# wwPDB EM Validation Summary Report (i)

Dec 11, 2022 – 05:16 pm GMT

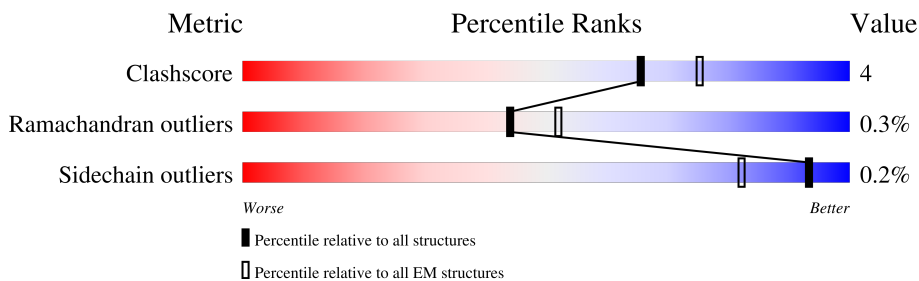|  |  |  |
|---|---|---|
| PDB ID | : | 6T63 |
| EMDB ID | : | EMD-10383 |
| Title | : | A model of the EIAV CA-SP hexamer (C2) from Gag-deltaMA tubes assembled at pH6 |
| Authors | : | Dick, R.A.; Xu, C.; Morado, D.R.; Kravchuk, V.; Ricana, C.L.; Lyddon, T.D.; Broad, A.M.; Feathers, J.R.; Johnson, M.C.; Vogt, V.M.; Perilla, J.R.; Briggs, J.A.G.; Schur, F.K.M. |
| Deposited on | : | 2019-10-17 |
| Resolution | : | 3.80 Å(reported) |
| Based on initial model | : | 2EIA |

# 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 3.80 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 |
|--------|------------------|-------|
| Clashscore | | 4 |
| Ramachandran outliers | | 0.3% |
| Sidechain outliers | | 0.2% |

*Worse*            *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|--------|--------------------------|--------------------------|
| Clashscore | 158937 | 4297 |
| 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 | 486 | 11%   39%   5%   55% |
| 1 | B | 486 | 7%   40%   •   55% |
| 1 | C | 486 | 10%   42%   •   55% |
| 1 | D | 486 | 14%   40%   5%   55% |
| 1 | E | 486 | 14%   40%   5%   55% |
| 1 | F | 486 | 5%   40%   •   55% |
| 1 | G | 486 | 9%   42%   •   55% |
| 1 | H | 486 | 9%   41%   •   55% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | I | 486 | 7% 41% · 55% |
| 1 | J | 486 | 11% 39% 5% 55% |
| 1 | K | 486 | 7% 40% · 55% |
| 1 | L | 486 | 10% 42% · 55% |
| 1 | M | 486 | 14% 40% 5% 55% |
| 1 | N | 486 | 14% 40% 5% 55% |
| 1 | O | 486 | 5% 40% · 55% |
| 1 | P | 486 | 9% 41% · 55% |
| 1 | Q | 486 | 9% 41% · 55% |
| 1 | R | 486 | 7% 41% · 55% |

# 2   Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 30978 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 Gag polyprotein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1721 | 1081 | 304 | 324 | 12 | | |
| 1 | B | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1721 | 1081 | 304 | 324 | 12 | | |
| 1 | C | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1721 | 1081 | 304 | 324 | 12 | | |
| 1 | F | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1721 | 1081 | 304 | 324 | 12 | | |
| 1 | D | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1721 | 1081 | 304 | 324 | 12 | | |
| 1 | H | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1721 | 1081 | 304 | 324 | 12 | | |
| 1 | I | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1721 | 1081 | 304 | 324 | 12 | | |
| 1 | E | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1721 | 1081 | 304 | 324 | 12 | | |
| 1 | G | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1721 | 1081 | 304 | 324 | 12 | | |
| 1 | J | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1721 | 1081 | 304 | 324 | 12 | | |
| 1 | K | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1721 | 1081 | 304 | 324 | 12 | | |
| 1 | L | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1721 | 1081 | 304 | 324 | 12 | | |
| 1 | O | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1721 | 1081 | 304 | 324 | 12 | | |
| 1 | M | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1721 | 1081 | 304 | 324 | 12 | | |
| 1 | Q | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1721 | 1081 | 304 | 324 | 12 | | |
| 1 | R | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1721 | 1081 | 304 | 324 | 12 | | |
| 1 | N | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1721 | 1081 | 304 | 324 | 12 | | |

*Continued on next page...*

*Continued from previous page...*

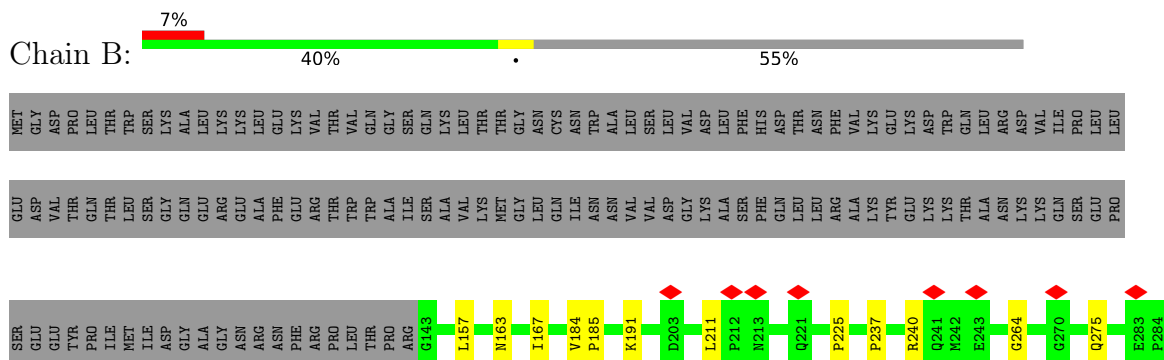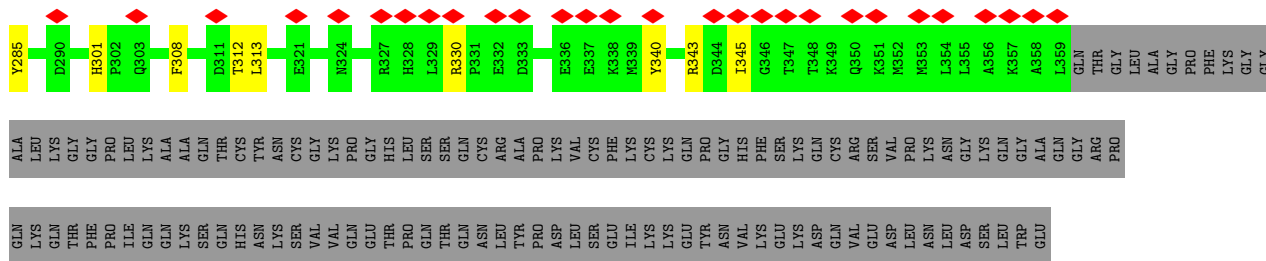| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 1 | P | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1721 | 1081 | 304 | 324 | 12 | | |

# 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.
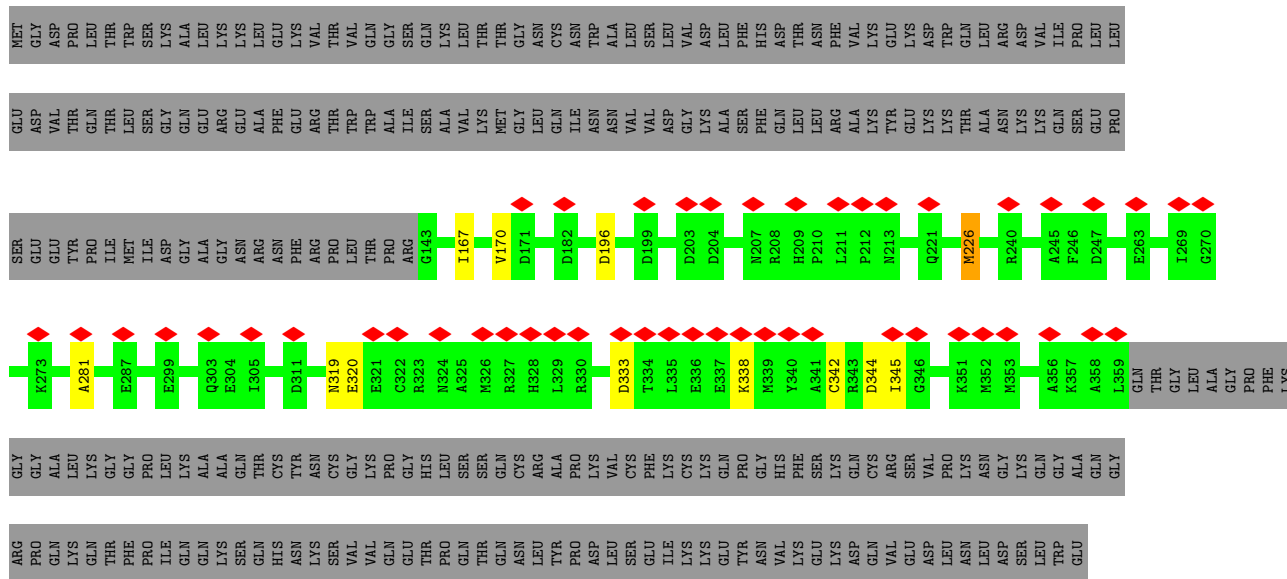
• Molecule 1: Gag polyprotein
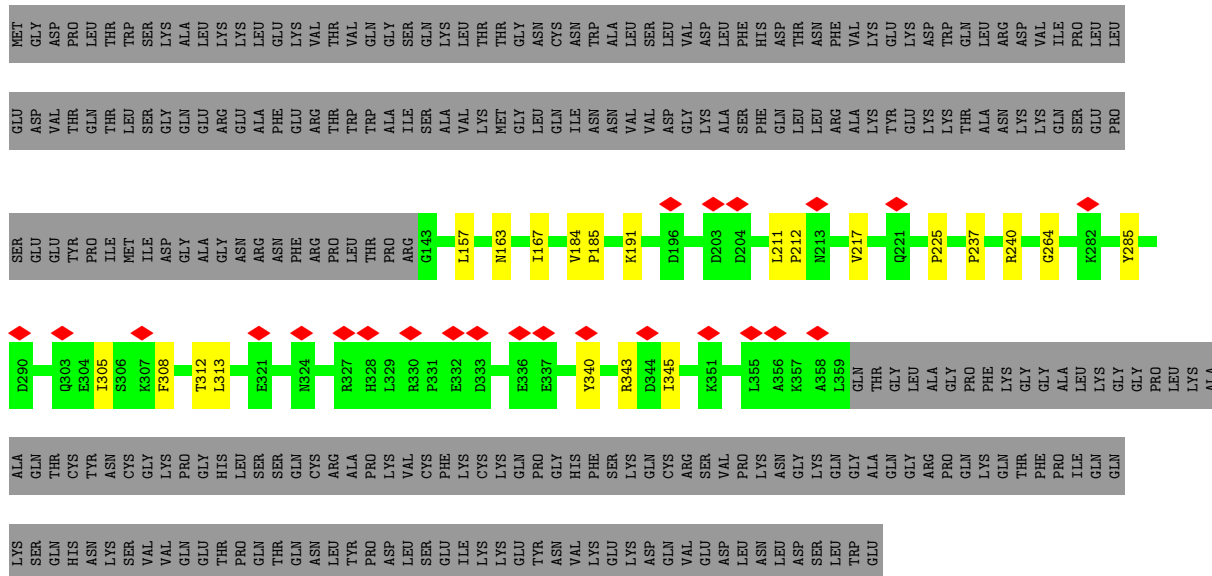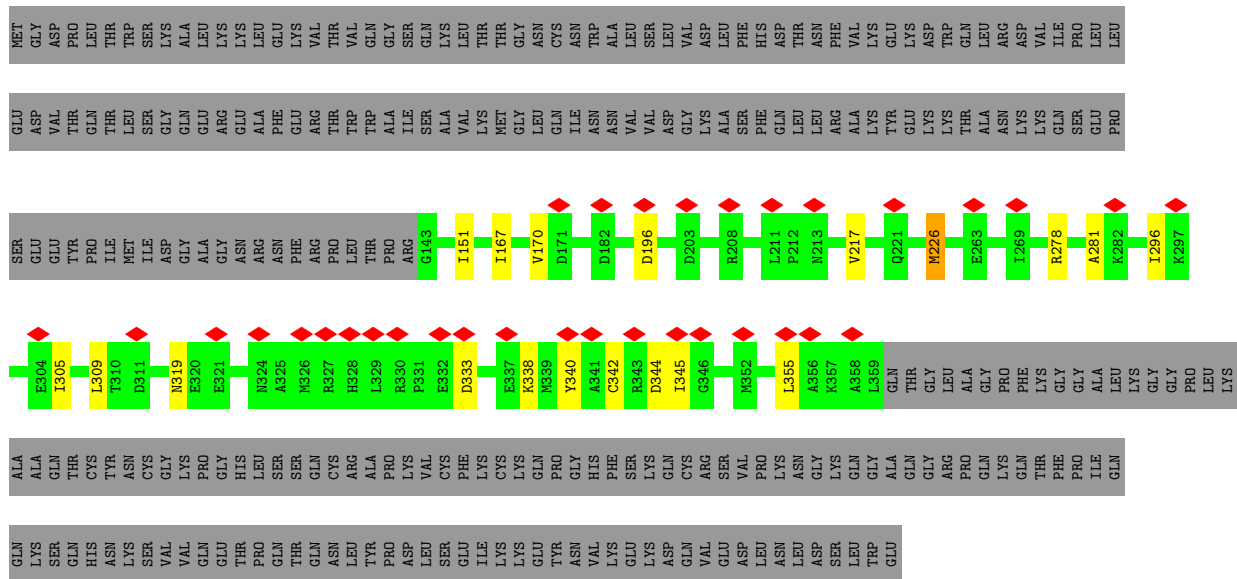


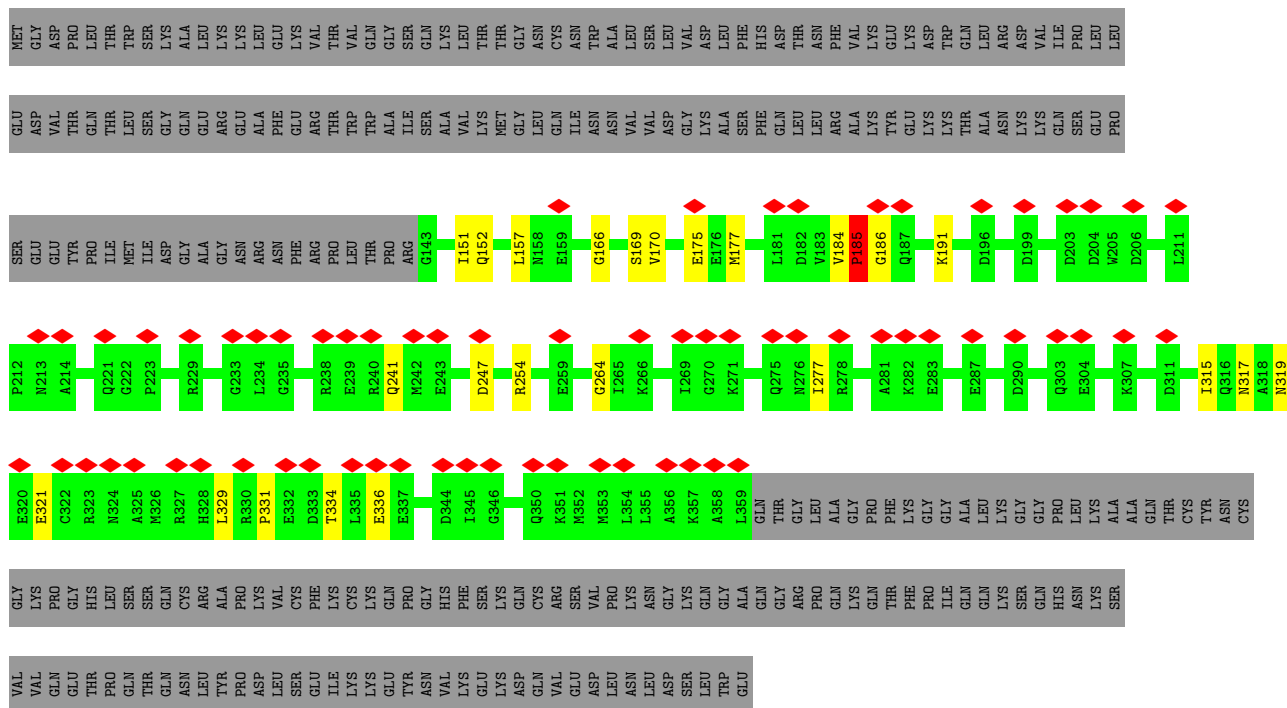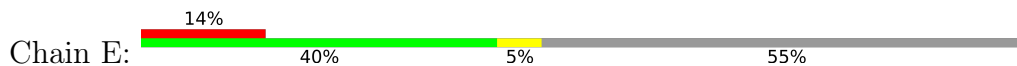• Molecule 1: Gag polyprotein

- Molecule 1: Gag polyprotein

Chain C:



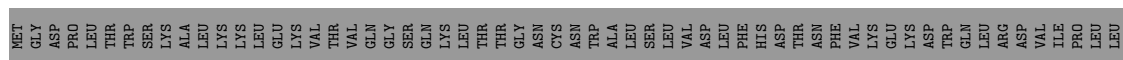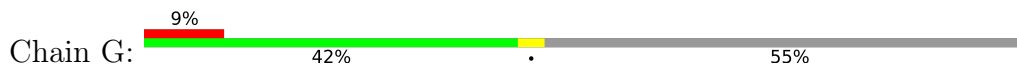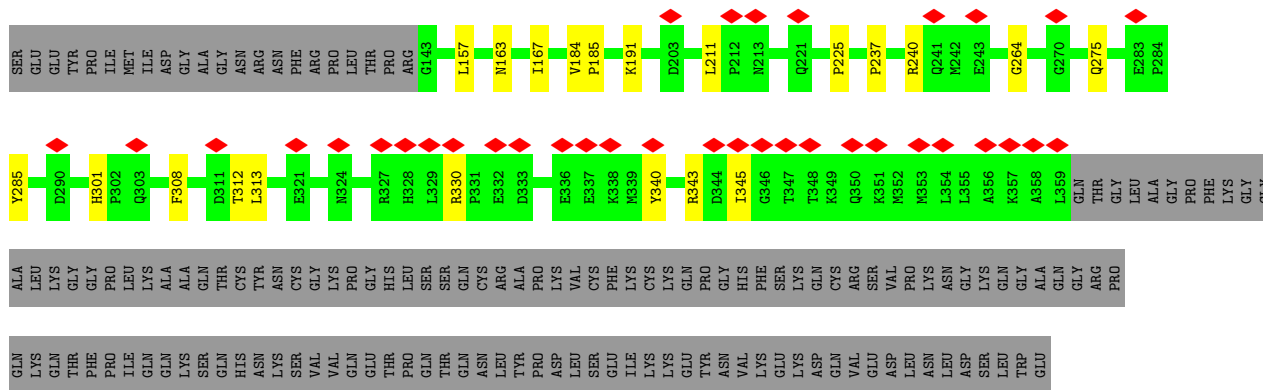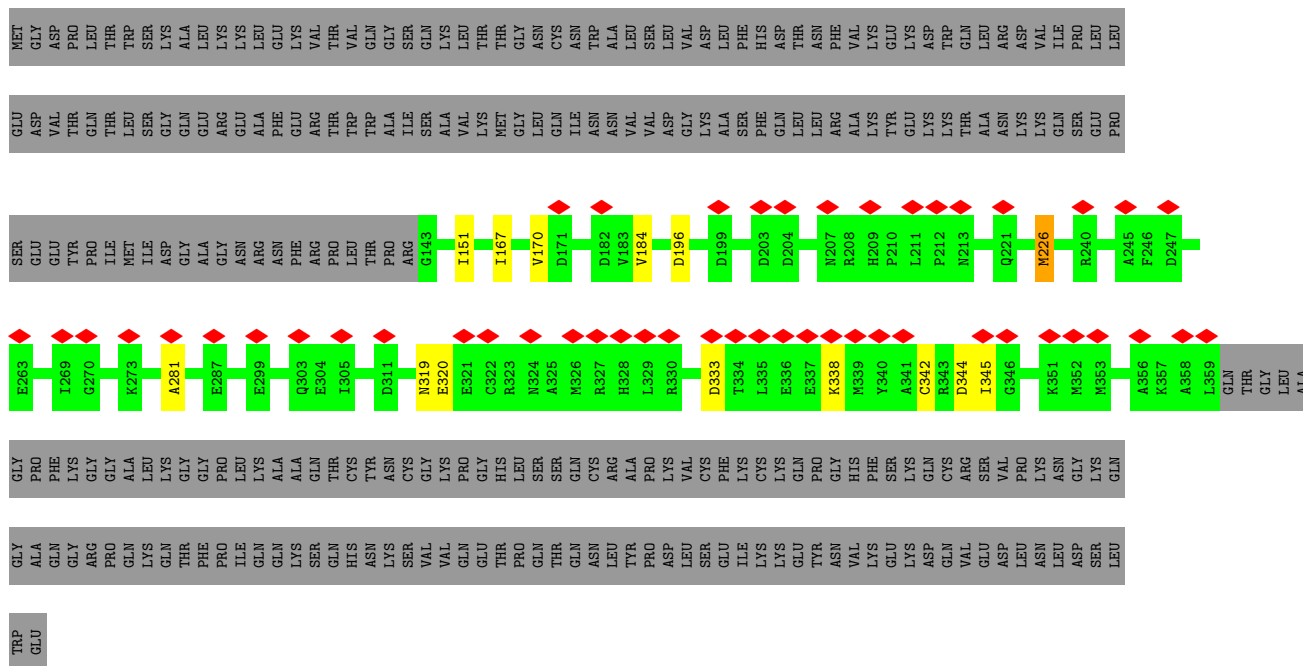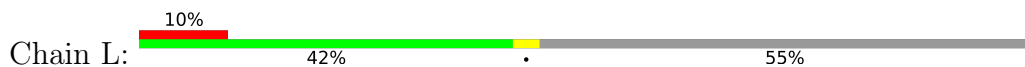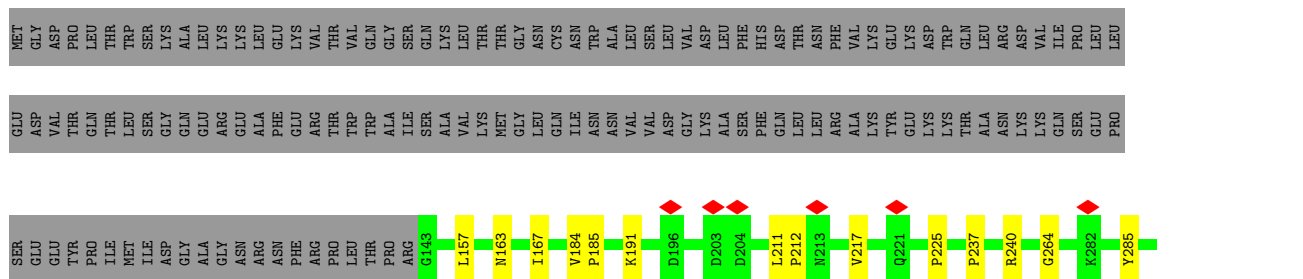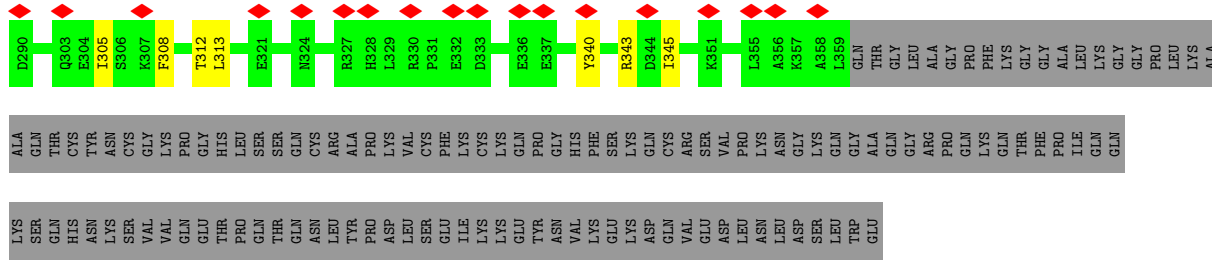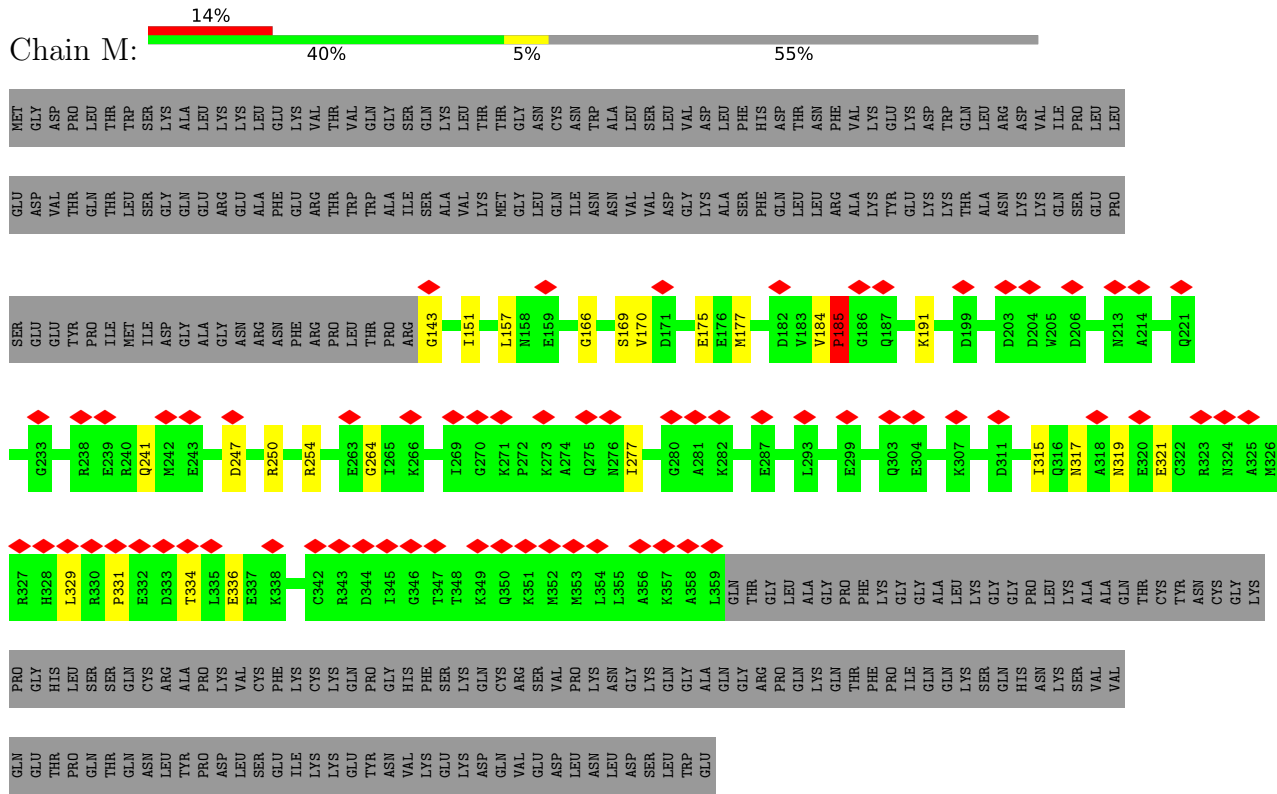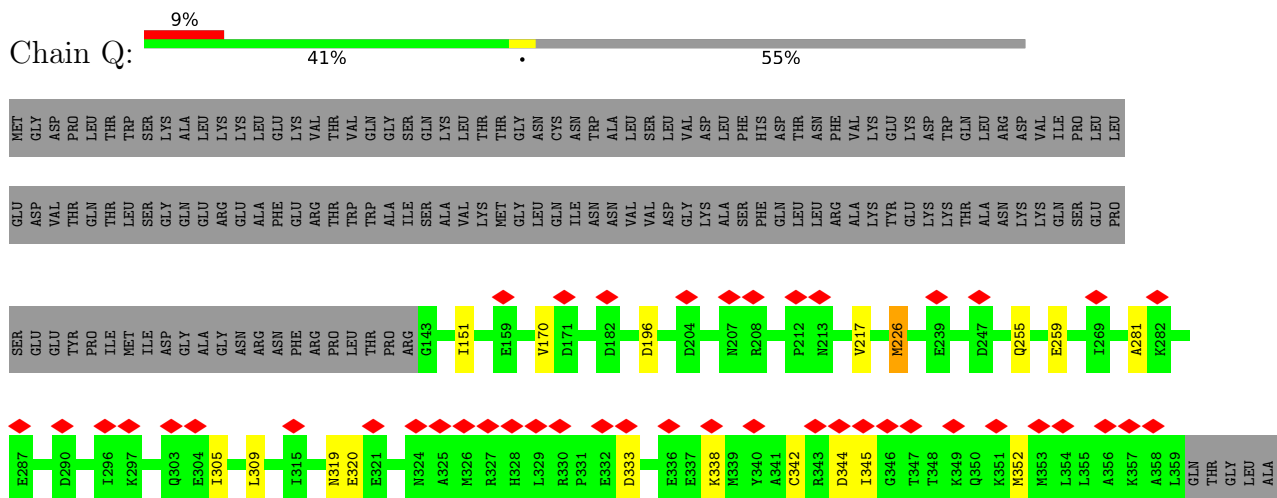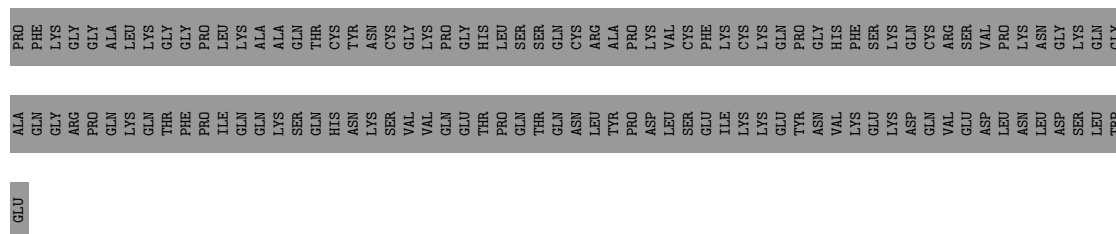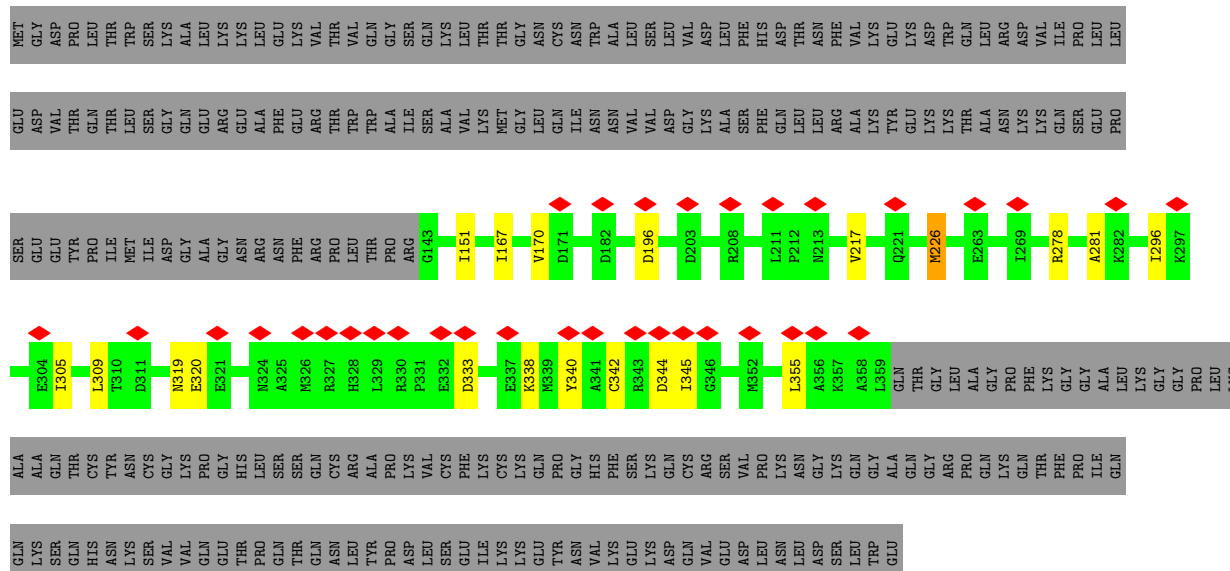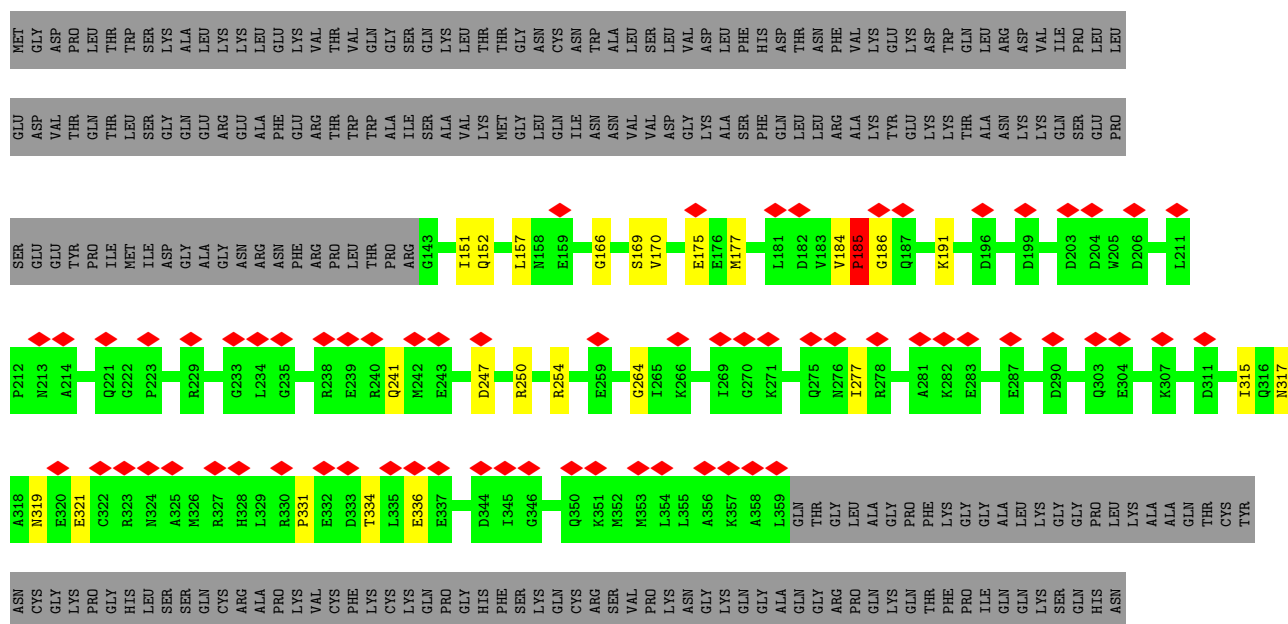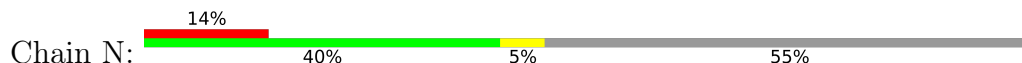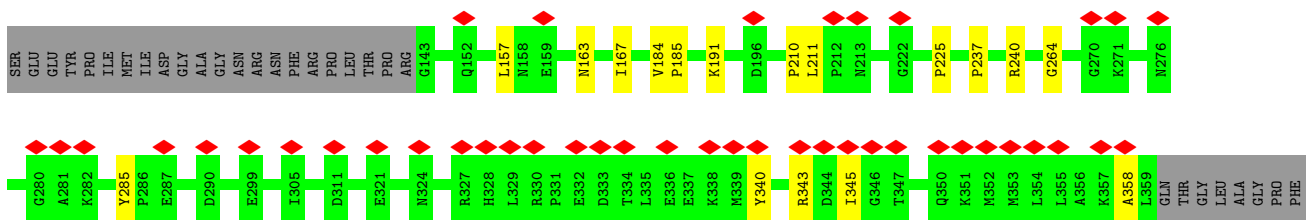- Molecule 1: Gag polyprotein

Chain F:

• Molecule 1: Gag polyprotein

Chain D:

14%

40%    5%    55%

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

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

SER GLU GLU TYR PRO ILE MET ILE ASP ALA GLY ASN ARG ASN PHE ARG PRO LEU THR PRO ARG **G143** **I151** **L157** **N158** **E159** **G166** **S169** **V170** **D171** **E175** **E176** **M177** **D182** **V183** **V184** **P185** **G186** **Q187** **K191** **D199** **D203** **D204** **W205** **D206** **N213** **A214** **Q221**

**G233** **R238** **E239** **R240** **Q241** **M242** **E243** **D247** **R254** **E263** **G264** **I265** **K266** **I269** **G270** **K271** **P272** **K273** **A274** **Q275** **N276** **I277** **G280** **A281** **K282** **E287** **L293** **E299** **Q303** **E304** **K307** **D311** **I315** **Q316** **N317** **A318** **N319** **E320** **E321** **C322** **R323** **N324** **A325** **M326** **R327** **H328**

**L329** **R330** **P331** **E332** **D333** **T334** **L335** **E336** **E337** **K338** **C342** **R343** **D344** **I345** **G346** **T347** **T348** **K349** **Q350** **K351** **M352** **M353** **L354** **L355** **A356** **K357** **A358** **L359** GLN THR GLY LEU ALA GLY PHE LYS GLY GLY ALA LEU LYS GLY GLY PRO LEU LYS ALA ALA GLN THR CYS TYR ASN CYS GLY LYS PRO GLY

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

THR PRO GLN THR GLN ASN LEU TYR PRO ASP LEU SER GLU ILE LYS LYS GLU TYR ASN VAL LYS GLU LYS ASP SER SER GLU TRP GLU

• Molecule 1: Gag polyprotein

Chain H:

9%

41%    •    55%

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

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

SER GLU GLU TYR PRO ILE MET ILE ASP ALA GLY ASN ARG ASN PHE ARG PRO LEU THR PRO ARG **G143** **I151** **E159** **V170** **D171** **D182** **V183** **V184** **D196** **D203** **D204** **N207** **R208** **P212** **N213** **V217** **M226** **E239** **D247** **E259** **I269** **A281** **K282**

**E287** **D290** **I296** **K297** **Q303** **E304** **I305** **L309** **I315** **N319** **E320** **E321** **N324** **A325** **M326** **R327** **H328** **L329** **R330** **P331** **E332** **D333** **E336** **E337** **K338** **M339** **Y340** **A341** **C342** **R343** **D344** **I345** **G346** **T347** **T348** **K349** **Q350** **K351** **M352** **M353** **L354** **L355** **A356** **K357** **A358** **L359** GLN THR GLY LEU ALA

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

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

TRP GLU

• Molecule 1: Gag polyprotein

Chain I:

7%

41%    •    55%

• Molecule 1: Gag polyprotein

Chain E:

14%

40%    5%    55%

• Molecule 1: Gag polyprotein

Chain G:

9%

42%    •    55%

• Molecule 1: Gag polyprotein

Chain J:

11%

39%    5%      55%

• Molecule 1: Gag polyprotein

Chain K:

7%

40%    •      55%

• Molecule 1: Gag polyprotein

Chain L:

10%

42% · 55%

• Molecule 1: Gag polyprotein

Chain O:

5%

40% · 55%

D290 Q303 E304 I305 S306 K307 F308 T312 L313 E321 N324 R327 H328 L329 R330 P331 E332 D333 E336 E337 Y340 R343 D344 I345 K351 L355 A356 K357 A358 L359 GLN THR GLY LEU ALA GLY PRO PHE LYS GLY GLY ALA LEU LYS GLY GLY PRO LEU LYS ALA

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

LYS SER GLN HIS LYS ASN LYS SER VAL VAL GLN GLU GLU THR PRO GLN THR GLN ASN LEU TYR PRO ASP LEU SER GLU ILE LYS LYS GLU TYR ASN VAL LYS GLU LYS ASP VAL GLU LEU ASN LEU ASP SER LEU TRP GLU

• Molecule 1: Gag polyprotein

14%

Chain M:                40%                 5%                      55%

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

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

SER GLU GLU TYR PRO ILE MET ILE ASP ALA GLY ALA ASN ARG ASN PRO LEU THR PRO ARG G143 I151 L157 N158 E159 G166 S169 V170 D171 E175 E176 M177 D182 V183 V184 P185 G186 Q187 K191 D199 D203 D204 W205 D206 N213 A214 Q221

G233 R238 E239 R240 Q241 M242 E243 D247 R250 R254 E263 G264 I265 K266 I269 G270 K271 P272 K273 A274 Q275 N276 I277 G280 A281 K282 E287 L293 E299 Q303 E304 K307 D311 I315 Q316 N317 A318 N319 E320 E321 C322 R323 N324 A325 M326

R327 H328 L329 R330 P331 E332 D333 T334 L335 E336 E337 K338 C342 R343 D344 I345 G346 T347 T348 K349 Q350 K351 M352 M353 L354 L355 A356 K357 A358 L359 GLN THR GLY LEU ALA GLY PRO PHE LYS GLY GLY ALA LEU LEU LYS SER GLY GLY PRO LEU LYS ALA ALA GLN THR CYS TYR ASN CYS GLY LYS

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

GLN GLU THR PRO GLN THR GLN ASN LEU TYR PRO ASP LEU SER GLU ILE LYS LYS GLU TYR ASN VAL LYS GLU LYS ASP VAL GLU LEU ASN LEU ASP SER LEU TRP GLU

• Molecule 1: Gag polyprotein

9%

Chain Q:                41%                 •                      55%

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

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

SER GLU GLU TYR PRO ILE MET ILE ASP ALA GLY ALA ASN ARG ASN PRO LEU THR PRO ARG G143 I151 E159 V170 D171 D182 D196 D204 N207 R208 P212 N213 V217 M226 E239 D247 Q255 E259 I269 A281 K282

E287 D290 I296 K297 Q303 E304 I305 L309 I315 N319 E320 E321 N324 A325 M326 R327 H328 L329 R330 P331 E332 D333 E336 E337 K338 M339 Y340 A341 C342 R343 D344 I345 G346 T347 T348 K349 Q350 K351 M352 M353 L354 L355 A356 K357 A358 L359 GLN THR GLY LEU ALA GLY

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

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

GLU

• Molecule 1: Gag polyprotein

Chain R:

7%
41% · 55%

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

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

SER GLU GLU TYR PRO ILE MET ILE ASP GLY ALA GLY ASN ARG ASN PHE ARG PRO LEU THR PRO ARG G143 I151 I167 V170 D171 D182 D196 D203 R208 L211 P212 N213 V217 Q221 M226 E263 I269 R278 A281 K282 I296 K297

E304 I305 L309 T310 D311 N319 E320 E321 N324 A325 M326 R327 H328 L329 R330 P331 E332 D333 E337 K338 M339 Y340 A341 C342 R343 D344 I345 G346 M352 L355 A356 K357 A358 L359 GLN THR GLY LEU ALA GLY PRO PHE LYS GLY LYS ALA LEU LYS GLY LYS LYS LEU LYS

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

GLN LYS SER GLN HIS ASN LYS SER VAL VAL GLN GLU THR PRO GLN THR GLN ASN LEU TYR PRO ASP LEU SER GLU ILE LYS LYS GLU TYR ASN VAL LYS GLU ASP GLN VAL GLU ASP LEU ASN LEU ASP SER LEU TRP GLU

• Molecule 1: Gag polyprotein

Chain N:

14%
40% 5% 55%

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

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

SER GLU GLU TYR PRO ILE MET ILE ASP GLY ALA GLY ASN ARG ASN ARG PRO LEU THR PRO ARG G143 I151 Q152 L157 N158 E159 G166 S169 V170 E175 E176 M177 L181 D182 V183 V184 P185 G186 Q187 K191 D196 D199 D203 D204 W205 D206 I211

P212 N213 A214 Q221 Q222 P223 R229 G233 L234 G235 R238 E239 R240 Q241 M242 E243 D247 R250 R254 E259 G264 I265 K266 I269 G270 K271 Q275 N276 I277 R278 A281 K282 E283 E287 D290 Q303 E304 K307 D311 I315 Q316 N317

A318 N319 E320 E321 C322 R323 N324 A325 M326 R327 H328 L329 R330 E332 D333 T334 L335 E336 E337 D344 I345 G346 Q350 K351 M352 M353 L354 L355 A356 K357 A358 L359 GLN THR GLY LEU ALA GLY PRO PHE LYS GLY GLY ALA LEU LYS GLY LYS LYS LEU LYS ALA ALA GLN THR CYS TYR

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

LYS SER VAL VAL GLN GLU THR PRO GLN THR GLN ASN LEU TYR PRO ASP LEU SER GLU ILE LYS LYS GLU TYR ASN VAL LYS GLU LYS ASP GLN VAL GLU ASP LEU ASN LEU ASP SER LEU TRP GLU

• Molecule 1: Gag polyprotein

Chain P:

9%

41%　　　　　•　　　　　55%

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

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

SER GLU GLU TYR PRO ILE MET ILE ASP ALA GLY ASN ARG ASN PHE ARG PRO LEU THR PRO ARG **G143** **Q152** **L157** **N158** **E159** **N163** **I167** **V184** **P185** **K191** **D196** **P210** **L211** **P212** **N213** **G222** **P225** **P237** **R240** **G264** **G270** **K271** **N276**

**G280** **A281** **K282** **Y285** **P286** **E287** **D290** **E299** **I305** **D311** **E321** **N324** **R327** **H328** **L329** **R330** **P331** **E332** **D333** **T334** **L335** **E336** **E337** **K338** **M339** **Y340** **R343** **D344** **I345** **G346** **T347** **Q350** **K351** **M352** **M353** **L354** **L355** **A356** **K357** **A358** **L359** GLN THR GLY LEU ALA GLY PRO PHE

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

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

# 4 Experimental information ⓘ

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SUBTOMOGRAM AVERAGING | Depositor |
| Imposed symmetry | POINT, C2 | Depositor |
| Number of subtomograms used | 112929 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF-correction was performed using NOVACTF | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose $(e^-/\text{Å}^2)$ | 3.4 | Depositor |
| Minimum defocus (nm) | -1500 | Depositor |
| Maximum defocus (nm) | -3500 | Depositor |
| Magnification | 130000 | Depositor |
| Image detector | GATAN K2 QUANTUM (4k x 4k) | Depositor |
| Maximum map value | 2.183 | Depositor |
| Minimum map value | -1.578 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.195 | Depositor |
| Recommended contour level | 0.499 | Depositor |
| Map size (Å) | 245.676, 245.676, 245.676 | wwPDB |
| Map dimensions | 236, 236, 236 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.041, 1.041, 1.041 | 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 | 0.31 | 0/1755 | 0.52 | 0/2375 |
| 1 | B | 0.31 | 0/1755 | 0.51 | 0/2375 |
| 1 | C | 0.30 | 0/1755 | 0.53 | 1/2375 (0.0%) |
| 1 | D | 0.31 | 0/1755 | 0.52 | 0/2375 |
| 1 | E | 0.31 | 0/1755 | 0.52 | 0/2375 |
| 1 | F | 0.31 | 0/1755 | 0.51 | 0/2375 |
| 1 | G | 0.31 | 0/1755 | 0.51 | 0/2375 |
| 1 | H | 0.31 | 0/1755 | 0.53 | 1/2375 (0.0%) |
| 1 | I | 0.30 | 0/1755 | 0.53 | 1/2375 (0.0%) |
| 1 | J | 0.31 | 0/1755 | 0.52 | 0/2375 |
| 1 | K | 0.31 | 0/1755 | 0.51 | 0/2375 |
| 1 | L | 0.30 | 0/1755 | 0.53 | 1/2375 (0.0%) |
| 1 | M | 0.31 | 0/1755 | 0.52 | 0/2375 |
| 1 | N | 0.31 | 0/1755 | 0.52 | 0/2375 |
| 1 | O | 0.31 | 0/1755 | 0.51 | 0/2375 |
| 1 | P | 0.31 | 0/1755 | 0.51 | 0/2375 |
| 1 | Q | 0.30 | 0/1755 | 0.53 | 1/2375 (0.0%) |
| 1 | R | 0.30 | 0/1755 | 0.53 | 1/2375 (0.0%) |
| All | All | 0.31 | 0/31590 | 0.52 | 6/42750 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|:---:|:---:|:---:|:---:|
| 1 | A | 0 | 1 |
| 1 | D | 0 | 1 |
| 1 | E | 0 | 1 |
| 1 | J | 0 | 1 |
| 1 | M | 0 | 1 |
| 1 | N | 0 | 1 |
| All | All | 0 | 6 |

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|-----------|---------|
| 1 | H | 196 | ASP | CB-CG-OD2 | 6.26 | 123.93 | 118.30 |
| 1 | R | 196 | ASP | CB-CG-OD2 | 6.24 | 123.92 | 118.30 |
| 1 | I | 196 | ASP | CB-CG-OD2 | 6.23 | 123.91 | 118.30 |
| 1 | L | 196 | ASP | CB-CG-OD2 | 6.18 | 123.86 | 118.30 |
| 1 | C | 196 | ASP | CB-CG-OD2 | 6.18 | 123.86 | 118.30 |

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------|
| 1 | A | 185 | PRO | Peptide |
| 1 | D | 185 | PRO | Peptide |
| 1 | E | 185 | PRO | Peptide |
| 1 | J | 185 | PRO | Peptide |
| 1 | M | 185 | PRO | Peptide |

## 5.2   Too-close contacts   (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 1721 | 0 | 1718 | 35 | 0 |
| 1 | B | 1721 | 0 | 1716 | 18 | 0 |
| 1 | C | 1721 | 0 | 1717 | 11 | 0 |
| 1 | D | 1721 | 0 | 1718 | 18 | 0 |
| 1 | E | 1721 | 0 | 1718 | 31 | 0 |
| 1 | F | 1721 | 0 | 1718 | 17 | 0 |
| 1 | G | 1721 | 0 | 1718 | 12 | 0 |
| 1 | H | 1721 | 0 | 1716 | 14 | 0 |
| 1 | I | 1721 | 0 | 1718 | 20 | 0 |
| 1 | J | 1721 | 0 | 1718 | 35 | 0 |
| 1 | K | 1721 | 0 | 1716 | 18 | 0 |
| 1 | L | 1721 | 0 | 1717 | 12 | 0 |
| 1 | M | 1721 | 0 | 1718 | 21 | 0 |
| 1 | N | 1721 | 0 | 1718 | 31 | 0 |
| 1 | O | 1721 | 0 | 1718 | 17 | 0 |

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | P | 1721 | 0 | 1718 | 13 | 0 |
| 1 | Q | 1721 | 0 | 1716 | 16 | 0 |
| 1 | R | 1721 | 0 | 1718 | 21 | 0 |
| All | All | 30978 | 0 | 30914 | 255 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 255 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------|--------|--------------------------|-------------------|
| 1:A:170:VAL:HG11 | 1:C:170:VAL:HG13 | 1.31 | 1.11 |
| 1:K:330:ARG:NH1 | 1:R:340:TYR:CD1 | 1.91 | 1.10 |
| 1:J:170:VAL:HG11 | 1:L:170:VAL:HG13 | 1.30 | 1.04 |
| 1:B:330:ARG:NH1 | 1:I:340:TYR:CD1 | 1.91 | 1.03 |
| 1:I:170:VAL:HG13 | 1:E:170:VAL:HG11 | 1.44 | 0.98 |

There are no symmetry-related clashes.

## 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 | 215/486 (44%) | 199 (93%) | 15 (7%) | 1 (0%) | 29 | 66 |
| 1 | B | 215/486 (44%) | 201 (94%) | 13 (6%) | 1 (0%) | 29 | 66 |
| 1 | C | 215/486 (44%) | 197 (92%) | 18 (8%) | 0 | 100 | 100 |
| 1 | D | 215/486 (44%) | 199 (93%) | 15 (7%) | 1 (0%) | 29 | 66 |
| 1 | E | 215/486 (44%) | 200 (93%) | 14 (6%) | 1 (0%) | 29 | 66 |
| 1 | F | 215/486 (44%) | 201 (94%) | 13 (6%) | 1 (0%) | 29 | 66 |
| 1 | G | 215/486 (44%) | 201 (94%) | 13 (6%) | 1 (0%) | 29 | 66 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | H | 215/486 (44%) | 197 (92%) | 18 (8%) | 0 | 100 | 100 |
| 1 | I | 215/486 (44%) | 197 (92%) | 18 (8%) | 0 | 100 | 100 |
| 1 | J | 215/486 (44%) | 199 (93%) | 15 (7%) | 1 (0%) | 29 | 66 |
| 1 | K | 215/486 (44%) | 201 (94%) | 13 (6%) | 1 (0%) | 29 | 66 |
| 1 | L | 215/486 (44%) | 197 (92%) | 18 (8%) | 0 | 100 | 100 |
| 1 | M | 215/486 (44%) | 200 (93%) | 14 (6%) | 1 (0%) | 29 | 66 |
| 1 | N | 215/486 (44%) | 200 (93%) | 14 (6%) | 1 (0%) | 29 | 66 |
| 1 | O | 215/486 (44%) | 201 (94%) | 13 (6%) | 1 (0%) | 29 | 66 |
| 1 | P | 215/486 (44%) | 201 (94%) | 13 (6%) | 1 (0%) | 29 | 66 |
| 1 | Q | 215/486 (44%) | 197 (92%) | 18 (8%) | 0 | 100 | 100 |
| 1 | R | 215/486 (44%) | 197 (92%) | 18 (8%) | 0 | 100 | 100 |
| All | All | 3870/8748 (44%) | 3585 (93%) | 273 (7%) | 12 (0%) | 44 | 74 |

5 of 12 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 185 | PRO |
| 1 | D | 185 | PRO |
| 1 | E | 185 | PRO |
| 1 | J | 185 | PRO |
| 1 | M | 185 | 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 | 187/421 (44%) | 187 (100%) | 0 | 100 | 100 |
| 1 | B | 187/421 (44%) | 187 (100%) | 0 | 100 | 100 |
| 1 | C | 187/421 (44%) | 186 (100%) | 1 (0%) | 88 | 94 |
| 1 | D | 187/421 (44%) | 187 (100%) | 0 | 100 | 100 |
| 1 | E | 187/421 (44%) | 187 (100%) | 0 | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------|-----------|----------|------|------|
| 1 | F | 187/421 (44%) | 187 (100%) | 0 | 100 | 100 |
| 1 | G | 187/421 (44%) | 187 (100%) | 0 | 100 | 100 |
| 1 | H | 187/421 (44%) | 186 (100%) | 1 (0%) | 88 | 94 |
| 1 | I | 187/421 (44%) | 186 (100%) | 1 (0%) | 88 | 94 |
| 1 | J | 187/421 (44%) | 187 (100%) | 0 | 100 | 100 |
| 1 | K | 187/421 (44%) | 187 (100%) | 0 | 100 | 100 |
| 1 | L | 187/421 (44%) | 186 (100%) | 1 (0%) | 88 | 94 |
| 1 | M | 187/421 (44%) | 187 (100%) | 0 | 100 | 100 |
| 1 | N | 187/421 (44%) | 187 (100%) | 0 | 100 | 100 |
| 1 | O | 187/421 (44%) | 187 (100%) | 0 | 100 | 100 |
| 1 | P | 187/421 (44%) | 187 (100%) | 0 | 100 | 100 |
| 1 | Q | 187/421 (44%) | 186 (100%) | 1 (0%) | 88 | 94 |
| 1 | R | 187/421 (44%) | 186 (100%) | 1 (0%) | 88 | 94 |
| All | All | 3366/7578 (44%) | 3360 (100%) | 6 (0%) | 93 | 97 |

5 of 6 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 226 | MET |
| 1 | Q | 226 | MET |
| 1 | R | 226 | MET |
| 1 | H | 226 | MET |
| 1 | C | 226 | MET |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 241 | GLN |
| 1 | P | 154 | ASN |
| 1 | Q | 207 | ASN |
| 1 | R | 248 | GLN |
| 1 | P | 279 | GLN |

### 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-10383. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

## 6.1   Orthogonal projections  ⓘ

### 6.1.1   Primary map



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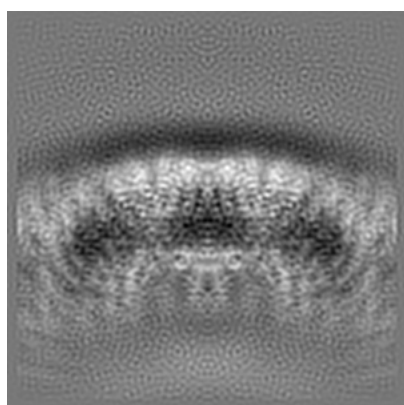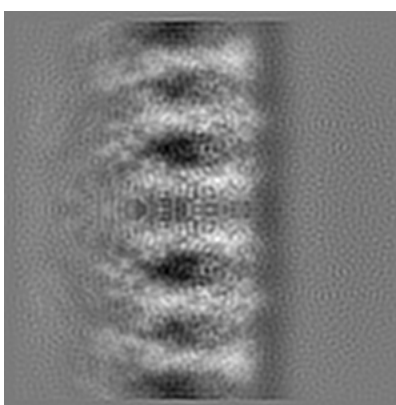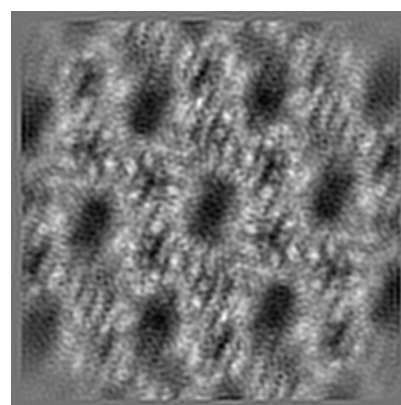
The images above show the map projected in three orthogonal directions.

## 6.2   Central slices  ⓘ
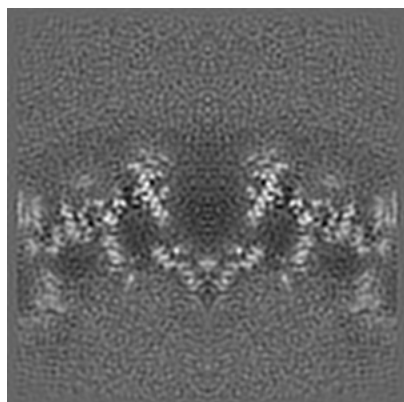
### 6.2.1   Primary map
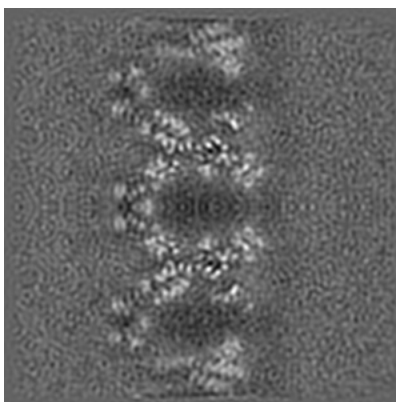


| X Index: 118 | Y Index: 118 | Z Index: 118 |
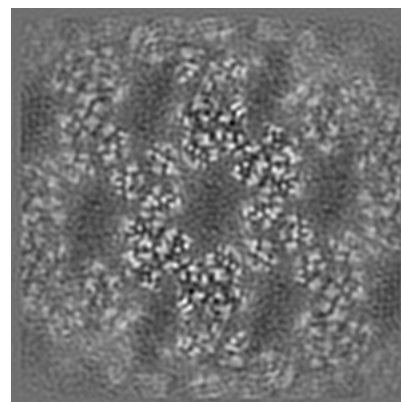
The images above show central slices of the map in three orthogonal directions.

## 6.3   Largest variance slices (i)

### 6.3.1   Primary map
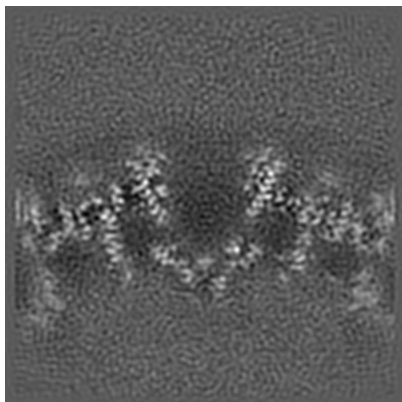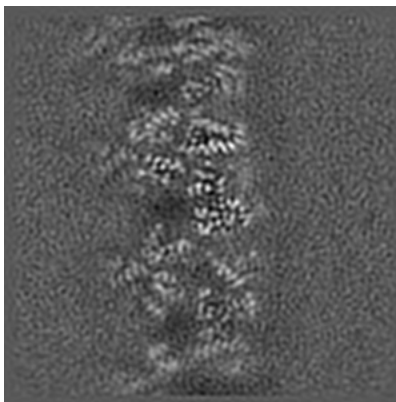


| X Index: 119 | Y Index: 157 | Z Index: 120 |
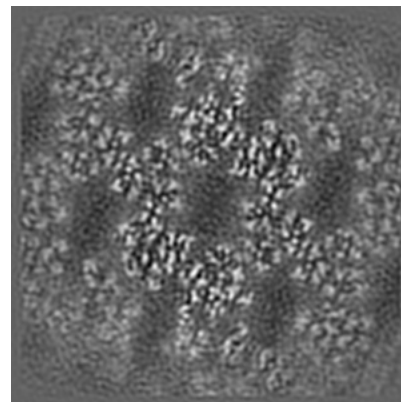
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4   Orthogonal surface views (i)

### 6.4.1   Primary map



| X | Y | Z |
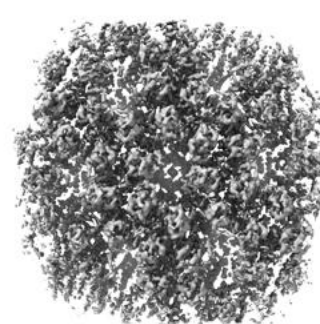
The images above show the 3D surface view of the map at the recommended contour level 0.499. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation (i)

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

# 7   Map analysis ⓘ

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

## 7.1   Map-value distribution ⓘ
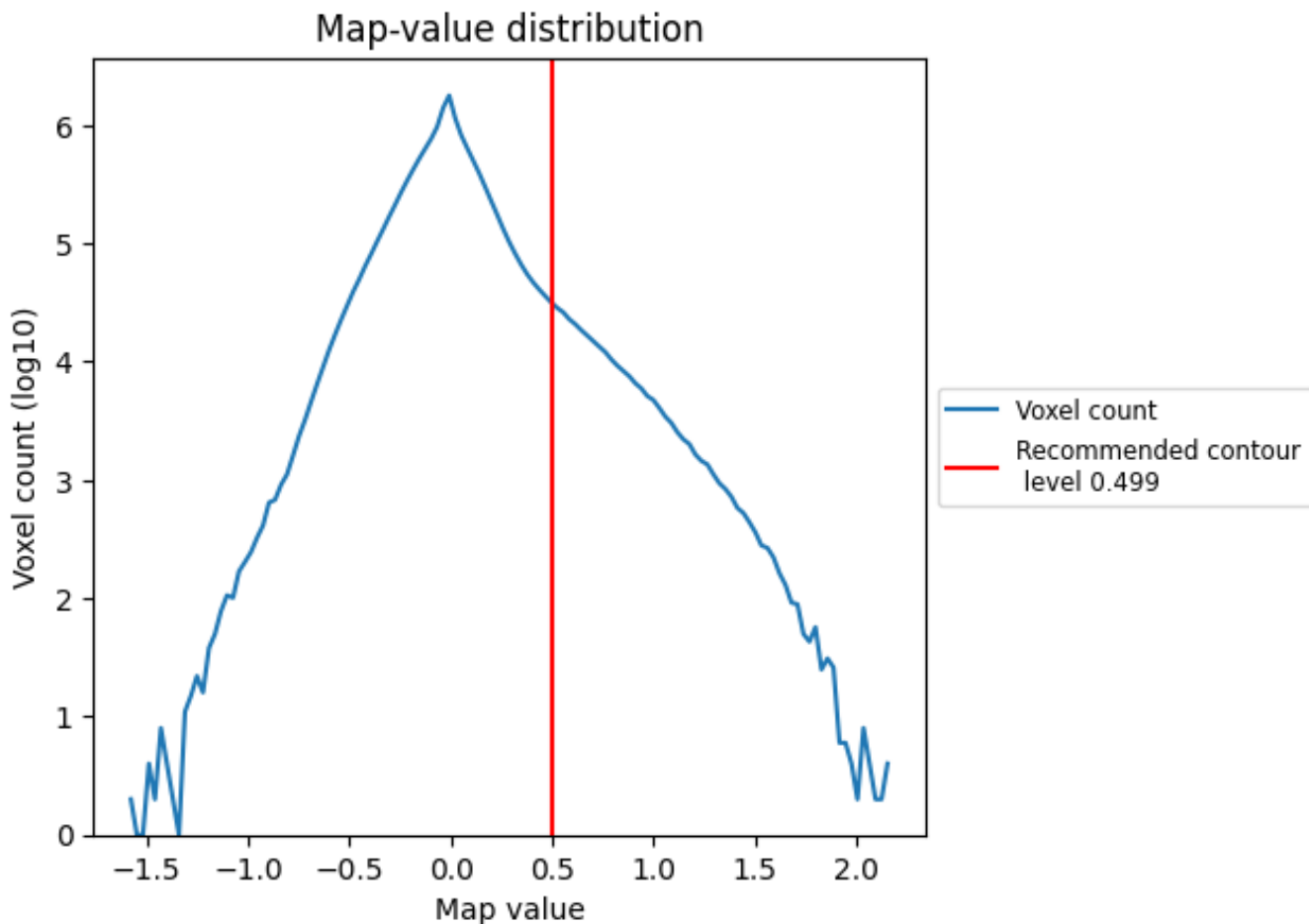


The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2   Volume estimate ⓘ
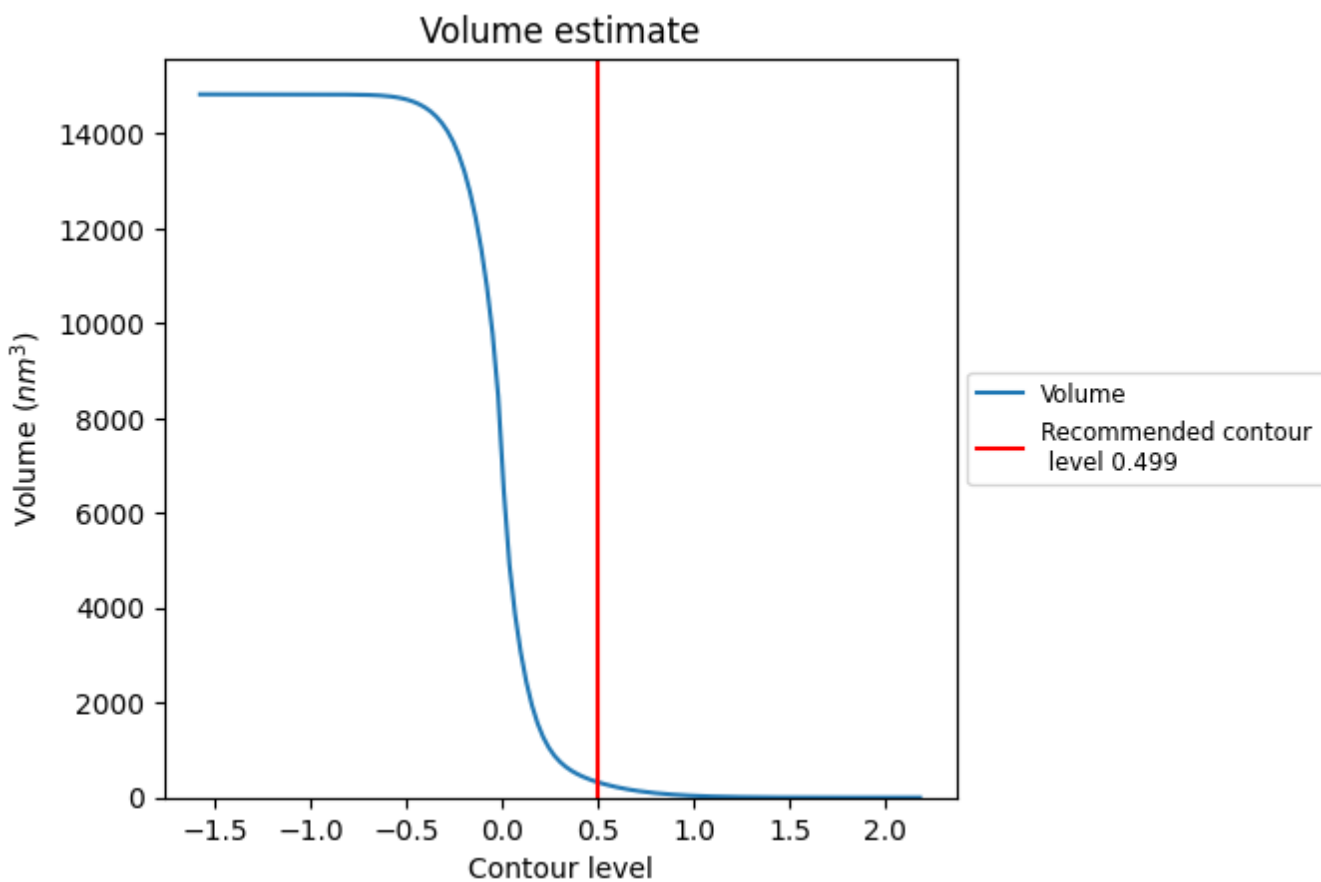


The volume at the recommended contour level is 325 nm$^3$; this corresponds to an approximate mass of 294 kDa.

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

## 7.3    Rotationally averaged power spectrum   ⓘ
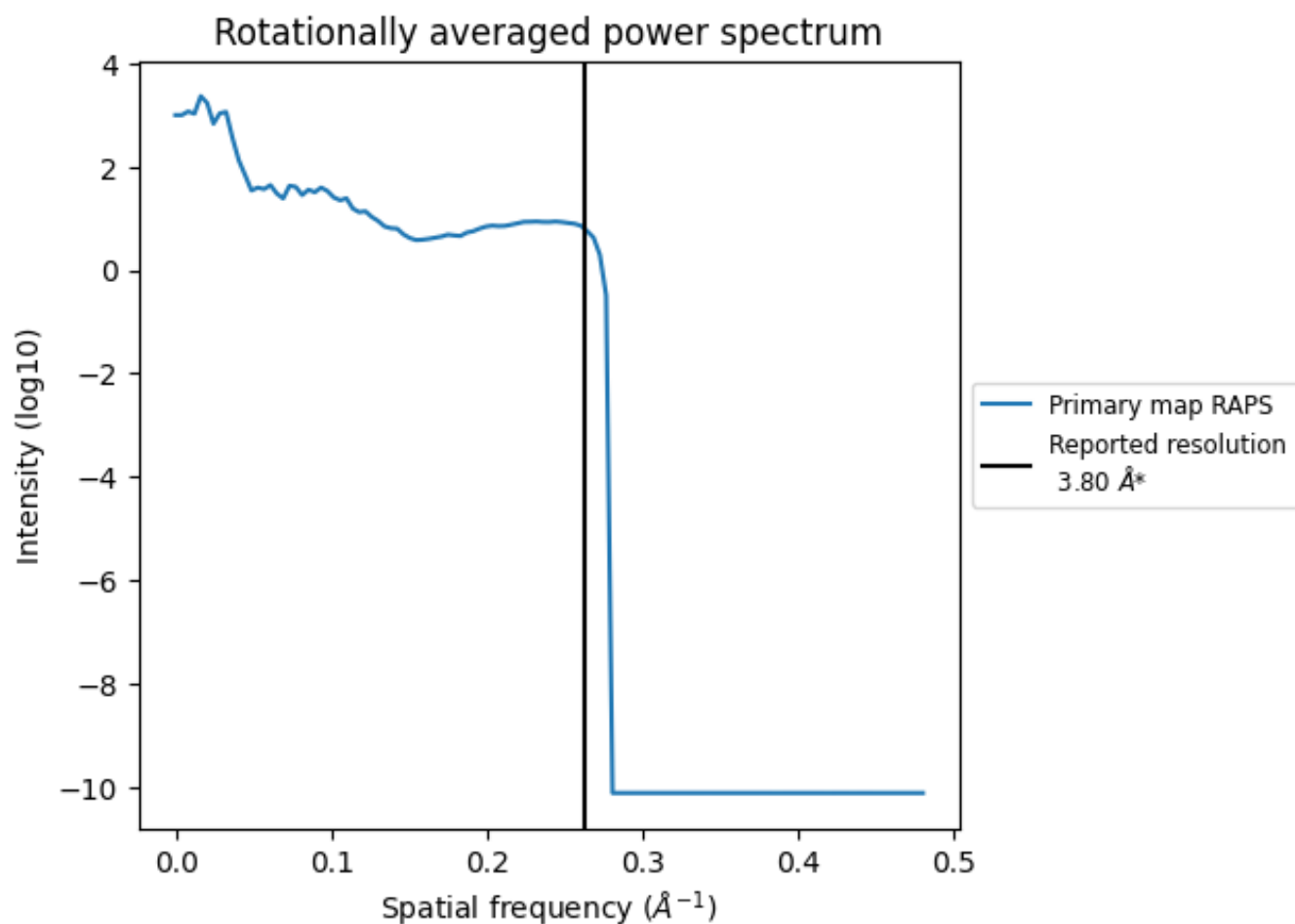


*Reported resolution corresponds to spatial frequency of 0.263 Å$^{-1}$

# 8   Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

# 9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-10383 and PDB model 6T63. Per-residue inclusion information can be found in section 3 on page 6.

## 9.1 Map-model overlay ⓘ



| X | Y | Z |
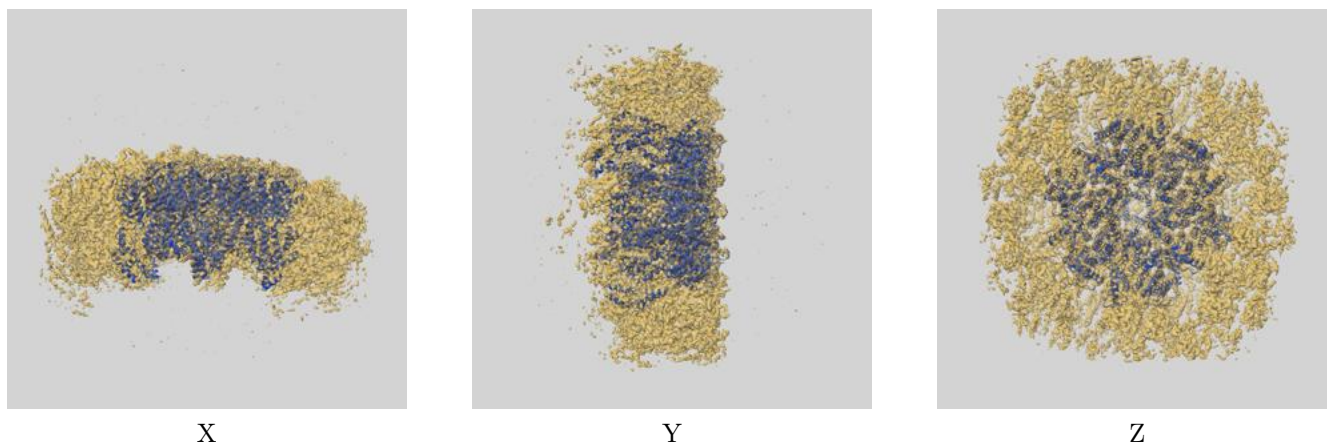
The images above show the 3D surface view of the map at the recommended contour level 0.499 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2    Q-score mapped to coordinate model ⓘ



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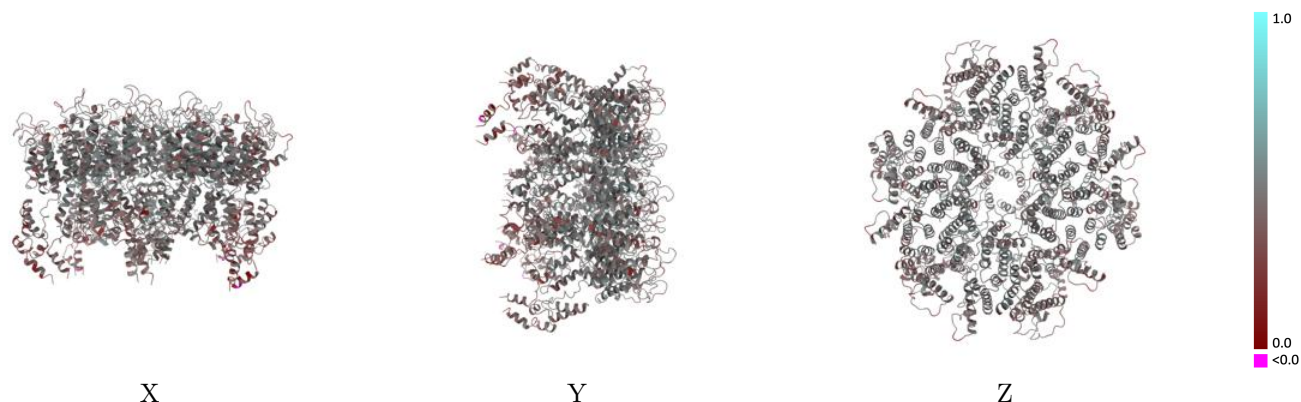
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3    Atom inclusion mapped to coordinate model ⓘ



X            Y            Z
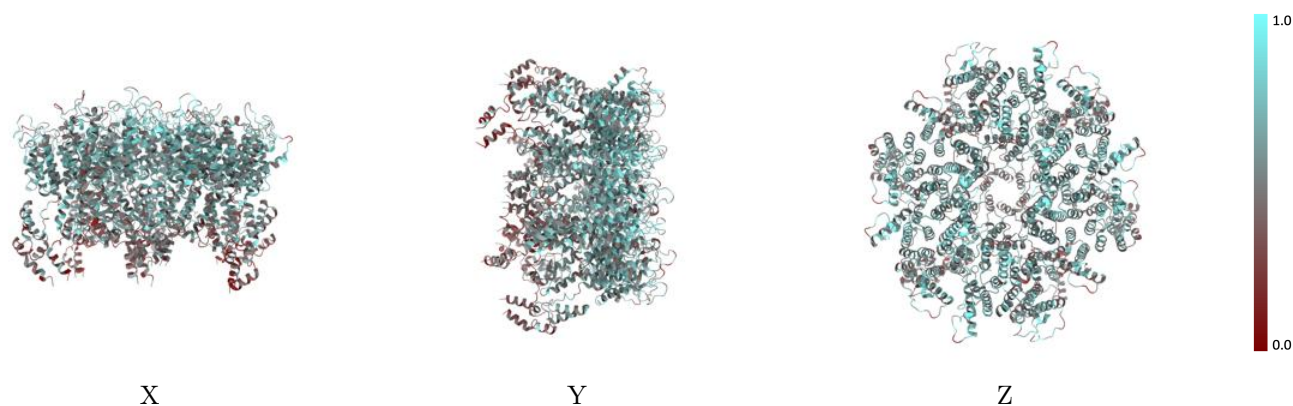
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.499).

## 9.4 Atom inclusion ⓘ
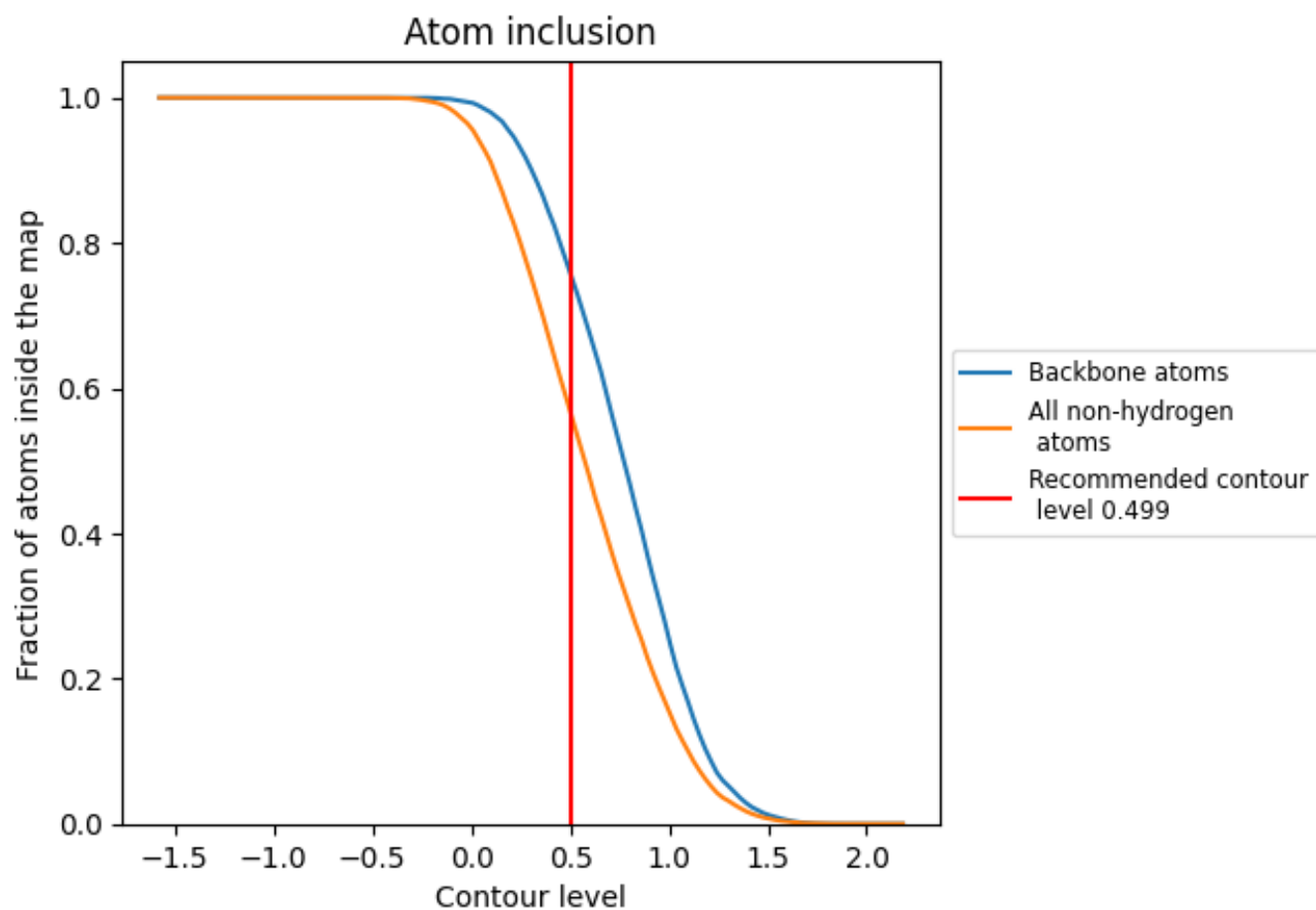


At the recommended contour level, 76% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.499) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|:-----:|:--------------:|:-------:|
| All | 0.5685 | 0.4350 |
| A | 0.5622 | 0.4630 |
| B | 0.5841 | 0.4220 |
| C | 0.5551 | 0.4090 |
| D | 0.5124 | 0.3900 |
| E | 0.5136 | 0.4130 |
| F | 0.6309 | 0.4830 |
| G | 0.5669 | 0.4390 |
| H | 0.5847 | 0.4260 |
| I | 0.6072 | 0.4650 |
| J | 0.5622 | 0.4670 |
| K | 0.5835 | 0.4190 |
| L | 0.5551 | 0.4080 |
| M | 0.5124 | 0.3880 |
| N | 0.5130 | 0.4160 |
| O | 0.6291 | 0.4840 |
| P | 0.5664 | 0.4400 |
| Q | 0.5859 | 0.4270 |
| R | 0.6072 | 0.4650 |

1.0

0.0
<0.0