# WORLDWIDE wwPDB PROTEIN DATA BANK

# Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 10:23 PM JST

| | | |
|---|---|---|
| PDB ID | : | 7F8W |
| EMDB ID | : | EMD-31494 |
| Title | : | Cryo-EM structure of the cholecystokinin receptor CCKBR in complex with gastrin-17 and Gq |
| Authors | : | Zhang, X.; He, C.; Wang, M.; Zhou, Q.; Yang, D.; Zhu, Y.; Wu, B.; Zhao, Q. |
| Deposited on | : | 2021-07-02 |
| Resolution | : | 3.10 Å(reported) |

# 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 3.10 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 | | 8 |
| Ramachandran outliers | | 0 |
| Sidechain outliers | | 0 |

*Worse*          *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
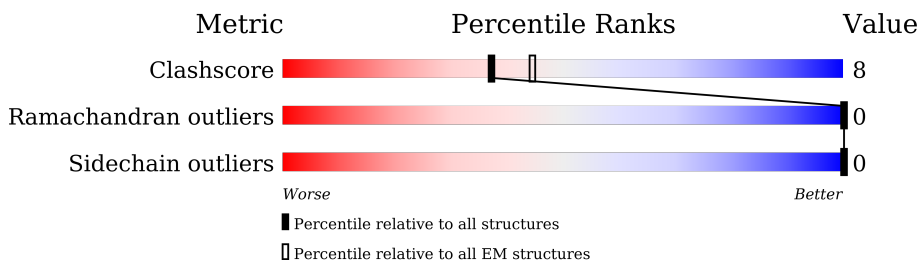
| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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 | 353 | 34% / 50% / 14% / 37% |
| 2 | B | 351 | 17% / 66% / 22% / 13% |
| 3 | C | 71 | 37% / 42% / · / 54% |
| 4 | D | 268 | 39% / 69% / 18% / 13% |
| 5 | E | 17 | 88% / 65% / 35% |
| 6 | R | 465 | 27% / 49% / 10% / 41% |

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# 2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 8486 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 Guanine nucleotide-binding protein G(q) subunit alpha.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|:---:|:---:|:---:|:---:|:---:|:---:|:---:|:---:|:---:|:---:|
| | | | Total | C | N | O | S | | |
| 1 | A | 224 | 1850 | 1180 | 318 | 343 | 9 | 0 | 0 |

There are 22 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|:---:|:---:|:---:|:---:|:---:|:---:|
| A | 1 | MET | - | initiating methionine | UNP P50148 |
| A | 2 | GLY | - | expression tag | UNP P50148 |
| A | 3 | CYS | - | expression tag | UNP P50148 |
| A | 4 | THR | - | expression tag | UNP P50148 |
| A | 5 | LEU | - | expression tag | UNP P50148 |
| A | 6 | SER | - | expression tag | UNP P50148 |
| A | 7 | ALA | - | expression tag | UNP P50148 |
| A | 8 | GLU | - | expression tag | UNP P50148 |
| A | 9 | ASP | - | expression tag | UNP P50148 |
| A | 10 | LYS | - | expression tag | UNP P50148 |
| A | 11 | ALA | - | expression tag | UNP P50148 |
| A | 12 | ALA | - | expression tag | UNP P50148 |
| A | 13 | VAL | - | expression tag | UNP P50148 |
| A | 14 | GLU | - | expression tag | UNP P50148 |
| A | 15 | ARG | - | expression tag | UNP P50148 |
| A | 16 | SER | - | expression tag | UNP P50148 |
| A | 17 | LYS | - | expression tag | UNP P50148 |
| A | 18 | MET | - | expression tag | UNP P50148 |
| A | 19 | ILE | - | expression tag | UNP P50148 |
| A | 20 | ASP | - | expression tag | UNP P50148 |
| A | 21 | ARG | - | expression tag | UNP P50148 |
| A | 22 | ASN | - | expression tag | UNP P50148 |

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 306 | Total 2347 | C 1453 | N 418 | O 456 | S 20 | 0 | 0 |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | -10 | MET | - | expression tag | UNP P62873 |
| B | -9 | HIS | - | expression tag | UNP P62873 |
| B | -8 | HIS | - | expression tag | UNP P62873 |
| B | -7 | HIS | - | expression tag | UNP P62873 |
| B | -6 | HIS | - | expression tag | UNP P62873 |
| B | -5 | HIS | - | expression tag | UNP P62873 |
| B | -4 | HIS | - | expression tag | UNP P62873 |
| B | -3 | GLY | - | expression tag | UNP P62873 |
| B | -2 | SER | - | expression tag | UNP P62873 |
| B | -1 | LEU | - | expression tag | UNP P62873 |
| B | 0 | LEU | - | expression tag | UNP P62873 |
| B | 1 | GLN | - | expression tag | UNP P62873 |

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 33 | Total 245 | C 156 | N 39 | O 48 | S 2 | 0 | 0 |

- Molecule 4 is a protein called scFv16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | D | 232 | Total 1783 | C 1131 | N 295 | O 347 | S 10 | 0 | 0 |

- Molecule 5 is a protein called Gastrin-17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | E | 17 | Total 133 | C 89 | N 20 | O 23 | S 1 | 0 | 0 |

- Molecule 6 is a protein called Gastrin/cholecystokinin type B receptor.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | S | | |
| 6 | R | 275 | 2128 | 1412 | 359 | 339 | 18 | 0 | 0 |

There are 48 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| R | -8 | ASP | - | expression tag | UNP P32239 |
| R | -7 | TYR | - | expression tag | UNP P32239 |
| R | -6 | LYS | - | expression tag | UNP P32239 |
| R | -5 | ASP | - | expression tag | UNP P32239 |
| R | -4 | ASP | - | expression tag | UNP P32239 |
| R | -3 | ASP | - | expression tag | UNP P32239 |
| R | -2 | ASP | - | expression tag | UNP P32239 |
| R | -1 | GLY | - | expression tag | UNP P32239 |
| R | 0 | ALA | - | expression tag | UNP P32239 |
| R | 1 | PRO | - | expression tag | UNP P32239 |
| R | 419 | GLU | - | expression tag | UNP P32239 |
| R | 420 | PHE | - | expression tag | UNP P32239 |
| R | 421 | LEU | - | expression tag | UNP P32239 |
| R | 422 | GLU | - | expression tag | UNP P32239 |
| R | 423 | VAL | - | expression tag | UNP P32239 |
| R | 424 | LEU | - | expression tag | UNP P32239 |
| R | 425 | PHE | - | expression tag | UNP P32239 |
| R | 426 | GLN | - | expression tag | UNP P32239 |
| R | 427 | GLY | - | expression tag | UNP P32239 |
| R | 428 | PRO | - | expression tag | UNP P32239 |
| R | 429 | TRP | - | expression tag | UNP P32239 |
| R | 430 | SER | - | expression tag | UNP P32239 |
| R | 431 | HIS | - | expression tag | UNP P32239 |
| R | 432 | PRO | - | expression tag | UNP P32239 |
| R | 433 | GLN | - | expression tag | UNP P32239 |
| R | 434 | PHE | - | expression tag | UNP P32239 |
| R | 435 | GLU | - | expression tag | UNP P32239 |
| R | 436 | LYS | - | expression tag | UNP P32239 |
| R | 437 | GLY | - | expression tag | UNP P32239 |
| R | 438 | GLY | - | expression tag | UNP P32239 |
| R | 439 | GLY | - | expression tag | UNP P32239 |
| R | 440 | SER | - | expression tag | UNP P32239 |
| R | 441 | GLY | - | expression tag | UNP P32239 |
| R | 442 | GLY | - | expression tag | UNP P32239 |
| R | 443 | GLY | - | expression tag | UNP P32239 |
| R | 444 | SER | - | expression tag | UNP P32239 |
| R | 445 | GLY | - | expression tag | UNP P32239 |

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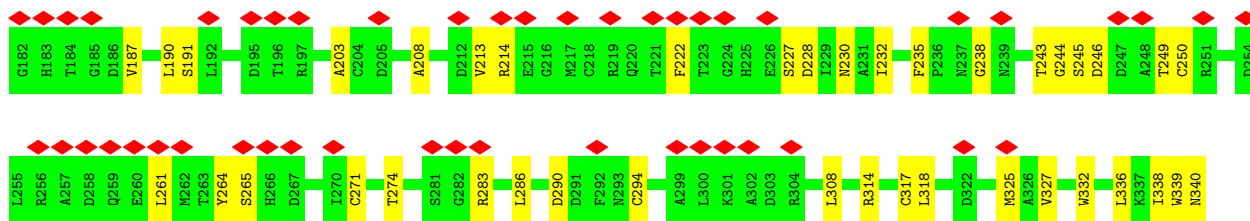| Chain | Residue | Modelled | Actual | Comment | Reference |
|:---:|:---:|:---:|:---:|:---:|:---:|
| R | 446 | GLY | - | expression tag | UNP P32239 |
| R | 447 | SER | - | expression tag | UNP P32239 |
| R | 448 | ALA | - | expression tag | UNP P32239 |
| R | 449 | TRP | - | expression tag | UNP P32239 |
| R | 450 | SER | - | expression tag | UNP P32239 |
| R | 451 | HIS | - | expression tag | UNP P32239 |
| R | 452 | PRO | - | expression tag | UNP P32239 |
| R | 453 | GLN | - | expression tag | UNP P32239 |
| R | 454 | PHE | - | expression tag | UNP P32239 |
| R | 455 | GLU | - | expression tag | UNP P32239 |
| R | 456 | LYS | - | expression tag | UNP P32239 |

# 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.

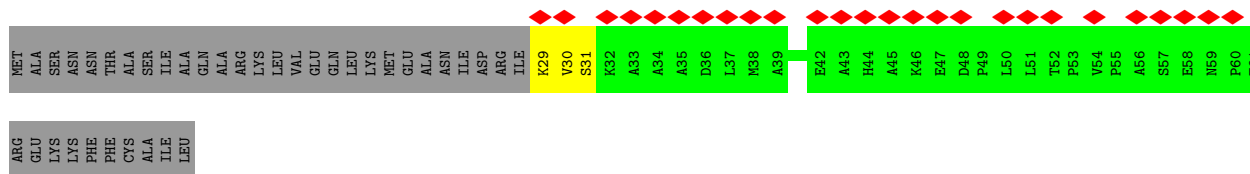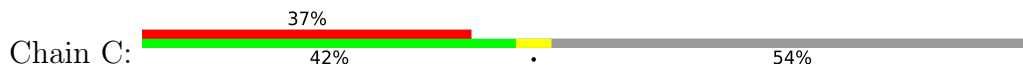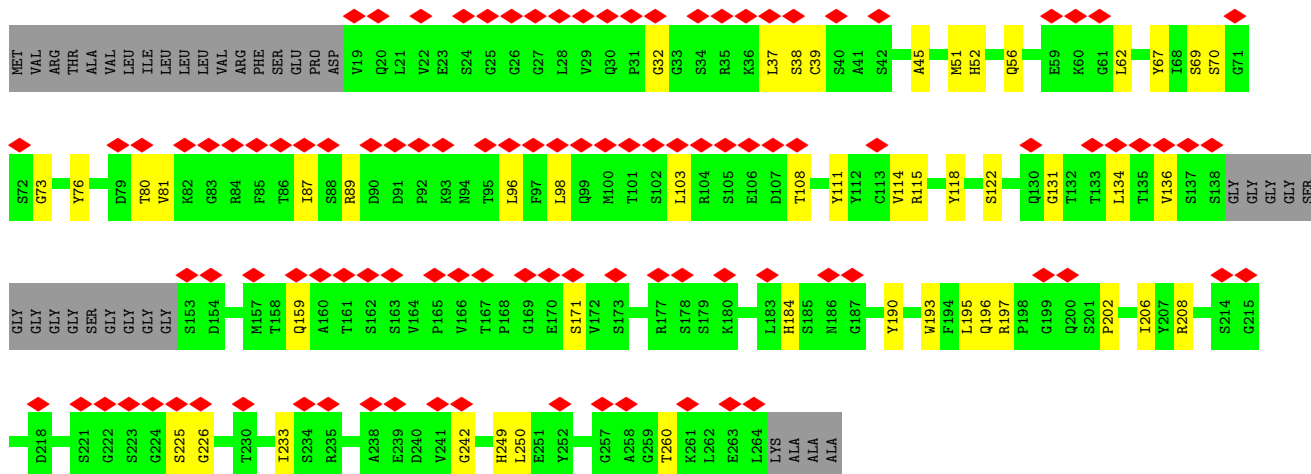• Molecule 1: Guanine nucleotide-binding protein G(q) subunit alpha



Chain A:

• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



Chain B:

G182 H183 T184 G185 D186 V187 L190 S191 L192 D195 T196 R197 A203 C204 D205 A208 D212 V213 R214 E215 G216 M217 C218 R219 Q220 T221 F222 T223 G224 H225 E226 S227 D228 I229 N230 A231 I232 F235 P236 N237 G238 N239 T243 G244 S245 D246 D247 A248 T249 C250 R251 D254

L255 R256 A257 D258 Q259 E260 L261 M262 T263 Y264 S265 H266 D267 I270 C271 T274 S281 G282 R283 L286 D290 D291 F292 N293 C294 A299 L300 K301 A302 D303 R304 L308 R314 C317 L318 D322 M325 A326 V327 W332 L336 K337 I338 W339 N340
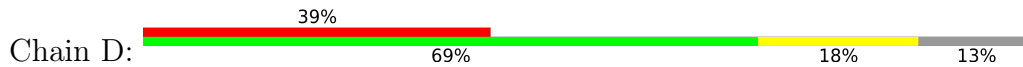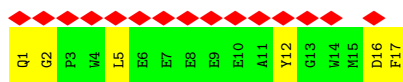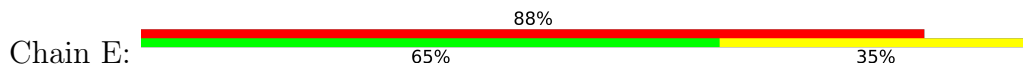
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain C:

MET ALA SER ASN ASN THR ALA SER ILE ALA GLN ALA ARG LYS LEU VAL GLU GLN LEU LYS MET GLU ALA ASN ILE ASP ARG ILE K29 V30 S31 K32 A33 A34 A35 D36 L37 M38 A39 E42 A43 H44 A45 K46 E47 D48 P49 L50 L51 T52 P53 V54 P55 A56 S57 E58 N59 P60 F61

ARG GLU LYS LYS PHE PHE CYS ALA ILE LEU

• Molecule 4: scFv16

Chain D:

MET VAL ARG THR ALA VAL LEU ILE LEU LEU LEU VAL ARG PHE SER GLU PRO ASP V19 Q20 L21 V22 E23 S24 G25 G26 G27 L28 V29 Q30 P31 G32 G33 S34 R35 K36 L37 S38 C39 S40 A41 S42 A45 M51 H52 Q56 E59 K60 G61 L62 Y67 I68 S69 S70 G71

S72 G73 Y76 D79 T80 V81 K82 G83 R84 F85 T86 I87 S88 R89 D90 D91 P92 K93 N94 T95 L96 F97 L98 Q99 M100 T101 S102 L103 R104 S105 E106 D107 T108 Y111 Y112 C113 V114 R115 Y118 S122 Q130 G131 T132 T133 L134 T135 V136 S137 S138 GLY GLY GLY SER

GLY GLY GLY SER GLY GLY GLY S153 D154 M157 T158 Q159 A160 T161 S162 S163 V164 P165 V166 T167 P168 G169 E170 S171 V172 S173 R177 S178 S179 K180 L183 H184 S185 N186 G187 Y190 W193 F194 L195 Q196 R197 P198 G199 Q200 S201 P202 I206 Y207 R208 S214 G215

D218 S221 G222 S223 G224 S225 G226 T230 I233 S234 R235 A238 E239 D240 V241 G242 H249 L250 E251 Y252 G257 A258 Q259 T260 K261 L262 E263 L264 LYS ALA ALA ALA

• Molecule 5: Gastrin-17

Chain E:

Q1 G2 P3 W4 L5 E6 E7 E8 E9 E10 A11 Y12 G13 W14 M15 D16 F17

• Molecule 6: Gastrin/cholecystokinin type B receptor

Chain R:

ASP TYR LYS ASP ASP ASP GLY ALA PRO GLU LEU LEU LYS LEU ASN ARG SER VAL GLN GLY THR GLY PRO PRO GLY ALA SER LEU CYS ARG PRO GLY ALA PRO LEU LEU ASN SER SER SER VAL GLY LEU LEU SER CYS GLU PRO PRO ARG ILE ARG GLY ALA GLY THR ARG GLU
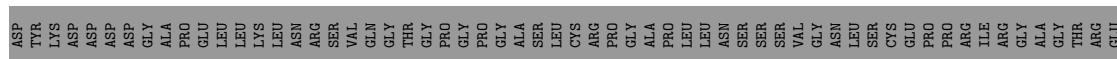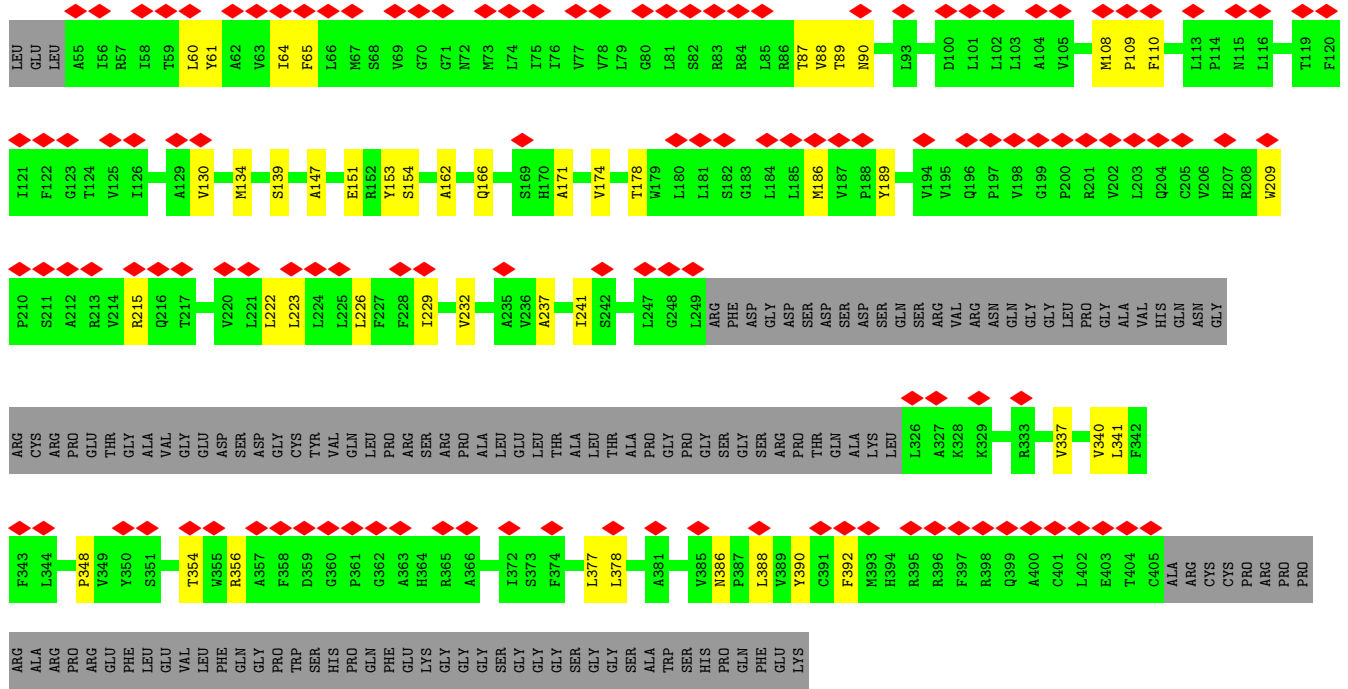
# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 354647 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose $(e^-/\text{Å}^2)$ | 1.75 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 0.180 | Depositor |
| Minimum map value | -0.108 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.003 | Depositor |
| Recommended contour level | 0.0252 | Depositor |
| Map size (Å) | 267.52, 267.52, 267.52 | wwPDB |
| Map dimensions | 256, 256, 256 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.045, 1.045, 1.045 | Depositor |

# 5 Model quality ⓘ

## 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NFA, PCA

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 | 0/1883 | 0.68 | 0/2532 |
| 2 | B | 0.29 | 0/2394 | 0.67 | 0/3248 |
| 3 | C | 0.27 | 0/251 | 0.54 | 0/342 |
| 4 | D | 0.31 | 0/1827 | 0.68 | 0/2477 |
| 5 | E | 0.30 | 0/119 | 0.50 | 0/165 |
| 6 | R | 0.32 | 0/2179 | 0.67 | 0/2977 |
| All | All | 0.30 | 0/8653 | 0.67 | 0/11741 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 1850 | 0 | 1851 | 43 | 0 |
| 2 | B | 2347 | 0 | 2249 | 48 | 0 |
| 3 | C | 245 | 0 | 240 | 2 | 0 |
| 4 | D | 1783 | 0 | 1719 | 31 | 0 |
| 5 | E | 133 | 0 | 101 | 4 | 0 |
| 6 | R | 2128 | 0 | 2256 | 28 | 0 |
| All | All | 8486 | 0 | 8416 | 139 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (139) 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) |
|---|---|---|---|
| 4:D:171:SER:HA | 4:D:233:ILE:O | 1.92 | 0.70 |
| 1:A:13:VAL:HG11 | 2:B:88:ASN:HD22 | 1.56 | 0.69 |
| 1:A:15:ARG:HH22 | 4:D:73:GLY:HA3 | 1.58 | 0.68 |
| 1:A:18:MET:HA | 1:A:21:ARG:HB2 | 1.76 | 0.68 |
| 1:A:34:LEU:HD22 | 1:A:218:THR:HB | 1.75 | 0.67 |
| 2:B:271:CYS:HB3 | 2:B:290:ASP:HB3 | 1.76 | 0.66 |
| 1:A:14:GLU:O | 1:A:17:LYS:HB2 | 1.96 | 0.65 |
| 1:A:183:ILE:HD13 | 2:B:117:LEU:HB3 | 1.78 | 0.65 |
| 4:D:52:HIS:HB2 | 4:D:114:VAL:HB | 1.79 | 0.65 |
| 2:B:46:ARG:HE | 2:B:48:ARG:HH12 | 1.44 | 0.64 |
| 2:B:59:TYR:HE2 | 2:B:75:GLN:HB3 | 1.61 | 0.64 |
| 2:B:132:ASN:HD22 | 4:D:45:ALA:HB2 | 1.63 | 0.64 |
| 6:R:60:LEU:HD22 | 6:R:377:LEU:HD21 | 1.82 | 0.62 |
| 1:A:17:LYS:HE2 | 2:B:89:LYS:HE2 | 1.83 | 0.61 |
| 1:A:188:PHE:HB2 | 1:A:195:PHE:HB3 | 1.81 | 0.61 |
| 2:B:325:MET:O | 2:B:340:ASN:ND2 | 2.35 | 0.60 |
| 5:E:5:LEU:HD21 | 5:E:12:TYR:H | 1.65 | 0.60 |
| 4:D:67:TYR:HB3 | 4:D:76:TYR:HB2 | 1.86 | 0.58 |
| 6:R:87:THR:H | 6:R:90:ASN:HB2 | 1.69 | 0.58 |
| 1:A:43:GLU:OE2 | 1:A:231:GLN:NE2 | 2.36 | 0.57 |
| 1:A:39:LEU:HD22 | 1:A:207:ARG:HH12 | 1.70 | 0.56 |
| 1:A:20:ASP:O | 1:A:24:ARG:N | 2.38 | 0.56 |
| 2:B:104:ALA:HB3 | 2:B:113:ALA:HB3 | 1.87 | 0.56 |
| 2:B:73:ALA:HB2 | 2:B:79:LEU:HD12 | 1.87 | 0.56 |
| 1:A:28:ARG:NH2 | 6:R:166:GLN:O | 2.39 | 0.56 |
| 2:B:38:ASP:O | 2:B:283:ARG:NH2 | 2.37 | 0.56 |
| 2:B:191:SER:HB3 | 2:B:232:ILE:HG23 | 1.89 | 0.55 |
| 2:B:294:CYS:HB2 | 2:B:308:LEU:HB2 | 1.88 | 0.55 |
| 4:D:103:LEU:HD21 | 4:D:134:LEU:HD21 | 1.89 | 0.55 |
| 1:A:18:MET:O | 1:A:22:ASN:N | 2.37 | 0.55 |
| 4:D:196:GLN:O | 4:D:242:GLY:HA3 | 2.07 | 0.55 |
| 2:B:70:LEU:HG | 2:B:82:TRP:HB2 | 1.90 | 0.54 |
| 6:R:130:VAL:O | 6:R:134:MET:HG2 | 2.08 | 0.53 |
| 1:A:28:ARG:HA | 1:A:31:ARG:HB2 | 1.89 | 0.53 |
| 4:D:69:SER:O | 4:D:89:ARG:NH1 | 2.41 | 0.53 |
| 1:A:224:VAL:O | 1:A:268:ASN:ND2 | 2.41 | 0.53 |
| 4:D:190:TYR:HB3 | 4:D:249:HIS:HB3 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:196:GLN:HB2 | 4:D:202:PRO:HB3 | 1.91 | 0.53 |
| 1:A:47:SER:OG | 1:A:51:LYS:NZ | 2.42 | 0.53 |
| 6:R:223:LEU:HD22 | 6:R:354:THR:HG21 | 1.90 | 0.53 |
| 4:D:37:LEU:HB2 | 4:D:98:LEU:HB3 | 1.92 | 0.52 |
| 1:A:188:PHE:N | 1:A:195:PHE:O | 2.42 | 0.52 |
| 1:A:183:ILE:HA | 1:A:199:ASP:O | 2.09 | 0.52 |
| 1:A:277:ILE:HG23 | 1:A:282:LEU:HD11 | 1.93 | 0.51 |
| 4:D:111:TYR:O | 4:D:131:GLY:HA2 | 2.11 | 0.51 |
| 2:B:274:THR:OG1 | 2:B:314:ARG:NH2 | 2.41 | 0.51 |
| 2:B:290:ASP:HA | 2:B:314:ARG:HB2 | 1.93 | 0.51 |
| 4:D:80:THR:HG23 | 4:D:81:VAL:HG23 | 1.93 | 0.51 |
| 2:B:245:SER:OG | 2:B:246:ASP:N | 2.44 | 0.51 |
| 1:A:247:ALA:HA | 1:A:250:ARG:HE | 1.75 | 0.50 |
| 4:D:184:HIS:HB2 | 4:D:250:LEU:HD11 | 1.93 | 0.50 |
| 5:E:16:ASP:OD1 | 6:R:356:ARG:NH2 | 2.43 | 0.50 |
| 1:A:226:LEU:HB3 | 1:A:268:ASN:HB2 | 1.93 | 0.50 |
| 4:D:195:LEU:HD22 | 4:D:197:ARG:HH11 | 1.75 | 0.50 |
| 1:A:13:VAL:HG21 | 2:B:88:ASN:HB3 | 1.92 | 0.50 |
| 1:A:274:GLU:O | 1:A:278:MET:HB2 | 2.12 | 0.50 |
| 2:B:232:ILE:HG13 | 2:B:243:THR:HG22 | 1.93 | 0.50 |
| 1:A:350:TYR:HA | 6:R:89:THR:HG21 | 1.94 | 0.49 |
| 2:B:249:THR:HG22 | 2:B:265:SER:HB2 | 1.94 | 0.49 |
| 1:A:37:LEU:HD12 | 1:A:200:VAL:HG21 | 1.94 | 0.49 |
| 1:A:189:ASP:OD1 | 1:A:189:ASP:N | 2.46 | 0.49 |
| 2:B:96:ARG:HH21 | 2:B:138:GLU:HG2 | 1.78 | 0.49 |
| 6:R:88:VAL:HG13 | 6:R:171:ALA:HB2 | 1.93 | 0.49 |
| 4:D:38:SER:HA | 4:D:96:LEU:O | 2.12 | 0.49 |
| 1:A:186:TYR:O | 1:A:196:ARG:HA | 2.13 | 0.49 |
| 6:R:139:SER:HA | 6:R:226:LEU:HD11 | 1.93 | 0.48 |
| 2:B:208:ALA:HB3 | 2:B:222:PHE:HB2 | 1.95 | 0.48 |
| 6:R:65:PHE:HD1 | 6:R:108:MET:HE2 | 1.78 | 0.48 |
| 2:B:261:LEU:HD12 | 3:C:30:VAL:HG21 | 1.96 | 0.48 |
| 4:D:87:ILE:HD12 | 4:D:98:LEU:HD13 | 1.95 | 0.48 |
| 6:R:61:TYR:HA | 6:R:64:ILE:HG22 | 1.96 | 0.47 |
| 6:R:64:ILE:HG23 | 6:R:108:MET:HE1 | 1.96 | 0.47 |
| 2:B:112:VAL:HG13 | 2:B:126:LEU:HD11 | 1.95 | 0.47 |
| 1:A:17:LYS:NZ | 2:B:52:ARG:O | 2.48 | 0.47 |
| 4:D:39:CYS:HB3 | 4:D:96:LEU:HB2 | 1.96 | 0.47 |
| 2:B:153:ASP:HB2 | 2:B:156:GLN:HB2 | 1.97 | 0.47 |
| 1:A:338:VAL:HA | 1:A:341:THR:HG22 | 1.97 | 0.47 |
| 2:B:213:VAL:HG12 | 2:B:214:ARG:HE | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:230:ASN:N | 2:B:244:GLY:O | 2.45 | 0.46 |
| 4:D:159:GLN:NE2 | 4:D:260:THR:OG1 | 2.43 | 0.46 |
| 1:A:226:LEU:HD22 | 1:A:267:LEU:HB3 | 1.98 | 0.46 |
| 1:A:183:ILE:HG13 | 1:A:200:VAL:HA | 1.98 | 0.46 |
| 2:B:81:ILE:O | 2:B:90:VAL:N | 2.49 | 0.46 |
| 2:B:187:VAL:HA | 2:B:203:ALA:HA | 1.97 | 0.46 |
| 2:B:168:LEU:HD22 | 2:B:213:VAL:HG13 | 1.97 | 0.45 |
| 4:D:56:GLN:HB2 | 4:D:62:LEU:HD23 | 1.97 | 0.45 |
| 4:D:122:SER:O | 4:D:208:ARG:NH2 | 2.49 | 0.45 |
| 2:B:250:CYS:HB2 | 2:B:264:TYR:HB2 | 1.98 | 0.45 |
| 4:D:32:GLY:N | 4:D:103:LEU:O | 2.49 | 0.45 |
| 4:D:108:THR:HG22 | 4:D:136:VAL:H | 1.81 | 0.45 |
| 1:A:240:ASN:HB2 | 1:A:243:GLU:HB3 | 1.98 | 0.45 |
| 2:B:168:LEU:O | 2:B:177:THR:N | 2.49 | 0.45 |
| 4:D:193:TRP:HB2 | 4:D:206:ILE:HB | 1.99 | 0.45 |
| 6:R:209:TRP:HB2 | 6:R:215:ARG:HD3 | 1.98 | 0.45 |
| 2:B:57:LYS:HB3 | 2:B:332:TRP:CD1 | 2.53 | 0.44 |
| 6:R:229:ILE:HA | 6:R:232:VAL:HG12 | 2.00 | 0.44 |
| 5:E:17:NFA:HZ | 6:R:222:LEU:HD21 | 1.99 | 0.44 |
| 2:B:78:LYS:HD3 | 2:B:78:LYS:HA | 1.85 | 0.44 |
| 2:B:145:TYR:O | 2:B:162:GLY:N | 2.47 | 0.44 |
| 2:B:129:ARG:O | 4:D:115:ARG:NH1 | 2.50 | 0.44 |
| 4:D:51:MET:HG3 | 4:D:96:LEU:HD21 | 1.99 | 0.44 |
| 6:R:337:VAL:O | 6:R:341:LEU:HB2 | 2.18 | 0.43 |
| 6:R:109:PRO:HG2 | 6:R:110:PHE:CD1 | 2.53 | 0.43 |
| 3:C:29:LYS:HG3 | 3:C:31:SER:H | 1.83 | 0.43 |
| 1:A:243:GLU:HA | 1:A:246:LYS:HB3 | 2.01 | 0.43 |
| 4:D:52:HIS:NE2 | 4:D:118:TYR:OH | 2.42 | 0.43 |
| 4:D:37:LEU:HD12 | 4:D:98:LEU:HD23 | 1.99 | 0.43 |
| 4:D:225:SER:OG | 4:D:226:GLY:N | 2.51 | 0.43 |
| 6:R:348:PRO:HG2 | 6:R:378:LEU:HD12 | 1.99 | 0.43 |
| 2:B:227:SER:OG | 2:B:228:ASP:N | 2.50 | 0.43 |
| 1:A:209:LYS:NZ | 2:B:228:ASP:OD2 | 2.31 | 0.43 |
| 2:B:61:MET:HG3 | 2:B:317:CYS:HB2 | 2.00 | 0.43 |
| 1:A:15:ARG:NH1 | 4:D:70:SER:O | 2.52 | 0.43 |
| 1:A:211:ILE:HD12 | 1:A:211:ILE:HA | 1.92 | 0.42 |
| 6:R:186:MET:HG2 | 6:R:189:TYR:HB2 | 2.00 | 0.42 |
| 6:R:153:TYR:HA | 6:R:241:ILE:HD11 | 2.00 | 0.42 |
| 5:E:1:PCA:HB2 | 5:E:2:GLY:H | 1.61 | 0.42 |
| 1:A:209:LYS:HD3 | 1:A:209:LYS:HA | 1.80 | 0.42 |
| 6:R:337:VAL:HA | 6:R:340:VAL:HG12 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:269:LYS:HA | 1:A:324:CYS:HA | 2.02 | 0.42 |
| 6:R:154:SER:HB3 | 6:R:162:ALA:HB2 | 2.01 | 0.42 |
| 2:B:47:THR:HA | 2:B:338:ILE:O | 2.20 | 0.42 |
| 2:B:327:VAL:HB | 2:B:339:TRP:O | 2.20 | 0.41 |
| 1:A:226:LEU:H | 1:A:268:ASN:HD22 | 1.68 | 0.41 |
| 2:B:70:LEU:HD11 | 2:B:336:LEU:HD21 | 2.01 | 0.41 |
| 2:B:158:VAL:HG13 | 2:B:190:LEU:HD21 | 2.02 | 0.41 |
| 2:B:286:LEU:HD22 | 2:B:318:LEU:HD11 | 2.02 | 0.41 |
| 4:D:108:THR:HA | 4:D:134:LEU:O | 2.20 | 0.41 |
| 6:R:388:LEU:HA | 6:R:392:PHE:HB2 | 2.01 | 0.41 |
| 6:R:237:ALA:O | 6:R:241:ILE:HG12 | 2.21 | 0.41 |
| 6:R:386:ASN:O | 6:R:390:TYR:HB2 | 2.21 | 0.41 |
| 1:A:31:ARG:HD3 | 1:A:31:ARG:HA | 1.89 | 0.41 |
| 1:A:269:LYS:HE2 | 1:A:325:ALA:HB2 | 2.03 | 0.41 |
| 2:B:121:CYS:HB3 | 2:B:139:LEU:HB2 | 2.03 | 0.41 |
| 1:A:350:TYR:OH | 6:R:166:GLN:OE1 | 2.33 | 0.40 |
| 2:B:235:PHE:HB3 | 2:B:238:GLY:H | 1.86 | 0.40 |
| 6:R:174:VAL:O | 6:R:178:THR:HG23 | 2.21 | 0.40 |
| 1:A:13:VAL:CG1 | 2:B:88:ASN:HD22 | 2.27 | 0.40 |
| 6:R:147:ALA:O | 6:R:151:GLU:HG2 | 2.22 | 0.40 |

There are no symmetry-related clashes.

## 5.3   Torsion angles (i)

### 5.3.1   Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 220/353 (62%) | 209 (95%) | 11 (5%) | 0 | 100 | 100 |
| 2 | B | 304/351 (87%) | 288 (95%) | 16 (5%) | 0 | 100 | 100 |
| 3 | C | 31/71 (44%) | 31 (100%) | 0 | 0 | 100 | 100 |
| 4 | D | 228/268 (85%) | 211 (92%) | 17 (8%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------|----------|---------|----------|------|------|
| 5 | E | 15/17 (88%) | 15 (100%) | 0 | 0 | 100 | 100 |
| 6 | R | 271/465 (58%) | 266 (98%) | 5 (2%) | 0 | 100 | 100 |
| All | All | 1069/1525 (70%) | 1020 (95%) | 49 (5%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------|-----------|----------|------|------|
| 1 | A | 204/320 (64%) | 204 (100%) | 0 | 100 | 100 |
| 2 | B | 254/293 (87%) | 254 (100%) | 0 | 100 | 100 |
| 3 | C | 26/58 (45%) | 26 (100%) | 0 | 100 | 100 |
| 4 | D | 197/217 (91%) | 197 (100%) | 0 | 100 | 100 |
| 5 | E | 8/12 (67%) | 8 (100%) | 0 | 100 | 100 |
| 6 | R | 232/383 (61%) | 232 (100%) | 0 | 100 | 100 |
| All | All | 921/1283 (72%) | 921 (100%) | 0 | 100 | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 268 | ASN |
| 2 | B | 132 | ASN |
| 4 | D | 159 | GLN |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------|------|-----------|--------|------|-----------|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 5 | PCA | E | 1 | 5 | 7,8,9 | 0.44 | 0 | 9,10,12 | 0.53 | 0 |
| 5 | NFA | E | 17 | 5 | 12,12,12 | 0.82 | 0 | 15,15,15 | 0.65 | 0 |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 5 | PCA | E | 1 | 5 | - | 0/0/11/13 | 0/1/1/1 |
| 5 | NFA | E | 17 | 5 | - | 1/8/8/8 | 0/1/1/1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 5 | E | 17 | NFA | NXT-C-CA-N |

There are no ring outliers.

2 monomers are involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5 | E | 1 | PCA | 1 | 0 |
| 5 | E | 17 | NFA | 1 | 0 |

## 5.5 Carbohydrates (i)

There are no monosaccharides 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-31494. 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 |
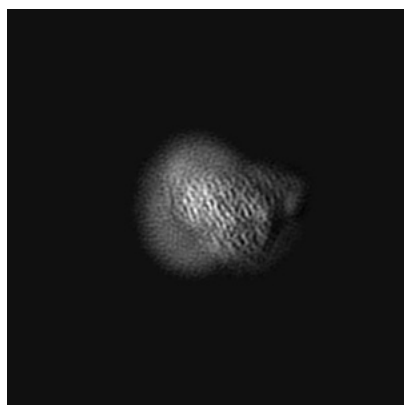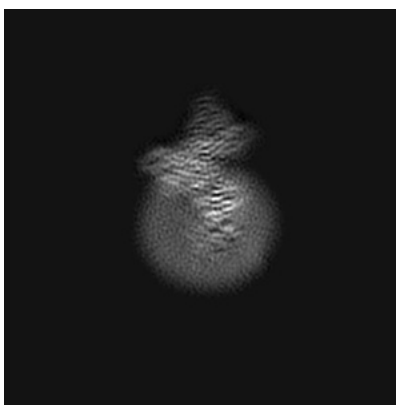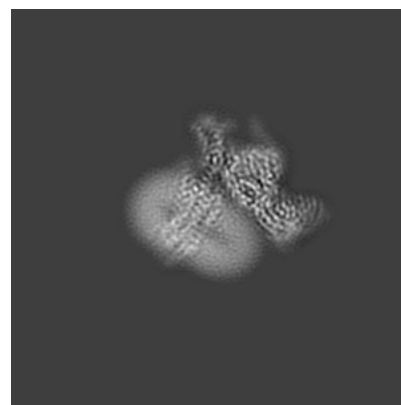
The images above show the map projected in three orthogonal directions.

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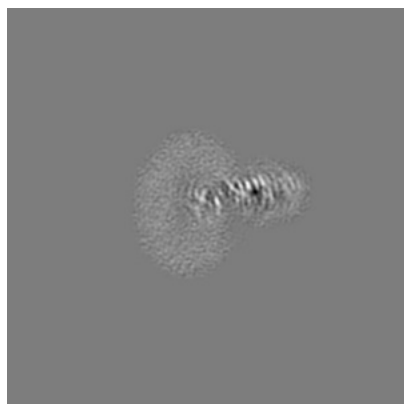
### 6.2.1 Primary map
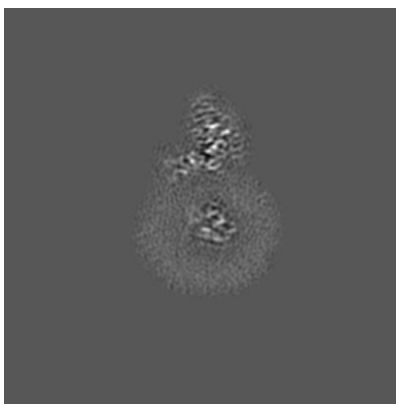


| X Index: 128 | Y Index: 128 | Z Index: 128 |
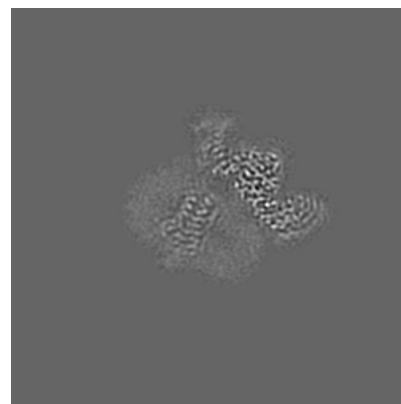
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices ⓘ

### 6.3.1 Primary map
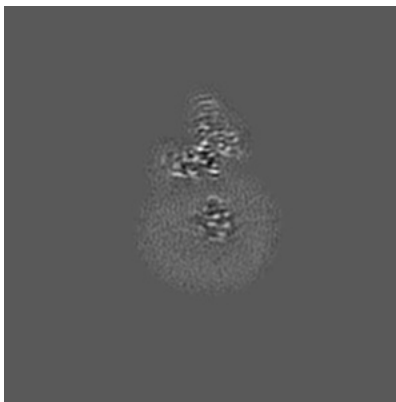


| X Index: 164 | Y Index: 131 | Z Index: 133 |
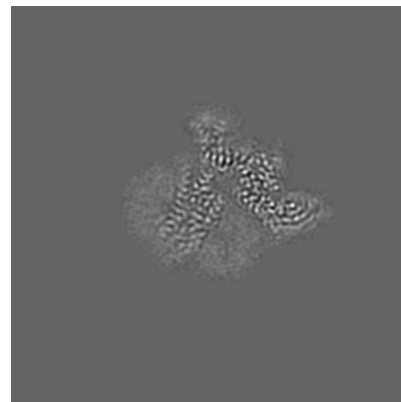
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views ⓘ

### 6.4.1 Primary map



| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.0252. 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 ⓘ
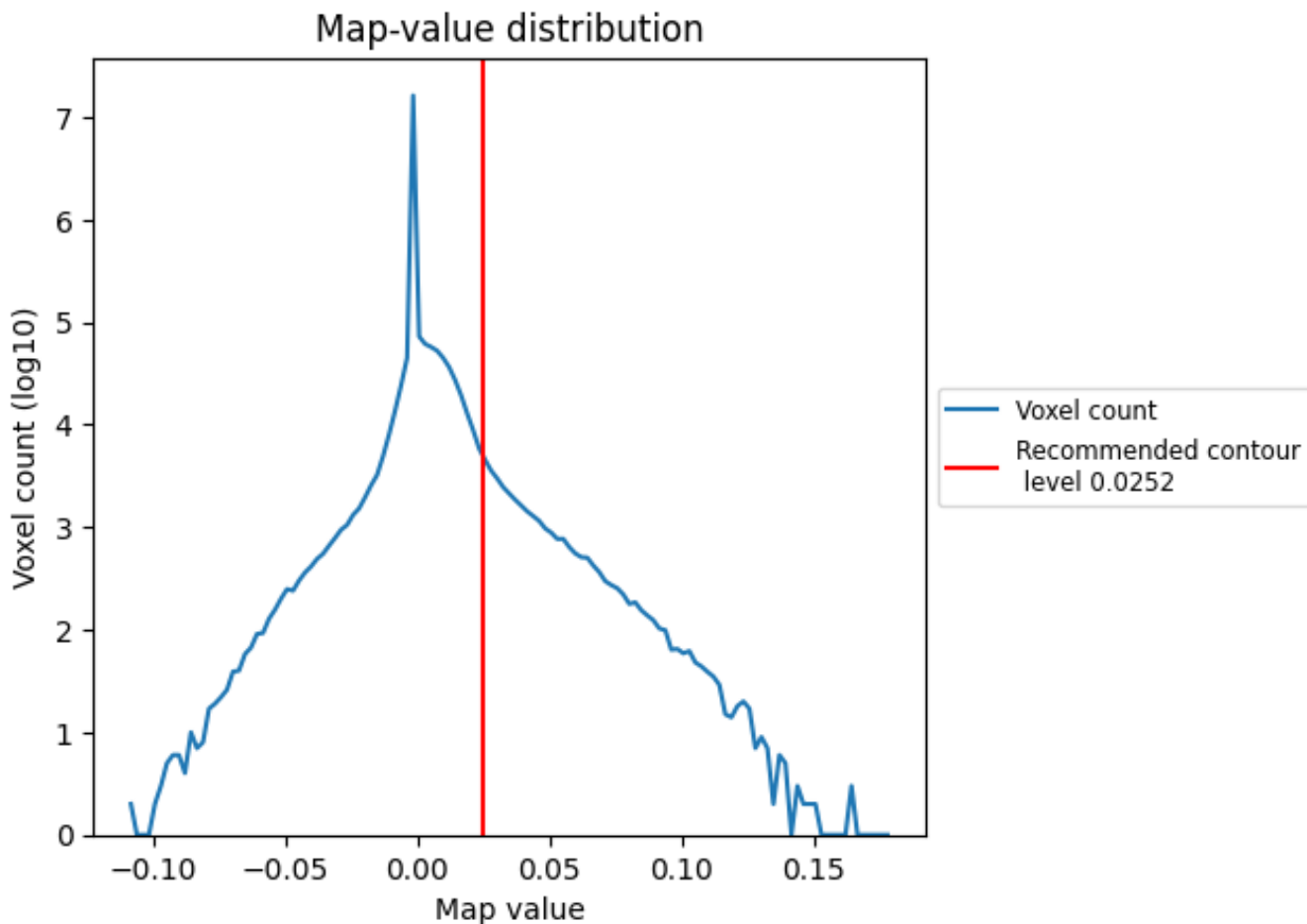


The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate ⓘ
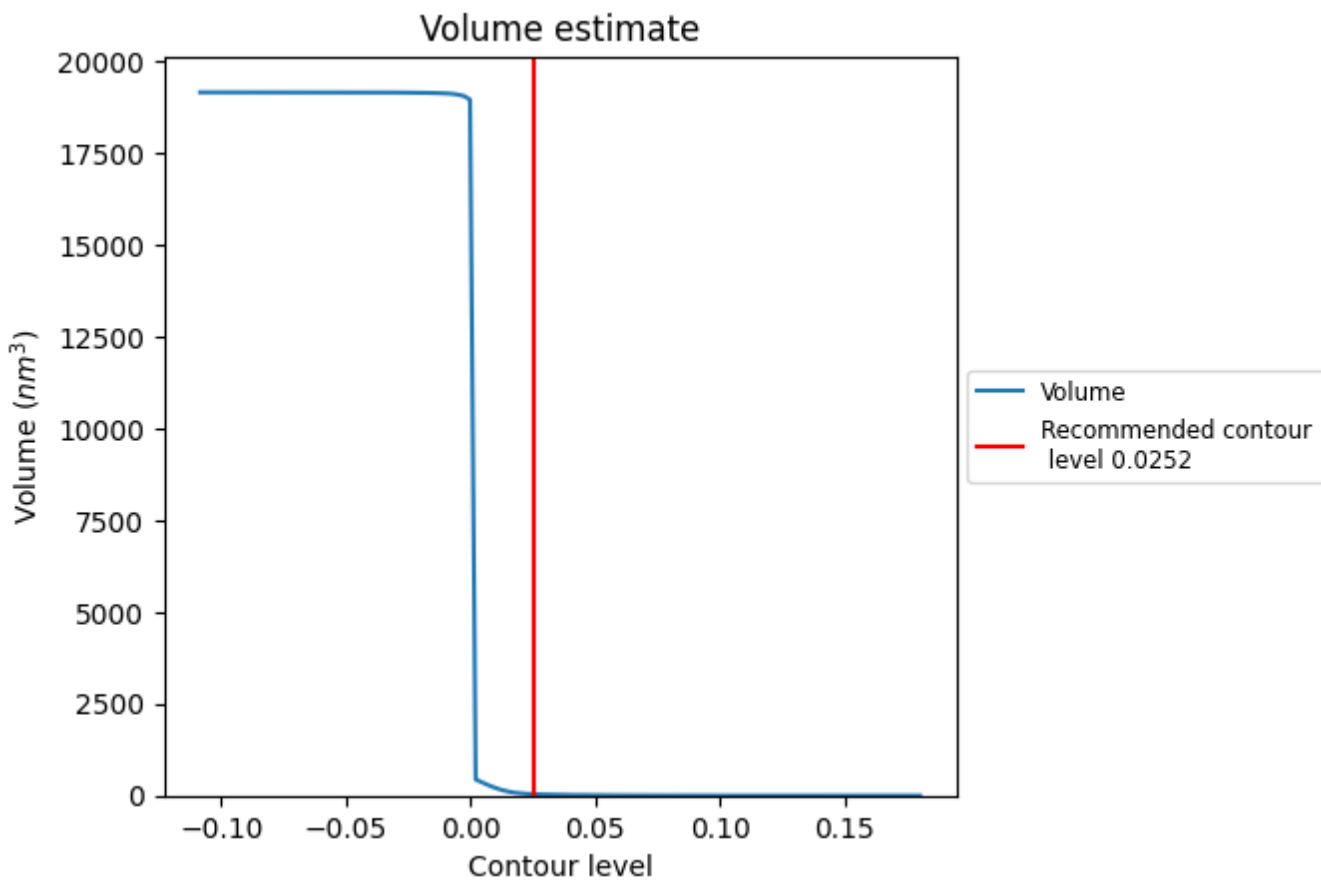


The volume at the recommended contour level is 38 nm$^3$; this corresponds to an approximate mass of 34 kDa.

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   ⓘ
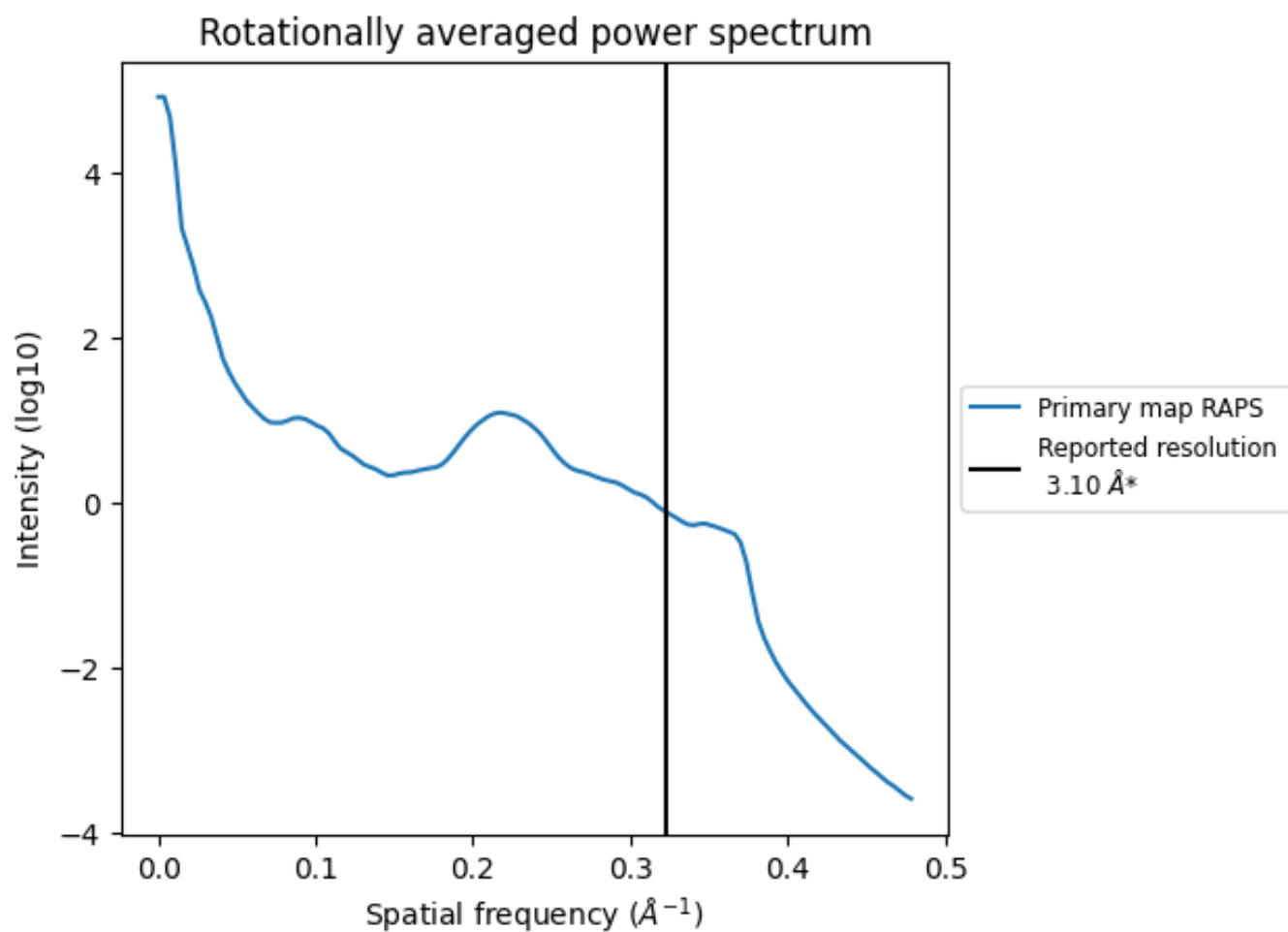


*Reported resolution corresponds to spatial frequency of 0.323 Å$^{-1}$

# 8 Fourier-Shell correlation ⓘ

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-31494 and PDB model 7F8W. Per-residue inclusion information can be found in section 3 on page 7.

## 9.1 Map-model overlay ⓘ
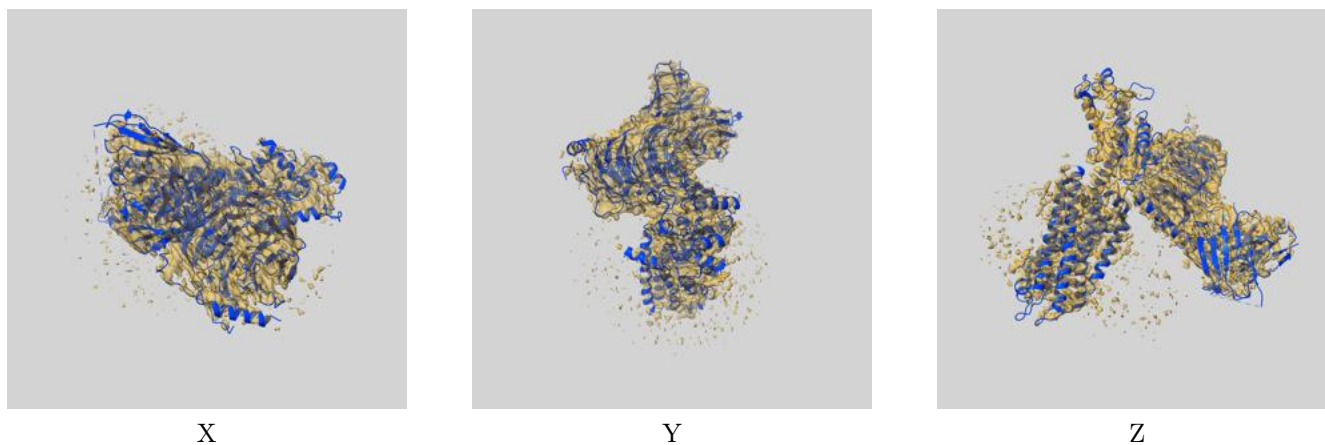


| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.0252 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 ⓘ
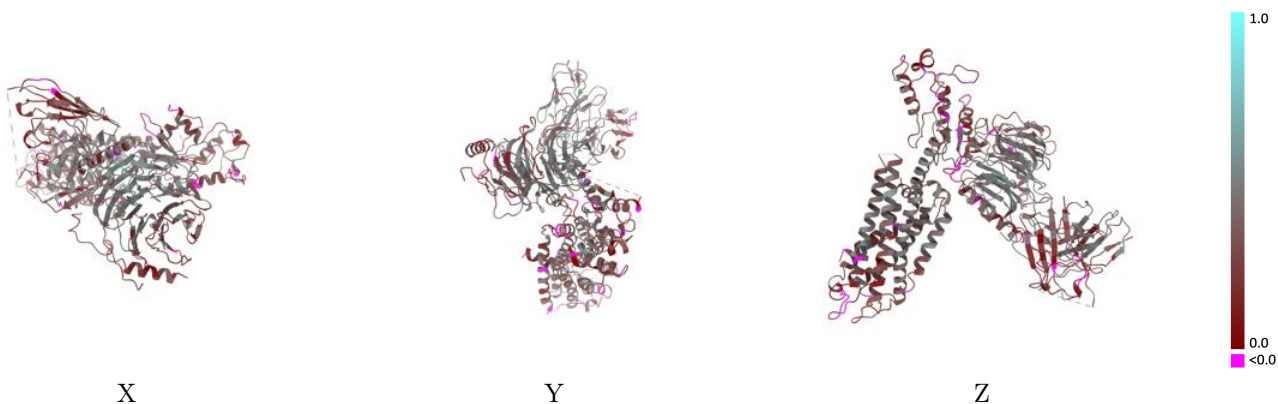


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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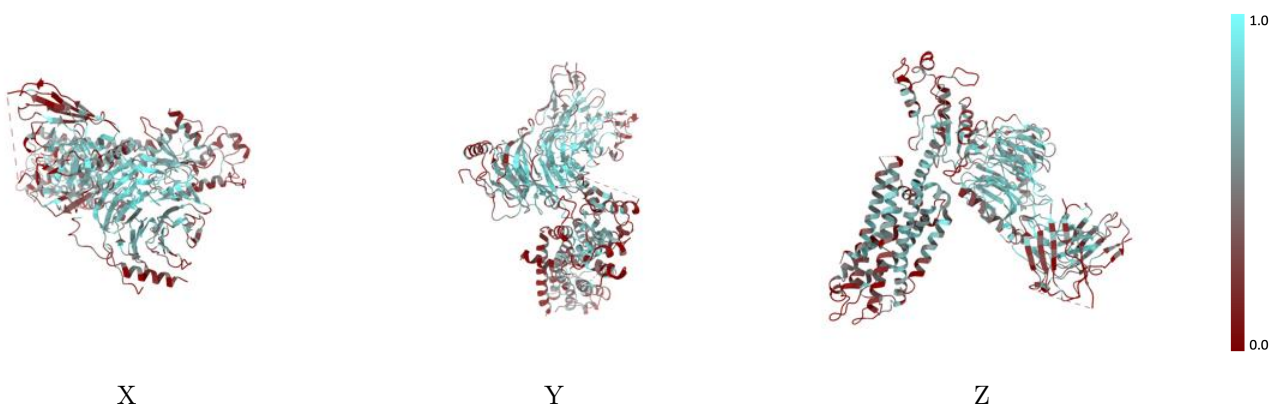


The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0252).

## 9.4   Atom inclusion ⓘ
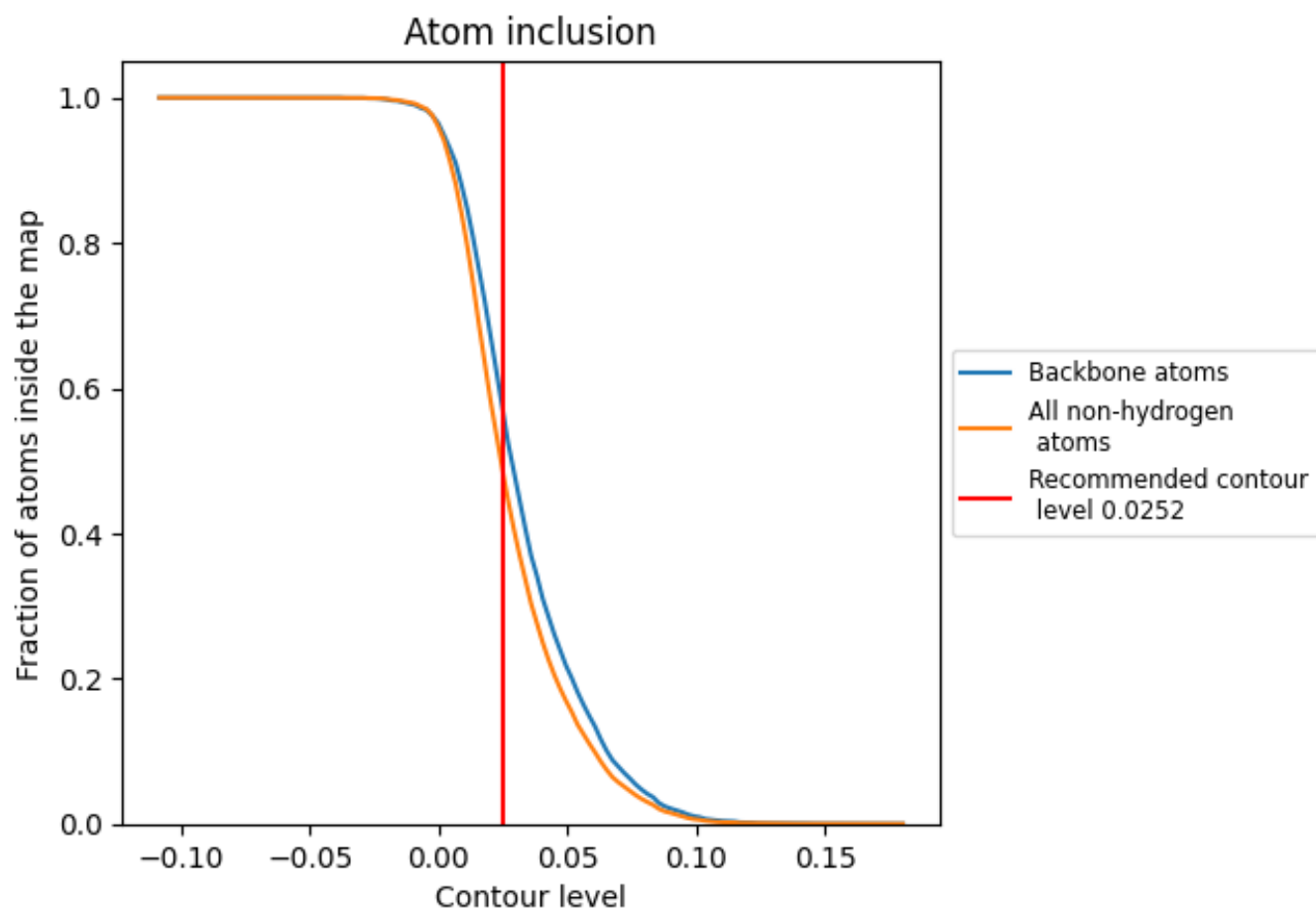


At the recommended contour level, 56% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0252) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|:-----:|:--------------:|:-------:|
| All | 0.4793 | 0.3350 |
| A | 0.3976 | 0.2750 |
| B | 0.6293 | 0.3870 |
| C | 0.2705 | 0.2680 |
| D | 0.4836 | 0.3490 |
| E | 0.1615 | 0.1240 |
| R | 0.4253 | 0.3380 |

1.0

0.0
<0.0