wwPDB EM Validation Summary Report

Oct 19, 2026 – 06:39 PM JST

PDB ID	:	9X6G / pdb_00009x6g
EMDB ID	:	EMD-66620
Title	:	Filament of mutant Escherichia coli CTP synthase fused with mEGFP
Authors	:	Yin, B.Q.; Hu, H.H.; Liu, J.L.
Deposited on	:	2025-10-15
Resolution	:	3.39 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 ⓘ symbol.

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

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

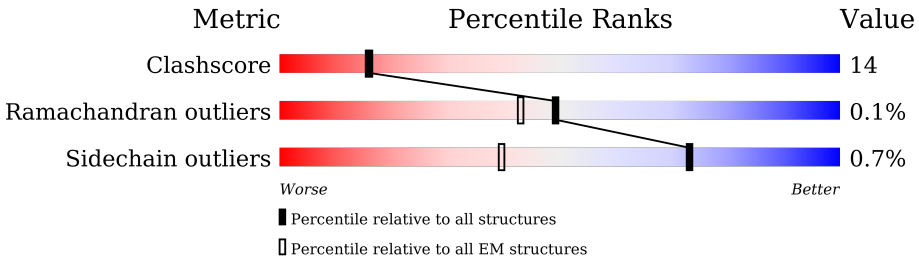
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

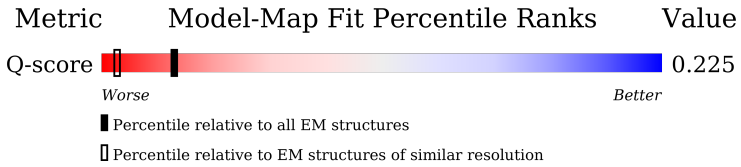
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.39 Å.

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





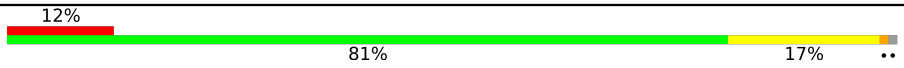
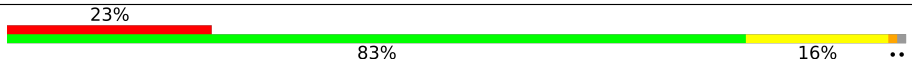
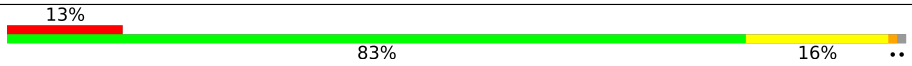
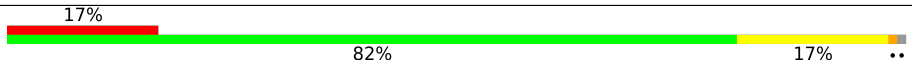
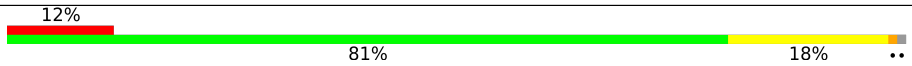
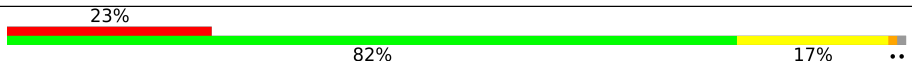
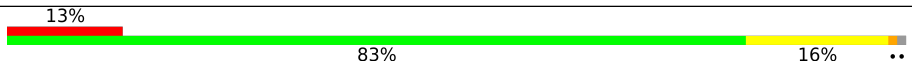
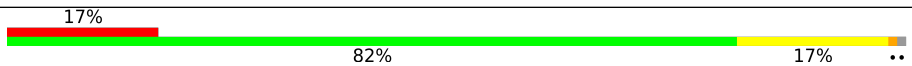
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14220 (2.89 - 3.89)

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	785	13% 82% 17%
1	B	785	12% 82% 17%
1	C	785	13% 82% 17%
1	D	785	12% 82% 17%

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Mol	Chain	Length	Quality of chain
1	E	785	
1	F	785	
1	G	785	
1	H	785	
1	I	785	
1	J	785	
1	K	785	
1	L	785	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 74028 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 mEGFP,CTP synthase,CTP synthase,CTP synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	781	Total 6169	C 3896	N 1086	O 1160	S 27	0	0
1	B	781	Total 6169	C 3896	N 1086	O 1160	S 27	0	0
1	C	781	Total 6169	C 3896	N 1086	O 1160	S 27	0	0
1	D	781	Total 6169	C 3896	N 1086	O 1160	S 27	0	0
1	E	781	Total 6169	C 3896	N 1086	O 1160	S 27	0	0
1	G	781	Total 6169	C 3896	N 1086	O 1160	S 27	0	0
1	I	781	Total 6169	C 3896	N 1086	O 1160	S 27	0	0
1	K	781	Total 6169	C 3896	N 1086	O 1160	S 27	0	0
1	F	781	Total 6169	C 3896	N 1086	O 1160	S 27	0	0
1	H	781	Total 6169	C 3896	N 1086	O 1160	S 27	0	0
1	J	781	Total 6169	C 3896	N 1086	O 1160	S 27	0	0
1	L	781	Total 6169	C 3896	N 1086	O 1160	S 27	0	0

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	263	ARG	ASN	conflict	UNP P0A7E5
A	360	ARG	GLU	conflict	UNP P0A7E5
A	361	ARG	GLY	conflict	UNP P0A7E5
A	493	GLU	SER	conflict	UNP P0A7E5
A	494	ARG	LEU	conflict	UNP P0A7E5
A	495	ARG	ASN	conflict	UNP P0A7E5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	774	HIS	-	expression tag	UNP P0A7E5
A	775	HIS	-	expression tag	UNP P0A7E5
A	776	HIS	-	expression tag	UNP P0A7E5
A	777	HIS	-	expression tag	UNP P0A7E5
A	778	HIS	-	expression tag	UNP P0A7E5
A	779	HIS	-	expression tag	UNP P0A7E5
A	780	HIS	-	expression tag	UNP P0A7E5
A	781	HIS	-	expression tag	UNP P0A7E5
A	782	HIS	-	expression tag	UNP P0A7E5
A	783	HIS	-	expression tag	UNP P0A7E5
A	784	HIS	-	expression tag	UNP P0A7E5
A	785	HIS	-	expression tag	UNP P0A7E5
B	263	ARG	ASN	conflict	UNP P0A7E5
B	360	ARG	GLU	conflict	UNP P0A7E5
B	361	ARG	GLY	conflict	UNP P0A7E5
B	493	GLU	SER	conflict	UNP P0A7E5
B	494	ARG	LEU	conflict	UNP P0A7E5
B	495	ARG	ASN	conflict	UNP P0A7E5
B	774	HIS	-	expression tag	UNP P0A7E5
B	775	HIS	-	expression tag	UNP P0A7E5
B	776	HIS	-	expression tag	UNP P0A7E5
B	777	HIS	-	expression tag	UNP P0A7E5
B	778	HIS	-	expression tag	UNP P0A7E5
B	779	HIS	-	expression tag	UNP P0A7E5
B	780	HIS	-	expression tag	UNP P0A7E5
B	781	HIS	-	expression tag	UNP P0A7E5
B	782	HIS	-	expression tag	UNP P0A7E5
B	783	HIS	-	expression tag	UNP P0A7E5
B	784	HIS	-	expression tag	UNP P0A7E5
B	785	HIS	-	expression tag	UNP P0A7E5
C	263	ARG	ASN	conflict	UNP P0A7E5
C	360	ARG	GLU	conflict	UNP P0A7E5
C	361	ARG	GLY	conflict	UNP P0A7E5
C	493	GLU	SER	conflict	UNP P0A7E5
C	494	ARG	LEU	conflict	UNP P0A7E5
C	495	ARG	ASN	conflict	UNP P0A7E5
C	774	HIS	-	expression tag	UNP P0A7E5
C	775	HIS	-	expression tag	UNP P0A7E5
C	776	HIS	-	expression tag	UNP P0A7E5
C	777	HIS	-	expression tag	UNP P0A7E5
C	778	HIS	-	expression tag	UNP P0A7E5
C	779	HIS	-	expression tag	UNP P0A7E5

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Chain	Residue	Modelled	Actual	Comment	Reference
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C	781	HIS	-	expression tag	UNP P0A7E5
C	782	HIS	-	expression tag	UNP P0A7E5
C	783	HIS	-	expression tag	UNP P0A7E5
C	784	HIS	-	expression tag	UNP P0A7E5
C	785	HIS	-	expression tag	UNP P0A7E5
D	263	ARG	ASN	conflict	UNP P0A7E5
D	360	ARG	GLU	conflict	UNP P0A7E5
D	361	ARG	GLY	conflict	UNP P0A7E5
D	493	GLU	SER	conflict	UNP P0A7E5
D	494	ARG	LEU	conflict	UNP P0A7E5
D	495	ARG	ASN	conflict	UNP P0A7E5
D	774	HIS	-	expression tag	UNP P0A7E5
D	775	HIS	-	expression tag	UNP P0A7E5
D	776	HIS	-	expression tag	UNP P0A7E5
D	777	HIS	-	expression tag	UNP P0A7E5
D	778	HIS	-	expression tag	UNP P0A7E5
D	779	HIS	-	expression tag	UNP P0A7E5
D	780	HIS	-	expression tag	UNP P0A7E5
D	781	HIS	-	expression tag	UNP P0A7E5
D	782	HIS	-	expression tag	UNP P0A7E5
D	783	HIS	-	expression tag	UNP P0A7E5
D	784	HIS	-	expression tag	UNP P0A7E5
D	785	HIS	-	expression tag	UNP P0A7E5
E	263	ARG	ASN	conflict	UNP P0A7E5
E	360	ARG	GLU	conflict	UNP P0A7E5
E	361	ARG	GLY	conflict	UNP P0A7E5
E	493	GLU	SER	conflict	UNP P0A7E5
E	494	ARG	LEU	conflict	UNP P0A7E5
E	495	ARG	ASN	conflict	UNP P0A7E5
E	774	HIS	-	expression tag	UNP P0A7E5
E	775	HIS	-	expression tag	UNP P0A7E5
E	776	HIS	-	expression tag	UNP P0A7E5
E	777	HIS	-	expression tag	UNP P0A7E5
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E	779	HIS	-	expression tag	UNP P0A7E5
E	780	HIS	-	expression tag	UNP P0A7E5
E	781	HIS	-	expression tag	UNP P0A7E5
E	782	HIS	-	expression tag	UNP P0A7E5
E	783	HIS	-	expression tag	UNP P0A7E5
E	784	HIS	-	expression tag	UNP P0A7E5
E	785	HIS	-	expression tag	UNP P0A7E5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	263	ARG	ASN	conflict	UNP P0A7E5
G	360	ARG	GLU	conflict	UNP P0A7E5
G	361	ARG	GLY	conflict	UNP P0A7E5
G	493	GLU	SER	conflict	UNP P0A7E5
G	494	ARG	LEU	conflict	UNP P0A7E5
G	495	ARG	ASN	conflict	UNP P0A7E5
G	774	HIS	-	expression tag	UNP P0A7E5
G	775	HIS	-	expression tag	UNP P0A7E5
G	776	HIS	-	expression tag	UNP P0A7E5
G	777	HIS	-	expression tag	UNP P0A7E5
G	778	HIS	-	expression tag	UNP P0A7E5
G	779	HIS	-	expression tag	UNP P0A7E5
G	780	HIS	-	expression tag	UNP P0A7E5
G	781	HIS	-	expression tag	UNP P0A7E5
G	782	HIS	-	expression tag	UNP P0A7E5
G	783	HIS	-	expression tag	UNP P0A7E5
G	784	HIS	-	expression tag	UNP P0A7E5
G	785	HIS	-	expression tag	UNP P0A7E5
I	263	ARG	ASN	conflict	UNP P0A7E5
I	360	ARG	GLU	conflict	UNP P0A7E5
I	361	ARG	GLY	conflict	UNP P0A7E5
I	493	GLU	SER	conflict	UNP P0A7E5
I	494	ARG	LEU	conflict	UNP P0A7E5
I	495	ARG	ASN	conflict	UNP P0A7E5
I	774	HIS	-	expression tag	UNP P0A7E5
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I	776	HIS	-	expression tag	UNP P0A7E5
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I	781	HIS	-	expression tag	UNP P0A7E5
I	782	HIS	-	expression tag	UNP P0A7E5
I	783	HIS	-	expression tag	UNP P0A7E5
I	784	HIS	-	expression tag	UNP P0A7E5
I	785	HIS	-	expression tag	UNP P0A7E5
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K	361	ARG	GLY	conflict	UNP P0A7E5
K	493	GLU	SER	conflict	UNP P0A7E5
K	494	ARG	LEU	conflict	UNP P0A7E5
K	495	ARG	ASN	conflict	UNP P0A7E5

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Chain	Residue	Modelled	Actual	Comment	Reference
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K	778	HIS	-	expression tag	UNP P0A7E5
K	779	HIS	-	expression tag	UNP P0A7E5
K	780	HIS	-	expression tag	UNP P0A7E5
K	781	HIS	-	expression tag	UNP P0A7E5
K	782	HIS	-	expression tag	UNP P0A7E5
K	783	HIS	-	expression tag	UNP P0A7E5
K	784	HIS	-	expression tag	UNP P0A7E5
K	785	HIS	-	expression tag	UNP P0A7E5
F	263	ARG	ASN	conflict	UNP P0A7E5
F	360	ARG	GLU	conflict	UNP P0A7E5
F	361	ARG	GLY	conflict	UNP P0A7E5
F	493	GLU	SER	conflict	UNP P0A7E5
F	494	ARG	LEU	conflict	UNP P0A7E5
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F	782	HIS	-	expression tag	UNP P0A7E5
F	783	HIS	-	expression tag	UNP P0A7E5
F	784	HIS	-	expression tag	UNP P0A7E5
F	785	HIS	-	expression tag	UNP P0A7E5
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H	777	HIS	-	expression tag	UNP P0A7E5
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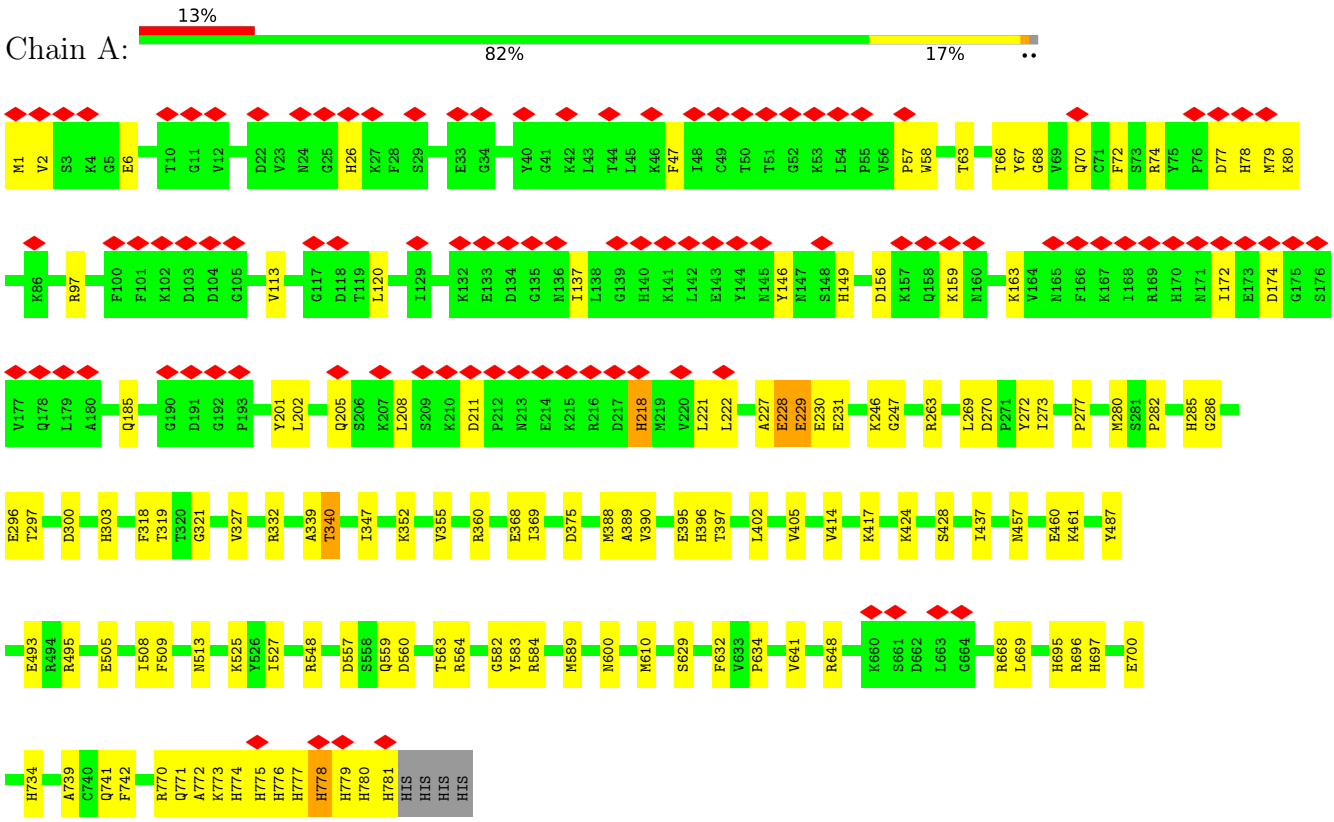
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Chain	Residue	Modelled	Actual	Comment	Reference
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H	782	HIS	-	expression tag	UNP P0A7E5
H	783	HIS	-	expression tag	UNP P0A7E5
H	784	HIS	-	expression tag	UNP P0A7E5
H	785	HIS	-	expression tag	UNP P0A7E5
J	263	ARG	ASN	conflict	UNP P0A7E5
J	360	ARG	GLU	conflict	UNP P0A7E5
J	361	ARG	GLY	conflict	UNP P0A7E5
J	493	GLU	SER	conflict	UNP P0A7E5
J	494	ARG	LEU	conflict	UNP P0A7E5
J	495	ARG	ASN	conflict	UNP P0A7E5
J	774	HIS	-	expression tag	UNP P0A7E5
J	775	HIS	-	expression tag	UNP P0A7E5
J	776	HIS	-	expression tag	UNP P0A7E5
J	777	HIS	-	expression tag	UNP P0A7E5
J	778	HIS	-	expression tag	UNP P0A7E5
J	779	HIS	-	expression tag	UNP P0A7E5
J	780	HIS	-	expression tag	UNP P0A7E5
J	781	HIS	-	expression tag	UNP P0A7E5
J	782	HIS	-	expression tag	UNP P0A7E5
J	783	HIS	-	expression tag	UNP P0A7E5
J	784	HIS	-	expression tag	UNP P0A7E5
J	785	HIS	-	expression tag	UNP P0A7E5
L	263	ARG	ASN	conflict	UNP P0A7E5
L	360	ARG	GLU	conflict	UNP P0A7E5
L	361	ARG	GLY	conflict	UNP P0A7E5
L	493	GLU	SER	conflict	UNP P0A7E5
L	494	ARG	LEU	conflict	UNP P0A7E5
L	495	ARG	ASN	conflict	UNP P0A7E5
L	774	HIS	-	expression tag	UNP P0A7E5
L	775	HIS	-	expression tag	UNP P0A7E5
L	776	HIS	-	expression tag	UNP P0A7E5
L	777	HIS	-	expression tag	UNP P0A7E5
L	778	HIS	-	expression tag	UNP P0A7E5
L	779	HIS	-	expression tag	UNP P0A7E5
L	780	HIS	-	expression tag	UNP P0A7E5
L	781	HIS	-	expression tag	UNP P0A7E5
L	782	HIS	-	expression tag	UNP P0A7E5
L	783	HIS	-	expression tag	UNP P0A7E5
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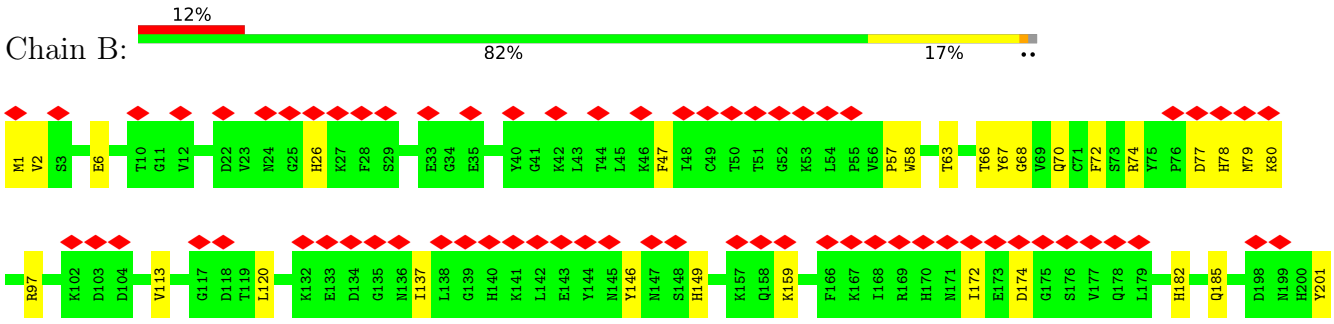
3 Residue-property plots (i)

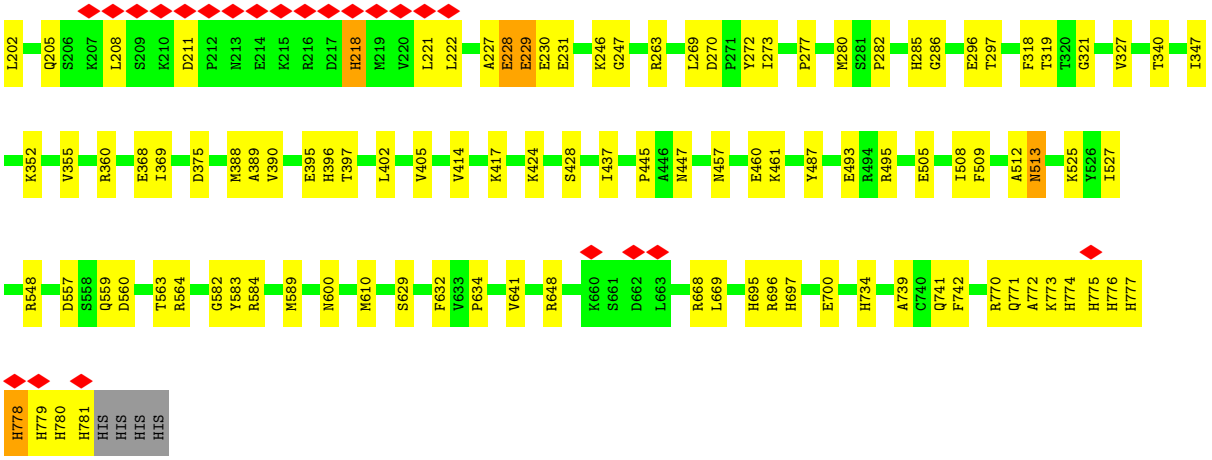
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: mEGFP,CTP synthase,CTP synthase,CTP synthase



• Molecule 1: mEGFP,CTP synthase,CTP synthase,CTP synthase

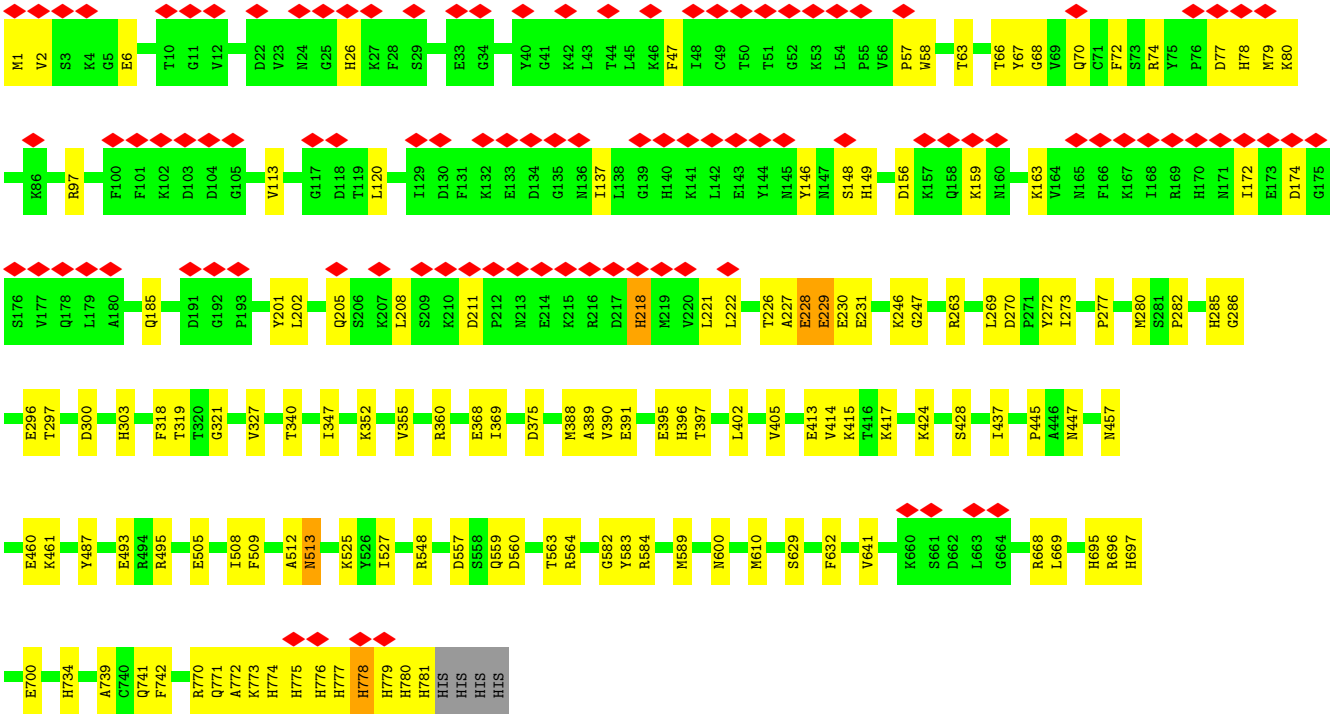




• Molecule 1: mEGFP,CTP synthase,CTP synthase,CTP synthase

Chain C:

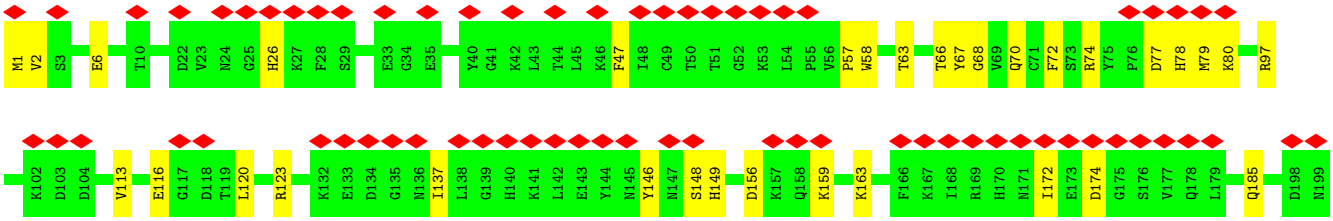


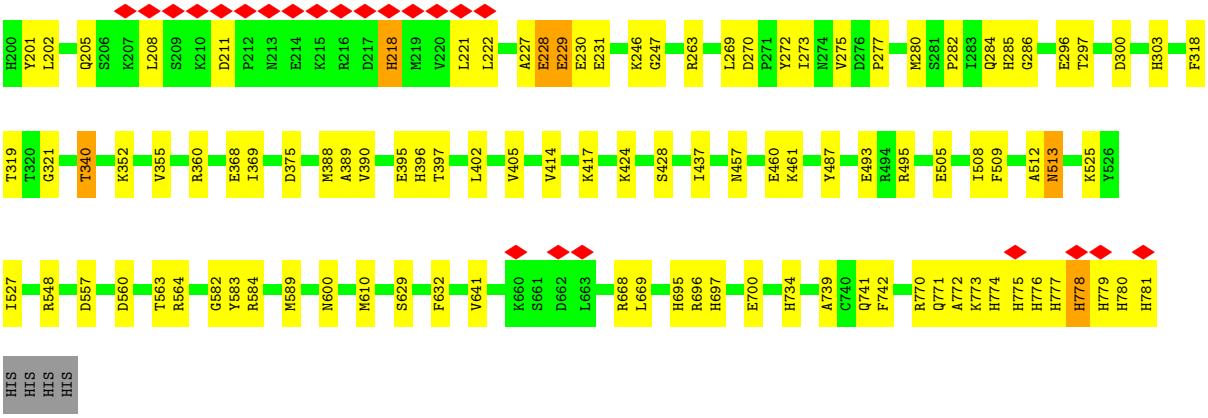


• Molecule 1: mEGFP,CTP synthase,CTP synthase,CTP synthase

Chain D:



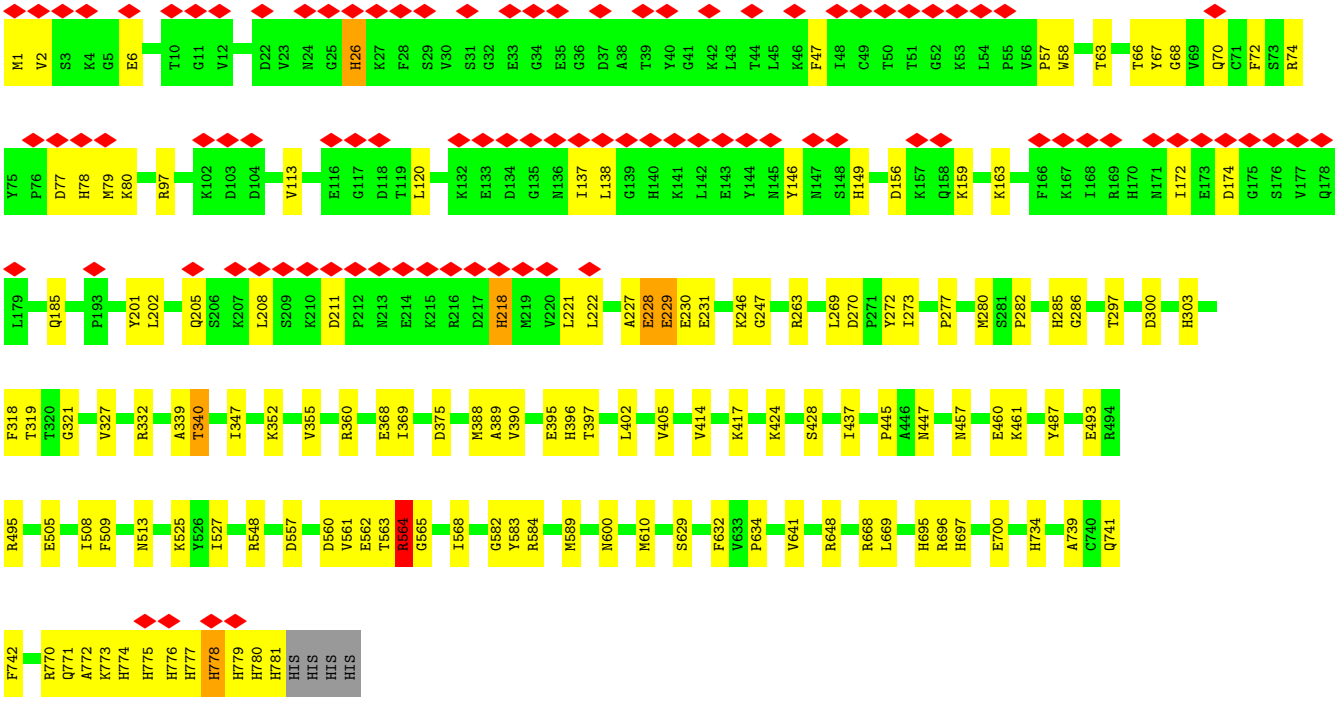




• Molecule 1: mEGFP,CTP synthase,CTP synthase,CTP synthase

Chain E:

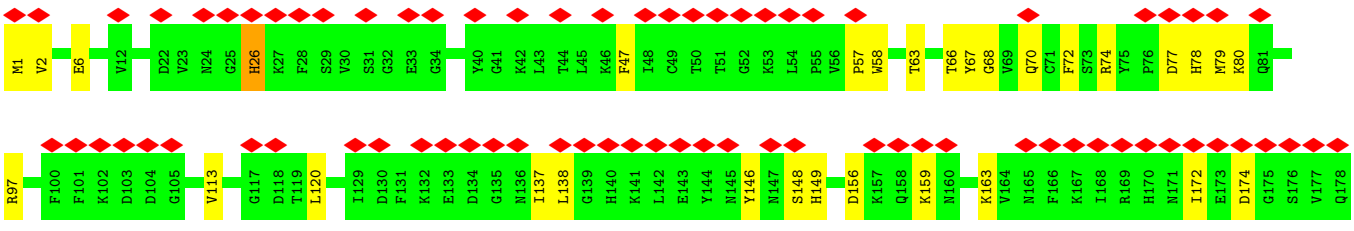


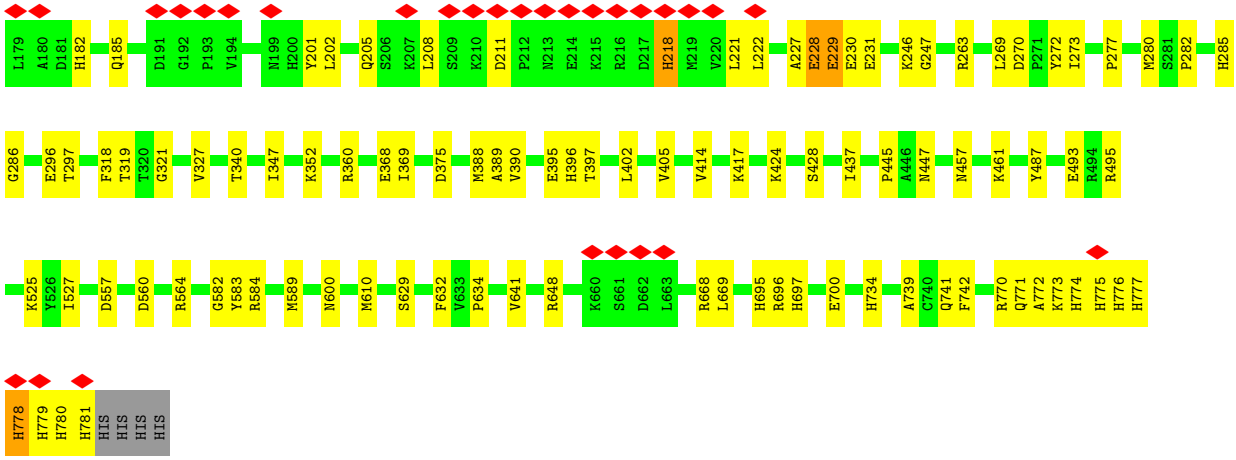


• Molecule 1: mEGFP,CTP synthase,CTP synthase,CTP synthase

Chain G:



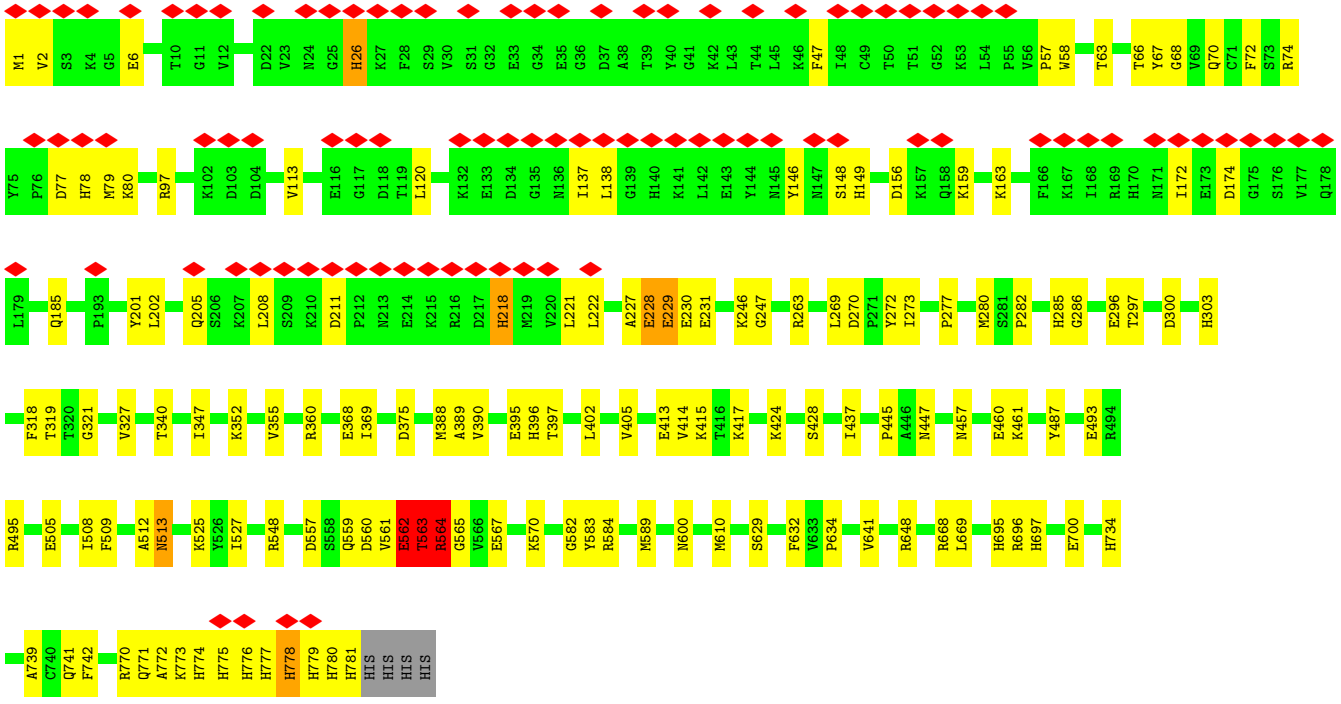




• Molecule 1: mEGFP,CTP synthase,CTP synthase,CTP synthase

Chain I:

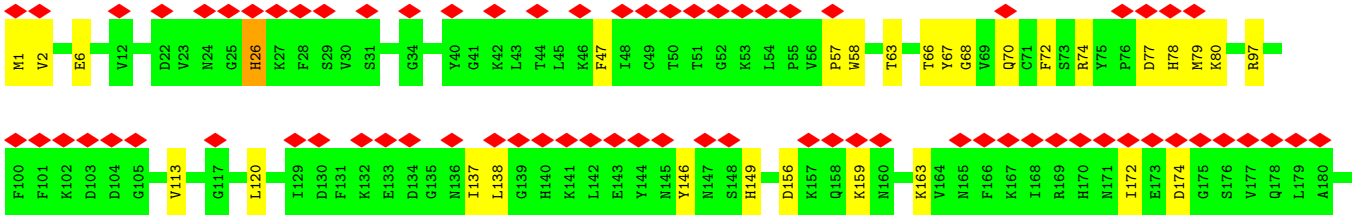


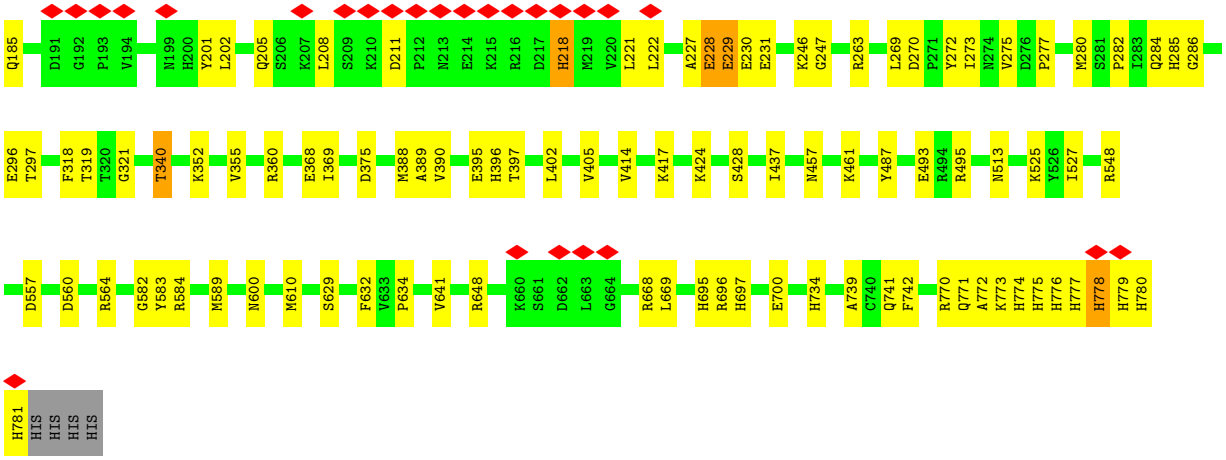


• Molecule 1: mEGFP,CTP synthase,CTP synthase,CTP synthase

Chain K:



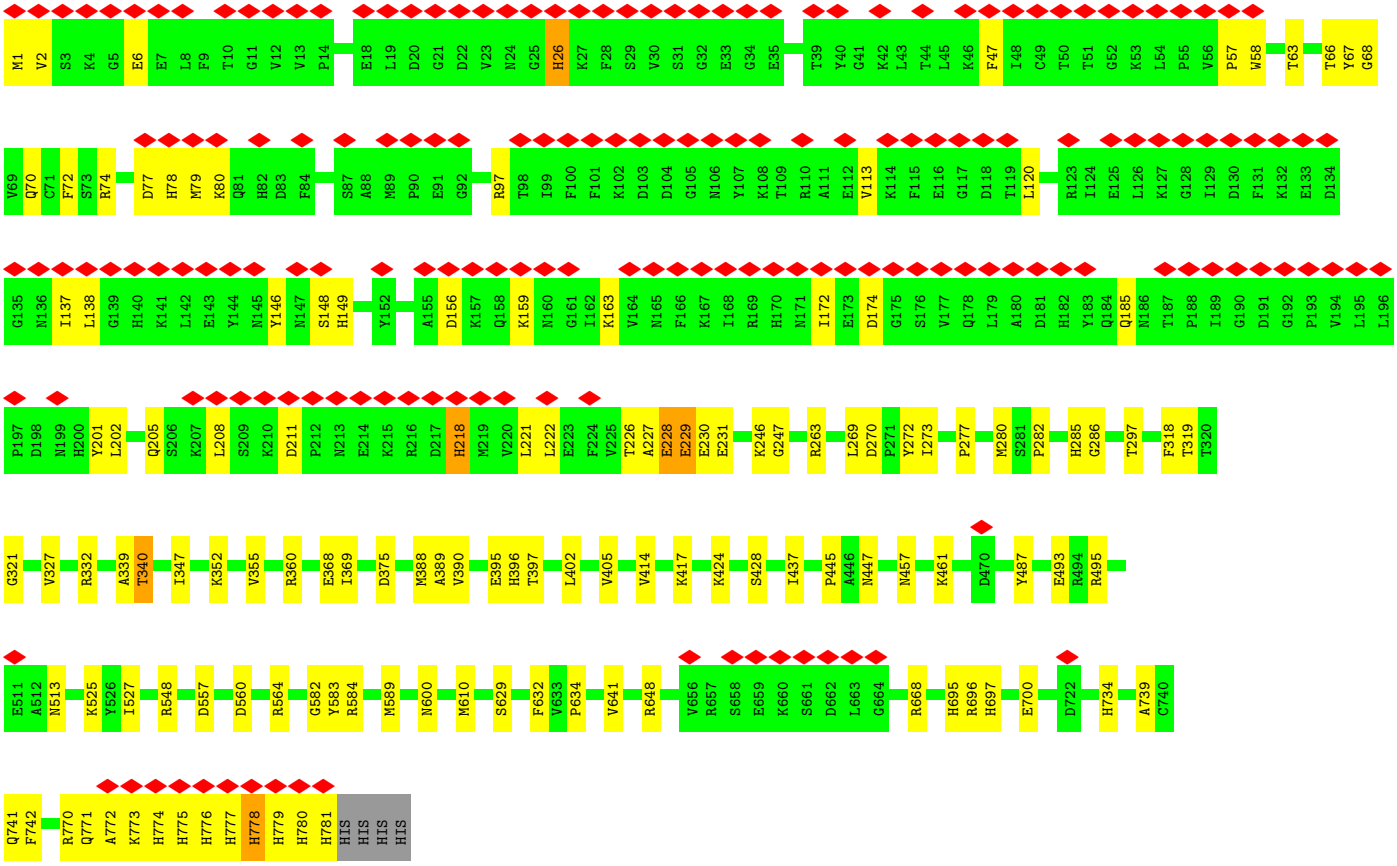




• Molecule 1: mEGFP,CTP synthase,CTP synthase,CTP synthase

Chain F:

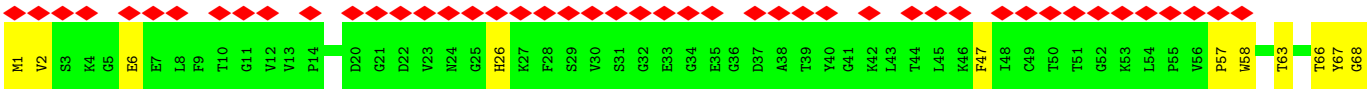


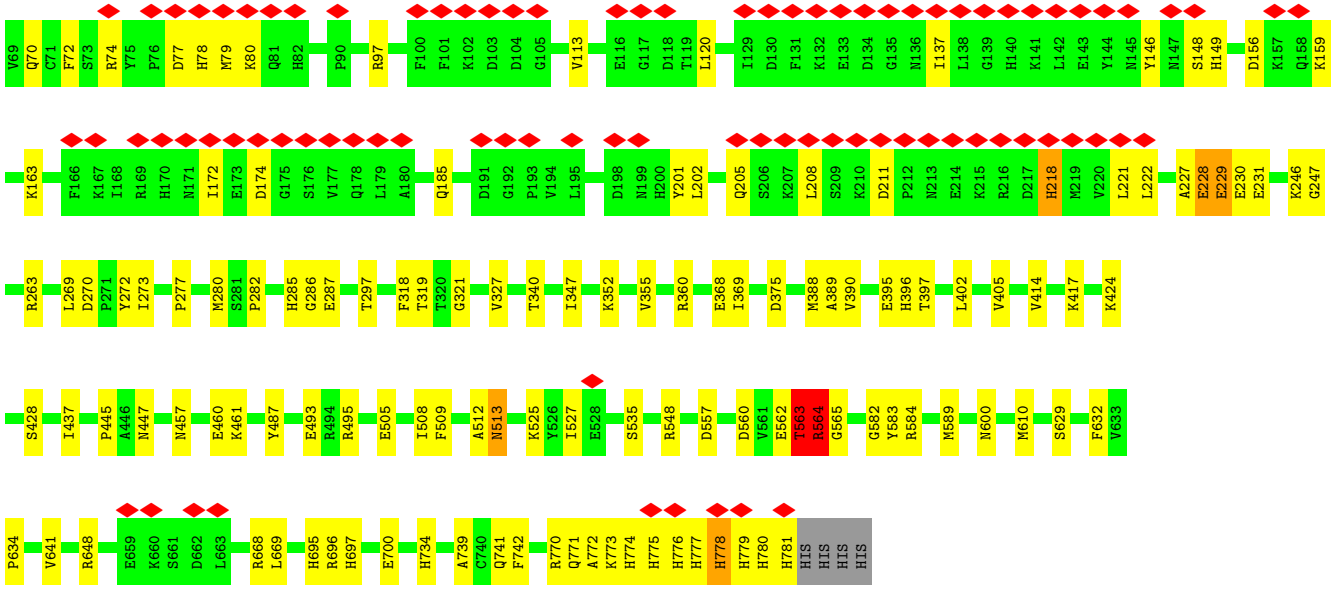


• Molecule 1: mEGFP,CTP synthase,CTP synthase,CTP synthase

Chain H:



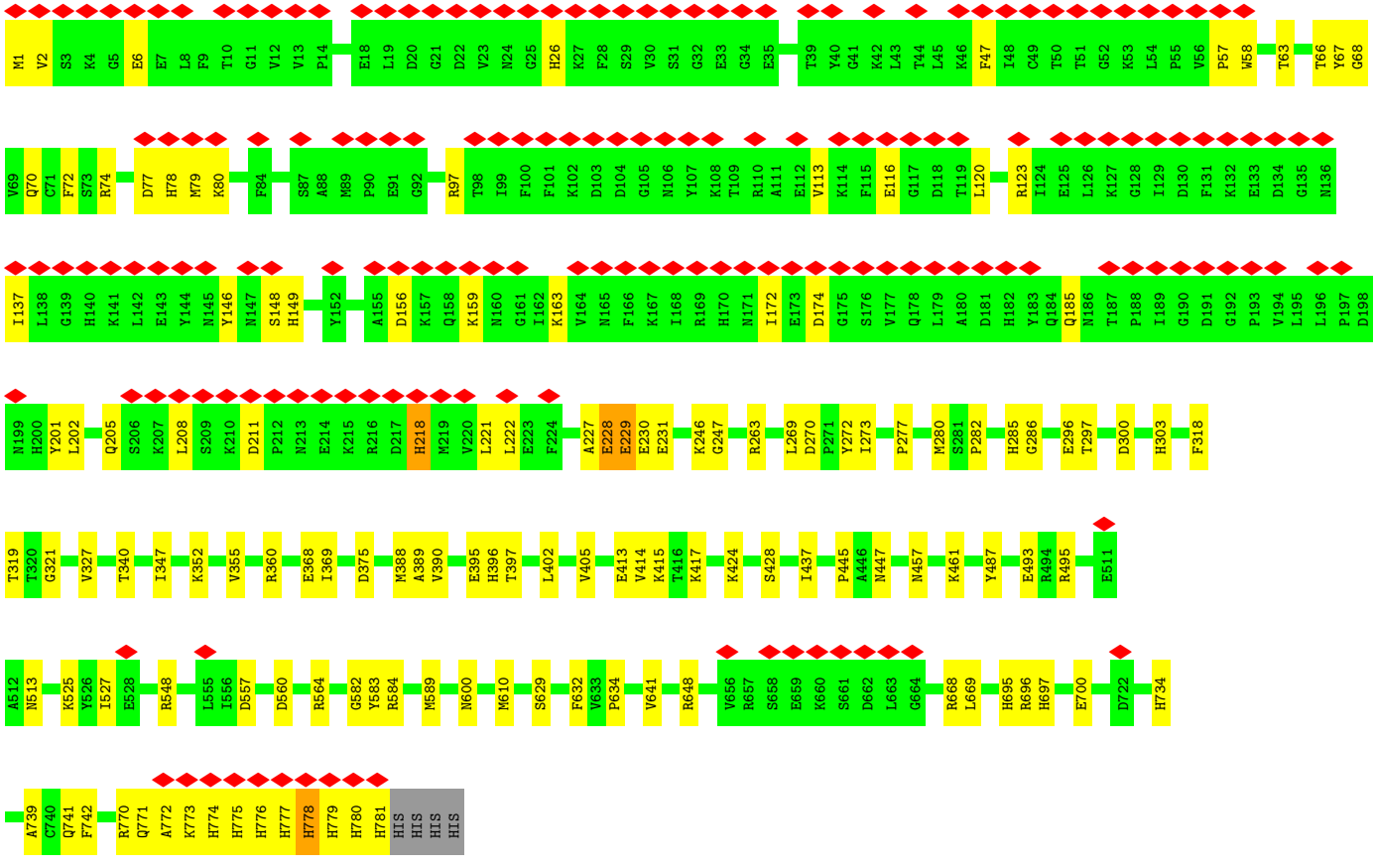




• Molecule 1: mEGFP,CTP synthase,CTP synthase,CTP synthase

Chain J:

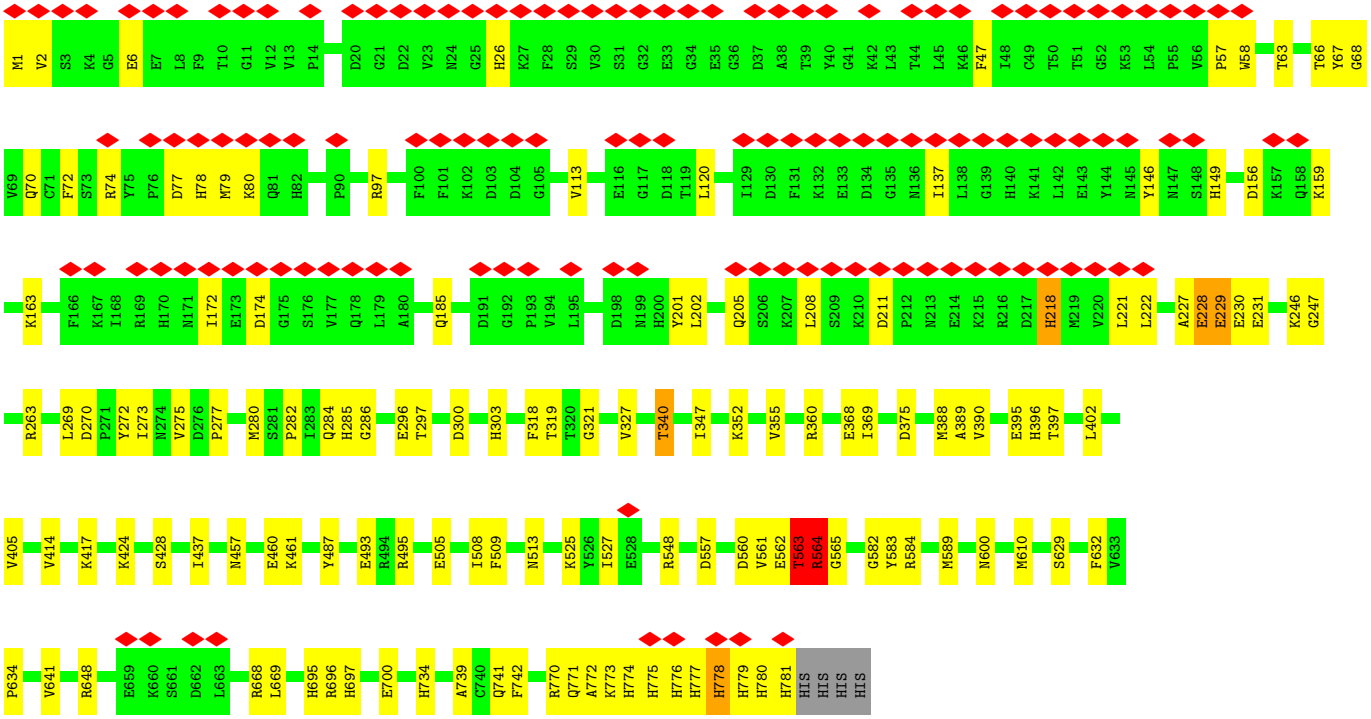




• Molecule 1: mEGFP,CTP synthase,CTP synthase,CTP synthase

Chain L:




M1 V2 S3 K4 G5 E6 E7 L8 F9 T10 G11 V12 V13 P14 D20 G21 D22 V23 N24 G25 H26 K27 F28 S29 V30 S31 G32 E33 G34 E35 G36 D37 A38 T39 Y40 G41 K42 L43 T44 L45 K46 F47 I48 C49 T50 T51 G52 K53 L54 P55 V56 P57 W58 T63 T66 Y67 G68
V69 Q70 C71 F72 S73 R74 Y75 P76 D77 H78 M79 K80 Q81 H82 P90 R97 F100 F101 K102 D103 D104 G105 V113 E116 G117 D118 T119 L120 I129 D130 F131 K132 E133 D134 G135 N136 I137 L138 G139 H140 K141 L142 E143 Y144 N145 Y146 N147 S148 H149 D156 K157 Q158 K159
K163 F166 K167 I168 R169 H170 N171 I172 E173 D174 G175 S176 V177 Q178 L179 A180 Q185 D191 G192 P193 V194 L195 D198 N199 H200 Y201 L202 Q205 S206 K207 L208 S209 K210 D211 P212 N213 E214 K215 R216 D217 H218 M219 V220 L221 L222 A227 E228 E229 E230 E231 K246 G247
R263 L269 D270 P271 Y272 I273 N274 V275 D276 P277 M280 S281 P282 I283 Q284 H285 G286 E296 T297 D300 H303 F318 T319 T320 G321 V327 T340 I347 K352 V355 R360 E368 I369 D375 M388 A389 V390 E395 H396 T397 L402
V405 V414 K417 K424 S428 I437 N457 E460 K461 Y487 E493 R494 R495 E505 I508 F509 N513 K525 Y526 I527 E528 R548 D557 D560 V561 E562 T563 R564 G565 G582 Y583 R584 M589 N600 M610 S629 F632 V633
P634 V641 R648 E659 K660 S661 D662 L663 R668 L669 H695 R696 H697 E700 H734 A739 C740 Q741 F742 R770 Q771 A772 K773 H774 H775 H776 H777 H778 H779 H780 H781 HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	161302	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.603	Depositor
Minimum map value	-0.227	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.0415	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.72	0/6297	1.05	3/8519 (0.0%)
1	B	0.72	0/6297	1.05	4/8519 (0.0%)
1	C	0.72	0/6297	1.05	3/8519 (0.0%)
1	D	0.72	0/6297	1.05	3/8519 (0.0%)
1	E	0.72	0/6297	1.05	4/8519 (0.0%)
1	F	0.72	0/6297	1.05	3/8519 (0.0%)
1	G	0.72	0/6297	1.05	4/8519 (0.0%)
1	H	0.72	0/6297	1.05	3/8519 (0.0%)
1	I	0.72	0/6297	1.05	5/8519 (0.1%)
1	J	0.72	0/6297	1.05	3/8519 (0.0%)
1	K	0.72	0/6297	1.05	3/8519 (0.0%)
1	L	0.72	0/6297	1.05	5/8519 (0.1%)
All	All	0.72	0/75564	1.05	43/102228 (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
1	E	0	1
1	H	0	1
1	I	0	1
1	L	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	218	HIS	N-CA-C	6.24	116.80	108.38
1	C	218	HIS	N-CA-C	6.23	116.80	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	218	HIS	N-CA-C	6.23	116.80	108.38
1	B	218	HIS	N-CA-C	6.22	116.78	108.38
1	J	218	HIS	N-CA-C	6.22	116.78	108.38

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	564	ARG	Sidechain
1	H	564	ARG	Sidechain
1	I	564	ARG	Sidechain
1	L	564	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6169	0	6124	229	0
1	B	6169	0	6124	233	0
1	C	6169	0	6124	227	0
1	D	6169	0	6124	229	0
1	E	6169	0	6124	226	0
1	F	6169	0	6124	191	0
1	G	6169	0	6124	191	0
1	H	6169	0	6124	228	0
1	I	6169	0	6124	234	0
1	J	6169	0	6124	186	0
1	K	6169	0	6124	186	0
1	L	6169	0	6124	230	0
All	All	74028	0	73488	2128	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 2128 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:509:PHE:CD2	1:I:509:PHE:HB2	1.50	1.46
1:D:509:PHE:HB2	1:I:509:PHE:CD2	1.50	1.43
1:C:509:PHE:CD2	1:H:509:PHE:HB2	1.62	1.35
1:H:340:THR:HB	1:J:285:HIS:NE2	1.44	1.32
1:C:509:PHE:HB2	1:H:509:PHE:CD2	1.62	1.32

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	779/785 (99%)	759 (97%)	20 (3%)	0	100	100
1	B	779/785 (99%)	759 (97%)	20 (3%)	0	100	100
1	C	779/785 (99%)	759 (97%)	20 (3%)	0	100	100
1	D	779/785 (99%)	759 (97%)	20 (3%)	0	100	100
1	E	779/785 (99%)	757 (97%)	22 (3%)	0	100	100
1	F	779/785 (99%)	759 (97%)	20 (3%)	0	100	100
1	G	779/785 (99%)	759 (97%)	20 (3%)	0	100	100
1	H	779/785 (99%)	756 (97%)	21 (3%)	2 (0%)	36	65
1	I	779/785 (99%)	756 (97%)	20 (3%)	3 (0%)	30	59
1	J	779/785 (99%)	759 (97%)	20 (3%)	0	100	100
1	K	779/785 (99%)	759 (97%)	20 (3%)	0	100	100
1	L	779/785 (99%)	756 (97%)	21 (3%)	2 (0%)	36	65
All	All	9348/9420 (99%)	9097 (97%)	244 (3%)	7 (0%)	49	78

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	563	THR

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Mol	Chain	Res	Type
1	L	563	THR
1	I	564	ARG
1	H	563	THR
1	H	564	ARG

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	672/676 (99%)	668 (99%)	4 (1%)	78	80
1	B	672/676 (99%)	668 (99%)	4 (1%)	78	80
1	C	672/676 (99%)	668 (99%)	4 (1%)	78	80
1	D	672/676 (99%)	667 (99%)	5 (1%)	76	78
1	E	672/676 (99%)	668 (99%)	4 (1%)	78	80
1	F	672/676 (99%)	668 (99%)	4 (1%)	78	80
1	G	672/676 (99%)	669 (100%)	3 (0%)	84	83
1	H	672/676 (99%)	665 (99%)	7 (1%)	68	75
1	I	672/676 (99%)	665 (99%)	7 (1%)	68	75
1	J	672/676 (99%)	669 (100%)	3 (0%)	84	83
1	K	672/676 (99%)	668 (99%)	4 (1%)	78	80
1	L	672/676 (99%)	665 (99%)	7 (1%)	68	75
All	All	8064/8112 (99%)	8008 (99%)	56 (1%)	73	78

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	562	GLU
1	L	564	ARG
1	F	26	HIS
1	L	563	THR
1	L	26	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 169 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	178	GLN
1	J	149	HIS
1	F	600	ASN
1	H	178	GLN
1	J	768	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

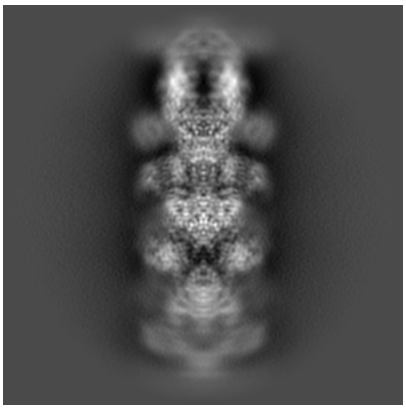
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-66620. These allow visual inspection of the internal detail of the map and identification of artifacts.

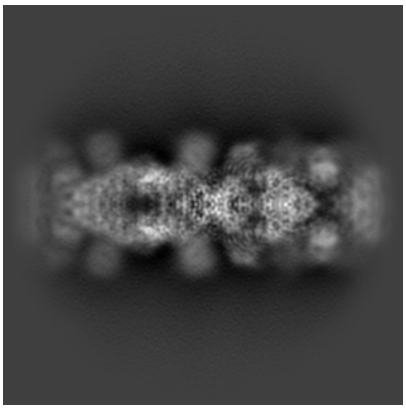
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

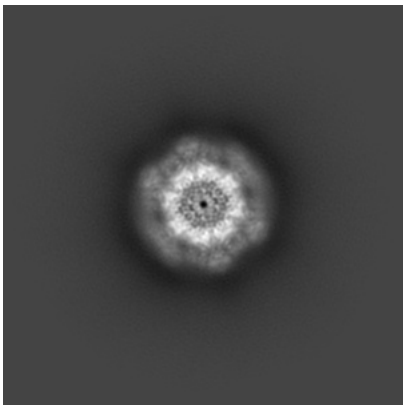
6.1.1 Primary map



X

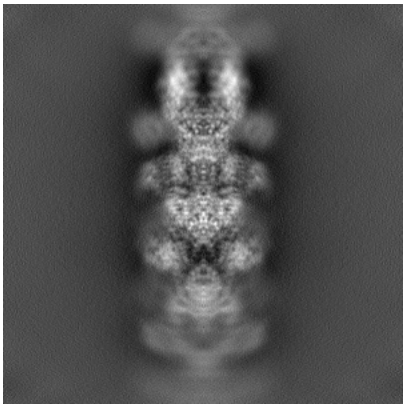


Y

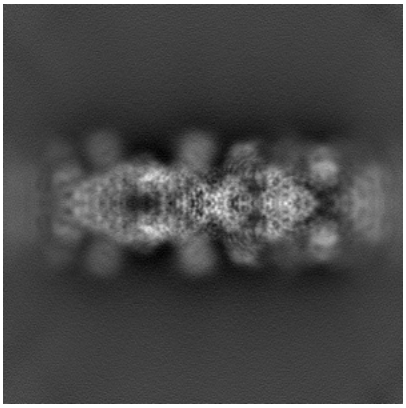


Z

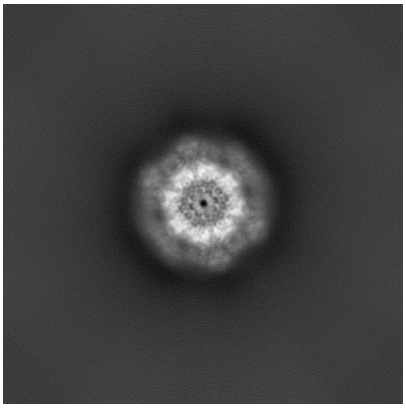
6.1.2 Raw map



X



Y

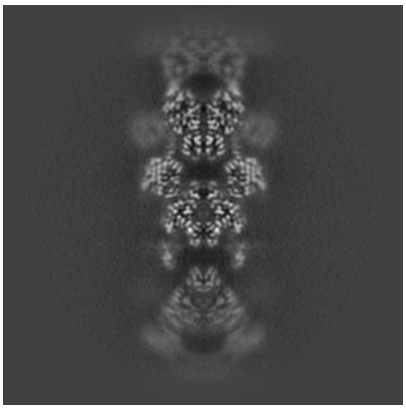


Z

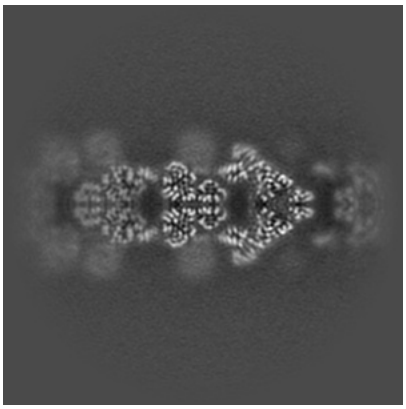
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

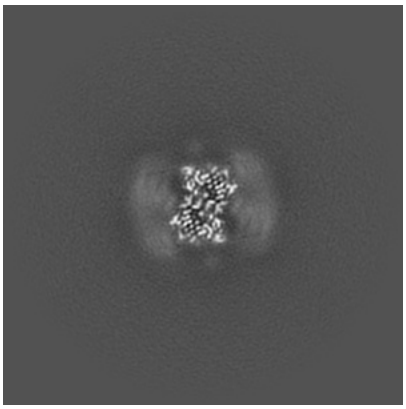
6.2.1 Primary map



X Index: 180

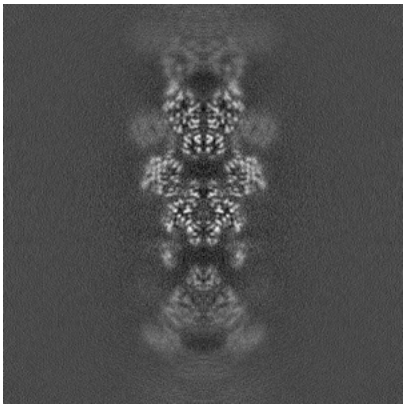


Y Index: 180

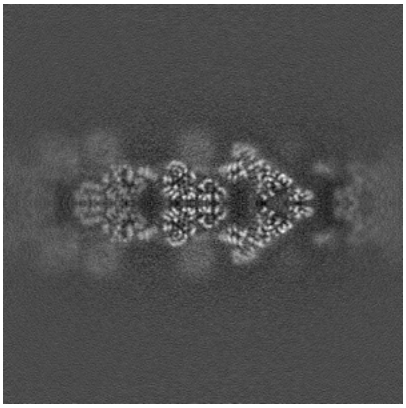


Z Index: 180

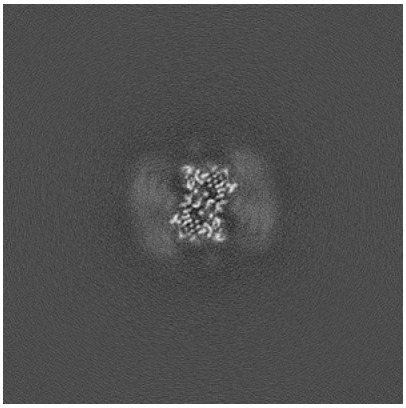
6.2.2 Raw map



X Index: 180



Y Index: 180

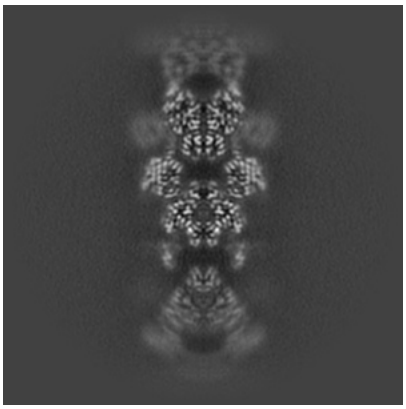


Z Index: 180

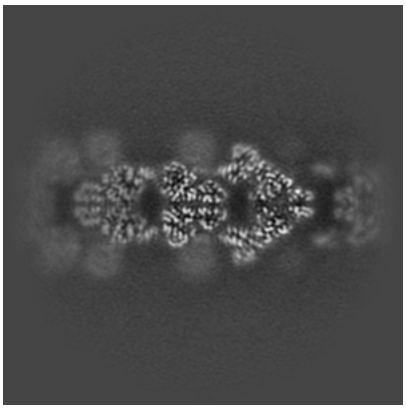
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

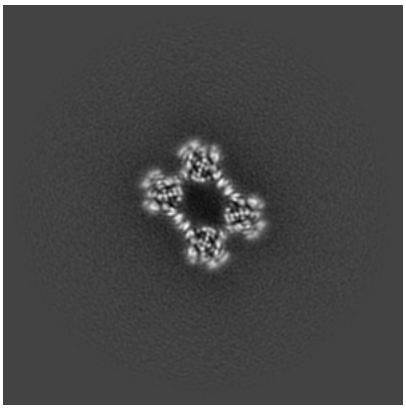
6.3.1 Primary map



X Index: 180

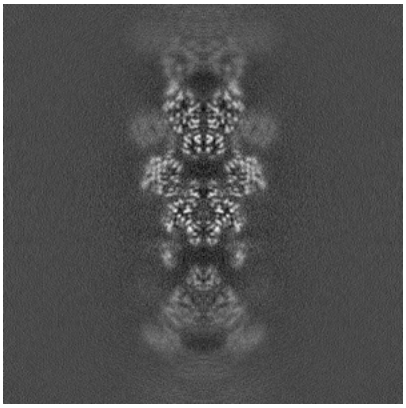


Y Index: 179

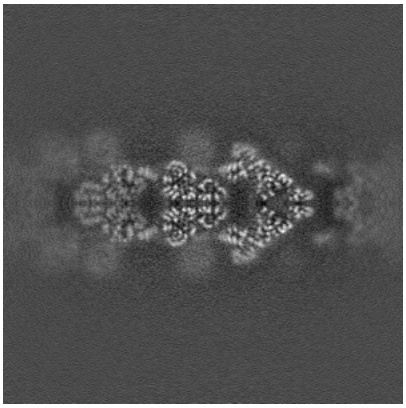


Z Index: 211

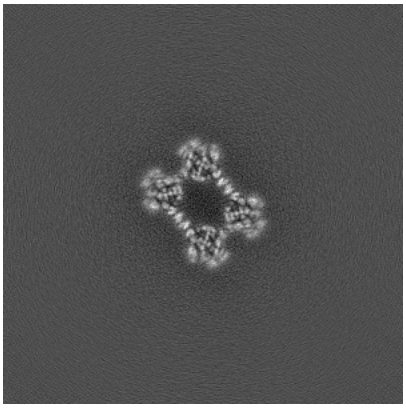
6.3.2 Raw map



X Index: 180



Y Index: 180

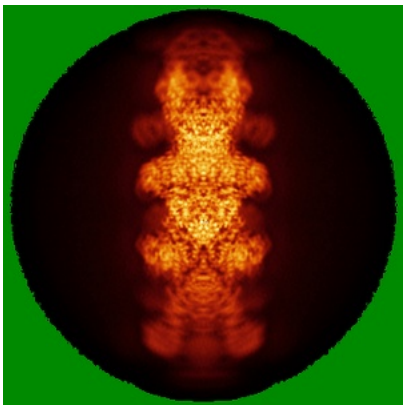


Z Index: 211

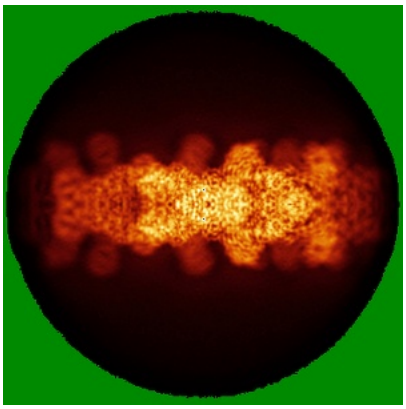
The images above show the largest variance slices of the map in three orthogonal directions.

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

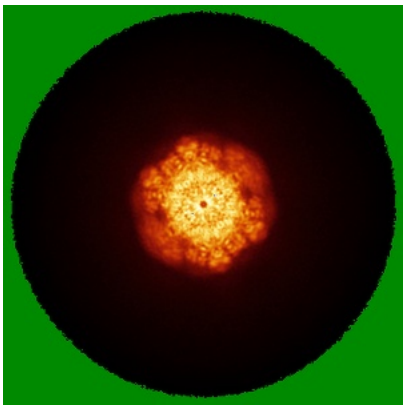
6.4.1 Primary map



X

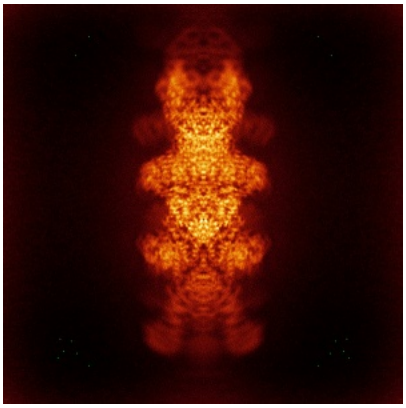


Y

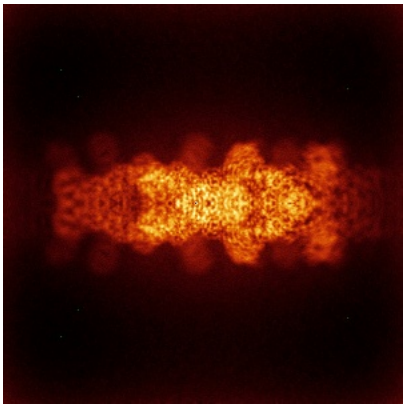


Z

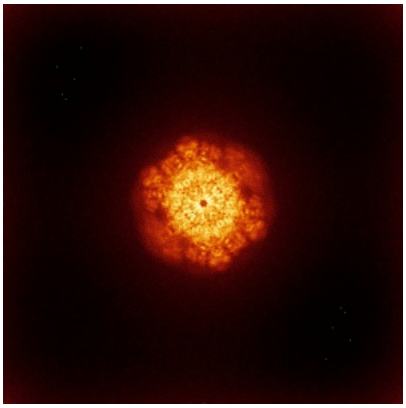
6.4.2 Raw map



X



Y

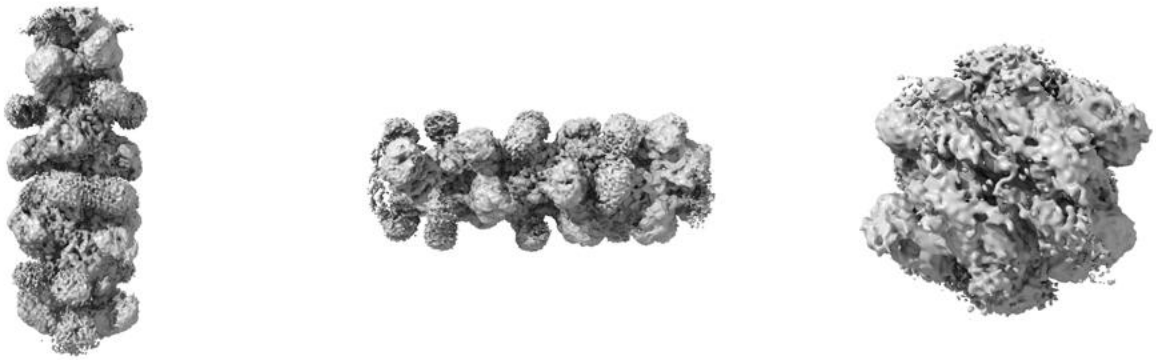


Z

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)

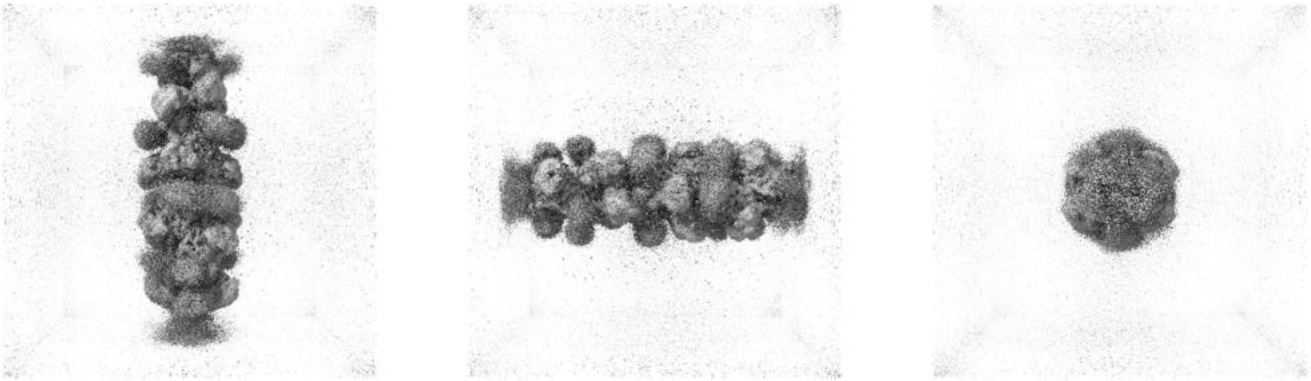
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0415. 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.

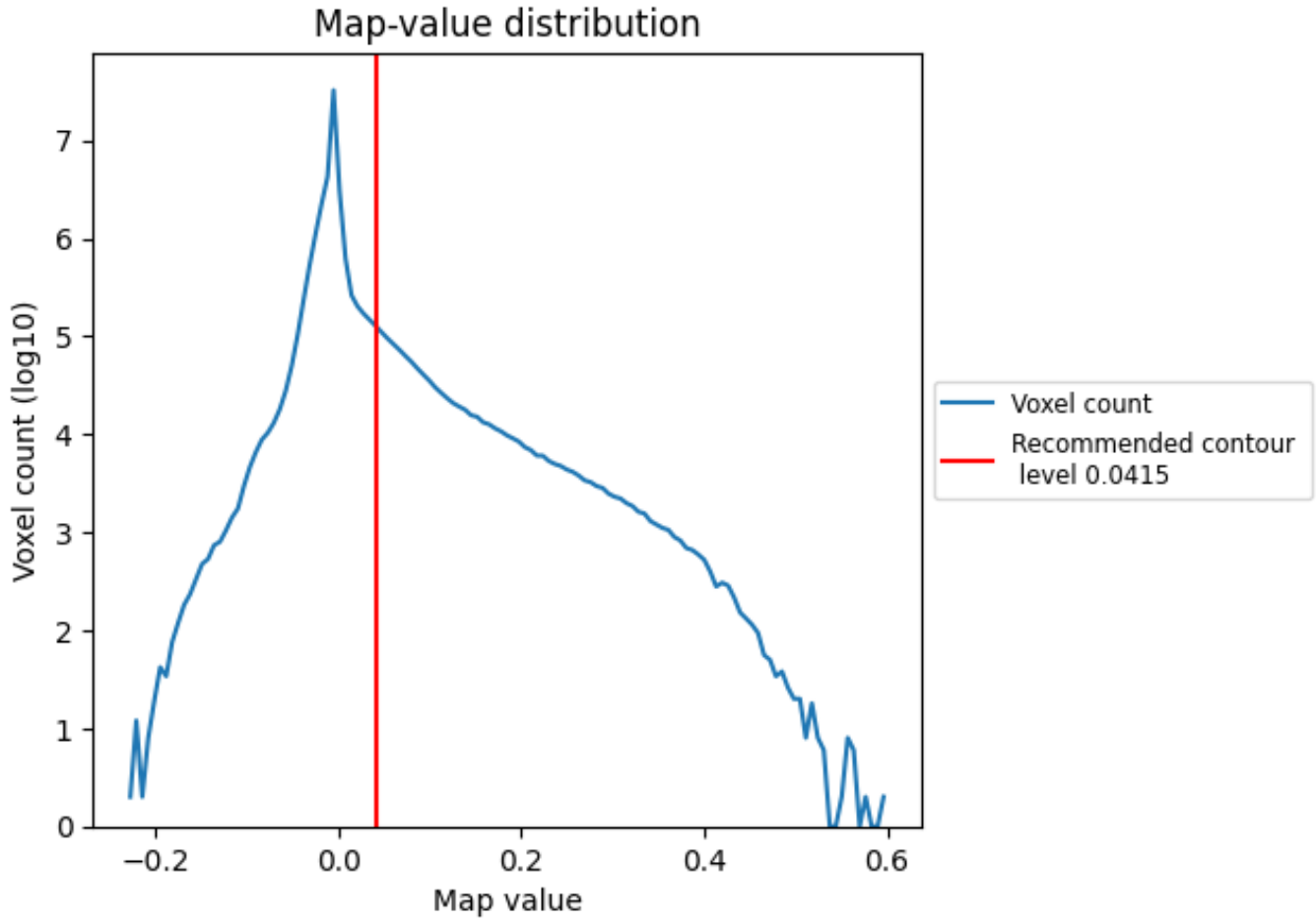
6.6 Mask visualisation (i)

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

7 Map analysis

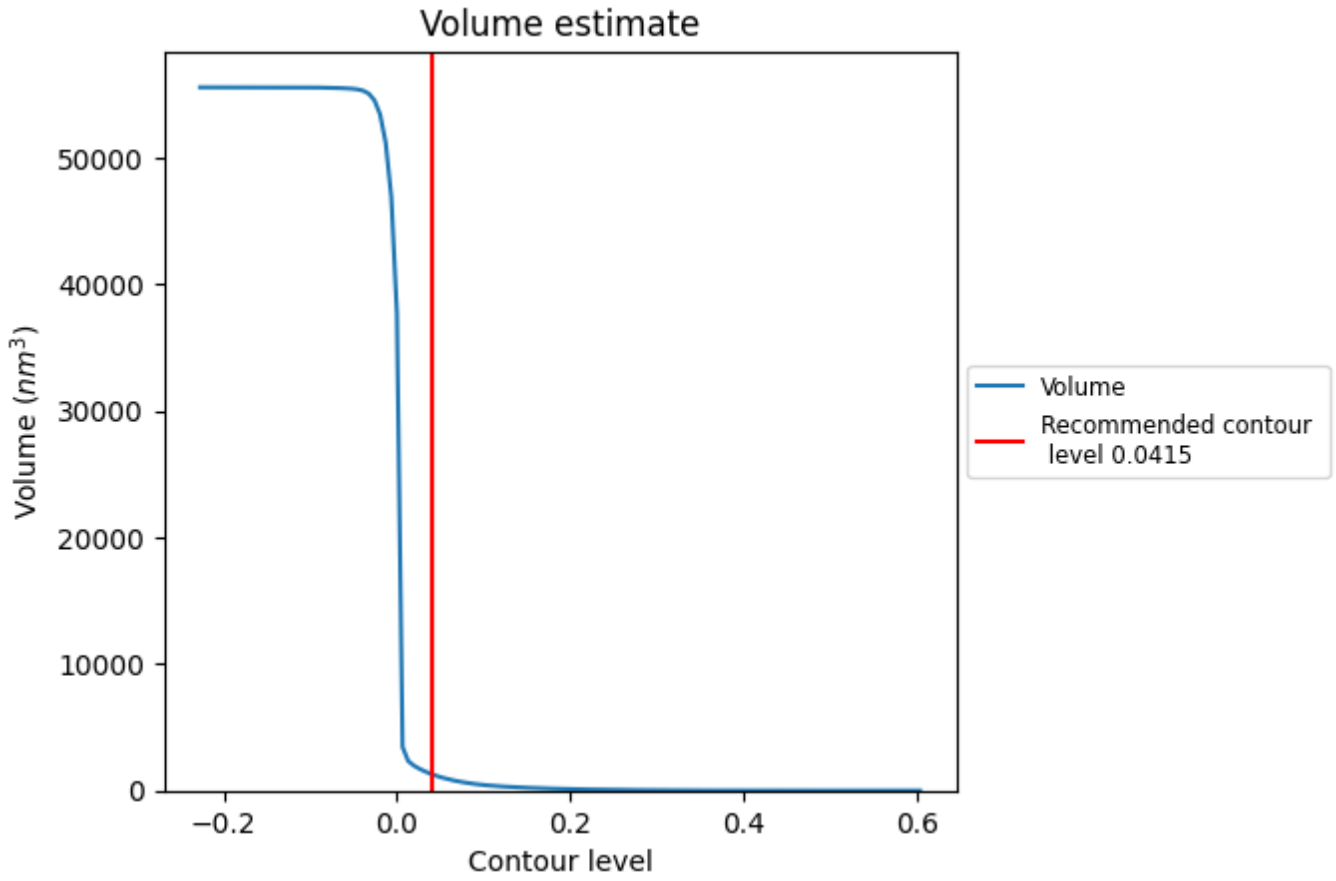
This section contains the results of statistical analysis of the map.

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.

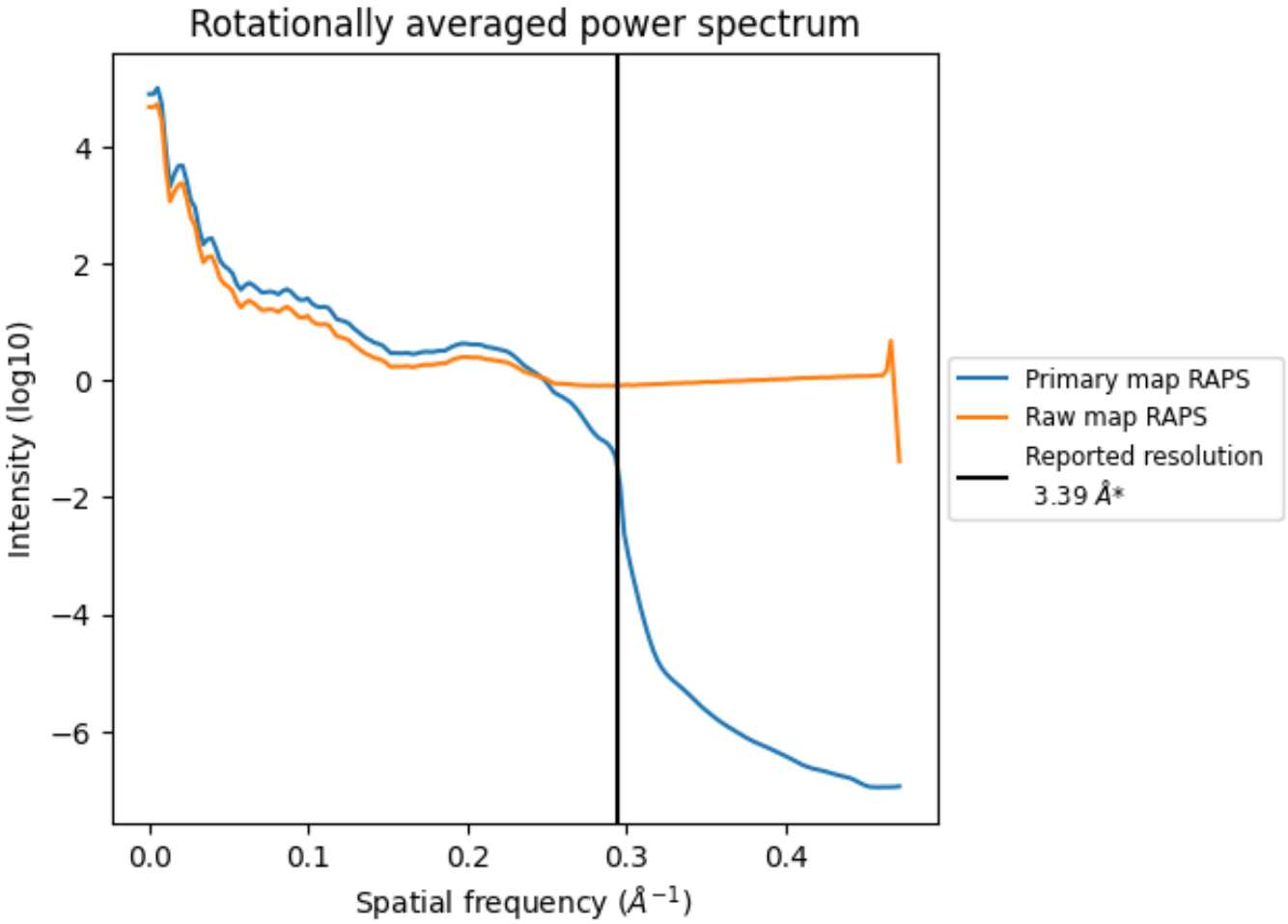
7.2 Volume estimate (i)



The volume at the recommended contour level is 1260 nm^3; this corresponds to an approximate mass of 1138 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)

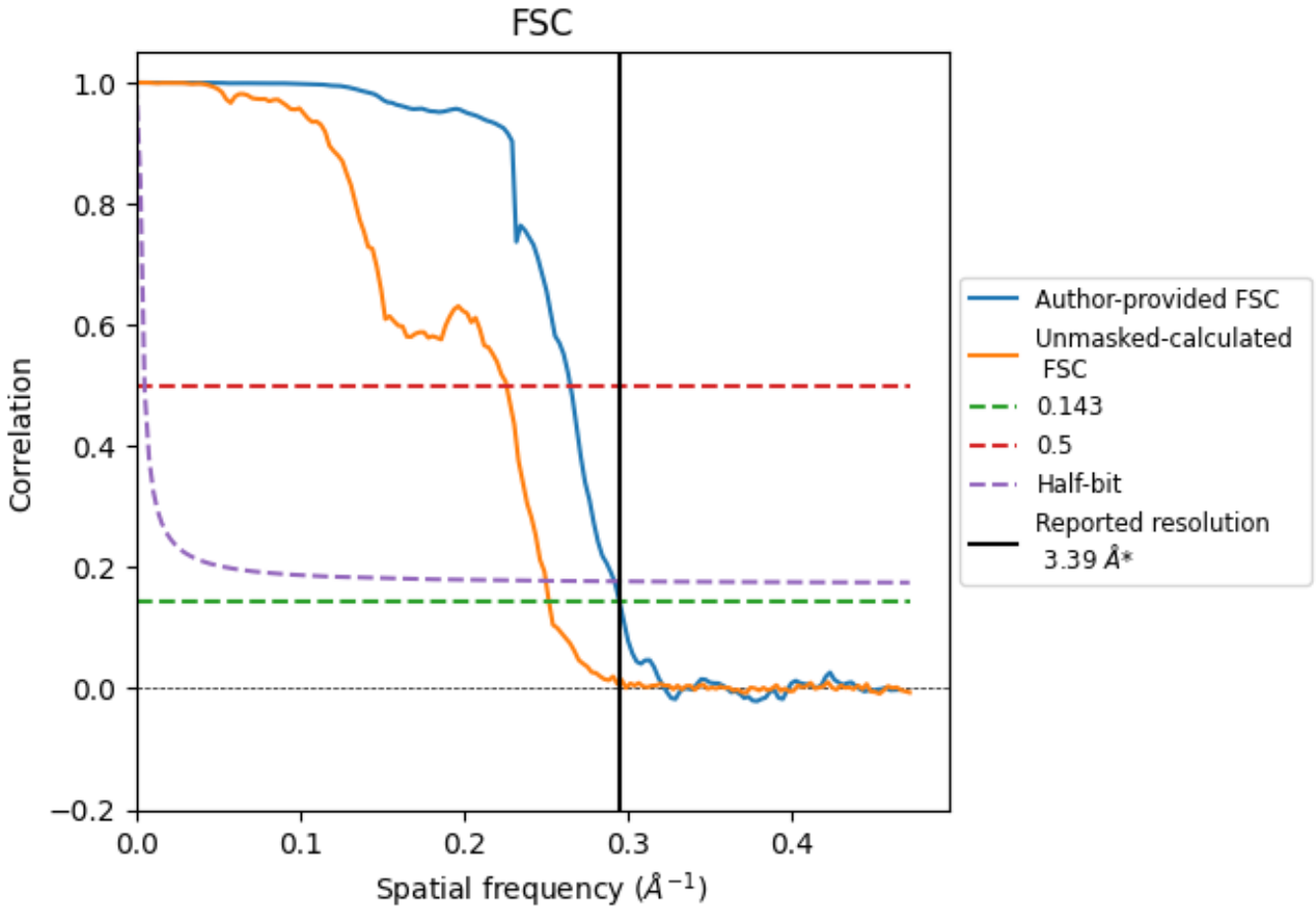


*Reported resolution corresponds to spatial frequency of 0.295 Å^{-1}

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 0.295 $Å^{-1}$

8.2 Resolution estimates (i)

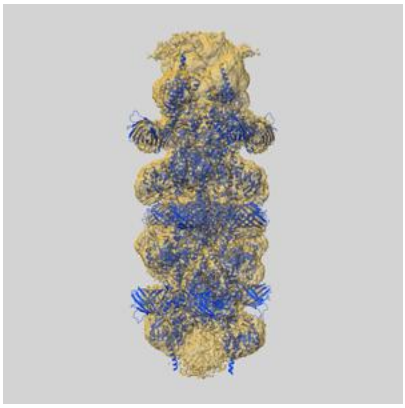
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.39	-	-
Author-provided FSC curve	3.39	3.78	3.43
Unmasked-calculated*	3.97	4.43	4.00

*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 3.97 differs from the reported value 3.39 by more than 10 %

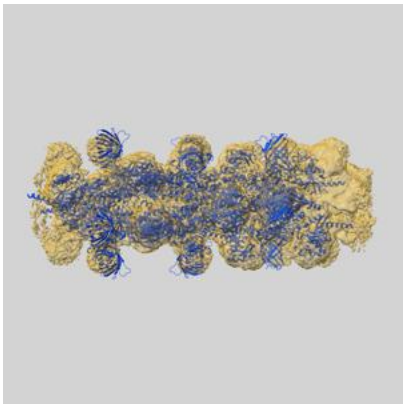
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-66620 and PDB model 9X6G. Per-residue inclusion information can be found in section 3 on page 10.

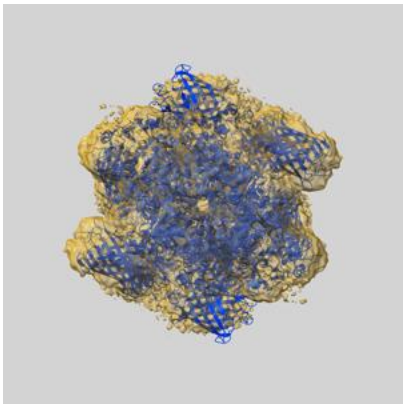
9.1 Map-model overlay



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0415 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.

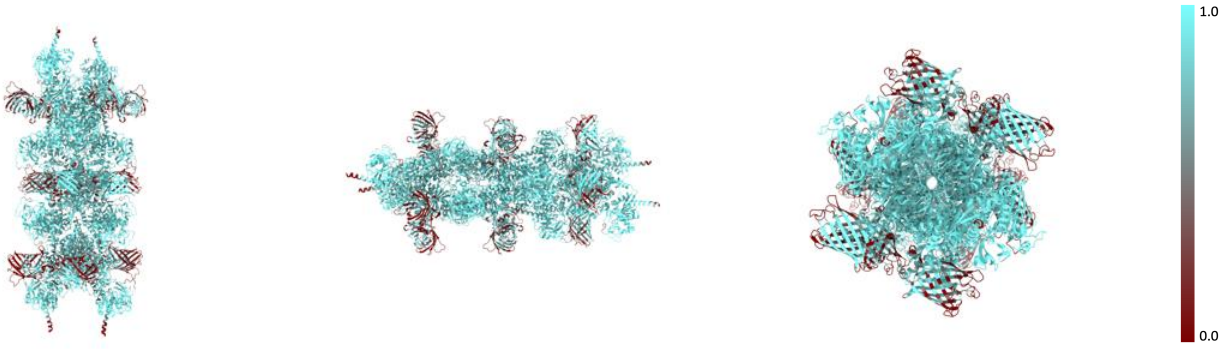
9.2 Q-score mapped to coordinate model



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.

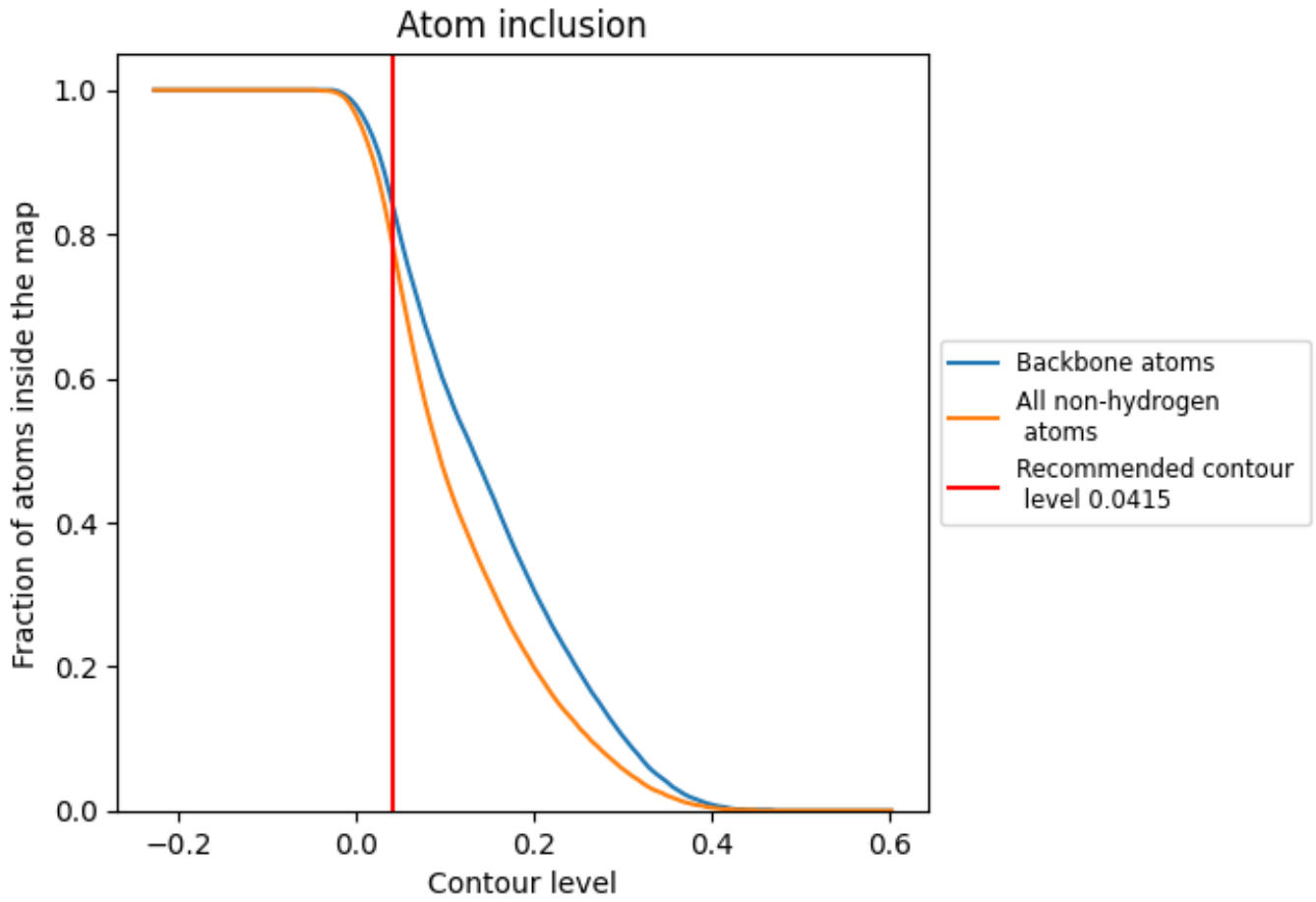
9.3 Atom inclusion mapped to coordinate model



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 (0.0415).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 78% 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 (0.0415) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7850	0.2250
A	0.8200	0.2790
B	0.8230	0.2690
C	0.8170	0.2730
D	0.8240	0.2690
E	0.8120	0.2600
F	0.7000	0.1220
G	0.8120	0.2360
H	0.7440	0.1900
I	0.8100	0.2550
J	0.6980	0.1220
K	0.8140	0.2360
L	0.7440	0.1890

