wwPDB EM Validation Summary Report (i)

Dec 5, 2024 – 02:55 PM JST

PDB ID	:	8YVF
EMDB ID	:	EMD-39599
Title	:	cryo-EM structure of carboxysomal midi-shell: assembly from CsoS4A/4B/1A/1B/1C/1D and CsoS2 C-terminal co-expression (T=9 Q=12)
Authors	:	Wang, P.; Li, J.X.; Li, T.P.; Li, K.; Ng, P.C.; Wang, S.M.; Chriscoli, V.; Basle, A.; Marles-Wright, J.; Zhang, Y.Z.; Liu, L.N.
Deposited on	:	2024-03-28
Resolution	:	2.99 Å(reported)

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

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

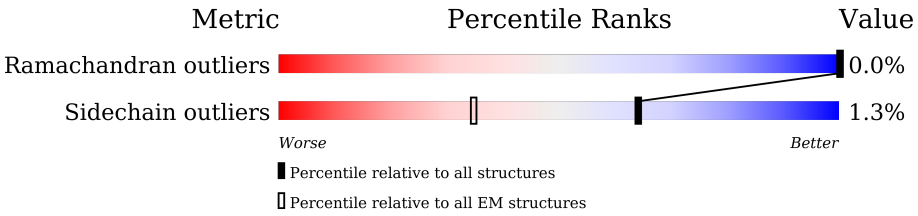
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.99 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	207382	16835
Sidechain outliers	206894	16415

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	0	98	94% 6%
1	2	98	92% • 6%
1	3	98	94% 6%
1	5	98	94% 6%
1	6	98	94% 6%
1	7	98	93% • 6%
1	8	98	94% 6%
1	9	98	94% 6%
1	A	98	94% 6%

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Mol	Chain	Length	Quality of chain
1	A1	98	93% • 6%
1	B	98	93% • 6%
1	C	98	92% • 6%
1	D	98	94% 6%
1	E	98	94% 6%
1	F	98	93% • 6%
1	G	98	94% 6%
1	H	98	94% 6%
1	I	98	93% • 6%
1	J	98	93% • 6%
1	K	98	93% • 6%
1	L	98	92% • 6%
1	M	98	93% • 6%
1	N	98	93% • 6%
1	O	98	93% • 6%
1	P	98	93% • 6%
1	Q	98	93% • 6%
1	R	98	93% • 6%
1	S	98	94% 6%
1	T	98	94% 6%
1	U	98	94% 6%
1	V	98	93% • 6%
1	W	98	94% 6%
1	X	98	94% 6%
1	Y	98	93% • 6%

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Mol	Chain	Length	Quality of chain
1	Z	98	94% 6%
1	a	98	92% 6%
1	b	98	94% 6%
1	c	98	94% 6%
1	d	98	94% 6%
1	e	98	92% 6%
1	f	98	93% 6%
1	g	98	93% 6%
1	h	98	94% 6%
1	i	98	94% 6%
1	j	98	92% 6%
1	k	98	93% 6%
1	l	98	93% 6%
1	m	98	92% 6%
1	n	98	94% 6%
1	o	98	93% 6%
1	p	98	94% 6%
1	q	98	94% 6%
1	r	98	92% 6%
1	s	98	94% 6%
1	t	98	94% 6%
1	u	98	94% 6%
1	v	98	94% 6%
2	1	83	95%
2	4	83	95%

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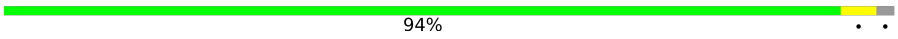
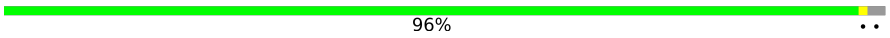
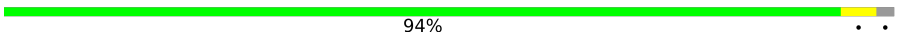
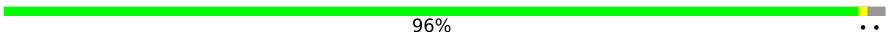
Mol	Chain	Length	Quality of chain
2	w	83	
2	x	83	
2	y	83	
2	z	83	
3	A2	279	
3	A3	279	
3	A4	279	
3	A5	279	
3	A6	279	
3	A7	279	
3	X1	279	
3	X2	279	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 47066 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Major carboxysome shell protein CsoS1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	2	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	3	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	5	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	6	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	7	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	8	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	9	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	A	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	B	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	C	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	D	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	E	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	F	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	G	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	H	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	I	92	Total	C	N	O	S	0	0
			656	408	123	122	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	K	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	L	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	M	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	N	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	O	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	P	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	Q	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	R	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	S	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	T	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	U	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	V	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	W	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	X	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	Y	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	Z	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	a	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	b	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	c	92	Total	C	N	O	S	0	0
			656	408	123	122	3		
1	d	92	Total	C	N	O	S	0	0
			656	408	123	122	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	e	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	f	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	g	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	h	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	i	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	j	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	k	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	l	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	m	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	n	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	o	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	p	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	q	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	r	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	s	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	t	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	u	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	v	92	Total 656	C 408	N 123	O 122	S 3	0	0
1	A1	92	Total 656	C 408	N 123	O 122	S 3	0	0

- Molecule 2 is a protein called Carboxysome shell vertex protein CsoS4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	4	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	w	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	x	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	y	81	Total	C	N	O	S	0	0
			608	386	105	112	5		
2	z	81	Total	C	N	O	S	0	0
			608	386	105	112	5		

- Molecule 3 is a protein called Carboxysome assembly protein CsoS2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A2	123	Total	C	N	O	S	0	0
			908	546	178	179	5		
3	A3	120	Total	C	N	O	S	0	0
			884	534	171	174	5		
3	A4	115	Total	C	N	O	S	0	0
			842	506	162	169	5		
3	A5	118	Total	C	N	O	S	0	0
			862	519	166	172	5		
3	A6	136	Total	C	N	O	S	0	0
			1000	602	196	197	5		
3	A7	117	Total	C	N	O	S	0	0
			856	517	164	171	4		
3	X1	48	Total	C	N	O	S	0	0
			337	199	55	81	2		
3	X2	48	Total	C	N	O	S	0	0
			337	199	55	81	2		

There are 8 discrepancies between the modelled and reference sequences:

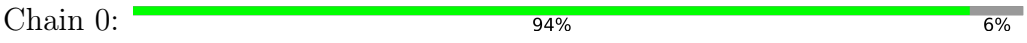
Chain	Residue	Modelled	Actual	Comment	Reference
A2	591	MET	-	initiating methionine	UNP O85041
A3	591	MET	-	initiating methionine	UNP O85041
A4	591	MET	-	initiating methionine	UNP O85041
A5	591	MET	-	initiating methionine	UNP O85041
A6	591	MET	-	initiating methionine	UNP O85041
A7	591	MET	-	initiating methionine	UNP O85041
X1	591	MET	-	initiating methionine	UNP O85041
X2	591	MET	-	initiating methionine	UNP O85041

3 Residue-property plots (i)

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

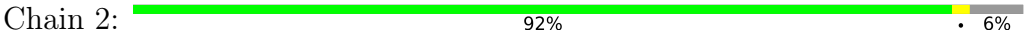
- Molecule 1: Major carboxysome shell protein CsoS1A

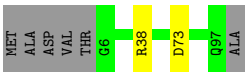
Chain 0:



- Molecule 1: Major carboxysome shell protein CsoS1A

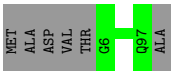
Chain 2:





- Molecule 1: Major carboxysome shell protein CsoS1A

Chain 3:

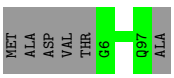


- Molecule 1: Major carboxysome shell protein CsoS1A

Chain 5:

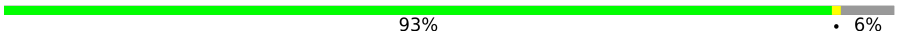
- Molecule 1: Major carboxysome shell protein CsoS1A

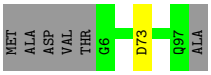
Chain 6:



- Molecule 1: Major carboxysome shell protein CsoS1A

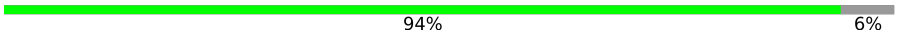
Chain 7:

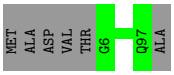




• Molecule 1: Major carboxysome shell protein CsoS1A

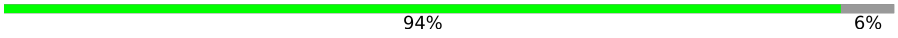
Chain 8:





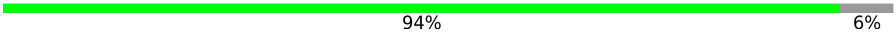
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain 9:



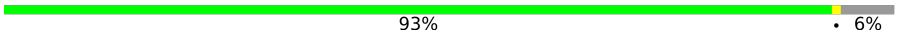
• Molecule 1: Major carboxysome shell protein CsoS1A

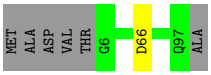
Chain A:



• Molecule 1: Major carboxysome shell protein CsoS1A

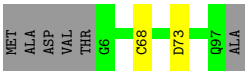
Chain B:





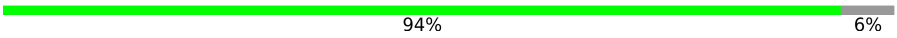
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain C:



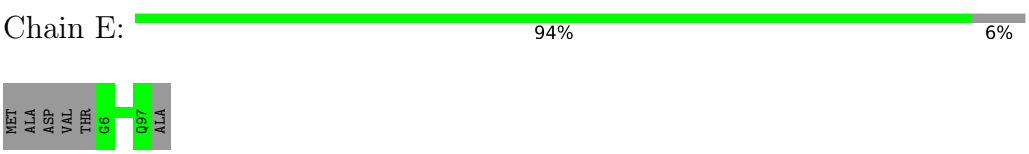
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain D:



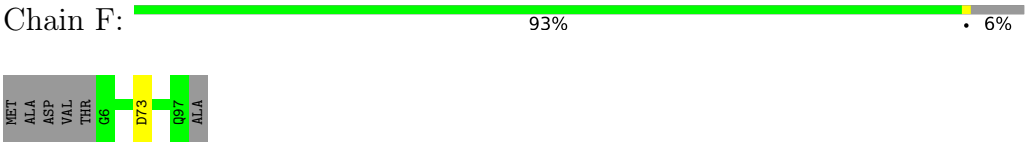
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain E:



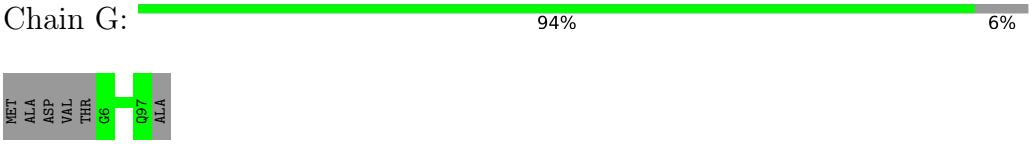
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain F:



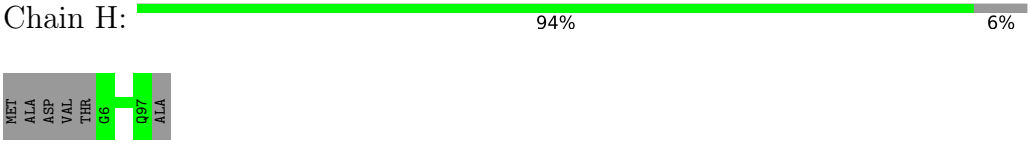
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain G:



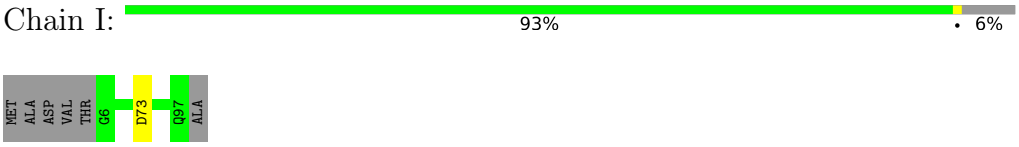
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain H:



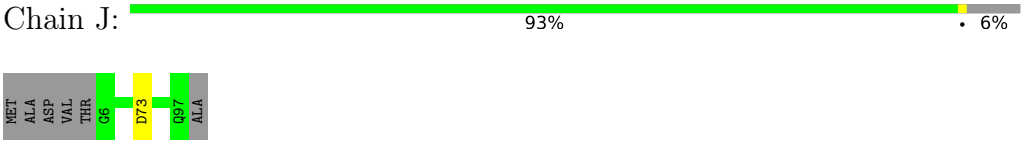
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain I:



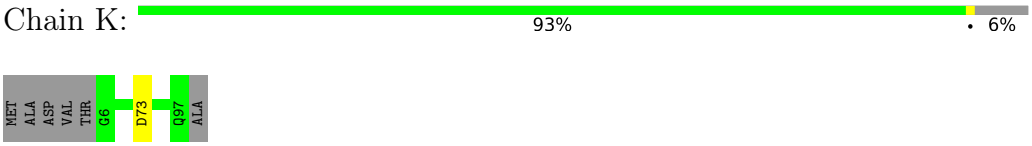
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain J:



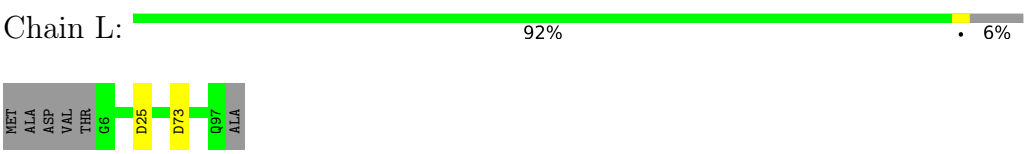
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain K:



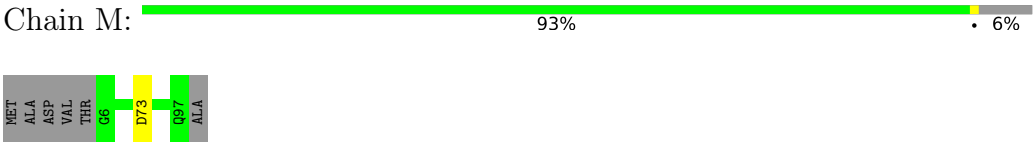
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain L:



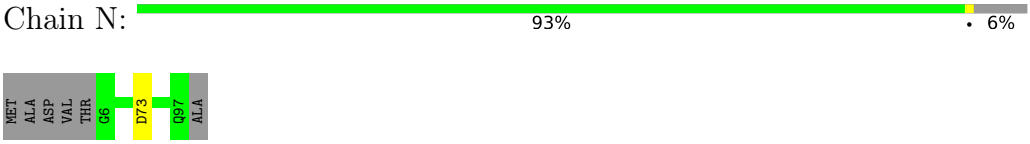
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain M:



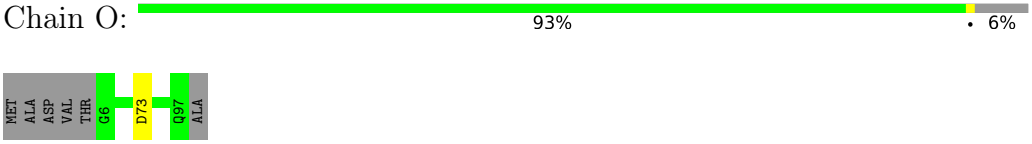
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain N:



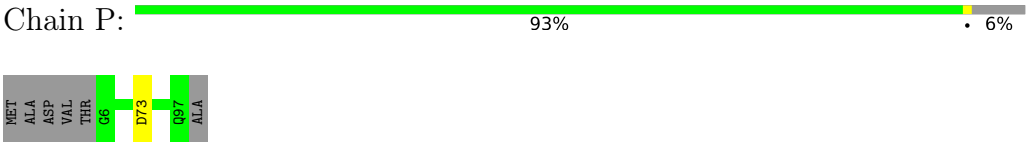
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain O:



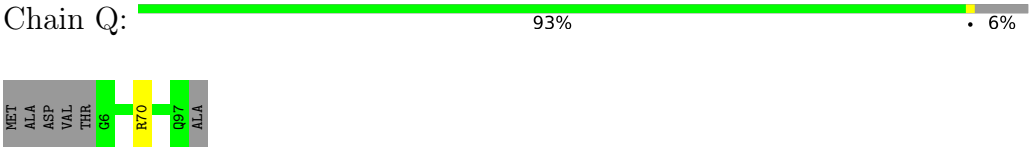
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain P:



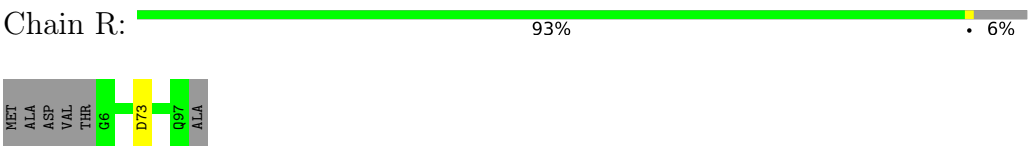
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain Q:



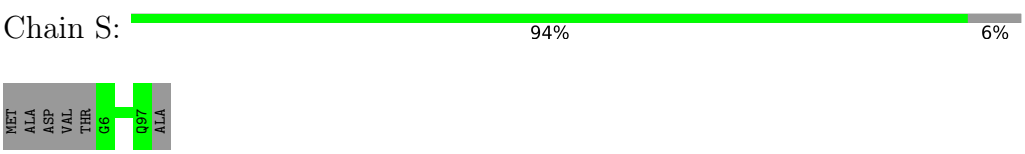
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain R:



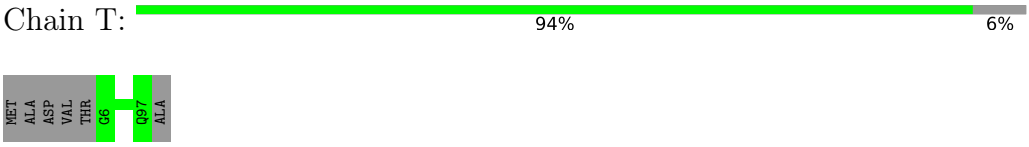
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain S:



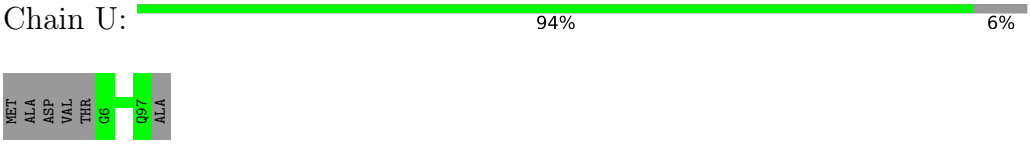
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain T:



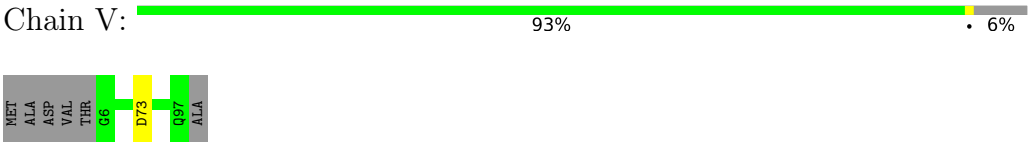
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain U:



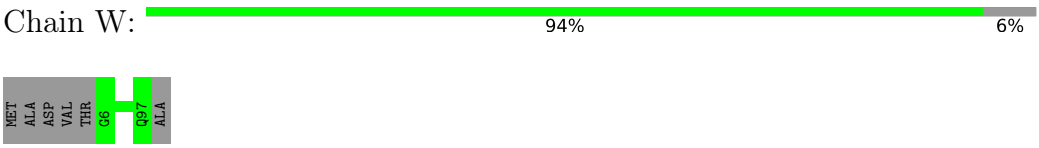
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain V:



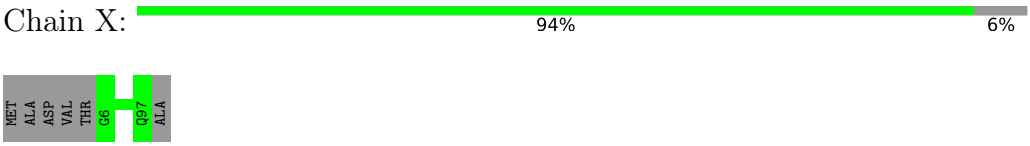
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain W:



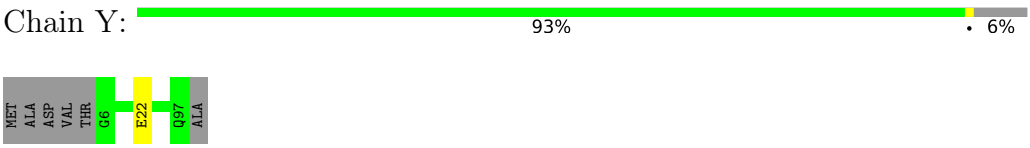
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain X:



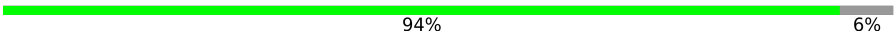
• Molecule 1: Major carboxysome shell protein CsoS1A

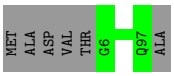
Chain Y:



• Molecule 1: Major carboxysome shell protein CsoS1A

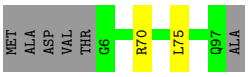
Chain Z:





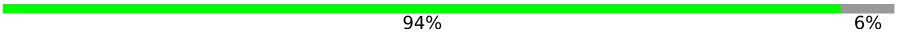
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain a:



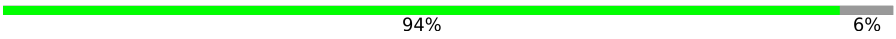
• Molecule 1: Major carboxysome shell protein CsoS1A

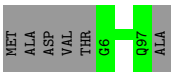
Chain b:



• Molecule 1: Major carboxysome shell protein CsoS1A

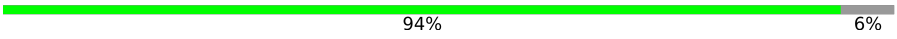
Chain c:

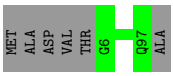




• Molecule 1: Major carboxysome shell protein CsoS1A

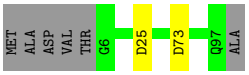
Chain d:





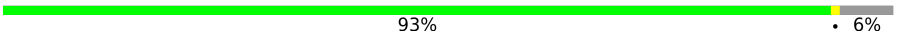
• Molecule 1: Major carboxysome shell protein CsoS1A

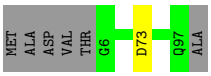
Chain e:



• Molecule 1: Major carboxysome shell protein CsoS1A

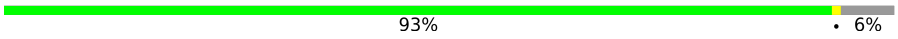
Chain f:

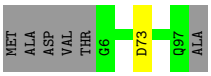




• Molecule 1: Major carboxysome shell protein CsoS1A

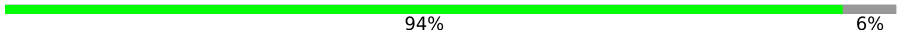
Chain g:





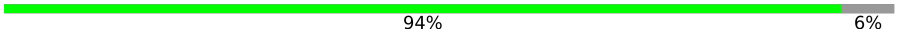
• Molecule 1: Major carboxysome shell protein CsoS1A

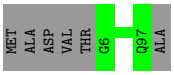
Chain h:



• Molecule 1: Major carboxysome shell protein CsoS1A

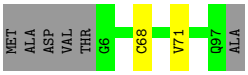
Chain i:





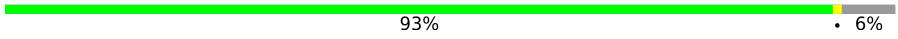
• Molecule 1: Major carboxysome shell protein CsoS1A

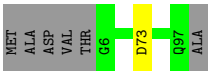
Chain j:



• Molecule 1: Major carboxysome shell protein CsoS1A

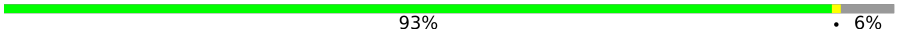
Chain k:

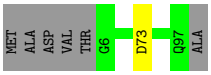




• Molecule 1: Major carboxysome shell protein CsoS1A

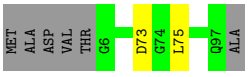
Chain l:





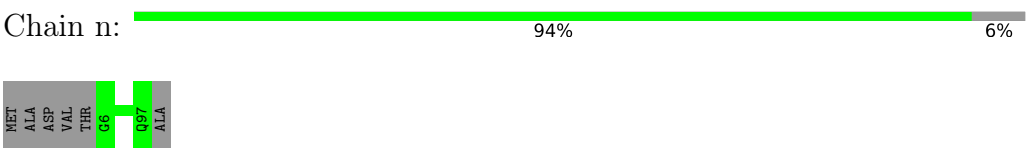
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain m:



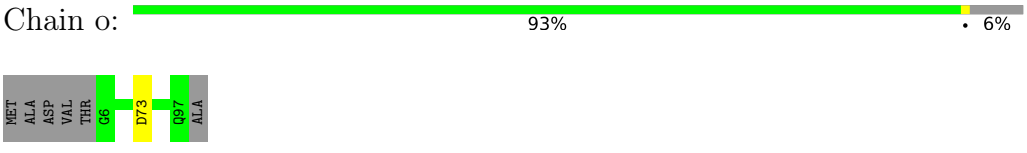
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain n:



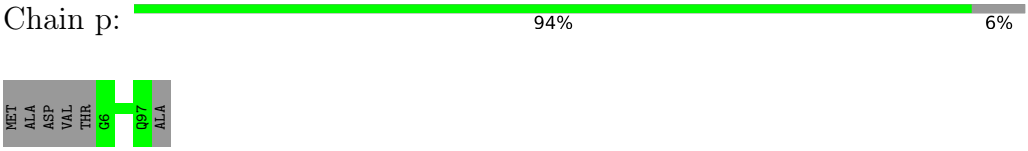
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain o:



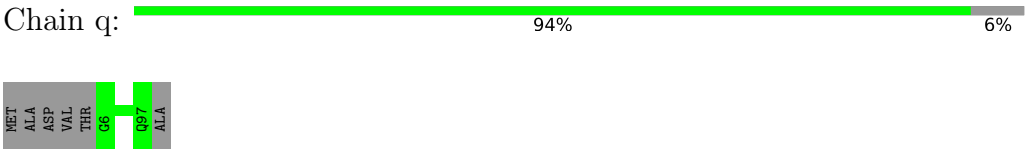
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain p:



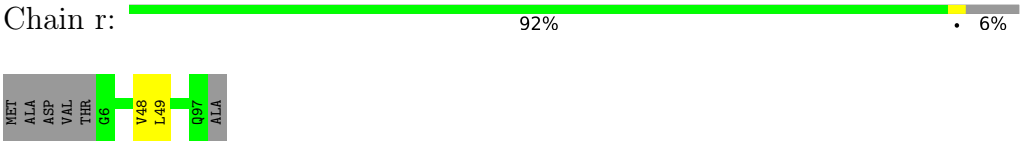
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain q:



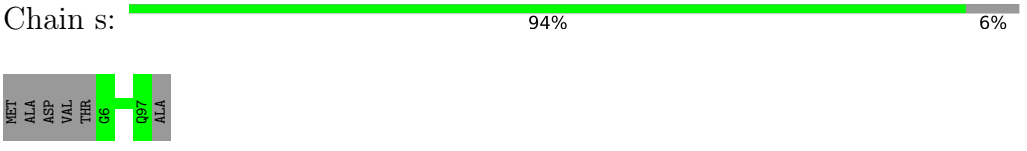
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain r:



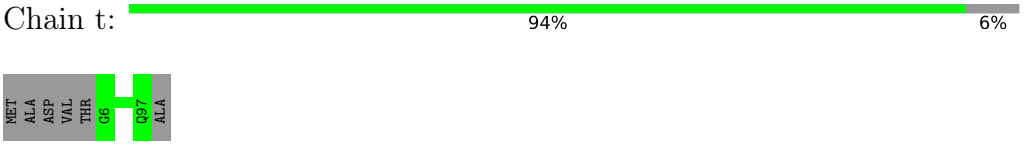
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain s:



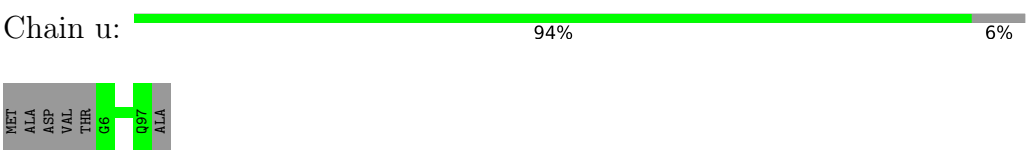
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain t:



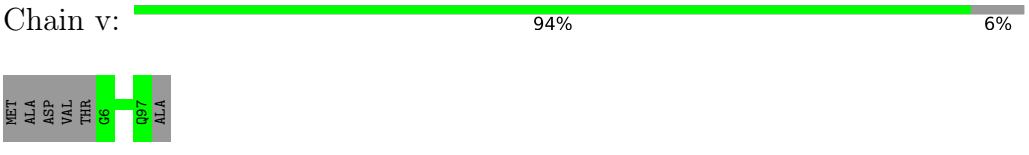
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain u:



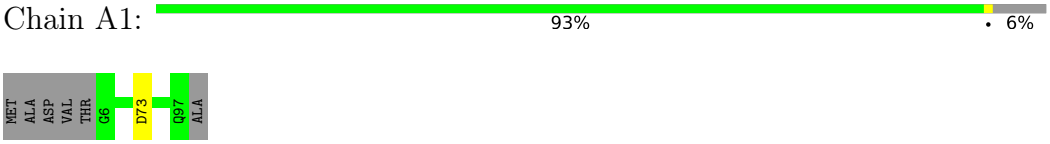
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain v:



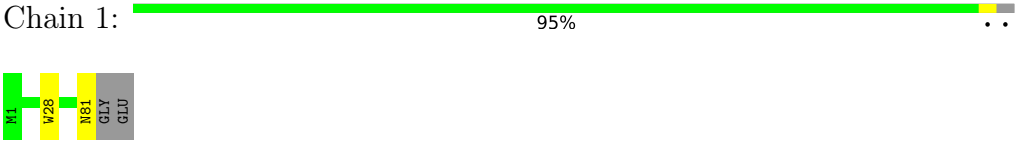
• Molecule 1: Major carboxysome shell protein CsoS1A

Chain A1:



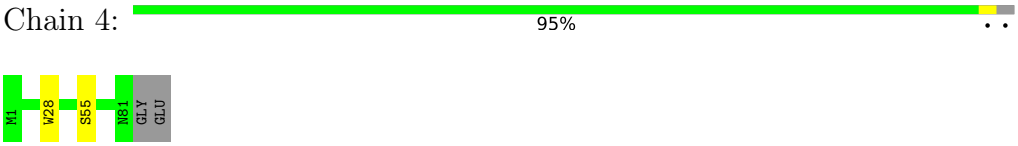
• Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain 1:



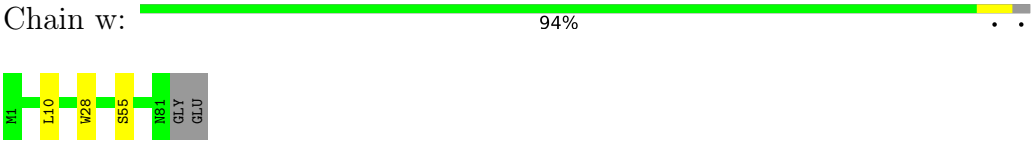
• Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain 4:



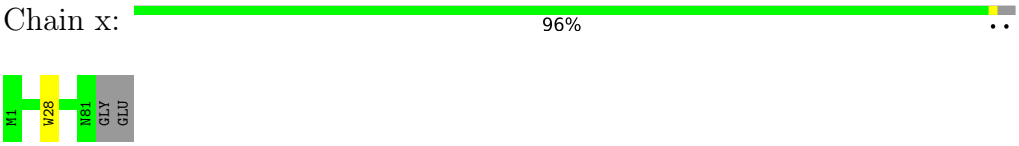
• Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain w:



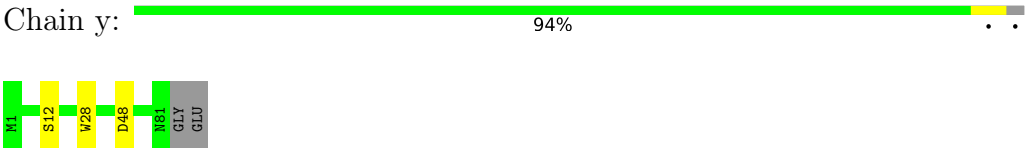
• Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain x:



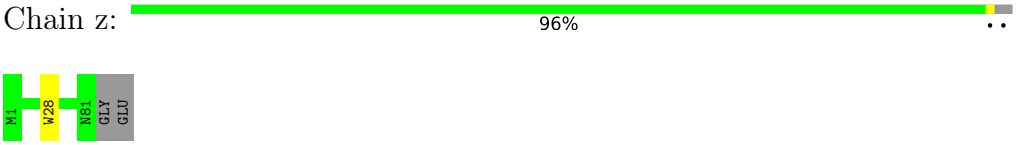
• Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain y:



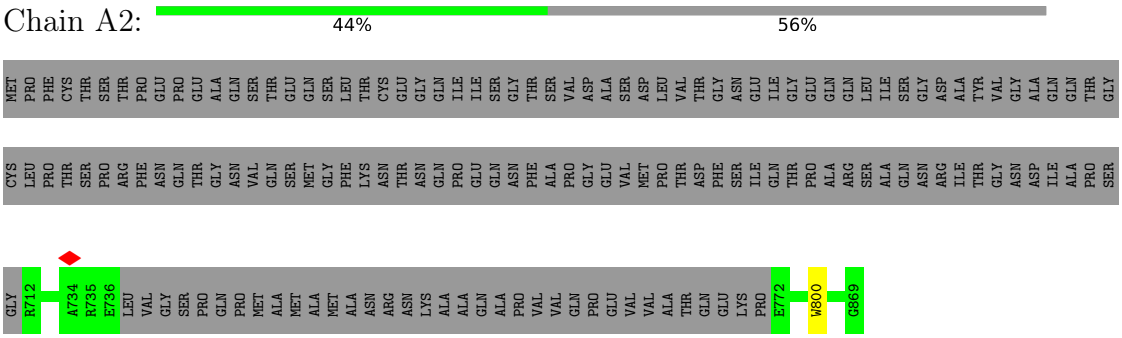
• Molecule 2: Carboxysome shell vertex protein CsoS4A

Chain z:



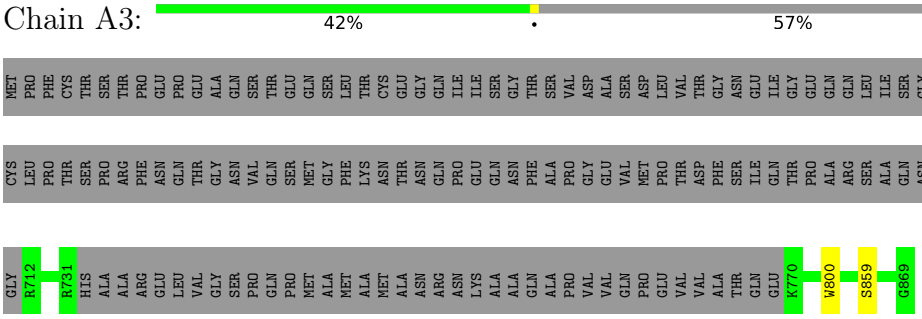
• Molecule 3: Carboxysome assembly protein CsoS2B

Chain A2:



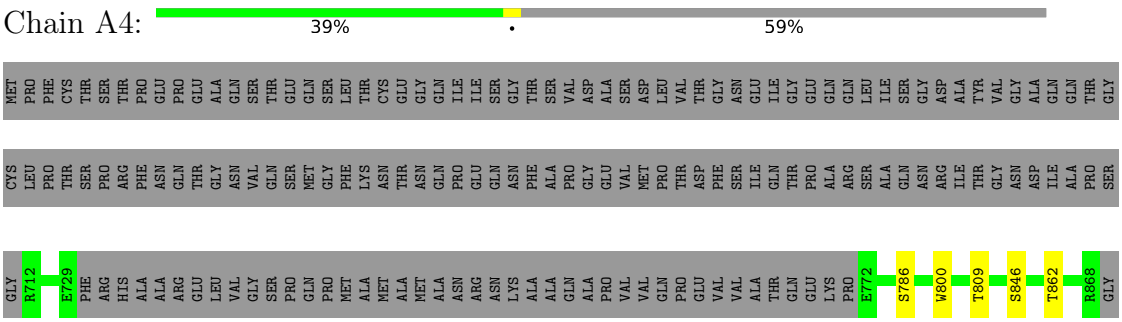
• Molecule 3: Carboxysome assembly protein CsoS2B

Chain A3:



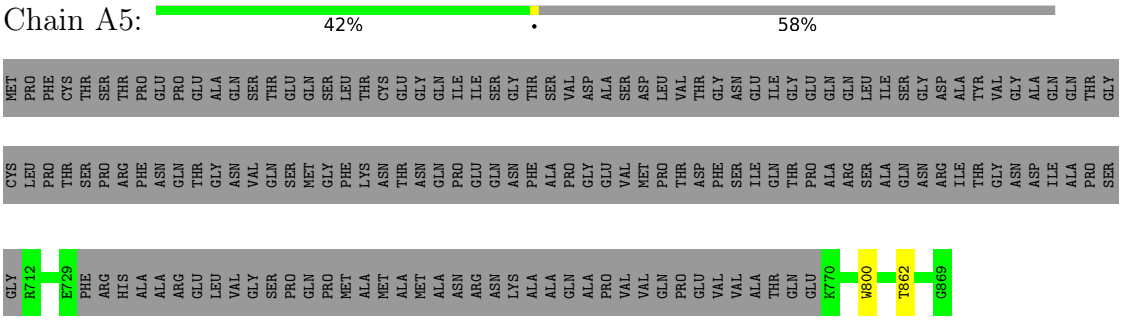
• Molecule 3: Carboxysome assembly protein CsoS2B

Chain A4:



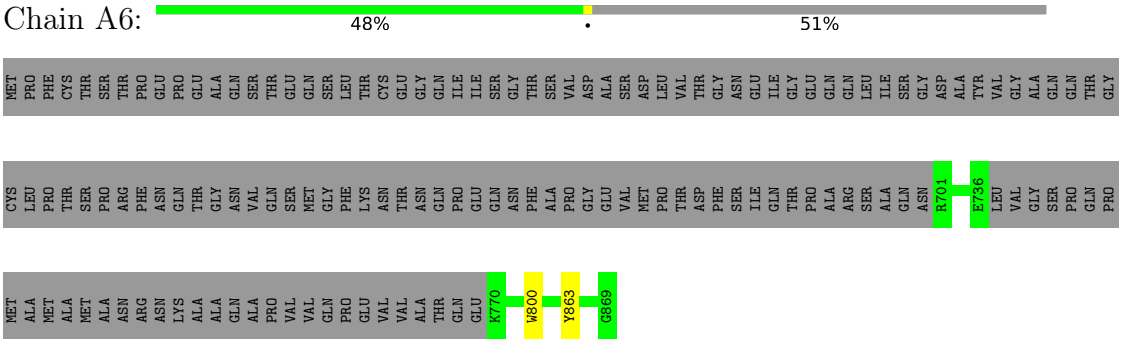
• Molecule 3: Carboxysome assembly protein CsoS2B

Chain A5:



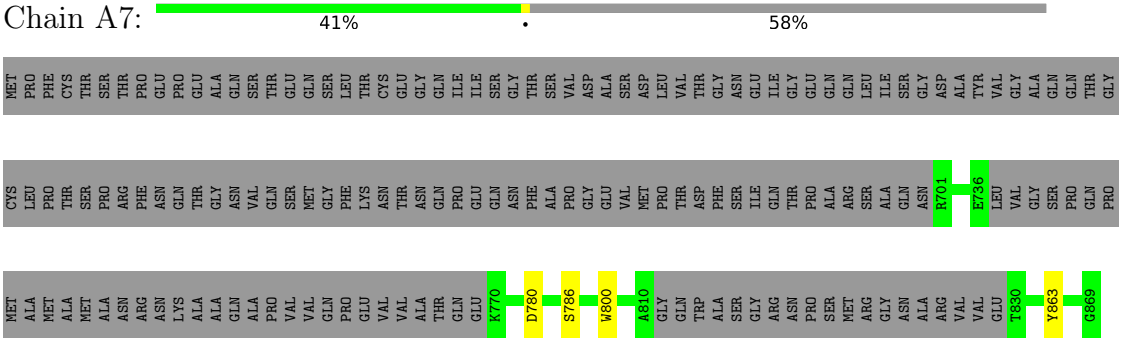
• Molecule 3: Carboxysome assembly protein CsoS2B

Chain A6:



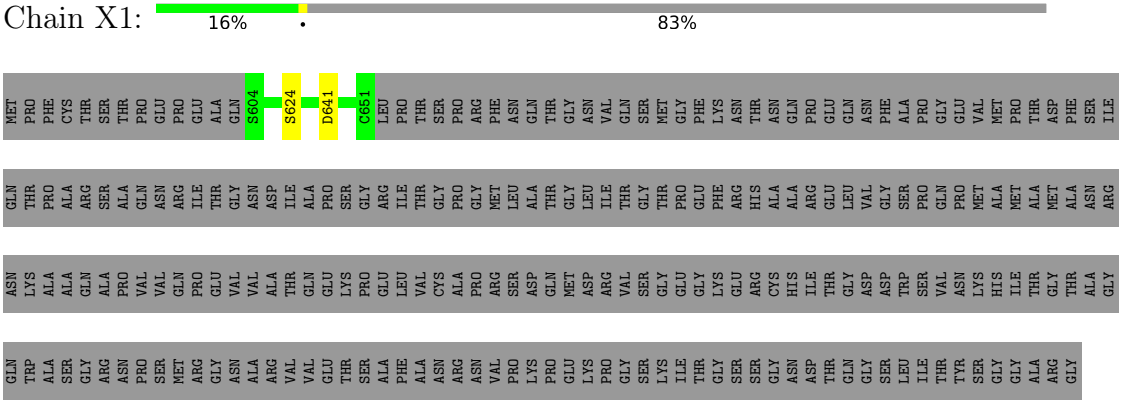
• Molecule 3: Carboxysome assembly protein CsoS2B

Chain A7:



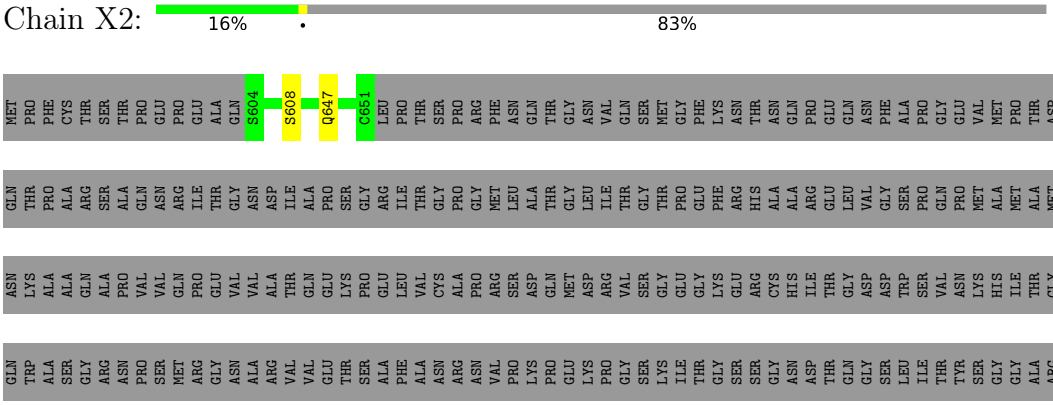
• Molecule 3: Carboxysome assembly protein CsoS2B

Chain X1:



• Molecule 3: Carboxysome assembly protein CsoS2B

Chain X2:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3655	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.0	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.598	Depositor
Minimum map value	-0.684	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.157	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	423.87695, 428.9231, 483.16925	wwPDB
Map dimensions	336, 340, 383	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2615385, 1.2615385, 1.2615385	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.33	0/662	0.61	0/897
1	2	0.32	0/662	0.60	0/897
1	3	0.39	0/662	0.69	0/897
1	5	0.38	0/662	0.64	0/897
1	6	0.31	0/662	0.59	0/897
1	7	0.33	0/662	0.62	0/897
1	8	0.38	0/662	0.61	0/897
1	9	0.29	0/662	0.58	0/897
1	A	0.31	0/662	0.60	0/897
1	A1	0.30	0/662	0.60	0/897
1	B	0.41	0/662	0.72	0/897
1	C	0.40	0/662	0.70	0/897
1	D	0.28	0/662	0.57	0/897
1	E	0.34	0/662	0.67	0/897
1	F	0.29	0/662	0.61	1/897 (0.1%)
1	G	0.39	0/662	0.68	0/897
1	H	0.26	0/662	0.55	0/897
1	I	0.36	0/662	0.67	0/897
1	J	0.42	0/662	0.70	1/897 (0.1%)
1	K	0.42	0/662	0.67	0/897
1	L	0.39	0/662	0.66	0/897
1	M	0.44	0/662	0.73	0/897
1	N	0.40	0/662	0.70	0/897
1	O	0.41	0/662	0.75	0/897
1	P	0.36	0/662	0.67	0/897
1	Q	0.37	0/662	0.67	0/897
1	R	0.35	0/662	0.68	0/897
1	S	0.31	0/662	0.64	0/897
1	T	0.30	0/662	0.60	0/897
1	U	0.46	0/662	0.76	0/897
1	V	0.35	0/662	0.66	0/897
1	W	0.41	0/662	0.68	0/897
1	X	0.40	0/662	0.70	0/897
1	Y	0.47	0/662	0.73	0/897

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	Z	0.32	0/662	0.61	0/897
1	a	0.37	0/662	0.66	0/897
1	b	0.31	0/662	0.60	0/897
1	c	0.39	0/662	0.67	0/897
1	d	0.27	0/662	0.53	0/897
1	e	0.41	0/662	0.68	0/897
1	f	0.31	0/662	0.61	0/897
1	g	0.31	0/662	0.59	0/897
1	h	0.27	0/662	0.55	0/897
1	i	0.29	0/662	0.58	0/897
1	j	0.35	0/662	0.64	0/897
1	k	0.36	0/662	0.67	0/897
1	l	0.36	0/662	0.64	0/897
1	m	0.38	0/662	0.64	1/897 (0.1%)
1	n	0.37	0/662	0.63	0/897
1	o	0.29	0/662	0.60	1/897 (0.1%)
1	p	0.31	0/662	0.57	0/897
1	q	0.33	0/662	0.64	0/897
1	r	0.34	0/662	0.66	0/897
1	s	0.34	0/662	0.66	0/897
1	t	0.32	0/662	0.60	0/897
1	u	0.32	0/662	0.62	0/897
1	v	0.32	0/662	0.63	0/897
2	1	0.33	0/620	0.58	0/843
2	4	0.37	0/620	0.64	0/843
2	w	0.48	0/620	0.60	0/843
2	x	0.28	0/620	0.48	0/843
2	y	0.39	0/620	0.60	0/843
2	z	0.34	0/620	0.56	0/843
3	A2	0.48	0/923	0.82	0/1243
3	A3	0.43	0/899	0.74	0/1211
3	A4	0.51	0/855	0.85	0/1153
3	A5	0.43	0/876	0.76	0/1181
3	A6	0.42	0/1017	0.73	0/1371
3	A7	0.47	0/869	0.80	0/1170
3	X1	0.49	0/337	0.76	0/456
3	X2	0.38	0/337	0.60	0/456
All	All	0.37	0/47567	0.66	4/64428 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	73	ASP	CB-CA-C	6.91	124.22	110.40
1	J	73	ASP	CB-CA-C	6.61	123.62	110.40
1	o	73	ASP	CB-CA-C	5.26	120.93	110.40
1	m	73	ASP	CB-CA-C	5.26	120.92	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	2	90/98 (92%)	90 (100%)	0	0	100	100
1	3	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	5	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	6	90/98 (92%)	90 (100%)	0	0	100	100
1	7	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	8	90/98 (92%)	90 (100%)	0	0	100	100
1	9	90/98 (92%)	90 (100%)	0	0	100	100
1	A	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	A1	90/98 (92%)	90 (100%)	0	0	100	100
1	B	90/98 (92%)	90 (100%)	0	0	100	100
1	C	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	D	90/98 (92%)	90 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	90/98 (92%)	90 (100%)	0	0	100	100
1	F	90/98 (92%)	90 (100%)	0	0	100	100
1	G	90/98 (92%)	90 (100%)	0	0	100	100
1	H	90/98 (92%)	90 (100%)	0	0	100	100
1	I	90/98 (92%)	90 (100%)	0	0	100	100
1	J	90/98 (92%)	90 (100%)	0	0	100	100
1	K	90/98 (92%)	90 (100%)	0	0	100	100
1	L	90/98 (92%)	90 (100%)	0	0	100	100
1	M	90/98 (92%)	90 (100%)	0	0	100	100
1	N	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	O	90/98 (92%)	90 (100%)	0	0	100	100
1	P	90/98 (92%)	90 (100%)	0	0	100	100
1	Q	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	R	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	S	90/98 (92%)	90 (100%)	0	0	100	100
1	T	90/98 (92%)	90 (100%)	0	0	100	100
1	U	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	V	90/98 (92%)	90 (100%)	0	0	100	100
1	W	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	X	90/98 (92%)	90 (100%)	0	0	100	100
1	Y	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	Z	90/98 (92%)	90 (100%)	0	0	100	100
1	a	90/98 (92%)	90 (100%)	0	0	100	100
1	b	90/98 (92%)	90 (100%)	0	0	100	100
1	c	90/98 (92%)	90 (100%)	0	0	100	100
1	d	90/98 (92%)	90 (100%)	0	0	100	100
1	e	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	f	90/98 (92%)	90 (100%)	0	0	100	100
1	g	90/98 (92%)	90 (100%)	0	0	100	100
1	h	90/98 (92%)	90 (100%)	0	0	100	100
1	i	90/98 (92%)	88 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	j	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	k	90/98 (92%)	90 (100%)	0	0	100	100
1	l	90/98 (92%)	90 (100%)	0	0	100	100
1	m	90/98 (92%)	90 (100%)	0	0	100	100
1	n	90/98 (92%)	90 (100%)	0	0	100	100
1	o	90/98 (92%)	90 (100%)	0	0	100	100
1	p	90/98 (92%)	90 (100%)	0	0	100	100
1	q	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	r	90/98 (92%)	88 (98%)	2 (2%)	0	100	100
1	s	90/98 (92%)	90 (100%)	0	0	100	100
1	t	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
1	u	90/98 (92%)	90 (100%)	0	0	100	100
1	v	90/98 (92%)	89 (99%)	1 (1%)	0	100	100
2	1	79/83 (95%)	77 (98%)	2 (2%)	0	100	100
2	4	79/83 (95%)	78 (99%)	0	1 (1%)	10	39
2	w	79/83 (95%)	75 (95%)	3 (4%)	1 (1%)	10	39
2	x	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
2	y	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
2	z	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
3	A2	119/279 (43%)	113 (95%)	6 (5%)	0	100	100
3	A3	116/279 (42%)	111 (96%)	5 (4%)	0	100	100
3	A4	111/279 (40%)	106 (96%)	5 (4%)	0	100	100
3	A5	114/279 (41%)	107 (94%)	7 (6%)	0	100	100
3	A6	132/279 (47%)	130 (98%)	2 (2%)	0	100	100
3	A7	111/279 (40%)	105 (95%)	6 (5%)	0	100	100
3	X1	46/279 (16%)	44 (96%)	2 (4%)	0	100	100
3	X2	46/279 (16%)	45 (98%)	1 (2%)	0	100	100
All	All	6399/8316 (77%)	6324 (99%)	73 (1%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	4	55	SER

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Mol	Chain	Res	Type
2	w	55	SER

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	0	63/67 (94%)	63 (100%)	0	100	100
1	2	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	3	63/67 (94%)	63 (100%)	0	100	100
1	5	63/67 (94%)	63 (100%)	0	100	100
1	6	63/67 (94%)	63 (100%)	0	100	100
1	7	63/67 (94%)	62 (98%)	1 (2%)	58	82
1	8	63/67 (94%)	63 (100%)	0	100	100
1	9	63/67 (94%)	63 (100%)	0	100	100
1	A	63/67 (94%)	63 (100%)	0	100	100
1	A1	63/67 (94%)	62 (98%)	1 (2%)	58	82
1	B	63/67 (94%)	62 (98%)	1 (2%)	58	82
1	C	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	D	63/67 (94%)	63 (100%)	0	100	100
1	E	63/67 (94%)	63 (100%)	0	100	100
1	F	63/67 (94%)	63 (100%)	0	100	100
1	G	63/67 (94%)	63 (100%)	0	100	100
1	H	63/67 (94%)	63 (100%)	0	100	100
1	I	63/67 (94%)	62 (98%)	1 (2%)	58	82
1	J	63/67 (94%)	63 (100%)	0	100	100
1	K	63/67 (94%)	62 (98%)	1 (2%)	58	82
1	L	63/67 (94%)	61 (97%)	2 (3%)	34	67
1	M	63/67 (94%)	62 (98%)	1 (2%)	58	82
1	N	63/67 (94%)	62 (98%)	1 (2%)	58	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	O	63/67 (94%)	62 (98%)	1 (2%)	58 82
1	P	63/67 (94%)	62 (98%)	1 (2%)	58 82
1	Q	63/67 (94%)	62 (98%)	1 (2%)	58 82
1	R	63/67 (94%)	62 (98%)	1 (2%)	58 82
1	S	63/67 (94%)	63 (100%)	0	100 100
1	T	63/67 (94%)	63 (100%)	0	100 100
1	U	63/67 (94%)	63 (100%)	0	100 100
1	V	63/67 (94%)	62 (98%)	1 (2%)	58 82
1	W	63/67 (94%)	63 (100%)	0	100 100
1	X	63/67 (94%)	63 (100%)	0	100 100
1	Y	63/67 (94%)	62 (98%)	1 (2%)	58 82
1	Z	63/67 (94%)	63 (100%)	0	100 100
1	a	63/67 (94%)	61 (97%)	2 (3%)	34 67
1	b	63/67 (94%)	63 (100%)	0	100 100
1	c	63/67 (94%)	63 (100%)	0	100 100
1	d	63/67 (94%)	63 (100%)	0	100 100
1	e	63/67 (94%)	61 (97%)	2 (3%)	34 67
1	f	63/67 (94%)	62 (98%)	1 (2%)	58 82
1	g	63/67 (94%)	62 (98%)	1 (2%)	58 82
1	h	63/67 (94%)	63 (100%)	0	100 100
1	i	63/67 (94%)	63 (100%)	0	100 100
1	j	63/67 (94%)	61 (97%)	2 (3%)	34 67
1	k	63/67 (94%)	62 (98%)	1 (2%)	58 82
1	l	63/67 (94%)	62 (98%)	1 (2%)	58 82
1	m	63/67 (94%)	62 (98%)	1 (2%)	58 82
1	n	63/67 (94%)	63 (100%)	0	100 100
1	o	63/67 (94%)	63 (100%)	0	100 100
1	p	63/67 (94%)	63 (100%)	0	100 100
1	q	63/67 (94%)	63 (100%)	0	100 100
1	r	63/67 (94%)	61 (97%)	2 (3%)	34 67
1	s	63/67 (94%)	63 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	t	63/67 (94%)	63 (100%)	0	100	100
1	u	63/67 (94%)	63 (100%)	0	100	100
1	v	63/67 (94%)	63 (100%)	0	100	100
2	1	66/67 (98%)	64 (97%)	2 (3%)	36	69
2	4	66/67 (98%)	65 (98%)	1 (2%)	60	83
2	w	66/67 (98%)	64 (97%)	2 (3%)	36	69
2	x	66/67 (98%)	65 (98%)	1 (2%)	60	83
2	y	66/67 (98%)	63 (96%)	3 (4%)	23	57
2	z	66/67 (98%)	65 (98%)	1 (2%)	60	83
3	A2	95/223 (43%)	94 (99%)	1 (1%)	70	87
3	A3	94/223 (42%)	92 (98%)	2 (2%)	48	77
3	A4	90/223 (40%)	85 (94%)	5 (6%)	17	49
3	A5	92/223 (41%)	90 (98%)	2 (2%)	47	76
3	A6	105/223 (47%)	103 (98%)	2 (2%)	52	79
3	A7	91/223 (41%)	87 (96%)	4 (4%)	24	58
3	X1	38/223 (17%)	36 (95%)	2 (5%)	19	51
3	X2	38/223 (17%)	36 (95%)	2 (5%)	19	51
All	All	4630/6005 (77%)	4568 (99%)	62 (1%)	64	85

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	j	71	VAL
3	A7	800	TRP
2	w	28	TRP
3	A7	786	SER
3	X2	608	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	X1	607	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

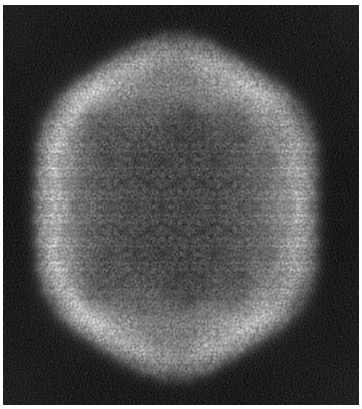
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39599. These allow visual inspection of the internal detail of the map and identification of artifacts.

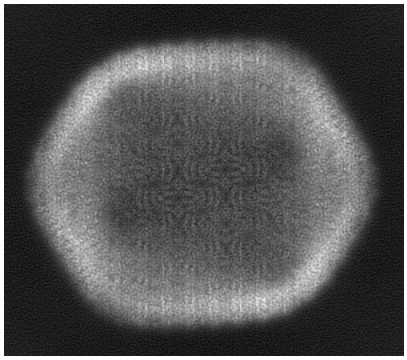
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

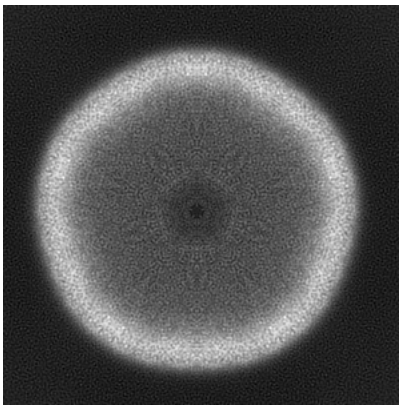
6.1.1 Primary map



X

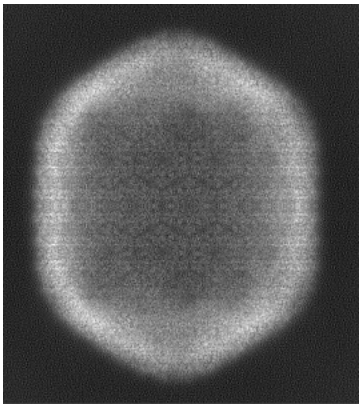


Y

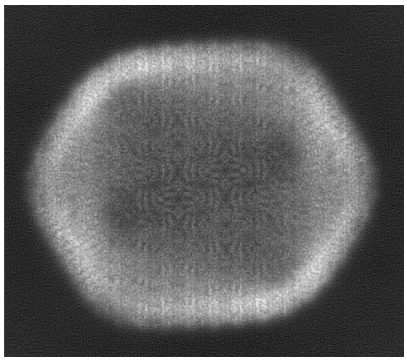


Z

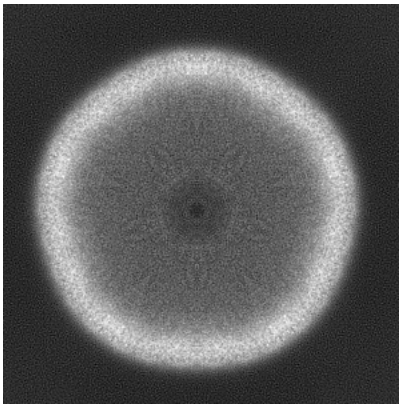
6.1.2 Raw map



X



Y

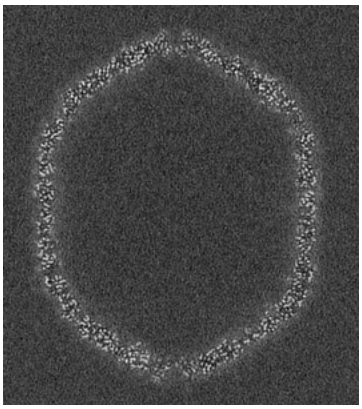


Z

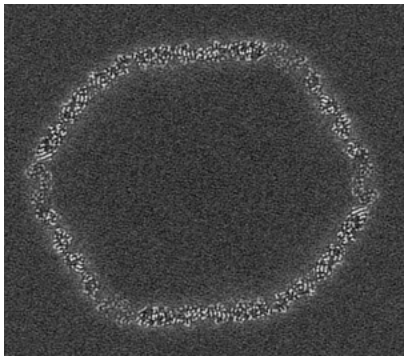
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

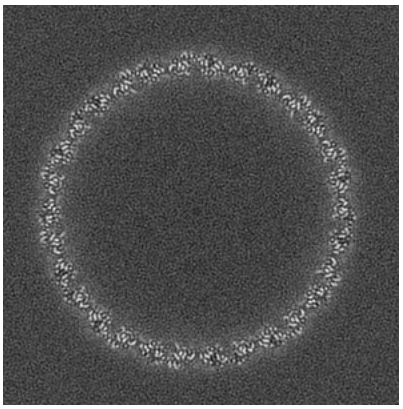
6.2.1 Primary map



X Index: 168

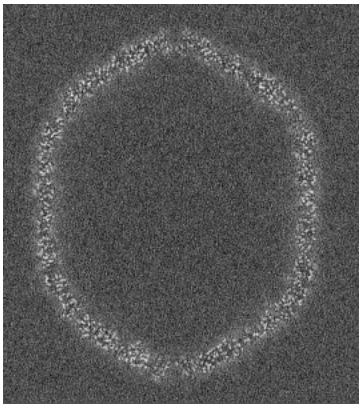


Y Index: 170

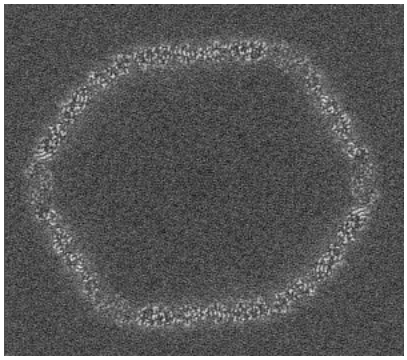


Z Index: 191

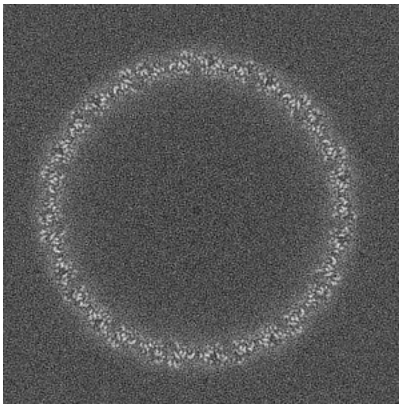
6.2.2 Raw map



X Index: 168



Y Index: 170

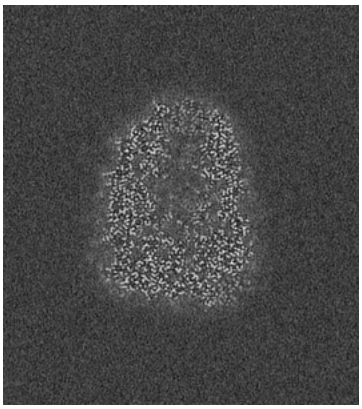


Z Index: 191

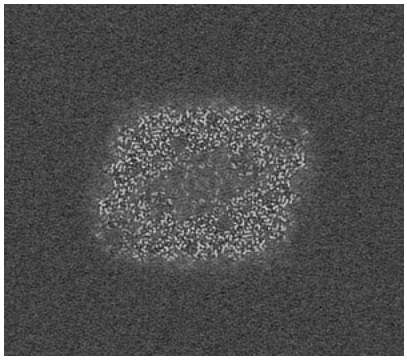
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

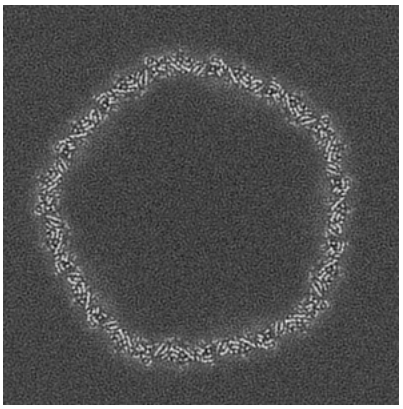
6.3.1 Primary map



X Index: 279

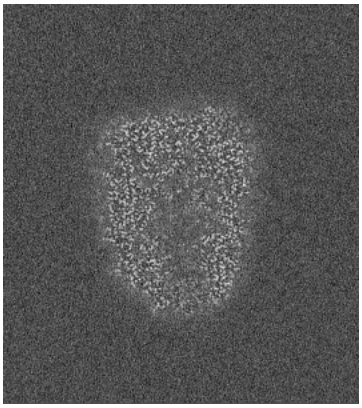


Y Index: 50

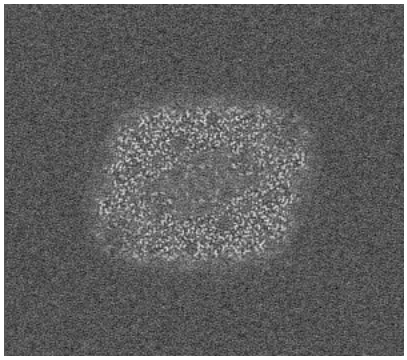


Z Index: 136

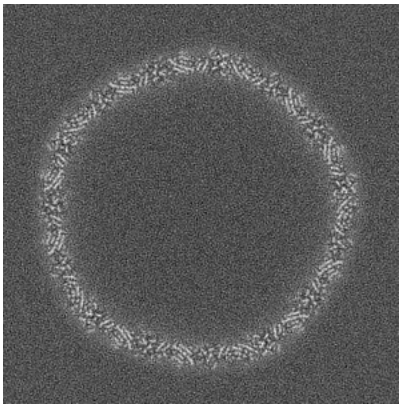
6.3.2 Raw map



X Index: 49



Y Index: 50

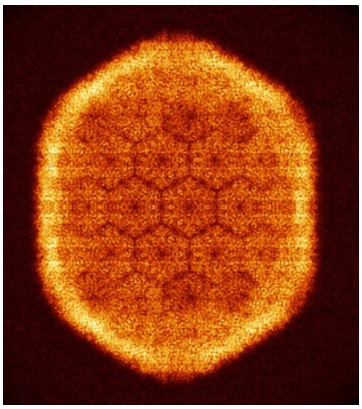


Z Index: 226

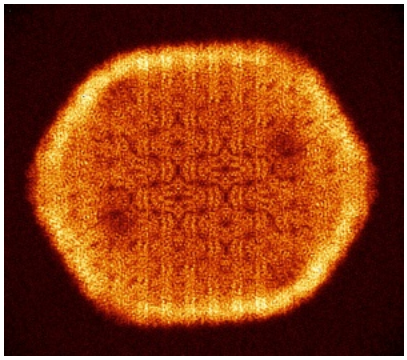
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

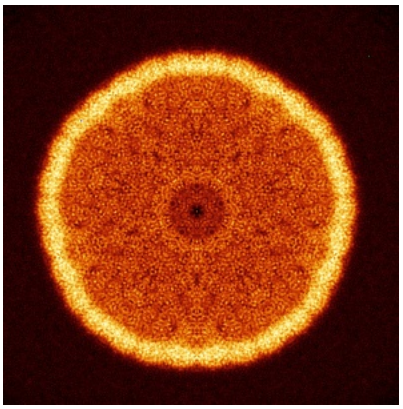
6.4.1 Primary map



X

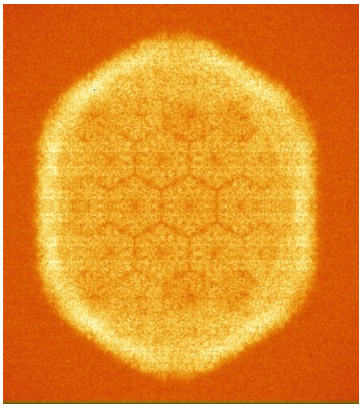


Y

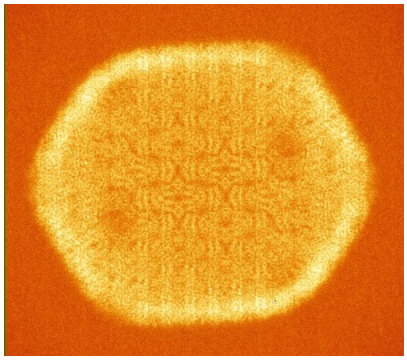


Z

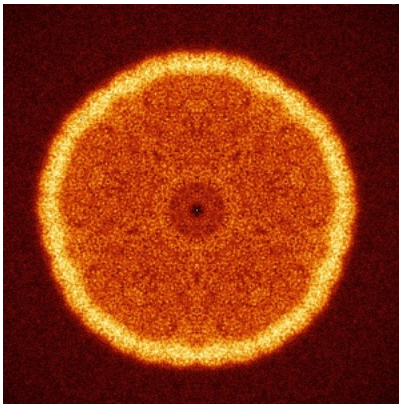
6.4.2 Raw map



X



Y

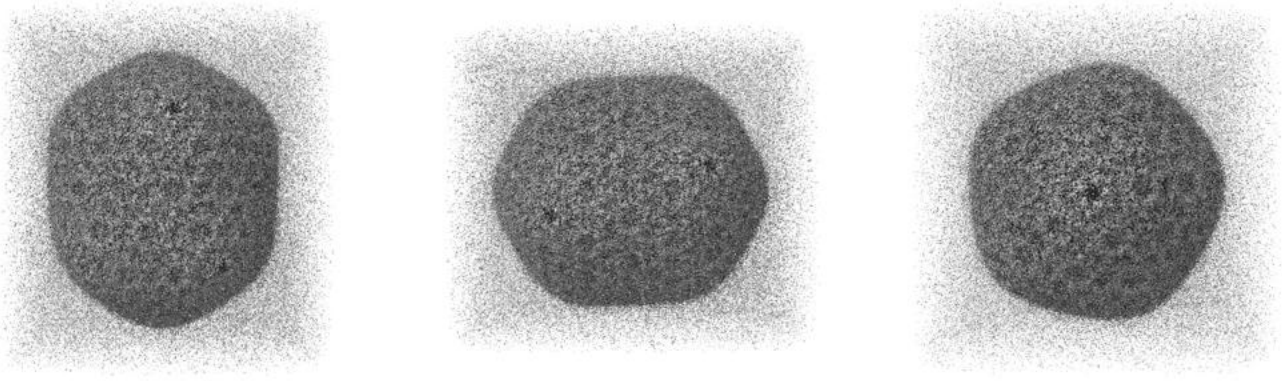


Z

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

6.5 Orthogonal surface views (i)

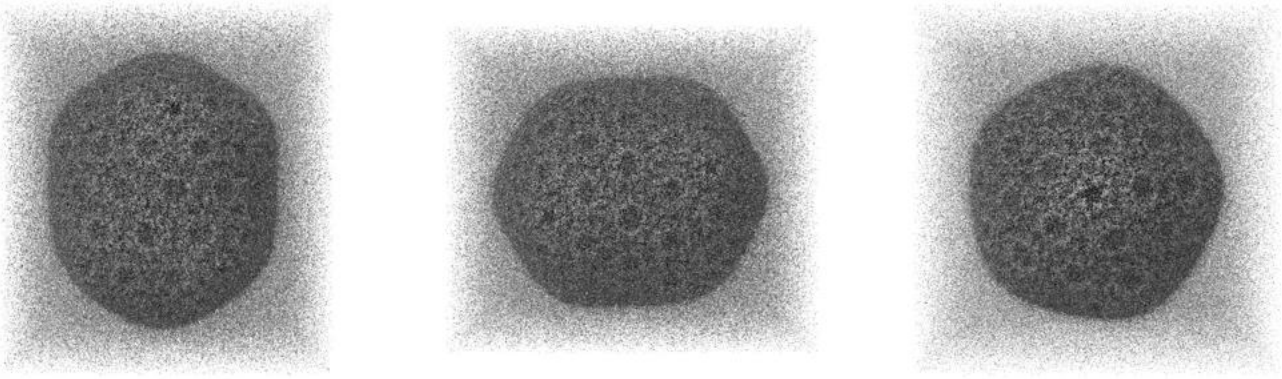
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

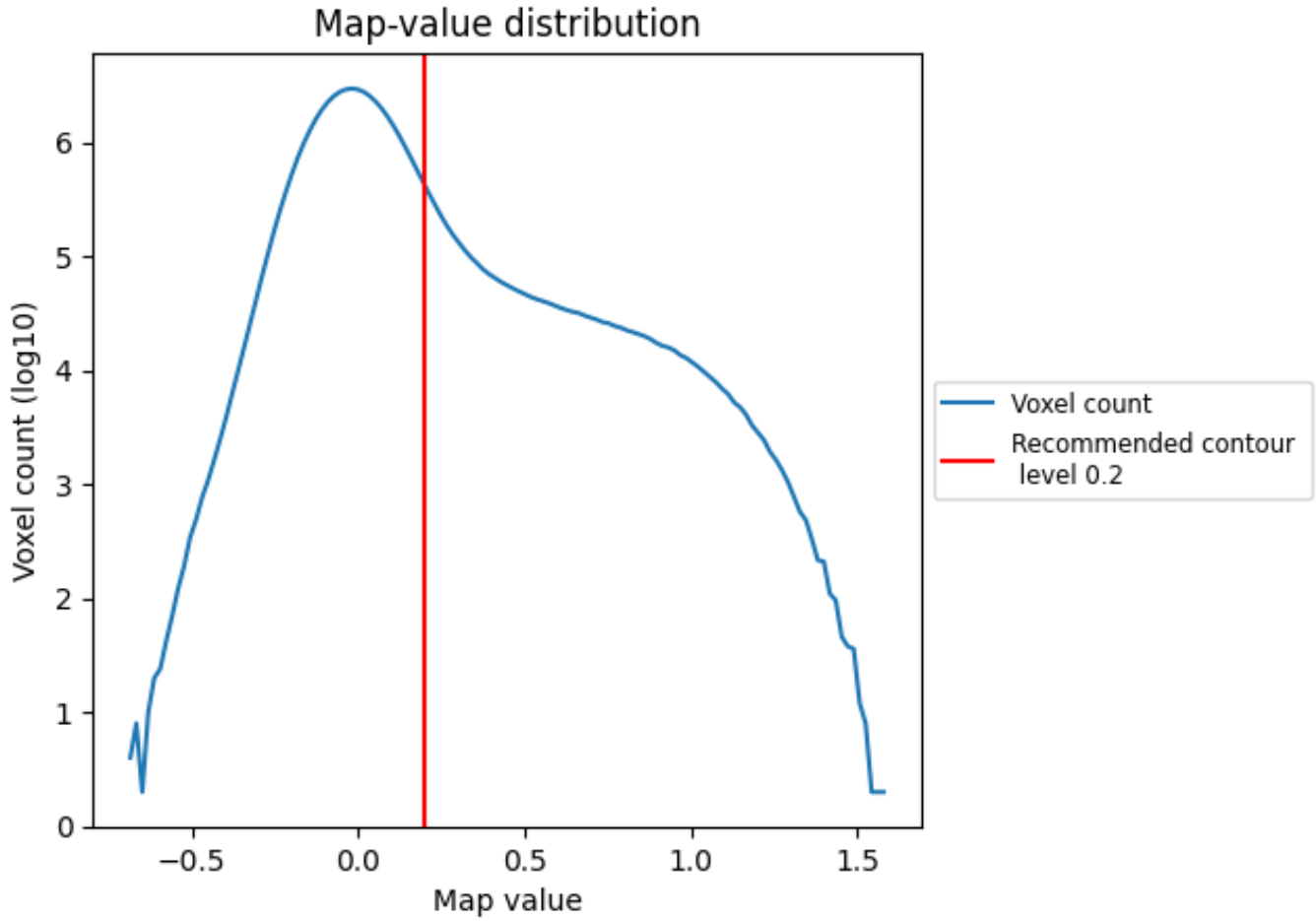
6.6 Mask visualisation (i)

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

7 Map analysis

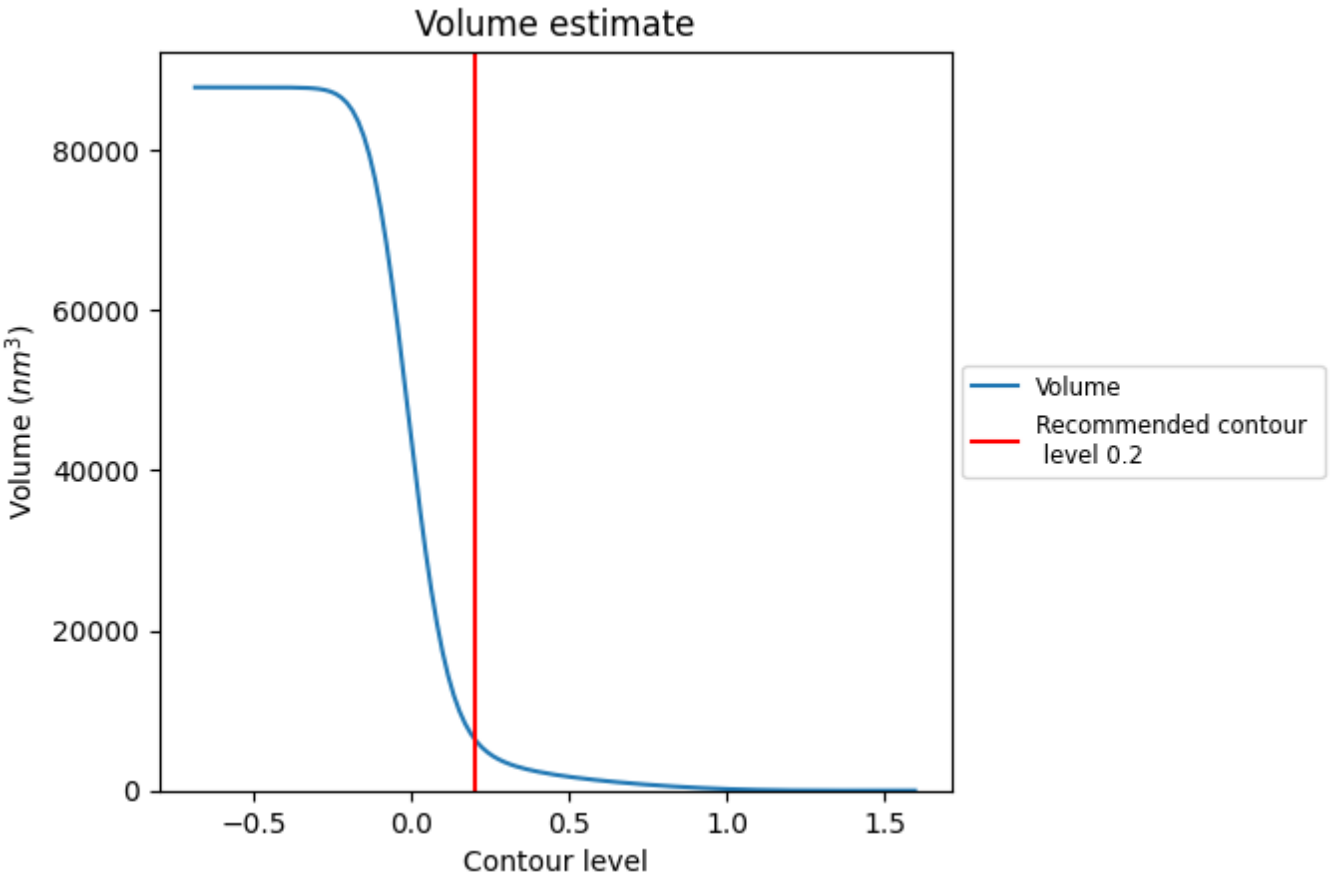
This section contains the results of statistical analysis of the map.

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 6548 nm^3; this corresponds to an approximate mass of 5915 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

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

8 Fourier-Shell correlation (i)

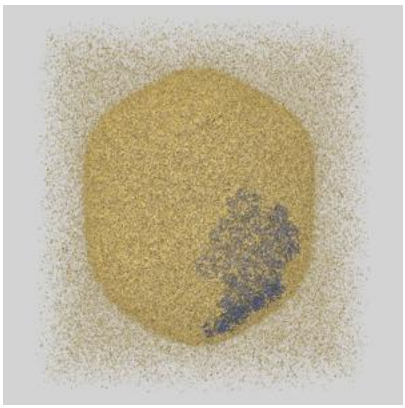
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

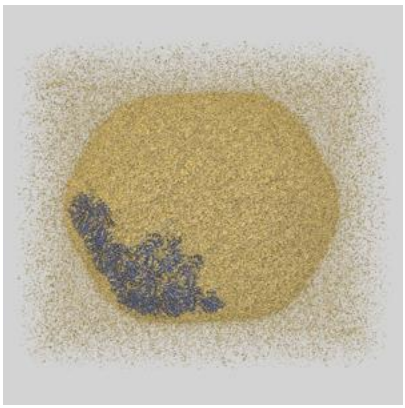
This section contains information regarding the fit between EMDB map EMD-39599 and PDB model 8YVF. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlays

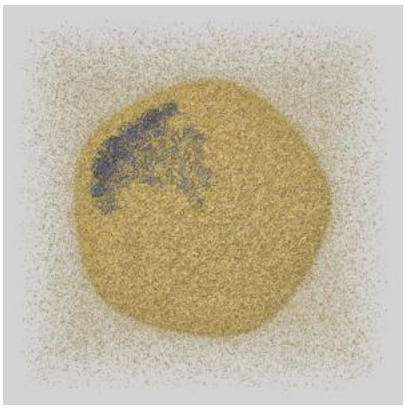
9.1.1 Map-model overlay



X

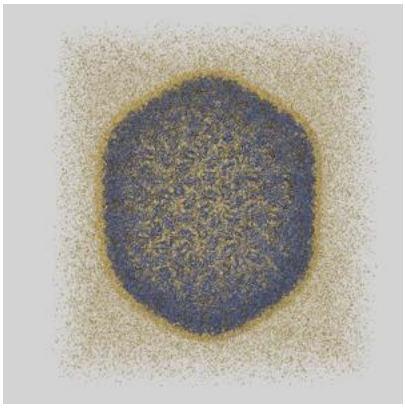


Y

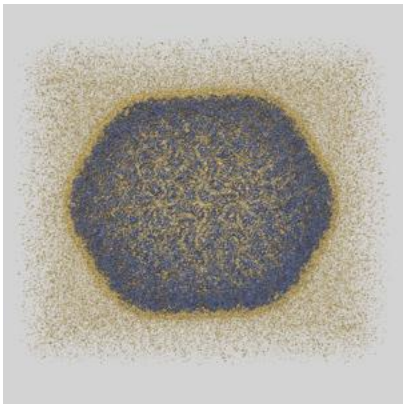


Z

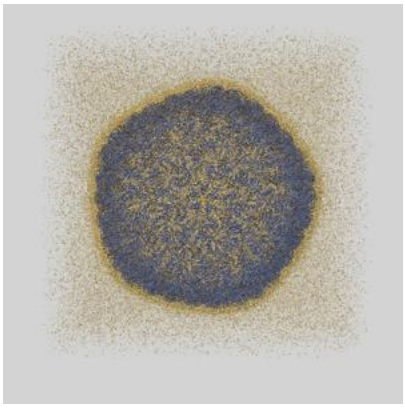
9.1.2 Map-model assembly overlay



X



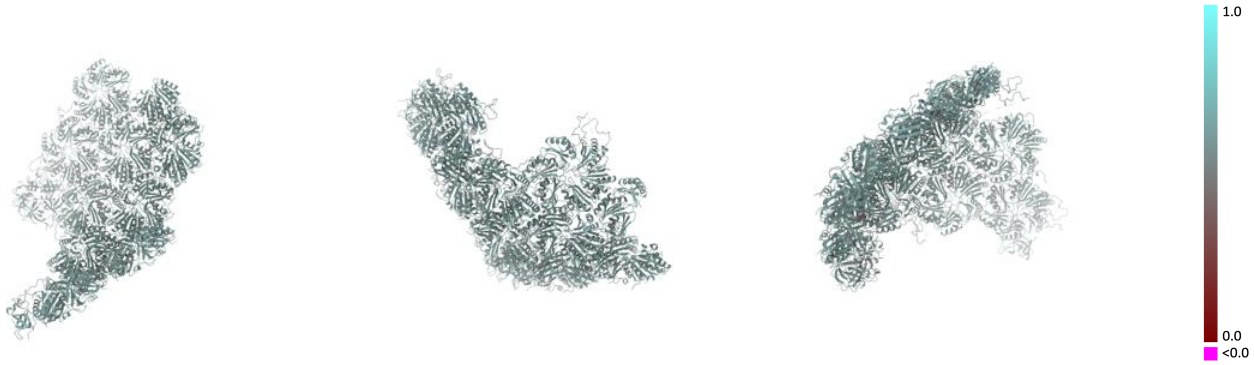
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

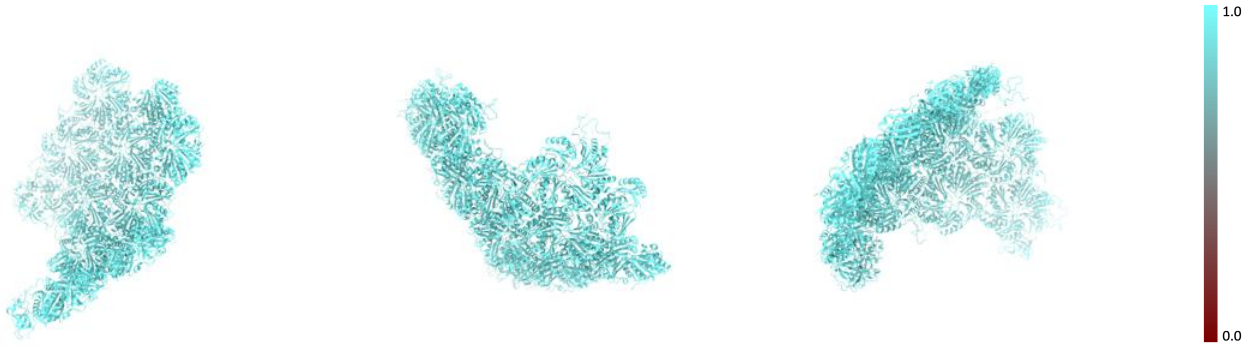
9.2 Q-score mapped to coordinate model



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.

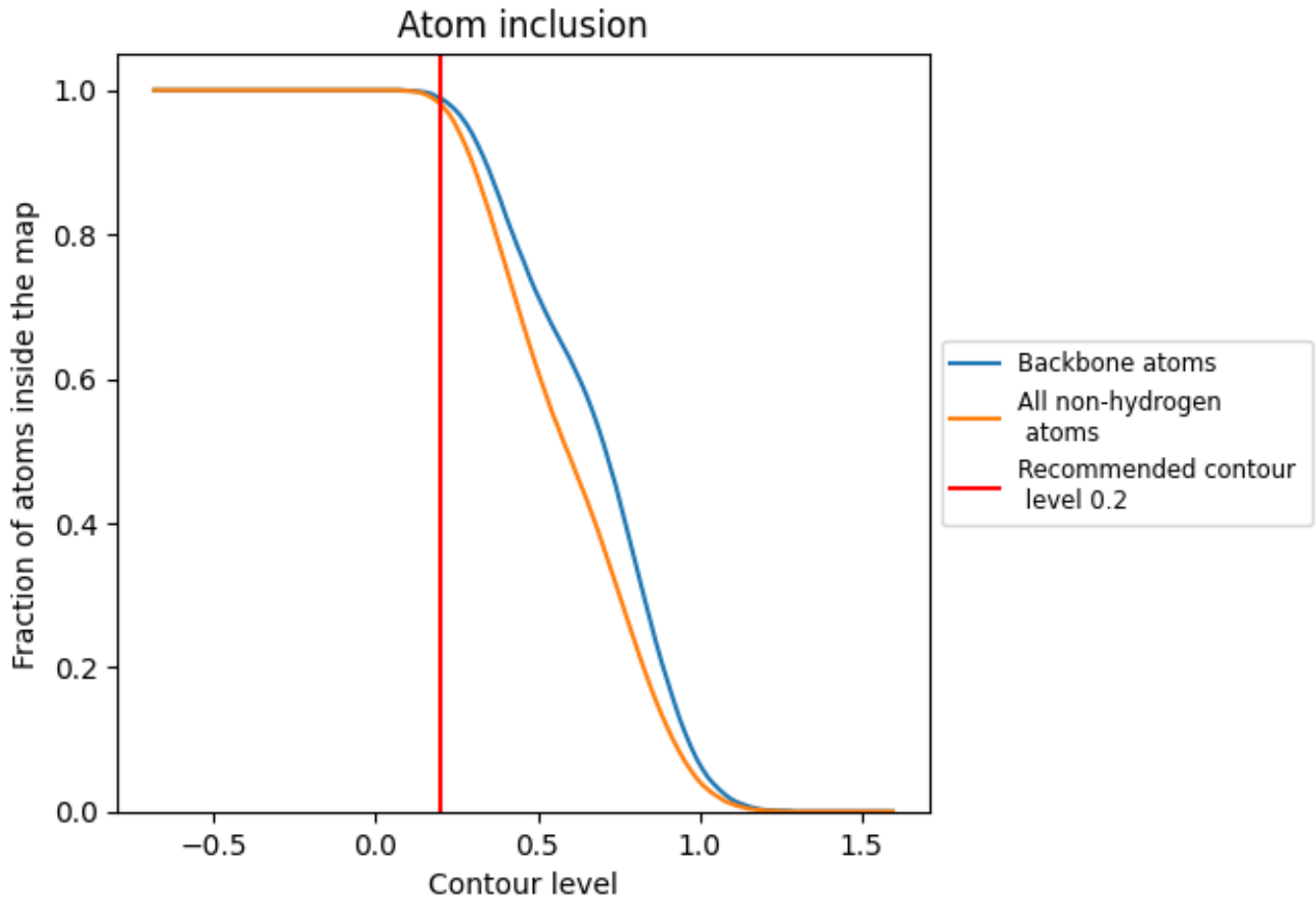
9.3 Atom inclusion mapped to coordinate model



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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9810	0.5690
0	0.9810	0.5710
1	0.9570	0.5590
2	0.9890	0.5760
3	0.9880	0.5720
4	0.9630	0.5640
5	0.9890	0.5750
6	0.9910	0.5740
7	0.9950	0.5800
8	0.9910	0.5790
9	0.9910	0.5690
A	0.9860	0.5770
A1	0.9840	0.5740
A2	0.9320	0.5410
A3	0.9510	0.5340
A4	0.9480	0.5330
A5	0.9680	0.5420
A6	0.9480	0.5330
A7	0.9390	0.5190
B	0.9840	0.5770
C	0.9940	0.5820
D	0.9940	0.5800
E	0.9940	0.5760
F	0.9940	0.5880
G	0.9910	0.5740
H	0.9970	0.5820
I	0.9880	0.5790
J	0.9940	0.5790
K	0.9860	0.5740
L	0.9880	0.5780
M	0.9810	0.5760
N	0.9950	0.5720
O	0.9970	0.5750
P	0.9970	0.5740
Q	0.9860	0.5880

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
R	0.9880	0.5820
S	0.9940	0.5730
T	0.9920	0.5770
U	0.9770	0.5710
V	0.9910	0.5790
W	0.9950	0.5730
X	0.9920	0.5770
X1	0.9410	0.5290
X2	0.9520	0.5390
Y	0.9780	0.5680
Z	0.9890	0.5810
a	0.9860	0.5710
b	0.9920	0.5750
c	0.9860	0.5750
d	0.9880	0.5810
e	0.9890	0.5710
f	0.9950	0.5780
g	0.9940	0.5780
h	0.9880	0.5750
i	0.9880	0.5740
j	0.9920	0.5760
k	0.9950	0.5720
l	0.9810	0.5710
m	0.9880	0.5720
n	0.9910	0.5740
o	0.9880	0.5730
p	0.9910	0.5740
q	0.9980	0.5780
r	0.9950	0.5740
s	0.9950	0.5760
t	0.9860	0.5710
u	0.9910	0.5790
v	0.9810	0.5660
w	0.9250	0.5490
x	0.9430	0.5490
y	0.9350	0.5560
z	0.9300	0.5480