Full wwPDB EM Validation Report (i)

May 30, 2023 – 12:35 PM EDT

PDB ID	:	8CXH
EMDB ID	:	EMD-27056
Title	:	Structures of Zika Virus in Complex with Antibodies Targeting E Dimer Epitopes and Basis for Neutralization Efficacy
Authors	:	Liu, W.; Zhang, X.K.; Gong, D.Y.; Dai, X.H.; Sharma, A.; Zhang, T.H.; Rey, F.; Zhou, Z.H.
Deposited on	:	2022-05-21
Resolution	:	3.20 Å(reported)

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

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

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

The following versions of software and data (see references (i)) were used in the production of this report:
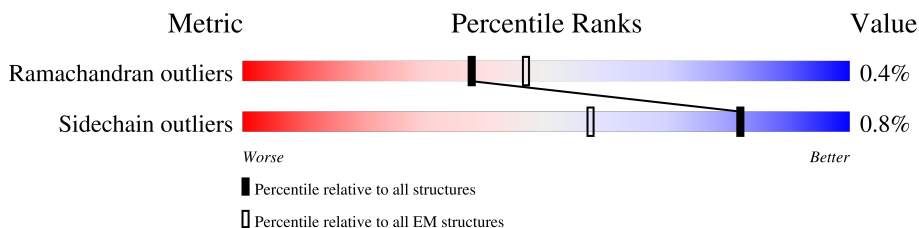
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 3.20 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.
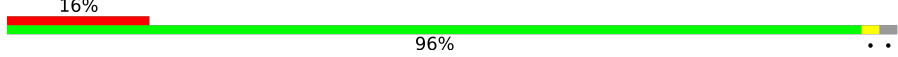
Metric	Percentile Ranks	Value
Ramachandran outliers		0.4%
Sidechain outliers		0.8%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

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

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	639	76% • 23%
1	B	639	76% 23%
1	C	639	77% • 22%
2	D	3423	• 98%
2	E	3423	• 98%
2	F	3423	• 98%
3	H	128	20% 98% ••
3	h	128	25% 98% ••
4	L	110	13% 96% ••

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	l	110	16% ▬▬▬▬▬▬▬▬ 96%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 16634 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 Ankyrin repeat family A protein 2,Envelope E protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	491	Total	C	N	O	S	0	0
			3714	2339	644	701	30		
1	B	491	Total	C	N	O	S	0	0
			3714	2339	644	701	30		
1	C	501	Total	C	N	O	S	0	0
			3790	2384	657	718	31		

- Molecule 2 is a protein called Membrane M protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	75	Total	C	N	O	S	0	0
			600	391	105	103	1		
2	E	75	Total	C	N	O	S	0	0
			600	391	105	103	1		
2	F	75	Total	C	N	O	S	0	0
			600	391	105	103	1		

- Molecule 3 is a protein called C10 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	127	Total	C	N	O	S	0	0
			1021	650	169	197	5		
3	h	127	Total	C	N	O	S	0	0
			1021	650	169	197	5		

- Molecule 4 is a protein called C10 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	108	Total	C	N	O	S	0	0
			787	488	134	162	3		
4	l	108	Total	C	N	O	S	0	0
			787	488	134	162	3		

WORLDWIDE PDB
PROTEIN DATA BANK

3 Residue-property plots ⓘ

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: Ankyrin repeat family A protein 2,Envelope E protein

Chain A:

• Molecule 1: Ankyrin repeat family A protein 2,Envelope E protein

Chain B:

• Molecule 1: Ankyrin repeat family A protein 2,Envelope E protein

Chain C:

• Molecule 2: Membrane M protein

Chain D:

98%

| MET LYS ASN PRO LYS LYS SER GLY GLY PHE ARG ILE ASN MET LEU LYS ARG GLY VAL ALA ARG VAL SER PRO PHE GLY GLY LEU LYS ARG LEU PRO ALA GLY LEU LEU LEU GLY HIS GLY PRO ILE ARG MET VAL LEU ALA ILE LEU ALA PHE LEU ARG PHE THR ALA ILE LYS |

| PRO SER LEU GLY LEU ILE ASN ARG TRP GLY SER VAL GLY LYS LYS GLU ALA MET GLU ILE ILE LYS LYS PHE LYS ASP LEU ALA ALA MET LEU ARG ILE ILE ASN ALA ARG LYS GLU LYS ARG ARG ALA ASP SER VAL ILE VAL GLY LEU LEU THR THR ALA |

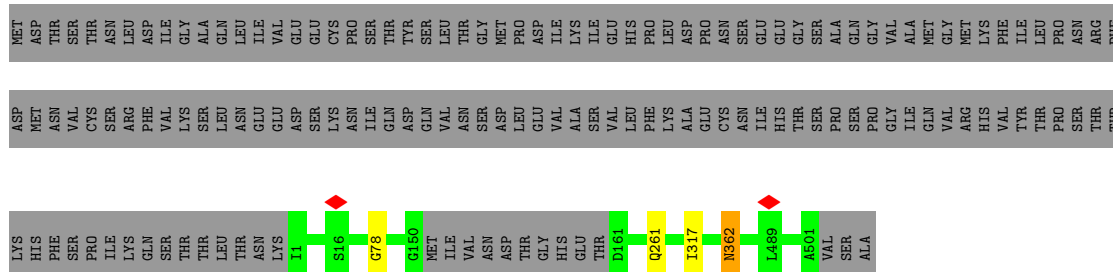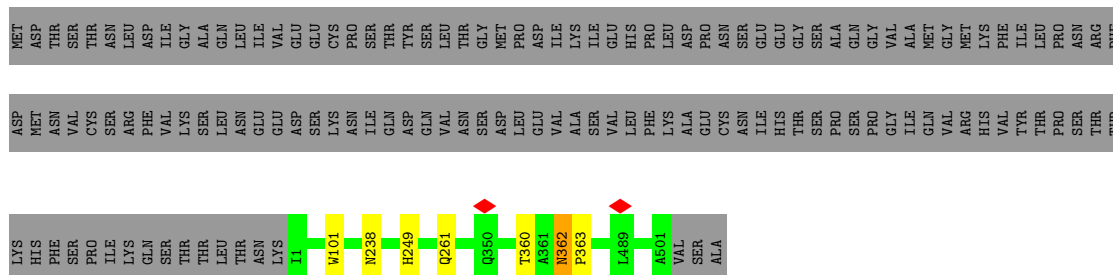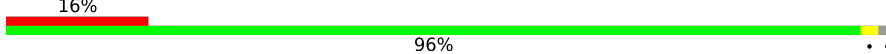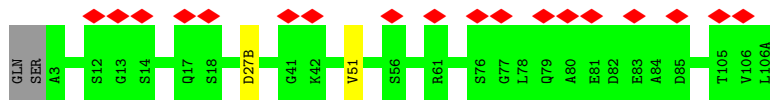| MET ALA ALA GLU VAL THR ARG ARG GLY SER ALA TYR TYR MET TYR LEU ASP ARG ASN ASP ALA GLY GLU ALA ILE SER PHE PRO THR THR LEU GLY MET ASN LYS CYS TYR ILE GLN ILE MET ASP LEU GLY HIS MET CYS ASP ALA THR MET SER TYR GLU CYS PRO MET LEU ASP GLU |

| GLY VAL GLU PRO ASP ASP VAL ASP CYS TRP CYS ASN THR THR SER THR TRP VAL VAL TYR GLY THR CYS HIS HIS LYS GLY GLU ALA ARG ARG SER ARG **A1** **E24** **S75** ILE ARG ALA CYS ILE GLY VAL VAL SER ASN ARG ASP PHE VAL GLU GLY MET SER GLY GLY THR TRP |

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

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

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

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

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

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

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

| LEU GLY LYS ILE HIS ILE PHE GLY ALA ALA PHE LYS SER LEU PHE GLY GLY MET SER TRP PHE SER GLN ILE LEU ILE GLY THR LEU LEU MET TRP LEU GLY LEU ASN THR LYS ASN GLY SER ILE SER LEU MET CYS LEU ALA LEU GLY GLY VAL LEU ILE PHE LEU SER THR |

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

| ILE SER SER VAL SER ARG MET GLU ASN ILE MET TRP ARG SER VAL GLU GLY GLU LEU ASN ALA ILE LEU GLU GLU ASN GLY VAL GLN LEU THR VAL VAL VAL GLY SER VAL LYS ASN PRO MET TRP ARG GLY PRO GLN ARG LEU PRO VAL PRO VAL ASN GLU LEU PRO HIS GLY TRP LYS |

| ALA TRP GLY LYS SER TYR PHE VAL ARG ALA ALA LYS THR ASN ASN SER PHE VAL VAL ASP GLY ASP THR LEU LYS GLU CYS PRO LEU LYS HIS ARG ALA TRP ASN SER PHE LEU VAL GLU ASP HIS GLY PHE GLY VAL PHE HIS THR SER VAL TRP LEU LYS VAL ARG GLU ASP TYR SER |

| LEU GLU CYS ASP PRO ALA VAL ILE GLY THR ALA VAL LYS GLY LYS GLU ALA VAL HIS SER ASP LEU GLY TYR TRP ILE GLU SER GLU LYS ASN ASP THR TRP ARG LEU LYS ARG ALA HIS LEU ILE GLU MET LYS THR CYS GLU TRP PRO LYS SER HIS THR LEU TRP THR ASP GLY ILE |

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

| SER LEU ARG THR THR THR ALA SER GLY LYS LEU ILE THR GLU TRP CYS CYS ARG GLU CYS THR MET PRO PRO LEU SER PHE ARG ALA LYS ASP GLY CYS TRP TYR GLY MET GLU ILE ARG PRO ARG LYS GLU PRO GLU SER ASN LEU VAL ARG SER MET VAL THR ALA GLY SER THR ASP |

| HIS MET ASP HIS PHE SER LEU GLY VAL LEU VAL ILE LEU LEU MET VAL GLN GLU GLY LEU LYS LYS ARG MET THR THR LYS ILE ILE SER THR MET ALA VAL LEU VAL LEU ALA MET ILE LEU GLY GLY PHE SER MET SER ASP LEU ALA LYS LEU ILE ILE LEU MET GLY ALA THR |

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

LEU MET VAL ILE ASN GLY PHE ALA LEU ALA TRP LEU ALA ILE ARG ALA MET VAL VAL PRO ARG THR ASP ASN ILE THR LEU ILE LEU ALA ALA LEU THR PRO LEU ALA ARG GLY THR LEU VAL ALA TRP ARG GLY LEU ALA THR CYS GLY PHE MET LEU SER

LEU LYS GLY GLY SER VAL LYS LYS GLY ASN LEU PRO VAL MET LEU GLY THR ALA LEU ARG ALA VAL ALA LEU ASP PRO ILE ASN VAL VAL GLY LEU LEU LEU LEU THR ARG SER GLY LYS ARG SER TRP PRO SER GLU VAL VAL LEU THR ALA VAL GLY LEU ILE CYS ALA LEU ALA

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

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

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

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

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

LEU THR VAL LEU ASP LEU HIS PRO GLY ALA GLY LYS THR ARG ARG VAL LEU PRO GLU ILE VAL ARG GLU ALA ILE LYS THR ARG LEU ARG THR VAL ILE LEU ALA PRO THR ARG VAL VAL ALA ALA GLU MET GLU GLU ALA LEU ARG GLY LEU PRO VAL ARG TYR MET THR THR ALA VAL

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

GLU ALA ALA ALA ILE PHE MET THR ALA THR PRO PRO GLY THR ARG ASP ALA PHE PRO ASP SER ASN SER PRO ILE MET ASP THR GLU VAL GLU VAL PRO GLU ARG ALA TRP SER SER GLY PHE ASP TRP VAL THR ASP HIS SER GLY LYS THR VAL TRP PHE VAL PRO SER VAL ARG ASN

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

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

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

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

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

LEU GLU THR ILE MET LEU LEU GLY LEU LEU GLY THR VAL SER LEU GLY ILE PHE PHE VAL LEU MET ARG ASN LYS GLY ILE GLY LYS MET GLY PHE GLY MET VAL THR LEU GLY ALA SER ALA TRP LEU MET TRP LEU SER GLU ILE GLU PRO ALA ARG ILE ALA CYS VAL LEU ILE VAL

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

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

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

- Molecule 2: Membrane M protein

Chain E: 98%

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

GLY VAL GLU PRO ASP ASP VAL ASP CYS TRP CYS ASN THR SER THR TRP VAL VAL TYR GLY THR CYS HIS LYS GLU GLY ALA ARG ARG SER ARG **A1** **R15** **S75** ILE ARG CYS ILE GLY VAL SER ASN ARG ASP PHE VAL GLU MET SER GLY GLY THR TRP

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

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

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

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

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

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

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

LEU GLY LYS ILE HIS ILE PHE GLY ALA ALA PHE SER LYS SER LEU PHE GLY GLY MET SER PHE SER GLN ILE LEU ILE GLY THR LEU LEU MET TRP LEU GLY LEU ASN THR LYS ASN GLY SER ILE SER LEU MET CYS LEU ALA LEU GLY GLY VAL LEU ILE PHE LEU SER THR

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

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

ALA TRP GLY LYS SER TYR PHE VAL ARG ALA LYS THR ASN ASN SER PHE VAL VAL ASP GLY ASP THR LEU LYS GLU CYS PRO LEU LYS HIS ARG ALA TRP ASN SER PHE LEU VAL GLU HIS GLY PHE VAL PHE HIS THR SER VAL TRP LEU LYS VAL ARG GLU ASP ALA ASP TYR SER

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

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

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

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

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

LEU MET VAL LEU ILE ASN GLY PHE ALA LEU TRP LEU ALA HIS ILE ALA ARG ALA MET VAL LEU VAL PRO ARG ASP THR ASP ILE THR LEU ALA ILE SER ALA ALA ALA LEU THR PRO LEU ALA ARG GLU GLY SER MET LEU LEU ALA LEU ALA THR CYS GLY GLY PHE MET LEU LEU SER

LEU LYS GLY LYS SER GLY SER VAL LYS LYS ASN LEU PRO PHE MET LEU LEU THR ALA LEU ARG MET VAL ASP ARG THR ALA ILE ASN VAL GLY LEU LEU LEU THR ARG SER GLY LYS ARG SER TRP PRO PRO SER GLU VAL LEU THR ALA VAL GLY LEU ILE CYS ALA LEU ALA

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

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

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

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

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

LEU THR VAL LEU ASP LEU HIS PRO GLY ALA GLY LYS THR ARG ARG VAL LEU PRO GLU ILE VAL ARG GLU ALA ILE LYS THR ARG LEU ARG THR VAL ILE LEU ALA PRO THR ARG VAL VAL ALA ALA GLU MET GLU GLU ALA LEU ARG GLY LEU PRO VAL ARG TYR MET THR THR ALA VAL

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

GLU ALA ALA ALA ILE PHE MET THR ALA THR PRO PRO GLY THR ARG ASP ALA PHE PRO ASP SER ASN SER PRO ILE MET ASP THR GLU VAL GLU VAL PRO GLU ARG ALA TRP SER SER GLY PHE ASP TRP VAL THR ASP HIS SER GLY LYS THR VAL TRP PHE VAL PRO SER VAL ARG ASN

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

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

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

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

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

LEU GLU THR ILE MET LEU LEU GLY LEU LEU GLY THR VAL SER LEU GLY ILE PHE PHE VAL LEU MET ARG ASN LYS GLY ILE GLY LYS MET GLY PHE GLY MET VAL THR LEU GLY ALA SER ALA TRP LEU MET TRP LEU SER GLU ILE GLU PRO ALA ARG ILE ALA CYS VAL LEU ILE VAL

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

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

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

GLY ILE MET LYS ASN PRO VAL VAL ASP GLY ILE VAL VAL THR ASP ILE ASP THR MET THR ILE ASP PRO GLN VAL GLU LYS LYS MET GLY GLN VAL LEU LEU ILE ALA VAL ALA VAL SER SER ALA ILE LEU SER ARG THR ALA TRP GLY TRP GLY GLU ALA GLY ALA LEU ILE THR ALA

ALA THR SER THR LEU TRP GLU GLY ASN PRO ASN ARG TYR TRP ASN SER SER THR ALA THR SER LEU CYS ASN ILE PHE ARG GLY SER TYR LEU ALA GLY ALA SER LEU ILE TYR THR VAL THR ARG ASN ALA GLY LEU VAL LYS ARG ARG GLY GLY GLY THR GLY GLU THR LEU GLY GLU

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

• Molecule 2: Membrane M protein

Chain F: 98%

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

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

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

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

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

GLY ASP SER ILE VAL ILE GLY VAL GLU GLY LYS ILE THR HIS HIS TRP HIS ARG SER SER THR ILE GLY LYS ALA PHE GLU THR ALA THR VAL ARG GLY ALA ILE THR ASN LYS ASN GLY SER ILE VAL LEU GLY ASP ALA TRP ASP GLY SER PHE GLY VAL GLY ALA LEU ASN SER LEU GLY

LYS GLY ILE ILE HIS GLN ILE PHE GLY ALA ALA PHE LYS LEU PHE GLY GLY MET SER TRP PHE SER GLN ILE LEU GLY THR LEU MET TRP LEU GLY ASN TRP LEU LYS ASN GLY SER ILE SER LEU MET CYS ALA LEU GLY VAL PHE LEU SER THR ALA VAL

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

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

GLY LYS SER TYR PHE VAL ARG ALA ALA LYS THR ASN ASN SER PHE VAL VAL ASP GLY ASP THR LEU LYS GLU CYS PRO LEU LYS HIS ARG ALA TRP ASN SER PHE LEU VAL GLU ASP HIS GLY PHE GLY VAL PHE HIS THR SER VAL TRP LEU LYS VAL ARG GLU ASP TYR SER LEU GLU

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

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

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

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

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

VAL LEU ILE GLY PHE ALA LEU ALA TRP LEU ALA ILE ARG ALA MET VAL VAL PRO ARG THR ASP ASN ILE LEU ILE LEU ALA LEU THR PRO LEU ARG GLY THR LEU LEU ALA TRP ARG ALA GLY LEU THR CYS GLY GLY PHE MET LEU LEU SER LEU LYS

GLY LYS GLY SER VAL LYS ASN LEU PRO PHE VAL MET ALA LEU GLY LEU THR ALA VAL ARG VAL ASP LEU LEU LEU THR ARG GLY SER GLY TRP PRO PRO SER GLU VAL LEU THR ALA VAL GLY LEU CYS ALA LEU ALA GLY

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

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

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

• Molecule 3: C10 heavy chain

20%

Chain H:

98%

E1 V2 Q3 L4 S7 G8 A9 E10 V11 K12 K13 K23 A40 P41 G42 E46 Q61 Q64 D65 D72 T73 S74 R83 S84 E85 Y100J Q105 T110 V111 S112 SER

• Molecule 3: C10 heavy chain

25%

Chain h:

98%

E1 V2 Q3 S7 G8 A9 E10 V11 K12 K13 P14 G15 A16 S17 A40 P41 G42 Q43 Q61 Q64 D65 R71 D72 T73 S74 E81 R83 S84 E85 D86 T87 Y100J Q105 V109 T110 V111 S112 SER

• Molecule 4: C10 light chain

13%

Chain L:

96%

GLN SER A3 S14 Q17 S18 I19 D27B H39 P40 G41 K42 A43 V51 G77 A80 E81 D82 E83 A84 D85 V106 L106A

• Molecule 4: C10 light chain

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1094250	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 $(e^-/\text{Å}^2)$	26	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	22.275	Depositor
Minimum map value	-12.363	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	265.0, 265.0, 265.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.47	0/3791	0.56	1/5128 (0.0%)
1	B	0.43	0/3791	0.57	1/5128 (0.0%)
1	C	0.53	2/3869 (0.1%)	0.61	3/5236 (0.1%)
2	D	0.34	0/615	0.47	0/838
2	E	0.33	0/615	0.45	0/838
2	F	0.32	0/615	0.44	0/838
3	H	0.30	0/1050	0.45	0/1427
3	h	0.28	0/1050	0.46	0/1427
4	L	0.34	0/805	0.50	0/1093
4	l	0.43	0/805	0.50	0/1093
All	All	0.43	2/17006 (0.0%)	0.55	5/23046 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	238	ASN	C-O	-5.68	1.12	1.23
1	C	238	ASN	CA-C	-5.64	1.38	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	101	TRP	CA-CB-CG	8.24	129.36	113.70
1	C	360	THR	N-CA-C	-6.92	92.33	111.00
1	B	362	ASN	N-CA-C	-6.77	92.72	111.00
1	A	362	ASN	C-N-CD	6.36	141.75	128.40
1	C	362	ASN	C-N-CD	6.10	141.20	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts   ⓘ

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

5.3   Torsion angles   ⓘ

5.3.1   Protein backbone   ⓘ

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	487/639 (76%)	424 (87%)	61 (12%)	2 (0%)	34	69
1	B	487/639 (76%)	433 (89%)	51 (10%)	3 (1%)	25	64
1	C	499/639 (78%)	443 (89%)	54 (11%)	2 (0%)	34	69
2	D	73/3423 (2%)	66 (90%)	7 (10%)	0	100	100
2	E	73/3423 (2%)	65 (89%)	8 (11%)	0	100	100
2	F	73/3423 (2%)	66 (90%)	7 (10%)	0	100	100
3	H	125/128 (98%)	119 (95%)	6 (5%)	0	100	100
3	h	125/128 (98%)	122 (98%)	3 (2%)	0	100	100
4	L	106/110 (96%)	101 (95%)	4 (4%)	1 (1%)	17	56
4	l	106/110 (96%)	100 (94%)	5 (5%)	1 (1%)	17	56
All	All	2154/12662 (17%)	1939 (90%)	206 (10%)	9 (0%)	38	69

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	362	ASN
1	A	261	GLN
1	B	261	GLN
4	l	51	VAL
1	A	349	MET
4	L	51	VAL
1	B	78	GLY
1	C	261	GLN
1	C	363	PRO

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	A	399/534 (75%)	394 (99%)	5 (1%)	69	87
1	B	399/534 (75%)	398 (100%)	1 (0%)	92	96
1	C	408/534 (76%)	406 (100%)	2 (0%)	88	95
2	D	64/2832 (2%)	63 (98%)	1 (2%)	62	84
2	E	64/2832 (2%)	63 (98%)	1 (2%)	62	84
2	F	64/2832 (2%)	64 (100%)	0	100	100
3	H	107/108 (99%)	106 (99%)	1 (1%)	78	91
3	h	107/108 (99%)	105 (98%)	2 (2%)	57	81
4	L	88/90 (98%)	87 (99%)	1 (1%)	73	88
4	l	88/90 (98%)	87 (99%)	1 (1%)	73	88
All	All	1788/10494 (17%)	1773 (99%)	15 (1%)	82	93

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	ASP
1	A	246	LYS
1	A	249	HIS
1	A	295	MET
1	A	426	ASP
2	D	24	GLU
3	H	100(J)	TYR
4	L	27(B)	ASP
1	B	317	ILE
2	E	15	ARG
3	h	71	ARG
3	h	100(J)	TYR
4	l	27(B)	ASP
1	C	249	HIS
1	C	362	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	163	ASN
1	A	249	HIS
1	A	344	GLN
1	A	399	HIS
2	D	7	HIS
4	L	38	GLN
4	L	39	HIS
1	B	85	GLN
1	B	103	ASN
1	B	266	HIS
1	B	446	HIS
1	B	447	GLN
2	E	7	HIS
2	E	39	ASN
4	l	37	GLN
4	l	38	GLN
4	l	39	HIS
1	C	77	GLN
1	C	103	ASN
1	C	134	ASN
1	C	147	GLN
1	C	148	HIS
1	C	158	HIS
1	C	163	ASN
1	C	266	HIS
1	C	447	GLN
1	C	465	GLN
2	F	7	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-27056. 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 ⓘ
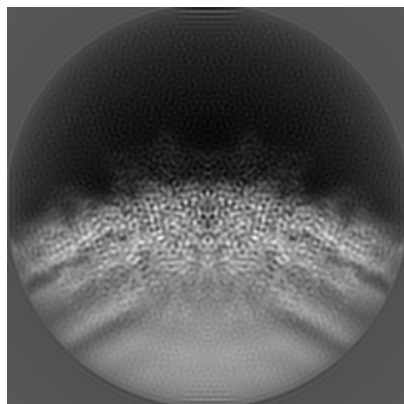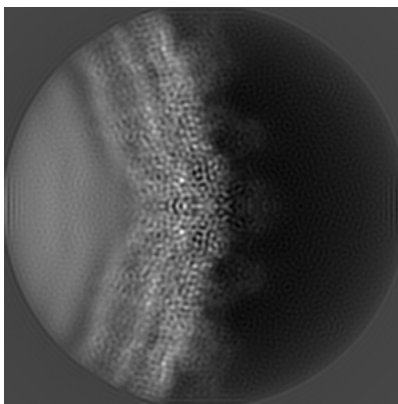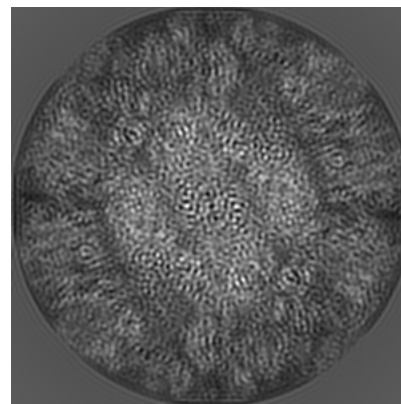
6.1.1 Primary map

| X | Y | Z |

6.1.2 Raw map

| X | Y | Z |
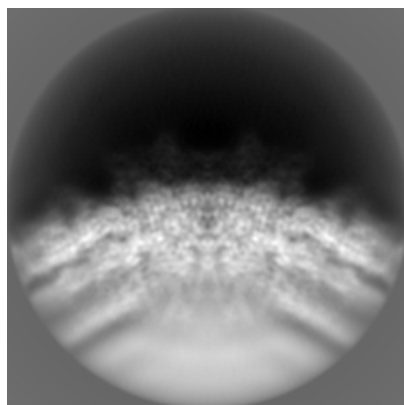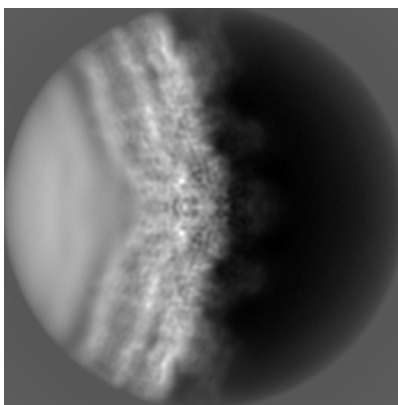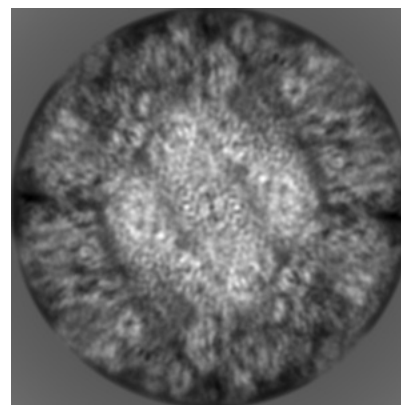
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
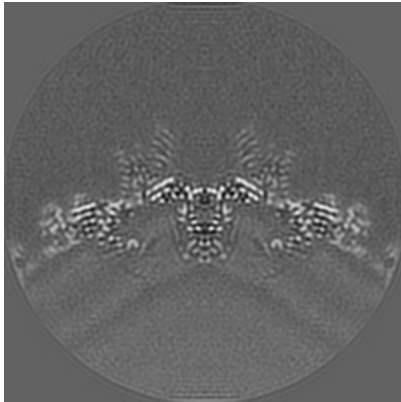
6.2.1 Primary map
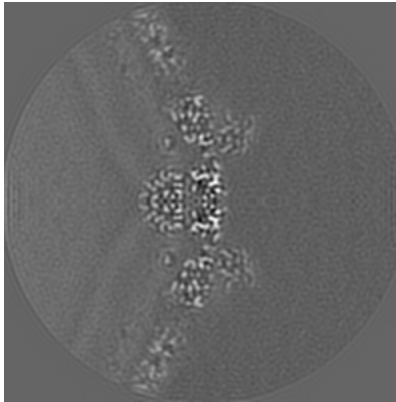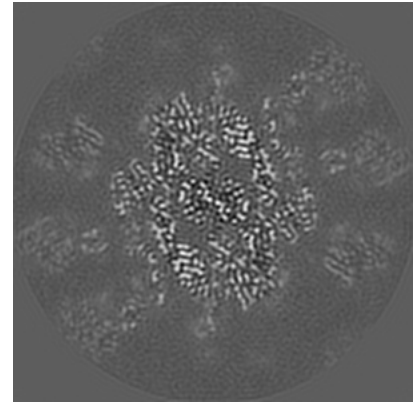
| X Index: 125 | Y Index: 125 | Z Index: 125 |

6.2.2 Raw map
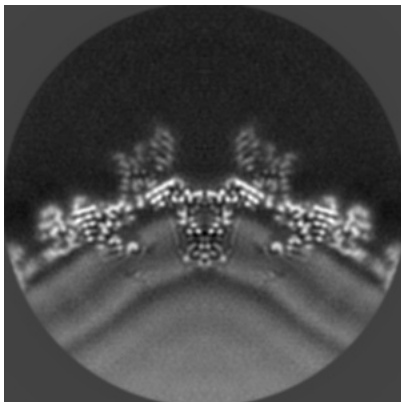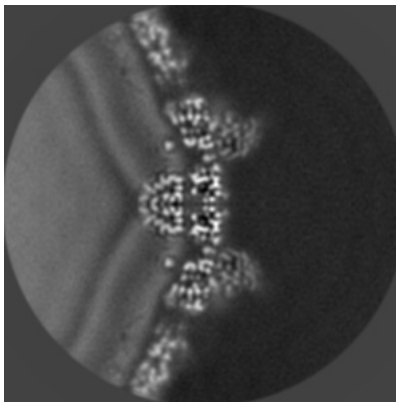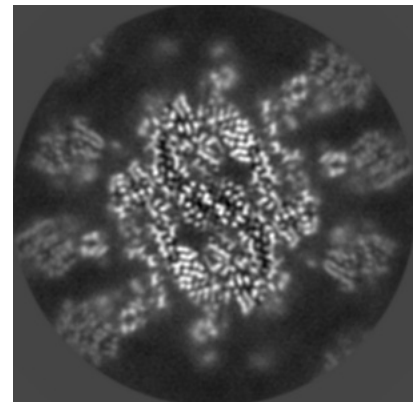
| X Index: 125 | Y Index: 125 | Z Index: 125 |

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
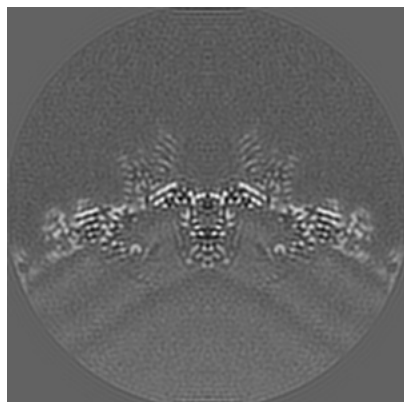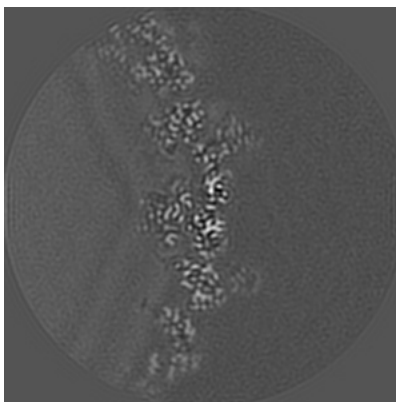
| X Index: 125 | Y Index: 134 | Z Index: 110 |
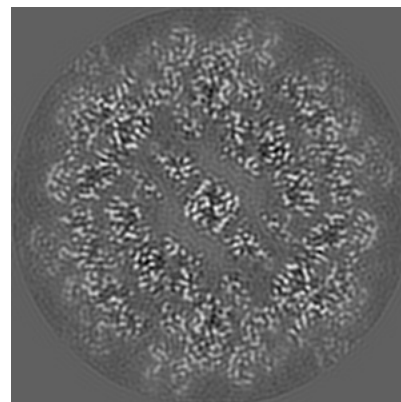
6.3.2 Raw map
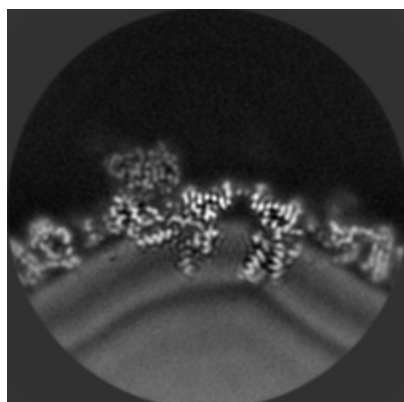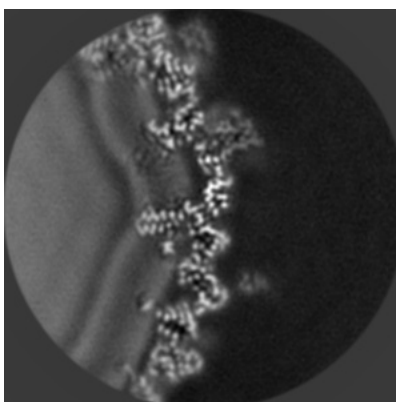
| X Index: 140 | Y Index: 138 | Z Index: 115 |
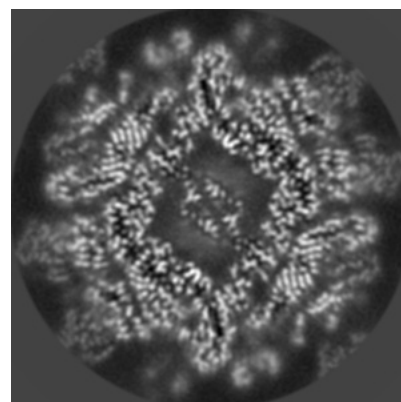
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map
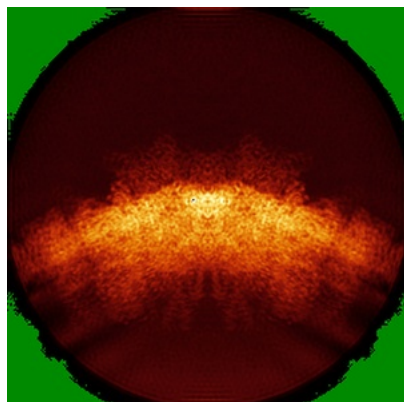
X
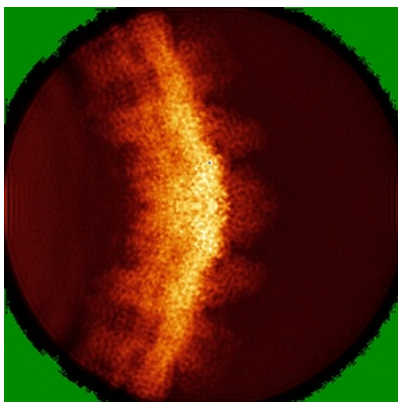
Y
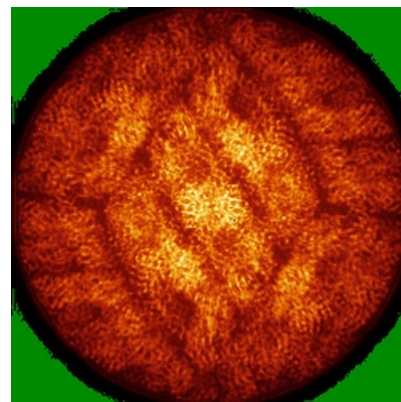
Z

6.4.2 Raw map

X

Y

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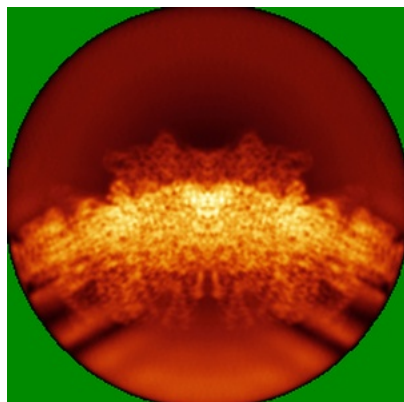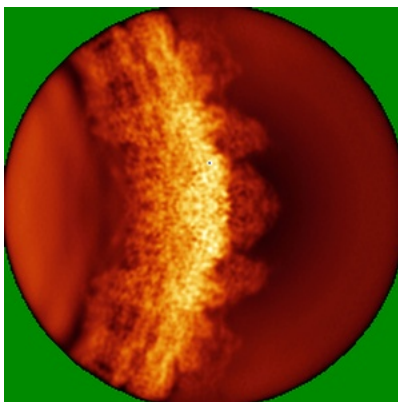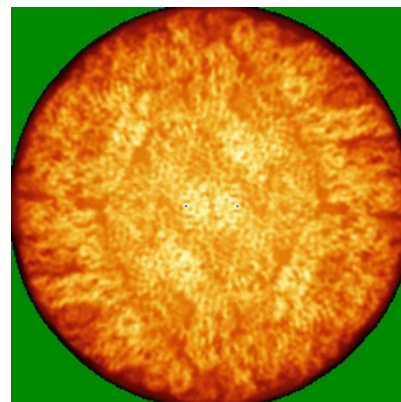
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

| X | Y | Z |
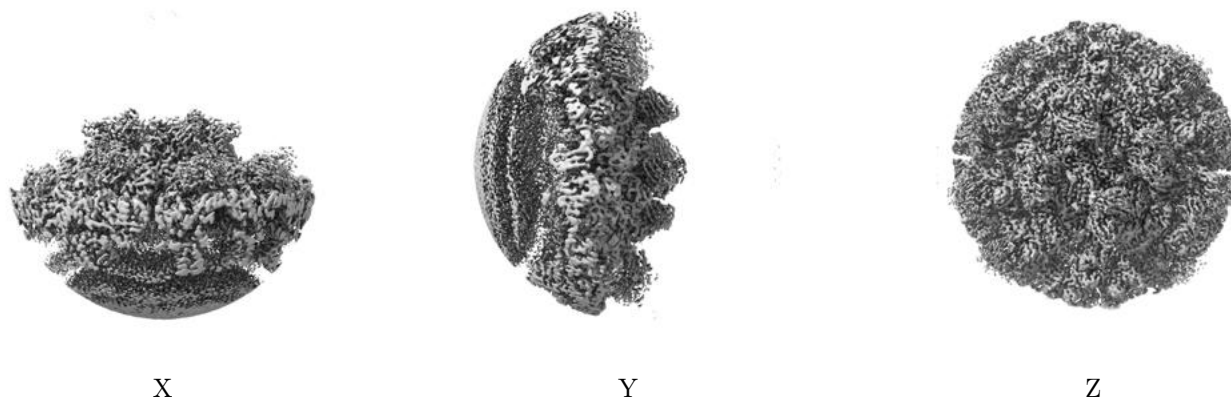
The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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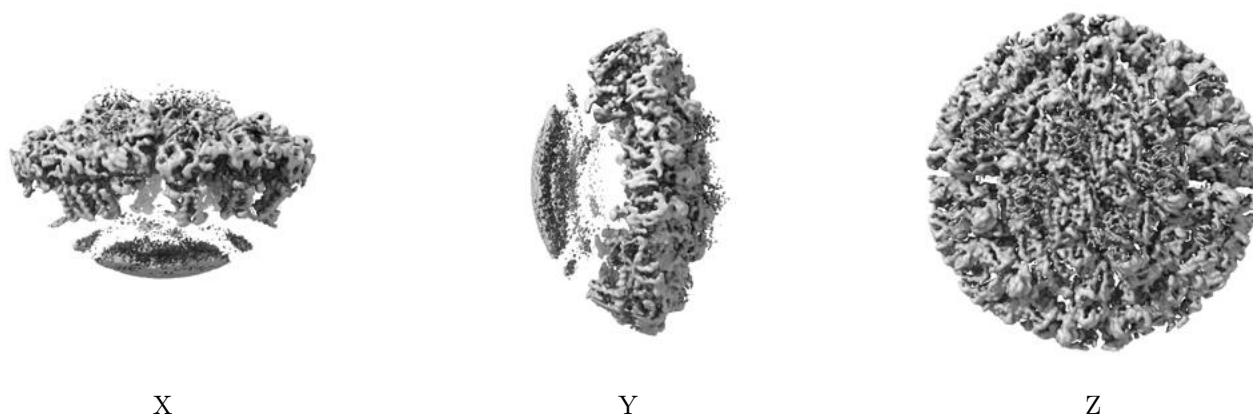
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation ⓘ

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure

- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1 emd_27056_msk_1.map ⓘ
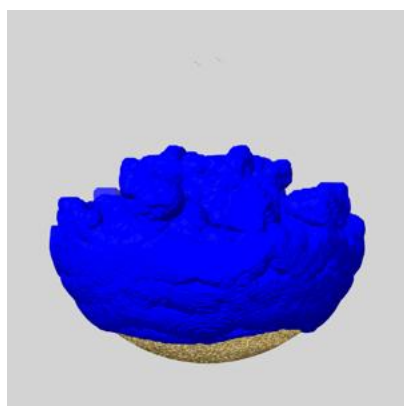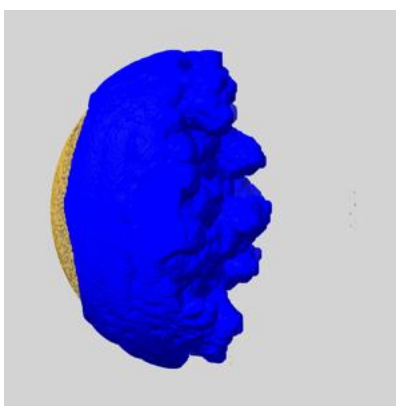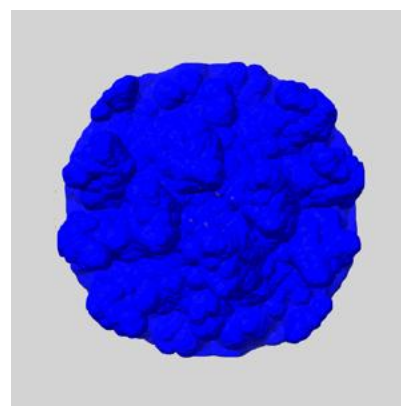
X   Y   Z

7 Map analysis (i)

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

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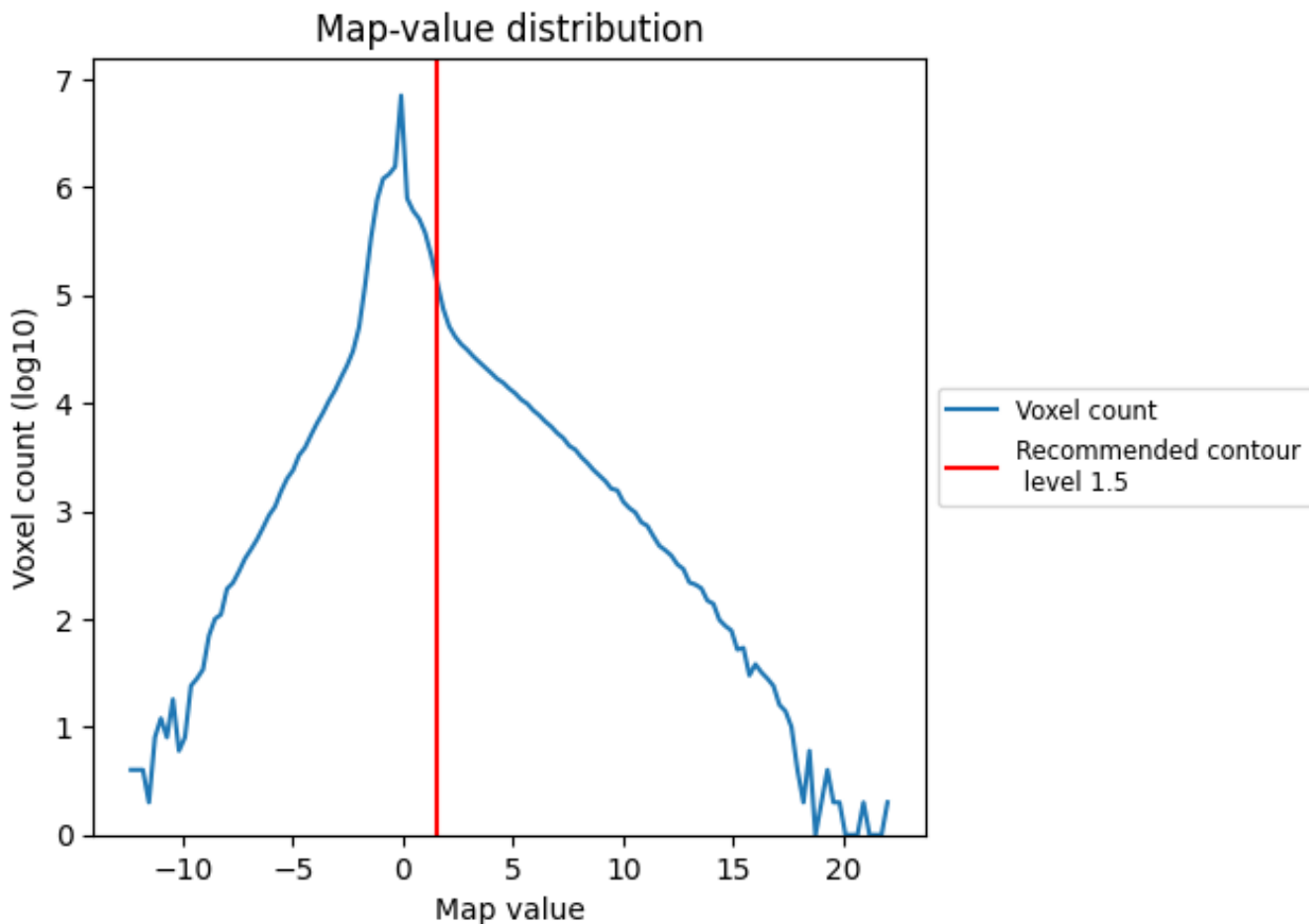
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
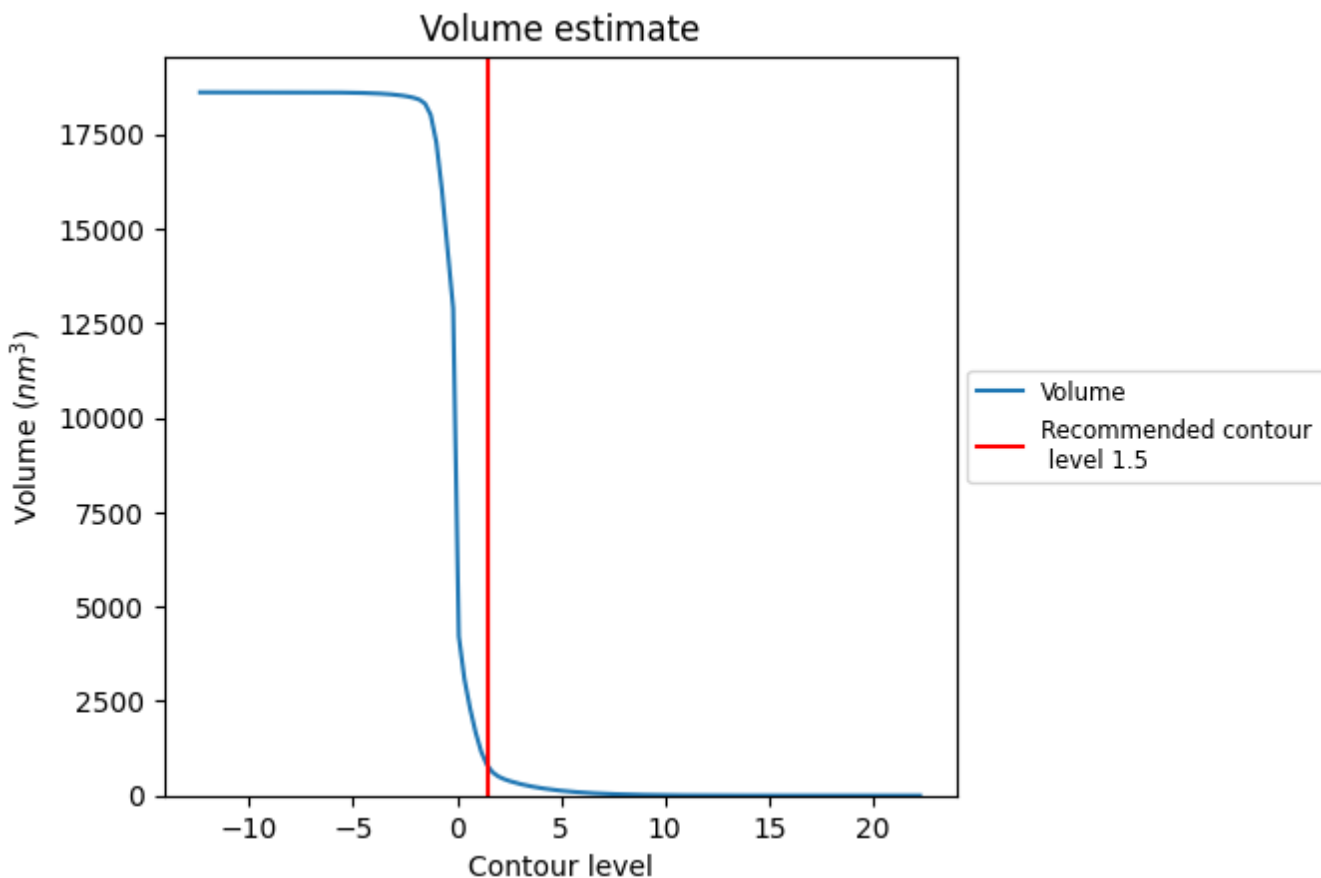
The volume at the recommended contour level is 769 nm^3; this corresponds to an approximate mass of 695 kDa.

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)
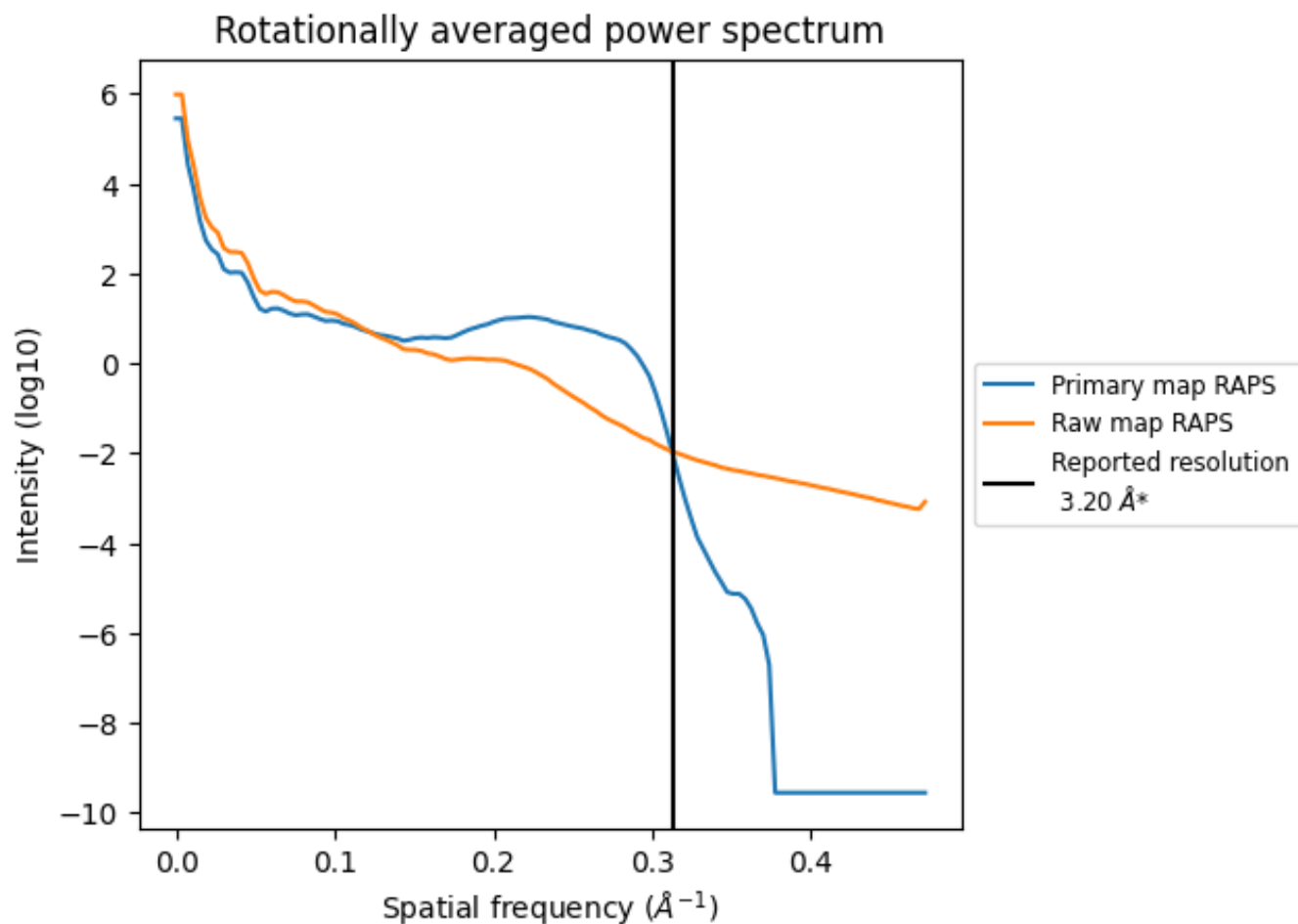
*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 ⓘ
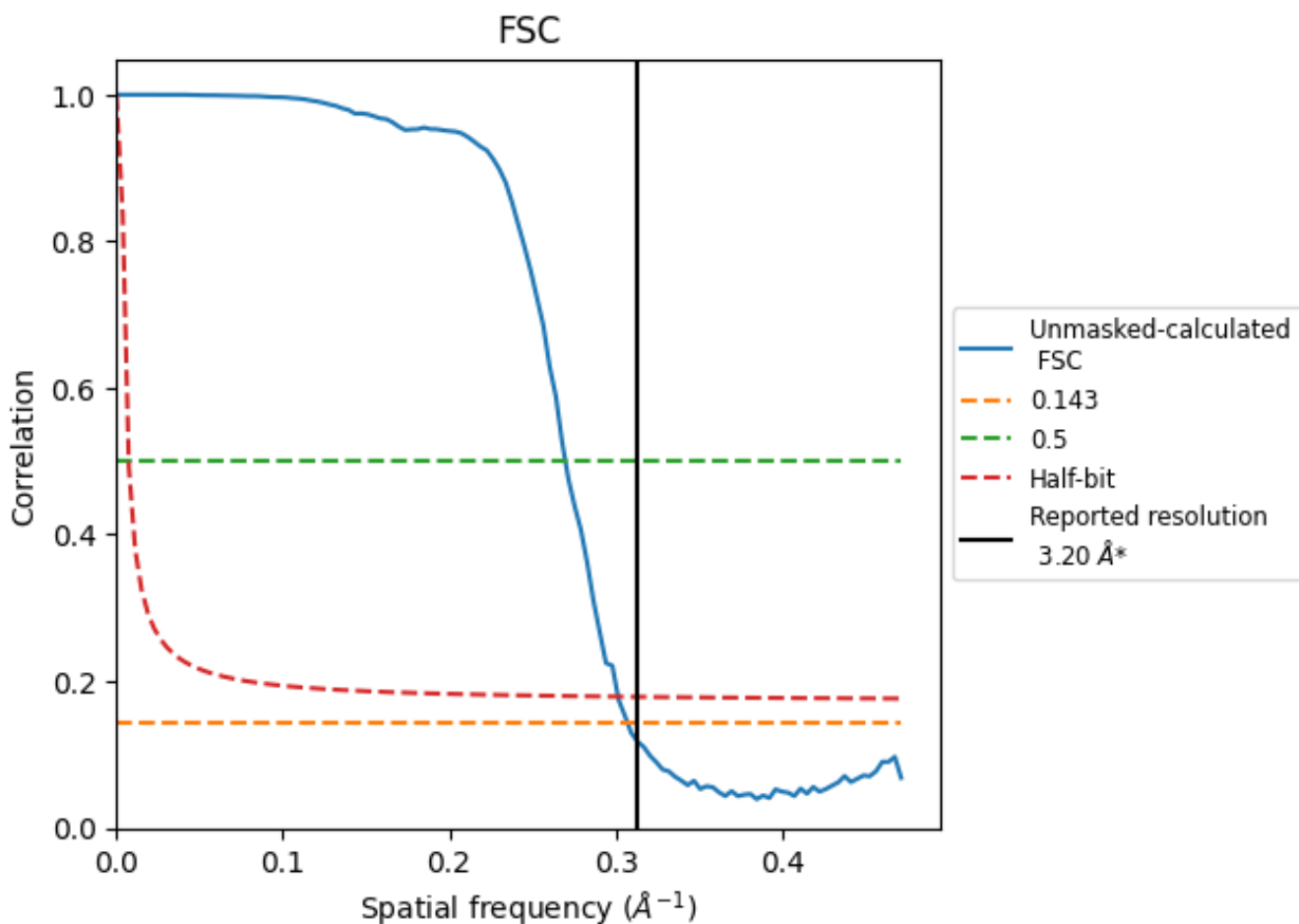
*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.26	3.71	3.32

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-27056 and PDB model 8CXH. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay ⓘ

X	Y	Z
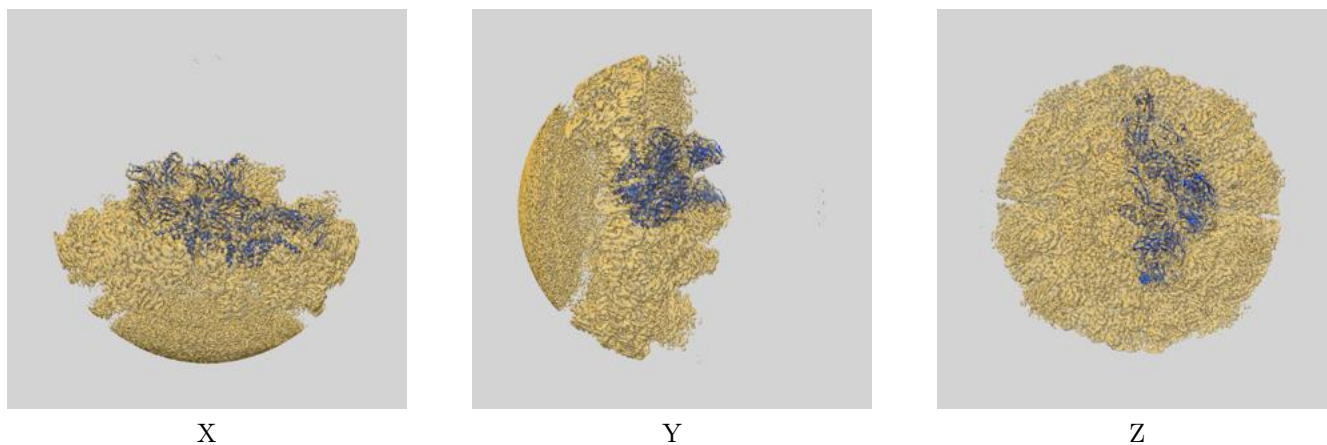
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model　ⓘ

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
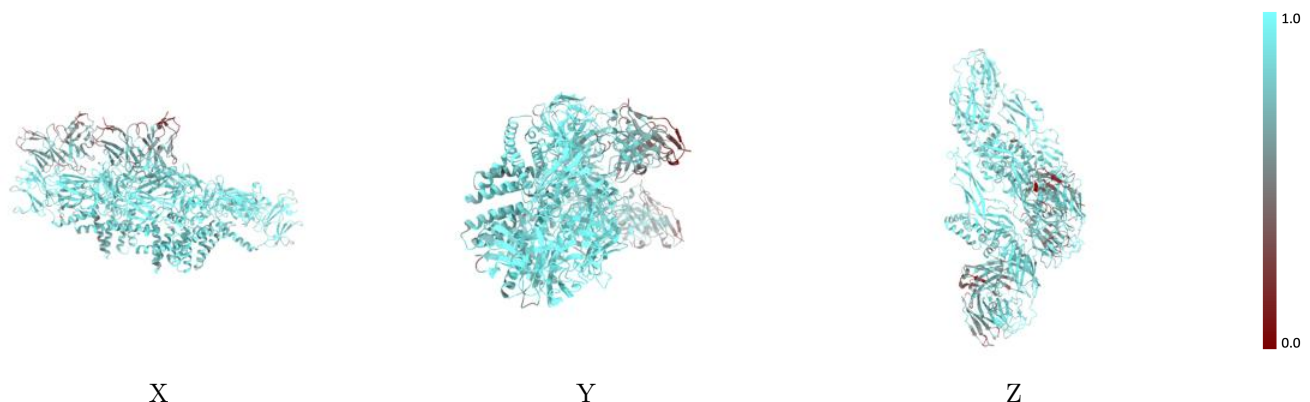
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.5).

9.4 Atom inclusion ⓘ
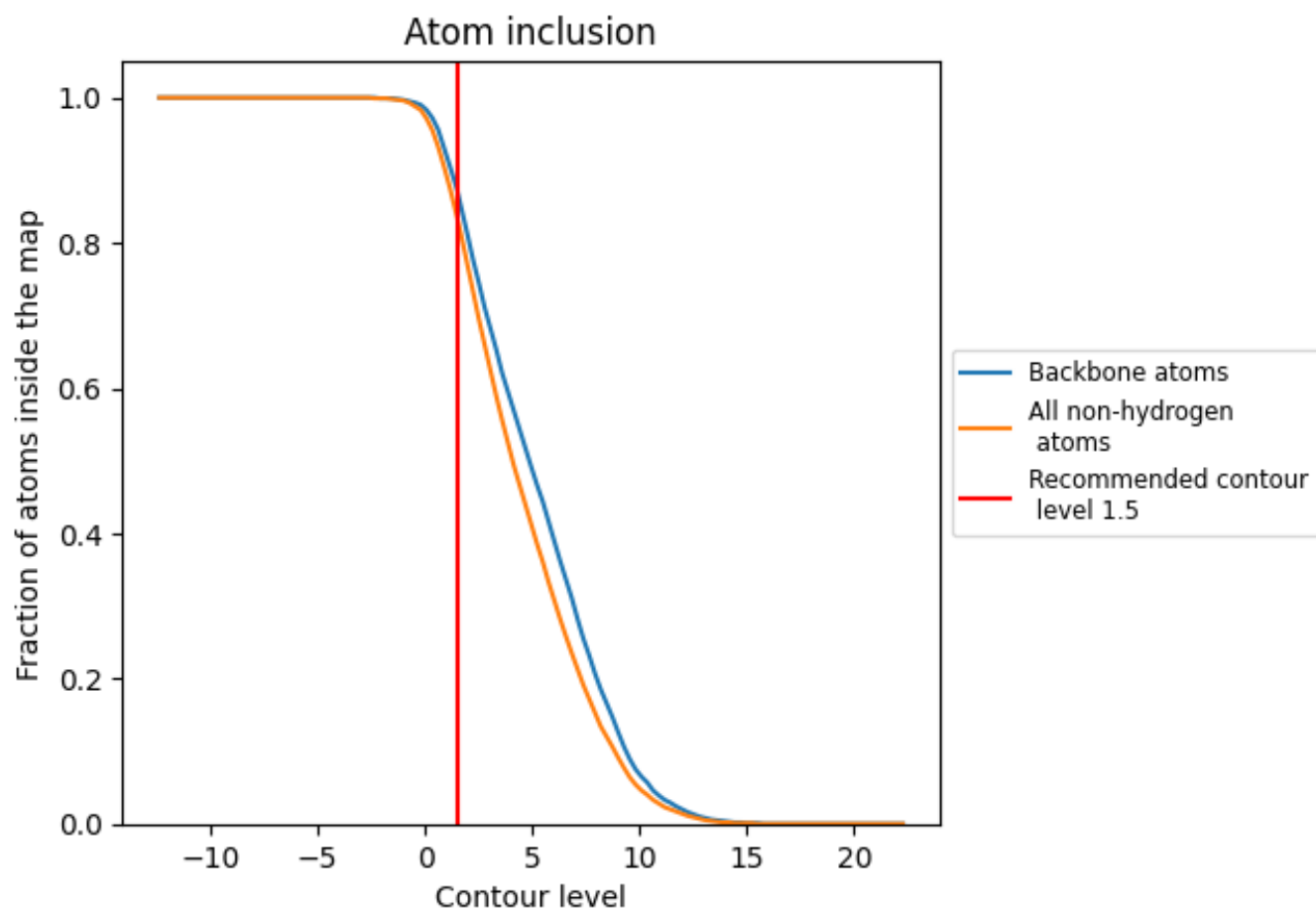
Atom inclusion

At the recommended contour level, 87% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8360	0.5350
A	0.8960	0.5450
B	0.8850	0.5330
C	0.8850	0.5330
D	0.9010	0.5610
E	0.8940	0.5420
F	0.9040	0.5450
H	0.6520	0.5300
L	0.6610	0.5310
h	0.5990	0.5090
l	0.6660	0.5320

1.0

0.0
<0.0