# wwPDB EM Validation Summary Report

Nov 6, 2022 – 09:38 AM EST

| | | |
|---|---|---|
| PDB ID | : | 6D7T |
| EMDB ID | : | EMD-7825 |
| Title | : | Cryo-EM structure of human TRPV6-Y467A in complex with 2-Aminoethoxydiphenyl borate (2-APB) |
| Authors | : | Singh, A.K.; Saotome, K.; McGoldrick, L.L.; Sobolevsky, A.I. |
| Deposited on | : | 2018-04-25 |
| Resolution | : | 4.44 Å(reported) |

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

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

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

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

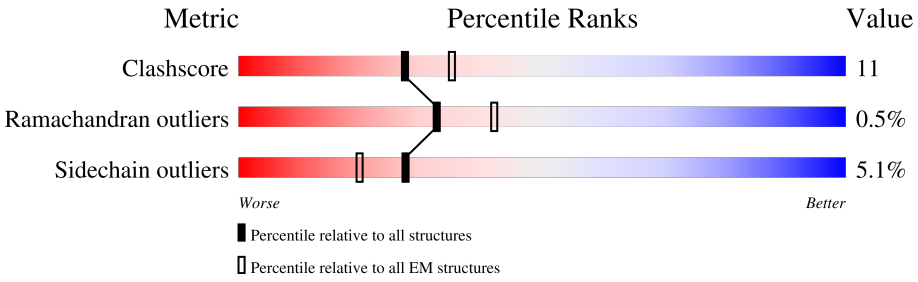
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.2 |

# 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 4.44 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) |
|---|---|---|
| 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 | 742 | 33% 57% 23% · 18% |
| 1 | B | 742 | 33% 57% 23% · 18% |
| 1 | C | 742 | 33% 56% 24% · 18% |
| 1 | D | 742 | 32% 57% 23% · 18% |

## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 19654 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 Transient receptor potential cation channel subfamily V member 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 611 | Total | C | N | O | S | 0 | 0 |
| | | | 4896 | 3162 | 830 | 864 | 40 | | |
| 1 | B | 611 | Total | C | N | O | S | 0 | 0 |
| | | | 4896 | 3162 | 830 | 864 | 40 | | |
| 1 | C | 611 | Total | C | N | O | S | 0 | 0 |
| | | | 4896 | 3162 | 830 | 864 | 40 | | |
| 1 | D | 611 | Total | C | N | O | S | 0 | 0 |
| | | | 4896 | 3162 | 830 | 864 | 40 | | |

There are 72 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 467 | ALA | TYR | engineered mutation | UNP Q9H1D0 |
| A | 726 | LEU | - | expression tag | UNP Q9H1D0 |
| A | 727 | VAL | - | expression tag | UNP Q9H1D0 |
| A | 728 | PRO | - | expression tag | UNP Q9H1D0 |
| A | 729 | ARG | - | expression tag | UNP Q9H1D0 |
| A | 730 | GLY | - | expression tag | UNP Q9H1D0 |
| A | 731 | SER | - | expression tag | UNP Q9H1D0 |
| A | 732 | ALA | - | expression tag | UNP Q9H1D0 |
| A | 733 | ALA | - | expression tag | UNP Q9H1D0 |
| A | 734 | ALA | - | expression tag | UNP Q9H1D0 |
| A | 735 | TRP | - | expression tag | UNP Q9H1D0 |
| A | 736 | SER | - | expression tag | UNP Q9H1D0 |
| A | 737 | HIS | - | expression tag | UNP Q9H1D0 |
| A | 738 | PRO | - | expression tag | UNP Q9H1D0 |
| A | 739 | GLN | - | expression tag | UNP Q9H1D0 |
| A | 740 | PHE | - | expression tag | UNP Q9H1D0 |
| A | 741 | GLU | - | expression tag | UNP Q9H1D0 |
| A | 742 | LYS | - | expression tag | UNP Q9H1D0 |
| B | 467 | ALA | TYR | engineered mutation | UNP Q9H1D0 |
| B | 726 | LEU | - | expression tag | UNP Q9H1D0 |
| B | 727 | VAL | - | expression tag | UNP Q9H1D0 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 728 | PRO | - | expression tag | UNP Q9H1D0 |
| B | 729 | ARG | - | expression tag | UNP Q9H1D0 |
| B | 730 | GLY | - | expression tag | UNP Q9H1D0 |
| B | 731 | SER | - | expression tag | UNP Q9H1D0 |
| B | 732 | ALA | - | expression tag | UNP Q9H1D0 |
| B | 733 | ALA | - | expression tag | UNP Q9H1D0 |
| B | 734 | ALA | - | expression tag | UNP Q9H1D0 |
| B | 735 | TRP | - | expression tag | UNP Q9H1D0 |
| B | 736 | SER | - | expression tag | UNP Q9H1D0 |
| B | 737 | HIS | - | expression tag | UNP Q9H1D0 |
| B | 738 | PRO | - | expression tag | UNP Q9H1D0 |
| B | 739 | GLN | - | expression tag | UNP Q9H1D0 |
| B | 740 | PHE | - | expression tag | UNP Q9H1D0 |
| B | 741 | GLU | - | expression tag | UNP Q9H1D0 |
| B | 742 | LYS | - | expression tag | UNP Q9H1D0 |
| C | 467 | ALA | TYR | engineered mutation | UNP Q9H1D0 |
| C | 726 | LEU | - | expression tag | UNP Q9H1D0 |
| C | 727 | VAL | - | expression tag | UNP Q9H1D0 |
| C | 728 | PRO | - | expression tag | UNP Q9H1D0 |
| C | 729 | ARG | - | expression tag | UNP Q9H1D0 |
| C | 730 | GLY | - | expression tag | UNP Q9H1D0 |
| C | 731 | SER | - | expression tag | UNP Q9H1D0 |
| C | 732 | ALA | - | expression tag | UNP Q9H1D0 |
| C | 733 | ALA | - | expression tag | UNP Q9H1D0 |
| C | 734 | ALA | - | expression tag | UNP Q9H1D0 |
| C | 735 | TRP | - | expression tag | UNP Q9H1D0 |
| C | 736 | SER | - | expression tag | UNP Q9H1D0 |
| C | 737 | HIS | - | expression tag | UNP Q9H1D0 |
| C | 738 | PRO | - | expression tag | UNP Q9H1D0 |
| C | 739 | GLN | - | expression tag | UNP Q9H1D0 |
| C | 740 | PHE | - | expression tag | UNP Q9H1D0 |
| C | 741 | GLU | - | expression tag | UNP Q9H1D0 |
| C | 742 | LYS | - | expression tag | UNP Q9H1D0 |
| D | 467 | ALA | TYR | engineered mutation | UNP Q9H1D0 |
| D | 726 | LEU | - | expression tag | UNP Q9H1D0 |
| D | 727 | VAL | - | expression tag | UNP Q9H1D0 |
| D | 728 | PRO | - | expression tag | UNP Q9H1D0 |
| D | 729 | ARG | - | expression tag | UNP Q9H1D0 |
| D | 730 | GLY | - | expression tag | UNP Q9H1D0 |
| D | 731 | SER | - | expression tag | UNP Q9H1D0 |
| D | 732 | ALA | - | expression tag | UNP Q9H1D0 |
| D | 733 | ALA | - | expression tag | UNP Q9H1D0 |

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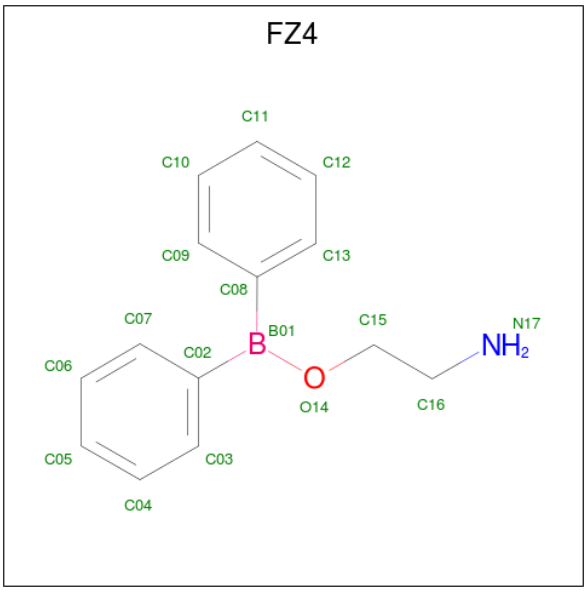
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | 734 | ALA | - | expression tag | UNP Q9H1D0 |
| D | 735 | TRP | - | expression tag | UNP Q9H1D0 |
| D | 736 | SER | - | expression tag | UNP Q9H1D0 |
| D | 737 | HIS | - | expression tag | UNP Q9H1D0 |
| D | 738 | PRO | - | expression tag | UNP Q9H1D0 |
| D | 739 | GLN | - | expression tag | UNP Q9H1D0 |
| D | 740 | PHE | - | expression tag | UNP Q9H1D0 |
| D | 741 | GLU | - | expression tag | UNP Q9H1D0 |
| D | 742 | LYS | - | expression tag | UNP Q9H1D0 |

- Molecule 2 is 2-aminoethyl diphenylborinate (three-letter code: FZ4) (formula: $C_{14}H_{16}BNO$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 2 | A | 1 | Total | B | C | N | O | 0 |
| | | | 17 | 1 | 14 | 1 | 1 | |
| 2 | B | 1 | Total | B | C | N | O | 0 |
| | | | 17 | 1 | 14 | 1 | 1 | |
| 2 | C | 1 | Total | B | C | N | O | 0 |
| | | | 17 | 1 | 14 | 1 | 1 | |
| 2 | D | 1 | Total | B | C | N | O | 0 |
| | | | 17 | 1 | 14 | 1 | 1 | |

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

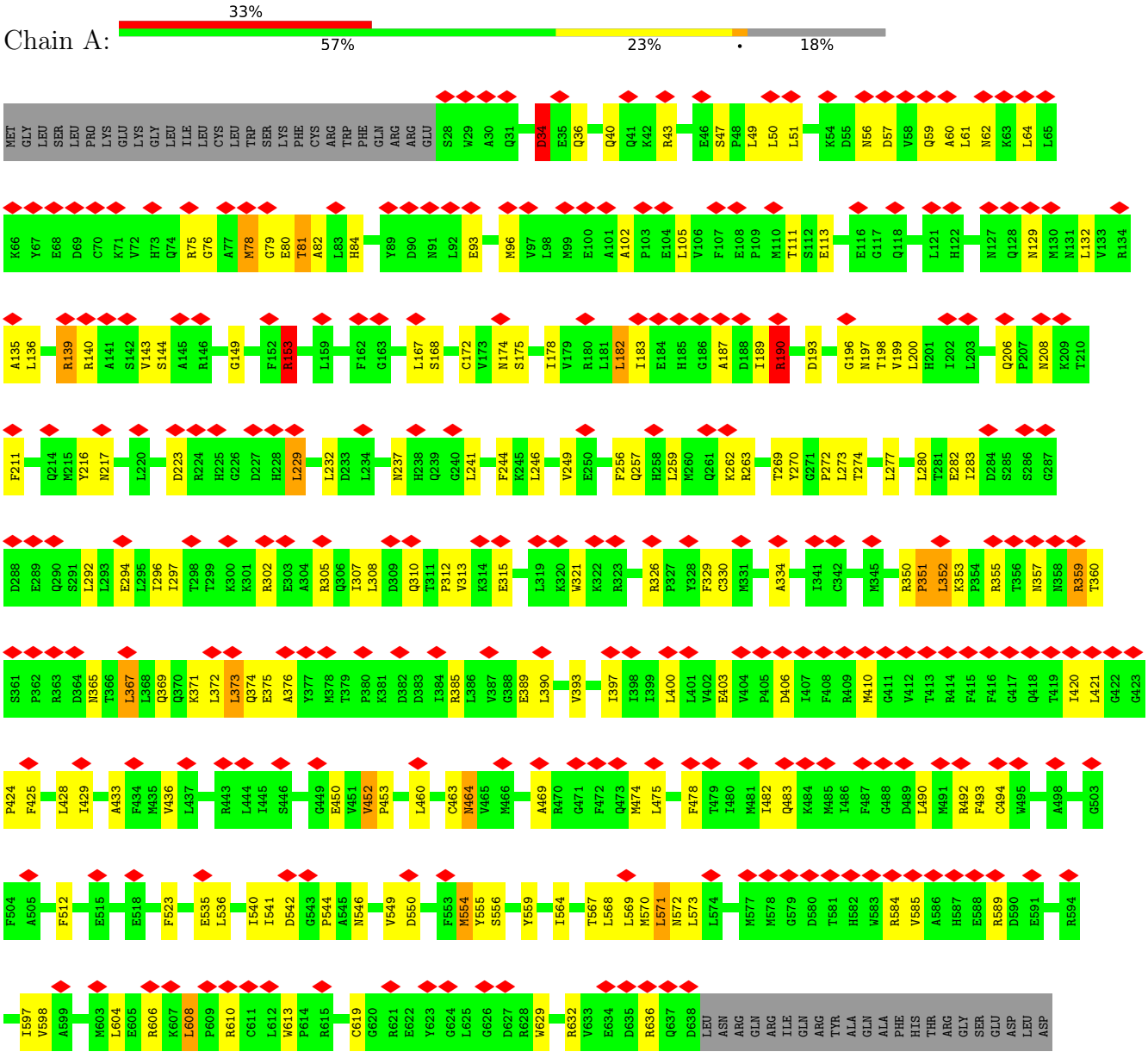
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 3 | A | 2 | Total | Ca | 0 |
| | | | 2 | 2 | |

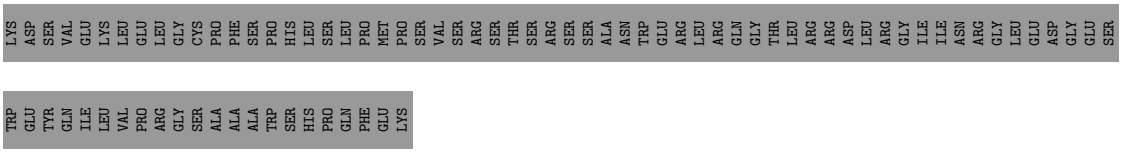
# 3 Residue-property plots (i)

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: Transient receptor potential cation channel subfamily V member 6

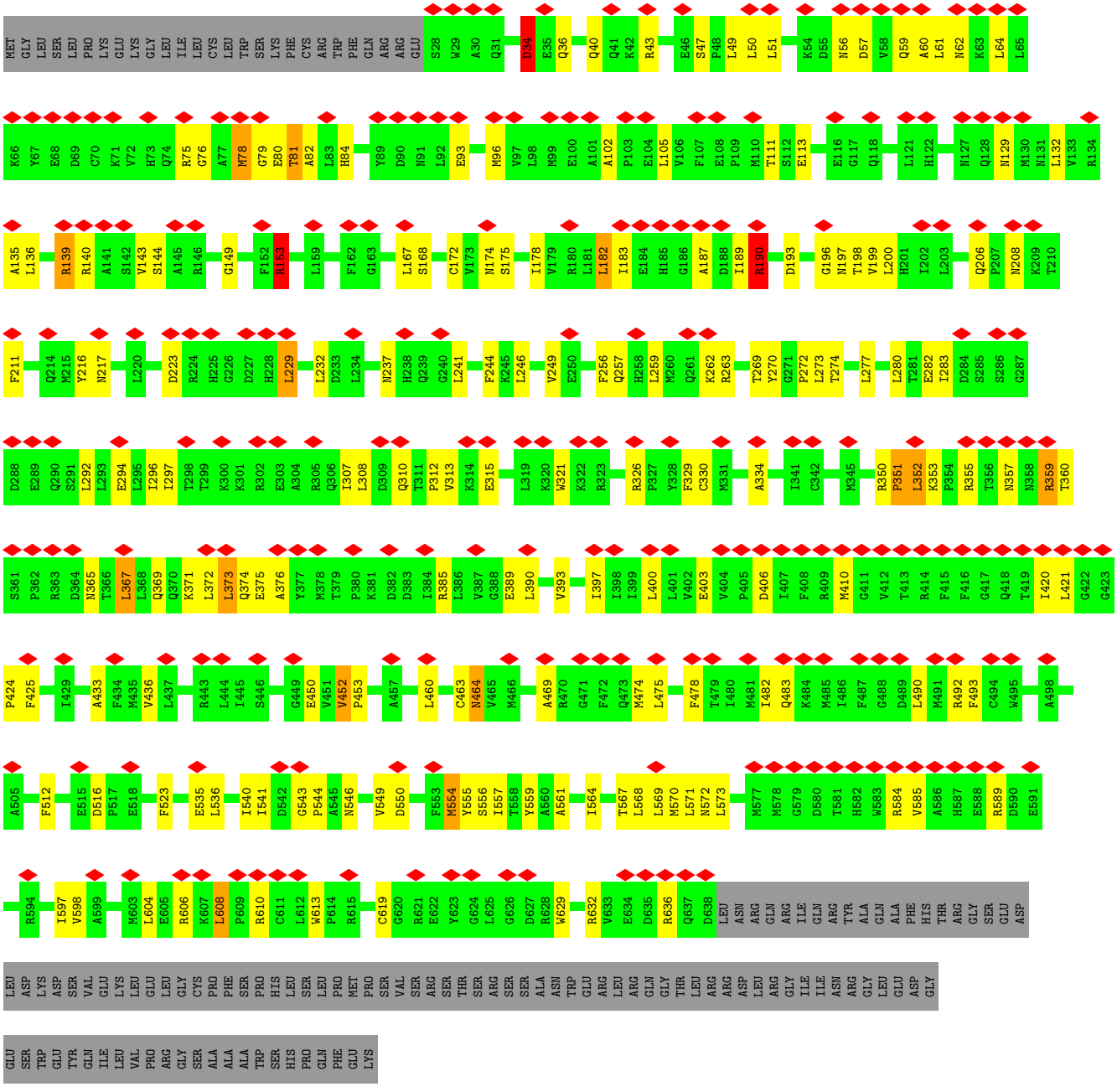
Chain A:





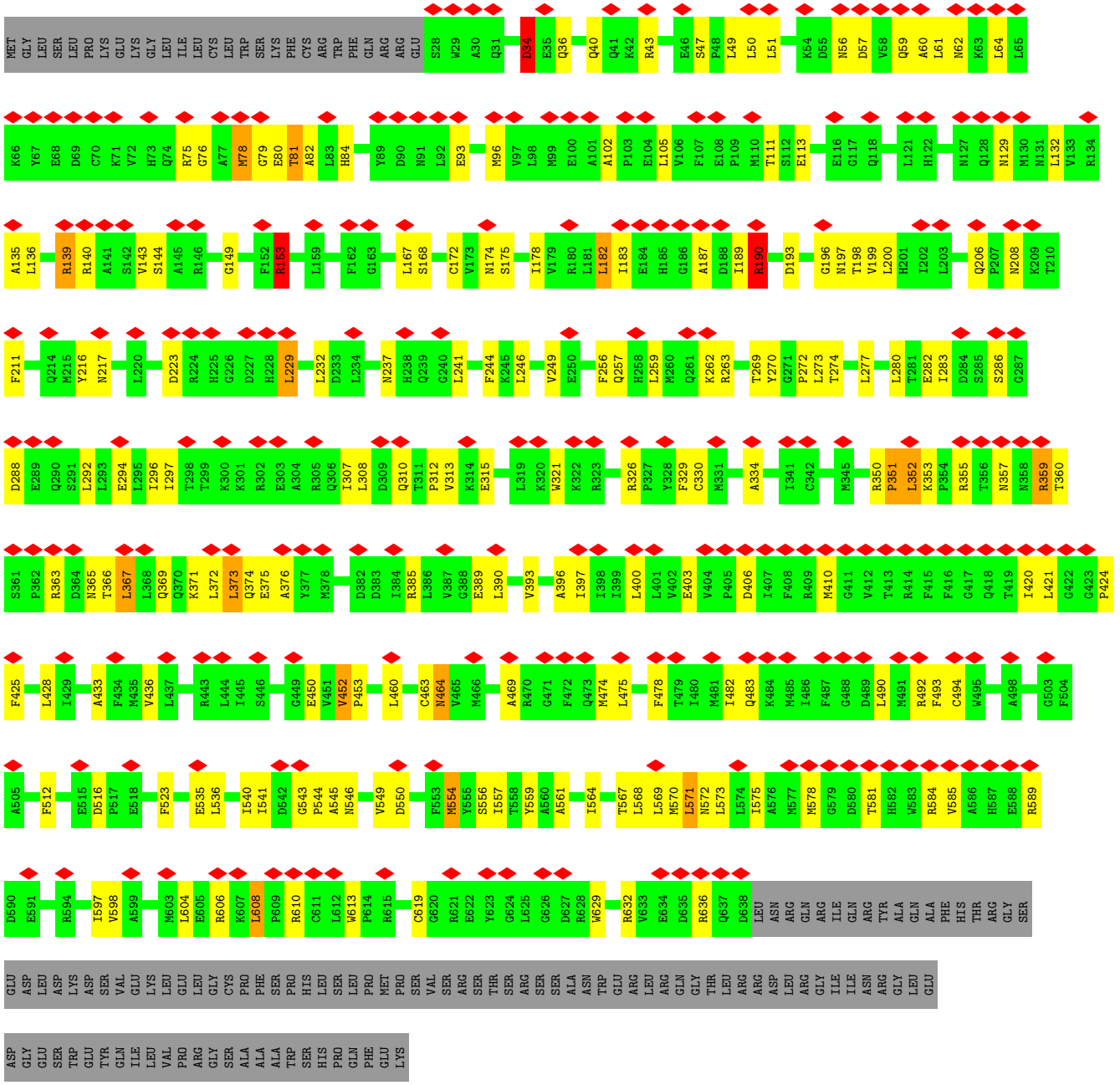

• Molecule 1: Transient receptor potential cation channel subfamily V member 6

Chain B:

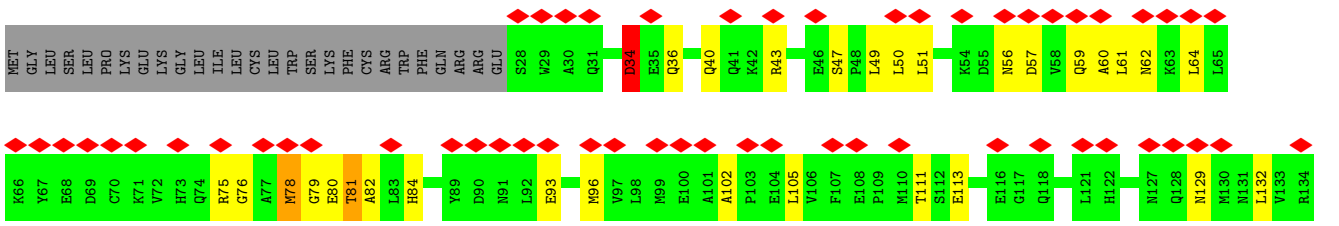

• Molecule 1: Transient receptor potential cation channel subfamily V member 6

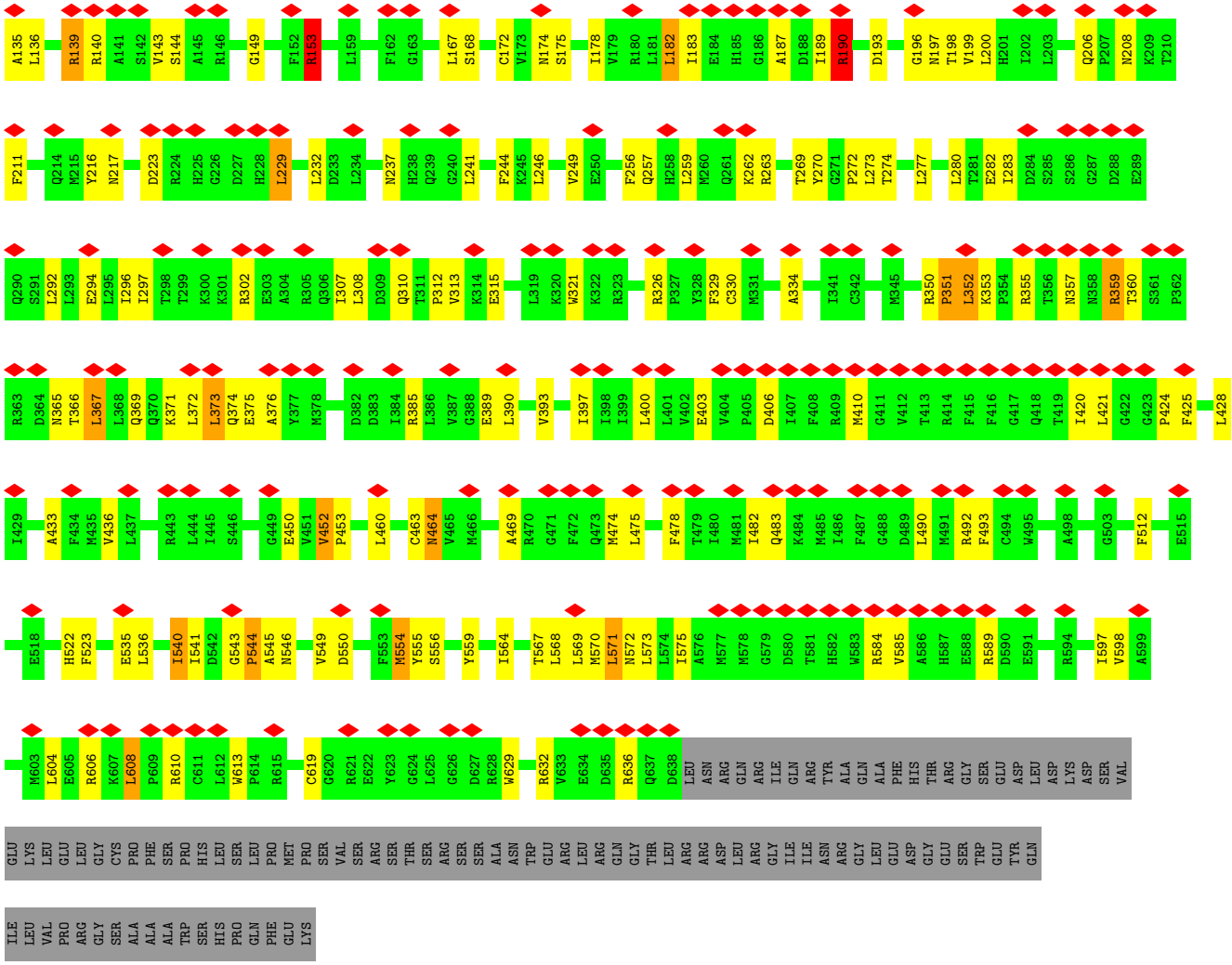
Chain C:



• Molecule 1: Transient receptor potential cation channel subfamily V member 6

Chain D:


A135 L136 R139 R140 A141 S142 V143 S144 A145 R146 G149 F152 R153 L159 F162 G163 L167 S168 C172 V173 N174 S175 I178 V179 R180 L181 L182 I183 E184 H185 G186 A187 D188 I189 R190 D193 G196 N197 T198 V199 L200 H201 I202 L203 Q206 P207 N208 K209 T210
F211 Q214 M215 Y216 N217 D223 R224 H225 G226 D227 H228 L229 L232 D233 L234 N237 H238 Q239 G240 L241 F244 K245 L246 V249 E250 F256 Q257 H258 L259 M260 Q261 K262 R263 T269 Y270 G271 P272 L273 T274 L277 L280 T281 E282 I283 D284 S285 S286 G287 D288 E289
Q290 S291 L292 L293 E294 L295 T296 I297 T298 T299 K300 K301 R302 E303 A304 R305 Q306 I307 L308 D309 Q310 T311 P312 V313 K314 E315 L319 K320 W321 K322 R323 R326 P327 Y328 F329 C330 M331 A334 I341 C342 M345 R350 P351 L352 K353 P354 R355 T356 N357 N358 R359 T360 S361 P362
R363 D364 N365 T366 L367 L368 Q369 Q370 K371 L372 L373 Q374 E375 A376 Y377 M378 D382 D383 I384 R385 L386 V387 G388 E389 L390 V393 I397 I398 I399 L400 L401 V402 E403 V404 P405 D406 I407 F408 R409 M410 G411 V412 T413 R414 F415 F416 G417 Q418 T419 I420 L421 G422 G423 P424 F425 L428
I429 A433 F434 M435 V436 L437 R443 L444 I445 S446 G449 E450 V451 V452 P453 L460 C463 N464 V465 M466 A469 R470 G471 F472 Q473 M474 L475 F478 T479 I480 M481 I482 Q483 K484 M485 I486 F487 G488 D489 L490 M491 R492 F493 C494 W495 A498 G503 F512 E515
E518 H522 F523 E535 L536 I540 I541 D542 G543 P544 A545 N546 V549 D550 F553 M554 Y555 S556 Y559 I564 T567 L568 L569 M570 L571 N572 L573 L574 I575 A576 M577 M578 G579 D580 T581 H582 W583 R584 V585 A586 H587 E588 R589 D590 E591 R594 I597 V598 A599
M603 L604 E605 R606 K607 L608 P609 R610 C611 L612 W613 P614 R615 C619 G620 R621 E622 Y623 G624 L625 G626 D627 R628 W629 R632 V633 E634 D635 R636 Q637 D638
LEU ASN ARG GLN ARG ILE GLN ARG TYR ALA GLN ALA PHE HIS THR ARG GLY SER GLU ASP LEU ASP LYS ASP SER VAL
GLU LYS LEU GLU LEU GLY CYS PRO PHE SER PRO HIS LEU SER LEU PRO MET PRO SER VAL SER ARG SER THR SER ARG SER SER ALA ASN TRP GLU ARG LEU ARG ARG GLN GLY THR LEU ARG ARG ASP LEU ARG GLY ILE ILE ASN ARG GLY LEU GLU ASP GLY GLU SER TRP GLU TYR GLN
ILE LEU VAL PRO ARG GLY SER ALA ALA ALA TRP SER HIS PRO GLN PHE GLU LYS

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 77460 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TECNAI 20 | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/Å^2$) | 43.0 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.200 | Depositor |
| Minimum map value | -0.111 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.009 | Depositor |
| Recommended contour level | 0.0669 | Depositor |
| Map size (Å) | 248.88, 248.88, 248.88 | wwPDB |
| Map dimensions | 204, 204, 204 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.22, 1.22, 1.22 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, FZ4

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 | 0.48 | 1/5008 (0.0%) | 0.79 | 15/6795 (0.2%) |
| 1 | B | 0.48 | 1/5008 (0.0%) | 0.79 | 15/6795 (0.2%) |
| 1 | C | 0.49 | 1/5008 (0.0%) | 0.78 | 15/6795 (0.2%) |
| 1 | D | 0.54 | 2/5008 (0.0%) | 0.80 | 19/6795 (0.3%) |
| All | All | 0.50 | 5/20032 (0.0%) | 0.79 | 64/27180 (0.2%) |

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 | 3 |
| 1 | B | 0 | 3 |
| 1 | C | 0 | 4 |
| 1 | D | 0 | 4 |
| All | All | 0 | 14 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | D | 544 | PRO | C-N | 17.00 | 1.73 | 1.34 |
| 1 | C | 540 | ILE | C-N | -10.15 | 1.10 | 1.34 |
| 1 | D | 540 | ILE | C-N | 9.40 | 1.55 | 1.34 |
| 1 | A | 540 | ILE | C-N | 7.56 | 1.51 | 1.34 |
| 1 | B | 540 | ILE | C-N | 7.56 | 1.51 | 1.34 |

The worst 5 of 64 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 190 | ARG | NE-CZ-NH2 | 10.29 | 125.44 | 120.30 |
| 1 | D | 190 | ARG | NE-CZ-NH2 | 10.27 | 125.44 | 120.30 |
| 1 | A | 190 | ARG | NE-CZ-NH2 | 10.23 | 125.41 | 120.30 |
| 1 | C | 190 | ARG | NE-CZ-NH2 | 10.23 | 125.41 | 120.30 |
| 1 | D | 372 | LEU | CA-CB-CG | 8.06 | 133.84 | 115.30 |

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 129 | ASN | Peptide |
| 1 | A | 223 | ASP | Peptide |
| 1 | A | 351 | PRO | Peptide |
| 1 | B | 129 | ASN | Peptide |
| 1 | B | 223 | ASP | 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 | 4896 | 0 | 4954 | 110 | 0 |
| 1 | B | 4896 | 0 | 4954 | 109 | 0 |
| 1 | C | 4896 | 0 | 4953 | 119 | 0 |
| 1 | D | 4896 | 0 | 4953 | 123 | 0 |
| 2 | A | 17 | 0 | 0 | 0 | 0 |
| 2 | B | 17 | 0 | 0 | 0 | 0 |
| 2 | C | 17 | 0 | 0 | 0 | 0 |
| 2 | D | 17 | 0 | 0 | 0 | 0 |
| 3 | A | 2 | 0 | 0 | 0 | 0 |
| All | All | 19654 | 0 | 19814 | 428 | 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 11.

The worst 5 of 428 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:D:544:PRO:C | 1:D:545:ALA:N | 1.73 | 1.42 |
| 1:D:535:GLU:OE1 | 1:D:541:ILE:HB | 1.54 | 1.06 |
| 1:D:535:GLU:CD | 1:D:541:ILE:HB | 1.93 | 0.88 |
| 1:B:535:GLU:HG3 | 1:C:559:TYR:HE2 | 1.58 | 0.68 |
| 1:A:535:GLU:HG3 | 1:B:559:TYR:HE2 | 1.58 | 0.68 |

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 | 609/742 (82%) | 541 (89%) | 65 (11%) | 3 (0%) | 29 | 68 |
| 1 | B | 609/742 (82%) | 540 (89%) | 66 (11%) | 3 (0%) | 29 | 68 |
| 1 | C | 609/742 (82%) | 541 (89%) | 64 (10%) | 4 (1%) | 22 | 62 |
| 1 | D | 609/742 (82%) | 540 (89%) | 66 (11%) | 3 (0%) | 29 | 68 |
| All | All | 2436/2968 (82%) | 2162 (89%) | 261 (11%) | 13 (0%) | 32 | 68 |

5 of 13 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 585 | VAL |
| 1 | B | 585 | VAL |
| 1 | C | 585 | VAL |
| 1 | D | 585 | VAL |
| 1 | C | 545 | ALA |

### 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 | 529/645 (82%) | 502 (95%) | 27 (5%) | 24 50 |
| 1 | B | 529/645 (82%) | 502 (95%) | 27 (5%) | 24 50 |
| 1 | C | 529/645 (82%) | 502 (95%) | 27 (5%) | 24 50 |
| 1 | D | 529/645 (82%) | 502 (95%) | 27 (5%) | 24 50 |
| All | All | 2116/2580 (82%) | 2008 (95%) | 108 (5%) | 27 50 |

5 of 108 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 81 | THR |
| 1 | C | 410 | MET |
| 1 | D | 421 | LEU |
| 1 | C | 136 | LEU |
| 1 | C | 190 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 208 | ASN |
| 1 | D | 546 | ASN |
| 1 | B | 546 | ASN |
| 1 | C | 206 | GLN |
| 1 | C | 208 | ASN |

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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 | $\#\|Z\| > 2$ |
| 2 | FZ4 | B | 801 | 1 | 16,18,18 | 0.74 | 0 | 17,22,22 | 1.50 | 2 (11%) |
| 2 | FZ4 | C | 801 | 1 | 16,18,18 | 0.75 | 0 | 17,22,22 | 1.52 | 2 (11%) |
| 2 | FZ4 | D | 801 | 1 | 16,18,18 | 0.76 | 0 | 17,22,22 | 1.51 | 2 (11%) |
| 2 | FZ4 | A | 801 | 1 | 16,18,18 | 0.75 | 0 | 17,22,22 | 1.51 | 2 (11%) |

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 |
|---|---|---|---|---|---|---|---|
| 2 | FZ4 | B | 801 | 1 | - | 7/12/12/12 | 0/2/2/2 |
| 2 | FZ4 | C | 801 | 1 | - | 7/12/12/12 | 0/2/2/2 |
| 2 | FZ4 | D | 801 | 1 | - | 7/12/12/12 | 0/2/2/2 |
| 2 | FZ4 | A | 801 | 1 | - | 7/12/12/12 | 0/2/2/2 |

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | C | 801 | FZ4 | C13-C08-C09 | 3.24 | 120.51 | 116.88 |
| 2 | D | 801 | FZ4 | C13-C08-C09 | 3.23 | 120.49 | 116.88 |
| 2 | A | 801 | FZ4 | C13-C08-C09 | 3.22 | 120.48 | 116.88 |
| 2 | B | 801 | FZ4 | C13-C08-C09 | 3.22 | 120.48 | 116.88 |
| 2 | D | 801 | FZ4 | C07-C02-C03 | 3.20 | 120.46 | 116.88 |

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | A | 801 | FZ4 | O14-B01-C02-C03 |
| 2 | A | 801 | FZ4 | O14-B01-C02-C07 |
| 2 | A | 801 | FZ4 | C02-B01-O14-C15 |
| 2 | A | 801 | FZ4 | C08-B01-O14-C15 |
| 2 | A | 801 | FZ4 | O14-C15-C16-N17 |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 1 | D | 1 |
| 1 | C | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | D | 544:PRO | C | 545:ALA | N | 1.73 |
| 1 | C | 540:ILE | C | 541:ILE | N | 1.10 |

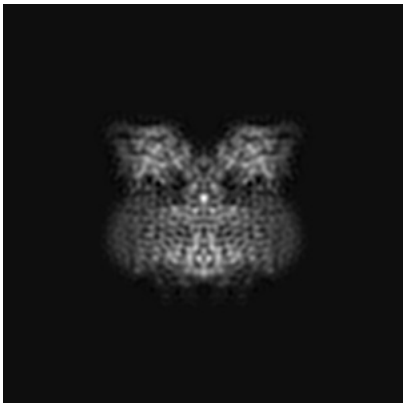
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7825. These allow visual inspection of the internal detail of the map and identification of artifacts.

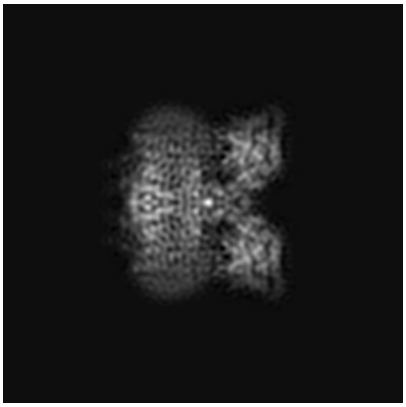
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

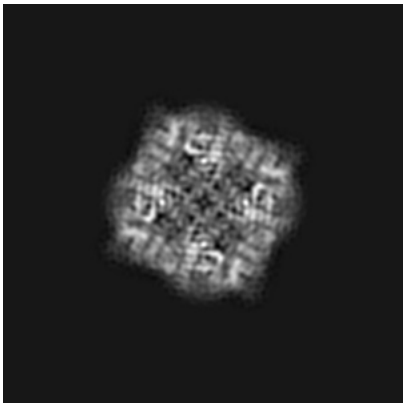
### 6.1.1 Primary map



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: 102

Y Index: 102

Z Index: 102

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: 102

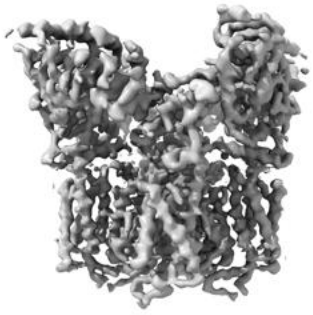
Y Index: 102

Z Index: 122

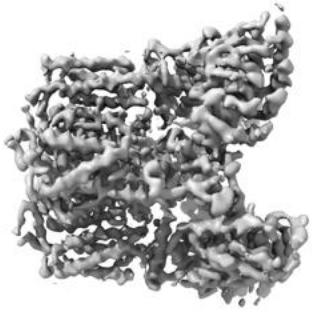
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views (i)

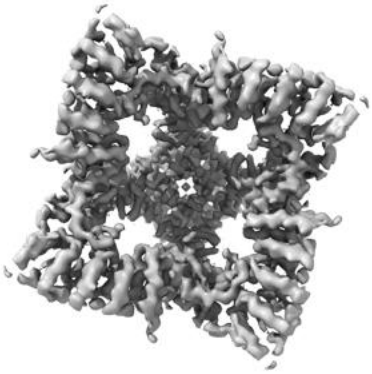
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0669. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

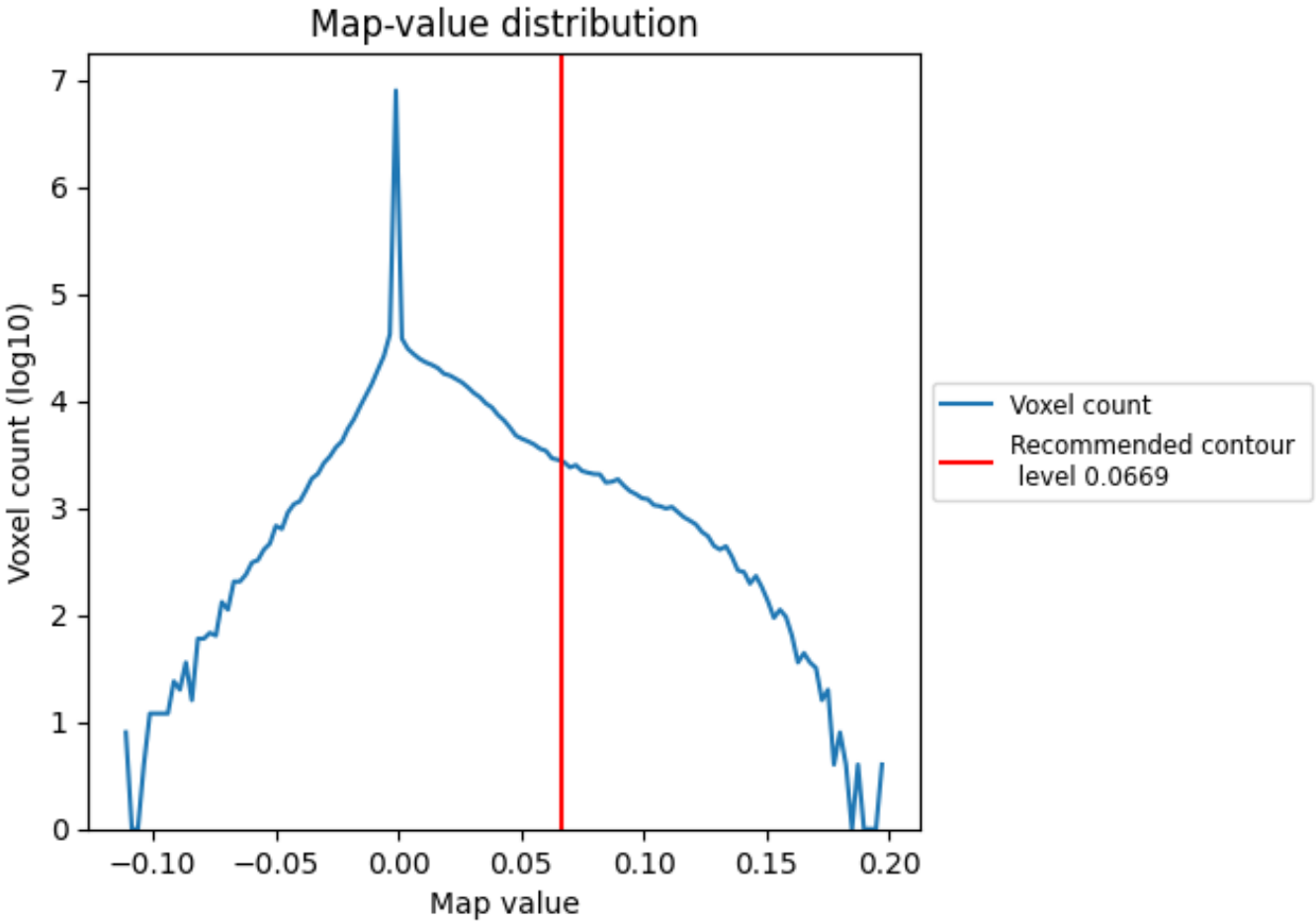
## 6.5 Mask visualisation (i)

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

# 7 Map analysis

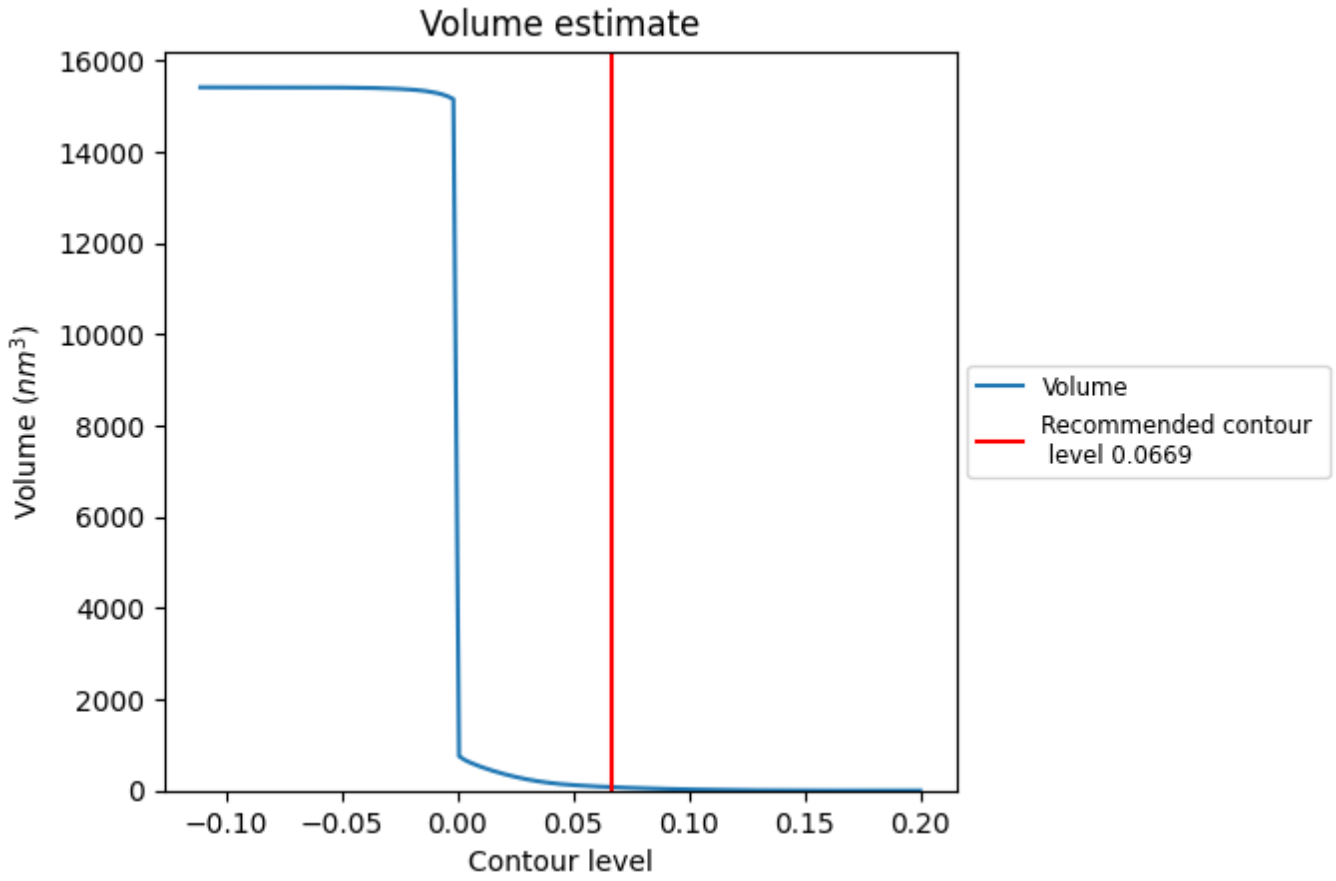
This section contains the results of statistical analysis of the map.

## 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.

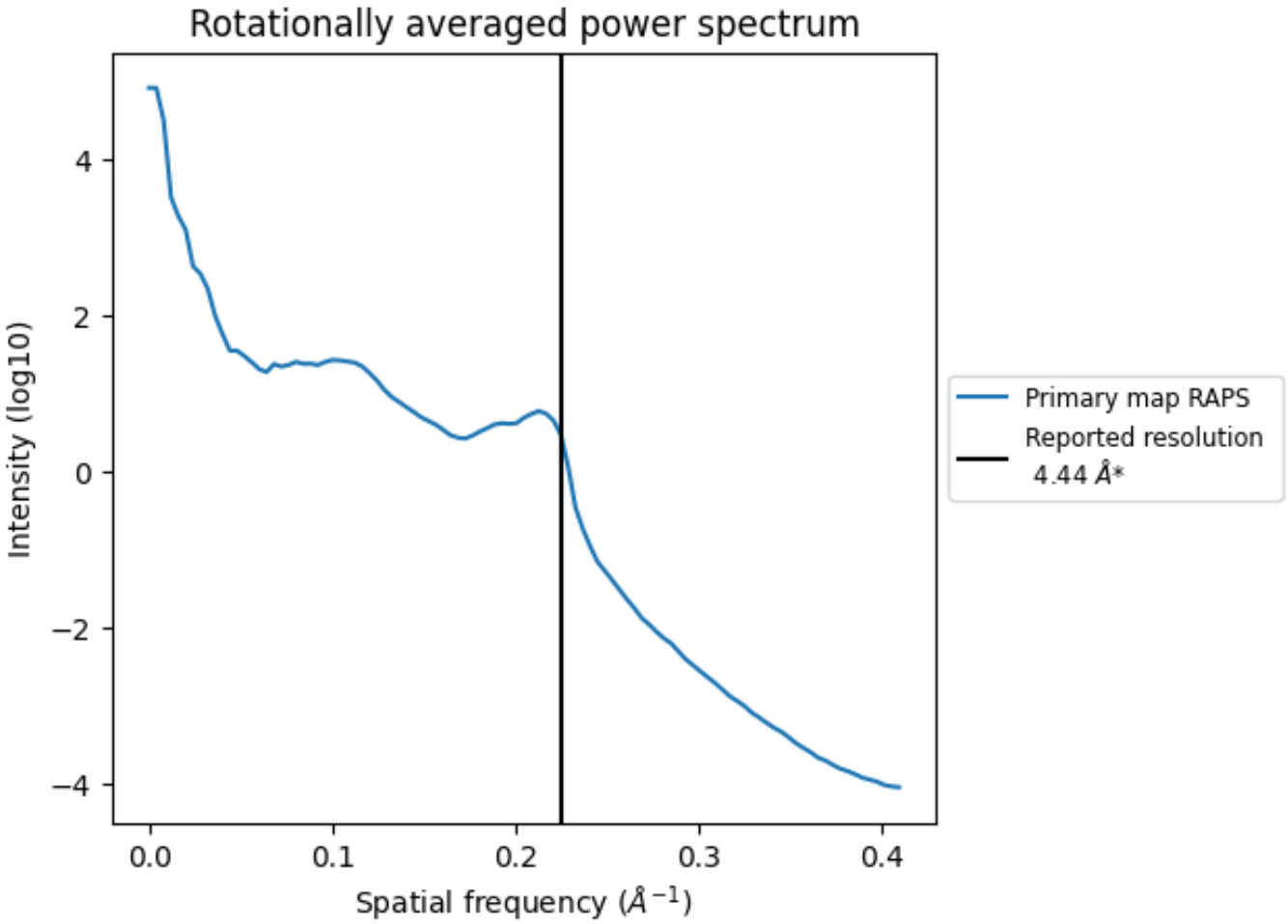
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 74 $nm^3$; this corresponds to an approximate mass of 67 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 0.225 $Å^{-1}$

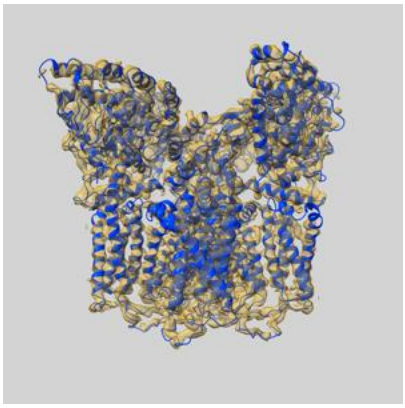
# 8 Fourier-Shell correlation (i)

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

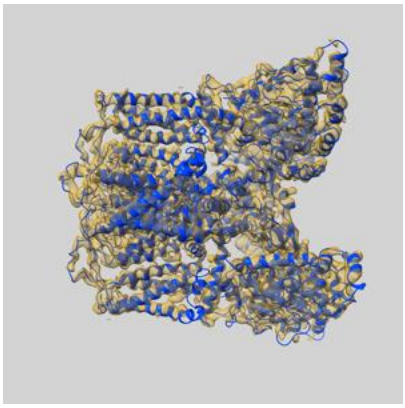
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7825 and PDB model 6D7T. Per-residue inclusion information can be found in section 3 on page 7.

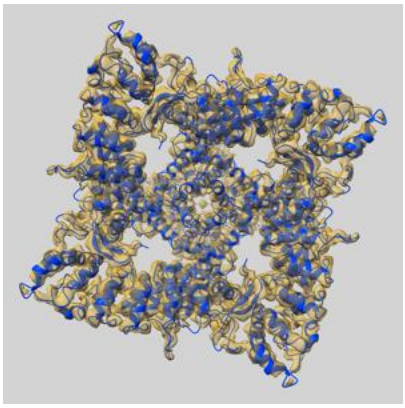
## 9.1 Map-model overlay



X



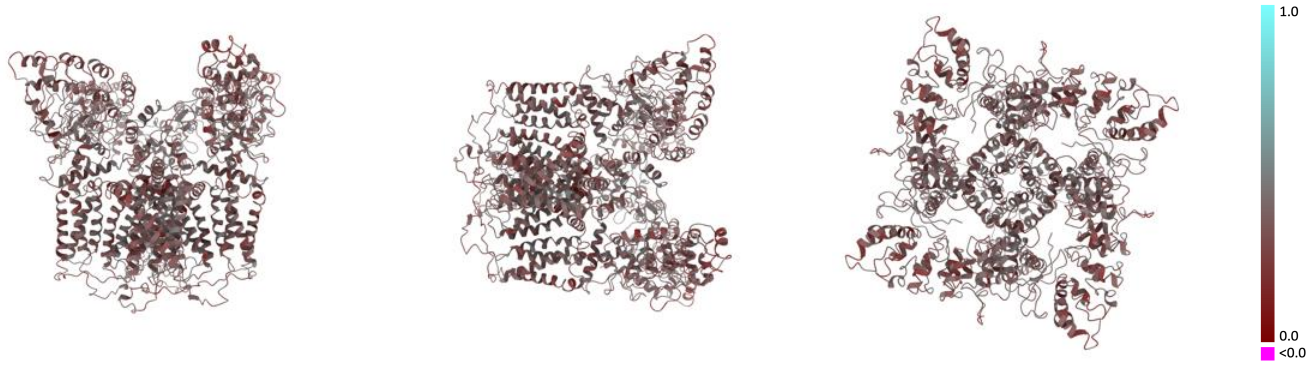
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0669 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

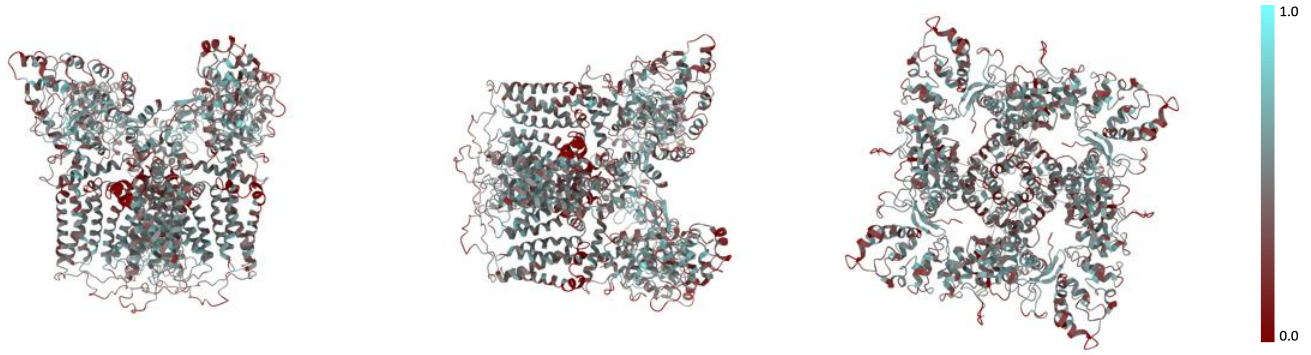
## 9.2 Q-score mapped to coordinate model (i)




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.

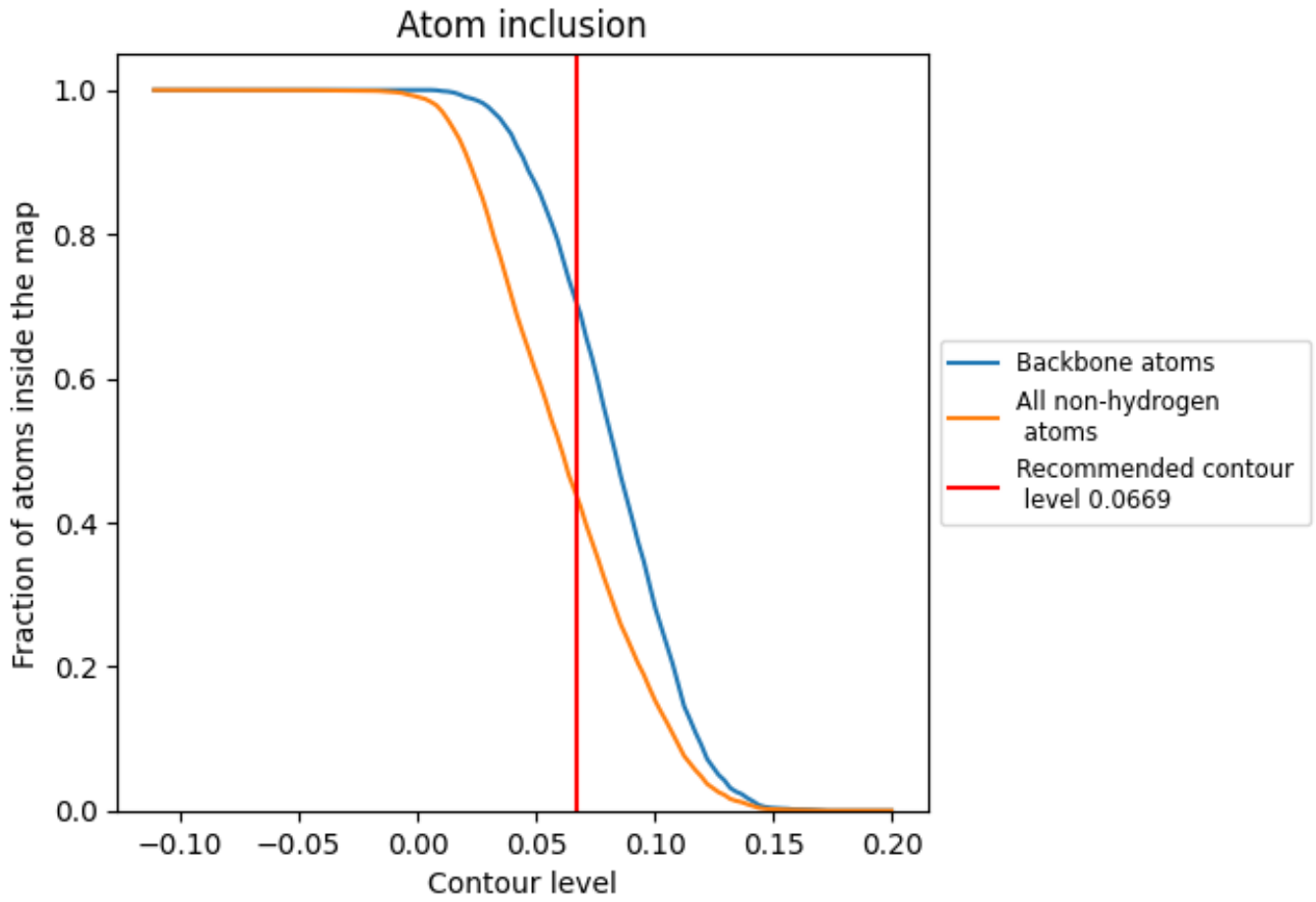
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.0669).

## 9.4 Atom inclusion (i)




At the recommended contour level, 71% of all backbone atoms, 44% 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 (0.0669) and Q-score for the entire model and for each chain.


| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.4379 | 0.3540 |
| A | 0.4375 | 0.3540 |
| B | 0.4381 | 0.3540 |
| C | 0.4389 | 0.3530 |
| D | 0.4371 | 0.3540 |