



wwPDB EM Validation Summary Report ⓘ

Jun 8, 2026 – 04:19 PM JST

PDB ID : 9VGU / pdb_00009vgu
EMDB ID : EMD-65051
Title : Cryo-EM structure of CagX-CagY complex with C16 symmetry
Authors : Mok, C.Y.; Chu, H.Y.; Au, S.W.N.
Deposited on : 2025-06-15
Resolution : 2.87 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.dev132
MolProbity : 4-5-2 with Phenix2.0
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) : 2.49

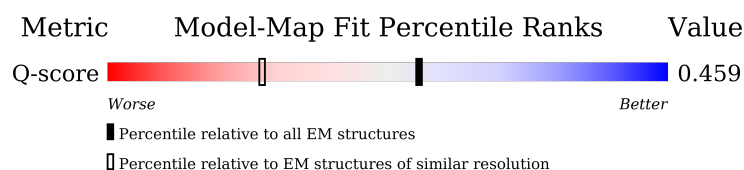
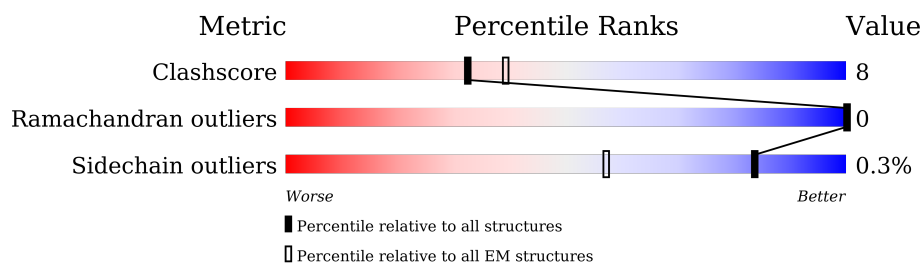
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.87 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.








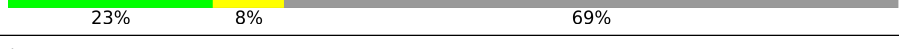

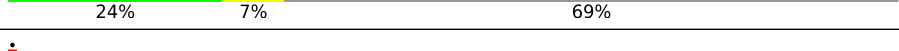
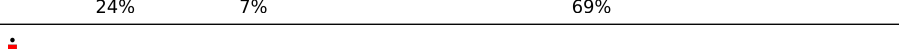
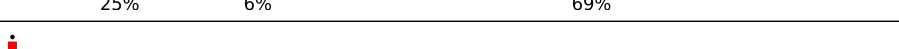















Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12062 (2.37 - 3.37)

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	495	
1	BX	495	
1	CX	495	
1	DX	495	

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Mol	Chain	Length	Quality of chain
1	EX	495	
1	FX	495	
1	GX	495	
1	HX	495	
1	IX	495	
1	JX	495	
1	KX	495	
1	LX	495	
1	MX	495	
1	NX	495	
1	OX	495	
1	PX	495	
2	AY	441	
2	BY	441	
2	CY	441	
2	DY	441	
2	EY	441	
2	FY	441	
2	GY	441	
2	HY	441	
2	IY	441	
2	JY	441	
2	KY	441	
2	LY	441	
2	MY	441	

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Mol	Chain	Length	Quality of chain
2	NY	441	<div><div><div></div><div></div><div></div></div><div>15% . 83%</div></div>
2	OY	441	<div><div><div></div><div></div><div></div></div><div>15% . 83%</div></div>
2	PY	441	<div><div><div></div><div></div><div></div></div><div>14% . 83%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 58955 atoms, of which 29419 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 X.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	AX	153	Total	C	H	N	O	S	0	0
			2488	794	1243	213	236	2		
1	BX	153	Total	C	H	N	O	S	0	0
			2493	794	1248	213	236	2		
1	CX	153	Total	C	H	N	O	S	0	0
			2493	794	1248	213	236	2		
1	EX	153	Total	C	H	N	O	S	0	0
			2493	794	1248	213	236	2		
1	DX	153	Total	C	H	N	O	S	0	0
			2493	794	1248	213	236	2		
1	FX	153	Total	C	H	N	O	S	0	0
			2493	794	1248	213	236	2		
1	GX	153	Total	C	H	N	O	S	0	0
			2493	794	1248	213	236	2		
1	HX	153	Total	C	H	N	O	S	0	0
			2493	794	1248	213	236	2		
1	IX	153	Total	C	H	N	O	S	0	0
			2493	794	1248	213	236	2		
1	JX	153	Total	C	H	N	O	S	0	0
			2493	794	1248	213	236	2		
1	KX	153	Total	C	H	N	O	S	0	0
			2493	794	1248	213	236	2		
1	LX	153	Total	C	H	N	O	S	0	0
			2493	794	1248	213	236	2		
1	MX	153	Total	C	H	N	O	S	0	0
			2493	794	1248	213	236	2		
1	NX	153	Total	C	H	N	O	S	0	0
			2493	794	1248	213	236	2		
1	OX	153	Total	C	H	N	O	S	0	0
			2493	794	1248	213	236	2		
1	PX	153	Total	C	H	N	O	S	0	0
			2493	794	1248	213	236	2		

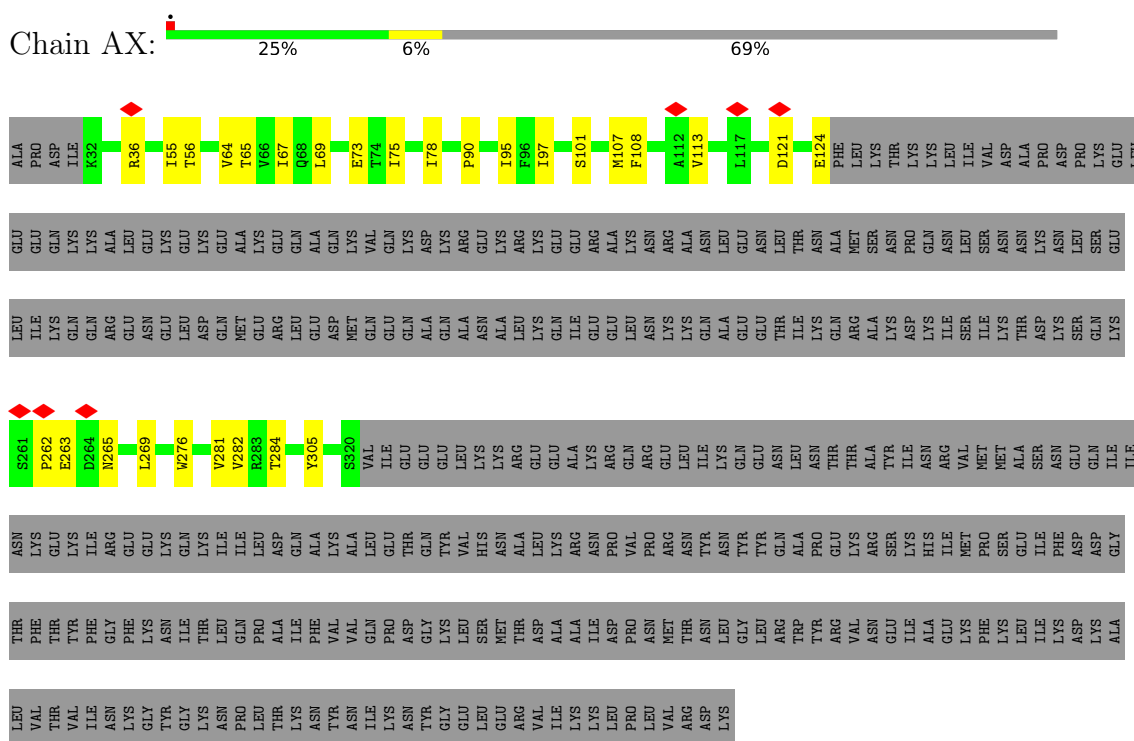
- Molecule 2 is a protein called Type IV secretion system apparatus protein CagY.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	AY	76	Total	C	H	N	O	S	0	0
			1192	369	591	104	125	3		
2	BY	76	Total	C	H	N	O	S	0	0
			1192	369	591	104	125	3		
2	CY	76	Total	C	H	N	O	S	0	0
			1192	369	591	104	125	3		
2	EY	76	Total	C	H	N	O	S	0	0
			1192	369	591	104	125	3		
2	DY	76	Total	C	H	N	O	S	0	0
			1192	369	591	104	125	3		
2	FY	76	Total	C	H	N	O	S	0	0
			1192	369	591	104	125	3		
2	GY	76	Total	C	H	N	O	S	0	0
			1192	369	591	104	125	3		
2	HY	76	Total	C	H	N	O	S	0	0
			1192	369	591	104	125	3		
2	IY	76	Total	C	H	N	O	S	0	0
			1192	369	591	104	125	3		
2	JY	76	Total	C	H	N	O	S	0	0
			1192	369	591	104	125	3		
2	KY	76	Total	C	H	N	O	S	0	0
			1192	369	591	104	125	3		
2	LY	76	Total	C	H	N	O	S	0	0
			1192	369	591	104	125	3		
2	MY	76	Total	C	H	N	O	S	0	0
			1192	369	591	104	125	3		
2	NY	76	Total	C	H	N	O	S	0	0
			1192	369	591	104	125	3		
2	OY	76	Total	C	H	N	O	S	0	0
			1192	369	591	104	125	3		
2	PY	76	Total	C	H	N	O	S	0	0
			1192	369	591	104	125	3		

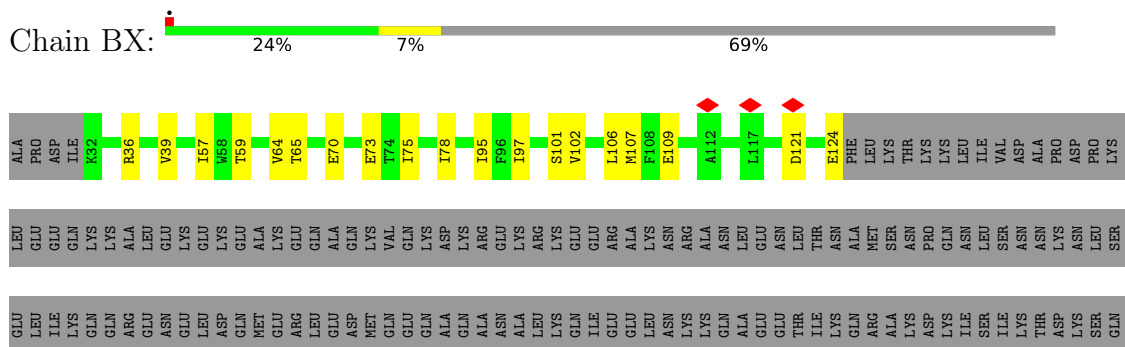
3 Residue-property plots [i](#)

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: Cag pathogenicity island protein X



- Molecule 1: Cag pathogenicity island protein X



[illegible]

- Molecule 1: Cag pathogenicity island protein X

[illegible]

- Molecule 1: Cag pathogenicity island protein X

[illegible]

GLY	LEU	ARG	TRP	TYR	ARG	VAL	ASN	GLU	ILE	ALA	GLY	LYS	LYS	PHE	LYS	LEU	ILE	LYS	ASP	ASN	ALA	LEU	VAL	THR	VAL	ILE	ASN	GLY	LYS	TYR	THR	LEU	PRO	ASN	LEU	THR	LYS	ASN	TYR	ILE	LYS	ASN	GLY	GLY	LEU	LEU	ARG	VAL	ILE	LYS	LYS	LYS	LEU	PRO	LEU	VAL	ARG	ASP	LYS
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- Molecule 1: Cag pathogenicity island protein X

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GLU LEU GLU LEU GLN GLN LYS LYS ALA ALA LEU LEU LYS GLU LYS GLU LYS LYS ASP ASP LYS LYS ARG ARG LYS LYS ARG LYS ASN ASN ALA ALA ARG ARG ASN ASN LEU LEU GLU GLU LEU LEU THR THR ASN ASN ALA ALA SER SER ASN ASN PRO PRO GLN GLN ASN ASN LEU LEU SER SER ASN ASN LYS LYS LYS LYS

SER	GLU	LEU	ILE	LYS	GLN	GLN	ARG	GLU	ASN	GLU	LEU	ASP	GLN	MET	GLU	ARG	LEU	GLU	ASP	MET	GLN	GLU	GLN	ALA	ALA	ALA	ALA	LEU	LYS	LYS	LYS	GLN	ALA	GLU	GLU	THR	ILE	LYS	GLN	ARG	ALA	LYS	ASP	LYS	ILE	ILE	SER	ILE	LYS	THR	ASP	LYS	LYS	FRP
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GLN	LYS	S261	P282	E263	D264	L269	S272	V282	R283	T284	R294	T295	A296	N300	F301	Y305	L306	T307	Y312	P313	Q314	R315	H316	S320	VAL	ILE	GLU	GLU	GLU	LEU	LYS	LYS	LYS	ARG	ARG	GLU	GLU	GLU	ALA	LYS	ARG	GLN	GLN	GLU	ASN	LEU	LEU	ASN	THR
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ALA	TYR	ILE	ASN	ARG	VAL	MET	ALA	ALA	SER	ASN	GLU	GLN	ILE	ILE	ASN	LYS	GLU	LYS	ILE	ILE	ARG	GLU	GLU	LYS	GLN	GLN	LYS	ILE	ILE	LEU	ASP	GLN	ALA	ALA	LYS	ALA	ALA	LEU	LEU	THR	GLU	GLN	TYR	TYR	VAL	HIS	ASN	ASN	ALA	LEU	LYS	ARG	ASN	PRO	VAL	PRO	PRO	ARG	ASN	TYR	ASN	TYR	GLN	ALA	ALA	PRO	THR
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LYS ARG SER LYS HIS ILE MET PRO GLU ILE PHE ASP ASP GLY THR PHE THR TYR PHE PHE PHE LYS ASN ILE LEU THR LEU GLN PRO ALA ILE PHE VAL VAL GLN PRO ASP GLY LYS LEU SER MET THR ASP ALA ALA ILE ASP PRO ASN MET THR ASN LEU GLY LEU ARG TRP TYR ARG

VAL	ASN	GLU	ILE	ALA	GLU	LYS	PHE	LEU	LEU	ILE	LYS	ASP	LYS	ALA	LEU	VAL	THR	VAL	ILE	ASN	LYS	GLY	TYR	GLY	GLY	ASN	ASN	PRO	PRO	LEU	THR	LYS	ASN	TYR	ASN	GLY	GLU	LEU	GLU	ARG	VAL	ILE	LYS	LYS	LEU	PRO	LEU	VAL	ARG	ASP	ILE
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- Molecule 1: Cag pathogenicity island protein X



ALA	ASP	K32	I46	L49	D51	I55	T56	L61	V64	V66	I67	E73	T74	I75	I78	I79	T80	N83	L95	P96	I97	S101	V102	M105	L106	M107	F108	E109	A112	V113	L117	D121	E124	PHE	LEU	LEU	THR	LVS	LVS
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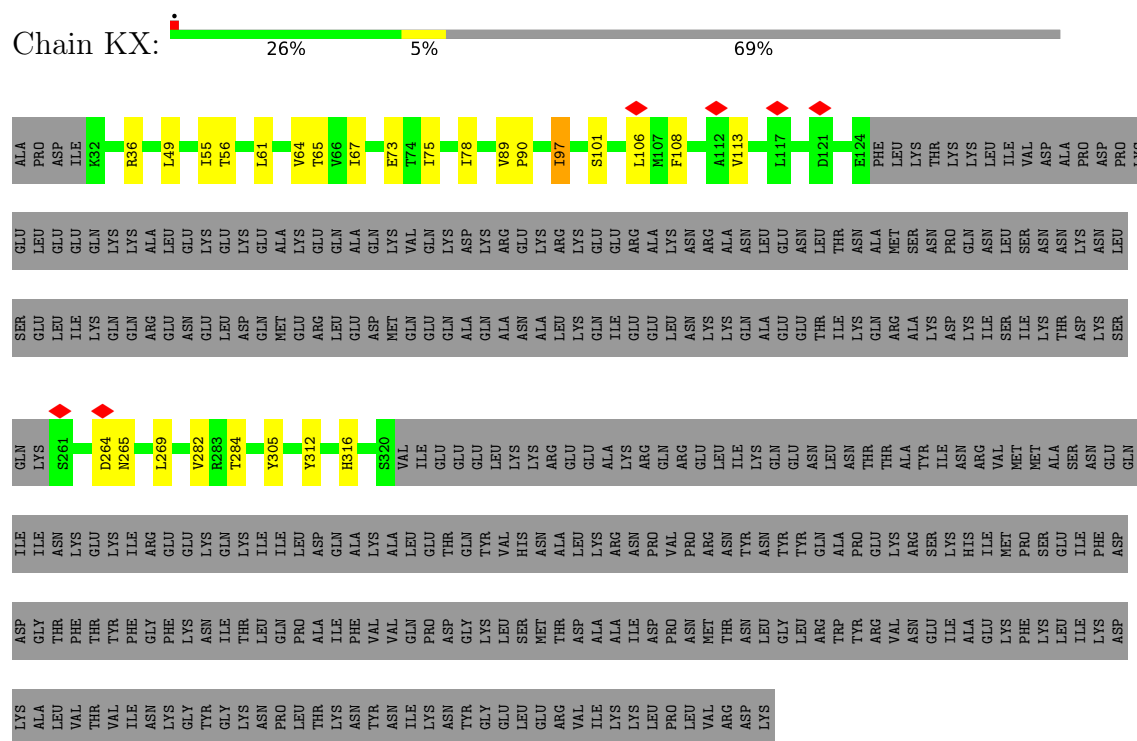
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ASN	LEU	SER	ASN	ASN	LYS	ASN	LEU	SER	GLU	LEU	ILE	LYS	GLN	ARG	ASN	GLU	LEU	ASP	GLN	MET	GLU	ARG	LEU	GLY	LEU	ASP	MET	GLN	GLU	GLN	ALA	ALA	ALA	ASN	ALA	LYS	LEU	GLN	LYS	ILE	ILE	GLU	GLU	LEU	ASN	LYS	GLN	ARG	ALA	LYS	ASP	ASP
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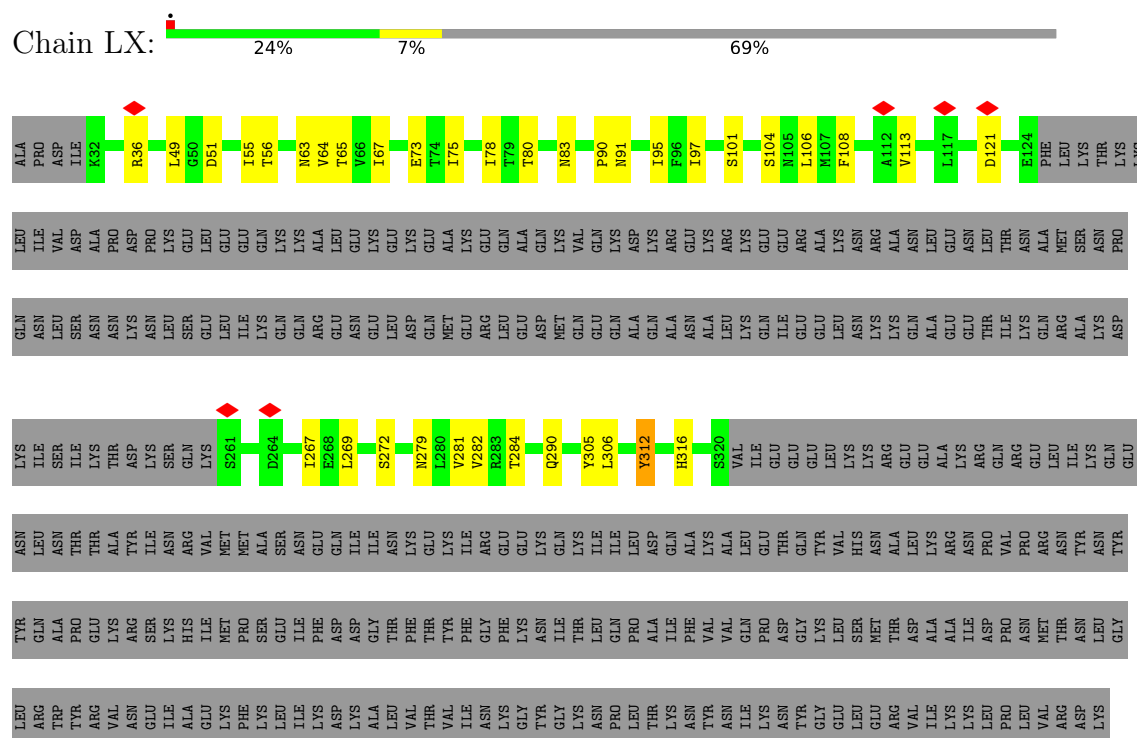
ILE	ILE	ILE	LYS	THR	ASP	LYS	SER	SER	GLN	GLY	S261	S262	E263	D264	N265	L269	S272	W276	V282	R283	T284	L288	V289	Q290	Y305	E311	Y312	H316	S320	VAL	ILE	GLU	GLU	GLU	LEU	LYS	LYS	ARG	GLU	GLU	ALA	LYS	ARG	GLN	ARG	GLU	LEU	ILE	LYS	LYS	GLN	GLU
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ASN	LEU	ASN	THR	THR	ALA	TYR	ILE	ASN	ARG	VAL	MET	MET	ALA	ASN	SER	GLY	GLN	ILE	ILE	ASN	LYS	GLY	ILE	ARG	GLU	GLU	LYS	GLN	LYS	ILE	ILE	THR	GLN	VAL	ASN	LEU	LYS	ALA	ASN	ARG	PRO	ASN	TYR	ASN	TYR
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TTR	GLN	ALA	PRO	GLU	GLY	LYS	ARG	SER	SER	HIS	ILE	ILE	MET	PRO	SER	GLU	ILE	ASP	ASP	PHE	ASP	GLY	PHE	LYS	ASN	ILE	THR	GLN	PRO	ALA	ILE	PHE	VAL	VAL	GLN	PRO	ASP	GLY	LYS	LYS	LEU	SER	MET	THR	ASP	ALA	ALA	ILE	ILE	ASP	PRO	ASN	ASN	ASN	LEU	CT
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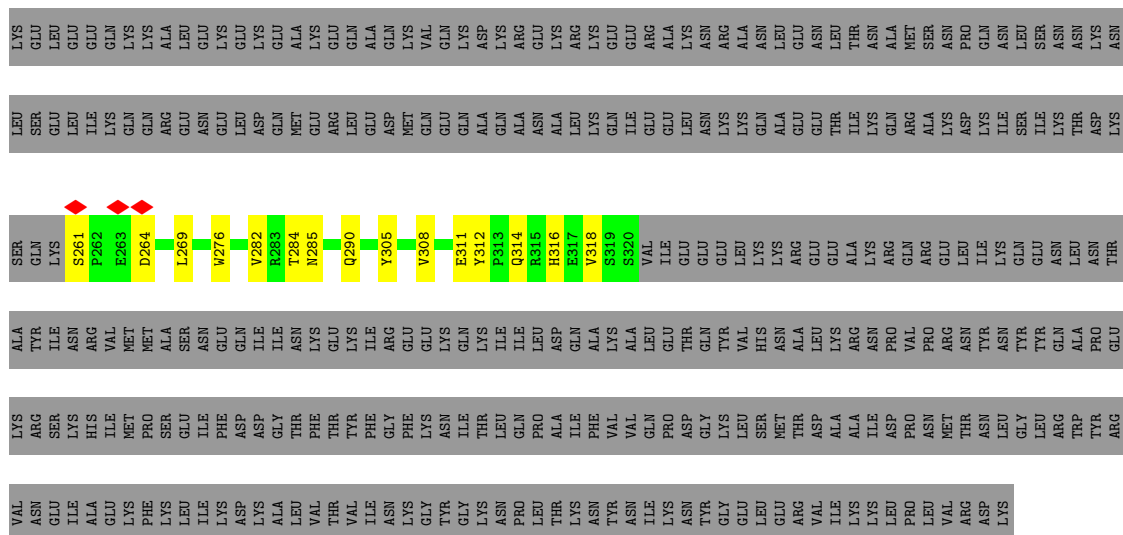
• Molecule 1: Cag pathogenicity island protein X



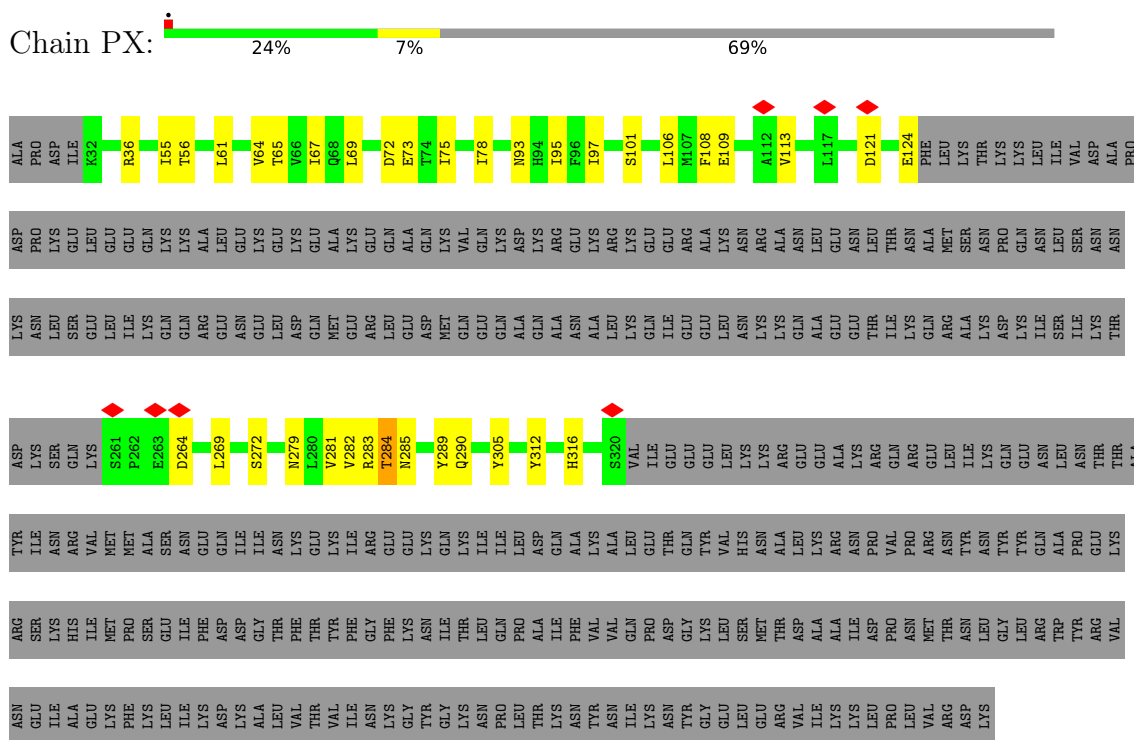
• Molecule 1: Cag pathogenicity island protein X



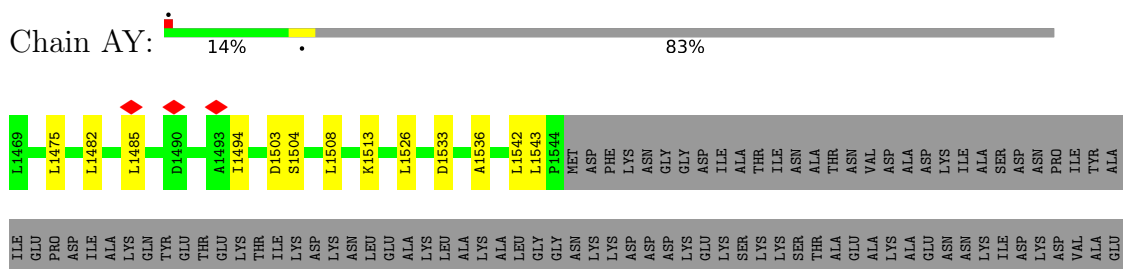


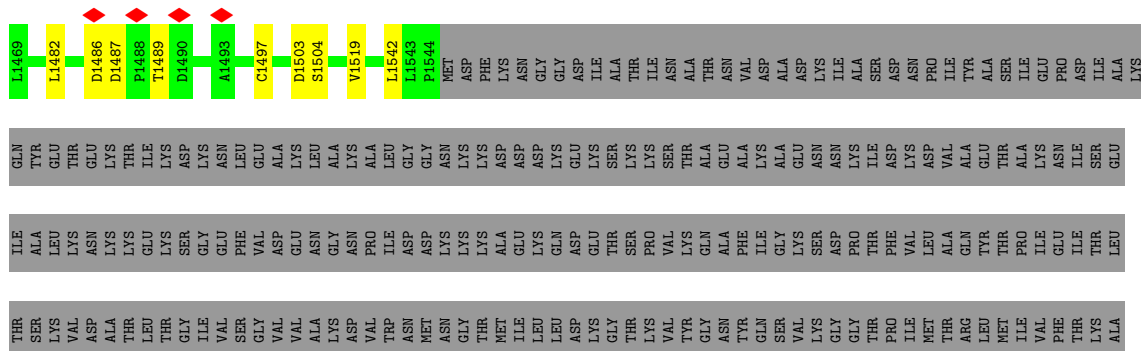


- Molecule 1: Cag pathogenicity island protein X



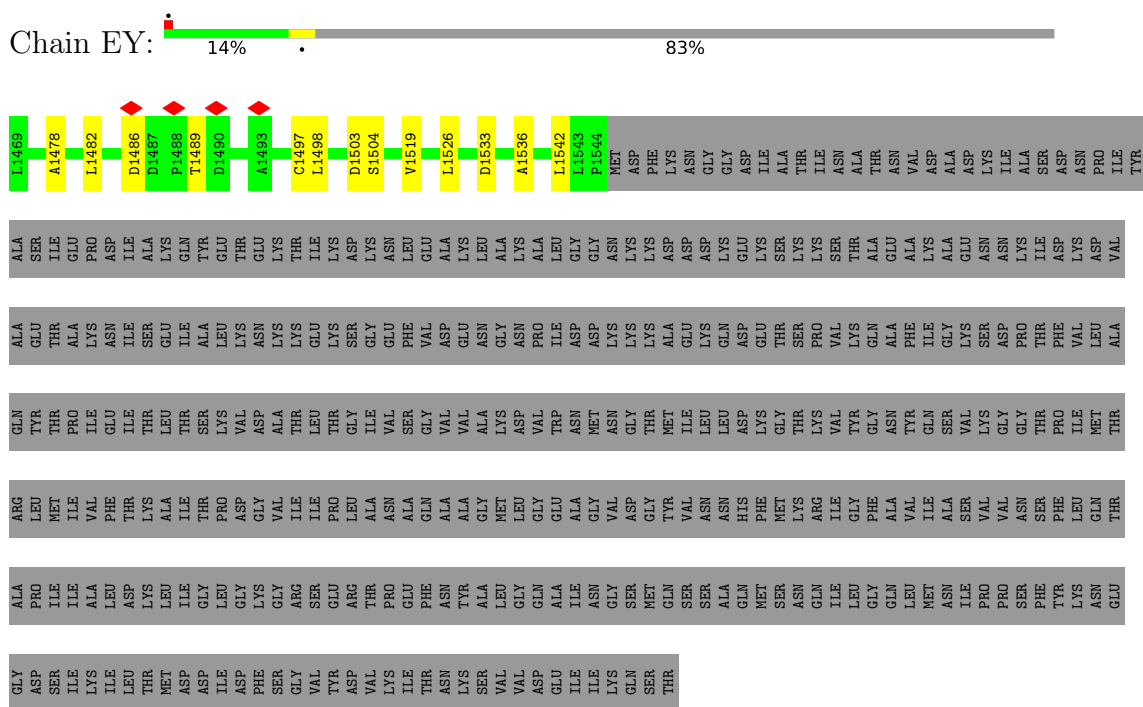
- Molecule 2: Type IV secretion system apparatus protein CagY



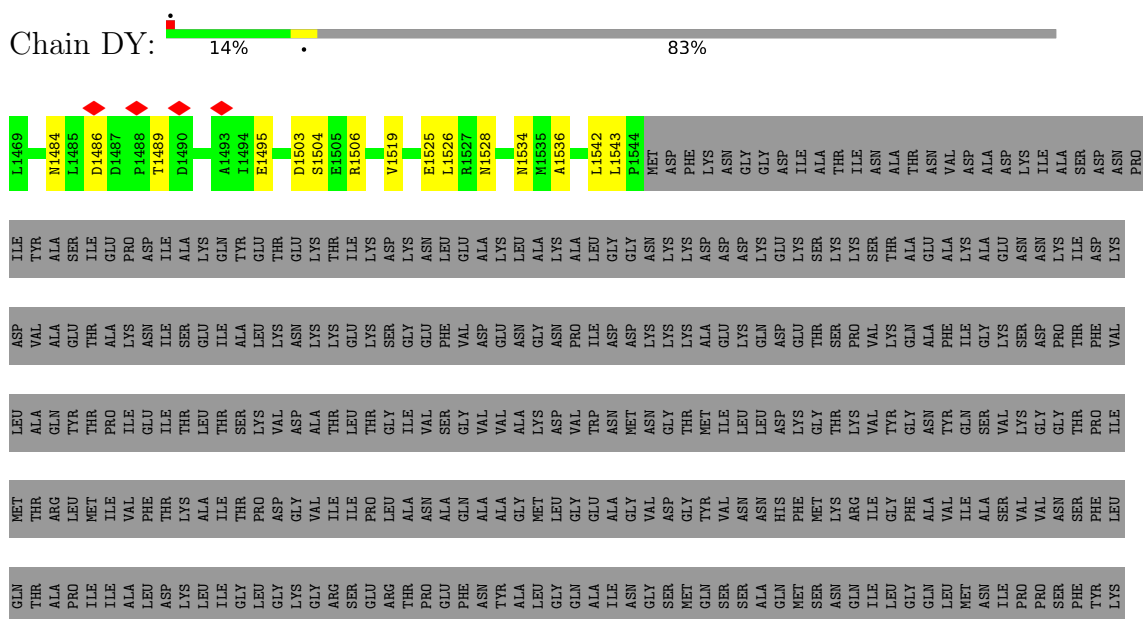


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- Molecule 2: Type IV secretion system apparatus protein CagY



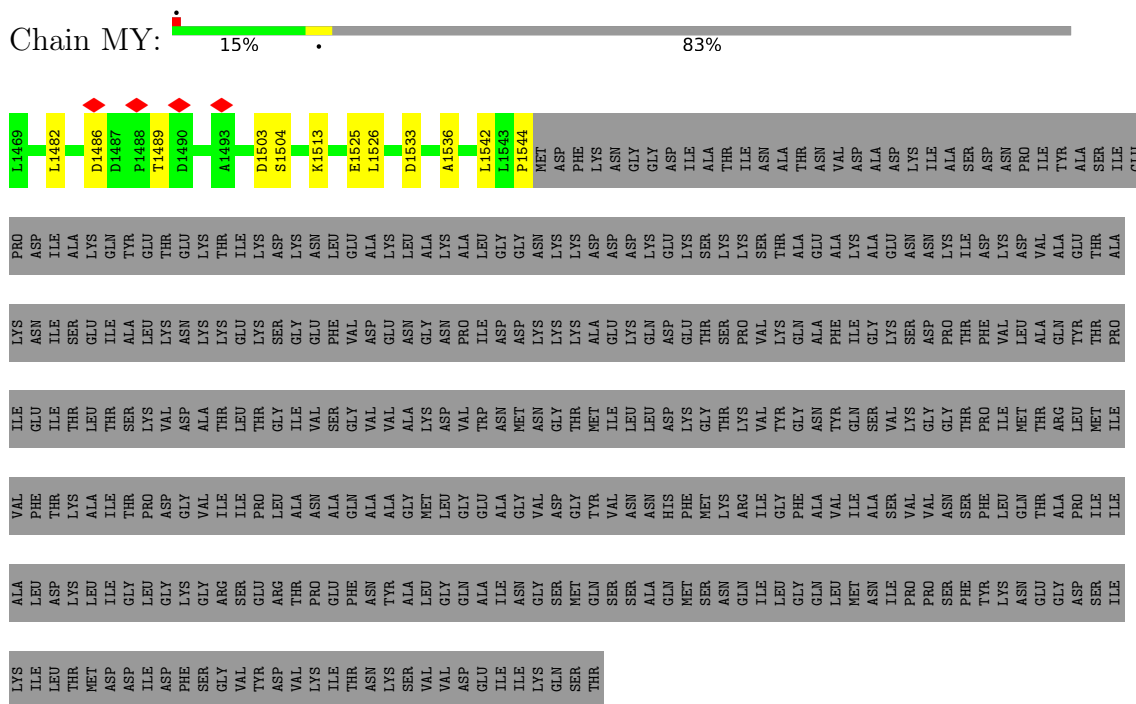
- Molecule 2: Type IV secretion system apparatus protein CagY



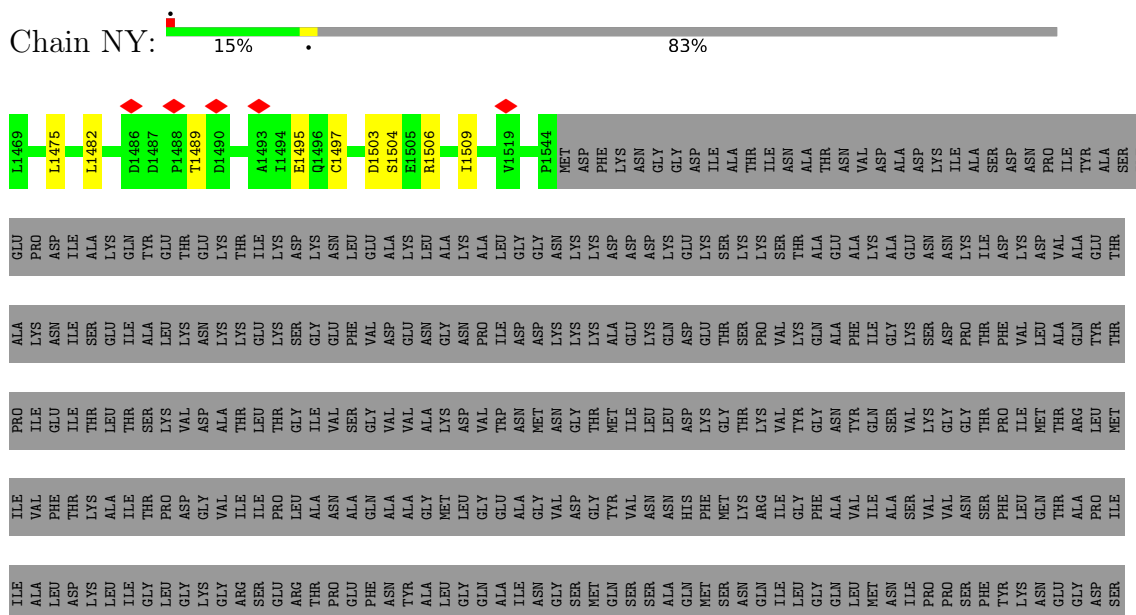


[illegible]

- Molecule 2: Type IV secretion system apparatus protein CagY



- Molecule 2: Type IV secretion system apparatus protein CagY



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	406996	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS TALOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.764	Depositor
Minimum map value	-1.067	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.171	Depositor
Map size (Å)	292.16, 292.16, 292.16	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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	0.15	0/1270	0.34	0/1719
1	BX	0.15	0/1270	0.32	0/1719
1	CX	0.15	0/1270	0.33	0/1719
1	DX	0.15	0/1270	0.33	0/1719
1	EX	0.15	0/1270	0.32	0/1719
1	FX	0.14	0/1270	0.30	0/1719
1	GX	0.15	0/1270	0.34	0/1719
1	HX	0.15	0/1270	0.33	0/1719
1	IX	0.15	0/1270	0.33	0/1719
1	JX	0.14	0/1270	0.32	0/1719
1	KX	0.14	0/1270	0.31	0/1719
1	LX	0.14	0/1270	0.31	0/1719
1	MX	0.14	0/1270	0.31	0/1719
1	NX	0.15	0/1270	0.32	0/1719
1	OX	0.16	0/1270	0.34	0/1719
1	PX	0.15	0/1270	0.37	0/1719
2	AY	0.11	0/607	0.29	0/818
2	BY	0.13	0/607	0.29	0/818
2	CY	0.10	0/607	0.25	0/818
2	DY	0.14	0/607	0.35	0/818
2	EY	0.12	0/607	0.29	0/818
2	FY	0.13	0/607	0.30	0/818
2	GY	0.11	0/607	0.29	0/818
2	HY	0.12	0/607	0.29	0/818
2	IY	0.12	0/607	0.29	0/818
2	JY	0.11	0/607	0.25	0/818
2	KY	0.12	0/607	0.30	0/818
2	LY	0.12	0/607	0.31	0/818
2	MY	0.13	0/607	0.31	0/818
2	NY	0.12	0/607	0.28	0/818
2	OY	0.10	0/607	0.26	0/818
2	PY	0.12	0/607	0.29	0/818
All	All	0.14	0/30032	0.32	0/40592

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AX	1245	1243	1246	24	0
1	BX	1245	1248	1246	22	0
1	CX	1245	1248	1246	29	0
1	DX	1245	1248	1246	24	0
1	EX	1245	1248	1246	32	0
1	FX	1245	1248	1246	24	0
1	GX	1245	1248	1246	27	0
1	HX	1245	1248	1246	33	0
1	IX	1245	1248	1246	24	0
1	JX	1245	1248	1246	30	0
1	KX	1245	1248	1246	23	0
1	LX	1245	1248	1246	29	0
1	MX	1245	1248	1246	24	0
1	NX	1245	1248	1246	28	0
1	OX	1245	1248	1246	32	0
1	PX	1245	1248	1246	34	0
2	AY	601	591	588	11	0
2	BY	601	591	588	9	0
2	CY	601	591	588	7	0
2	DY	601	591	588	13	0
2	EY	601	591	588	13	0
2	FY	601	591	588	8	0
2	GY	601	591	588	10	0
2	HY	601	591	588	7	0
2	IY	601	591	588	10	0
2	JY	601	591	588	8	0
2	KY	601	591	588	9	0
2	LY	601	591	588	8	0
2	MY	601	591	588	11	0
2	NY	601	591	588	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	OY	601	591	588	8	0
2	PY	601	591	588	11	0
All	All	29536	29419	29344	499	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 8.

The worst 5 of 499 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:JX:106:LEU:HD11	2:KY:1542:LEU:HD23	1.51	0.90
1:GX:307:THR:OG1	1:HX:290:GLN:OE1	1.95	0.83
1:LX:106:LEU:HD11	2:MY:1542:LEU:HD23	1.59	0.82
1:HX:106:LEU:HD11	2:IY:1542:LEU:HD21	1.62	0.81
1:MX:307:THR:OG1	1:NX:290:GLN:NE2	2.15	0.80

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	149/495 (30%)	139 (93%)	10 (7%)	0	100	100
1	BX	149/495 (30%)	135 (91%)	14 (9%)	0	100	100
1	CX	149/495 (30%)	134 (90%)	15 (10%)	0	100	100
1	DX	149/495 (30%)	135 (91%)	14 (9%)	0	100	100
1	EX	149/495 (30%)	138 (93%)	11 (7%)	0	100	100
1	FX	149/495 (30%)	137 (92%)	12 (8%)	0	100	100
1	GX	149/495 (30%)	133 (89%)	16 (11%)	0	100	100
1	HX	149/495 (30%)	134 (90%)	15 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	IX	149/495 (30%)	137 (92%)	12 (8%)	0	100	100
1	JX	149/495 (30%)	136 (91%)	13 (9%)	0	100	100
1	KX	149/495 (30%)	138 (93%)	11 (7%)	0	100	100
1	LX	149/495 (30%)	135 (91%)	14 (9%)	0	100	100
1	MX	149/495 (30%)	139 (93%)	10 (7%)	0	100	100
1	NX	149/495 (30%)	137 (92%)	12 (8%)	0	100	100
1	OX	149/495 (30%)	137 (92%)	12 (8%)	0	100	100
1	PX	149/495 (30%)	135 (91%)	14 (9%)	0	100	100
2	AY	74/441 (17%)	73 (99%)	1 (1%)	0	100	100
2	BY	74/441 (17%)	72 (97%)	2 (3%)	0	100	100
2	CY	74/441 (17%)	73 (99%)	1 (1%)	0	100	100
2	DY	74/441 (17%)	73 (99%)	1 (1%)	0	100	100
2	EY	74/441 (17%)	72 (97%)	2 (3%)	0	100	100
2	FY	74/441 (17%)	72 (97%)	2 (3%)	0	100	100
2	GY	74/441 (17%)	73 (99%)	1 (1%)	0	100	100
2	HY	74/441 (17%)	71 (96%)	3 (4%)	0	100	100
2	IY	74/441 (17%)	73 (99%)	1 (1%)	0	100	100
2	JY	74/441 (17%)	72 (97%)	2 (3%)	0	100	100
2	KY	74/441 (17%)	72 (97%)	2 (3%)	0	100	100
2	LY	74/441 (17%)	73 (99%)	1 (1%)	0	100	100
2	MY	74/441 (17%)	72 (97%)	2 (3%)	0	100	100
2	NY	74/441 (17%)	73 (99%)	1 (1%)	0	100	100
2	OY	74/441 (17%)	73 (99%)	1 (1%)	0	100	100
2	PY	74/441 (17%)	74 (100%)	0	0	100	100
All	All	3568/14976 (24%)	3340 (94%)	228 (6%)	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	141/451 (31%)	141 (100%)	0	100	100
1	BX	141/451 (31%)	140 (99%)	1 (1%)	76	90
1	CX	141/451 (31%)	141 (100%)	0	100	100
1	DX	141/451 (31%)	140 (99%)	1 (1%)	76	90
1	EX	141/451 (31%)	141 (100%)	0	100	100
1	FX	141/451 (31%)	140 (99%)	1 (1%)	76	90
1	GX	141/451 (31%)	141 (100%)	0	100	100
1	HX	141/451 (31%)	139 (99%)	2 (1%)	59	83
1	IX	141/451 (31%)	140 (99%)	1 (1%)	76	90
1	JX	141/451 (31%)	141 (100%)	0	100	100
1	KX	141/451 (31%)	140 (99%)	1 (1%)	76	90
1	LX	141/451 (31%)	140 (99%)	1 (1%)	76	90
1	MX	141/451 (31%)	140 (99%)	1 (1%)	76	90
1	NX	141/451 (31%)	141 (100%)	0	100	100
1	OX	141/451 (31%)	141 (100%)	0	100	100
1	PX	141/451 (31%)	140 (99%)	1 (1%)	76	90
2	AY	67/371 (18%)	67 (100%)	0	100	100
2	BY	67/371 (18%)	67 (100%)	0	100	100
2	CY	67/371 (18%)	67 (100%)	0	100	100
2	DY	67/371 (18%)	67 (100%)	0	100	100
2	EY	67/371 (18%)	67 (100%)	0	100	100
2	FY	67/371 (18%)	67 (100%)	0	100	100
2	GY	67/371 (18%)	66 (98%)	1 (2%)	57	82
2	HY	67/371 (18%)	67 (100%)	0	100	100
2	IY	67/371 (18%)	67 (100%)	0	100	100
2	JY	67/371 (18%)	67 (100%)	0	100	100
2	KY	67/371 (18%)	67 (100%)	0	100	100
2	LY	67/371 (18%)	67 (100%)	0	100	100
2	MY	67/371 (18%)	67 (100%)	0	100	100
2	NY	67/371 (18%)	67 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	OY	67/371 (18%)	67 (100%)	0	100	100
2	PY	67/371 (18%)	67 (100%)	0	100	100
All	All	3328/13152 (25%)	3317 (100%)	11 (0%)	84	95

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	KX	97	ILE
1	LX	312	TYR
1	PX	284	THR
1	MX	38	ARG
1	HX	284	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	LX	297	GLN
1	MX	63	ASN
1	PX	94	HIS
1	NX	290	GLN
1	OX	94	HIS

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.

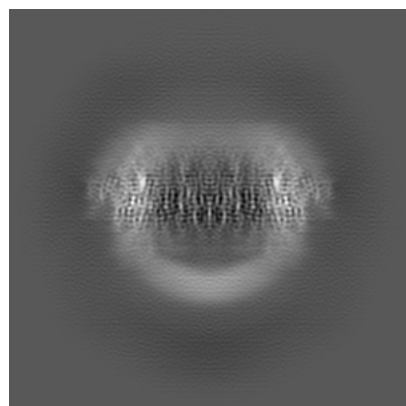
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65051. These allow visual inspection of the internal detail of the map and identification of artifacts.

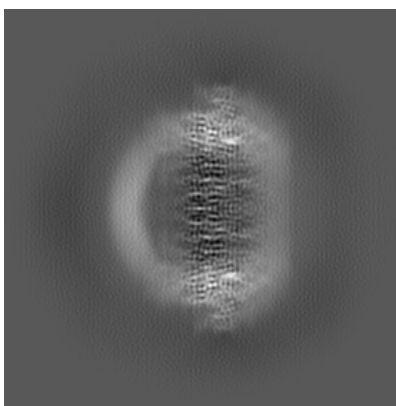
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

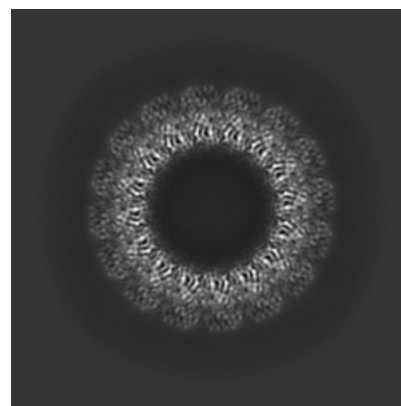
6.1.1 Primary map



X

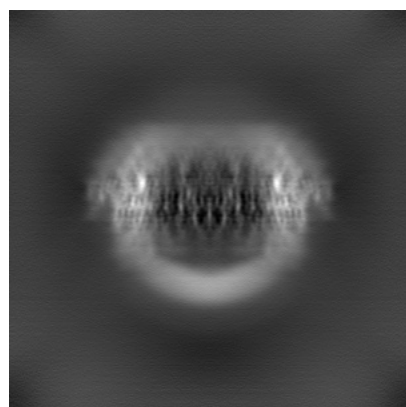


Y

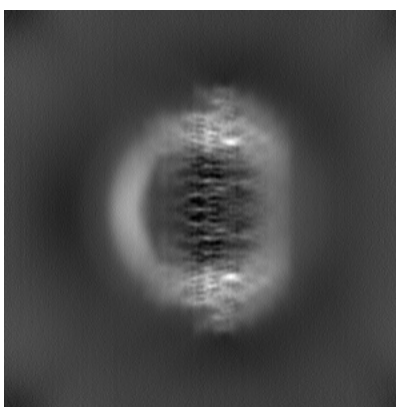


Z

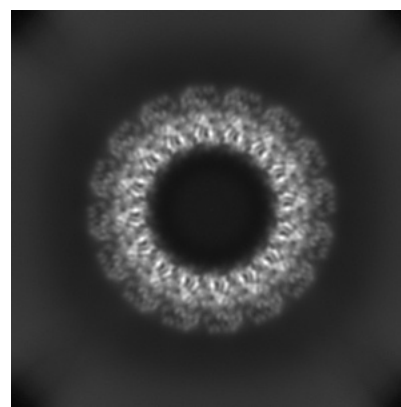
6.1.2 Raw map



X



Y

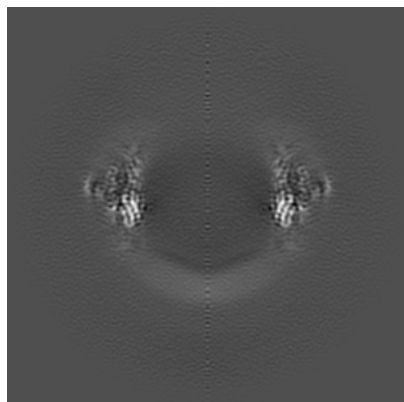


Z

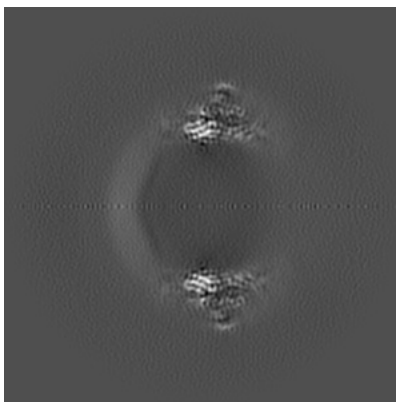
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

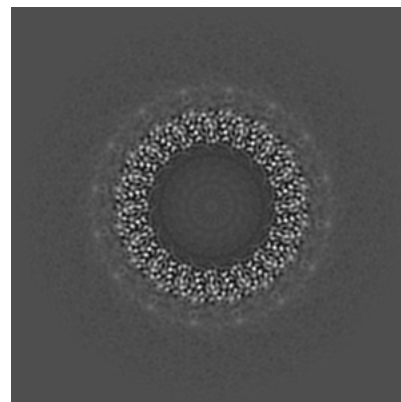
6.2.1 Primary map



X Index: 176

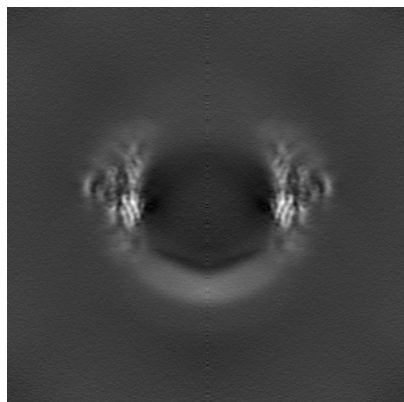


Y Index: 176

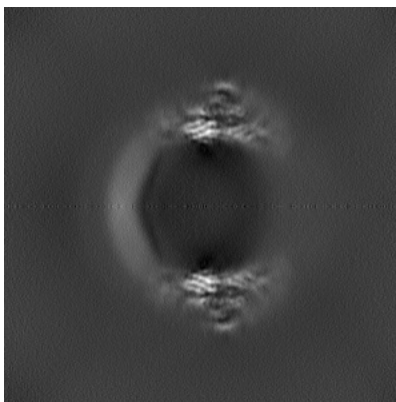


Z Index: 176

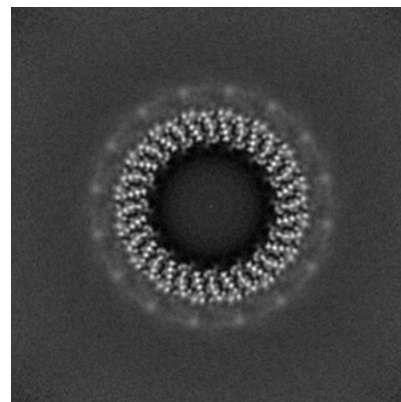
6.2.2 Raw map



X Index: 176



Y Index: 176

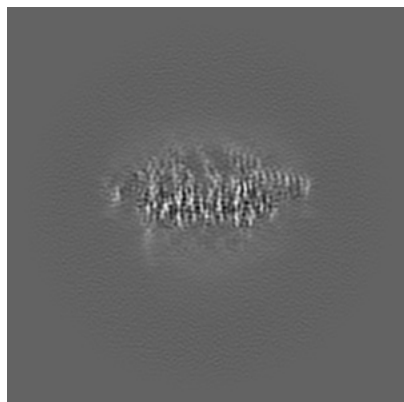


Z Index: 176

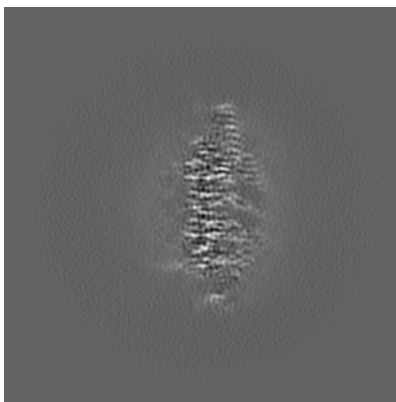
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

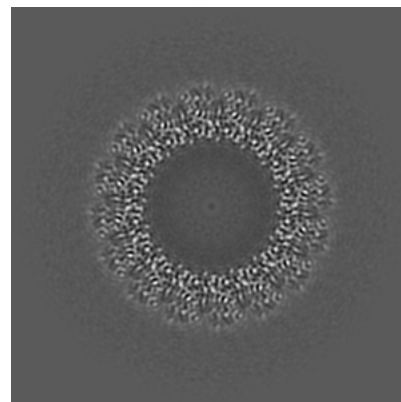
6.3.1 Primary map



X Index: 237

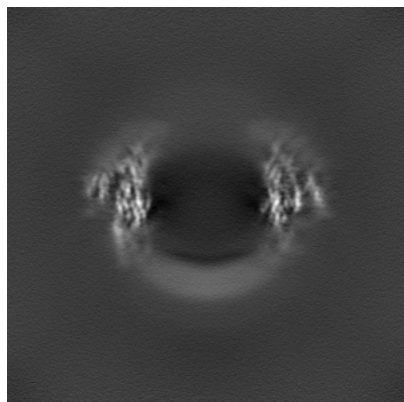


Y Index: 115

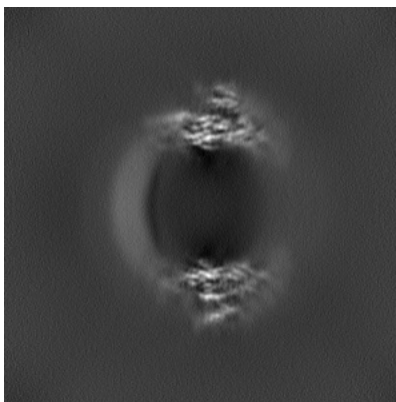


Z Index: 185

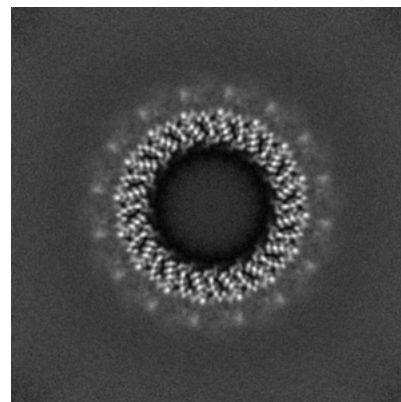
6.3.2 Raw map



X Index: 151



Y Index: 151

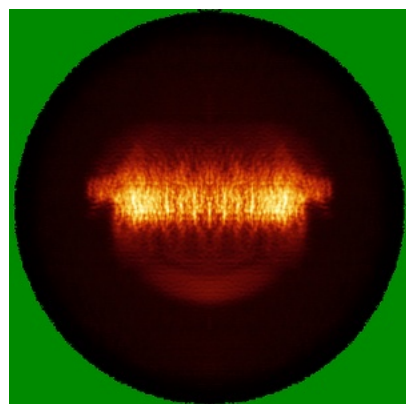


Z Index: 178

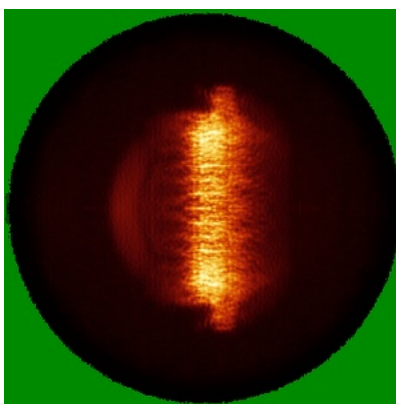
The images above show the largest variance slices of the map in three orthogonal directions.

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

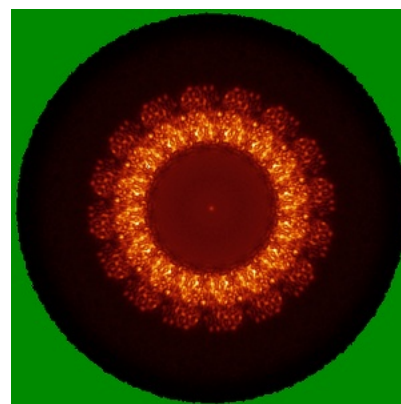
6.4.1 Primary map



X

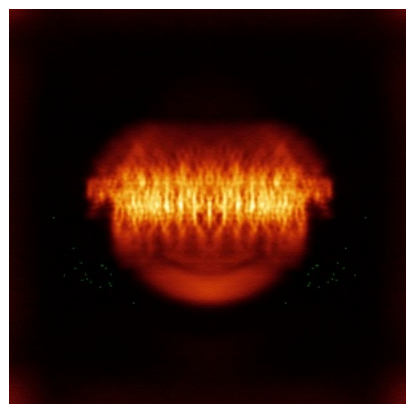


Y

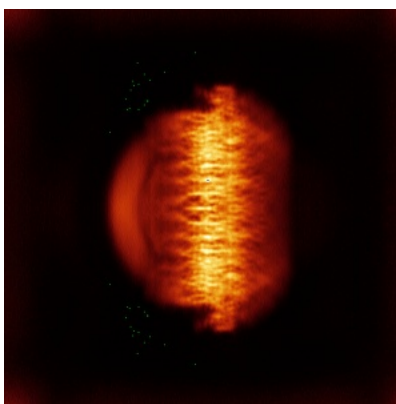


Z

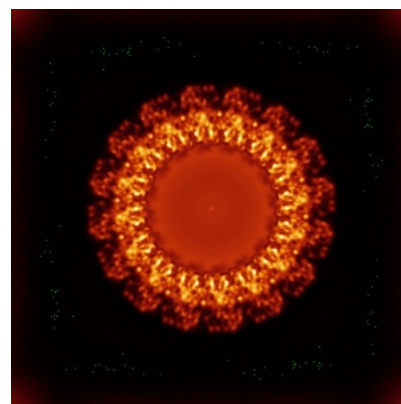
6.4.2 Raw map



X



Y

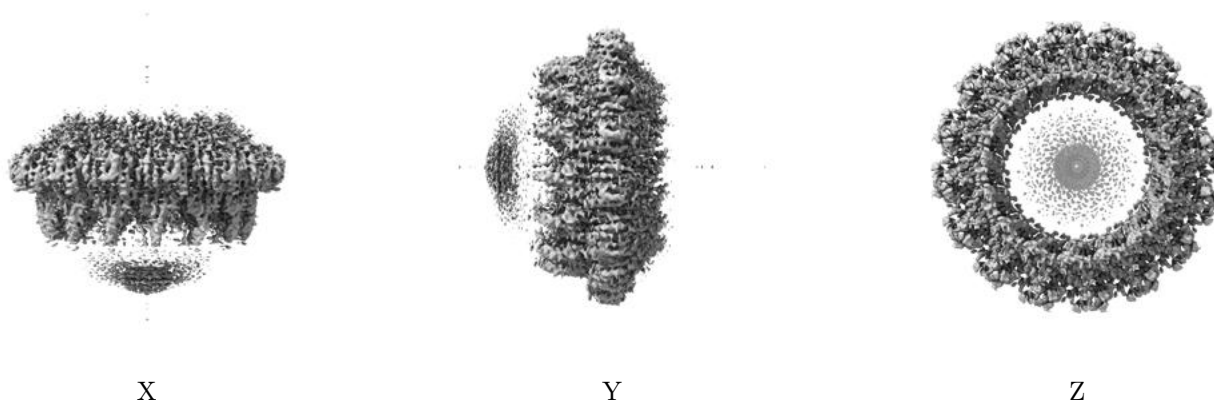


Z

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.

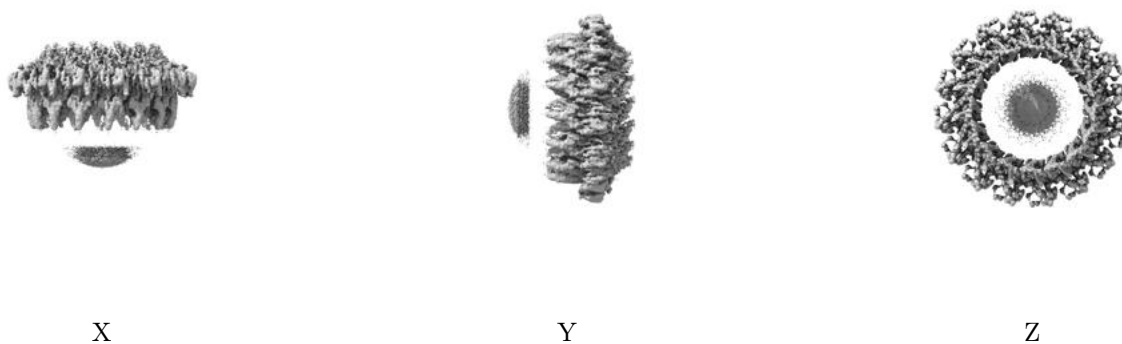
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.171. 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



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.

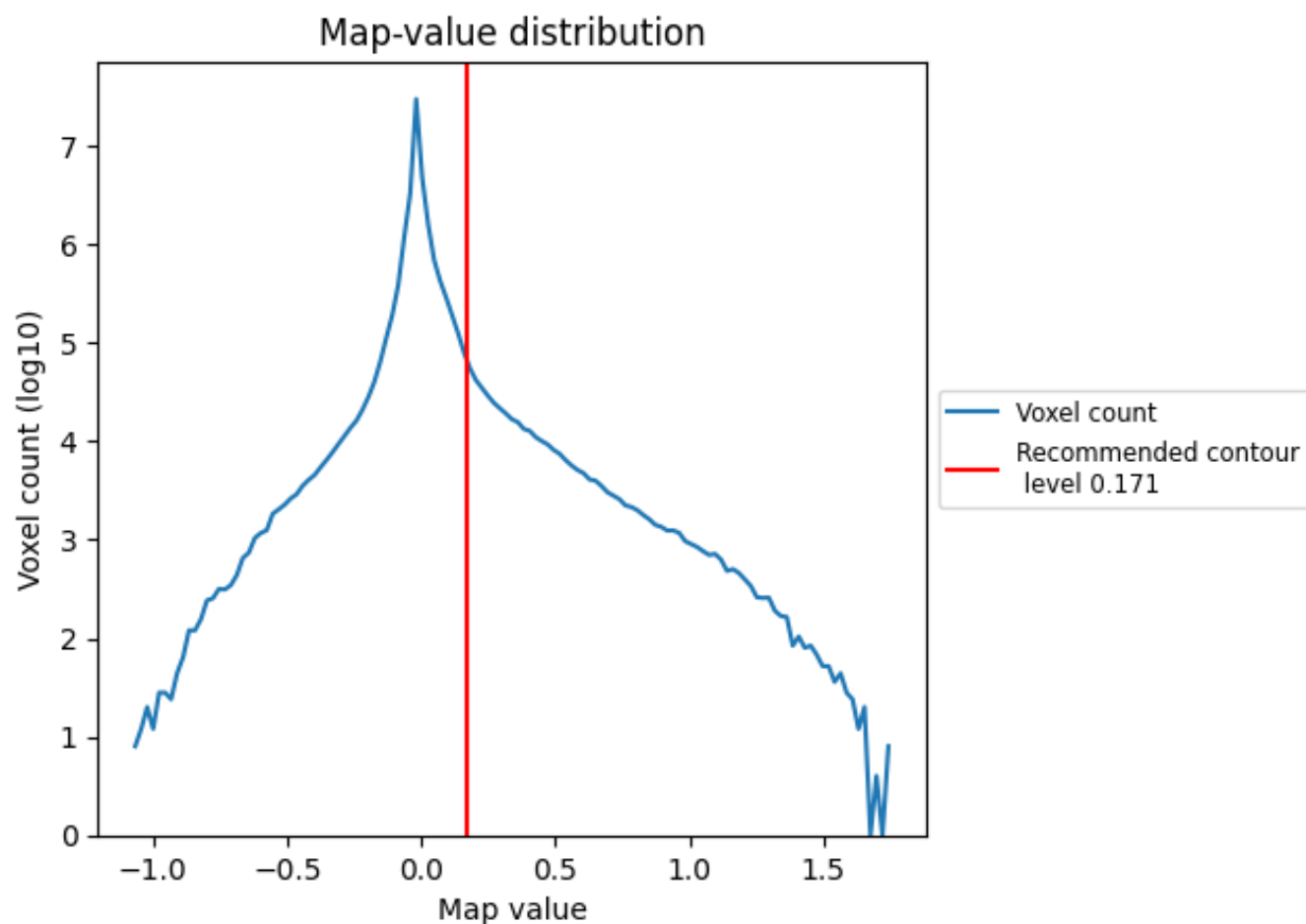
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

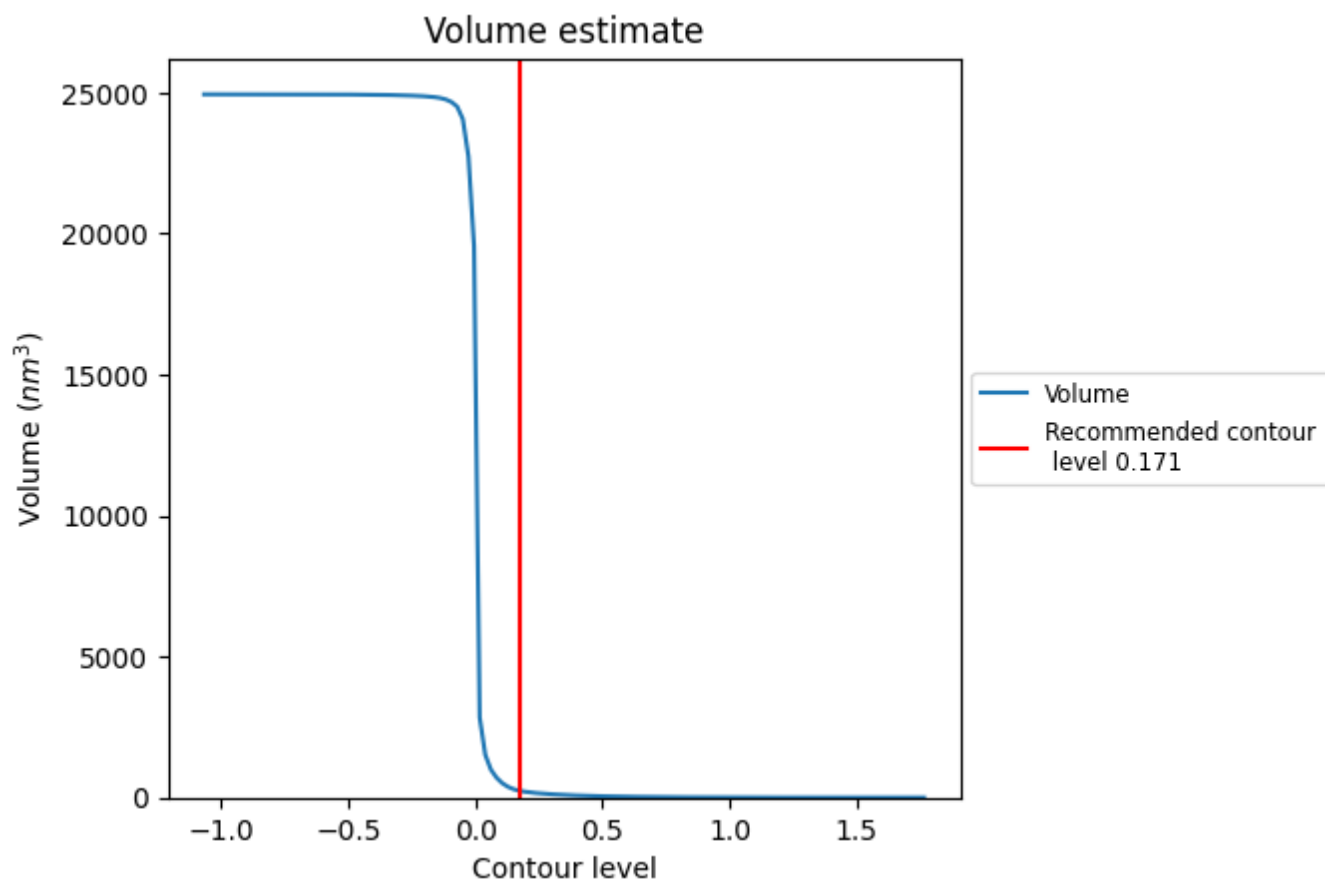
This section contains the results of statistical analysis of the map.

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.

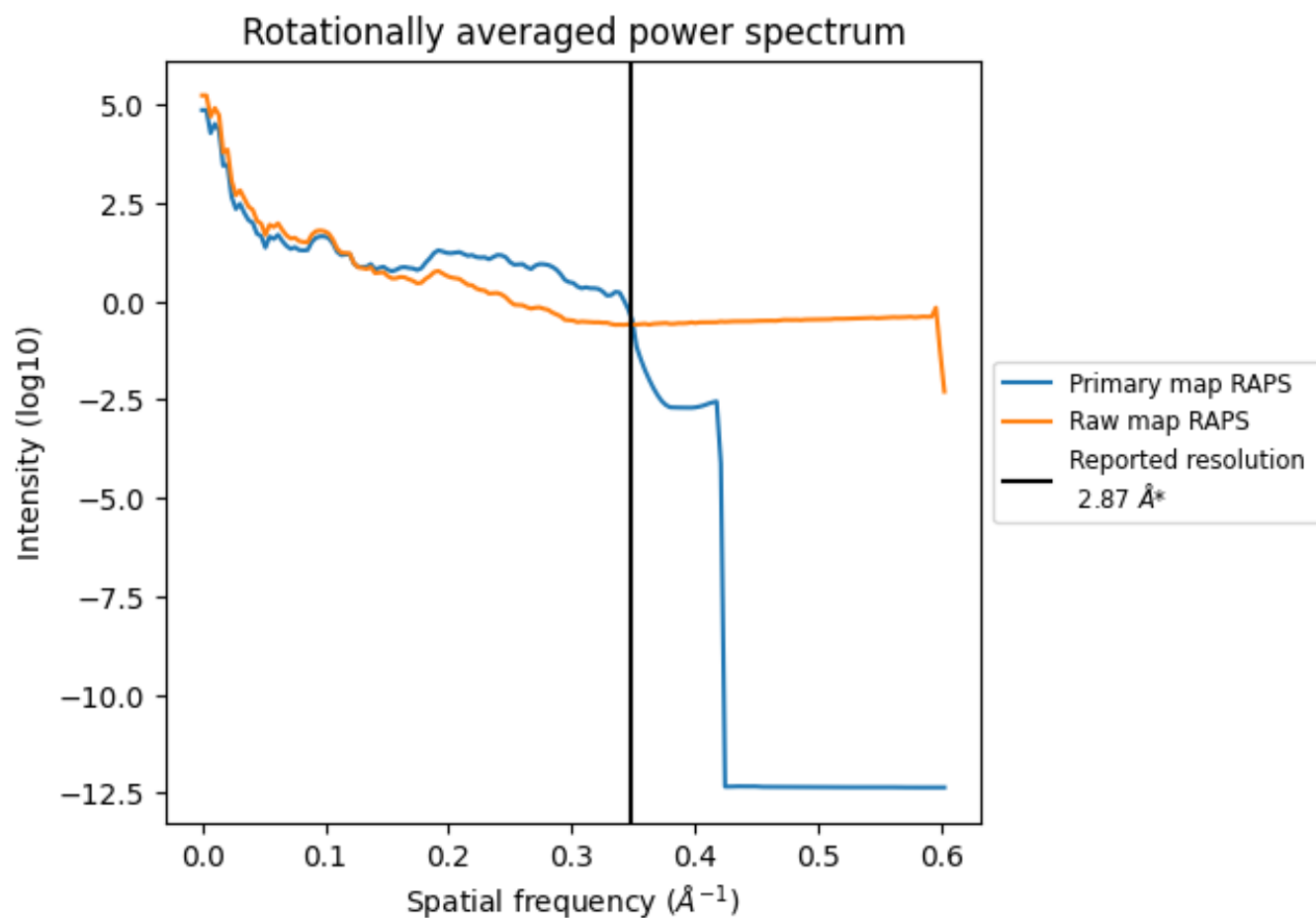
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 247 nm³; this corresponds to an approximate mass of 223 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 ⓘ

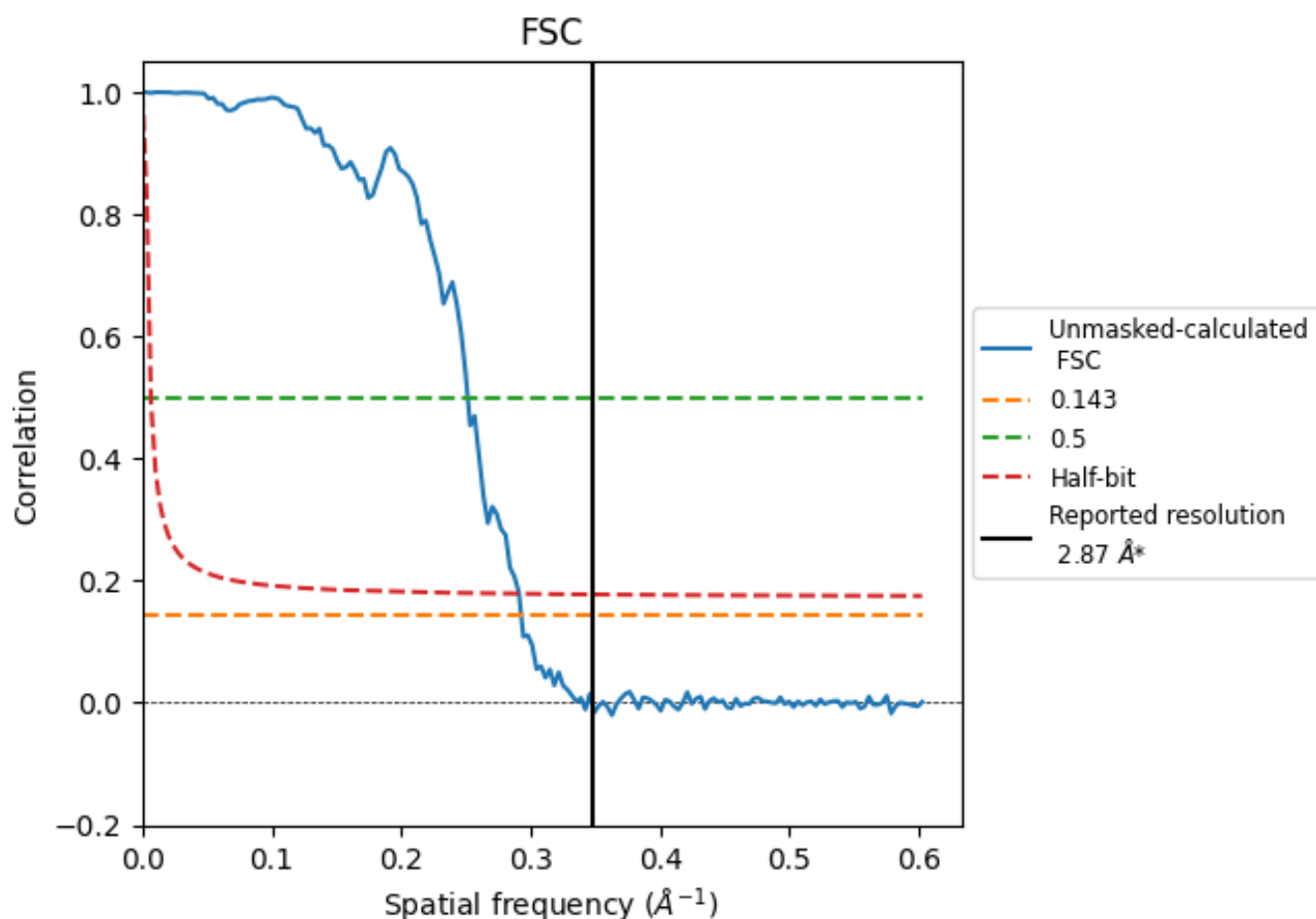


*Reported resolution corresponds to spatial frequency of 0.348 \AA^{-1}

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 0.348 \AA^{-1}

8.2 Resolution estimates [i](#)

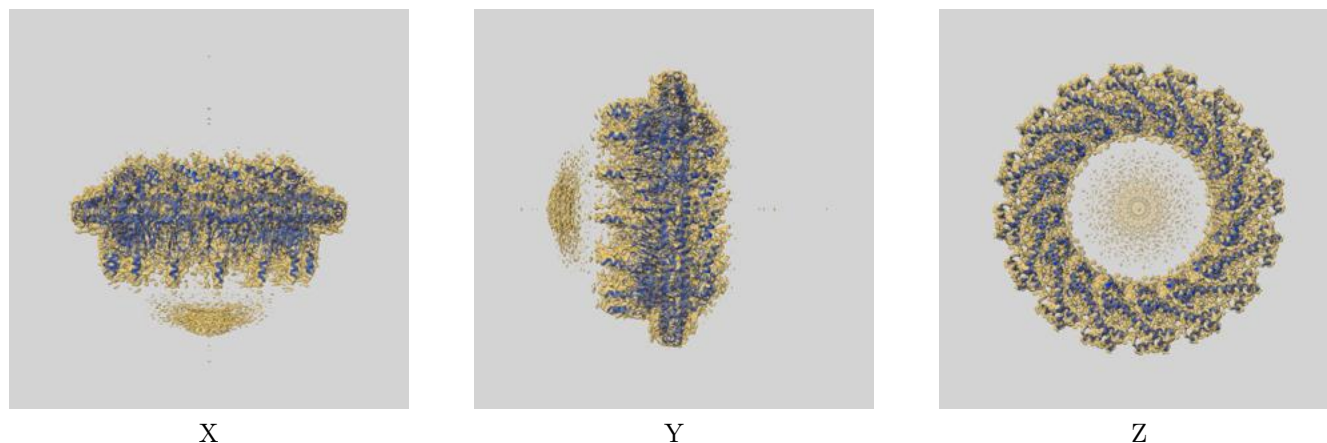
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.42	3.98	3.44

*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 3.42 differs from the reported value 2.87 by more than 10 %

9 Map-model fit [i](#)

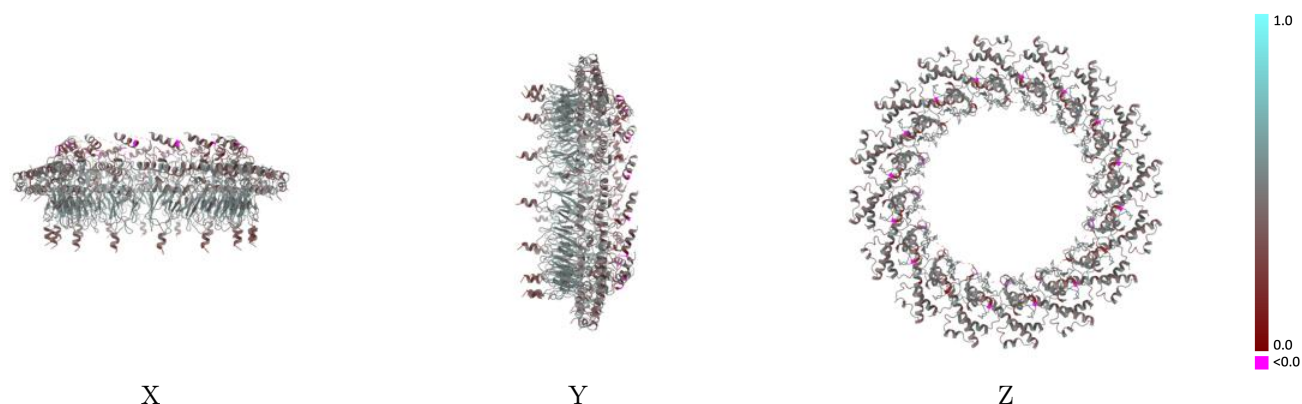
This section contains information regarding the fit between EMDB map EMD-65051 and PDB model 9VGU. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



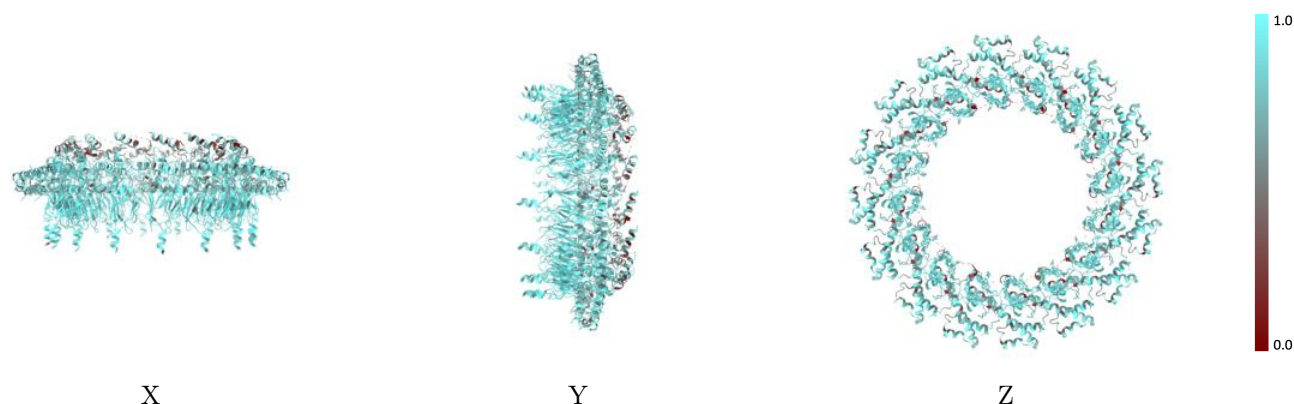
The images above show the 3D surface view of the map at the recommended contour level 0.171 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



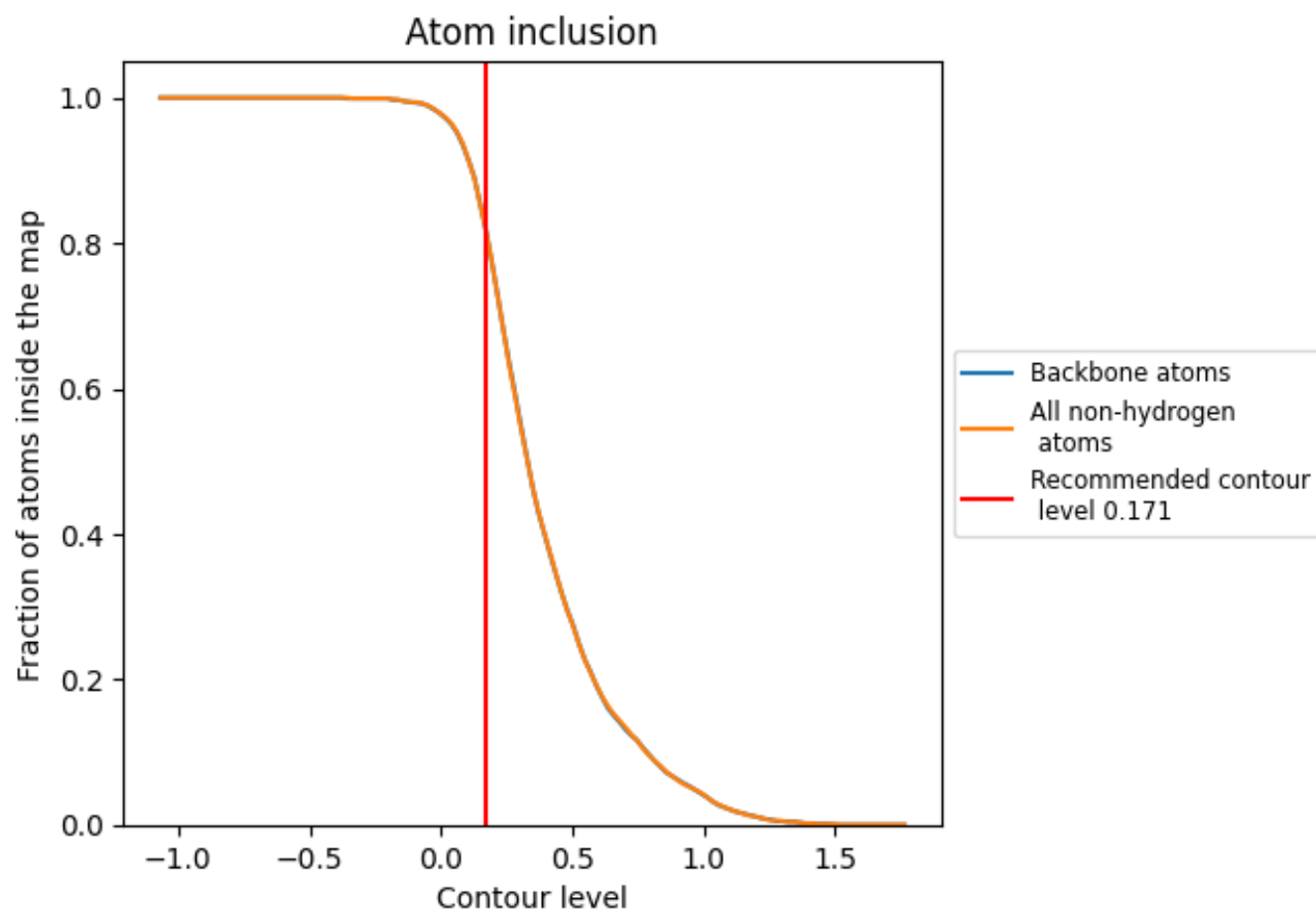
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.171).



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 82% 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 (0.171) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8180	 0.4590
AX	 0.8390	 0.4690
AY	 0.7890	 0.4410
BX	 0.8390	 0.4670
BY	 0.7810	 0.4430
CX	 0.8380	 0.4650
CY	 0.7810	 0.4430
DX	 0.8360	 0.4680
DY	 0.7740	 0.4350
EX	 0.8390	 0.4710
EY	 0.7930	 0.4400
FX	 0.8420	 0.4690
FY	 0.7790	 0.4360
GX	 0.8330	 0.4660
GY	 0.7720	 0.4410
HX	 0.8290	 0.4670
HY	 0.7720	 0.4360
IX	 0.8420	 0.4730
IY	 0.7860	 0.4450
JX	 0.8440	 0.4690
JY	 0.7790	 0.4330
KX	 0.8360	 0.4700
KY	 0.7790	 0.4380
LX	 0.8350	 0.4690
LY	 0.7880	 0.4440
MX	 0.8460	 0.4710
MY	 0.7890	 0.4400
NX	 0.8370	 0.4660
NY	 0.7760	 0.4400
OX	 0.8360	 0.4670
OY	 0.7810	 0.4380
PX	 0.8400	 0.4680
PY	 0.7780	 0.4420

