# Full wwPDB EM Validation Report

Dec 30, 2024 – 01:58 PM EST

| | | |
|---|---|---|
| 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.

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

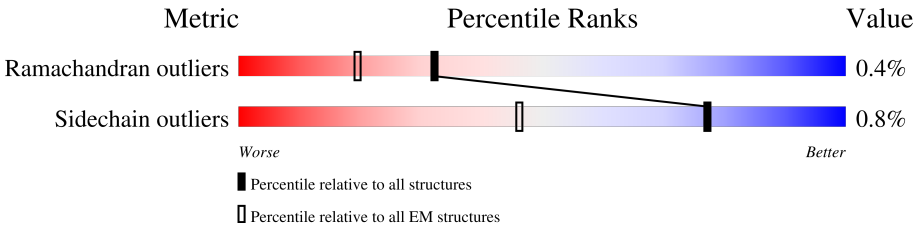
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev113 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA,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

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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 | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 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% ·· |

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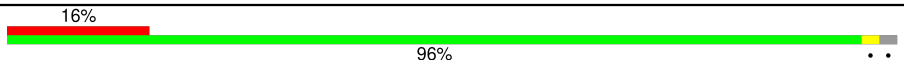
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | l | 110 |   |

# 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.

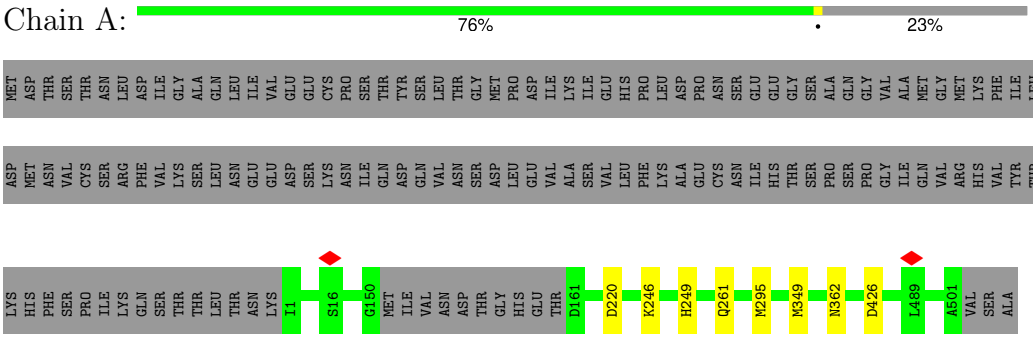
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | L | 108 | Total | C | N | O | S | 0 | 0 |
| | | | 787 | 488 | 134 | 162 | 3 | | |
| 4 | l | 108 | Total | C | N | O | S | 0 | 0 |
| | | | 787 | 488 | 134 | 162 | 3 | | |

# 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.

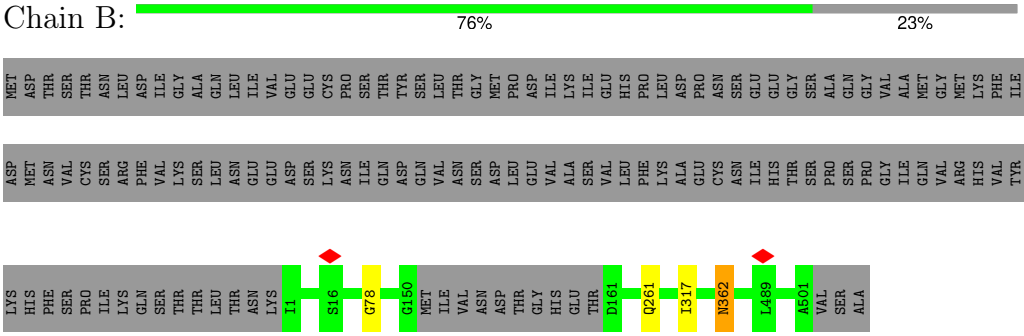
• Molecule 1: Ankyrin repeat family A protein 2,Envelope E protein

Chain A:



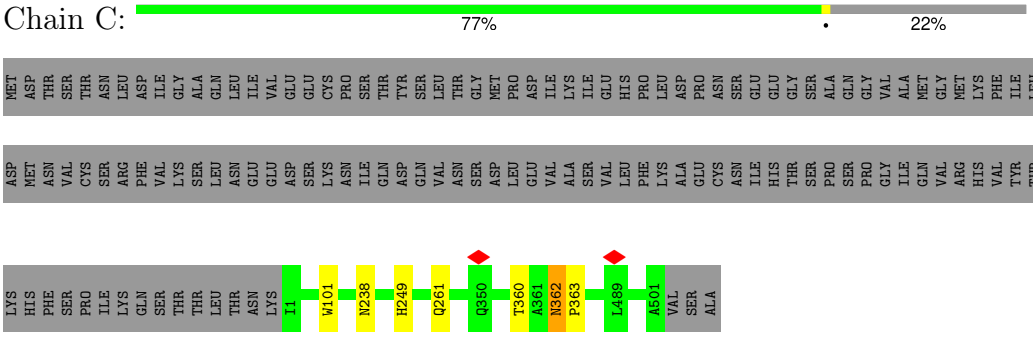

• Molecule 1: Ankyrin repeat family A protein 2,Envelope E protein

Chain B:



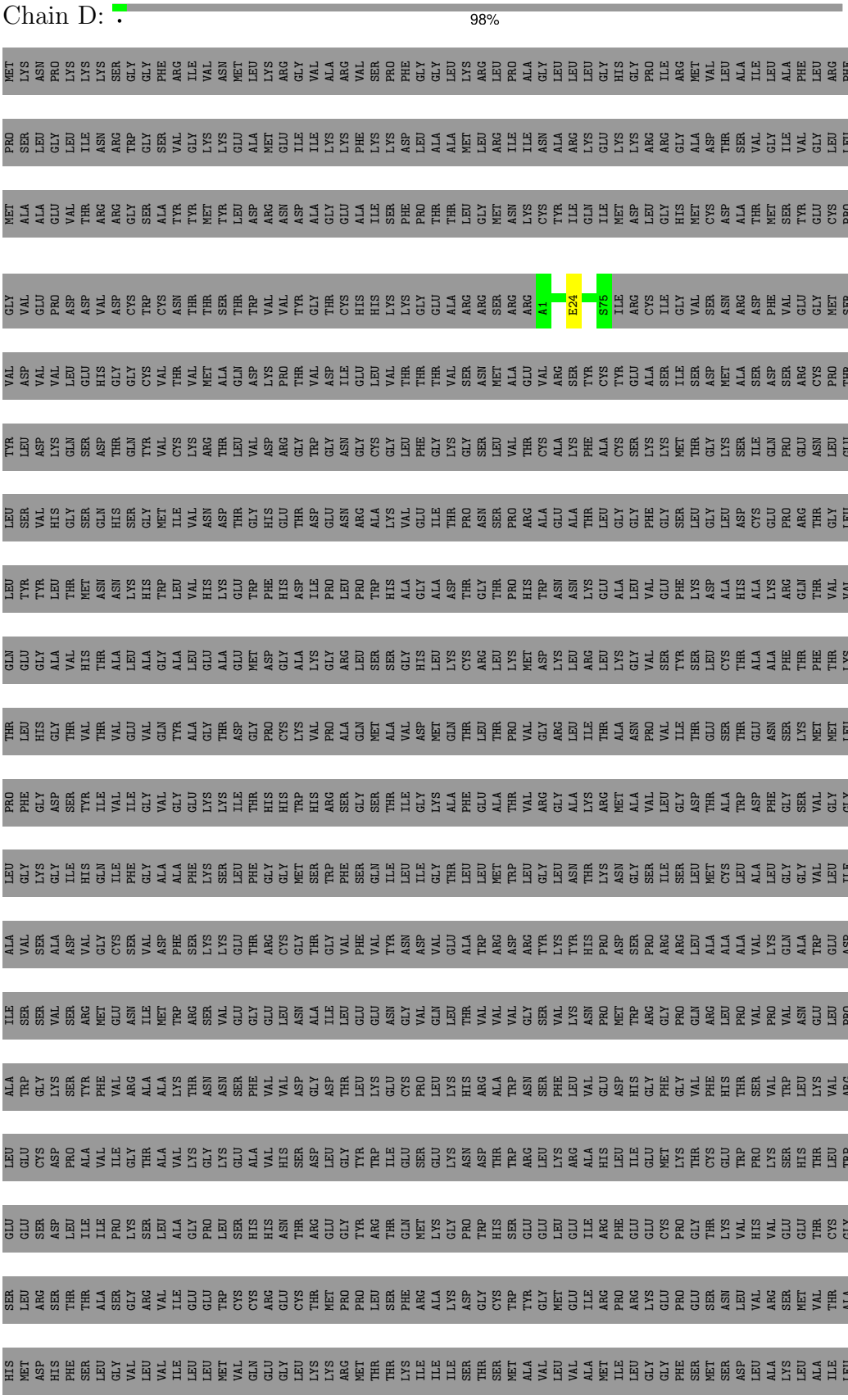

• Molecule 1: Ankyrin repeat family A protein 2,Envelope E protein

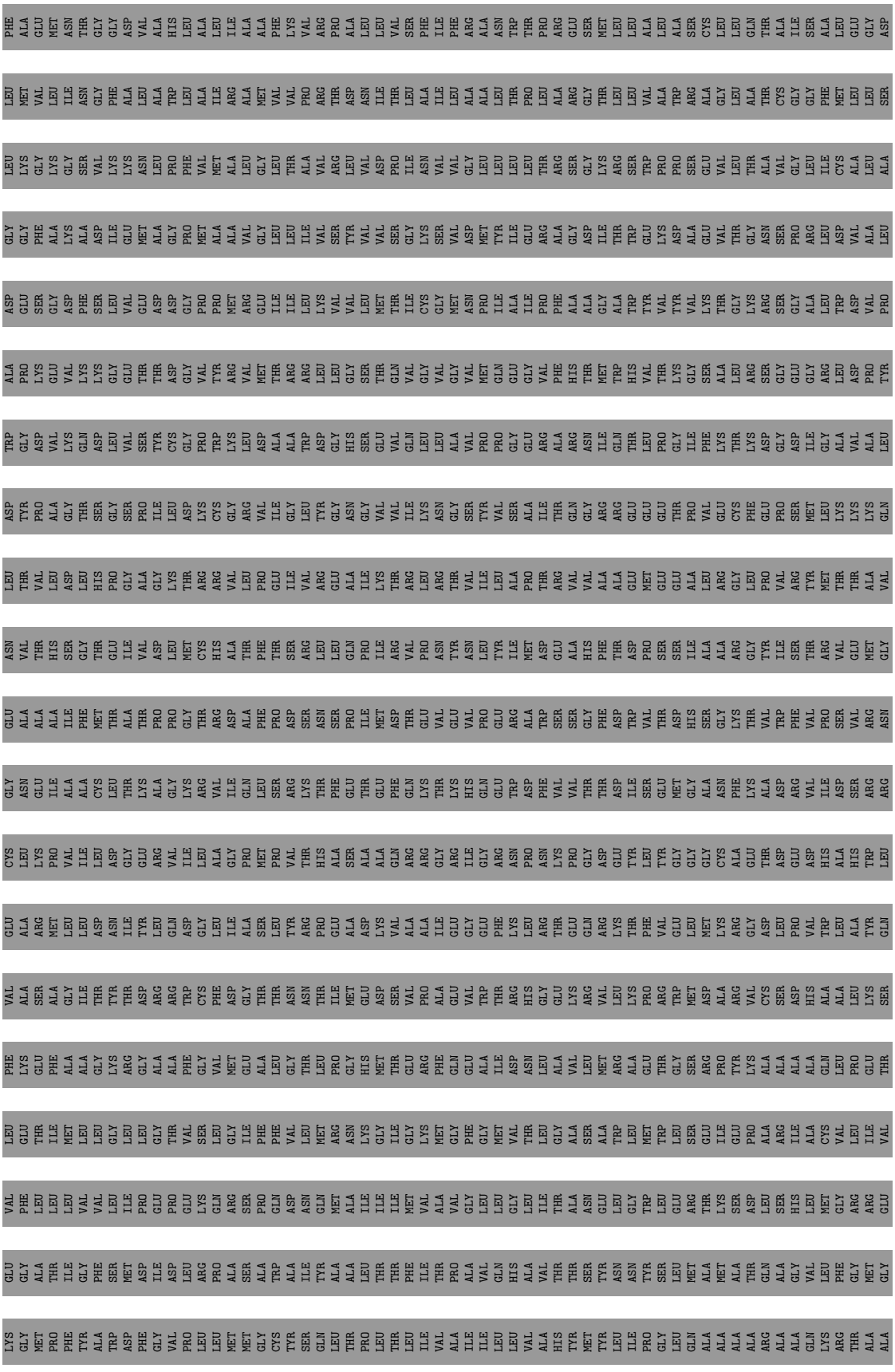
Chain C:

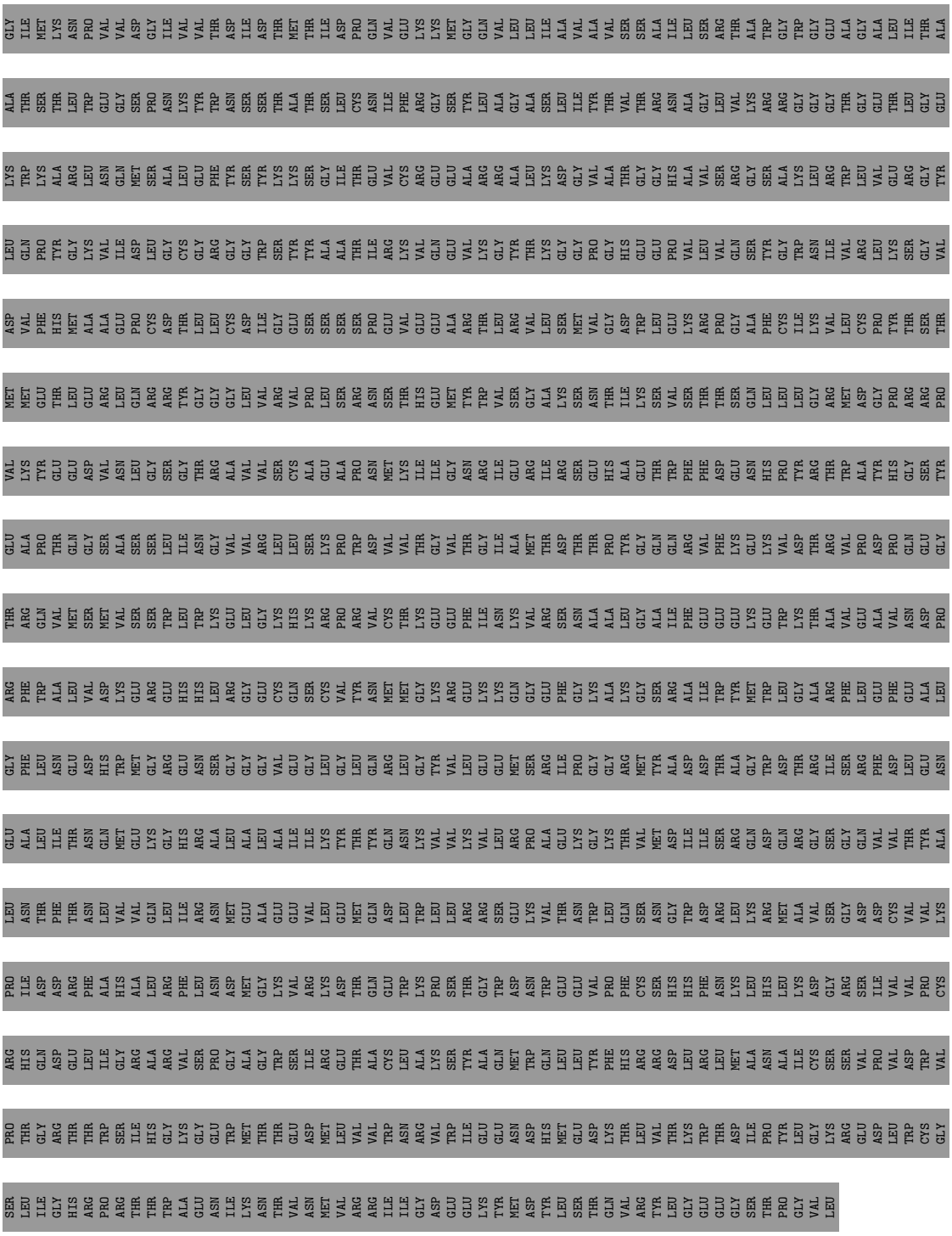


• Molecule 2: Membrane M protein

Chain D:



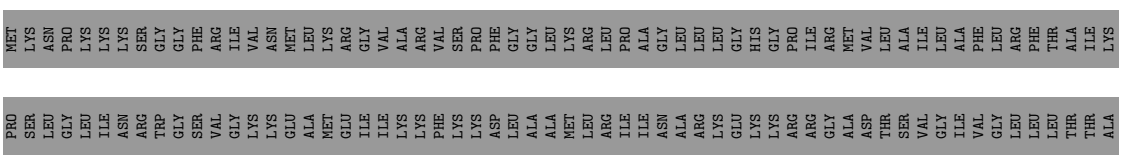

PHE ALA GLU MET ASN THR GLY GLY ASP VAL ALA HIS LEU ALA LEU ILE ILE ALA ALA ALA PHE LYS VAL ARG PRO ALA LEU LEU VAL SER PHE ILE PHE ARG ALA ASN TRP THR PRO ARG GLU SER MET LEU LEU ALA LEU ALA SER CYS LEU LEU GLN THR ALA ILE SER ALA LEU GLU GLY ASP
LEU MET VAL LEU ILE ASN GLY PHE ALA LEU ALA ALA TRP LEU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



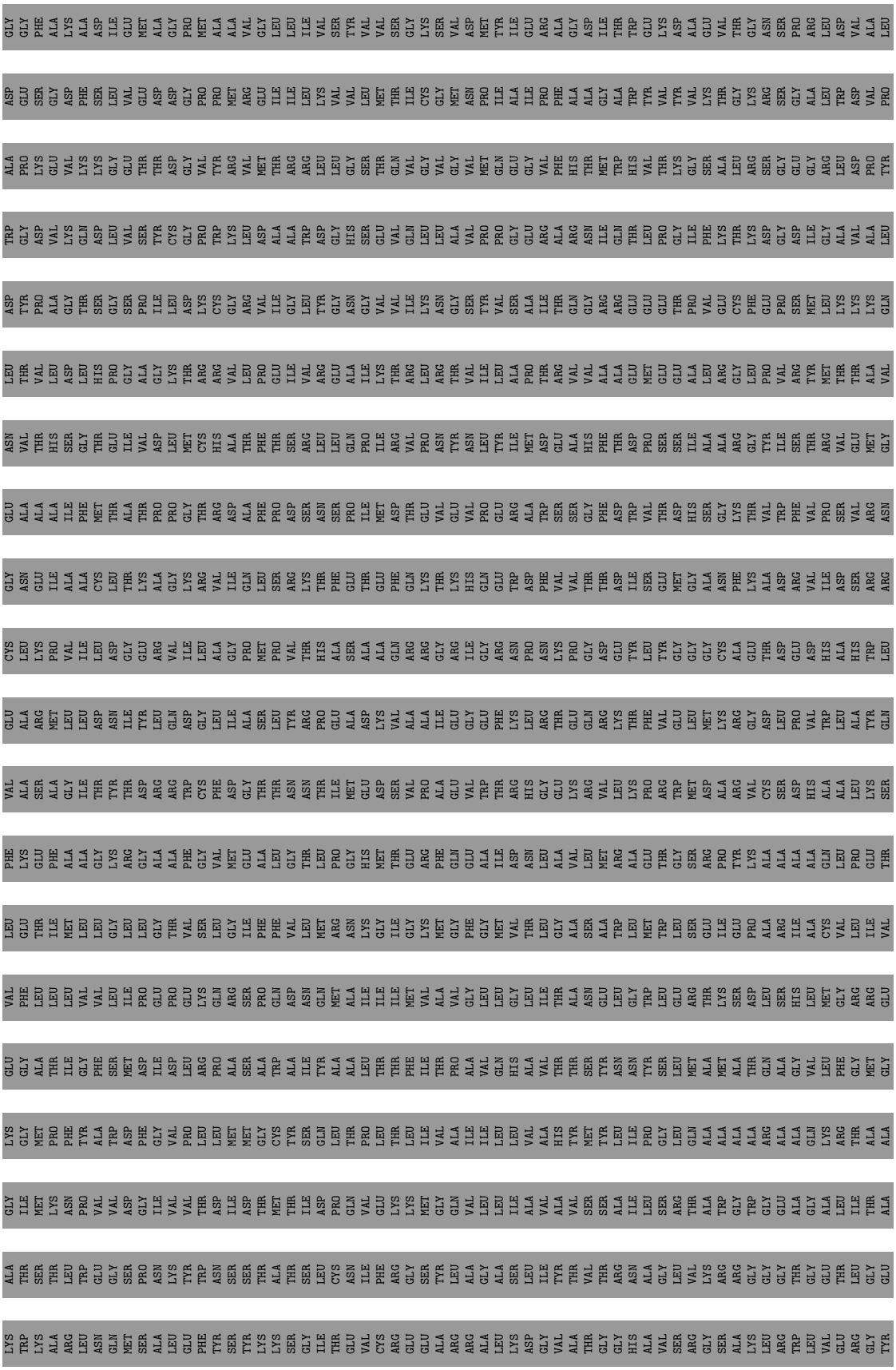

• Molecule 2: Membrane M protein

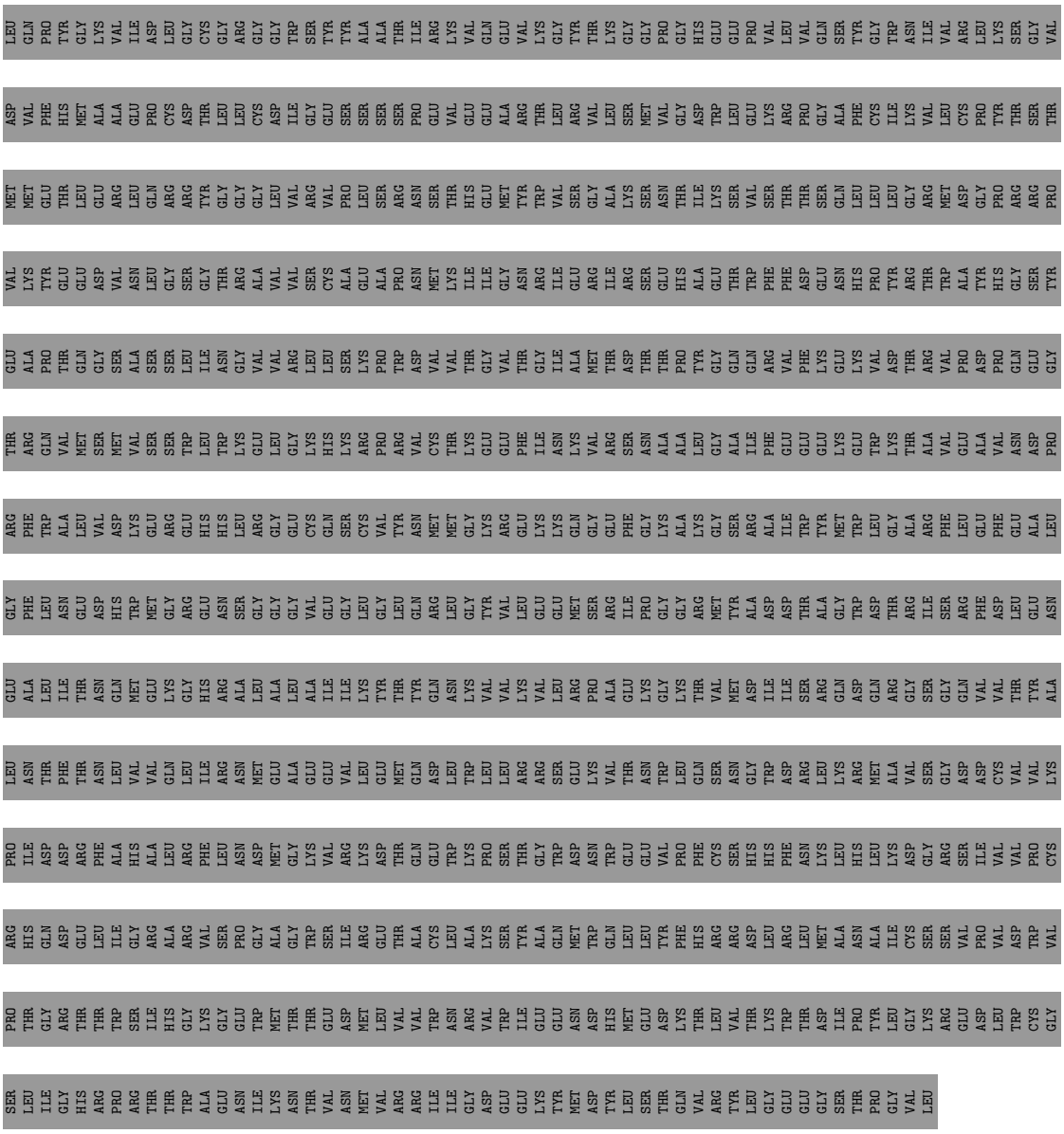
Chain E:



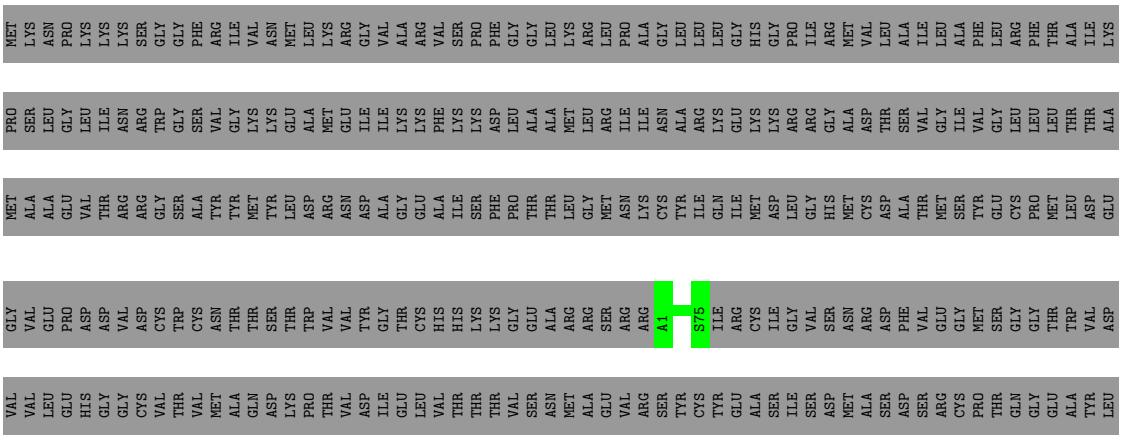
A1
R15
S75

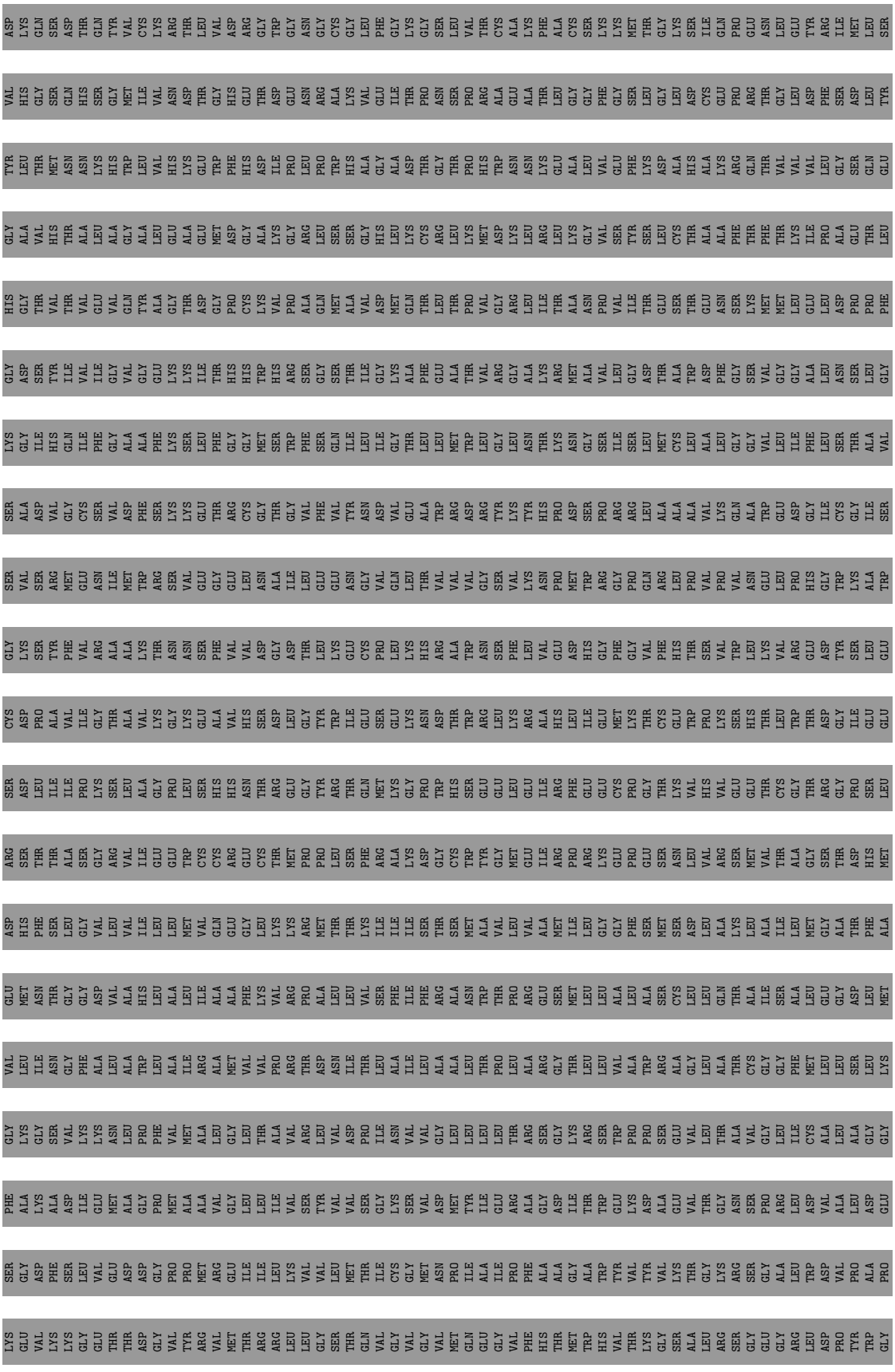


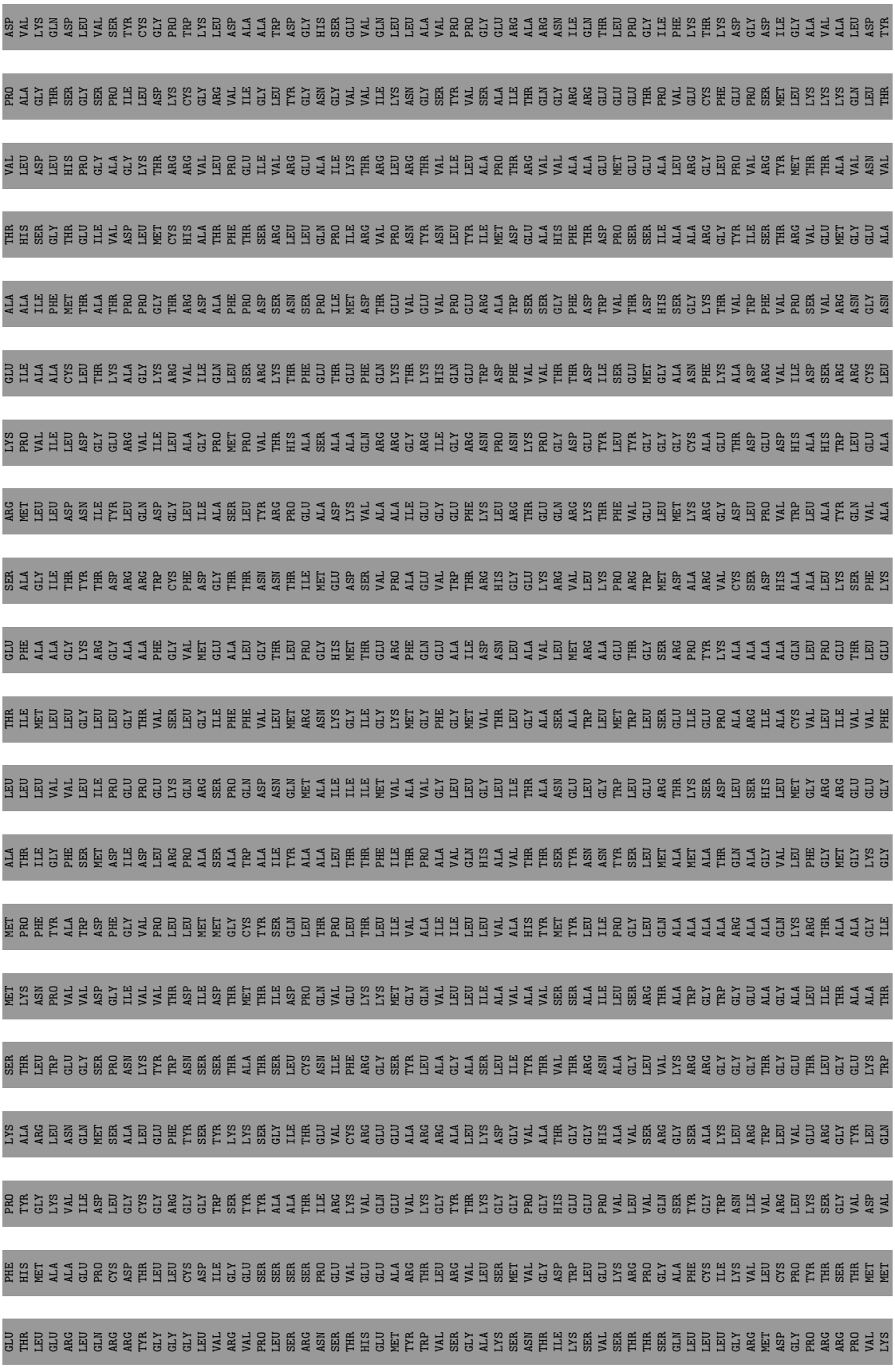


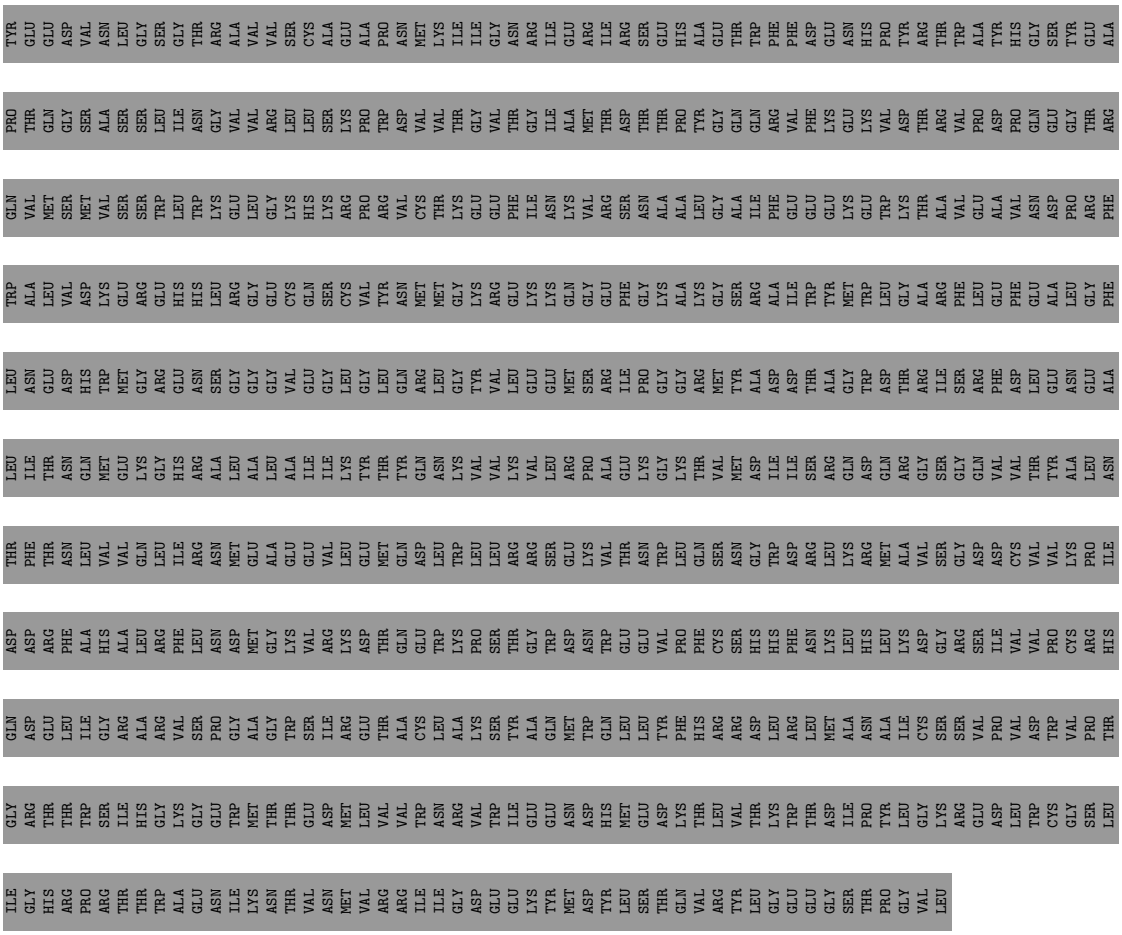
• Molecule 2: Membrane M protein

Chain F: 98%



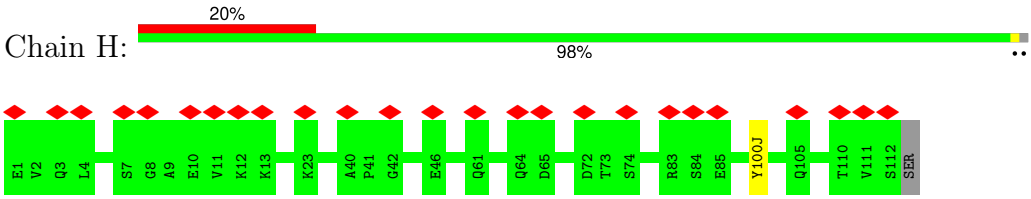



ASP VAL LYS GLN ASP LEU VAL SER TYR CYS GLY PRO TRP LYS LEU ASP ALA ALA TRP ASP GLY HIS SER GLU VAL GLN LEU LEU ALA VAL PRO PRO GLY GLU ARG ALA ARG ASN ILE GLN THR LEU PRO GLY ILE PHE LYS THR LYS ASP GLY ALA VAL ALA LEU ASP TYR
PRO ALA GLY THR SER GLY SER PRO ILE LEU ASP LYS CYS GLY ARG VAL ILE GLY LEU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



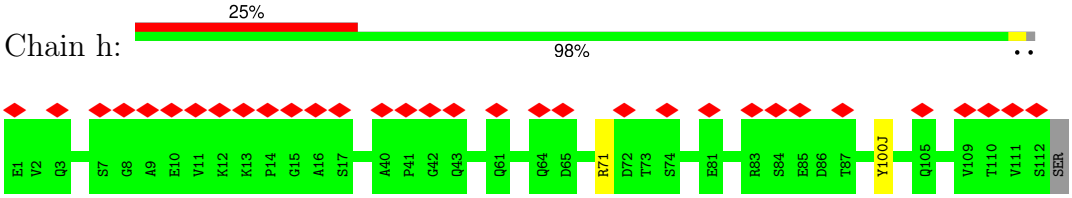

• Molecule 3: C10 heavy chain

Chain H:



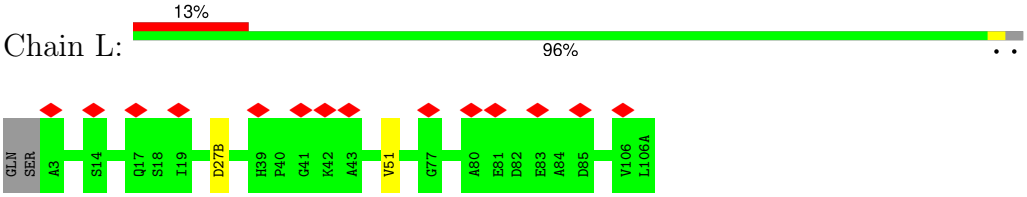

• Molecule 3: C10 heavy chain

Chain h:



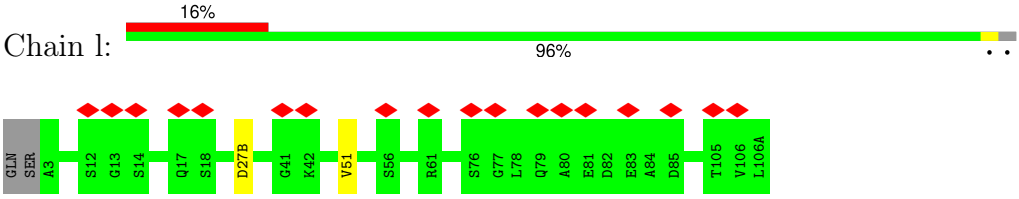

• Molecule 4: C10 light chain

Chain L:



• Molecule 4: C10 light chain

Chain l:



# 4 Experimental information (i)

| 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 ($e^-/Å^2$) | 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

## 5.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 1 | A | 0.47 | 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%) | 30 | 64 |
| 1 | B | 487/639 (76%) | 433 (89%) | 51 (10%) | 3 (1%) | 22 | 57 |
| 1 | C | 499/639 (78%) | 443 (89%) | 54 (11%) | 2 (0%) | 30 | 64 |
| 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%) | 14 | 49 |
| 4 | l | 106/110 (96%) | 100 (94%) | 5 (5%) | 1 (1%) | 14 | 49 |
| All | All | 2154/12662 (17%) | 1939 (90%) | 206 (10%) | 9 (0%) | 32 | 64 |

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 (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 399/534 (75%) | 394 (99%) | 5 (1%) | 65 83 |
| 1 | B | 399/534 (75%) | 398 (100%) | 1 (0%) | 91 96 |
| 1 | C | 408/534 (76%) | 406 (100%) | 2 (0%) | 86 93 |
| 2 | D | 64/2832 (2%) | 63 (98%) | 1 (2%) | 58 79 |
| 2 | E | 64/2832 (2%) | 63 (98%) | 1 (2%) | 58 79 |
| 2 | F | 64/2832 (2%) | 64 (100%) | 0 | 100 100 |
| 3 | H | 107/108 (99%) | 106 (99%) | 1 (1%) | 75 89 |
| 3 | h | 107/108 (99%) | 105 (98%) | 2 (2%) | 52 76 |
| 4 | L | 88/90 (98%) | 87 (99%) | 1 (1%) | 70 86 |
| 4 | l | 88/90 (98%) | 87 (99%) | 1 (1%) | 70 86 |
| All | All | 1788/10494 (17%) | 1773 (99%) | 15 (1%) | 77 90 |

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 (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

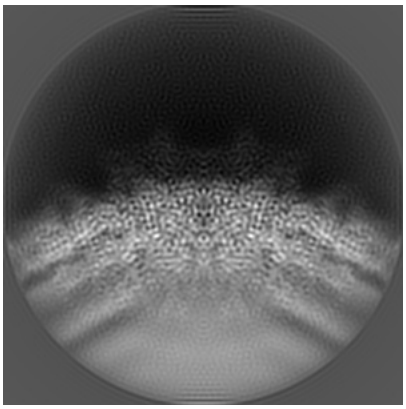
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27056. These allow visual inspection of the internal detail of the map and identification of artifacts.

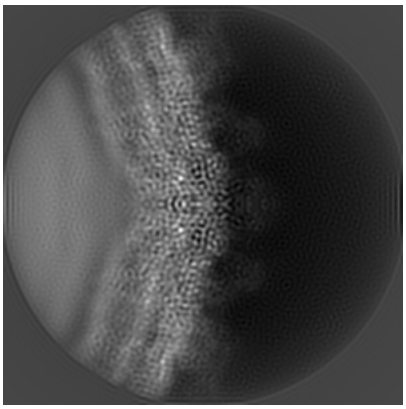
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

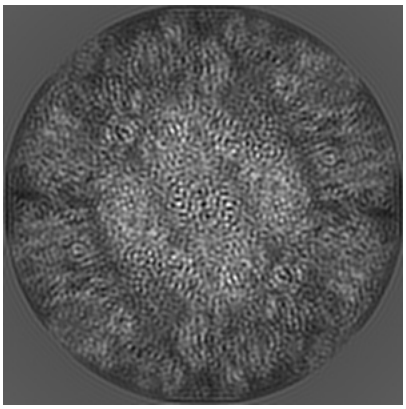
### 6.1.1 Primary map



X

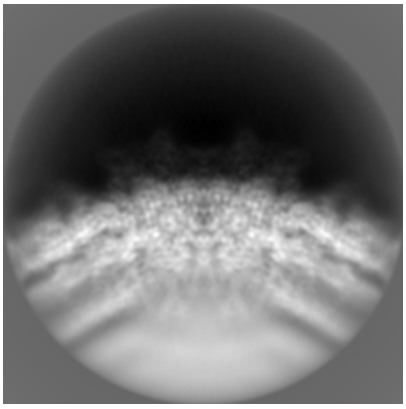


Y

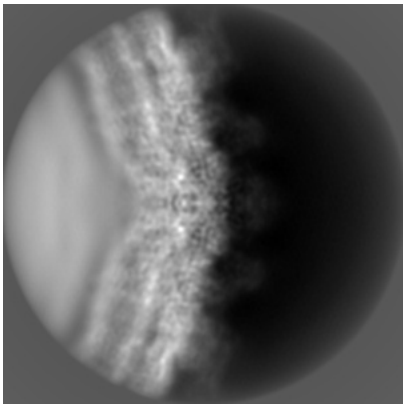


Z

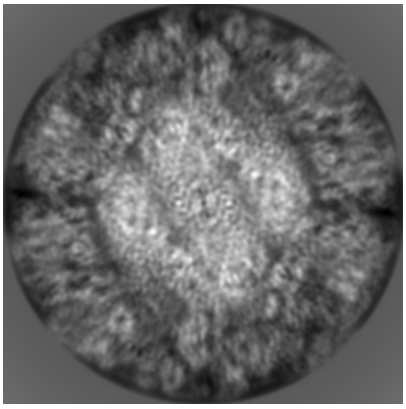
### 6.1.2 Raw map



X



Y

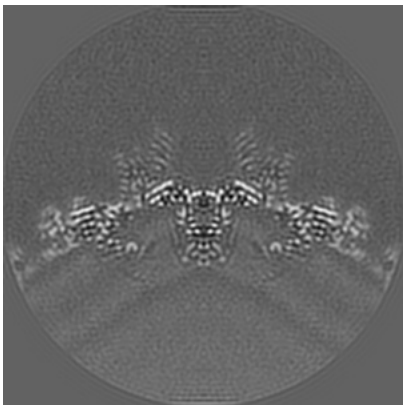


Z

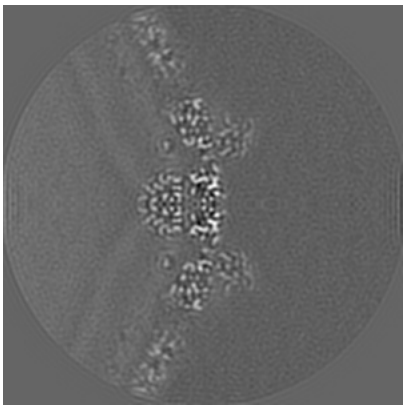
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

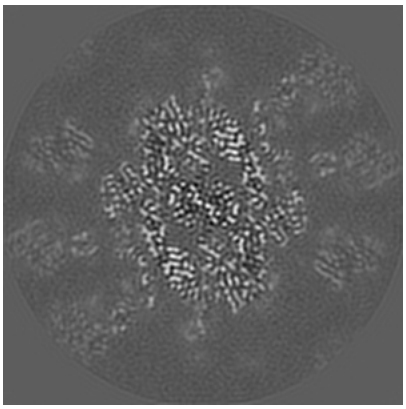
### 6.2.1 Primary map



X Index: 125

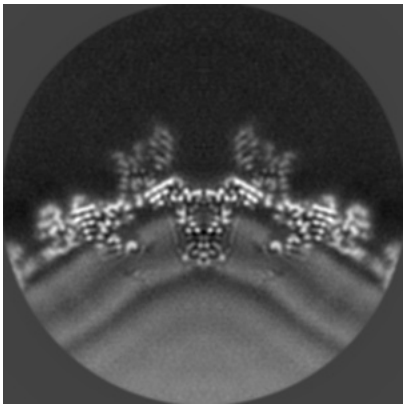


Y Index: 125

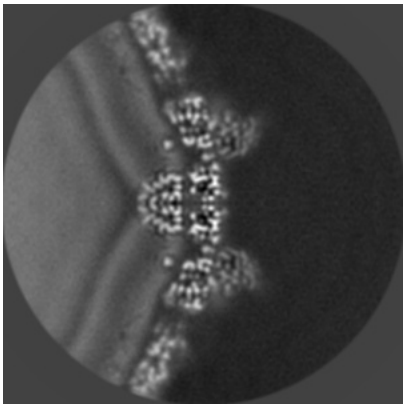


Z Index: 125

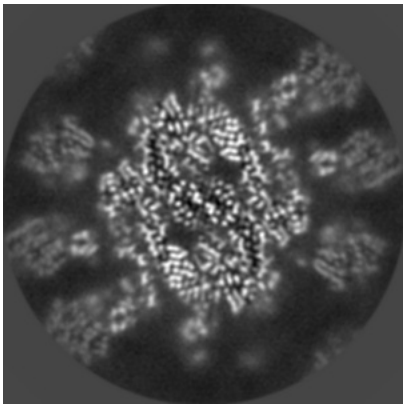
### 6.2.2 Raw map



X Index: 125



Y Index: 125

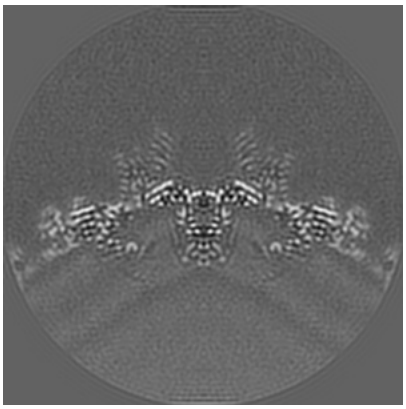


Z Index: 125

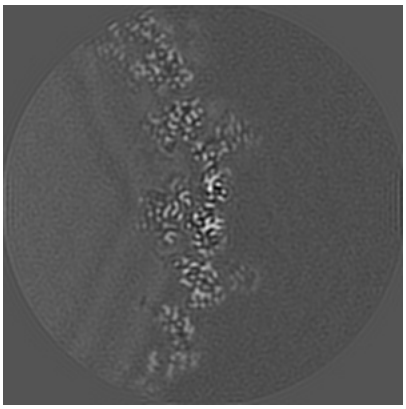
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

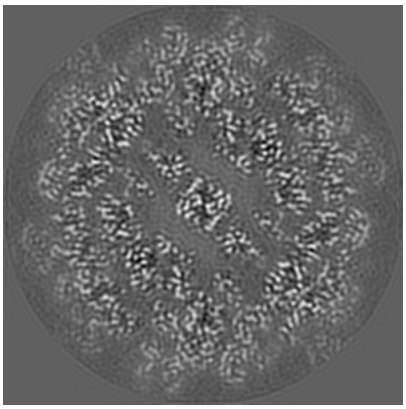
### 6.3.1 Primary map



X Index: 125

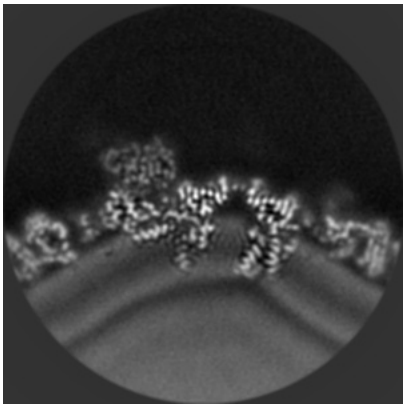


Y Index: 134

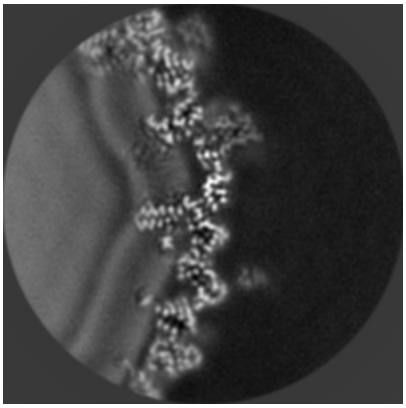


Z Index: 110

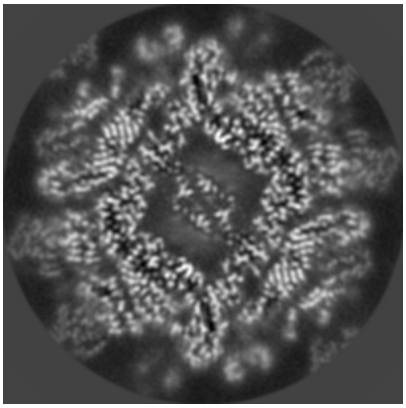
### 6.3.2 Raw map



X Index: 140



Y Index: 138

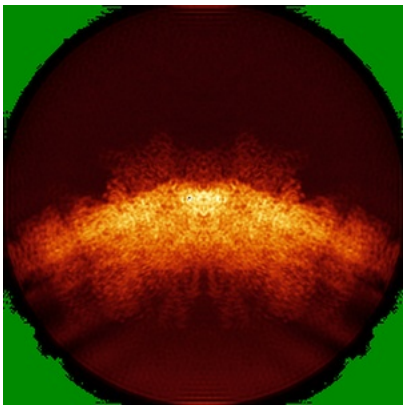


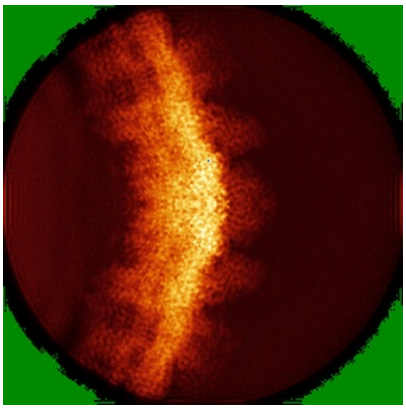
Z Index: 115

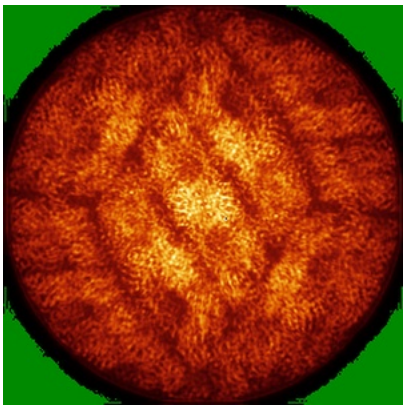
The images above show the largest variance slices of the map in three orthogonal directions.

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

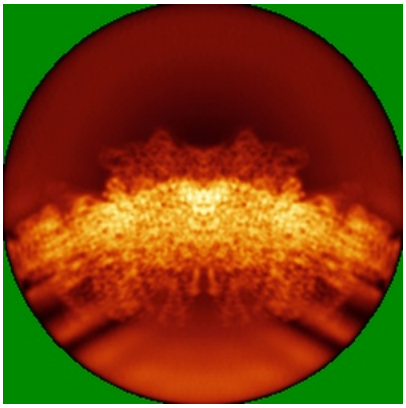
### 6.4.1 Primary map

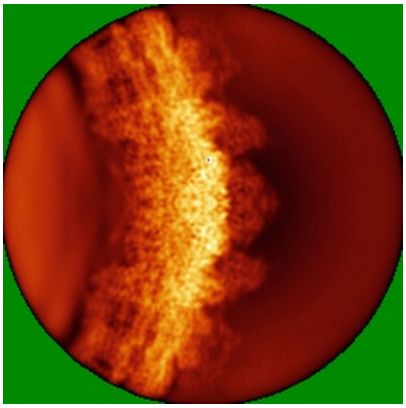

X

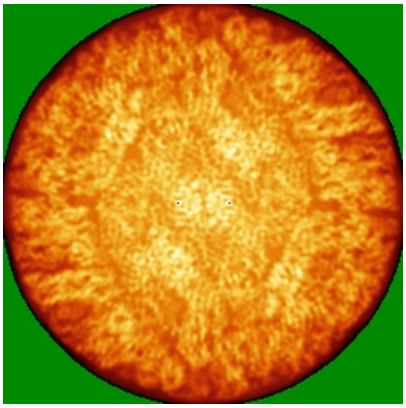

Y


Z

### 6.4.2 Raw map


X

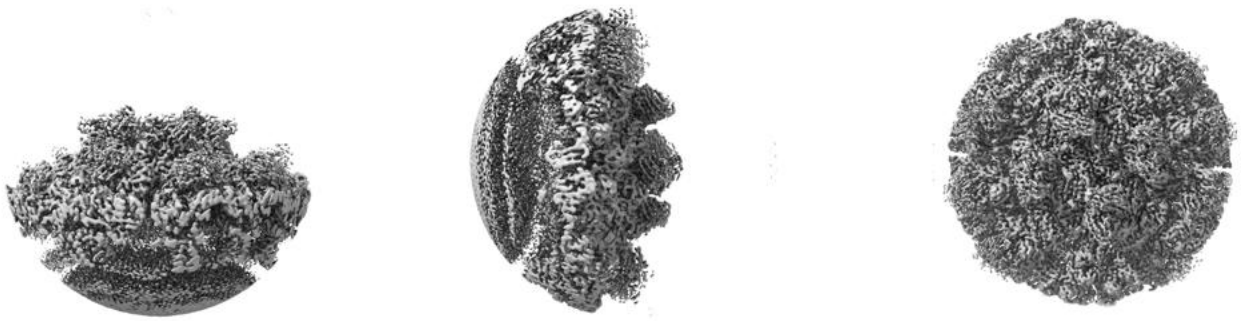

Y


Z

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

## 6.5 Orthogonal surface views (i)

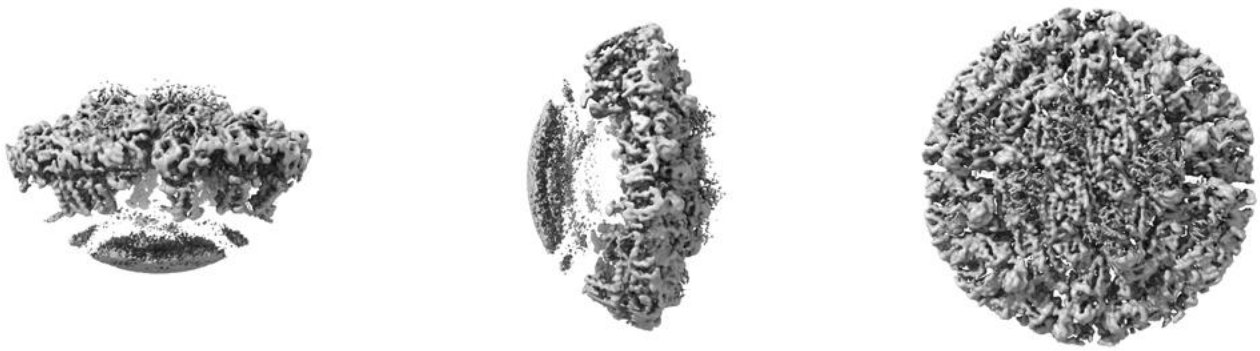
### 6.5.1 Primary map



X Y Z

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

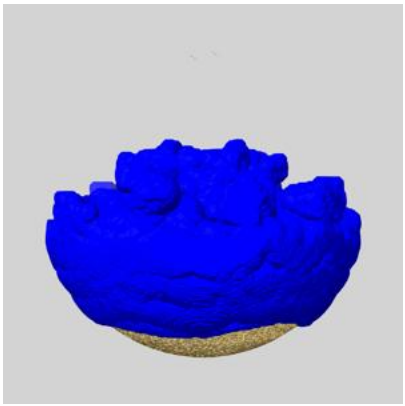
## 6.6 Mask visualisation (i)

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

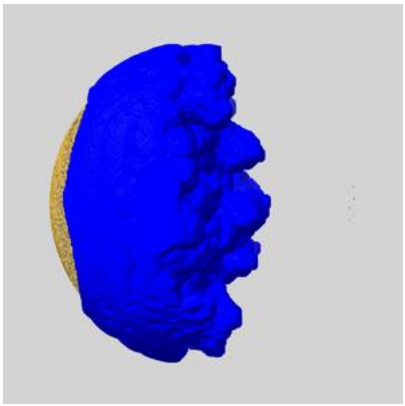
A mask typically either:

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

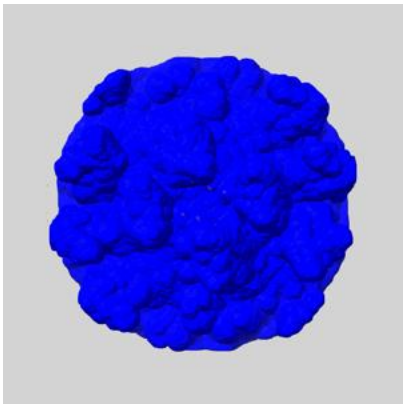
### 6.6.1 emd_27056_msk_1.map (i)



X



Y

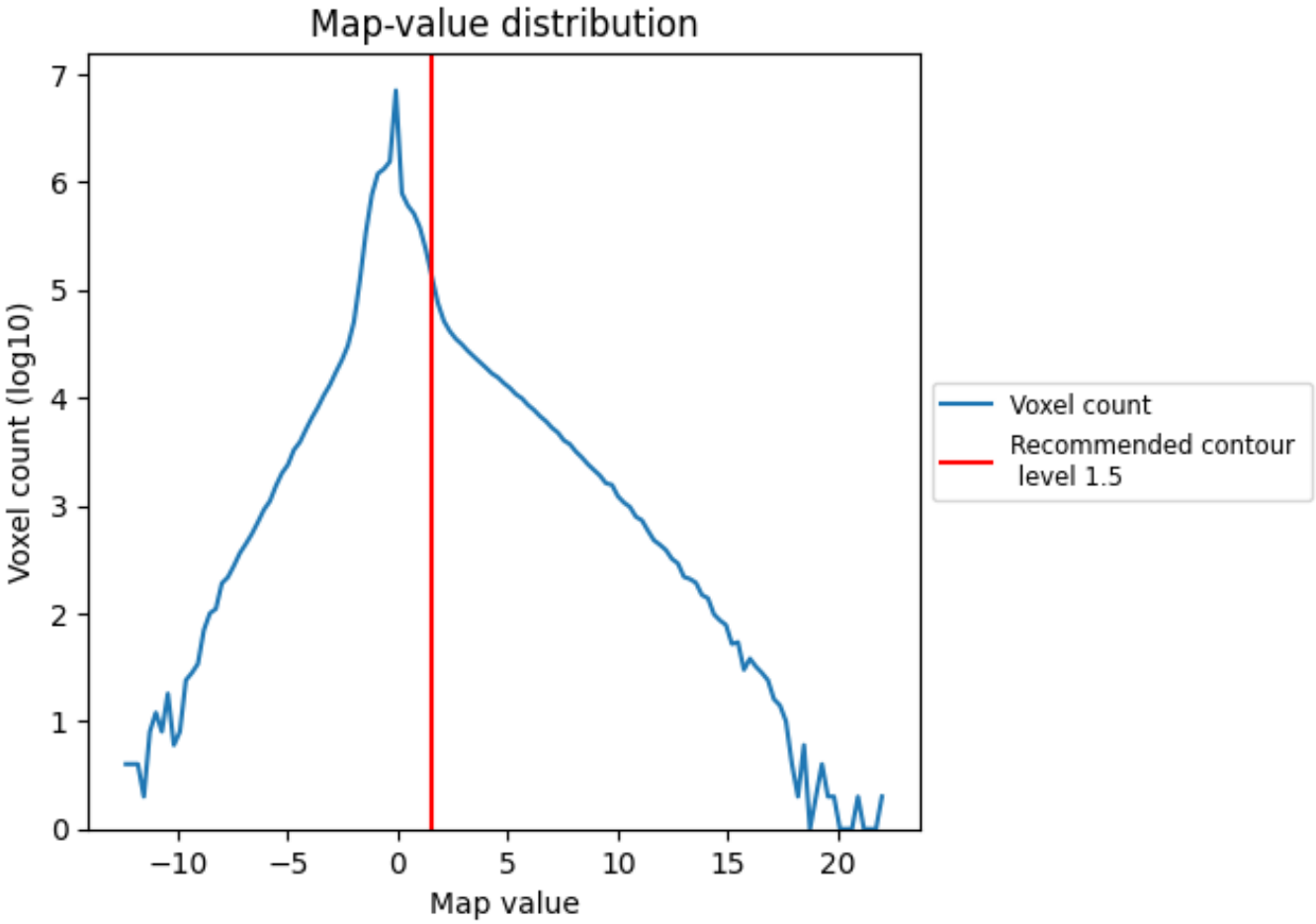


Z

# 7 Map analysis

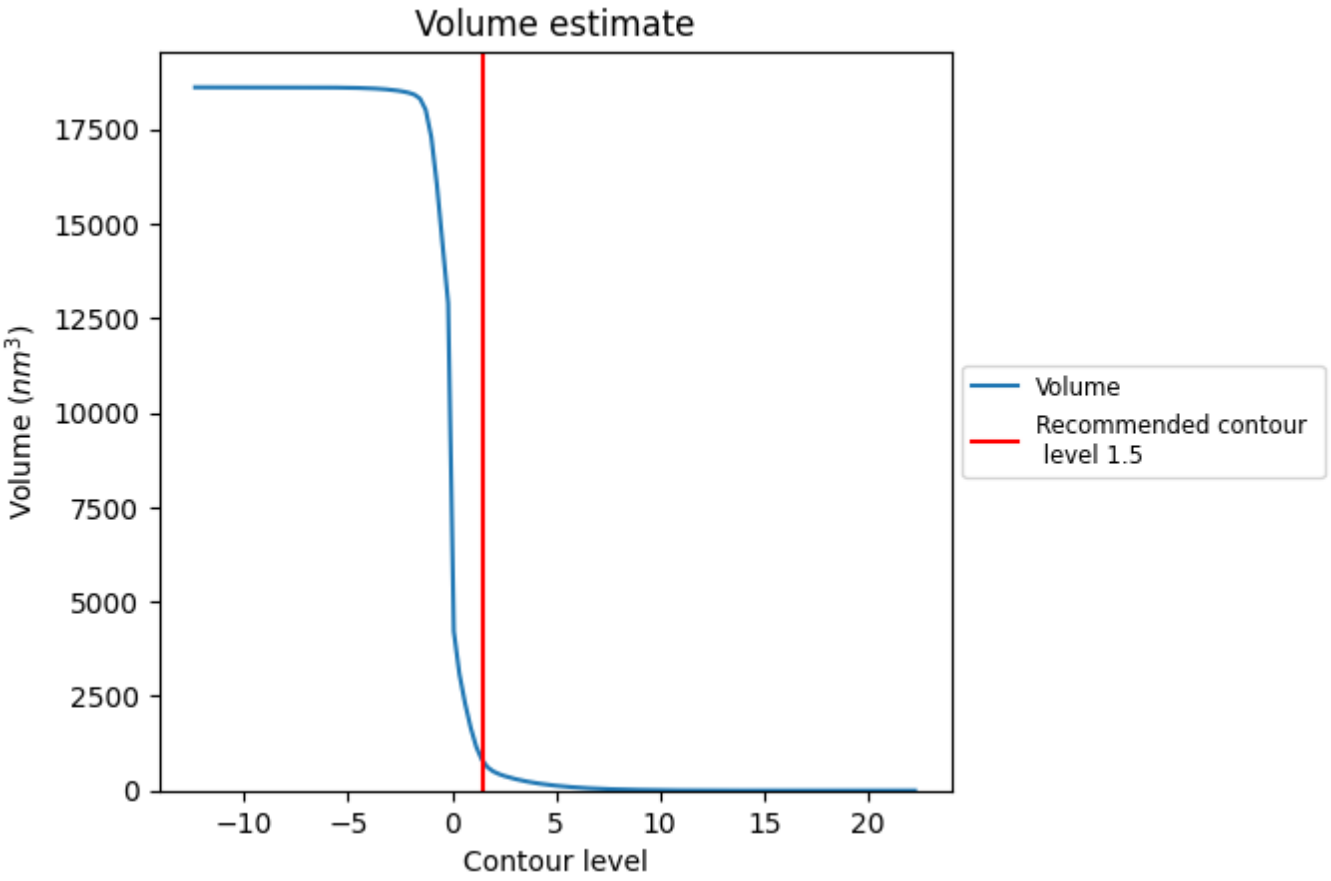
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

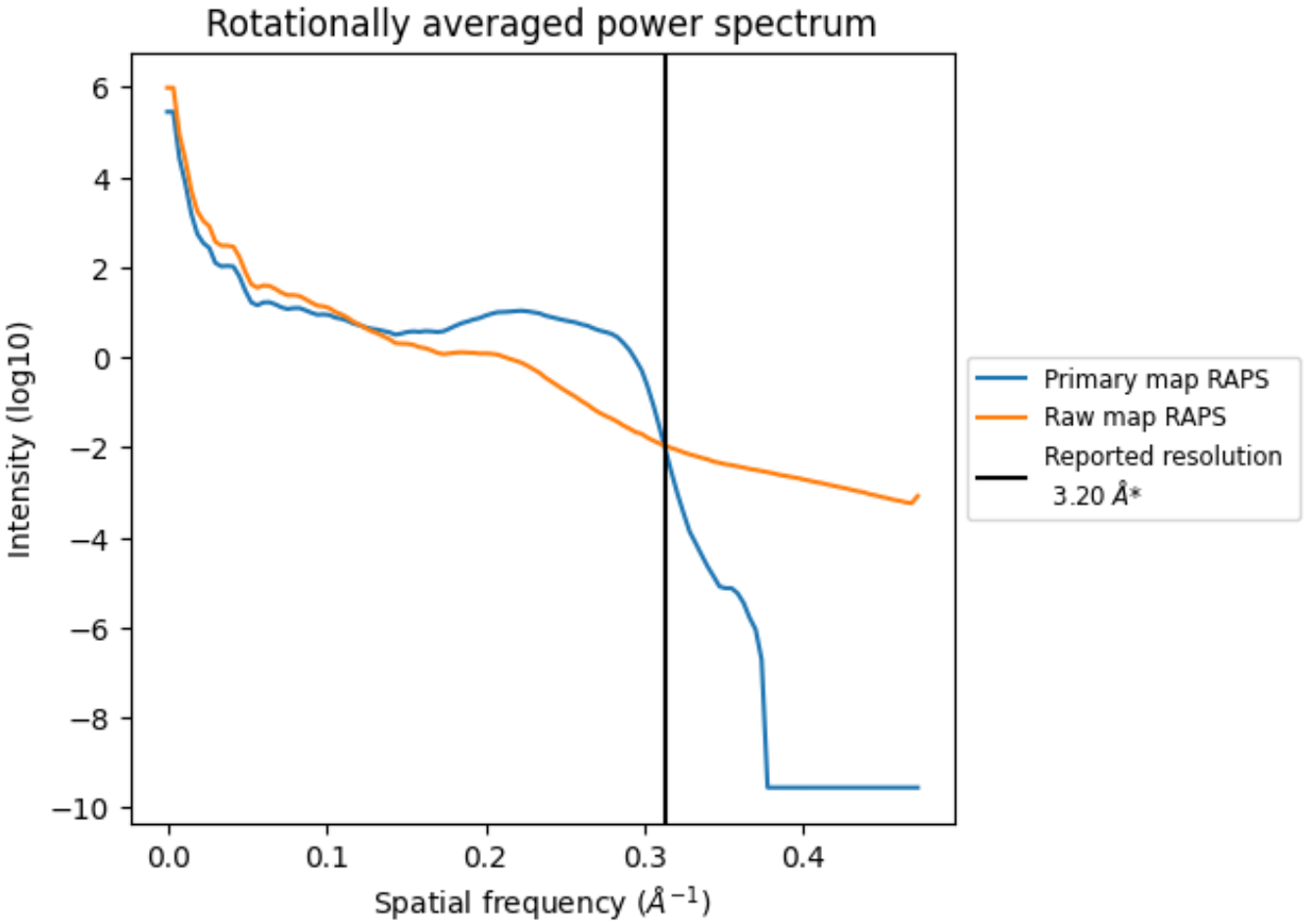
## 7.2 Volume estimate




The volume at the recommended contour level is 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)

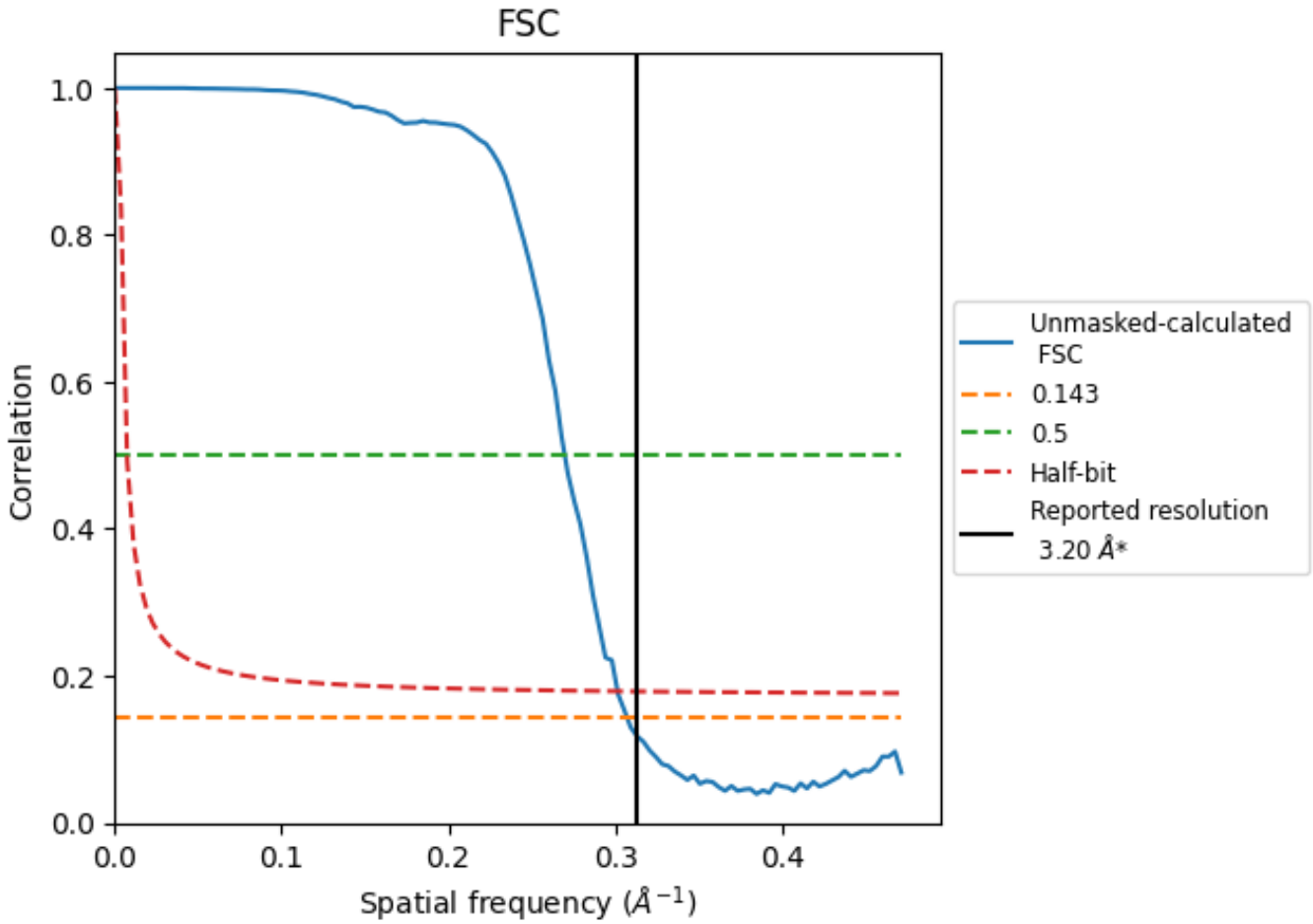



*Reported resolution corresponds to spatial frequency of 0.312 Å$^{-1}$

# 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)

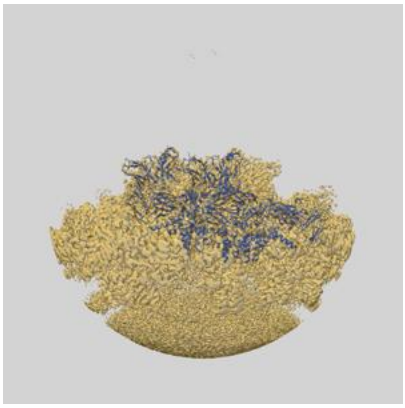
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.20 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 3.26 | 3.71 | 3.32 |

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

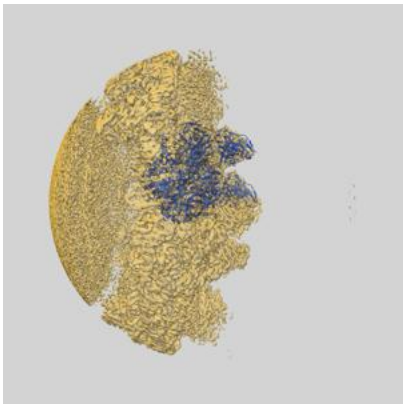
# 9 Map-model fit

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.

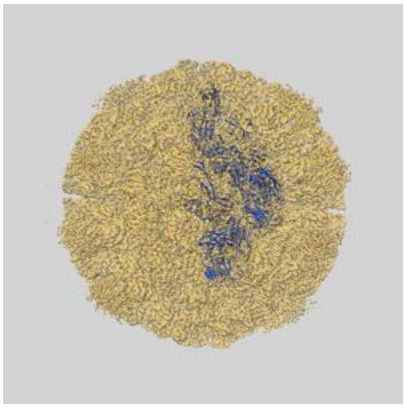
## 9.1 Map-model overlay



X



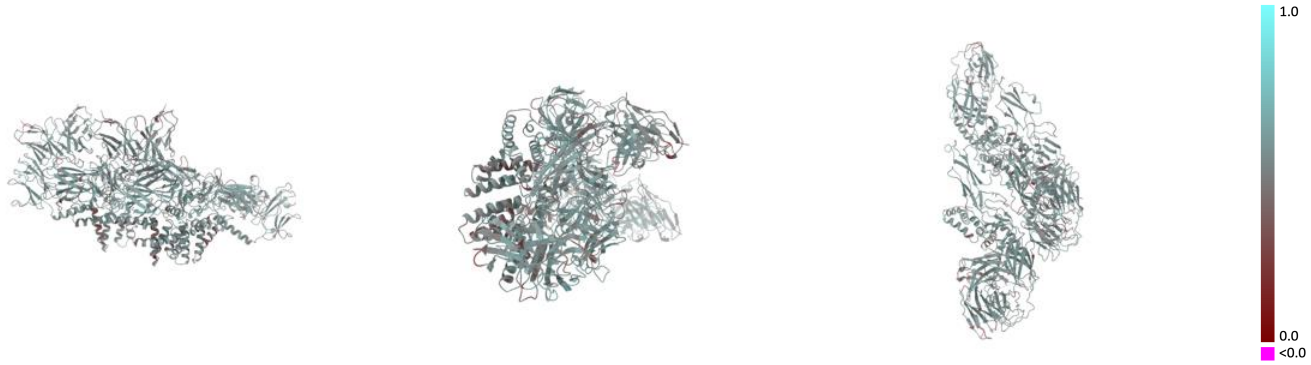
Y



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.

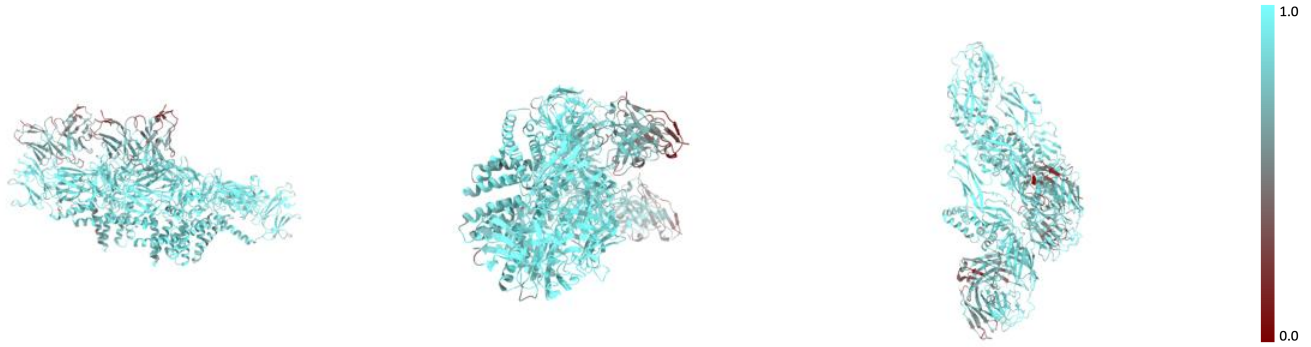
## 9.2 Q-score mapped to coordinate model




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.

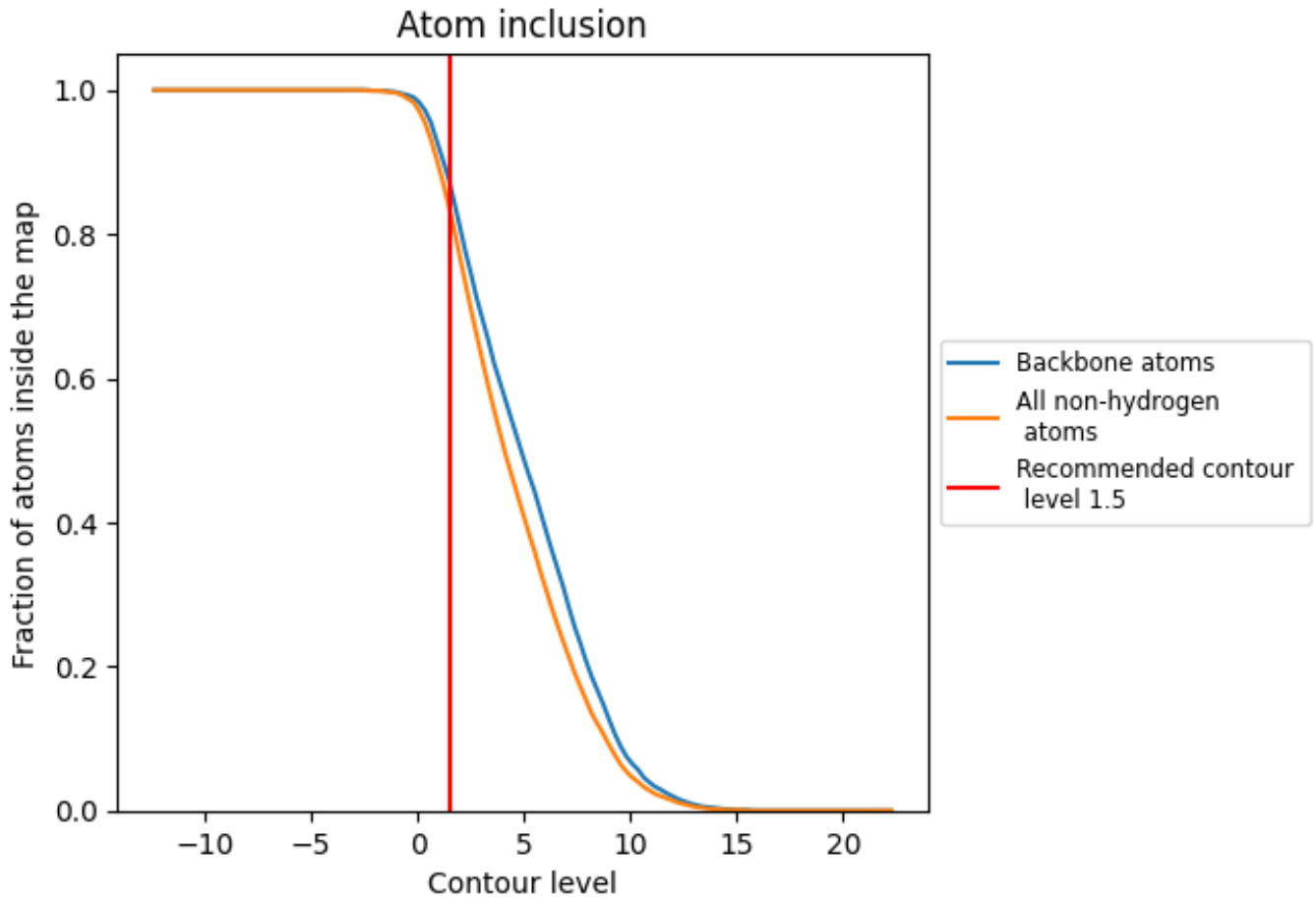
## 9.3 Atom inclusion mapped to coordinate model




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 (i)




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

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 |