



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 11:42 AM EDT

PDB ID : 6X6L
EMDB ID : EMD-22077
Title : Cryo-EM Structure of CagX and CagY within the dCag3 Helicobacter pylori PR
Authors : Sheedlo, M.J.; Chung, J.M.; Sawhney, N.; Durie, C.L.; Cover, T.L.; Ohi, M.D.; Lacy, D.B.
Deposited on : 2020-05-28
Resolution : 3.00 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.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) : 2.39

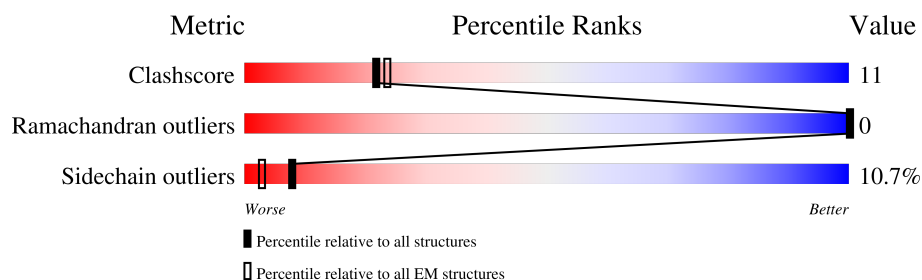
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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








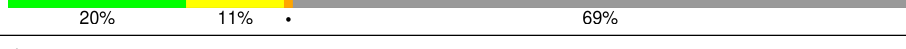

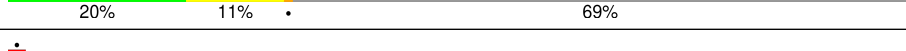
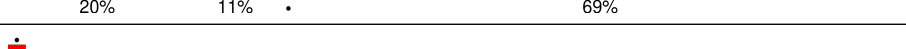
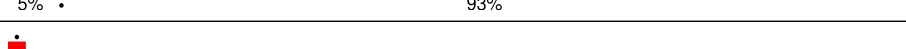
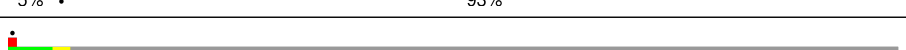
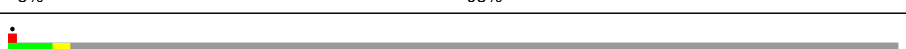

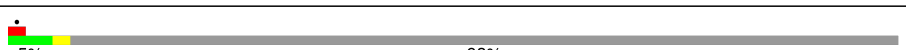
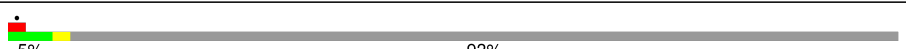


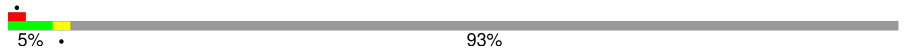
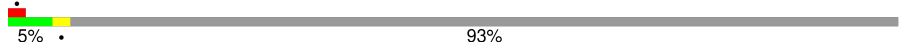
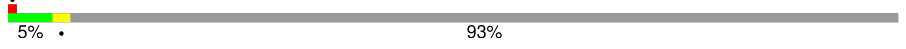
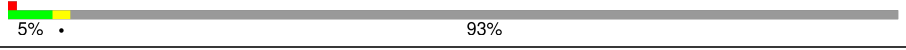
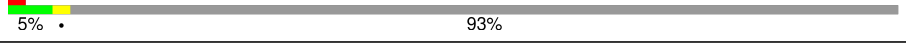
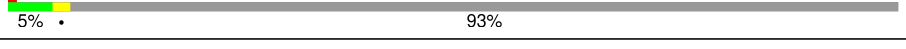


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AX	521	
1	BX	521	
1	CX	521	
1	DX	521	
1	EX	521	
1	FX	521	
1	GX	521	
1	HX	521	

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Mol	Chain	Length	Quality of chain
1	IX	521	 20% 10% 69%
1	JX	521	 20% 10% 69%
1	KX	521	 19% 11% 69%
1	LX	521	 19% 11% 69%
1	MX	521	 21% 10% 69%
1	NX	521	 20% 11% 69%
1	OX	521	 19% 11% 69%
1	PX	521	 20% 11% 69%
1	QX	521	 20% 11% 69%
2	AY	1927	 5% 93%
2	BY	1927	 5% 93%
2	CY	1927	 5% 93%
2	DY	1927	 5% 93%
2	EY	1927	 5% 93%
2	FY	1927	 5% 93%
2	GY	1927	 5% 93%
2	HY	1927	 5% 93%
2	IY	1927	 5% 93%
2	JY	1927	 5% 93%
2	KY	1927	 5% 93%
2	LY	1927	 5% 93%
2	MY	1927	 5% 93%
2	NY	1927	 5% 93%
2	OY	1927	 5% 93%
2	PY	1927	 5% 93%

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Mol	Chain	Length	Quality of chain
2	QY	1927	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>5% .</div><div>93%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 40613 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 Cag pathogenicity island protein (Cag8).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	BX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	CX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	DX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	EX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	FX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	GX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	HX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	IX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	JX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	KX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	LX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	MX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	NX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	OX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	PX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	QX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AX	?	-	GLU	deletion	UNP O25263
AX	516	GLU	LEU	conflict	UNP O25263
BX	?	-	GLU	deletion	UNP O25263
BX	516	GLU	LEU	conflict	UNP O25263
CX	?	-	GLU	deletion	UNP O25263
CX	516	GLU	LEU	conflict	UNP O25263
DX	?	-	GLU	deletion	UNP O25263
DX	516	GLU	LEU	conflict	UNP O25263
EX	?	-	GLU	deletion	UNP O25263
EX	516	GLU	LEU	conflict	UNP O25263
FX	?	-	GLU	deletion	UNP O25263
FX	516	GLU	LEU	conflict	UNP O25263
GX	?	-	GLU	deletion	UNP O25263
GX	516	GLU	LEU	conflict	UNP O25263
HX	?	-	GLU	deletion	UNP O25263
HX	516	GLU	LEU	conflict	UNP O25263
IX	?	-	GLU	deletion	UNP O25263
IX	516	GLU	LEU	conflict	UNP O25263
JX	?	-	GLU	deletion	UNP O25263
JX	516	GLU	LEU	conflict	UNP O25263
KX	?	-	GLU	deletion	UNP O25263
KX	516	GLU	LEU	conflict	UNP O25263
LX	?	-	GLU	deletion	UNP O25263
LX	516	GLU	LEU	conflict	UNP O25263
MX	?	-	GLU	deletion	UNP O25263
MX	516	GLU	LEU	conflict	UNP O25263
NX	?	-	GLU	deletion	UNP O25263
NX	516	GLU	LEU	conflict	UNP O25263
OX	?	-	GLU	deletion	UNP O25263
OX	516	GLU	LEU	conflict	UNP O25263
PX	?	-	GLU	deletion	UNP O25263
PX	516	GLU	LEU	conflict	UNP O25263
QX	?	-	GLU	deletion	UNP O25263
QX	516	GLU	LEU	conflict	UNP O25263

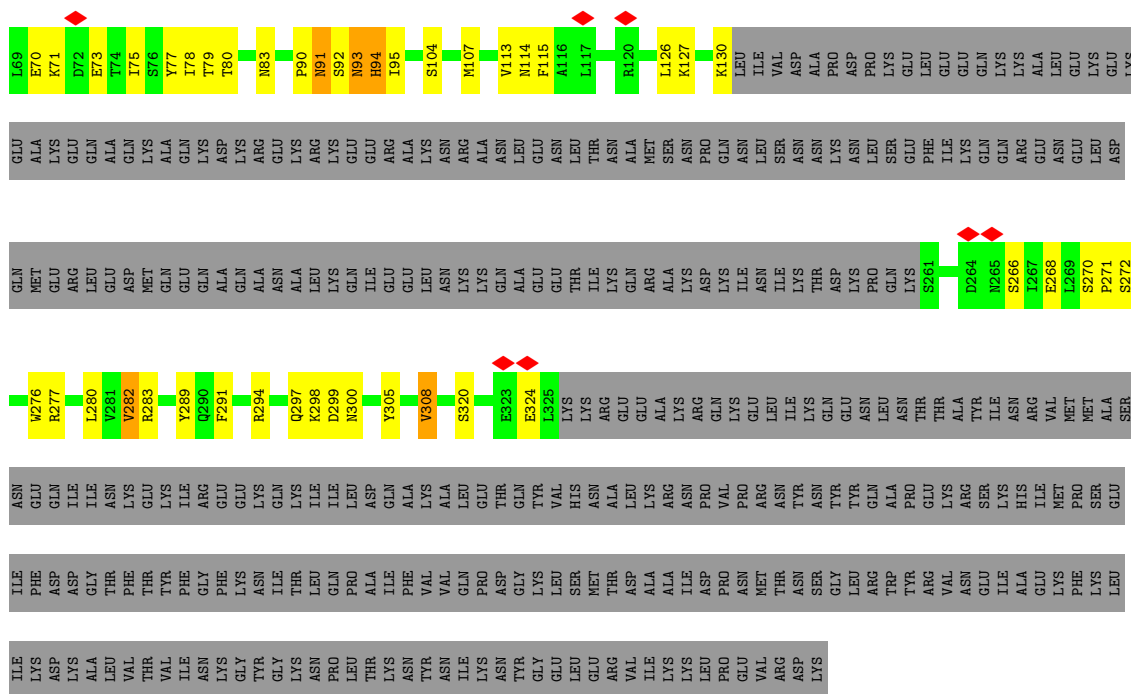
- Molecule 2 is a protein called Cag pathogenicity island protein (Cag7).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AY	135	Total	C	N	O	S	0	0
			1050	649	177	220	4		
2	BY	135	Total	C	N	O	S	0	0
			1050	649	177	220	4		

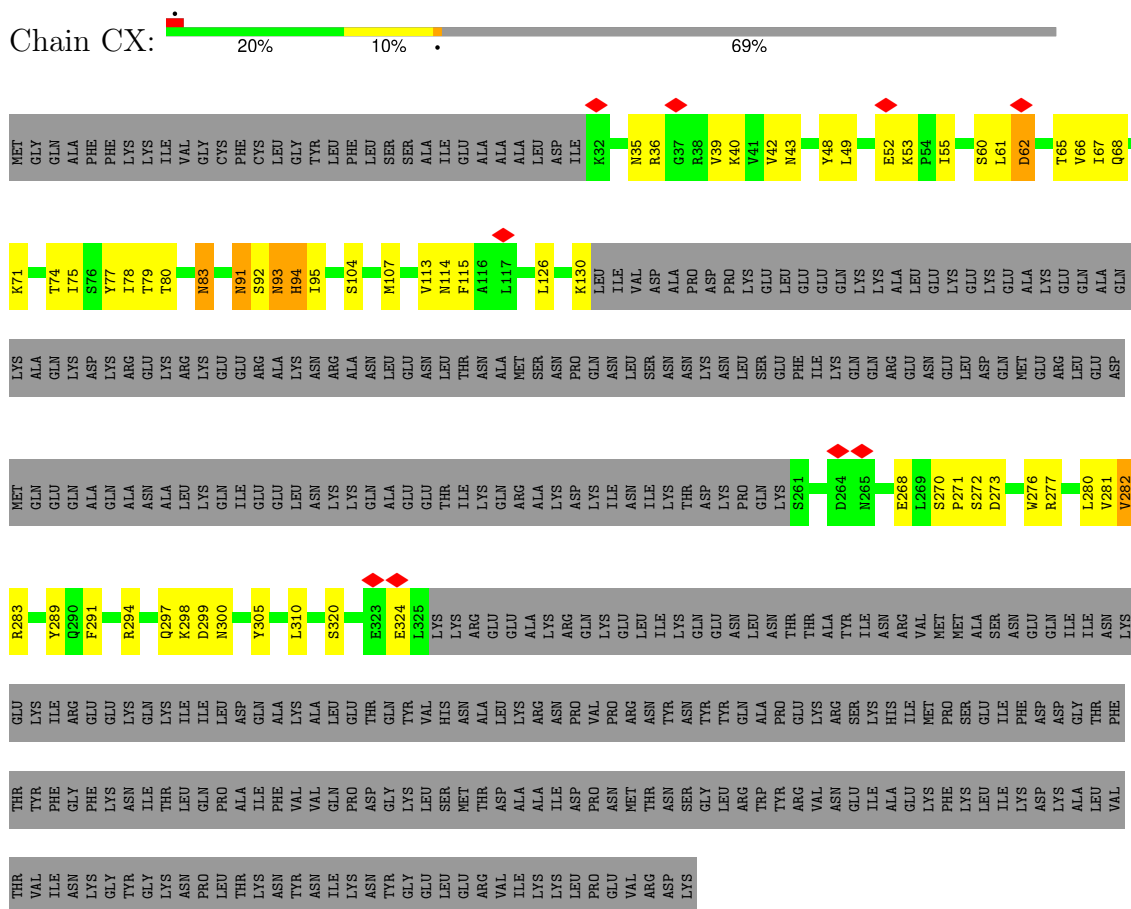
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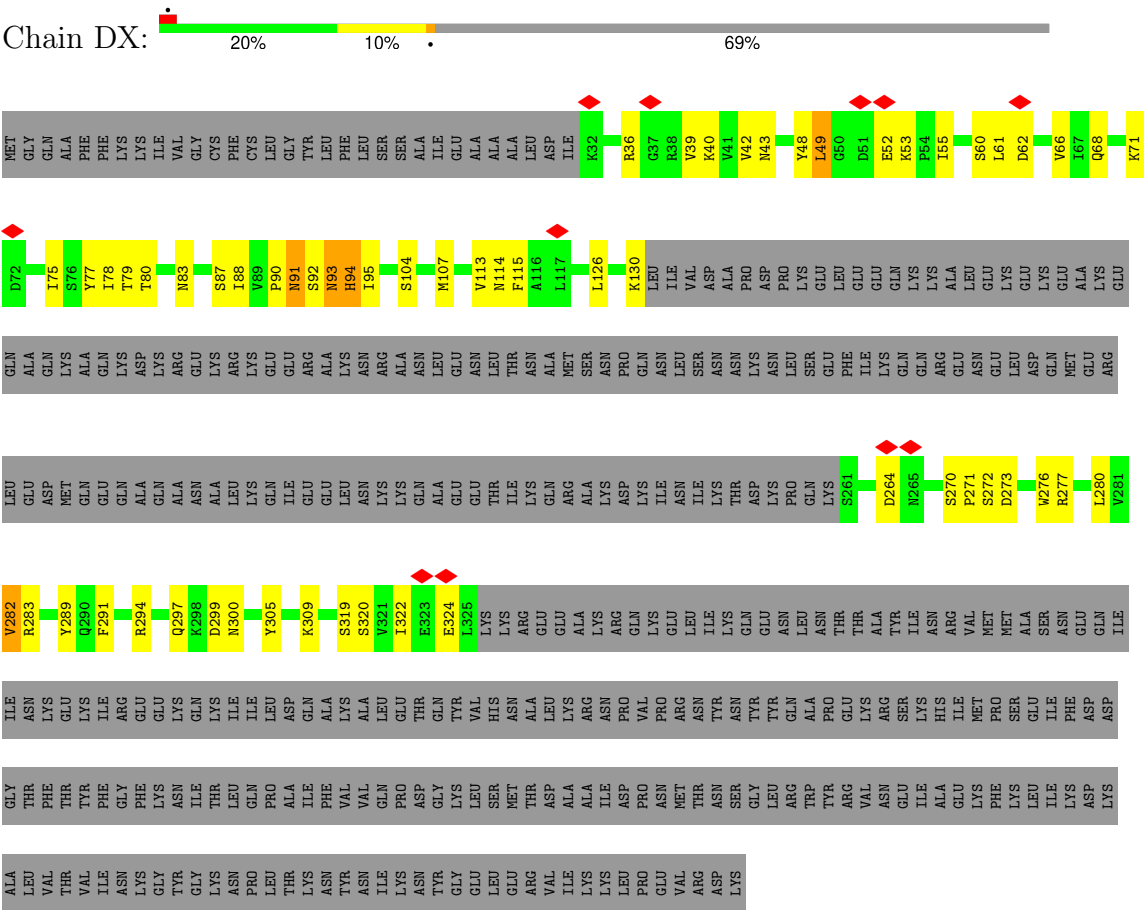
Mol	Chain	Residues	Atoms					AltConf	Trace
2	CY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	DY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	EY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	FY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	GY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	HY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	IY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	JY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	KY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	LY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	MY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	NY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	OY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	PY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	QY	135	Total 1050	C 649	N 177	O 220	S 4	0	0



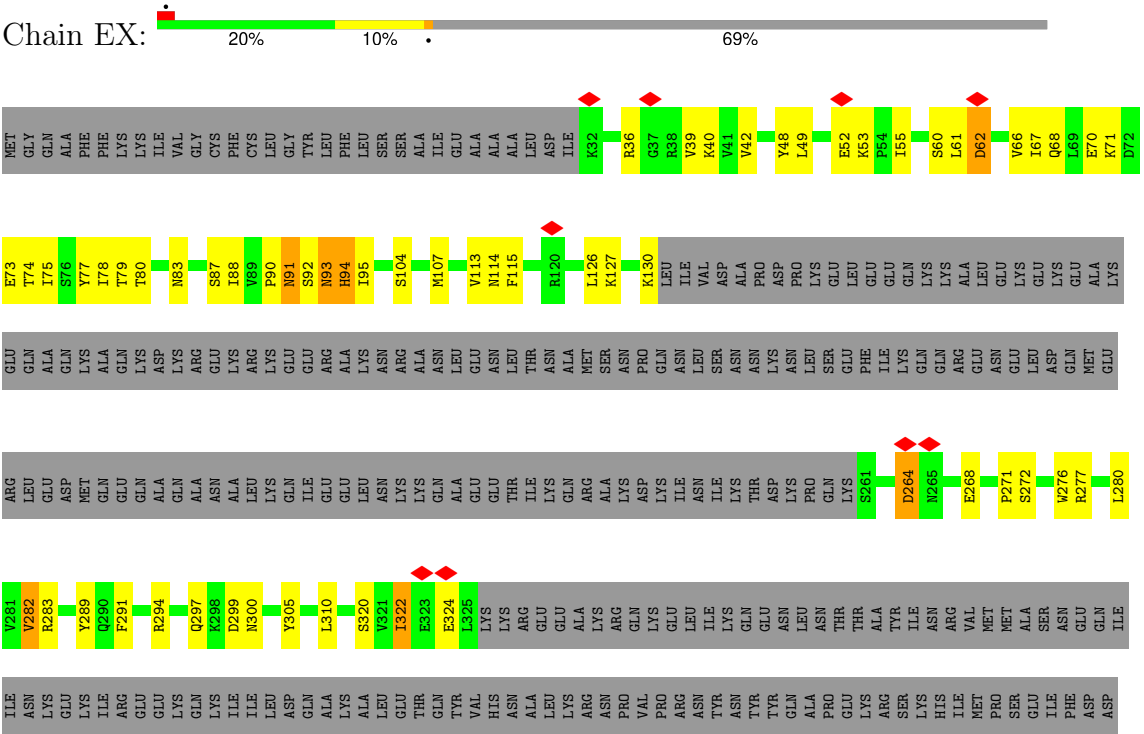
- Molecule 1: Cag pathogenicity island protein (Cag8)

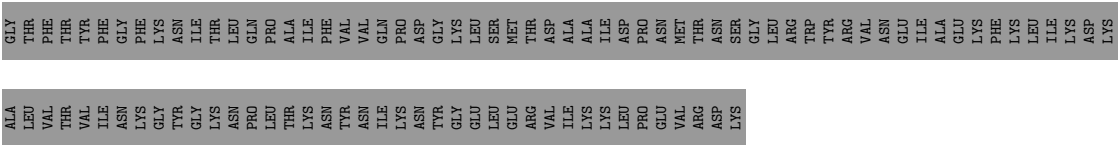


- Molecule 1: Cag pathogenicity island protein (Cag8)

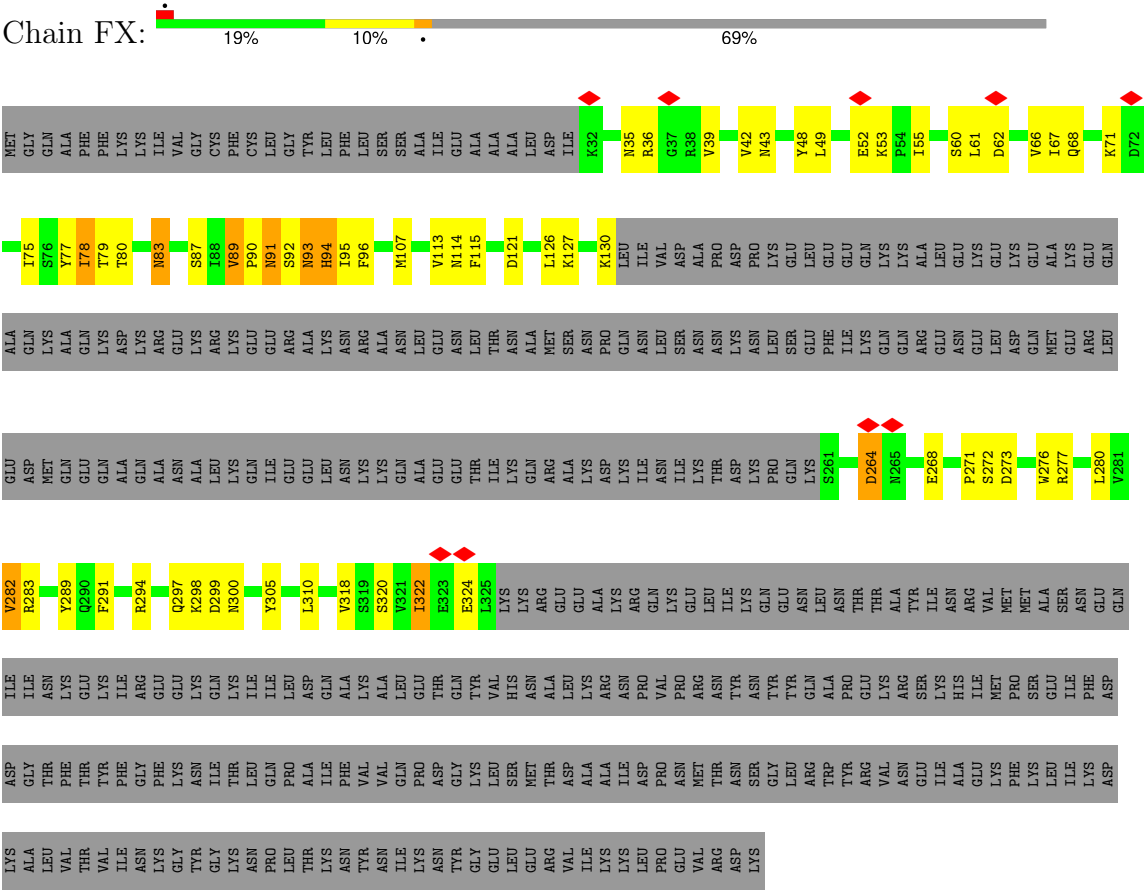


● Molecule 1: Cag pathogenicity island protein (Cag8)

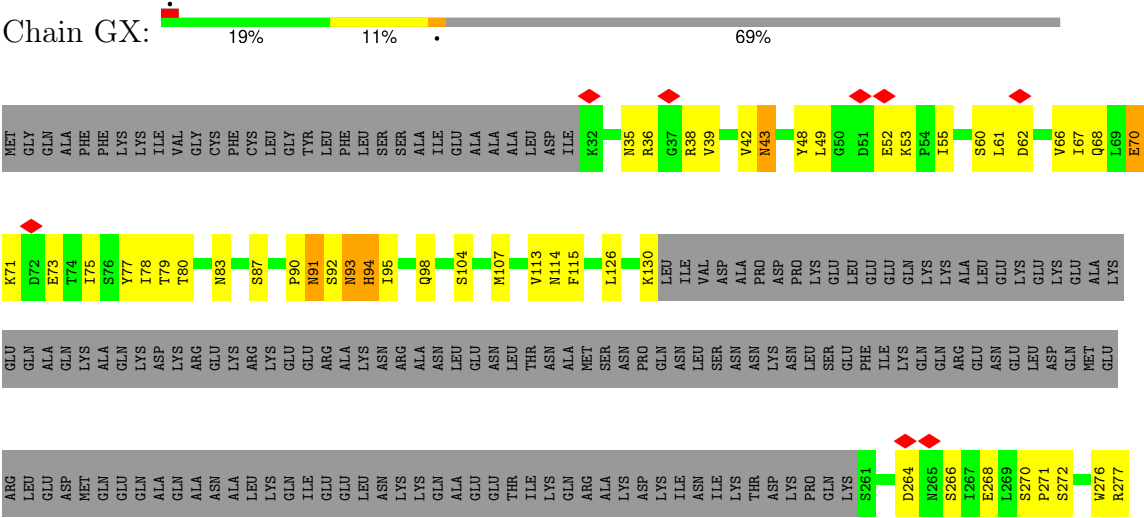


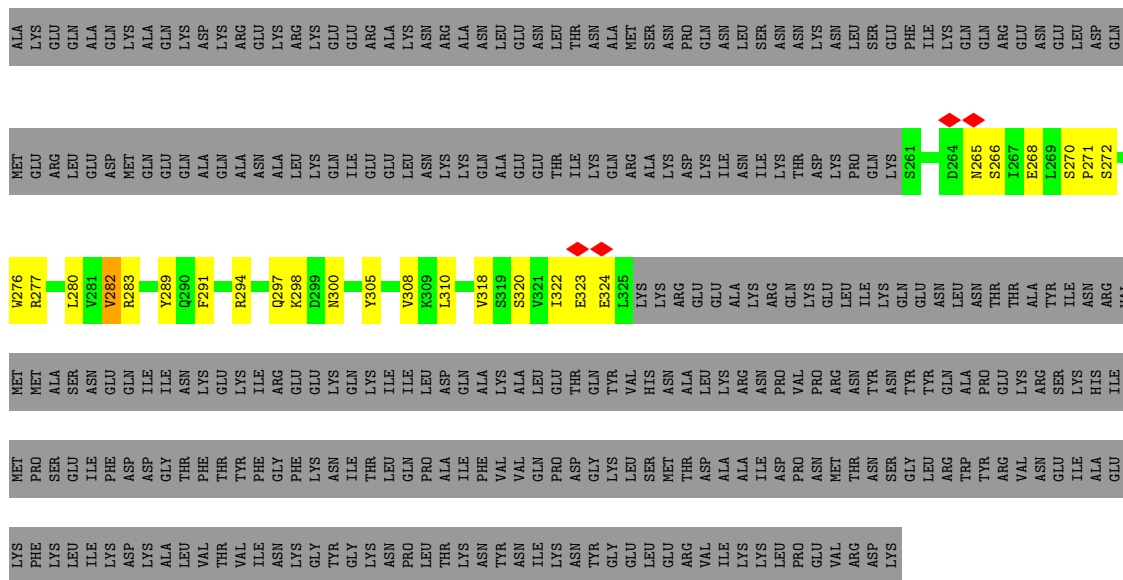


• Molecule 1: Cag pathogenicity island protein (Cag8)

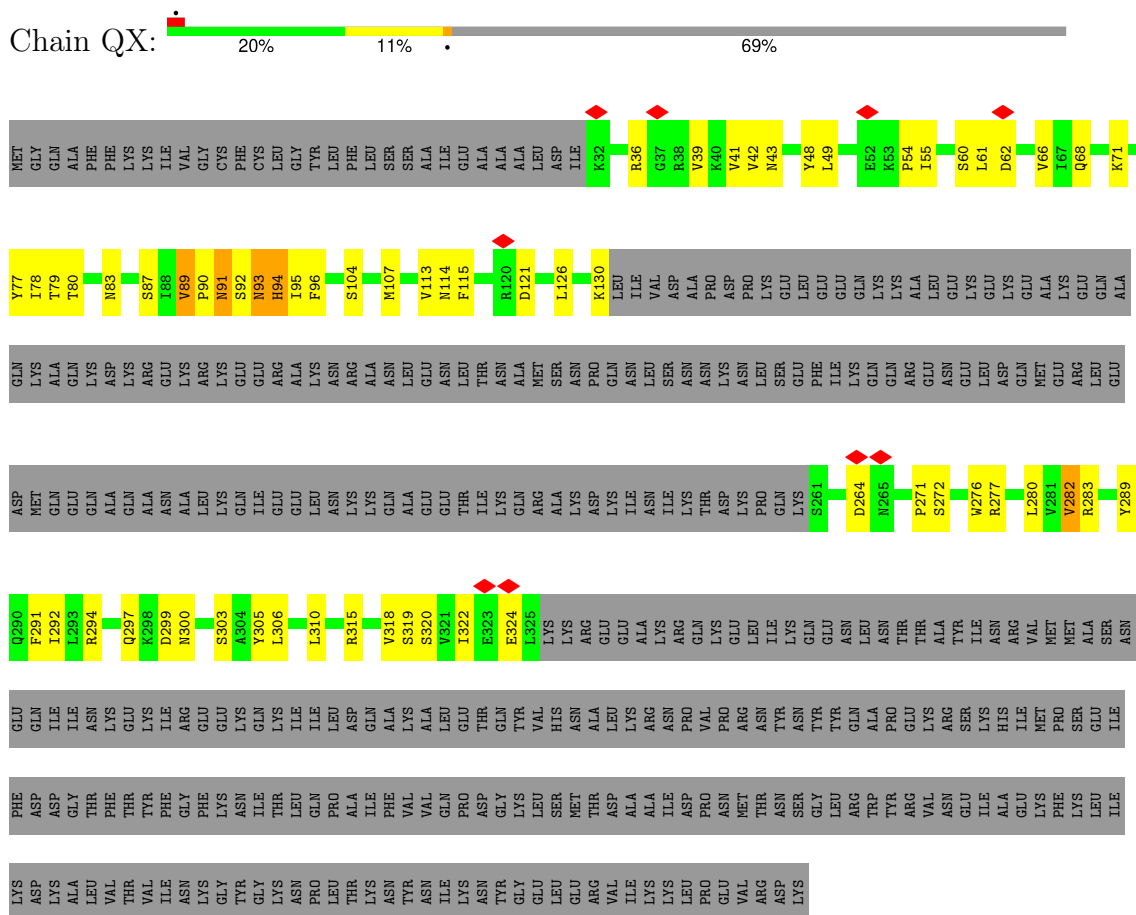


• Molecule 1: Cag pathogenicity island protein (Cag8)





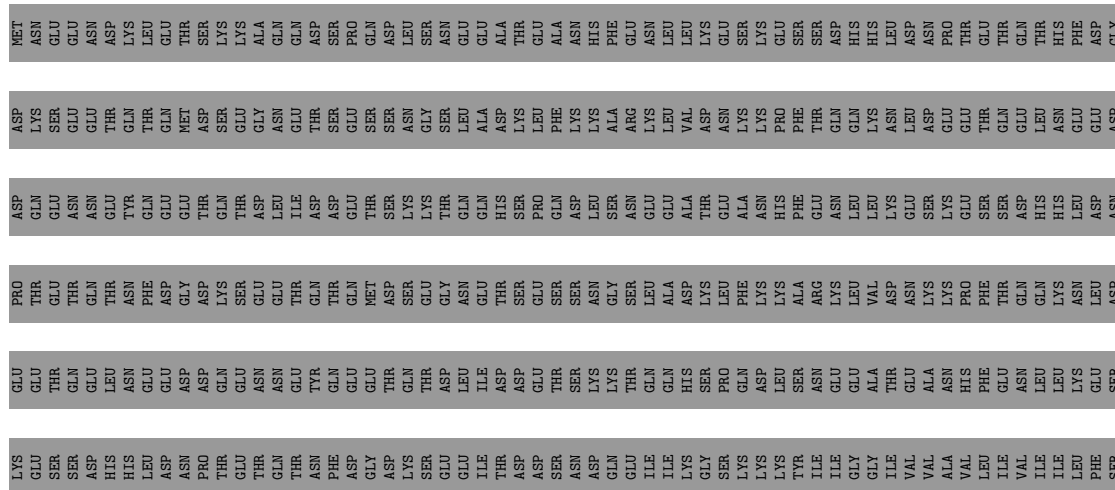
- Molecule 1: Cag pathogenicity island protein (Cag8)



- Molecule 2: Cag pathogenicity island protein (Cag7)











[illegible]

- Molecule 2: Cag pathogenicity island protein (Cag7)

[illegible]





[illegible]

- Molecule 2: Cag pathogenicity island protein (Cag7)

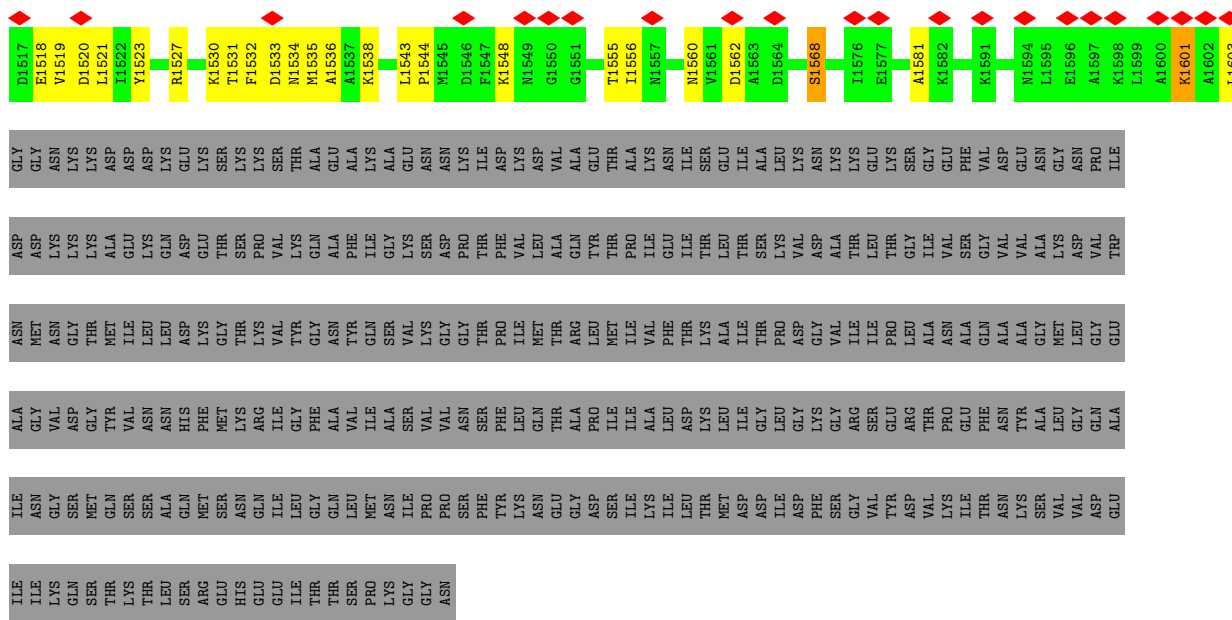
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- Molecule 2: Cag pathogenicity island protein (Cag7)

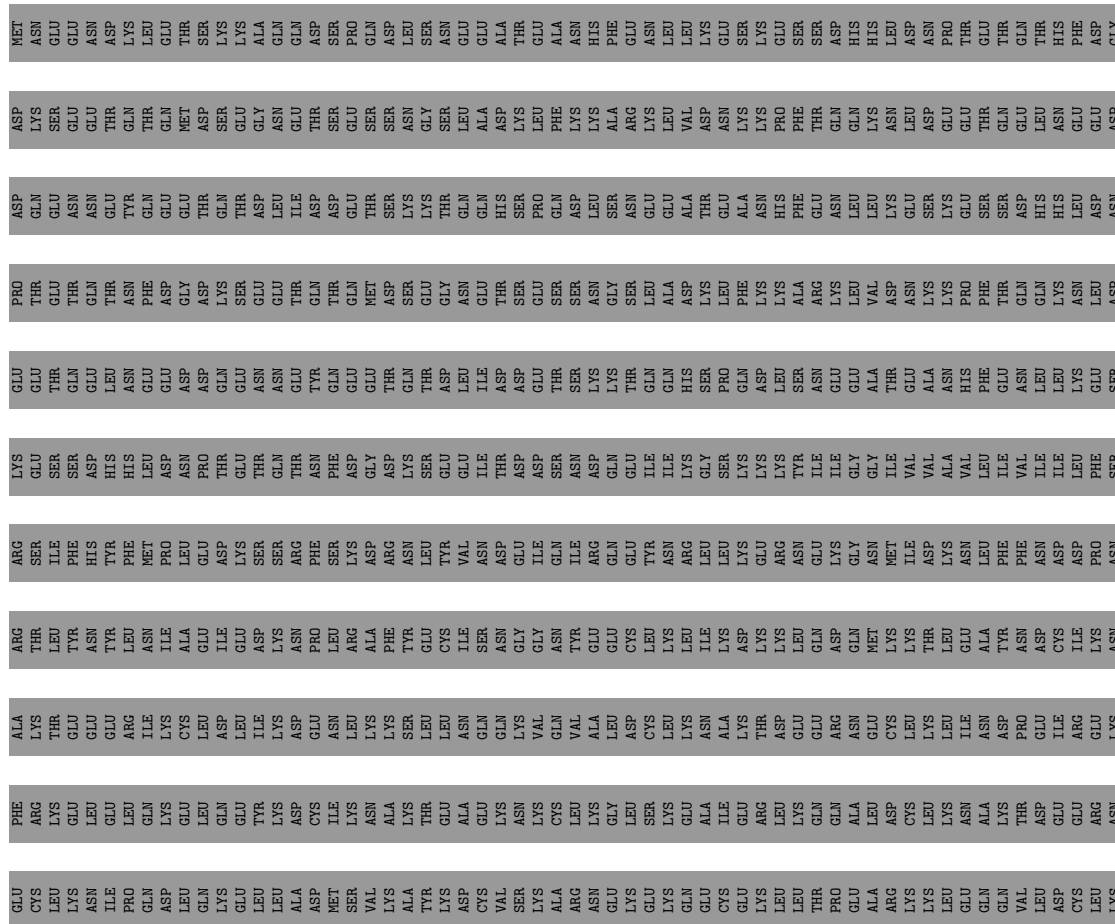
[illegible]







- Molecule 2: Cag pathogenicity island protein (Cag7)





ILE	LYS	GLN	SER	THR	LYS	THR	LEU	SER	ARG	GLU	HIS	GLU	GLU	ILE	THR	THR	SER	PRO	LYS	GLY	GLY	ASN
ASN	GLY	MET	GLN	SER	SER	ALA	MET	ASN	GLN	ILE	GLY	GLY	LEU	MET	ASN	ILE	PRO	PRO	PHE	THR	LYS	ASN

- Molecule 2: Cag pathogenicity island protein (Cag7)

[illegible]

- Molecule 2: Cag pathogenicity island protein (Cag7)



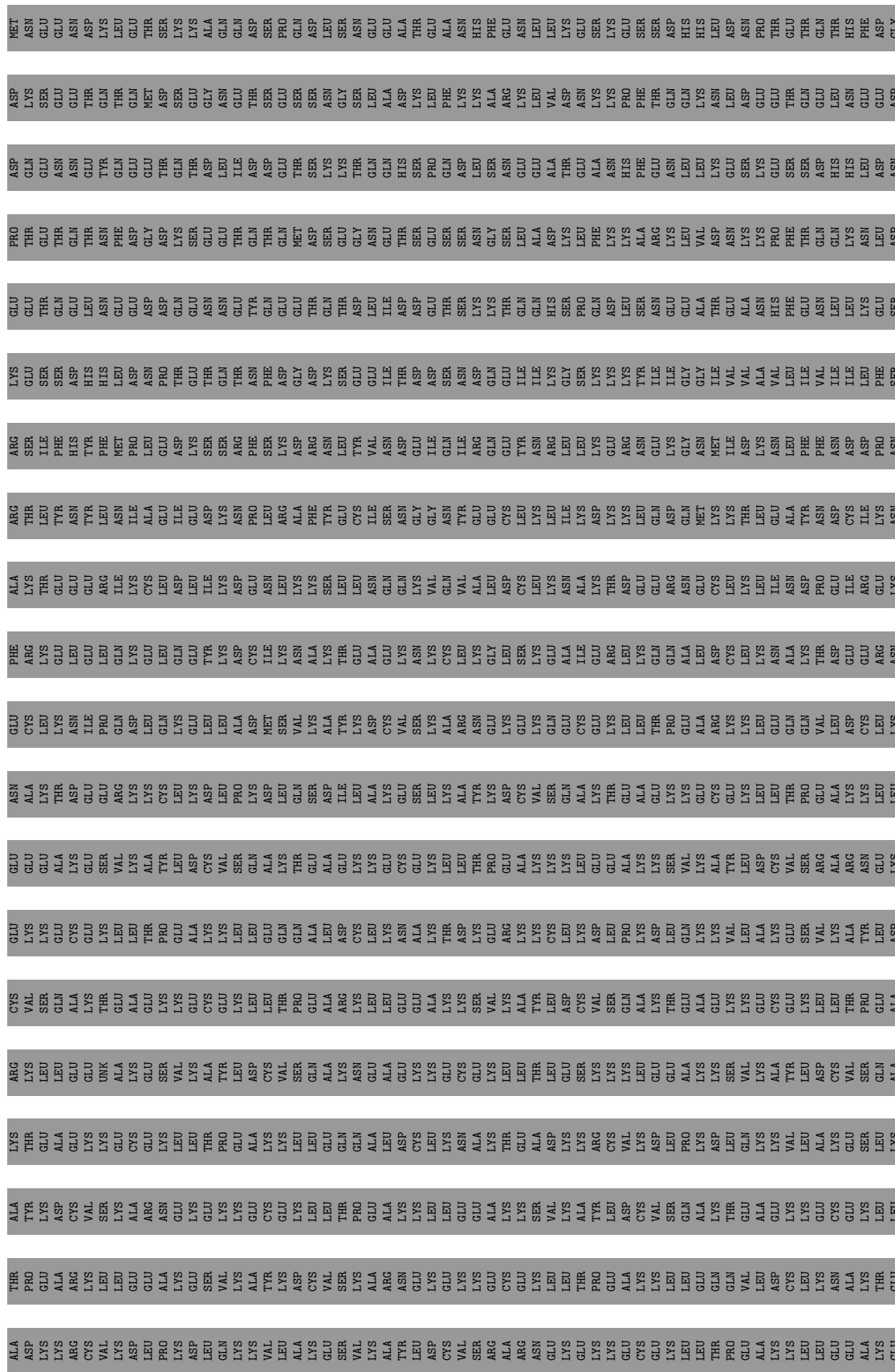


[illegible]

- Molecule 2: Cag pathogenicity island protein (Cag7)

[illegible]

- Molecule 2: Cag pathogenicity island protein (Cag7)



[illegible]







SER	GLN
MET	SER
GLN	THR
LYS	LYS
SER	THR
THR	LEU
ALA	SER
GLN	ARG
MET	GLU
SER	HIS
ASN	GLU
GLN	GLU
ILE	ILE
LEU	THR
GLY	THR
GLN	SER
LEU	PRO
MET	LYS
ASN	GLY
ILE	GLY
PRO	ASN
THR	
SER	
PHE	
TYR	
LYS	
ASN	
GLU	
GLY	
ASP	
ASP	
SER	
ILE	
LYS	
ILE	
LEU	
THR	
THR	
MET	
ASP	
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ILE	
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PHE	
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ASP	
VAL	
LYS	
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LYS	

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GLU
GLU
ILE
THR
THR
SER
PRO
LYS
GLY
GLY
ASN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10477	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	510.0, 510.0, 510.0	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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	AX	0.41	0/1365	0.55	0/1845
1	BX	0.41	0/1365	0.54	0/1845
1	CX	0.40	0/1365	0.54	0/1845
1	DX	0.40	0/1365	0.54	0/1845
1	EX	0.41	0/1365	0.54	0/1845
1	FX	0.40	0/1365	0.54	0/1845
1	GX	0.41	0/1365	0.54	0/1845
1	HX	0.41	0/1365	0.55	0/1845
1	IX	0.40	0/1365	0.54	0/1845
1	JX	0.41	0/1365	0.54	0/1845
1	KX	0.41	0/1365	0.54	0/1845
1	LX	0.41	0/1365	0.54	0/1845
1	MX	0.40	0/1365	0.54	0/1845
1	NX	0.41	0/1365	0.54	0/1845
1	OX	0.41	0/1365	0.54	0/1845
1	PX	0.41	0/1365	0.54	0/1845
1	QX	0.41	0/1365	0.54	0/1845
2	AY	0.32	0/1061	0.48	0/1432
2	BY	0.32	0/1061	0.48	0/1432
2	CY	0.31	0/1061	0.49	0/1432
2	DY	0.32	0/1061	0.49	0/1432
2	EY	0.31	0/1061	0.49	0/1432
2	FY	0.32	0/1061	0.48	0/1432
2	GY	0.32	0/1061	0.51	0/1432
2	HY	0.32	0/1061	0.51	0/1432
2	IY	0.31	0/1061	0.47	0/1432
2	JY	0.32	0/1061	0.50	0/1432
2	KY	0.32	0/1061	0.52	1/1432 (0.1%)
2	LY	0.31	0/1061	0.48	0/1432
2	MY	0.31	0/1061	0.48	0/1432
2	NY	0.31	0/1061	0.51	1/1432 (0.1%)
2	OY	0.31	0/1061	0.49	0/1432
2	PY	0.31	0/1061	0.51	0/1432
2	QY	0.32	0/1061	0.50	0/1432

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.37	0/41242	0.52	2/55709 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	KY	1521	LEU	CA-CB-CG	6.10	129.33	115.30
2	NY	1521	LEU	CA-CB-CG	5.59	128.16	115.30

There are no chirality outliers.

There are no planarity outliers.

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	AX	1339	0	1355	40	0
1	BX	1339	0	1355	43	0
1	CX	1339	0	1355	42	0
1	DX	1339	0	1355	40	0
1	EX	1339	0	1355	44	0
1	FX	1339	0	1355	43	0
1	GX	1339	0	1355	42	0
1	HX	1339	0	1355	42	0
1	IX	1339	0	1355	37	0
1	JX	1339	0	1355	42	0
1	KX	1339	0	1355	49	0
1	LX	1339	0	1355	46	0
1	MX	1339	0	1355	35	0
1	NX	1339	0	1355	43	0
1	OX	1339	0	1355	45	0
1	PX	1339	0	1355	41	0
1	QX	1339	0	1355	42	0
2	AY	1050	0	1038	26	0
2	BY	1050	0	1038	31	0
2	CY	1050	0	1038	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	DY	1050	0	1038	28	0
2	EY	1050	0	1038	27	0
2	FY	1050	0	1038	22	0
2	GY	1050	0	1038	25	0
2	HY	1050	0	1038	27	0
2	IY	1050	0	1038	28	0
2	JY	1050	0	1038	28	0
2	KY	1050	0	1038	31	0
2	LY	1050	0	1038	21	0
2	MY	1050	0	1038	29	0
2	NY	1050	0	1038	31	0
2	OY	1050	0	1038	26	0
2	PY	1050	0	1038	27	0
2	QY	1050	0	1038	24	0
All	All	40613	0	40681	925	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 11.

The worst 5 of 925 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:BX:126:LEU:O	1:BX:130:LYS:HB2	1.66	0.95
1:AX:126:LEU:O	1:AX:130:LYS:HB2	1.66	0.94
1:KX:126:LEU:O	1:KX:130:LYS:HB2	1.67	0.94
1:IX:126:LEU:O	1:IX:130:LYS:HB2	1.68	0.93
1:HX:126:LEU:O	1:HX:130:LYS:HB2	1.68	0.93

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	AX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	BX	160/521 (31%)	156 (98%)	4 (2%)	0	100	100
1	CX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	DX	160/521 (31%)	155 (97%)	5 (3%)	0	100	100
1	EX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	FX	160/521 (31%)	153 (96%)	7 (4%)	0	100	100
1	GX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	HX	160/521 (31%)	155 (97%)	5 (3%)	0	100	100
1	IX	160/521 (31%)	153 (96%)	7 (4%)	0	100	100
1	JX	160/521 (31%)	155 (97%)	5 (3%)	0	100	100
1	KX	160/521 (31%)	155 (97%)	5 (3%)	0	100	100
1	LX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	MX	160/521 (31%)	155 (97%)	5 (3%)	0	100	100
1	NX	160/521 (31%)	155 (97%)	5 (3%)	0	100	100
1	OX	160/521 (31%)	153 (96%)	7 (4%)	0	100	100
1	PX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	QX	160/521 (31%)	153 (96%)	7 (4%)	0	100	100
2	AY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100
2	BY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	CY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	DY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	EY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	FY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	GY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	HY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100
2	IY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	JY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	KY	133/1927 (7%)	129 (97%)	4 (3%)	0	100	100
2	LY	133/1927 (7%)	129 (97%)	4 (3%)	0	100	100
2	MY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	NY	133/1927 (7%)	129 (97%)	4 (3%)	0	100	100
2	OY	133/1927 (7%)	129 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	PY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	QY	133/1927 (7%)	129 (97%)	4 (3%)	0	100	100
All	All	4981/41616 (12%)	4801 (96%)	180 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AX	152/469 (32%)	134 (88%)	18 (12%)	4	19
1	BX	152/469 (32%)	137 (90%)	15 (10%)	6	26
1	CX	152/469 (32%)	137 (90%)	15 (10%)	6	26
1	DX	152/469 (32%)	136 (90%)	16 (10%)	5	23
1	EX	152/469 (32%)	137 (90%)	15 (10%)	6	26
1	FX	152/469 (32%)	133 (88%)	19 (12%)	3	17
1	GX	152/469 (32%)	134 (88%)	18 (12%)	4	19
1	HX	152/469 (32%)	135 (89%)	17 (11%)	5	21
1	IX	152/469 (32%)	135 (89%)	17 (11%)	5	21
1	JX	152/469 (32%)	136 (90%)	16 (10%)	5	23
1	KX	152/469 (32%)	135 (89%)	17 (11%)	5	21
1	LX	152/469 (32%)	134 (88%)	18 (12%)	4	19
1	MX	152/469 (32%)	137 (90%)	15 (10%)	6	26
1	NX	152/469 (32%)	137 (90%)	15 (10%)	6	26
1	OX	152/469 (32%)	134 (88%)	18 (12%)	4	19
1	PX	152/469 (32%)	134 (88%)	18 (12%)	4	19
1	QX	152/469 (32%)	136 (90%)	16 (10%)	5	23
2	AY	115/1724 (7%)	102 (89%)	13 (11%)	4	21
2	BY	115/1724 (7%)	100 (87%)	15 (13%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	CY	115/1724 (7%)	103 (90%)	12 (10%)	5	23
2	DY	115/1724 (7%)	103 (90%)	12 (10%)	5	23
2	EY	115/1724 (7%)	103 (90%)	12 (10%)	5	23
2	FY	115/1724 (7%)	100 (87%)	15 (13%)	3	16
2	GY	115/1724 (7%)	100 (87%)	15 (13%)	3	16
2	HY	115/1724 (7%)	104 (90%)	11 (10%)	7	27
2	IY	115/1724 (7%)	103 (90%)	12 (10%)	5	23
2	JY	115/1724 (7%)	105 (91%)	10 (9%)	8	32
2	KY	115/1724 (7%)	103 (90%)	12 (10%)	5	23
2	LY	115/1724 (7%)	106 (92%)	9 (8%)	10	36
2	MY	115/1724 (7%)	104 (90%)	11 (10%)	7	27
2	NY	115/1724 (7%)	106 (92%)	9 (8%)	10	36
2	OY	115/1724 (7%)	102 (89%)	13 (11%)	4	21
2	PY	115/1724 (7%)	107 (93%)	8 (7%)	12	41
2	QY	115/1724 (7%)	102 (89%)	13 (11%)	4	21
All	All	4539/37281 (12%)	4054 (89%)	485 (11%)	8	22

5 of 485 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	OX	32	LYS
2	NY	1481	CYS
2	AY	1503	ASP
2	MY	1555	THR
2	QY	1481	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
2	FY	1549	ASN
2	PY	1476	HIS
2	HY	1583	GLN
2	OY	1594	ASN
2	QY	1549	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

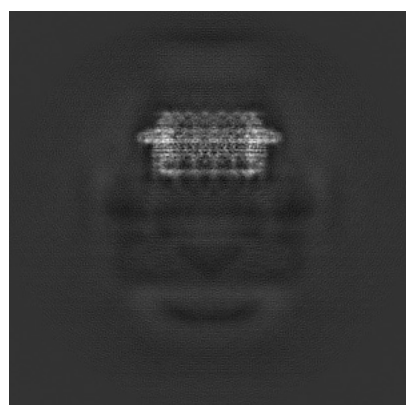
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22077. These allow visual inspection of the internal detail of the map and identification of artifacts.

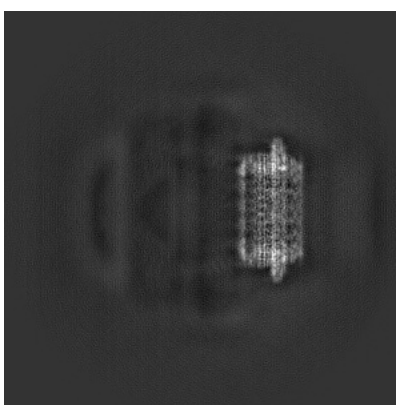
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

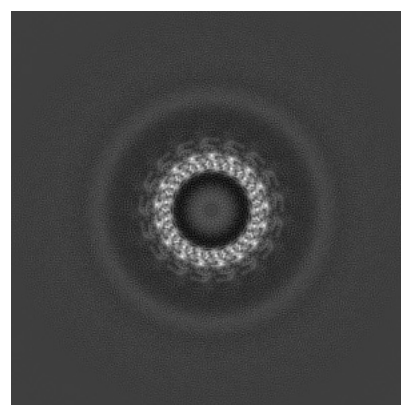
6.1.1 Primary map



X



Y

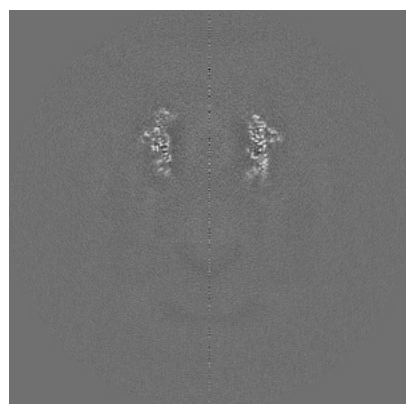


Z

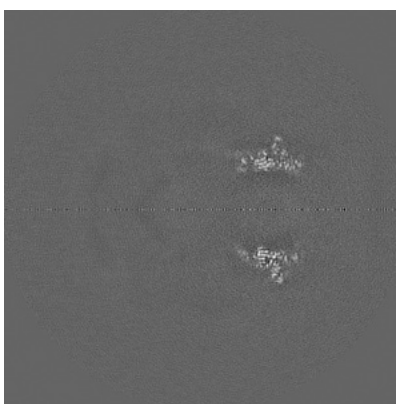
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

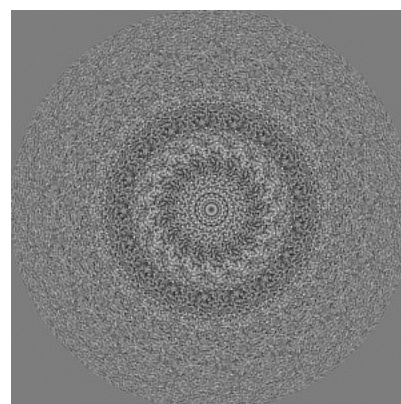
6.2.1 Primary map



X Index: 255



Y Index: 255



Z Index: 255

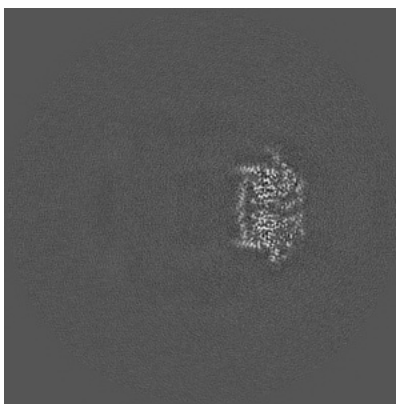
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

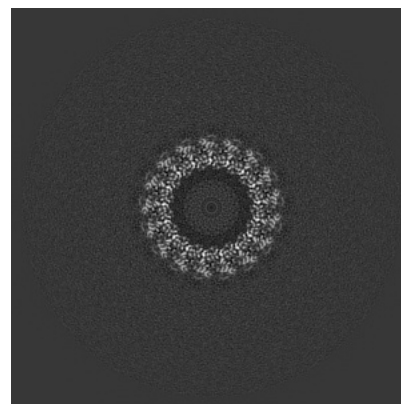
6.3.1 Primary map



X Index: 309



Y Index: 307

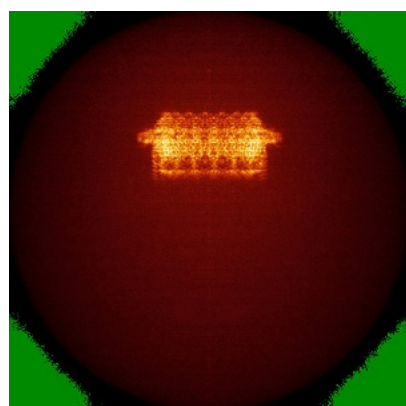


Z Index: 342

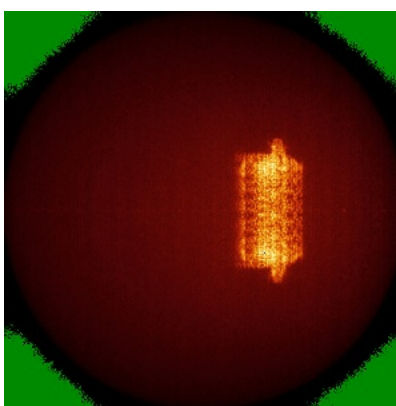
The images above show the largest variance slices of the map in three orthogonal directions.

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

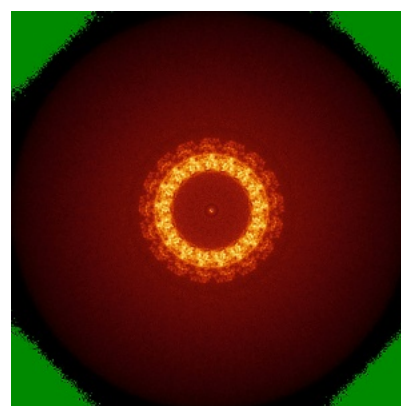
6.4.1 Primary map



X



Y

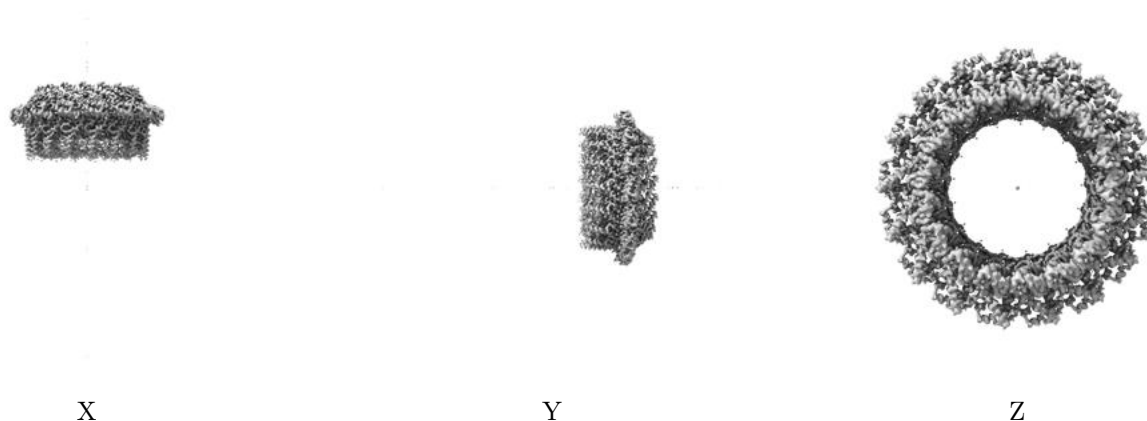


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

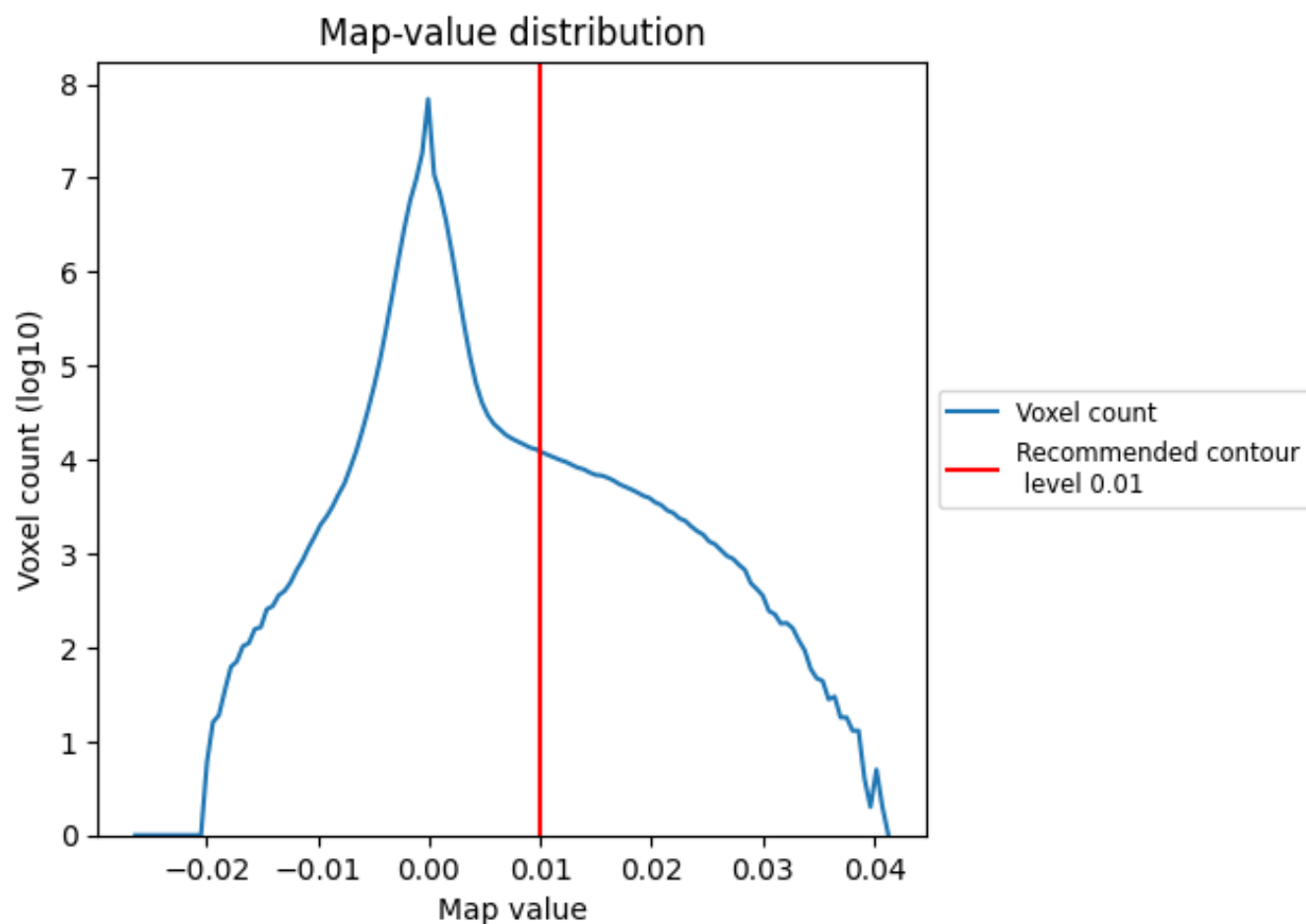
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

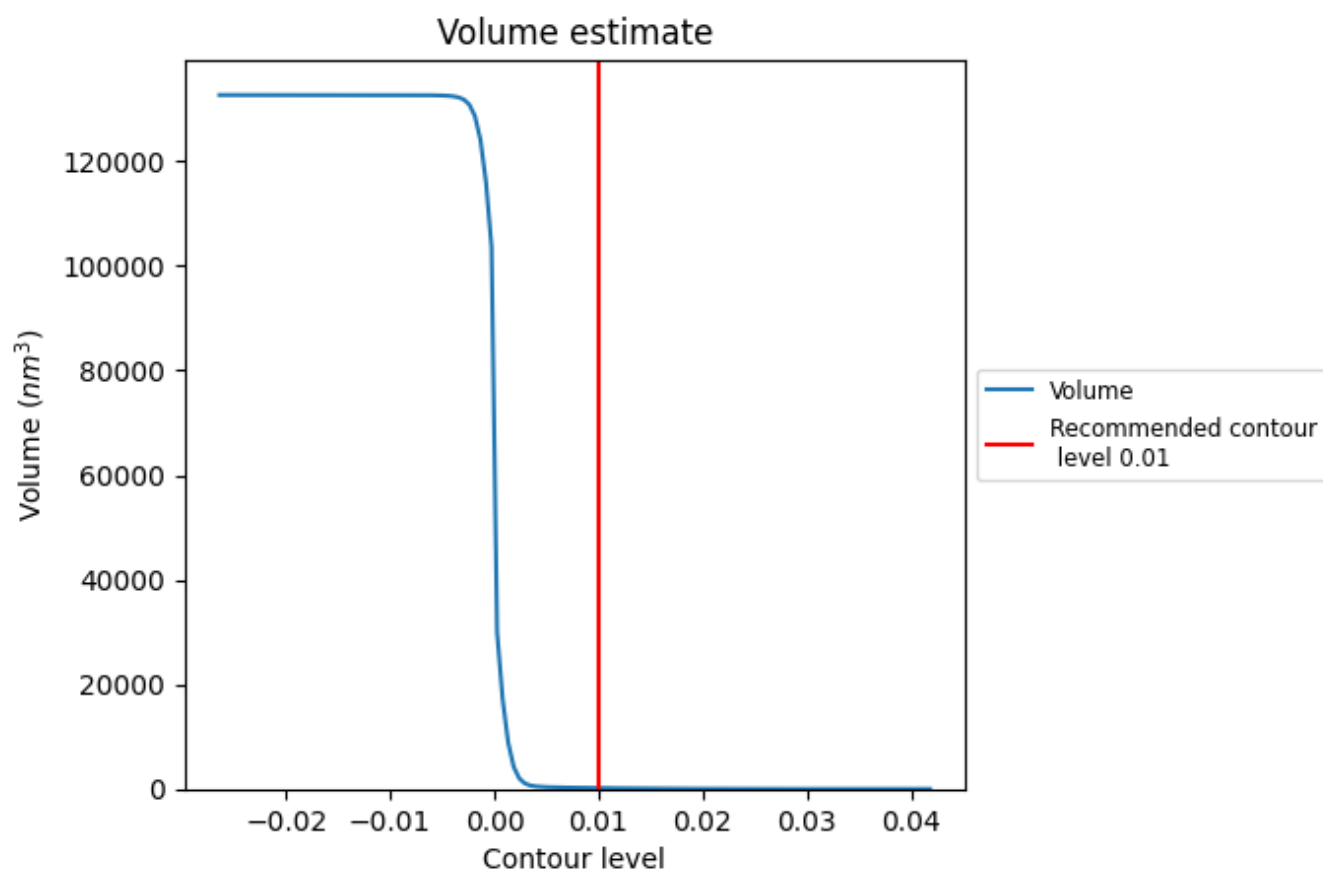
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

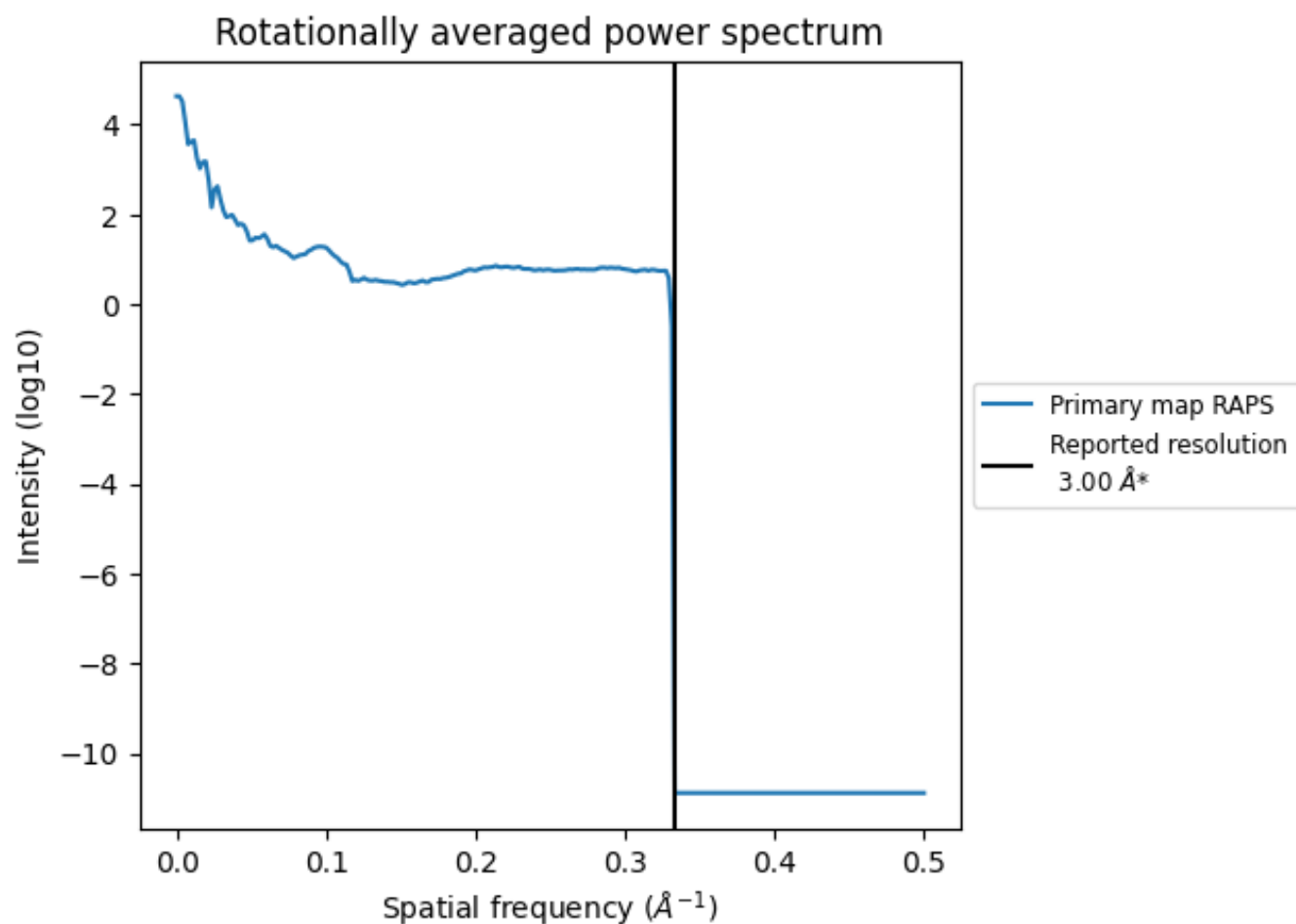
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 175 nm³; this corresponds to an approximate mass of 158 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

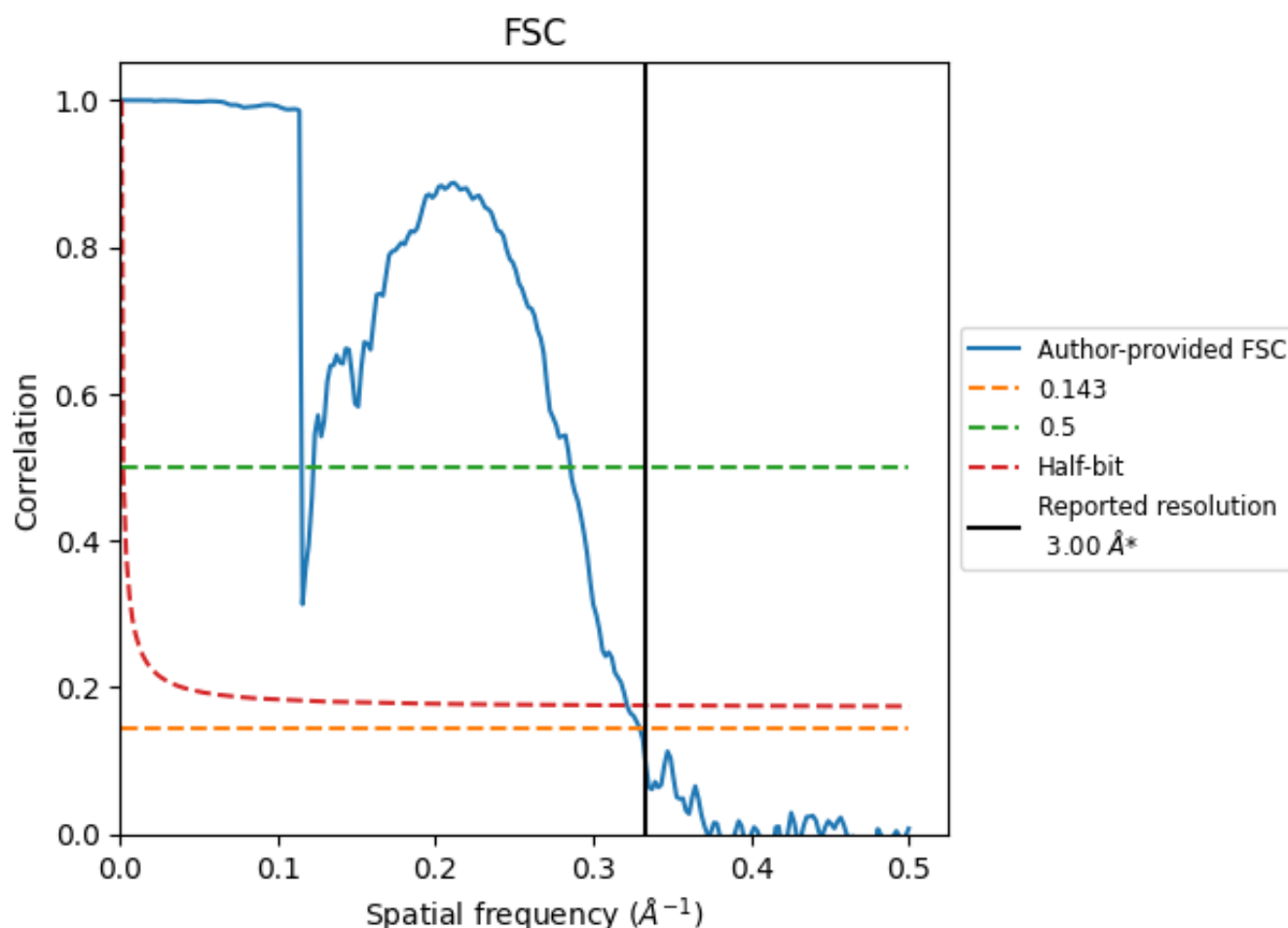


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

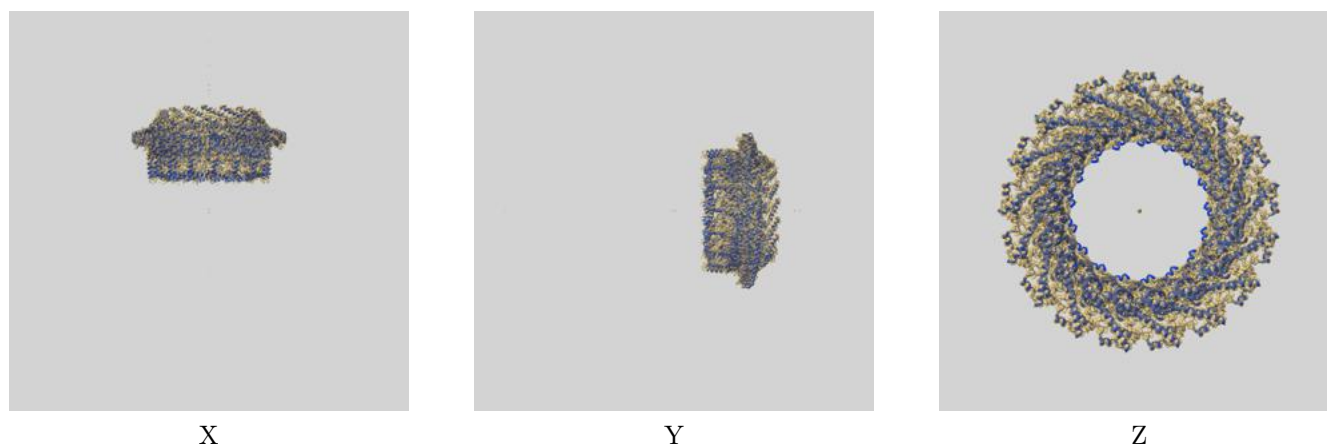
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.03	8.69	3.11
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

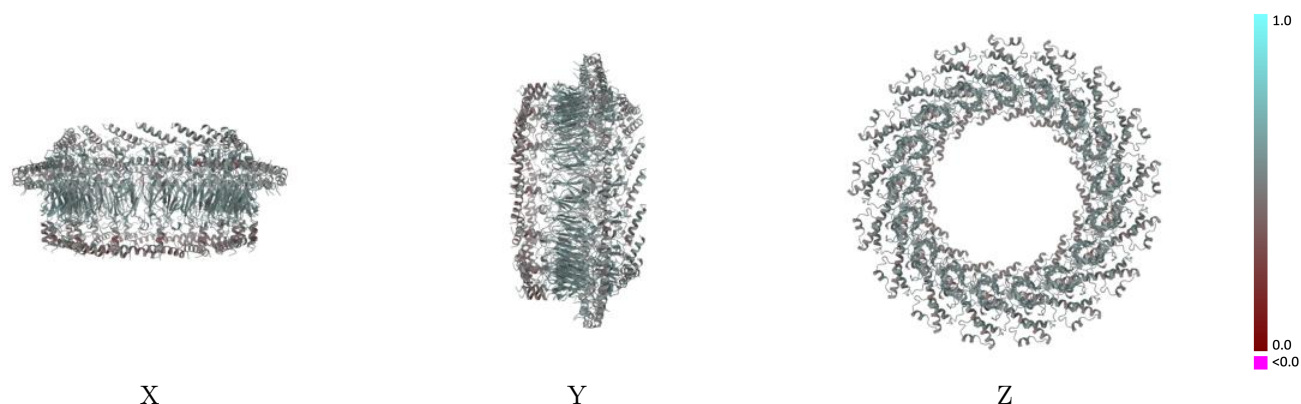
This section contains information regarding the fit between EMDB map EMD-22077 and PDB model 6X6L. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



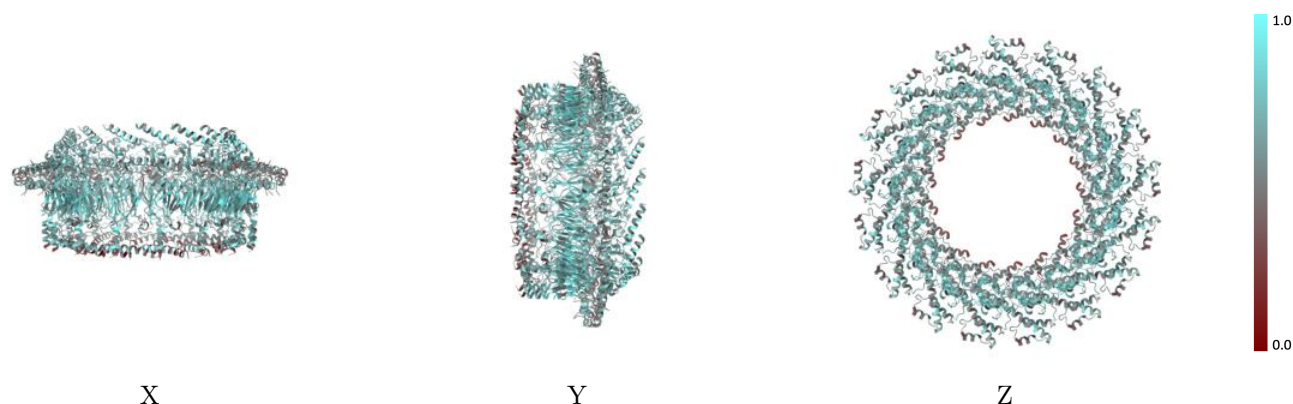
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



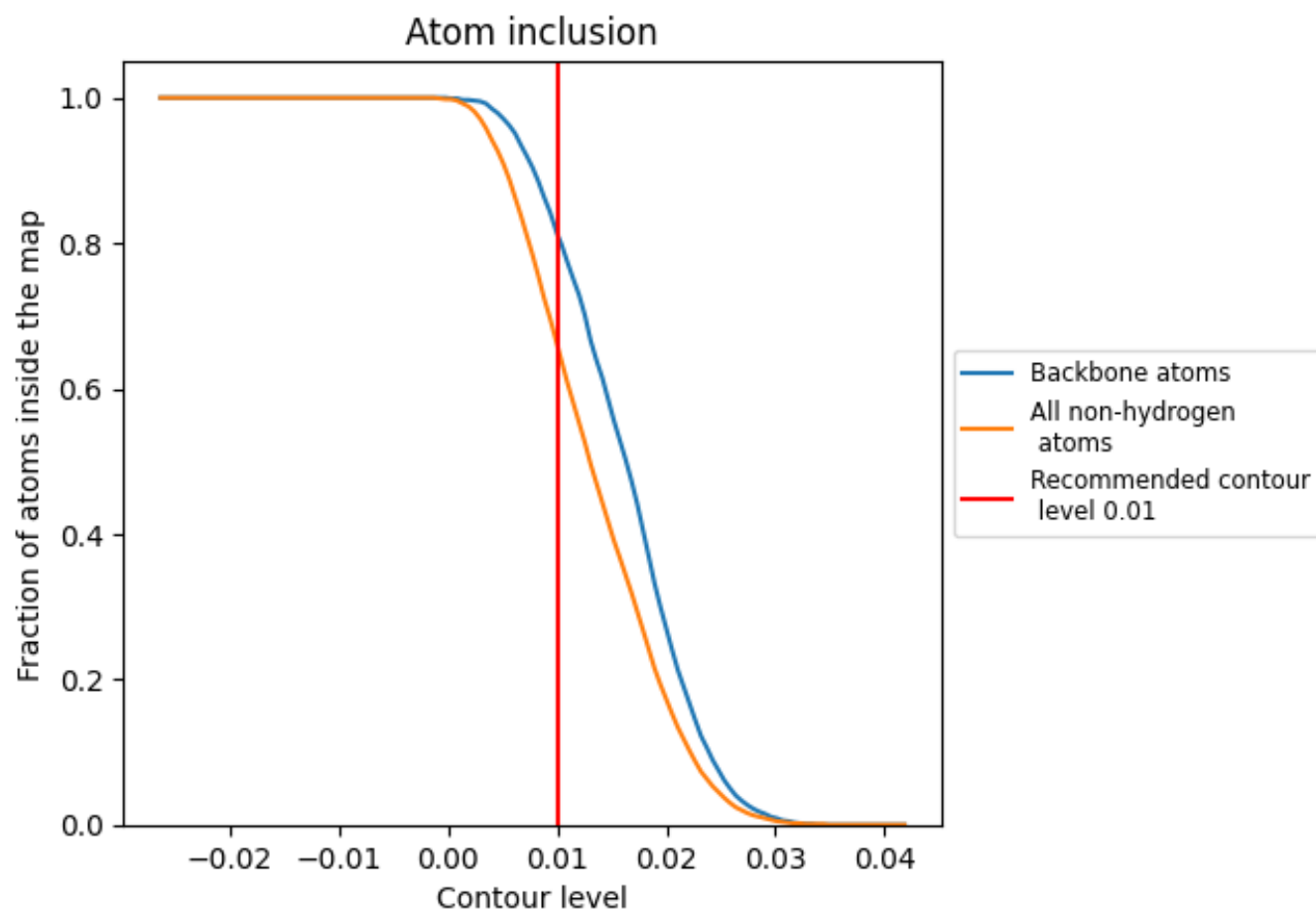
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6590	 0.5180
AX	 0.7300	 0.5370
AY	 0.5760	 0.4950
BX	 0.7260	 0.5360
BY	 0.5740	 0.4950
CX	 0.7260	 0.5370
CY	 0.5720	 0.4940
DX	 0.7230	 0.5340
DY	 0.5760	 0.4950
EX	 0.7240	 0.5360
EY	 0.5780	 0.4920
FX	 0.7300	 0.5340
FY	 0.5710	 0.4930
GX	 0.7180	 0.5330
GY	 0.5720	 0.4920
HX	 0.7270	 0.5340
HY	 0.5840	 0.4940
IX	 0.7250	 0.5350
IY	 0.5680	 0.4940
JX	 0.7290	 0.5360
JY	 0.5700	 0.4950
KX	 0.7240	 0.5370
KY	 0.5730	 0.4940
LX	 0.7290	 0.5360
LY	 0.5720	 0.4930
MX	 0.7240	 0.5370
MY	 0.5740	 0.4940
NX	 0.7240	 0.5390
NY	 0.5730	 0.4950
OX	 0.7300	 0.5400
OY	 0.5740	 0.4960
PX	 0.7270	 0.5380
PY	 0.5800	 0.4940
QX	 0.7260	 0.5380
QY	 0.5730	 0.4950

