Index: 250



Y Index: 250

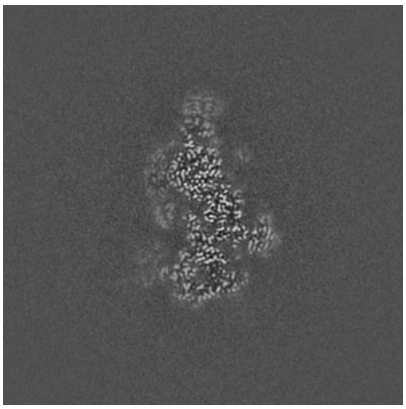


Z Index: 250

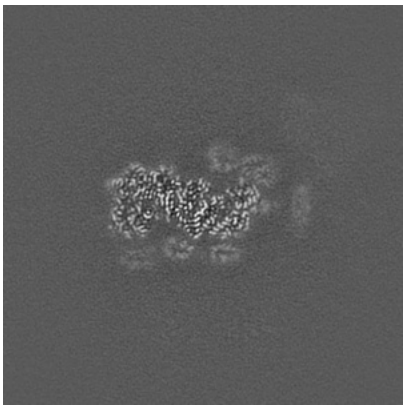
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

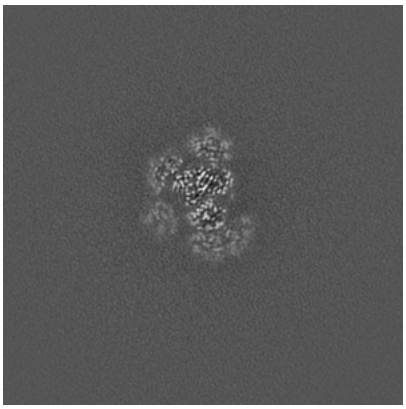
6.3.1 Primary map



X Index: 239

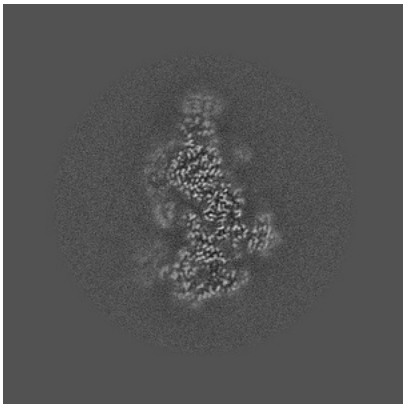


Y Index: 270

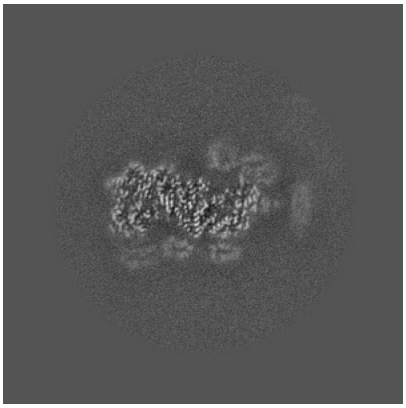


Z Index: 233

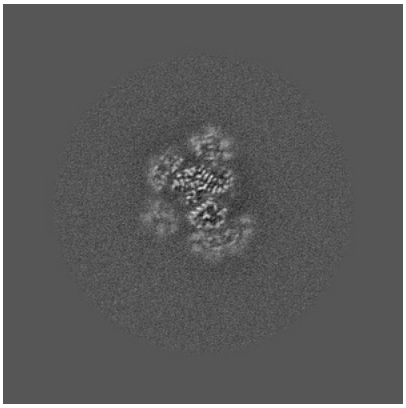
6.3.2 Raw map



X Index: 239



Y Index: 269



Z Index: 234

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

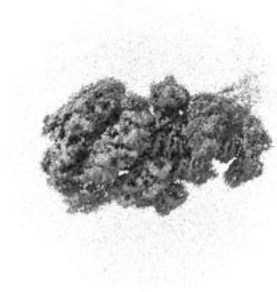
Y

Z

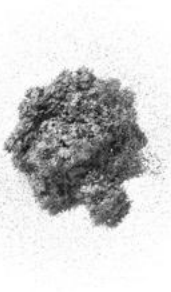
The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X



Y



Z

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

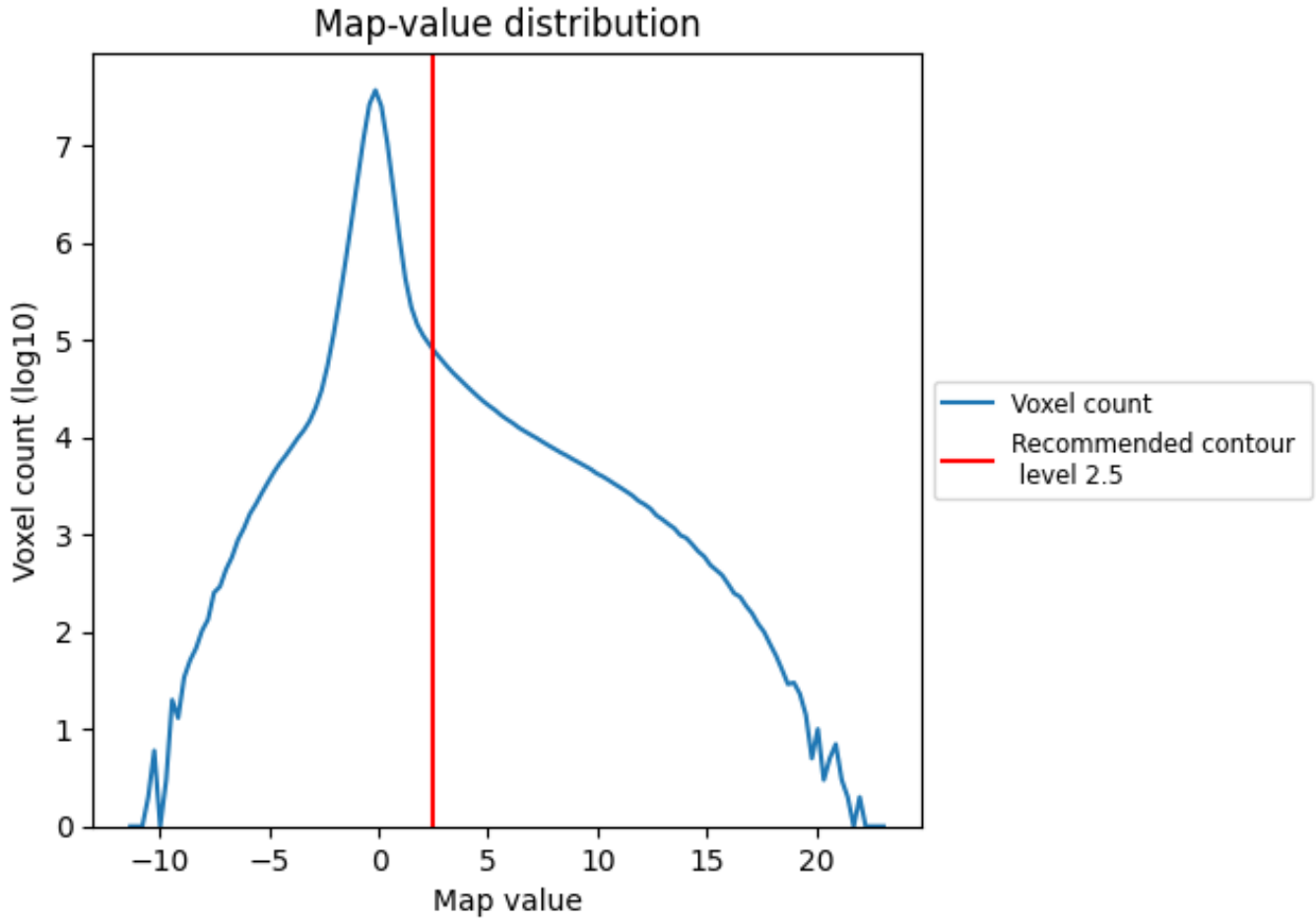
6.5 Mask visualisation (i)

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

7 Map analysis

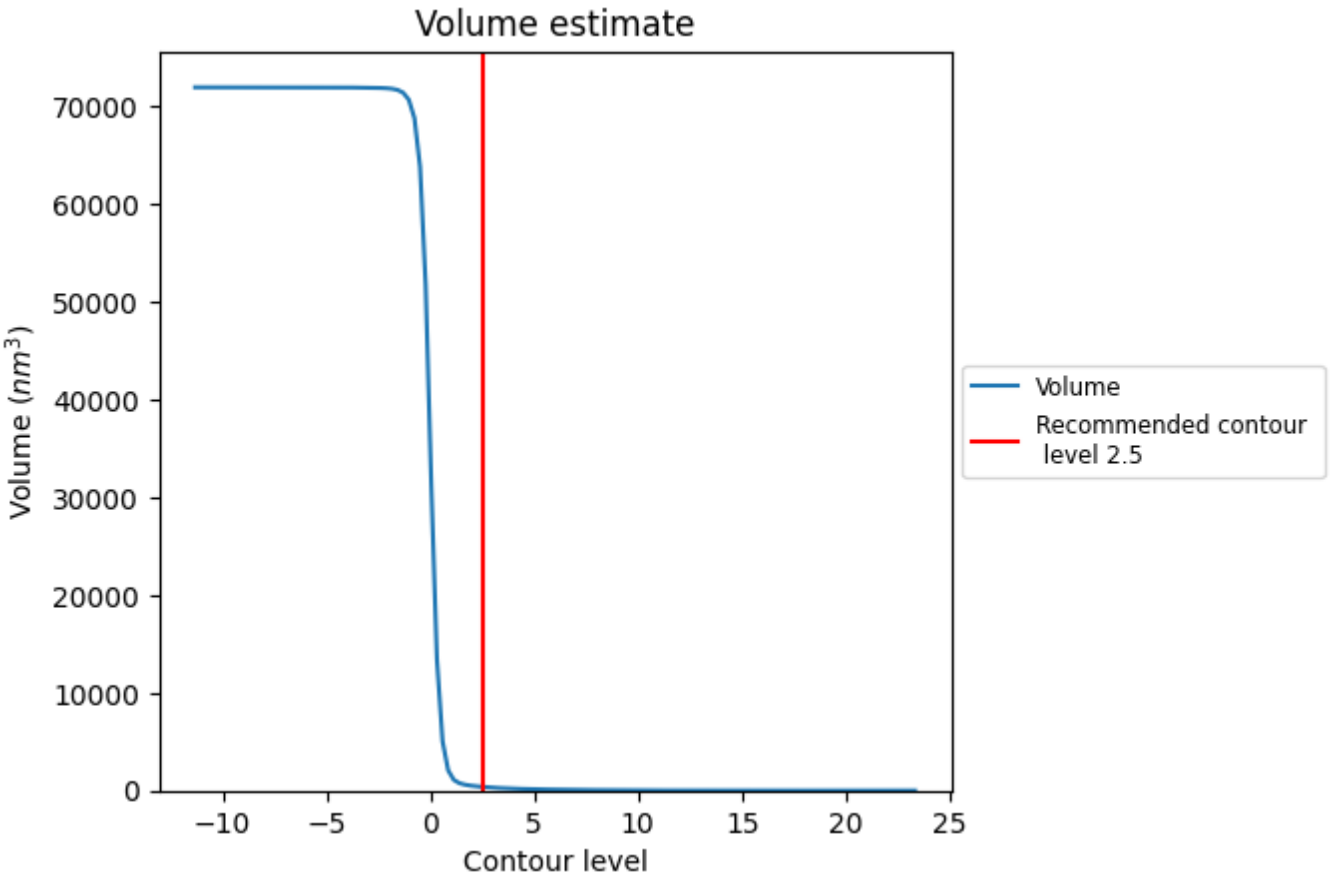
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

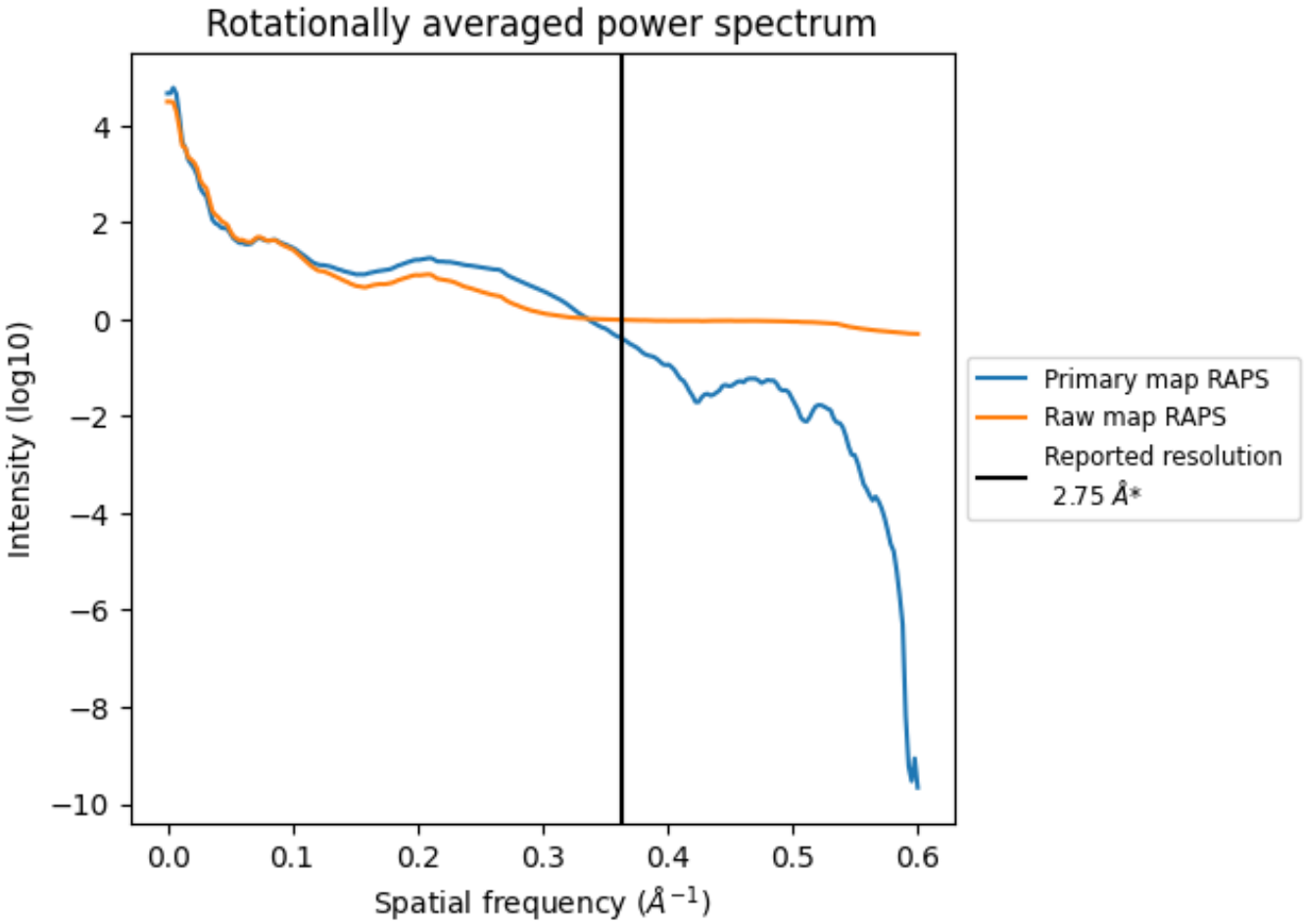
7.2 Volume estimate



The volume at the recommended contour level is 378 nm^3; this corresponds to an approximate mass of 341 kDa.

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

7.3 Rotationally averaged power spectrum (i)

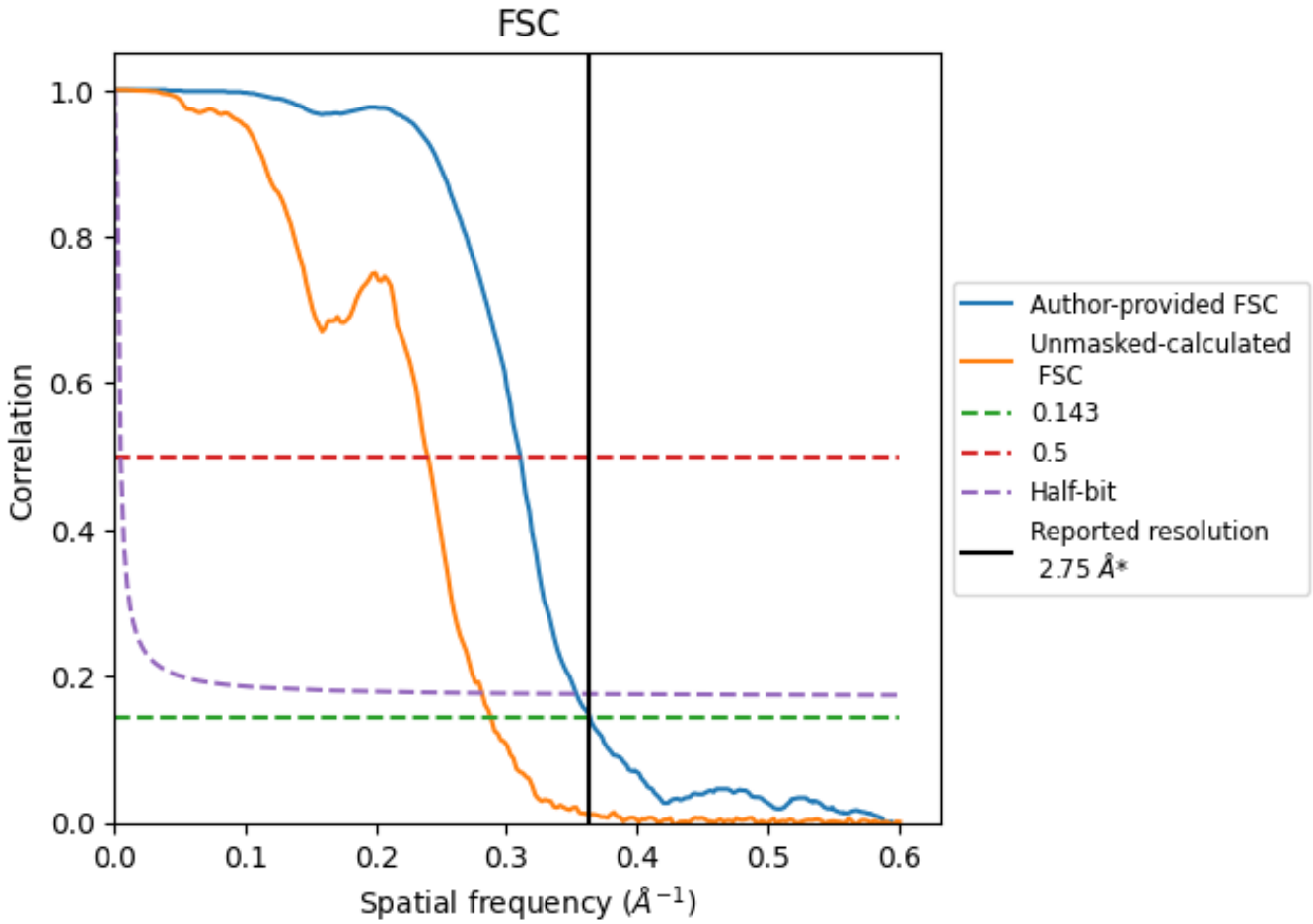


*Reported resolution corresponds to spatial frequency of 0.364 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.364 Å^{-1}

8.2 Resolution estimates (i)

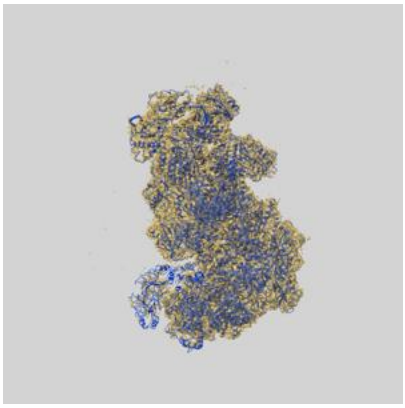
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.75	-	-
Author-provided FSC curve	2.75	3.22	2.83
Unmasked-calculated*	3.47	4.17	3.55

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.47 differs from the reported value 2.75 by more than 10 %

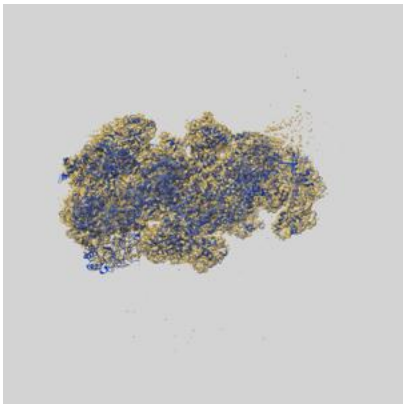
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10102 and PDB model 6S6B. Per-residue inclusion information can be found in section 3 on page 9.

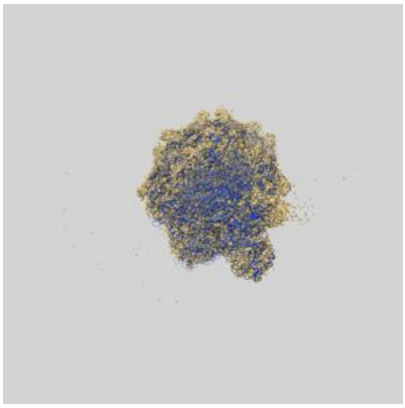
9.1 Map-model overlay



X



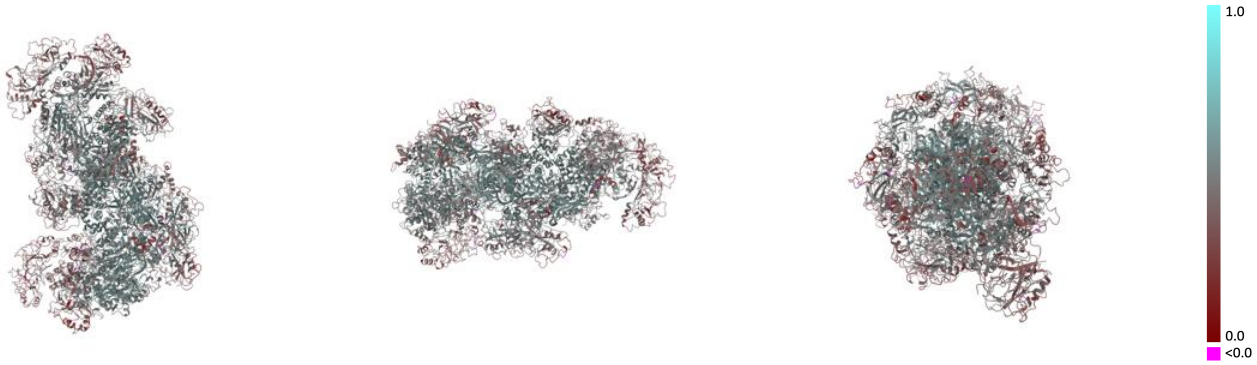
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

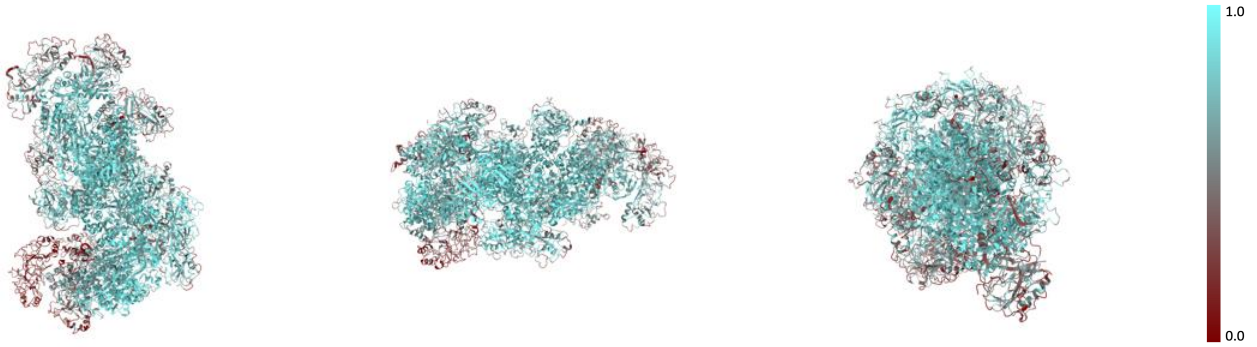
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

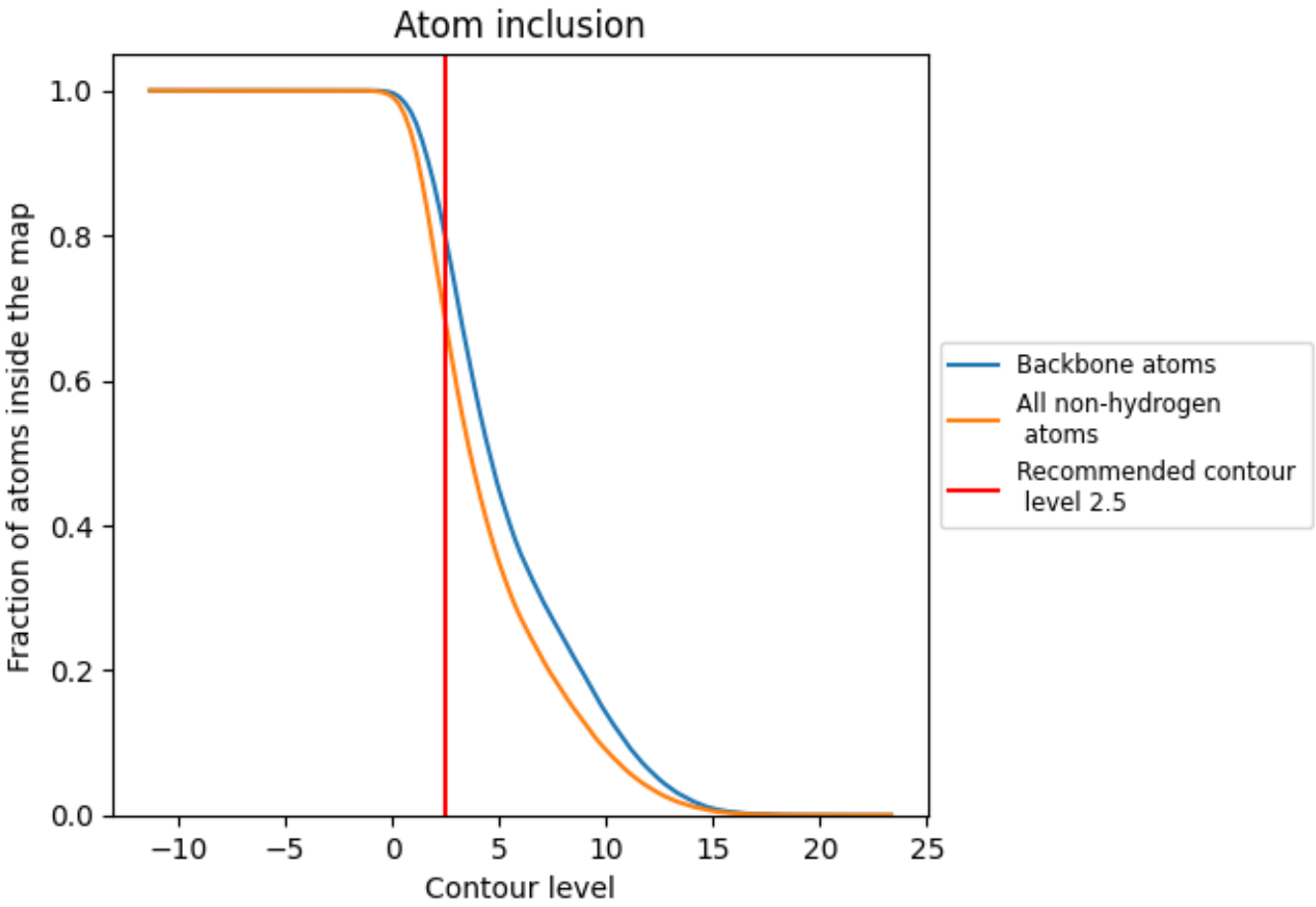
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6786	0.4560
A	0.8863	0.5510
B	0.8935	0.5500
C	0.8984	0.5540
D	0.9060	0.5590
E	0.8931	0.5620
F	0.8927	0.5630
G	0.8805	0.5460
H	0.8827	0.5440
I	0.8928	0.5510
J	0.8302	0.4970
K	0.8222	0.5080
L	0.7226	0.4260
M	0.8072	0.4620
N	0.6277	0.3960
O	0.6269	0.4060
P	0.4952	0.4130
Q	0.6623	0.4120
R	0.7027	0.3950
S	0.5004	0.3790
T	0.5769	0.3660
V	0.8933	0.5400
W	0.4113	0.3920
X	0.3657	0.3420
Y	0.1781	0.3390
Z	0.0567	0.3090
l	0.7454	0.4400
m	0.8028	0.4670
n	0.5923	0.3650
o	0.6549	0.4150
p	0.5703	0.4240
q	0.6961	0.4340
r	0.7506	0.4310
s	0.4805	0.4010
t	0.4474	0.3340

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
w	0.4577	0.3810
x	0.3010	0.3370
y	0.1516	0.3250
z	0.0758	0.3200