# Full wwPDB EM Validation Report ⓘ

Jan 7, 2023 – 01:34 PM EST

| | | |
|---|---|---|
| PDB ID | : | 8DDW |
| EMDB ID | : | EMD-27344 |
| Title | : | cryo-EM structure of TRPM3 ion channel in complex with Gbg, tethered by ALFA-nanobody |
| Authors | : | Zhao, C.; MacKinnon, R. |
| Deposited on | : | 2022-06-19 |
| Resolution | : | 4.70 Å(reported) |

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

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

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

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

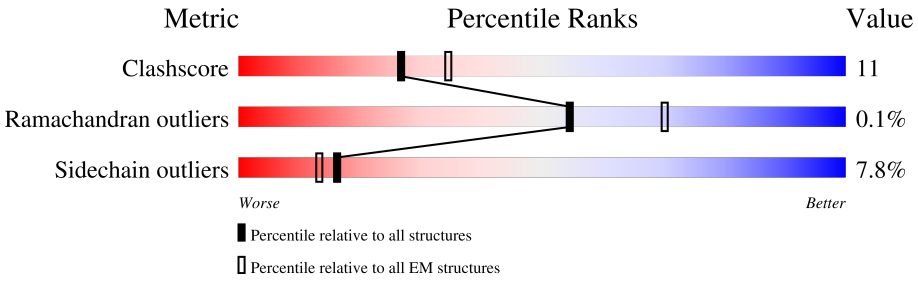
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | 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 4.70 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 | 1371 | 12% 36% 13% • 49% |
| 1 | B | 1371 | 20% 35% 14% • 49% |
| 1 | C | 1371 | 18% 37% 13% • 49% |
| 1 | D | 1371 | 12% 38% 13% • 48% |
| 2 | E | 17 | 12% 82% 18% |
| 2 | F | 17 | 18% 94% 6% |
| 2 | G | 17 | 24% 76% 24% |
| 2 | H | 17 | 18% 88% 12% |

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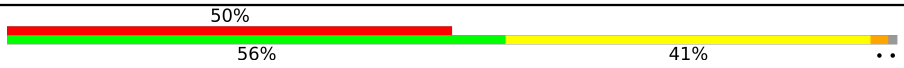
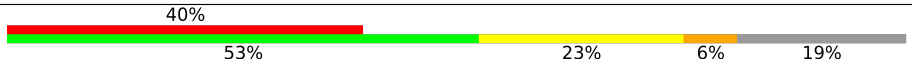
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | I | 339 |   |
| 4 | J | 70 |   |

# 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25869 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 M, member 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 695 | Total | C | N | O | S | 0 | 0 |
| | | | 5576 | 3553 | 972 | 1014 | 37 | | |
| 1 | B | 695 | Total | C | N | O | S | 0 | 0 |
| | | | 5576 | 3553 | 972 | 1014 | 37 | | |
| 1 | C | 695 | Total | C | N | O | S | 0 | 0 |
| | | | 5576 | 3553 | 972 | 1014 | 37 | | |
| 1 | D | 719 | Total | C | N | O | S | 0 | 0 |
| | | | 5765 | 3673 | 1003 | 1051 | 38 | | |

- Molecule 2 is a protein called Unidentified segment at the N-terminus of TRPM3.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 2 | E | 17 | Total | C | N | O | 0 | 0 |
| | | | 85 | 51 | 17 | 17 | | |
| 2 | F | 17 | Total | C | N | O | 0 | 0 |
| | | | 85 | 51 | 17 | 17 | | |
| 2 | G | 17 | Total | C | N | O | 0 | 0 |
| | | | 85 | 51 | 17 | 17 | | |
| 2 | H | 17 | Total | C | N | O | 0 | 0 |
| | | | 85 | 51 | 17 | 17 | | |

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | I | 337 | Total | C | N | O | S | 2 | 0 |
| | | | 2598 | 1603 | 466 | 506 | 23 | | |

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | J | 57 | Total | C | N | O | S | 0 | 0 |
| | | | 438 | 274 | 77 | 84 | 3 | | |

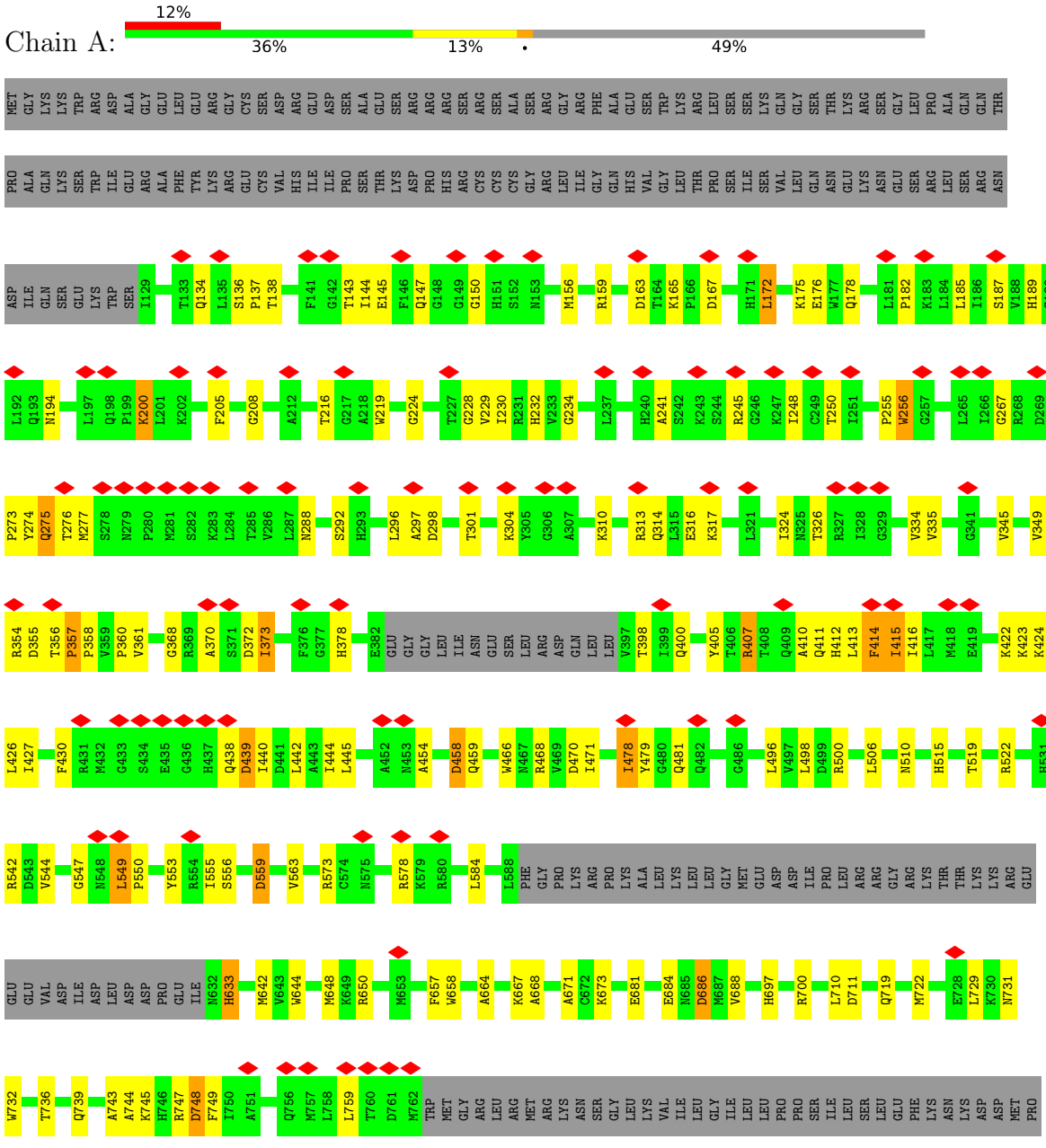
There is a discrepancy between the modelled and reference sequences:

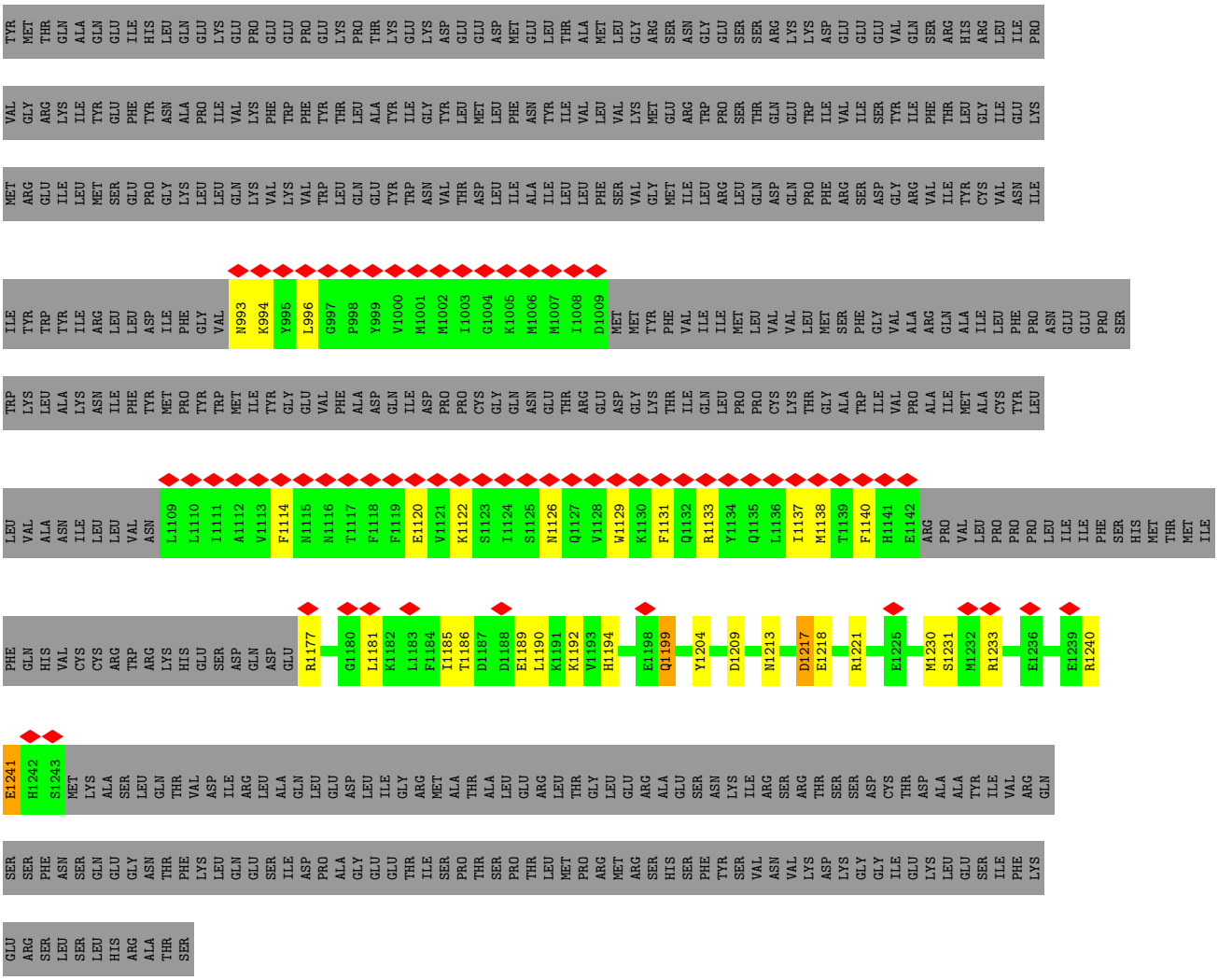
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| J | 68 | SER | CYS | engineered mutation | UNP P59768 |

# 3 Residue-property plots (i)

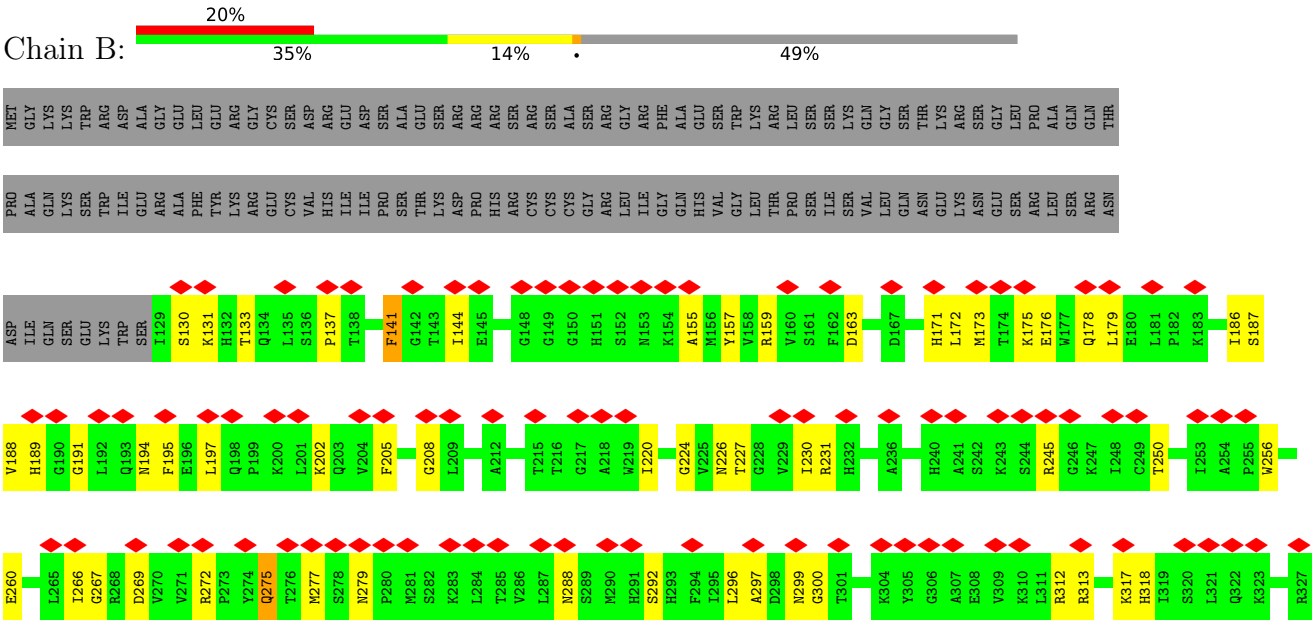
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

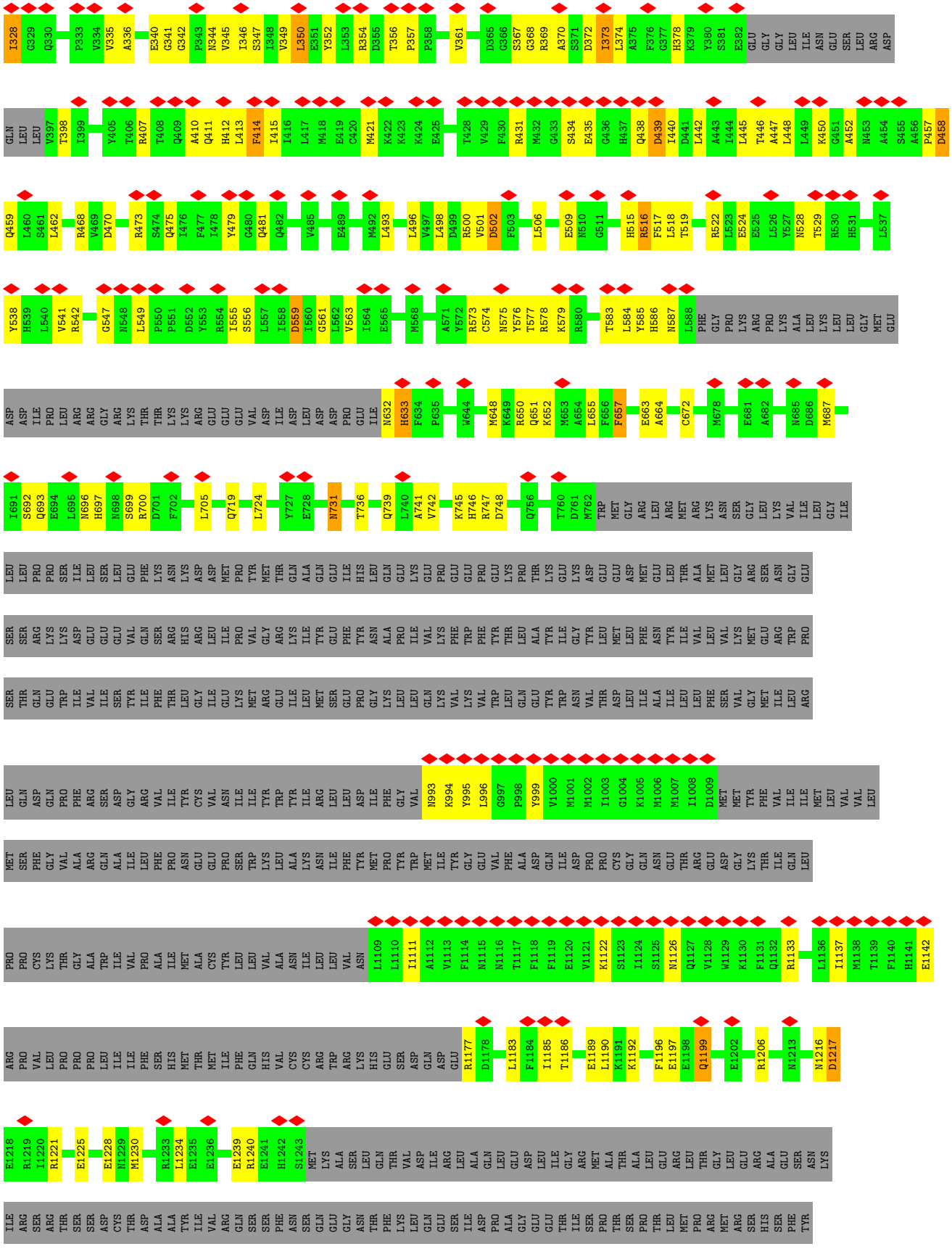
• Molecule 1: Transient receptor potential cation channel, subfamily M, member 3

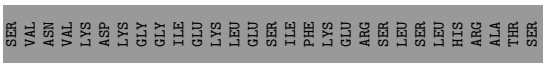




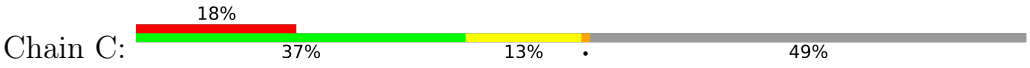
• Molecule 1: Transient receptor potential cation channel, subfamily M, member 3

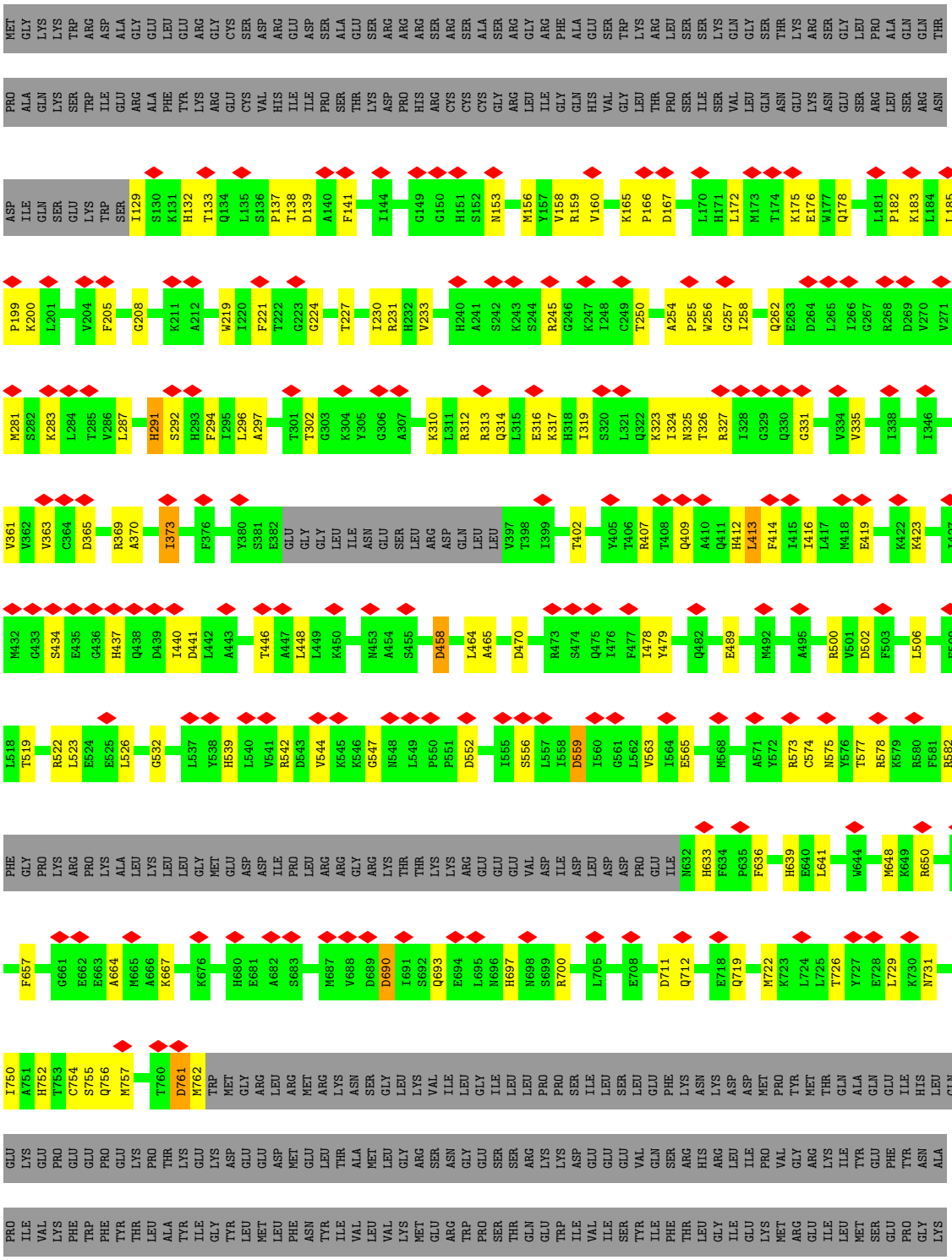


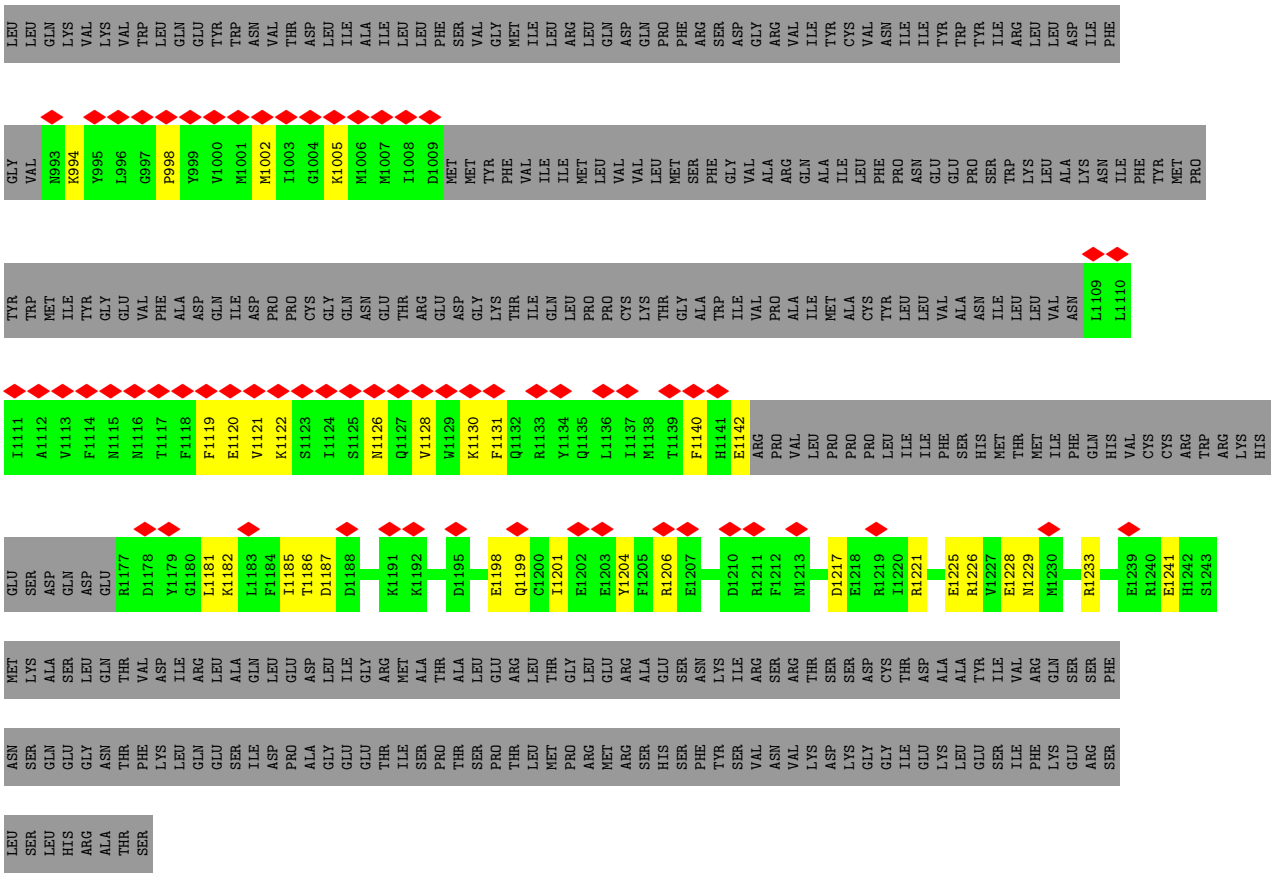

I328 G329 Q330 P333 V334 V335 A336 E340 G341 G342 P343 N344 V345 I346 S347 I348 V349 L350 E351 Y352 L353 R354 D355 T356 P357 P358 V361 D365 G366 S367 G368 R369 A370 S371 D372 I373 L374 A375 F376 G377 H378 K379 Y380 S381 E382 GLU GLY GLY GLY LEU LEU ILE ASN GLU SER LEU ARG ASP
GLN LEU LEU V397 T398 I399 Y405 T406 R407 T408 Q409 A410 Q411 H412 L413 F414 I415 T416 L417 M418 E419 C420 M421 K422 K423 K424 E425 T428 V429 F430 R431 M432 G433 S434 E435 G436 H437 Q438 D439 I440 D441 L442 A443 I444 L445 T446 A447 L448 L449 K450 G451 A452 N453 A454 S455 A456 P457 D458
Q459 L460 S461 L462 R468 V469 D470 R473 S474 Q475 I476 F477 I478 Y479 G480 Q481 Q482 V485 E489 M492 L493 L496 V497 L498 D499 R500 V501 D502 F503 L506 E509 N510 G511 H515 R516 F517 L518 T519 R522 L523 E524 E525 L526 Y527 N528 T529 R530 H531 L537
Y538 H539 L540 V541 R542 G547 N548 L549 P550 P551 D552 Y553 R554 I555 S556 L557 I558 D559 I560 G561 L562 V563 I564 E565 M568 A571 Y572 R573 C574 N575 Y576 T577 R578 K579 R580 T583 L584 Y585 H586 N587 L588 PHE GLY PRO LYS ARG PRO LYS ALA LEU LYS LEU LEU GLY MET GLU
ASP ASP ILE PRO LEU ARG ARG GLY ARG LYS THR THR LYS LYS ARG GLU GLU GLU VAL ASP ILE ASP LEU ASP ASP PRO GLU ILE N632 H633 F634 P635 W644 M648 K649 R650 Q651 K652 M653 A654 L655 F656 F657 E663 A664 C672 M678 E681 A682 N685 D686 M687
I691 S692 Q693 E694 L695 N696 H697 N698 S699 R700 D701 F702 L705 Q719 L724 Y727 E728 N731 T736 Q739 L740 A741 V742 K745 H746 R747 D748 Q756 T760 D761 M762 TRP MET GLY ARG LEU ARG MET ARG LYS ASN SER GLY LEU LYS VAL ILE LEU GLY ILE
LEU LEU PRO PRO SER ILE LEU SER LEU GLU PHE LYS ASN LYS ASP ASP MET PRO TYR MET THR GLN ALA GLN GLU ILE HIS LEU GLN GLU LYS GLU PRO GLU GLU PRO GLU LYS PRO THR LYS GLU LYS ASP GLU GLU ASP MET GLU LEU THR ALA MET LEU GLY ARG SER ASN GLY GLU
SER SER ARG LYS LYS ASP GLU GLU GLU VAL GLN SER ARG HIS ARG LEU ILE PRO VAL GLY ARG LYS ILE TYR GLU PHE TYR ASN ALA PRO ILE VAL LYS PHE TRP PHE TYR THR LEU ALA TYR ILE GLY TYR LEU MET LEU PHE ASN TYR ILE ILE VAL LEU VAL LYS MET GLU ARG TRP PRO
SER THR GLN GLU TRP ILE VAL ILE SER TYR ILE PHE THR LEU GLY ILE GLU LYS MET ARG GLU ILE LEU MET SER GLU PRO GLY LYS LEU LEU GLN LYS VAL LYS VAL TRP LEU GLN GLU TYR TRP ASN VAL THR ASP LEU ILE ALA ILE LEU LEU LEU PHE SER VAL GLY MET ILE LEU ARG
LEU GLN ASP GLN PRO PHE ARG SER ASP GLY ARG VAL ILE ILE TYR CYS VAL ASN ILE ILE TYR TRP TYR ILE ILE ARG LEU LEU ASP ILE PHE GLY VAL N993 K994 Y995 L996 G997 P998 Y999 V1000 M1001 M1002 I1003 G1004 K1005 M1006 M1007 I1008 D1009 MET MET TYR PHE VAL ILE ILE MET LEU VAL VAL LEU
MET SER PHE GLY VAL ALA ARG GLN ALA ILE LEU PHE PRO ASN GLU GLU PRO SER TRP LYS LEU ALA LYS ASN ILE PHE TYR MET PRO TYR TRP MET ILE TYR GLY GLU VAL PHE ALA ASP GLN ILE ASP PRO PRO CYS GLY GLN ASN GLU THR ARG GLU ASP GLY LYS THR ILE GLN LEU
PRO PRO CYS LYS THR GLY ALA TRP ILE VAL PRO ALA ILE MET ALA CYS TYR LEU LEU VAL ALA ASN ILE LEU LEU VAL ASN L1109 L1110 I1111 A1112 V1113 F1114 N1115 N1116 T1117 F1118 F1119 E1120 V1121 K1122 S1123 I1124 S1125 N1126 Q1127 V1128 W1129 K1130 F1131 Q1132 R1133 L1136 I1137 M1138 T1139 F1140 H1141 E1142
ARG PRO VAL LEU PRO PRO PRO LEU ILE ILE PHE SER HIS MET THR MET ILE PHE GLN HIS VAL CYS CYS ARG TRP ARG LYS HIS GLU SER ASP GLN ASP GLU R1177 D1178 L1183 F1184 I1185 T1186 E1189 L1190 K1191 K1192 F1196 E1197 E1198 Q1199 E1202 R1206 N1213 N1216 D1217
E1218 R1219 I1220 R1221 E1225 E1228 N1229 M1230 R1233 L1234 E1235 E1236 E1239 R1240 E1241 H1242 S1243 MET LYS ALA SER LEU GLN THR VAL ASP ILE ARG LEU ALA GLN LEU GLU ASP LEU ILE GLY ARG MET ALA THR ALA LEU GLU ARG LEU THR GLY LEU GLU ARG ALA GLU SER ASN LYS
ILE ARG SER THR SER SER ASP CYS THR ASP ALA ALA TYR ILE VAL ARG GLN SER SER PHE ASN SER GLN GLU GLY ASN THR PHE LYS LEU GLN GLU SER ILE ASP PRO ALA GLY GLU GLU THR ILE SER PRO THR SER PRO THR LEU MET PRO ARG MET ARG SER HIS SER PHE TYR



• Molecule 1: Transient receptor potential cation channel, subfamily M, member 3

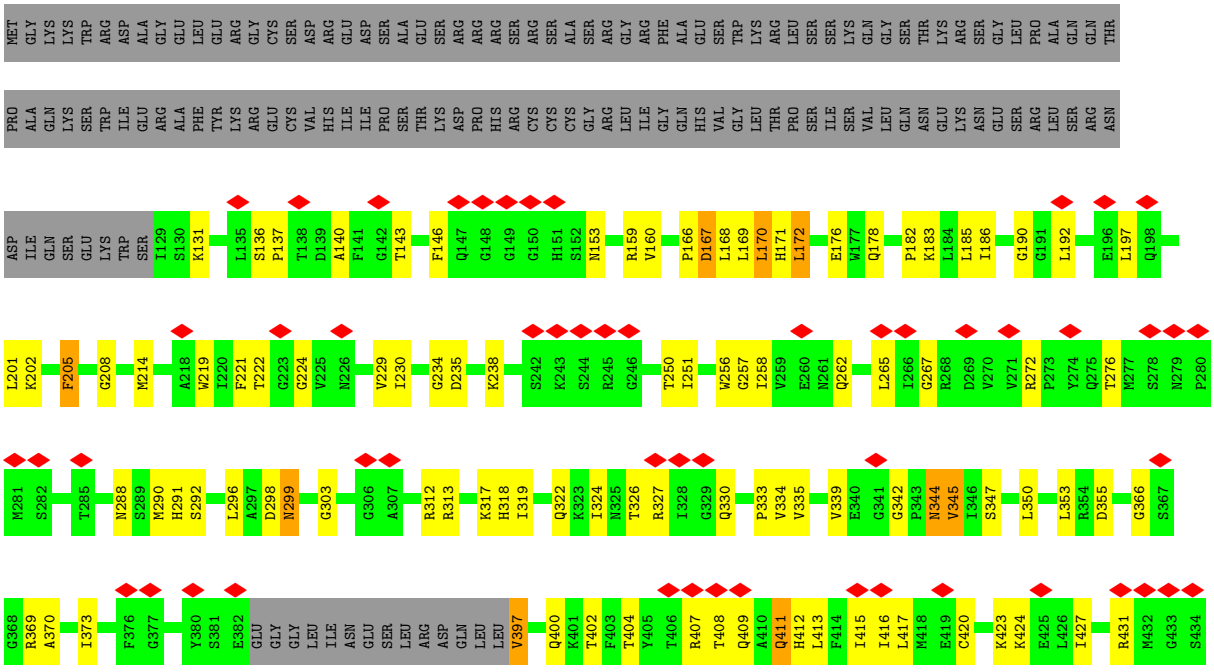


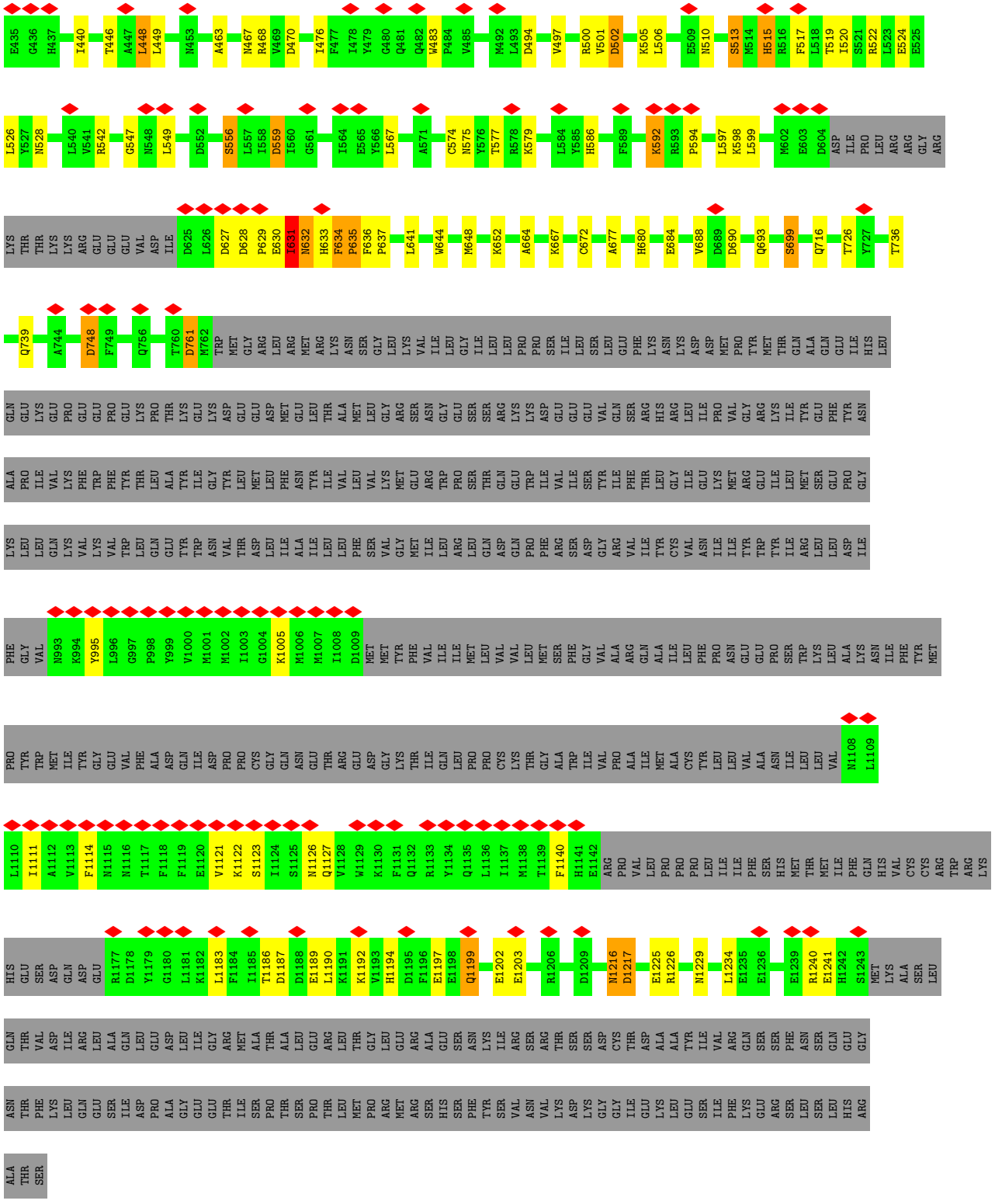





• Molecule 1: Transient receptor potential cation channel, subfamily M, member 3

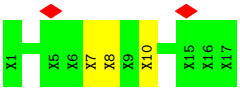
Chain D:



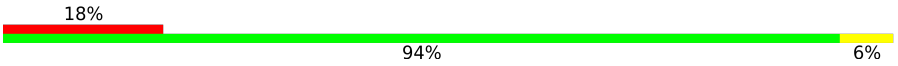

• Molecule 2: Unidentified segment at the N-terminus of TRPM3

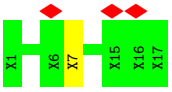
Chain E:




• Molecule 2: Unidentified segment at the N-terminus of TRPM3

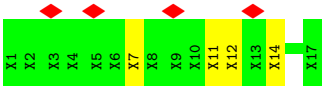
Chain F:



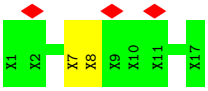

• Molecule 2: Unidentified segment at the N-terminus of TRPM3

Chain G:

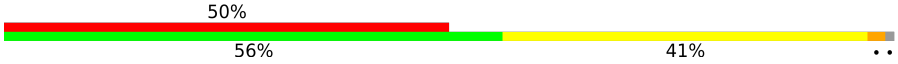

• Molecule 2: Unidentified segment at the N-terminus of TRPM3

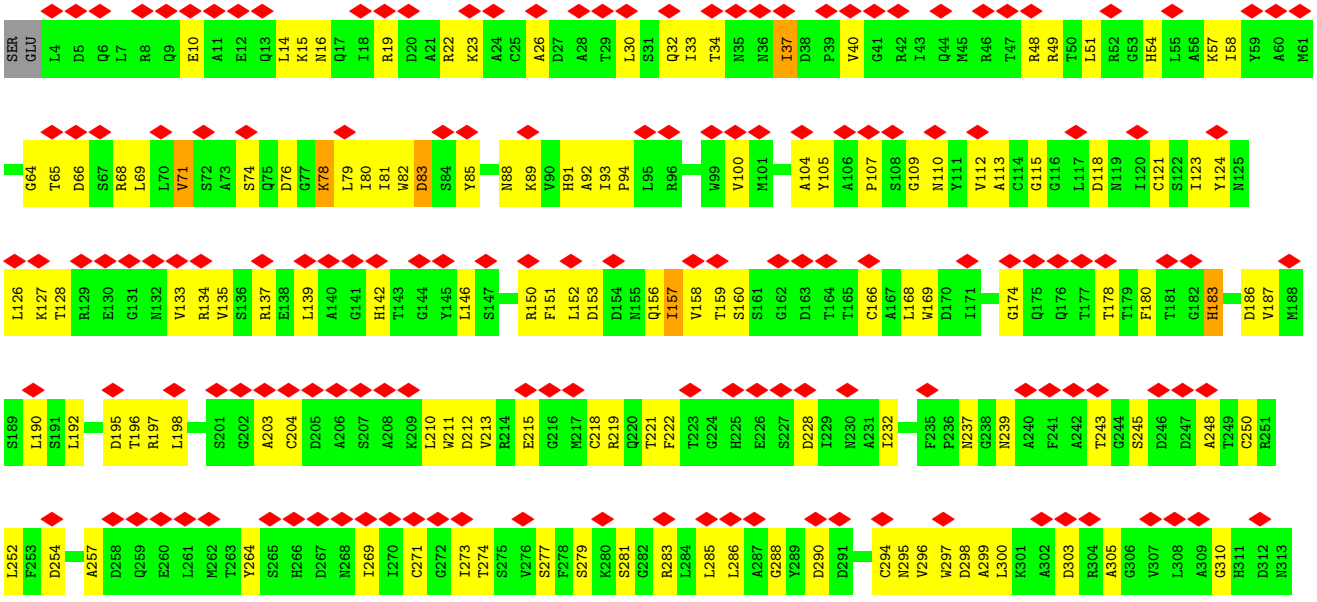
Chain H:

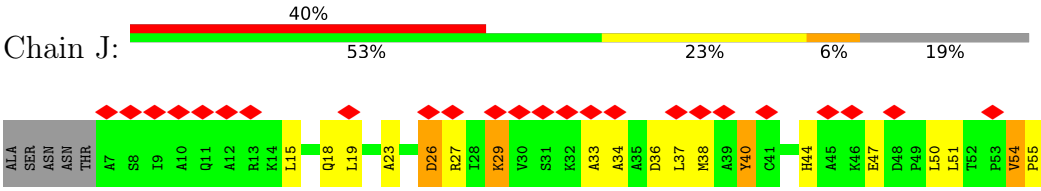

• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain I:




• Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 62171 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 51.4 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 2000 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 0.041 | Depositor |
| Minimum map value | -0.029 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.001 | Depositor |
| Recommended contour level | 0.011 | Depositor |
| Map size (Å) | 483.84003, 483.84003, 483.84003 | wwPDB |
| Map dimensions | 448, 448, 448 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.08, 1.08, 1.08 | 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 | 0.26 | 0/5686 | 0.46 | 0/7667 |
| 1 | B | 0.25 | 0/5686 | 0.45 | 0/7667 |
| 1 | C | 0.26 | 0/5686 | 0.46 | 0/7667 |
| 1 | D | 0.27 | 0/5879 | 0.46 | 0/7927 |
| 3 | I | 0.25 | 0/2651 | 0.54 | 0/3593 |
| 4 | J | 0.27 | 0/444 | 0.51 | 0/599 |
| All | All | 0.26 | 0/26032 | 0.47 | 0/35120 |

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 | 5576 | 0 | 5602 | 118 | 0 |
| 1 | B | 5576 | 0 | 5602 | 111 | 0 |
| 1 | C | 5576 | 0 | 5602 | 116 | 0 |
| 1 | D | 5765 | 0 | 5793 | 139 | 0 |
| 2 | E | 85 | 0 | 21 | 3 | 0 |
| 2 | F | 85 | 0 | 23 | 1 | 0 |
| 2 | G | 85 | 0 | 23 | 4 | 0 |
| 2 | H | 85 | 0 | 19 | 2 | 0 |
| 3 | I | 2598 | 0 | 2509 | 92 | 0 |
| 4 | J | 438 | 0 | 447 | 16 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| All | All | 25869 | 0 | 25641 | 568 | 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.

All (568) 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:629:PRO:HD2 | 1:D:631:ILE:HD13 | 1.52 | 0.89 |
| 1:A:356:THR:HB | 1:A:357:PRO:HD3 | 1.59 | 0.82 |
| 1:D:520:ILE:N | 1:D:632:ASN:HD21 | 1.83 | 0.76 |
| 3:I:54:HIS:HB2 | 3:I:334:SER:HB2 | 1.67 | 0.75 |
| 1:A:496:LEU:O | 1:A:650:ARG:NH1 | 2.23 | 0.72 |
| 1:D:205:PHE:HA | 1:D:440:ILE:HG13 | 1.73 | 0.71 |
| 1:B:205:PHE:HA | 1:B:440:ILE:HG13 | 1.73 | 0.71 |
| 1:A:439:ASP:OD1 | 1:A:439:ASP:N | 2.24 | 0.70 |
| 1:D:520:ILE:H | 1:D:632:ASN:ND2 | 1.90 | 0.70 |
| 3:I:51:LEU:HB3 | 3:I:54:HIS:HE1 | 1.57 | 0.70 |
| 3:I:252:LEU:HD22 | 3:I:299:ALA:HB1 | 1.73 | 0.70 |
| 1:D:520:ILE:H | 1:D:632:ASN:CG | 1.95 | 0.70 |
| 1:D:407:ARG:HB2 | 1:D:411:GLN:HB2 | 1.76 | 0.68 |
| 1:D:726:THR:HB | 1:D:1183:LEU:HB2 | 1.76 | 0.67 |
| 1:C:750:ILE:O | 1:C:756:GLN:NE2 | 2.28 | 0.66 |
| 1:D:629:PRO:O | 1:D:631:ILE:N | 2.29 | 0.66 |
| 1:B:1217:ASP:OD1 | 1:B:1217:ASP:N | 2.28 | 0.66 |
| 1:A:185:LEU:HB3 | 1:A:334:VAL:HG22 | 1.76 | 0.66 |
| 1:D:629:PRO:O | 1:D:630:GLU:HB2 | 1.95 | 0.66 |
| 1:C:1005:LYS:HD2 | 1:C:1121:VAL:HG13 | 1.78 | 0.65 |
| 3:I:160:SER:HB3 | 3:I:190:LEU:HD23 | 1.78 | 0.65 |
| 1:D:229:VAL:HG11 | 1:D:339:VAL:HB | 1.76 | 0.65 |
| 1:B:458:ASP:OD1 | 1:B:458:ASP:N | 2.30 | 0.65 |
| 1:B:346:ILE:HD12 | 1:B:374:LEU:HD21 | 1.78 | 0.65 |
| 1:C:502:ASP:OD1 | 1:C:502:ASP:N | 2.28 | 0.65 |
| 1:B:250:THR:HB | 1:B:292:SER:H | 1.61 | 0.65 |
| 1:D:631:ILE:HG23 | 1:D:632:ASN:N | 2.10 | 0.64 |
| 1:A:573:ARG:HH21 | 1:A:578:ARG:HD3 | 1.62 | 0.64 |
| 4:J:54:VAL:HG22 | 4:J:55:PRO:HD2 | 1.79 | 0.64 |
| 1:C:325:ASN:O | 1:C:327:ARG:NH1 | 2.30 | 0.64 |
| 1:A:350:LEU:HD22 | 1:A:354:ARG:HH11 | 1.63 | 0.64 |
| 3:I:239:ASN:ND2 | 4:J:36:ASP:OD2 | 2.31 | 0.64 |
| 1:D:513:SER:OG | 1:D:515:HIS:ND1 | 2.28 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:136:SER:O | 2:E:8:UNK:N | 2.32 | 0.63 |
| 1:B:573:ARG:HB3 | 1:B:578:ARG:HH22 | 1.63 | 0.63 |
| 1:D:506:LEU:O | 1:D:510:ASN:ND2 | 2.31 | 0.63 |
| 1:C:664:ALA:HA | 1:C:667:LYS:HD3 | 1.79 | 0.63 |
| 1:A:498:LEU:O | 1:A:500:ARG:NH1 | 2.30 | 0.63 |
| 1:B:208:GLY:HA3 | 1:B:440:ILE:HB | 1.80 | 0.63 |
| 1:D:517:PHE:O | 1:D:522:ARG:NH1 | 2.32 | 0.63 |
| 1:D:634:PHE:N | 1:D:634:PHE:CD1 | 2.67 | 0.63 |
| 1:A:407:ARG:HG3 | 1:A:411:GLN:HB2 | 1.80 | 0.63 |
| 1:B:498:LEU:O | 1:B:500:ARG:NH1 | 2.30 | 0.63 |
| 1:A:506:LEU:O | 1:A:510:ASN:ND2 | 2.31 | 0.62 |
| 3:I:166:CYS:HB2 | 3:I:180:PHE:HB2 | 1.80 | 0.62 |
| 1:B:559:ASP:OD1 | 1:B:559:ASP:N | 2.33 | 0.62 |
| 3:I:64:GLY:N | 3:I:69:LEU:O | 2.33 | 0.62 |
| 1:A:355:ASP:CG | 1:A:357:PRO:HD2 | 2.20 | 0.62 |
| 1:B:197:LEU:HD11 | 1:B:202:LYS:HB3 | 1.80 | 0.62 |
| 1:D:136:SER:O | 2:H:8:UNK:N | 2.33 | 0.62 |
| 3:I:104:ALA:HB3 | 3:I:113:ALA:HB3 | 1.81 | 0.62 |
| 3:I:51:LEU:HD23 | 3:I:336:LEU:HB3 | 1.80 | 0.62 |
| 1:A:335:VAL:HG23 | 1:A:360:PRO:HG2 | 1.82 | 0.61 |
| 1:A:137:PRO:HA | 2:E:7:UNK:HA | 1.82 | 0.61 |
| 1:A:743:ALA:O | 1:A:745:LYS:NZ | 2.33 | 0.61 |
| 1:D:1217:ASP:N | 1:D:1217:ASP:OD1 | 2.32 | 0.61 |
| 1:C:313:ARG:NH1 | 1:C:313:ARG:O | 2.33 | 0.61 |
| 1:B:651:GLN:HE21 | 1:B:655:LEU:HG | 1.65 | 0.61 |
| 1:C:556:SER:OG | 1:C:559:ASP:OD1 | 2.18 | 0.61 |
| 1:D:559:ASP:OD1 | 1:D:559:ASP:N | 2.31 | 0.61 |
| 1:B:502:ASP:OD1 | 1:B:502:ASP:N | 2.34 | 0.61 |
| 1:C:573:ARG:HE | 1:C:578:ARG:HH21 | 1.49 | 0.61 |
| 1:D:502:ASP:OD1 | 1:D:502:ASP:N | 2.32 | 0.61 |
| 1:D:520:ILE:N | 1:D:632:ASN:ND2 | 2.48 | 0.61 |
| 1:C:1221:ARG:NH1 | 1:C:1225:GLU:OE2 | 2.34 | 0.61 |
| 1:A:559:ASP:N | 1:A:559:ASP:OD1 | 2.33 | 0.60 |
| 1:D:634:PHE:O | 1:D:636:PHE:N | 2.34 | 0.60 |
| 1:A:445:LEU:HD23 | 1:A:471:ILE:HG13 | 1.83 | 0.60 |
| 1:C:719:GLN:HA | 1:C:722:MET:HE2 | 1.84 | 0.60 |
| 1:B:1142:GLU:HA | 1:B:1177:ARG:HH22 | 1.67 | 0.60 |
| 1:D:644:TRP:NE1 | 1:D:648:MET:SD | 2.74 | 0.60 |
| 3:I:218:CYS:O | 4:J:18:GLN:NE2 | 2.35 | 0.60 |
| 1:D:333:PRO:HB2 | 1:D:448:LEU:HD22 | 1.83 | 0.60 |
| 1:A:145:GLU:HG3 | 1:A:273:PRO:HA | 1.82 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:313:ARG:HG3 | 1:B:317:LYS:HE2 | 1.84 | 0.60 |
| 1:B:496:LEU:O | 1:B:650:ARG:NH1 | 2.34 | 0.60 |
| 1:A:1122:LYS:O | 1:A:1126:ASN:ND2 | 2.34 | 0.60 |
| 3:I:115:GLY:HA3 | 3:I:146:LEU:HD23 | 1.84 | 0.60 |
| 1:B:524:GLU:O | 1:B:528:ASN:ND2 | 2.32 | 0.59 |
| 1:A:224:GLY:H | 1:A:230:ILE:HD13 | 1.67 | 0.59 |
| 1:A:1240:ARG:NH1 | 1:D:1241:GLU:OE1 | 2.36 | 0.59 |
| 1:D:397:VAL:N | 1:D:400:GLN:OE1 | 2.35 | 0.59 |
| 1:C:690:ASP:OD1 | 1:C:690:ASP:N | 2.29 | 0.59 |
| 3:I:48:ARG:NE | 3:I:340:ASN:OD1 | 2.31 | 0.59 |
| 1:A:248:ILE:O | 1:A:292:SER:OG | 2.20 | 0.59 |
| 1:B:1133:ARG:HH21 | 1:B:1137:ILE:HD11 | 1.67 | 0.59 |
| 1:A:353:LEU:HD13 | 1:A:423:LYS:HB2 | 1.84 | 0.59 |
| 1:B:1122:LYS:O | 1:B:1126:ASN:ND2 | 2.36 | 0.59 |
| 1:C:748:ASP:N | 1:C:748:ASP:OD1 | 2.35 | 0.59 |
| 1:D:594:PRO:HB2 | 1:D:597:LEU:HB2 | 1.85 | 0.58 |
| 1:D:716:GLN:NE2 | 1:D:1199:GLN:OE1 | 2.32 | 0.58 |
| 1:D:267:GLY:H | 1:D:272:ARG:HH11 | 1.50 | 0.58 |
| 1:C:402:THR:OG1 | 1:C:409:GLN:OE1 | 2.22 | 0.58 |
| 1:A:1241:GLU:OE1 | 1:B:1240:ARG:NH2 | 2.35 | 0.58 |
| 1:A:644:TRP:NE1 | 1:A:648:MET:SD | 2.77 | 0.58 |
| 1:A:658:TRP:HE1 | 1:A:668:ALA:HB2 | 1.69 | 0.58 |
| 3:I:80:ILE:HA | 3:I:92:ALA:HA | 1.84 | 0.58 |
| 3:I:187:VAL:HA | 3:I:203:ALA:HA | 1.86 | 0.58 |
| 1:A:255:PRO:HA | 1:A:297:ALA:HB3 | 1.85 | 0.58 |
| 1:C:257:GLY:HA3 | 1:C:302:THR:HA | 1.85 | 0.58 |
| 1:C:506:LEU:O | 1:C:510:ASN:ND2 | 2.31 | 0.58 |
| 1:D:342:GLY:H | 1:D:345:VAL:HB | 1.69 | 0.58 |
| 1:B:439:ASP:HB2 | 1:B:442:LEU:HB2 | 1.85 | 0.58 |
| 1:B:493:LEU:HB2 | 1:B:522:ARG:HE | 1.69 | 0.58 |
| 1:B:1221:ARG:NH1 | 1:B:1225:GLU:OE2 | 2.37 | 0.58 |
| 1:D:313:ARG:NH2 | 1:D:355:ASP:OD2 | 2.36 | 0.58 |
| 1:A:187:SER:OG | 1:A:189:HIS:NE2 | 2.35 | 0.57 |
| 1:A:194:ASN:HA | 1:A:228:GLY:H | 1.68 | 0.57 |
| 1:C:542:ARG:O | 1:C:547:GLY:N | 2.37 | 0.57 |
| 1:C:697:HIS:HD2 | 1:C:700:ARG:HH12 | 1.51 | 0.57 |
| 3:I:310:GLY:O | 3:I:337:LYS:NZ | 2.37 | 0.57 |
| 1:C:1225:GLU:O | 1:C:1229:ASN:ND2 | 2.38 | 0.57 |
| 3:I:121:CYS:HB3 | 3:I:139:LEU:HB2 | 1.86 | 0.57 |
| 4:J:34:ALA:O | 4:J:38:MET:N | 2.33 | 0.57 |
| 1:B:189:HIS:NE2 | 1:B:352:TYR:OH | 2.34 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:365:ASP:HB3 | 1:C:431:ARG:HH22 | 1.69 | 0.57 |
| 1:D:1186:THR:HG22 | 1:D:1189:GLU:HG2 | 1.86 | 0.57 |
| 1:D:1190:LEU:O | 1:D:1194:HIS:ND1 | 2.38 | 0.57 |
| 3:I:264:TYR:OH | 3:I:299:ALA:O | 2.19 | 0.57 |
| 1:B:144:ILE:HG22 | 1:B:272:ARG:HB2 | 1.86 | 0.57 |
| 1:D:630:GLU:O | 1:D:631:ILE:HG22 | 2.04 | 0.56 |
| 1:C:458:ASP:OD1 | 1:C:458:ASP:N | 2.37 | 0.56 |
| 1:A:313:ARG:O | 1:A:313:ARG:NH1 | 2.39 | 0.56 |
| 1:A:993:ASN:OD1 | 1:A:996:LEU:N | 2.36 | 0.56 |
| 3:I:250:CYS:HB3 | 3:I:264:TYR:HB2 | 1.86 | 0.56 |
| 1:A:163:ASP:O | 1:A:165:LYS:NZ | 2.39 | 0.56 |
| 1:D:631:ILE:O | 1:D:633:HIS:ND1 | 2.39 | 0.56 |
| 4:J:29:LYS:O | 4:J:33:ALA:N | 2.37 | 0.56 |
| 1:A:143:THR:OG1 | 1:A:156:MET:SD | 2.63 | 0.56 |
| 1:B:144:ILE:HG13 | 1:B:155:ALA:HB3 | 1.88 | 0.56 |
| 1:B:173:MET:HB3 | 1:B:179:LEU:HD12 | 1.87 | 0.56 |
| 1:B:692:SER:O | 1:B:696:ASN:ND2 | 2.38 | 0.56 |
| 1:B:664:ALA:N | 1:B:1197:GLU:OE2 | 2.38 | 0.56 |
| 1:C:221:PHE:O | 1:C:312:ARG:NH2 | 2.38 | 0.56 |
| 1:A:748:ASP:OD1 | 1:A:748:ASP:N | 2.36 | 0.56 |
| 1:B:336:ALA:HB3 | 1:B:361:VAL:HG22 | 1.86 | 0.56 |
| 1:C:565:GLU:OE2 | 1:C:577:THR:OG1 | 2.19 | 0.56 |
| 1:C:1241:GLU:OE1 | 1:D:1240:ARG:NH2 | 2.38 | 0.56 |
| 1:D:574:CYS:SG | 1:D:575:ASN:N | 2.79 | 0.56 |
| 3:I:76:ASP:HB2 | 3:I:78:LYS:HE3 | 1.86 | 0.56 |
| 3:I:137:ARG:HH21 | 3:I:174:GLY:HA3 | 1.70 | 0.56 |
| 1:D:299:ASN:OD1 | 1:D:299:ASN:N | 2.39 | 0.56 |
| 3:I:248:ALA:HB1 | 3:I:269:ILE:HG22 | 1.88 | 0.56 |
| 1:A:355:ASP:O | 1:A:356:THR:C | 2.45 | 0.56 |
| 1:C:159:ARG:HA | 1:C:296:LEU:HB2 | 1.88 | 0.56 |
| 1:B:994:LYS:NZ | 1:B:995:TYR:OH | 2.39 | 0.55 |
| 3:I:326:ALA:HA | 4:J:50:LEU:HD21 | 1.87 | 0.55 |
| 3:I:126:LEU:HA | 3:I:133:VAL:HG22 | 1.89 | 0.55 |
| 3:I:128:THR:HG21 | 3:I:134:ARG:HG2 | 1.88 | 0.55 |
| 3:I:279:SER:OG | 3:I:283:ARG:N | 2.38 | 0.55 |
| 1:C:1122:LYS:O | 1:C:1126:ASN:ND2 | 2.40 | 0.55 |
| 1:A:430:PHE:HE1 | 1:A:438:GLN:HA | 1.71 | 0.55 |
| 1:B:137:PRO:HA | 2:F:7:UNK:HA | 1.88 | 0.55 |
| 1:D:238:LYS:HB2 | 1:D:290:MET:HG3 | 1.89 | 0.55 |
| 4:J:23:ALA:HA | 4:J:27:ARG:HH22 | 1.72 | 0.55 |
| 1:A:208:GLY:HA3 | 1:A:440:ILE:HB | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:275:GLN:NE2 | 1:B:277:MET:O | 2.34 | 0.55 |
| 1:C:175:LYS:O | 1:C:178:GLN:NE2 | 2.39 | 0.55 |
| 3:I:254:ASP:OD2 | 3:I:257:ALA:N | 2.40 | 0.55 |
| 1:B:577:THR:O | 1:B:579:LYS:NZ | 2.40 | 0.55 |
| 1:B:473:ARG:HB2 | 1:B:506:LEU:HD21 | 1.89 | 0.55 |
| 1:D:265:LEU:HA | 1:D:272:ARG:HD3 | 1.87 | 0.55 |
| 3:I:271:CYS:HB3 | 3:I:290:ASP:HB2 | 1.89 | 0.55 |
| 1:C:1181:LEU:HG | 1:C:1182:LYS:HG3 | 1.90 | 0.54 |
| 1:B:335:VAL:HB | 1:B:448:LEU:HD21 | 1.88 | 0.54 |
| 1:C:712:GLN:HG2 | 1:C:1204:TYR:HB2 | 1.88 | 0.54 |
| 1:D:257:GLY:O | 1:D:262:GLN:NE2 | 2.40 | 0.54 |
| 1:D:1189:GLU:HA | 1:D:1192:LYS:HD3 | 1.88 | 0.54 |
| 3:I:83:ASP:N | 3:I:88:ASN:O | 2.39 | 0.54 |
| 1:A:241:ALA:O | 1:B:1206:ARG:NH1 | 2.38 | 0.54 |
| 1:B:175:LYS:O | 1:B:178:GLN:NE2 | 2.41 | 0.54 |
| 1:A:175:LYS:O | 1:A:178:GLN:NE2 | 2.41 | 0.54 |
| 1:D:172:LEU:HD12 | 1:D:176:GLU:HB2 | 1.89 | 0.54 |
| 3:I:195:ASP:HB2 | 3:I:197:ARG:HH11 | 1.73 | 0.54 |
| 1:B:194:ASN:OD1 | 1:B:231:ARG:NH1 | 2.40 | 0.54 |
| 1:D:748:ASP:OD1 | 1:D:748:ASP:N | 2.33 | 0.54 |
| 1:A:439:ASP:HB2 | 1:A:442:LEU:HB2 | 1.90 | 0.54 |
| 1:A:697:HIS:HD2 | 1:A:700:ARG:HH12 | 1.55 | 0.54 |
| 1:C:413:LEU:HB3 | 1:C:416:ILE:HD11 | 1.90 | 0.54 |
| 1:D:592:LYS:NZ | 1:D:594:PRO:O | 2.41 | 0.54 |
| 3:I:331:SER:OG | 3:I:332:TRP:N | 2.39 | 0.54 |
| 1:A:454:ALA:O | 1:A:459:GLN:NE2 | 2.41 | 0.54 |
| 1:B:468:ARG:NH2 | 1:B:470:ASP:OD2 | 2.40 | 0.54 |
| 1:D:185:LEU:HB3 | 1:D:334:VAL:HG22 | 1.90 | 0.54 |
| 1:D:208:GLY:HA3 | 1:D:440:ILE:HB | 1.89 | 0.54 |
| 3:I:180:PHE:HZ | 3:I:213:VAL:HA | 1.73 | 0.54 |
| 1:C:255:PRO:HG2 | 1:C:258:ILE:HG13 | 1.90 | 0.53 |
| 3:I:112:VAL:HG23 | 3:I:126:LEU:HD11 | 1.89 | 0.53 |
| 3:I:285:LEU:O | 3:I:297:TRP:N | 2.41 | 0.53 |
| 1:A:256:TRP:HB2 | 1:A:296:LEU:HB3 | 1.90 | 0.53 |
| 1:C:711:ASP:HA | 1:C:752:HIS:HE2 | 1.72 | 0.53 |
| 1:C:353:LEU:HB3 | 1:C:423:LYS:HD2 | 1.90 | 0.53 |
| 1:D:629:PRO:C | 1:D:631:ILE:N | 2.61 | 0.53 |
| 1:D:634:PHE:O | 1:D:637:PRO:HD3 | 2.08 | 0.53 |
| 1:C:565:GLU:OE2 | 1:C:574:CYS:N | 2.39 | 0.53 |
| 1:D:137:PRO:HA | 2:H:7:UNK:HA | 1.90 | 0.53 |
| 3:I:298:ASP:HB3 | 3:I:303:ASP:H | 1.74 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:172:LEU:HD12 | 1:C:176:GLU:HB2 | 1.89 | 0.53 |
| 1:C:582:ARG:O | 1:C:586:HIS:HB2 | 2.08 | 0.53 |
| 1:D:353:LEU:HB3 | 1:D:423:LYS:HD2 | 1.91 | 0.53 |
| 1:C:349:VAL:HG23 | 1:C:361:VAL:HG21 | 1.91 | 0.53 |
| 3:I:232:ILE:HA | 3:I:243:THR:HA | 1.91 | 0.53 |
| 1:A:234:GLY:HA3 | 1:A:288:ASN:HD21 | 1.73 | 0.53 |
| 1:B:407:ARG:HG2 | 1:B:410:ALA:HB3 | 1.91 | 0.53 |
| 1:D:664:ALA:N | 1:D:1197:GLU:OE2 | 2.41 | 0.53 |
| 3:I:40:VAL:HG22 | 3:I:303:ASP:HB3 | 1.92 | 0.52 |
| 1:D:690:ASP:HA | 1:D:693:GLN:HE21 | 1.72 | 0.52 |
| 1:A:250:THR:HB | 1:A:292:SER:H | 1.75 | 0.52 |
| 1:C:470:ASP:OD1 | 1:C:470:ASP:N | 2.42 | 0.52 |
| 1:C:350:LEU:HD13 | 1:C:354:ARG:HH22 | 1.74 | 0.52 |
| 3:I:33:ILE:HG22 | 3:I:34:THR:HG23 | 1.91 | 0.52 |
| 1:C:137:PRO:HA | 2:G:7:UNK:HA | 1.92 | 0.52 |
| 1:D:258:ILE:HA | 1:D:303:GLY:HA2 | 1.92 | 0.52 |
| 1:D:627:ASP:O | 1:D:628:ASP:HB3 | 2.10 | 0.52 |
| 1:A:349:VAL:HG23 | 1:A:361:VAL:HG21 | 1.92 | 0.52 |
| 1:B:398:THR:HA | 1:B:414:PHE:HE2 | 1.75 | 0.52 |
| 1:B:672:CYS:HG | 1:B:699:SER:HG | 1.57 | 0.52 |
| 1:D:632:ASN:C | 1:D:632:ASN:HD22 | 2.13 | 0.52 |
| 3:I:15:LYS:HD3 | 3:I:19:ARG:HE | 1.73 | 0.52 |
| 1:D:224:GLY:O | 1:D:288:ASN:N | 2.36 | 0.51 |
| 1:A:550:PRO:HG2 | 1:A:553:TYR:HB2 | 1.92 | 0.51 |
| 1:A:1189:GLU:HA | 1:A:1192:LYS:HD3 | 1.93 | 0.51 |
| 3:I:118:ASP:OD1 | 3:I:118:ASP:N | 2.43 | 0.51 |
| 1:C:574:CYS:SG | 1:C:575:ASN:N | 2.83 | 0.51 |
| 1:C:761:ASP:OD1 | 1:C:761:ASP:N | 2.42 | 0.51 |
| 3:I:281:SER:HA | 4:J:40:TYR:CZ | 2.46 | 0.51 |
| 3:I:121:CYS:O | 3:I:139:LEU:N | 2.44 | 0.51 |
| 1:A:411:GLN:HE22 | 1:A:413:LEU:HG | 1.75 | 0.51 |
| 1:B:742:VAL:O | 1:B:745:LYS:NZ | 2.38 | 0.51 |
| 1:D:1005:LYS:HD2 | 1:D:1121:VAL:HG13 | 1.92 | 0.51 |
| 3:I:22:ARG:O | 3:I:26:ALA:N | 2.40 | 0.51 |
| 3:I:79:LEU:HB3 | 3:I:93:ILE:HB | 1.92 | 0.51 |
| 1:B:141:PHE:O | 1:B:269:ASP:N | 2.40 | 0.50 |
| 1:D:234:GLY:HA3 | 1:D:288:ASN:HD21 | 1.76 | 0.50 |
| 1:B:186:ILE:HB | 1:B:220:ILE:HG12 | 1.93 | 0.50 |
| 1:B:574:CYS:SG | 1:B:575:ASN:N | 2.84 | 0.50 |
| 1:C:129:ILE:HD12 | 1:C:132:HIS:HB2 | 1.93 | 0.50 |
| 1:C:559:ASP:OD1 | 1:C:559:ASP:N | 2.31 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:159:ARG:HA | 1:B:296:LEU:HB2 | 1.93 | 0.50 |
| 3:I:57:LYS:HB3 | 3:I:332:TRP:CG | 2.46 | 0.50 |
| 1:D:250:THR:HB | 1:D:292:SER:H | 1.76 | 0.50 |
| 3:I:69:LEU:HD21 | 3:I:81:ILE:HG23 | 1.93 | 0.50 |
| 1:B:157:TYR:OH | 1:B:267:GLY:O | 2.29 | 0.50 |
| 1:C:429:VAL:HB | 1:C:431:ARG:HH21 | 1.76 | 0.50 |
| 3:I:198:LEU:HD23 | 3:I:212:ASP:HA | 1.92 | 0.50 |
| 1:B:342:GLY:H | 1:B:345:VAL:HB | 1.76 | 0.50 |
| 1:C:323:LYS:HD3 | 1:C:331:GLY:HA2 | 1.93 | 0.50 |
| 1:C:419:GLU:O | 1:C:423:LYS:NZ | 2.45 | 0.50 |
| 1:D:201:LEU:HD21 | 1:D:366:GLY:HA3 | 1.93 | 0.50 |
| 3:I:37:ILE:HD12 | 3:I:283:ARG:HH22 | 1.75 | 0.50 |
| 3:I:151:PHE:HA | 3:I:157:ILE:HA | 1.93 | 0.50 |
| 1:D:221:PHE:O | 1:D:312:ARG:NH2 | 2.45 | 0.49 |
| 1:B:277:MET:HB2 | 1:C:511:GLY:HA3 | 1.93 | 0.49 |
| 1:B:470:ASP:OD1 | 1:B:470:ASP:N | 2.44 | 0.49 |
| 1:C:132:HIS:O | 2:G:12:UNK:N | 2.45 | 0.49 |
| 1:D:344:ASN:O | 1:D:347:SER:OG | 2.22 | 0.49 |
| 1:D:631:ILE:O | 1:D:632:ASN:C | 2.50 | 0.49 |
| 4:J:26:ASP:N | 4:J:26:ASP:OD1 | 2.45 | 0.49 |
| 1:A:353:LEU:HD11 | 1:A:427:ILE:HD11 | 1.93 | 0.49 |
| 1:C:139:ASP:H | 1:C:159:ARG:HD3 | 1.77 | 0.49 |
| 1:B:195:PHE:O | 1:B:231:ARG:NH2 | 2.45 | 0.49 |
| 1:D:761:ASP:N | 1:D:761:ASP:OD1 | 2.46 | 0.49 |
| 1:A:216:THR:HG1 | 1:A:466:TRP:HD1 | 1.60 | 0.49 |
| 1:B:446:THR:HG22 | 1:B:475:GLN:HG3 | 1.95 | 0.49 |
| 1:C:254:ALA:O | 1:C:297:ALA:N | 2.45 | 0.49 |
| 1:D:166:PRO:HA | 1:D:169:LEU:HD12 | 1.94 | 0.49 |
| 1:D:324:ILE:HG23 | 1:D:326:THR:H | 1.78 | 0.49 |
| 3:I:239:ASN:HB2 | 4:J:37:LEU:HD21 | 1.93 | 0.49 |
| 1:B:556:SER:OG | 1:B:559:ASP:OD1 | 2.23 | 0.49 |
| 4:J:44:HIS:ND1 | 4:J:47:GLU:OE2 | 2.46 | 0.49 |
| 4:J:47:GLU:N | 4:J:47:GLU:OE1 | 2.45 | 0.49 |
| 1:D:598:LYS:HG3 | 1:D:599:LEU:HD12 | 1.94 | 0.49 |
| 1:A:664:ALA:HA | 1:A:667:LYS:HD3 | 1.93 | 0.49 |
| 1:A:1241:GLU:HA | 1:B:1240:ARG:HH12 | 1.77 | 0.49 |
| 1:B:1189:GLU:HA | 1:B:1192:LYS:HD3 | 1.95 | 0.49 |
| 1:A:468:ARG:NH2 | 1:A:470:ASP:OD2 | 2.46 | 0.48 |
| 1:B:663:GLU:OE2 | 1:B:731:ASN:ND2 | 2.46 | 0.48 |
| 1:D:467:ASN:HB2 | 1:D:500:ARG:HH21 | 1.78 | 0.48 |
| 1:D:502:ASP:O | 1:D:505:LYS:HG2 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:577:THR:O | 1:D:579:LYS:NZ | 2.39 | 0.48 |
| 1:D:1122:LYS:O | 1:D:1126:ASN:ND2 | 2.32 | 0.48 |
| 3:I:245:SER:H | 3:I:273:ILE:HD12 | 1.78 | 0.48 |
| 3:I:48:ARG:NH2 | 3:I:340:ASN:O | 2.46 | 0.48 |
| 1:A:398:THR:HB | 1:A:414:PHE:HZ | 1.78 | 0.48 |
| 1:D:664:ALA:HA | 1:D:667:LYS:HD3 | 1.94 | 0.48 |
| 1:C:139:ASP:OD1 | 1:C:159:ARG:NH1 | 2.47 | 0.48 |
| 1:C:256:TRP:N | 1:C:297:ALA:O | 2.46 | 0.48 |
| 1:C:324:ILE:HG23 | 1:C:326:THR:H | 1.79 | 0.48 |
| 1:A:697:HIS:CD2 | 1:A:700:ARG:HH22 | 2.31 | 0.48 |
| 1:A:458:ASP:N | 1:A:458:ASP:OD1 | 2.45 | 0.48 |
| 1:C:363:VAL:O | 1:C:430:PHE:N | 2.46 | 0.48 |
| 1:D:630:GLU:HB3 | 1:D:633:HIS:HE1 | 1.79 | 0.48 |
| 1:A:407:ARG:HH12 | 1:A:410:ALA:HB3 | 1.78 | 0.48 |
| 1:A:673:LYS:HD3 | 1:A:744:ALA:HA | 1.96 | 0.48 |
| 1:B:561:GLY:HA3 | 1:B:576:TYR:HB2 | 1.95 | 0.48 |
| 1:B:741:ALA:O | 1:B:745:LYS:N | 2.47 | 0.48 |
| 1:C:577:THR:HB | 1:C:582:ARG:HH21 | 1.79 | 0.48 |
| 3:I:30:LEU:HD21 | 3:I:300:LEU:HG | 1.94 | 0.48 |
| 1:A:642:MET:HE2 | 1:A:671:ALA:HB2 | 1.95 | 0.48 |
| 1:A:1218:GLU:OE2 | 1:A:1221:ARG:NH2 | 2.44 | 0.48 |
| 1:C:185:LEU:HD22 | 1:C:319:ILE:HG21 | 1.95 | 0.48 |
| 1:C:156:MET:SD | 1:C:156:MET:N | 2.86 | 0.47 |
| 1:C:198:GLN:NE2 | 1:C:199:PRO:O | 2.47 | 0.47 |
| 1:B:256:TRP:N | 1:B:297:ALA:O | 2.46 | 0.47 |
| 1:B:745:LYS:HB3 | 1:B:747:ARG:HH12 | 1.78 | 0.47 |
| 1:C:697:HIS:CD2 | 1:C:700:ARG:HH22 | 2.32 | 0.47 |
| 1:D:1225:GLU:O | 1:D:1229:ASN:ND2 | 2.47 | 0.47 |
| 1:A:519:THR:H | 1:A:522:ARG:HB2 | 1.78 | 0.47 |
| 1:A:573:ARG:HE | 1:A:578:ARG:NH1 | 2.12 | 0.47 |
| 1:A:1185:ILE:HG21 | 1:A:1190:LEU:HD13 | 1.95 | 0.47 |
| 1:C:431:ARG:HG3 | 1:C:434:SER:HB2 | 1.95 | 0.47 |
| 1:D:186:ILE:HA | 1:D:335:VAL:HG12 | 1.96 | 0.47 |
| 1:A:400:GLN:OE1 | 1:A:400:GLN:N | 2.45 | 0.47 |
| 1:D:230:ILE:O | 1:D:288:ASN:ND2 | 2.48 | 0.47 |
| 1:D:319:ILE:HA | 1:D:322:GLN:HG2 | 1.97 | 0.47 |
| 1:A:313:ARG:NH1 | 1:A:317:LYS:HG3 | 2.30 | 0.47 |
| 1:A:358:PRO:HB2 | 1:A:426:LEU:HD12 | 1.96 | 0.47 |
| 1:B:260:GLU:OE2 | 1:B:279:ASN:ND2 | 2.48 | 0.47 |
| 1:D:140:ALA:HB3 | 1:D:159:ARG:HD3 | 1.95 | 0.47 |
| 1:D:250:THR:H | 1:D:292:SER:HB2 | 1.80 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:I:68:ARG:HG3 | 3:I:85:TYR:CD1 | 2.49 | 0.47 |
| 1:D:182:PRO:HG3 | 1:D:219:TRP:CG | 2.49 | 0.47 |
| 1:D:1187:ASP:OD1 | 1:D:1187:ASP:N | 2.39 | 0.47 |
| 1:D:1216:ASN:OD1 | 1:D:1216:ASN:N | 2.46 | 0.47 |
| 3:I:183:HIS:HD2 | 3:I:211:TRP:HE1 | 1.63 | 0.47 |
| 1:A:368:GLY:H | 1:A:372:ASP:HB2 | 1.80 | 0.47 |
| 1:B:188:VAL:O | 1:B:312:ARG:NH2 | 2.48 | 0.47 |
| 1:B:435:GLU:O | 1:B:438:GLN:NE2 | 2.47 | 0.47 |
| 1:D:160:VAL:O | 1:D:298:ASP:N | 2.38 | 0.47 |
| 1:D:176:GLU:O | 1:D:178:GLN:NE2 | 2.48 | 0.47 |
| 1:D:680:HIS:NE2 | 1:D:684:GLU:OE2 | 2.48 | 0.47 |
| 3:I:105:TYR:CE2 | 3:I:109:GLY:HA2 | 2.49 | 0.47 |
| 3:I:215:GLU:N | 3:I:215:GLU:OE1 | 2.48 | 0.47 |
| 1:B:515:HIS:O | 1:B:633:HIS:NE2 | 2.47 | 0.47 |
| 1:C:756:GLN:HE22 | 1:C:1130:LYS:HB3 | 1.80 | 0.47 |
| 1:C:1120:GLU:OE1 | 1:C:1120:GLU:N | 2.43 | 0.47 |
| 1:D:370:ALA:O | 1:D:373:ILE:HG12 | 2.15 | 0.47 |
| 1:C:754:CYS:HA | 1:C:757:MET:HG2 | 1.95 | 0.47 |
| 1:D:353:LEU:HD13 | 1:D:423:LYS:HB2 | 1.97 | 0.47 |
| 1:A:147:GLN:N | 1:A:274:TYR:O | 2.37 | 0.46 |
| 1:D:197:LEU:HD11 | 1:D:202:LYS:HB3 | 1.97 | 0.46 |
| 1:A:144:ILE:HG22 | 1:A:272:ARG:HB2 | 1.97 | 0.46 |
| 1:A:200:LYS:HA | 1:A:200:LYS:HD2 | 1.64 | 0.46 |
| 1:A:229:VAL:HA | 1:A:232:HIS:HD2 | 1.79 | 0.46 |
| 1:B:431:ARG:HE | 1:B:434:SER:HB3 | 1.80 | 0.46 |
| 1:C:544:VAL:HG21 | 1:C:563:VAL:HG22 | 1.96 | 0.46 |
| 1:A:542:ARG:HG3 | 1:A:547:GLY:HA2 | 1.97 | 0.46 |
| 1:B:299:ASN:OD1 | 1:B:299:ASN:N | 2.49 | 0.46 |
| 3:I:49:ARG:NH2 | 4:J:62:ARG:O | 2.47 | 0.46 |
| 1:A:301:THR:HB | 1:A:304:LYS:HG3 | 1.97 | 0.46 |
| 1:B:452:ALA:HB3 | 1:B:459:GLN:HE21 | 1.80 | 0.46 |
| 1:D:313:ARG:O | 1:D:313:ARG:NH1 | 2.49 | 0.46 |
| 1:D:402:THR:OG1 | 1:D:409:GLN:NE2 | 2.48 | 0.46 |
| 3:I:158:VAL:HG22 | 3:I:168:LEU:HD13 | 1.97 | 0.46 |
| 1:B:748:ASP:OD1 | 1:B:748:ASP:N | 2.49 | 0.46 |
| 1:C:129:ILE:HD13 | 2:G:14:UNK:HA | 1.98 | 0.46 |
| 1:D:631:ILE:CG2 | 1:D:632:ASN:N | 2.79 | 0.46 |
| 1:D:1111:ILE:HA | 1:D:1114:PHE:HB2 | 1.97 | 0.46 |
| 1:B:226:ASN:HB2 | 1:B:288:ASN:HA | 1.98 | 0.46 |
| 1:C:1217:ASP:OD1 | 1:C:1217:ASP:N | 2.47 | 0.46 |
| 3:I:281:SER:HB3 | 4:J:44:HIS:HD2 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:468:ARG:NH2 | 1:D:470:ASP:OD2 | 2.49 | 0.46 |
| 1:A:356:THR:O | 1:A:358:PRO:HD3 | 2.15 | 0.46 |
| 1:C:194:ASN:OD1 | 1:C:231:ARG:NH1 | 2.49 | 0.46 |
| 3:I:10:GLU:O | 3:I:14:LEU:N | 2.39 | 0.46 |
| 3:I:110:ASN:HD22 | 3:I:127:LYS:HD3 | 1.81 | 0.46 |
| 1:A:1177:ARG:HG3 | 1:A:1181:LEU:HD23 | 1.97 | 0.46 |
| 1:D:494:ASP:HA | 1:D:497:VAL:HG22 | 1.98 | 0.46 |
| 3:I:150:ARG:HB3 | 3:I:192:LEU:HD11 | 1.97 | 0.46 |
| 1:A:378:HIS:CE1 | 1:A:424:LYS:HB2 | 2.51 | 0.45 |
| 1:C:519:THR:HG23 | 1:C:522:ARG:HD2 | 1.98 | 0.45 |
| 3:I:65:THR:HG21 | 3:I:107:PRO:HA | 1.99 | 0.45 |
| 1:B:328:ILE:HG13 | 1:B:458:ASP:HA | 1.98 | 0.45 |
| 1:C:139:ASP:OD1 | 1:C:139:ASP:N | 2.49 | 0.45 |
| 1:B:171:HIS:O | 1:B:175:LYS:HB2 | 2.16 | 0.45 |
| 1:B:439:ASP:N | 1:B:439:ASP:OD1 | 2.50 | 0.45 |
| 1:C:245:ARG:NE | 1:D:1203:GLU:OE1 | 2.49 | 0.45 |
| 1:D:182:PRO:HD3 | 1:D:219:TRP:CE2 | 2.51 | 0.45 |
| 3:I:210:LEU:HB2 | 3:I:222:PHE:HE2 | 1.82 | 0.45 |
| 1:A:159:ARG:NH2 | 1:A:298:ASP:OD2 | 2.44 | 0.45 |
| 1:A:310:LYS:O | 1:A:314:GLN:HG2 | 2.17 | 0.45 |
| 1:B:189:HIS:CD2 | 1:B:352:TYR:HH | 2.31 | 0.45 |
| 1:B:350:LEU:O | 1:B:354:ARG:N | 2.40 | 0.45 |
| 1:D:567:LEU:HD22 | 1:D:677:ALA:HB1 | 1.98 | 0.45 |
| 3:I:328:ALA:HB2 | 3:I:338:ILE:HG23 | 1.98 | 0.45 |
| 1:D:497:VAL:HG12 | 1:D:526:LEU:HD23 | 1.98 | 0.45 |
| 3:I:156:GLN:HG3 | 3:I:168:LEU:HD11 | 1.97 | 0.45 |
| 1:B:378:HIS:HA | 1:B:421:MET:HE1 | 1.99 | 0.45 |
| 1:C:208:GLY:HA2 | 1:C:441:ASP:HB2 | 1.99 | 0.45 |
| 1:C:1198:GLU:HA | 1:C:1201:ILE:HG22 | 1.99 | 0.45 |
| 1:D:146:PHE:HD2 | 1:D:153:ASN:HB3 | 1.82 | 0.45 |
| 1:D:190:GLY:HA2 | 1:D:339:VAL:O | 2.17 | 0.45 |
| 1:D:672:CYS:O | 1:D:699:SER:OG | 2.35 | 0.45 |
| 3:I:204:CYS:HA | 3:I:228:ASP:HA | 1.98 | 0.45 |
| 1:A:747:ARG:HG2 | 1:A:1131:PHE:CG | 2.52 | 0.45 |
| 1:D:542:ARG:HG3 | 1:D:547:GLY:HA2 | 1.99 | 0.45 |
| 1:D:631:ILE:HD12 | 1:D:631:ILE:HA | 1.70 | 0.45 |
| 1:C:185:LEU:HD22 | 1:C:319:ILE:HD12 | 2.00 | 0.44 |
| 3:I:16:ASN:OD1 | 3:I:19:ARG:NH2 | 2.50 | 0.44 |
| 3:I:152:LEU:HB2 | 3:I:156:GLN:HB3 | 1.99 | 0.44 |
| 1:C:747:ARG:HG2 | 1:C:1131:PHE:CG | 2.52 | 0.44 |
| 1:C:750:ILE:O | 1:C:755:SER:OG | 2.35 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:159:ARG:HA | 1:D:296:LEU:HB2 | 1.99 | 0.44 |
| 1:D:520:ILE:HG13 | 1:D:632:ASN:ND2 | 2.31 | 0.44 |
| 1:B:538:TYR:HD1 | 1:B:555:ILE:HD11 | 1.83 | 0.44 |
| 1:C:153:ASN:ND2 | 1:C:291:HIS:O | 2.38 | 0.44 |
| 1:D:417:LEU:HA | 1:D:420:CYS:HB3 | 1.97 | 0.44 |
| 1:D:520:ILE:N | 1:D:632:ASN:OD1 | 2.40 | 0.44 |
| 1:A:729:LEU:HB3 | 1:A:732:TRP:CD1 | 2.52 | 0.44 |
| 1:B:1196:PHE:O | 1:B:1199:GLN:HG2 | 2.17 | 0.44 |
| 1:C:256:TRP:NE1 | 1:C:262:GLN:OE1 | 2.50 | 0.44 |
| 1:C:335:VAL:HB | 1:C:448:LEU:HD21 | 1.98 | 0.44 |
| 1:D:634:PHE:O | 1:D:635:PRO:C | 2.55 | 0.44 |
| 1:C:350:LEU:O | 1:C:354:ARG:N | 2.50 | 0.44 |
| 1:C:690:ASP:O | 1:C:693:GLN:HG2 | 2.17 | 0.44 |
| 1:D:183:LYS:HG2 | 1:D:324:ILE:HD11 | 2.00 | 0.44 |
| 1:D:470:ASP:N | 1:D:470:ASP:OD1 | 2.51 | 0.44 |
| 1:A:314:GLN:HA | 1:A:317:LYS:HD2 | 2.00 | 0.44 |
| 1:D:641:LEU:HD23 | 1:D:641:LEU:HA | 1.85 | 0.44 |
| 3:I:159:THR:HG1 | 3:I:169:TRP:HE1 | 1.66 | 0.44 |
| 3:I:283:ARG:HG2 | 4:J:51:LEU:HD22 | 1.98 | 0.44 |
| 1:A:356:THR:HB | 1:A:357:PRO:CD | 2.41 | 0.44 |
| 1:B:356:THR:HB | 1:B:357:PRO:HD3 | 2.00 | 0.44 |
| 1:B:1228:GLU:HB2 | 1:C:1226:ARG:NH1 | 2.33 | 0.44 |
| 1:D:631:ILE:O | 1:D:633:HIS:CG | 2.71 | 0.44 |
| 3:I:294[B]:CYS:SG | 3:I:295:ASN:N | 2.90 | 0.44 |
| 1:A:729:LEU:HB3 | 1:A:732:TRP:HD1 | 1.82 | 0.44 |
| 1:A:1199:GLN:HE21 | 1:A:1199:GLN:HB3 | 1.57 | 0.44 |
| 1:A:1230:MET:HG3 | 1:D:1234:LEU:HD22 | 1.99 | 0.44 |
| 1:C:313:ARG:NH1 | 1:C:316:GLU:HB2 | 2.33 | 0.44 |
| 1:C:1185:ILE:HD12 | 1:C:1185:ILE:HA | 1.85 | 0.44 |
| 3:I:274:THR:N | 3:I:288:GLY:O | 2.40 | 0.44 |
| 1:A:150:GLY:HA3 | 1:B:509:GLU:HG2 | 2.00 | 0.43 |
| 1:A:275:GLN:NE2 | 1:A:277:MET:H | 2.16 | 0.43 |
| 1:C:230:ILE:HA | 1:C:233:VAL:HG22 | 2.00 | 0.43 |
| 1:D:556:SER:OG | 1:D:559:ASP:OD1 | 2.26 | 0.43 |
| 3:I:286:LEU:HD21 | 3:I:327:VAL:HG21 | 2.00 | 0.43 |
| 1:A:134:GLN:N | 2:E:10:UNK:O | 2.36 | 0.43 |
| 1:A:229:VAL:HA | 1:A:232:HIS:CD2 | 2.54 | 0.43 |
| 1:A:994:LYS:HA | 1:A:1129:TRP:CZ2 | 2.53 | 0.43 |
| 3:I:37:ILE:H | 3:I:37:ILE:HG12 | 1.43 | 0.43 |
| 1:A:759:LEU:HB3 | 1:A:1137:ILE:HD12 | 2.00 | 0.43 |
| 1:B:340:GLU:HA | 1:B:367:SER:HB3 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:541:VAL:HG22 | 1:B:563:VAL:HG21 | 2.01 | 0.43 |
| 1:C:1228:GLU:HB2 | 1:D:1226:ARG:NH1 | 2.34 | 0.43 |
| 1:D:519:THR:HB | 1:D:632:ASN:OD1 | 2.18 | 0.43 |
| 3:I:210:LEU:HB3 | 3:I:219:ARG:HB2 | 2.00 | 0.43 |
| 1:A:245:ARG:HE | 1:B:1206:ARG:HG2 | 1.82 | 0.43 |
| 1:B:368:GLY:H | 1:B:372:ASP:HB2 | 1.82 | 0.43 |
| 1:B:542:ARG:O | 1:B:547:GLY:N | 2.51 | 0.43 |
| 1:D:170:LEU:HD22 | 1:D:318:HIS:CE1 | 2.53 | 0.43 |
| 3:I:34:THR:HB | 3:I:37:ILE:HD11 | 2.00 | 0.43 |
| 3:I:107:PRO:HG2 | 3:I:153:ASP:HA | 1.99 | 0.43 |
| 1:B:501:VAL:HG21 | 1:B:652:LYS:HG2 | 2.01 | 0.43 |
| 1:C:746:HIS:HE1 | 1:C:748:ASP:HB2 | 1.83 | 0.43 |
| 3:I:79:LEU:N | 3:I:93:ILE:O | 2.36 | 0.43 |
| 1:A:415:ILE:HD13 | 1:A:415:ILE:H | 1.83 | 0.43 |
| 1:C:183:LYS:HD3 | 1:C:465:ALA:HB1 | 2.01 | 0.43 |
| 1:D:221:PHE:HE1 | 1:D:251:ILE:HD12 | 1.83 | 0.43 |
| 1:A:1209:ASP:O | 1:A:1213:ASN:ND2 | 2.38 | 0.43 |
| 1:B:187:SER:OG | 1:B:189:HIS:NE2 | 2.45 | 0.43 |
| 1:B:1185:ILE:HD12 | 1:B:1185:ILE:HA | 1.93 | 0.43 |
| 1:D:476:ILE:HG22 | 1:D:483:TRP:HH2 | 1.83 | 0.43 |
| 1:D:501:VAL:HG21 | 1:D:652:LYS:HG2 | 2.01 | 0.43 |
| 1:A:544:VAL:HG21 | 1:A:563:VAL:HG22 | 2.00 | 0.43 |
| 1:B:578:ARG:HA | 1:B:578:ARG:HD3 | 1.77 | 0.43 |
| 3:I:323:ASP:HB2 | 3:I:325:MET:HG3 | 2.01 | 0.43 |
| 1:B:328:ILE:HD11 | 1:B:457:PRO:HB2 | 2.01 | 0.43 |
| 1:B:516:ARG:HA | 1:B:633:HIS:CE1 | 2.54 | 0.43 |
| 3:I:328:ALA:HA | 3:I:338:ILE:HA | 2.01 | 0.43 |
| 1:A:335:VAL:HG11 | 1:A:444:ILE:HG23 | 2.01 | 0.42 |
| 1:B:370:ALA:HA | 1:B:373:ILE:HG23 | 2.01 | 0.42 |
| 1:D:256:TRP:HB3 | 1:D:298:ASP:HA | 2.01 | 0.42 |
| 3:I:57:LYS:HB3 | 3:I:332:TRP:CD2 | 2.54 | 0.42 |
| 1:A:313:ARG:NH1 | 1:A:316:GLU:HB2 | 2.34 | 0.42 |
| 1:B:131:LYS:HD3 | 1:B:131:LYS:HA | 1.83 | 0.42 |
| 1:B:172:LEU:HD12 | 1:B:176:GLU:HB2 | 2.01 | 0.42 |
| 1:D:628:ASP:HB2 | 1:D:631:ILE:HB | 2.01 | 0.42 |
| 3:I:320:VAL:HG22 | 3:I:327:VAL:HG12 | 2.01 | 0.42 |
| 1:A:172:LEU:HG | 1:A:176:GLU:HB2 | 2.00 | 0.42 |
| 1:C:437:HIS:NE2 | 1:C:446:THR:HG21 | 2.35 | 0.42 |
| 1:A:422:LYS:HD2 | 1:A:423:LYS:HZ2 | 1.84 | 0.42 |
| 1:C:257:GLY:HA2 | 1:C:262:GLN:NE2 | 2.34 | 0.42 |
| 1:C:489:GLU:HB3 | 1:C:522:ARG:NH2 | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:446:THR:HA | 1:D:449:LEU:HB2 | 2.01 | 0.42 |
| 1:D:736:THR:OG1 | 1:D:739:GLN:NE2 | 2.52 | 0.42 |
| 3:I:58:ILE:HG12 | 3:I:74:SER:HB2 | 2.01 | 0.42 |
| 3:I:82:TRP:HA | 3:I:89:LYS:HA | 2.00 | 0.42 |
| 3:I:180:PHE:CD2 | 3:I:211:TRP:HB3 | 2.55 | 0.42 |
| 1:A:515:HIS:O | 1:A:633:HIS:NE2 | 2.52 | 0.42 |
| 1:B:250:THR:H | 1:B:292:SER:HB2 | 1.84 | 0.42 |
| 1:C:1187:ASP:OD1 | 1:C:1187:ASP:N | 2.52 | 0.42 |
| 1:D:631:ILE:C | 1:D:633:HIS:N | 2.70 | 0.42 |
| 3:I:124:TYR:HA | 3:I:135:VAL:HA | 2.00 | 0.42 |
| 1:A:478:ILE:HG13 | 1:A:481:GLN:NE2 | 2.34 | 0.42 |
| 1:A:686:ASP:OD1 | 1:A:686:ASP:N | 2.53 | 0.42 |
| 1:B:191:GLY:H | 1:B:341:GLY:H | 1.67 | 0.42 |
| 1:C:641:LEU:HB3 | 1:C:657:PHE:CD2 | 2.55 | 0.42 |
| 1:A:697:HIS:CD2 | 1:A:700:ARG:HH12 | 2.37 | 0.42 |
| 1:B:398:THR:HA | 1:B:414:PHE:CE2 | 2.54 | 0.42 |
| 1:B:224:GLY:H | 1:B:230:ILE:HD13 | 1.84 | 0.42 |
| 1:C:313:ARG:NH1 | 1:C:317:LYS:HG3 | 2.35 | 0.42 |
| 1:C:636:PHE:HB3 | 1:C:639:HIS:ND1 | 2.34 | 0.42 |
| 1:D:404:THR:HG22 | 1:D:408:THR:HA | 2.02 | 0.42 |
| 1:D:634:PHE:C | 1:D:636:PHE:N | 2.73 | 0.42 |
| 1:A:736:THR:OG1 | 1:A:739:GLN:NE2 | 2.53 | 0.42 |
| 1:C:165:LYS:HA | 1:C:166:PRO:HD3 | 1.92 | 0.42 |
| 1:B:349:VAL:HG23 | 1:B:361:VAL:HG21 | 2.02 | 0.42 |
| 1:B:697:HIS:CD2 | 1:B:700:ARG:HH12 | 2.37 | 0.42 |
| 1:A:470:ASP:OD1 | 1:A:470:ASP:N | 2.52 | 0.41 |
| 1:C:182:PRO:HG3 | 1:C:219:TRP:CD2 | 2.54 | 0.41 |
| 1:C:370:ALA:O | 1:C:373:ILE:HG12 | 2.20 | 0.41 |
| 3:I:329:THR:N | 3:I:337:LYS:O | 2.40 | 0.41 |
| 1:B:133:THR:HG21 | 1:B:300:GLY:HA3 | 2.02 | 0.41 |
| 1:B:407:ARG:HB3 | 1:B:411:GLN:HB2 | 2.02 | 0.41 |
| 1:C:245:ARG:NH2 | 1:D:1203:GLU:OE2 | 2.52 | 0.41 |
| 1:D:524:GLU:O | 1:D:528:ASN:ND2 | 2.40 | 0.41 |
| 1:C:729:LEU:HD23 | 1:C:729:LEU:HA | 1.96 | 0.41 |
| 1:D:313:ARG:NH1 | 1:D:317:LYS:HG3 | 2.36 | 0.41 |
| 1:A:267:GLY:H | 1:A:272:ARG:NH1 | 2.19 | 0.41 |
| 1:B:736:THR:N | 1:B:739:GLN:OE1 | 2.53 | 0.41 |
| 1:C:353:LEU:HD22 | 1:C:423:LYS:HB2 | 2.03 | 0.41 |
| 1:A:182:PRO:HD3 | 1:A:219:TRP:CE2 | 2.56 | 0.41 |
| 1:B:1234:LEU:HD21 | 1:C:1233:ARG:HB3 | 2.01 | 0.41 |
| 1:D:167:ASP:OD1 | 1:D:168:LEU:N | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:463:ALA:O | 1:D:467:ASN:N | 2.54 | 0.41 |
| 1:B:657:PHE:HD1 | 1:B:657:PHE:HA | 1.76 | 0.41 |
| 3:I:78:LYS:HA | 3:I:94:PRO:HA | 2.03 | 0.41 |
| 1:B:583:THR:O | 1:B:587:ASN:N | 2.51 | 0.41 |
| 1:C:281:MET:N | 1:C:281:MET:SD | 2.94 | 0.41 |
| 1:C:310:LYS:O | 1:C:314:GLN:HG2 | 2.21 | 0.41 |
| 1:C:998:PRO:O | 1:C:1002:MET:HG3 | 2.21 | 0.41 |
| 1:D:404:THR:HA | 1:D:408:THR:HA | 2.03 | 0.41 |
| 1:D:634:PHE:H | 1:D:634:PHE:HD1 | 1.66 | 0.41 |
| 1:A:553:TYR:CE2 | 1:A:555:ILE:HA | 2.56 | 0.41 |
| 1:A:573:ARG:NH2 | 1:A:578:ARG:HD3 | 2.34 | 0.41 |
| 1:A:1233:ARG:HB3 | 1:D:1234:LEU:HD21 | 2.03 | 0.41 |
| 1:B:447:ALA:HA | 1:B:450:LYS:HG2 | 2.03 | 0.41 |
| 1:C:313:ARG:HA | 1:C:313:ARG:HD2 | 1.86 | 0.41 |
| 1:D:424:LYS:HA | 1:D:427:ILE:HG13 | 2.02 | 0.41 |
| 1:D:1123:SER:O | 1:D:1127:GLN:HG2 | 2.21 | 0.41 |
| 1:A:710:LEU:HD22 | 1:A:749:PHE:CZ | 2.56 | 0.41 |
| 1:B:993:ASN:HB3 | 1:B:996:LEU:HB2 | 2.03 | 0.41 |
| 1:C:141:PHE:HB2 | 1:C:158:VAL:HG22 | 2.03 | 0.41 |
| 1:C:250:THR:H | 1:C:292:SER:HB2 | 1.86 | 0.41 |
| 1:C:464:LEU:O | 1:C:500:ARG:NH2 | 2.54 | 0.41 |
| 3:I:71:VAL:HG23 | 3:I:79:LEU:HG | 2.03 | 0.41 |
| 1:A:324:ILE:HG23 | 1:A:326:THR:H | 1.85 | 0.40 |
| 1:A:370:ALA:HA | 1:A:373:ILE:HG23 | 2.02 | 0.40 |
| 1:C:165:LYS:HA | 1:C:165:LYS:HD3 | 1.85 | 0.40 |
| 1:C:369:ARG:HG3 | 1:C:370:ALA:H | 1.86 | 0.40 |
| 3:I:183:HIS:CD2 | 3:I:211:TRP:HE1 | 2.39 | 0.40 |
| 4:J:15:LEU:O | 4:J:19:LEU:N | 2.49 | 0.40 |
| 1:A:1129:TRP:CH2 | 1:A:1133:ARG:HD2 | 2.57 | 0.40 |
| 1:A:1217:ASP:OD1 | 1:A:1217:ASP:N | 2.54 | 0.40 |
| 1:C:133:THR:HA | 2:G:11:UNK:HA | 2.03 | 0.40 |
| 1:C:224:GLY:H | 1:C:230:ILE:HD13 | 1.85 | 0.40 |
| 1:C:523:LEU:HA | 1:C:526:LEU:HD12 | 2.03 | 0.40 |
| 1:C:532:GLY:HA3 | 1:C:650:ARG:HH21 | 1.85 | 0.40 |
| 3:I:296:VAL:HB | 3:I:305:ALA:HB3 | 2.02 | 0.40 |
| 1:B:556:SER:N | 1:B:559:ASP:OD2 | 2.54 | 0.40 |
| 1:D:369:ARG:HA | 1:D:369:ARG:HD3 | 1.86 | 0.40 |
| 1:A:542:ARG:HD3 | 1:A:549:LEU:HD21 | 2.04 | 0.40 |
| 1:A:681:GLU:O | 1:A:684:GLU:HG2 | 2.20 | 0.40 |
| 1:A:1231:SER:HB2 | 1:B:1230:MET:HE2 | 2.03 | 0.40 |
| 1:C:747:ARG:HE | 1:C:1128:VAL:HA | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:747:ARG:HH21 | 1:C:1128:VAL:HG13 | 1.87 | 0.40 |
| 1:D:631:ILE:HG13 | 1:D:632:ASN:H | 1.87 | 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 | 683/1371 (50%) | 646 (95%) | 36 (5%) | 1 (0%) | 51 85 |
| 1 | B | 683/1371 (50%) | 653 (96%) | 30 (4%) | 0 | 100 100 |
| 1 | C | 683/1371 (50%) | 650 (95%) | 33 (5%) | 0 | 100 100 |
| 1 | D | 707/1371 (52%) | 670 (95%) | 35 (5%) | 2 (0%) | 41 76 |
| 3 | I | 337/339 (99%) | 308 (91%) | 29 (9%) | 0 | 100 100 |
| 4 | J | 55/70 (79%) | 47 (86%) | 8 (14%) | 0 | 100 100 |
| All | All | 3148/5893 (53%) | 2974 (94%) | 171 (5%) | 3 (0%) | 54 85 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 631 | ILE |
| 1 | D | 635 | PRO |
| 1 | A | 357 | PRO |

### 5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 610/1219 (50%) | 565 (93%) | 45 (7%) | 13 40 |
| 1 | B | 610/1219 (50%) | 555 (91%) | 55 (9%) | 9 32 |
| 1 | C | 610/1219 (50%) | 567 (93%) | 43 (7%) | 15 41 |
| 1 | D | 631/1219 (52%) | 583 (92%) | 48 (8%) | 13 39 |
| 3 | I | 282/282 (100%) | 260 (92%) | 22 (8%) | 12 38 |
| 4 | J | 46/57 (81%) | 42 (91%) | 4 (9%) | 10 34 |
| All | All | 2789/5215 (54%) | 2572 (92%) | 217 (8%) | 16 38 |

All (217) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 138 | THR |
| 1 | A | 167 | ASP |
| 1 | A | 172 | LEU |
| 1 | A | 200 | LYS |
| 1 | A | 205 | PHE |
| 1 | A | 256 | TRP |
| 1 | A | 272 | ARG |
| 1 | A | 275 | GLN |
| 1 | A | 276 | THR |
| 1 | A | 345 | VAL |
| 1 | A | 350 | LEU |
| 1 | A | 373 | ILE |
| 1 | A | 405 | TYR |
| 1 | A | 407 | ARG |
| 1 | A | 412 | HIS |
| 1 | A | 414 | PHE |
| 1 | A | 415 | ILE |
| 1 | A | 416 | ILE |
| 1 | A | 439 | ASP |
| 1 | A | 458 | ASP |
| 1 | A | 478 | ILE |
| 1 | A | 479 | TYR |
| 1 | A | 549 | LEU |
| 1 | A | 556 | SER |
| 1 | A | 559 | ASP |
| 1 | A | 584 | LEU |
| 1 | A | 633 | HIS |
| 1 | A | 657 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 686 | ASP |
| 1 | A | 688 | VAL |
| 1 | A | 711 | ASP |
| 1 | A | 719 | GLN |
| 1 | A | 722 | MET |
| 1 | A | 731 | ASN |
| 1 | A | 748 | ASP |
| 1 | A | 1114 | PHE |
| 1 | A | 1120 | GLU |
| 1 | A | 1138 | MET |
| 1 | A | 1140 | PHE |
| 1 | A | 1186 | THR |
| 1 | A | 1194 | HIS |
| 1 | A | 1199 | GLN |
| 1 | A | 1204 | TYR |
| 1 | A | 1217 | ASP |
| 1 | A | 1241 | GLU |
| 1 | B | 130 | SER |
| 1 | B | 141 | PHE |
| 1 | B | 163 | ASP |
| 1 | B | 227 | THR |
| 1 | B | 245 | ARG |
| 1 | B | 266 | ILE |
| 1 | B | 275 | GLN |
| 1 | B | 318 | HIS |
| 1 | B | 328 | ILE |
| 1 | B | 344 | ASN |
| 1 | B | 347 | SER |
| 1 | B | 350 | LEU |
| 1 | B | 369 | ARG |
| 1 | B | 373 | ILE |
| 1 | B | 412 | HIS |
| 1 | B | 413 | LEU |
| 1 | B | 414 | PHE |
| 1 | B | 415 | ILE |
| 1 | B | 439 | ASP |
| 1 | B | 445 | LEU |
| 1 | B | 458 | ASP |
| 1 | B | 462 | LEU |
| 1 | B | 479 | TYR |
| 1 | B | 481 | GLN |
| 1 | B | 502 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 516 | ARG |
| 1 | B | 517 | PHE |
| 1 | B | 518 | LEU |
| 1 | B | 519 | THR |
| 1 | B | 529 | THR |
| 1 | B | 549 | LEU |
| 1 | B | 559 | ASP |
| 1 | B | 584 | LEU |
| 1 | B | 585 | TYR |
| 1 | B | 586 | HIS |
| 1 | B | 632 | ASN |
| 1 | B | 633 | HIS |
| 1 | B | 648 | MET |
| 1 | B | 657 | PHE |
| 1 | B | 687 | MET |
| 1 | B | 693 | GLN |
| 1 | B | 705 | LEU |
| 1 | B | 719 | GLN |
| 1 | B | 724 | LEU |
| 1 | B | 731 | ASN |
| 1 | B | 746 | HIS |
| 1 | B | 999 | TYR |
| 1 | B | 1111 | ILE |
| 1 | B | 1183 | LEU |
| 1 | B | 1186 | THR |
| 1 | B | 1190 | LEU |
| 1 | B | 1199 | GLN |
| 1 | B | 1216 | ASN |
| 1 | B | 1217 | ASP |
| 1 | B | 1239 | GLU |
| 1 | C | 138 | THR |
| 1 | C | 160 | VAL |
| 1 | C | 167 | ASP |
| 1 | C | 197 | LEU |
| 1 | C | 200 | LYS |
| 1 | C | 205 | PHE |
| 1 | C | 227 | THR |
| 1 | C | 279 | ASN |
| 1 | C | 283 | LYS |
| 1 | C | 287 | LEU |
| 1 | C | 291 | HIS |
| 1 | C | 294 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 350 | LEU |
| 1 | C | 373 | ILE |
| 1 | C | 407 | ARG |
| 1 | C | 412 | HIS |
| 1 | C | 413 | LEU |
| 1 | C | 414 | PHE |
| 1 | C | 431 | ARG |
| 1 | C | 440 | ILE |
| 1 | C | 458 | ASP |
| 1 | C | 478 | ILE |
| 1 | C | 479 | TYR |
| 1 | C | 517 | PHE |
| 1 | C | 539 | HIS |
| 1 | C | 552 | ASP |
| 1 | C | 559 | ASP |
| 1 | C | 633 | HIS |
| 1 | C | 648 | MET |
| 1 | C | 690 | ASP |
| 1 | C | 726 | THR |
| 1 | C | 731 | ASN |
| 1 | C | 746 | HIS |
| 1 | C | 748 | ASP |
| 1 | C | 761 | ASP |
| 1 | C | 762 | MET |
| 1 | C | 994 | LYS |
| 1 | C | 1119 | PHE |
| 1 | C | 1140 | PHE |
| 1 | C | 1142 | GLU |
| 1 | C | 1186 | THR |
| 1 | C | 1199 | GLN |
| 1 | C | 1206 | ARG |
| 1 | D | 131 | LYS |
| 1 | D | 143 | THR |
| 1 | D | 167 | ASP |
| 1 | D | 170 | LEU |
| 1 | D | 171 | HIS |
| 1 | D | 172 | LEU |
| 1 | D | 192 | LEU |
| 1 | D | 205 | PHE |
| 1 | D | 214 | MET |
| 1 | D | 222 | THR |
| 1 | D | 235 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 276 | THR |
| 1 | D | 291 | HIS |
| 1 | D | 299 | ASN |
| 1 | D | 327 | ARG |
| 1 | D | 330 | GLN |
| 1 | D | 344 | ASN |
| 1 | D | 345 | VAL |
| 1 | D | 350 | LEU |
| 1 | D | 397 | VAL |
| 1 | D | 411 | GLN |
| 1 | D | 412 | HIS |
| 1 | D | 413 | LEU |
| 1 | D | 415 | ILE |
| 1 | D | 416 | ILE |
| 1 | D | 431 | ARG |
| 1 | D | 448 | LEU |
| 1 | D | 502 | ASP |
| 1 | D | 513 | SER |
| 1 | D | 515 | HIS |
| 1 | D | 549 | LEU |
| 1 | D | 556 | SER |
| 1 | D | 559 | ASP |
| 1 | D | 586 | HIS |
| 1 | D | 592 | LYS |
| 1 | D | 631 | ILE |
| 1 | D | 632 | ASN |
| 1 | D | 634 | PHE |
| 1 | D | 688 | VAL |
| 1 | D | 699 | SER |
| 1 | D | 748 | ASP |
| 1 | D | 761 | ASP |
| 1 | D | 995 | TYR |
| 1 | D | 1140 | PHE |
| 1 | D | 1199 | GLN |
| 1 | D | 1202 | GLU |
| 1 | D | 1216 | ASN |
| 1 | D | 1217 | ASP |
| 3 | I | 23 | LYS |
| 3 | I | 32 | GLN |
| 3 | I | 37 | ILE |
| 3 | I | 66 | ASP |
| 3 | I | 71 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | I | 78 | LYS |
| 3 | I | 83 | ASP |
| 3 | I | 91 | HIS |
| 3 | I | 100 | VAL |
| 3 | I | 123 | ILE |
| 3 | I | 142 | HIS |
| 3 | I | 157 | ILE |
| 3 | I | 178 | THR |
| 3 | I | 183 | HIS |
| 3 | I | 186 | ASP |
| 3 | I | 196 | THR |
| 3 | I | 221 | THR |
| 3 | I | 237 | ASN |
| 3 | I | 277 | SER |
| 3 | I | 321 | THR |
| 3 | I | 323 | ASP |
| 3 | I | 338 | ILE |
| 4 | J | 26 | ASP |
| 4 | J | 29 | LYS |
| 4 | J | 40 | TYR |
| 4 | J | 54 | VAL |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 134 | GLN |
| 1 | A | 198 | GLN |
| 1 | A | 275 | GLN |
| 1 | A | 288 | ASN |
| 1 | A | 318 | HIS |
| 1 | A | 378 | HIS |
| 1 | A | 481 | GLN |
| 1 | A | 490 | GLN |
| 1 | A | 510 | ASN |
| 1 | A | 539 | HIS |
| 1 | A | 696 | ASN |
| 1 | A | 697 | HIS |
| 1 | A | 716 | GLN |
| 1 | A | 719 | GLN |
| 1 | A | 739 | GLN |
| 1 | A | 1199 | GLN |
| 1 | B | 134 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 178 | GLN |
| 1 | B | 198 | GLN |
| 1 | B | 378 | HIS |
| 1 | B | 459 | GLN |
| 1 | B | 481 | GLN |
| 1 | B | 632 | ASN |
| 1 | B | 696 | ASN |
| 1 | B | 697 | HIS |
| 1 | B | 716 | GLN |
| 1 | B | 719 | GLN |
| 1 | B | 731 | ASN |
| 1 | B | 1116 | ASN |
| 1 | B | 1199 | GLN |
| 1 | B | 1242 | HIS |
| 1 | C | 134 | GLN |
| 1 | C | 178 | GLN |
| 1 | C | 240 | HIS |
| 1 | C | 330 | GLN |
| 1 | C | 378 | HIS |
| 1 | C | 481 | GLN |
| 1 | C | 697 | HIS |
| 1 | C | 704 | GLN |
| 1 | C | 712 | GLN |
| 1 | C | 719 | GLN |
| 1 | C | 756 | GLN |
| 1 | C | 1126 | ASN |
| 1 | C | 1242 | HIS |
| 1 | D | 153 | ASN |
| 1 | D | 314 | GLN |
| 1 | D | 409 | GLN |
| 1 | D | 548 | ASN |
| 1 | D | 660 | HIS |
| 1 | D | 693 | GLN |
| 1 | D | 696 | ASN |
| 1 | D | 719 | GLN |
| 1 | D | 739 | GLN |
| 1 | D | 1108 | ASN |
| 1 | D | 1115 | ASN |
| 1 | D | 1116 | ASN |
| 3 | I | 44 | GLN |
| 3 | I | 91 | HIS |
| 3 | I | 183 | HIS |

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no 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.

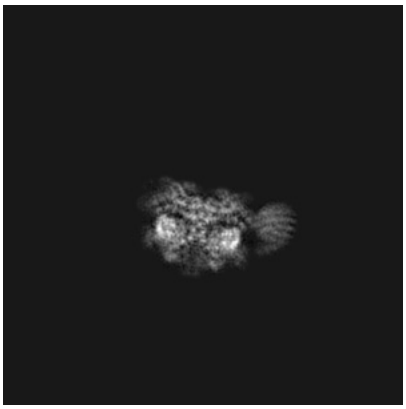
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27344. These allow visual inspection of the internal detail of the map and identification of artifacts.

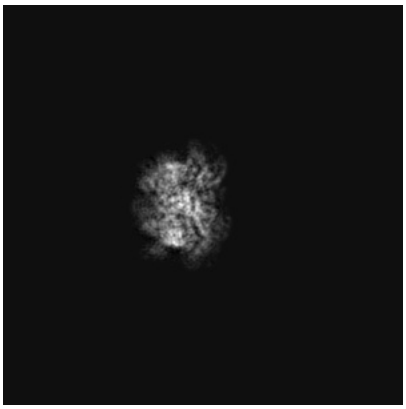
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

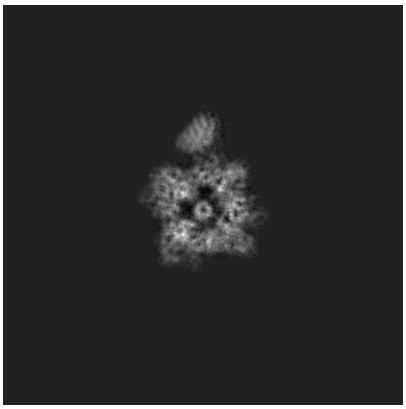
### 6.1.1 Primary map



X

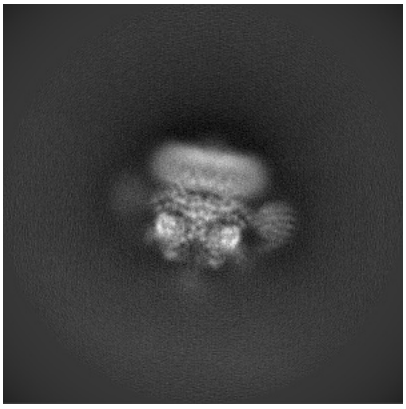


Y

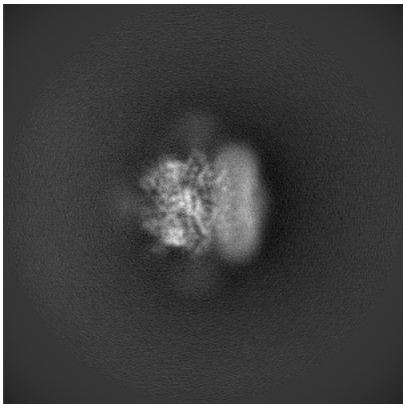


Z

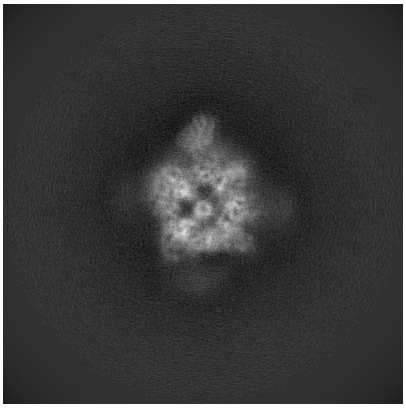
### 6.1.2 Raw map



X



Y



Z

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

## 6.2 Central slices (i)

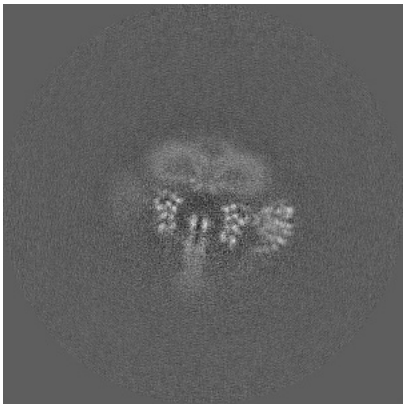
### 6.2.1 Primary map

X Index: 224

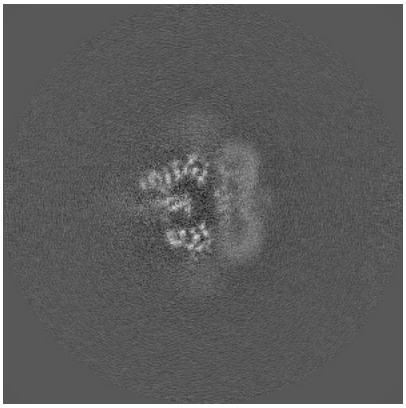
Y Index: 224

Z Index: 224

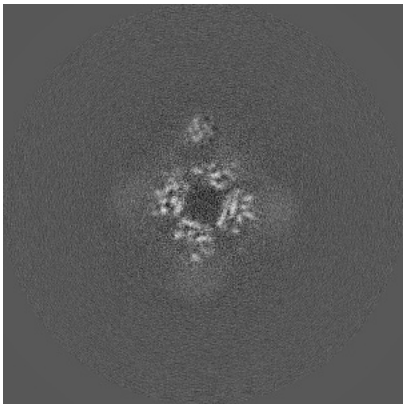
### 6.2.2 Raw map



X Index: 224



Y Index: 224



Z Index: 224

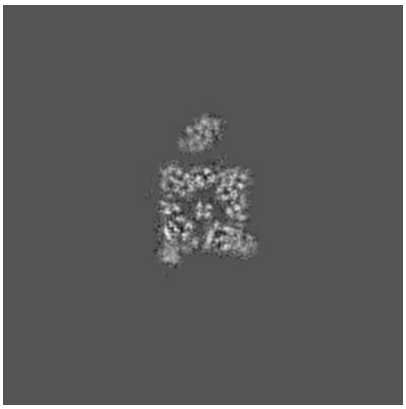
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

### 6.3.1 Primary map

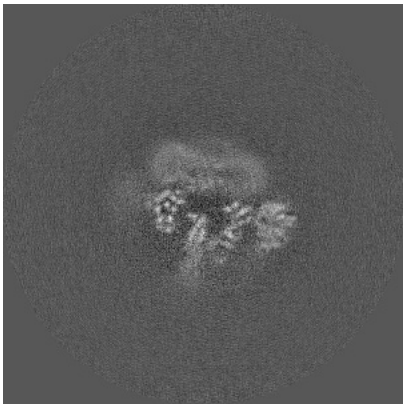
X Index: 229

Y Index: 191

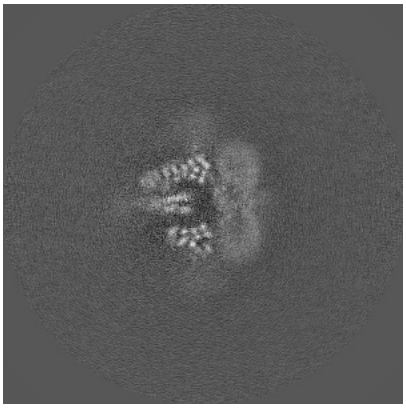


Z Index: 190

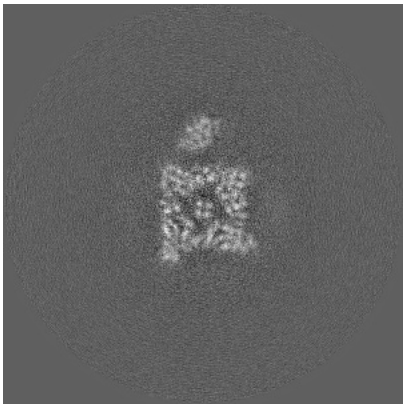
### 6.3.2 Raw map



X Index: 219



Y Index: 221

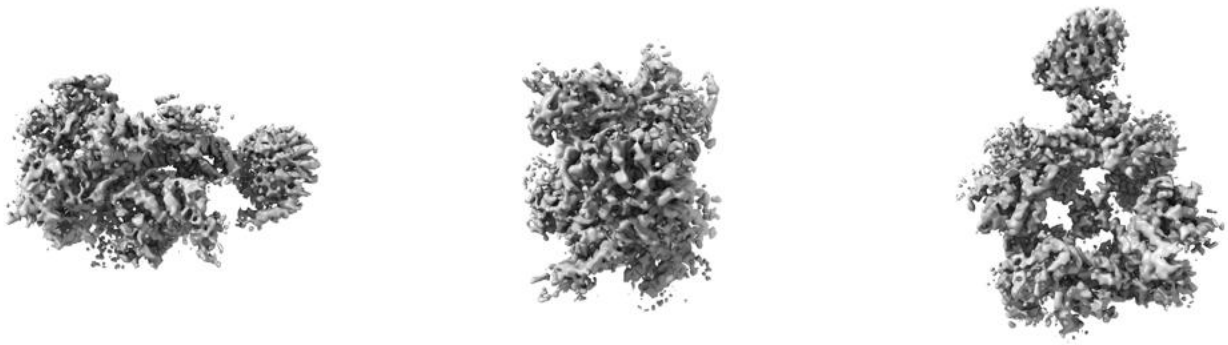


Z Index: 192

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

## 6.4 Orthogonal surface views (i)

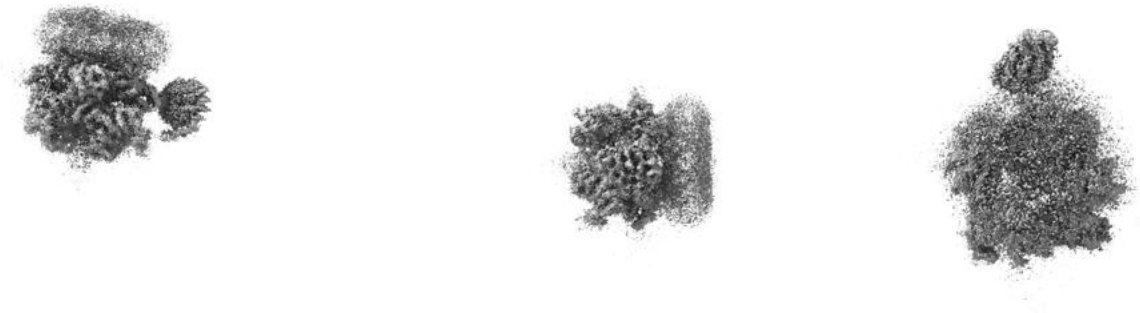
### 6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



X Y Z

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

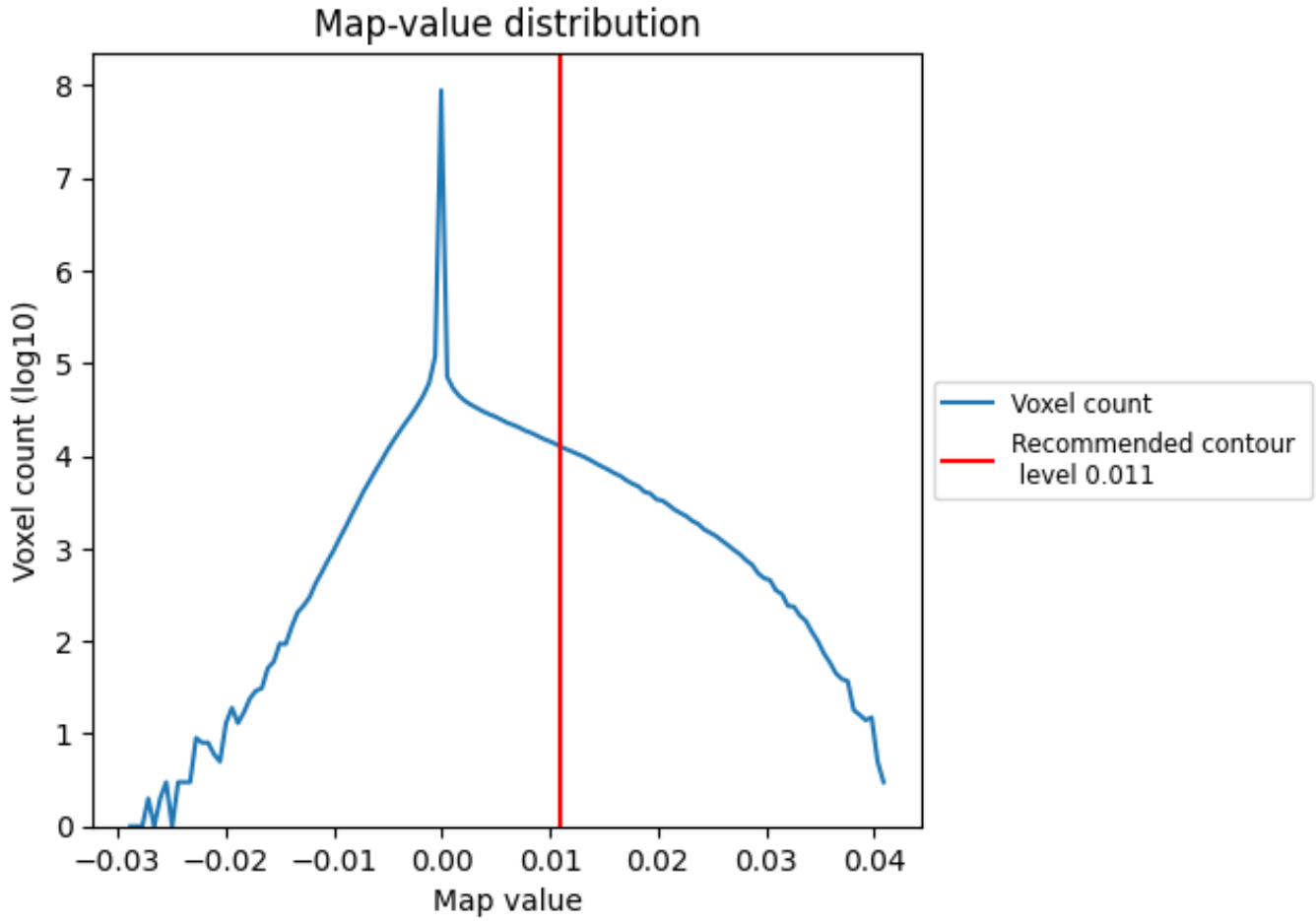
## 6.5 Mask visualisation (i)

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

# 7 Map analysis

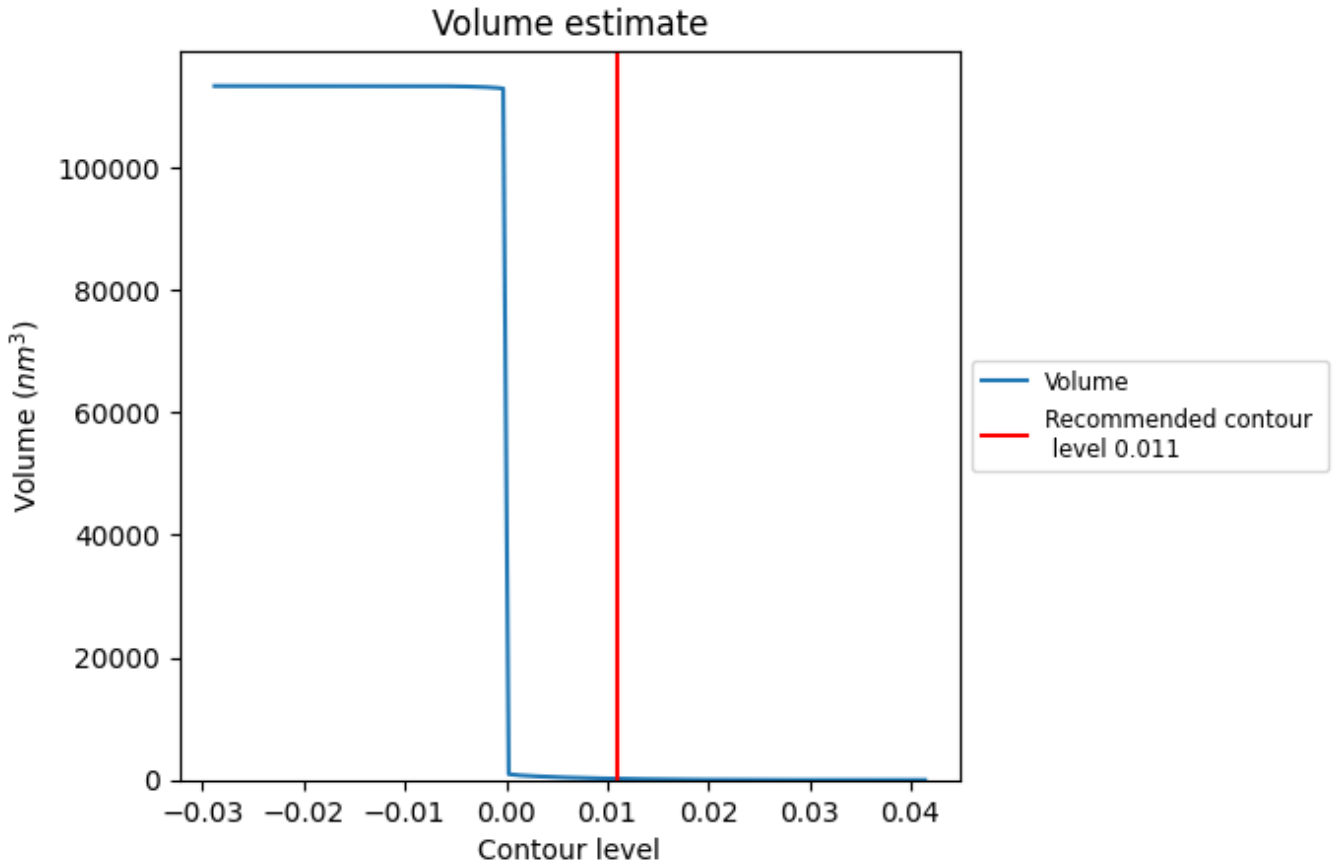
This section contains the results of statistical analysis of the map.

## 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.

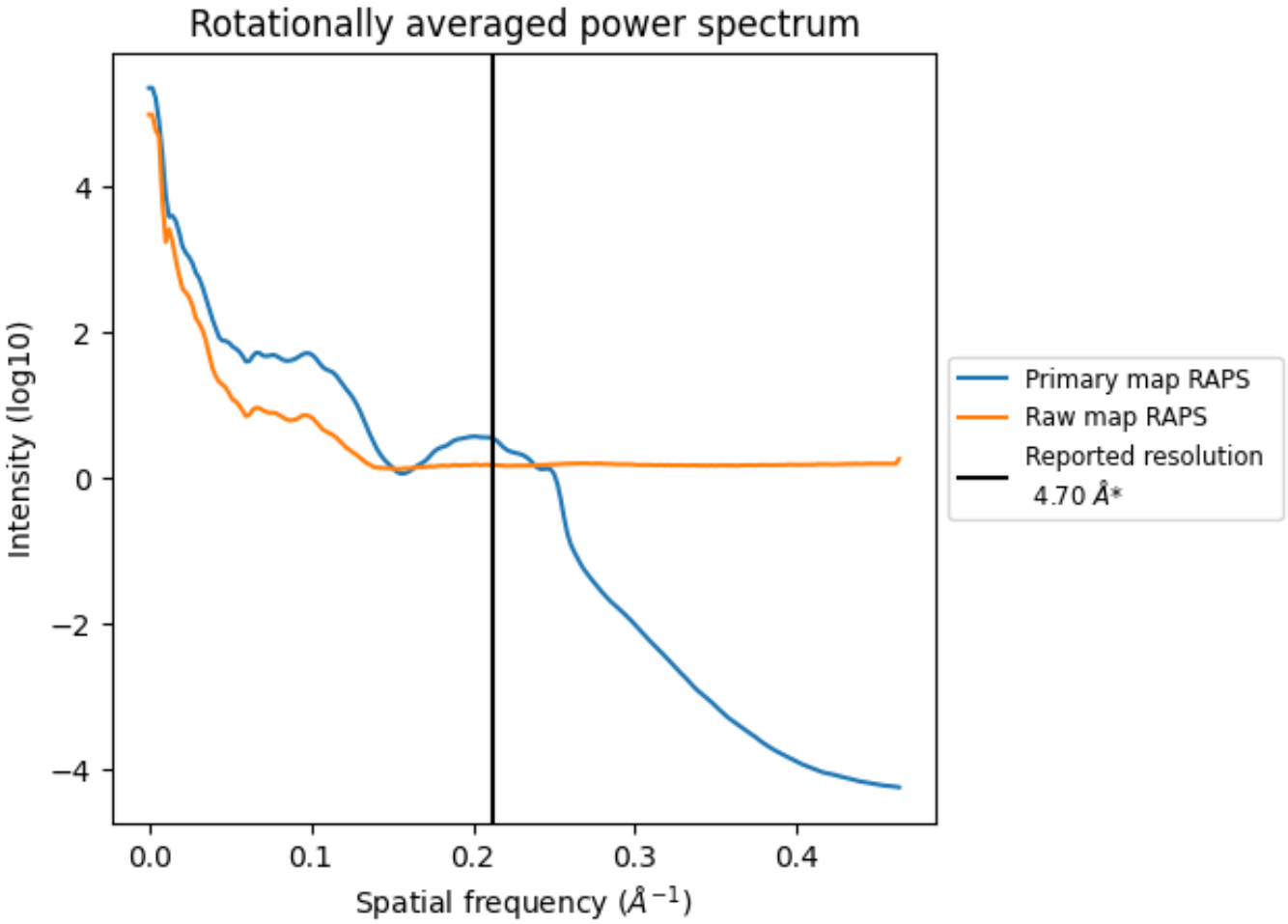
## 7.2 Volume estimate




The volume at the recommended contour level is 198 $nm^3$; this corresponds to an approximate mass of 179 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)

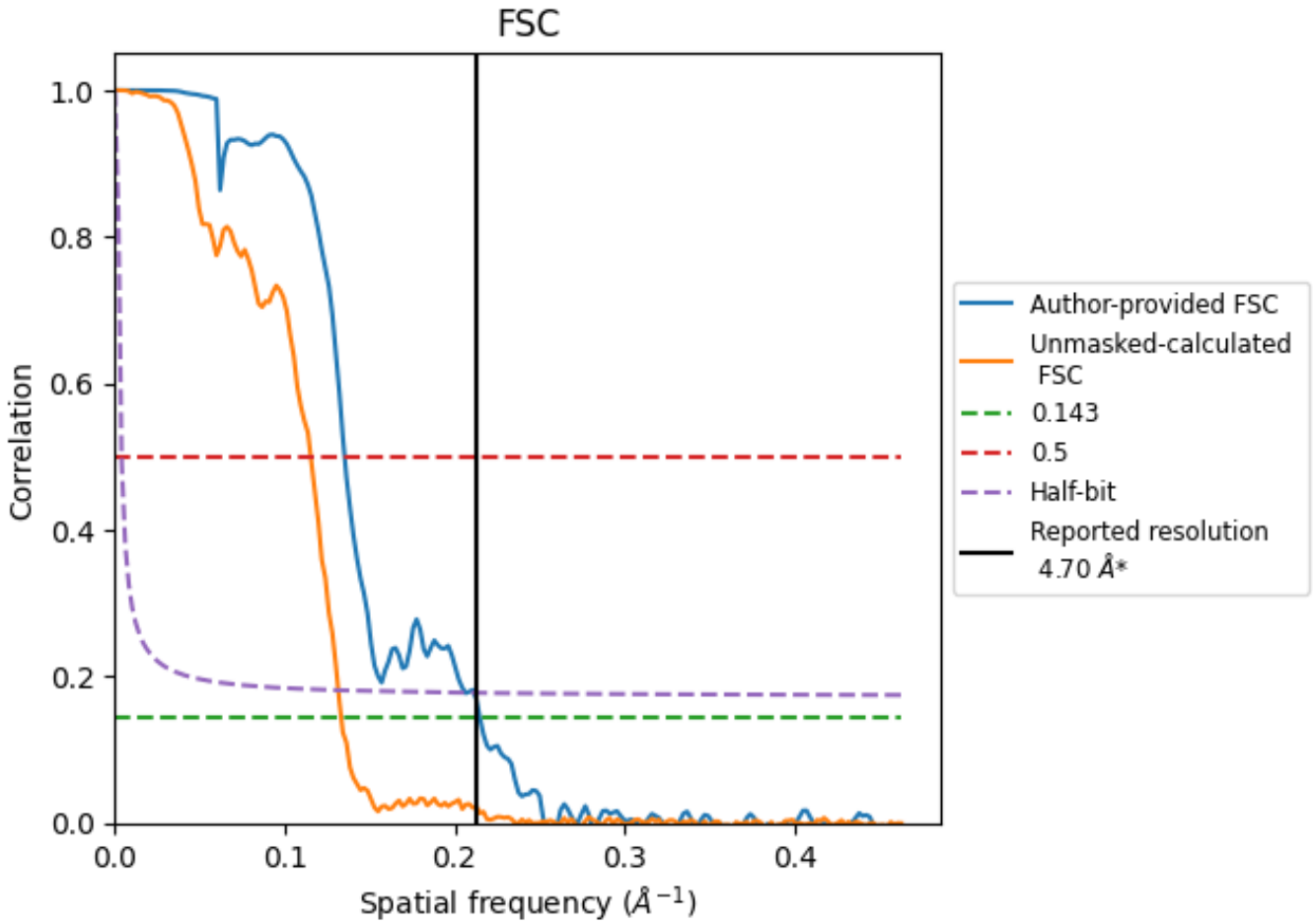



*Reported resolution corresponds to spatial frequency of 0.213 Å$^{-1}$

# 8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.213 Å$^{-1}$

## 8.2 Resolution estimates (i)

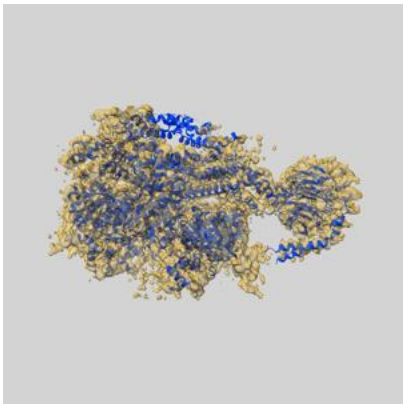
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 4.70 | - | - |
| Author-provided FSC curve | 4.65 | 7.39 | 4.84 |
| Unmasked-calculated* | 7.50 | 8.67 | 7.60 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.50 differs from the reported value 4.7 by more than 10 %

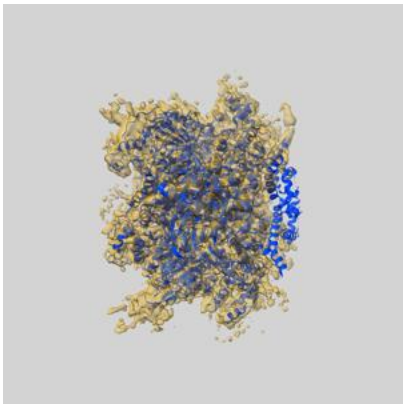
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27344 and PDB model 8DDW. Per-residue inclusion information can be found in section 3 on page 6.

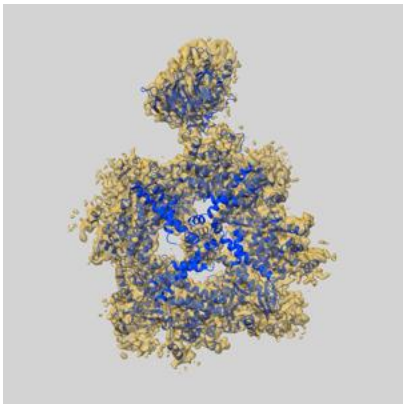
## 9.1 Map-model overlay



X



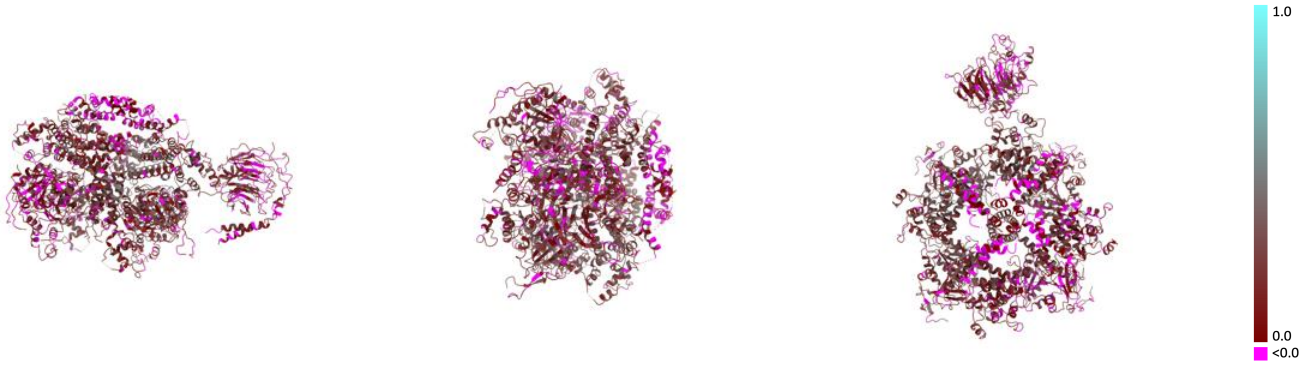
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011 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.

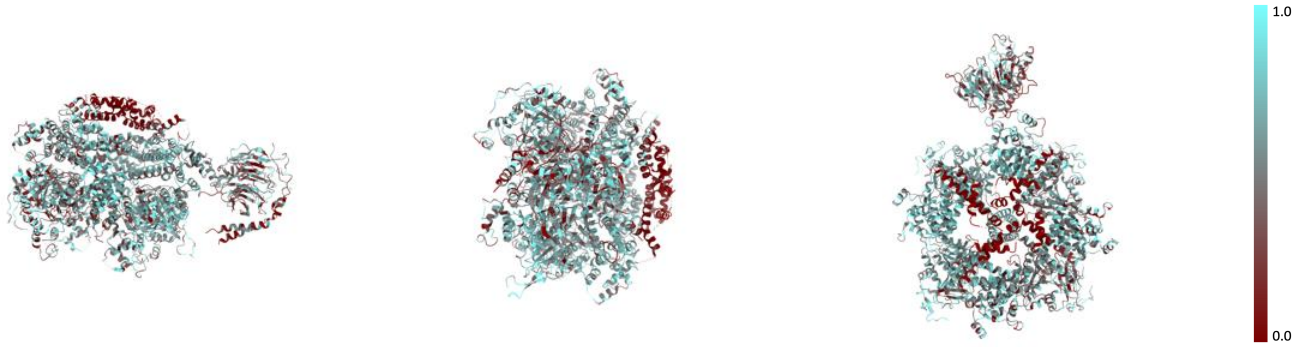
## 9.2 Q-score mapped to coordinate model (i)




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.

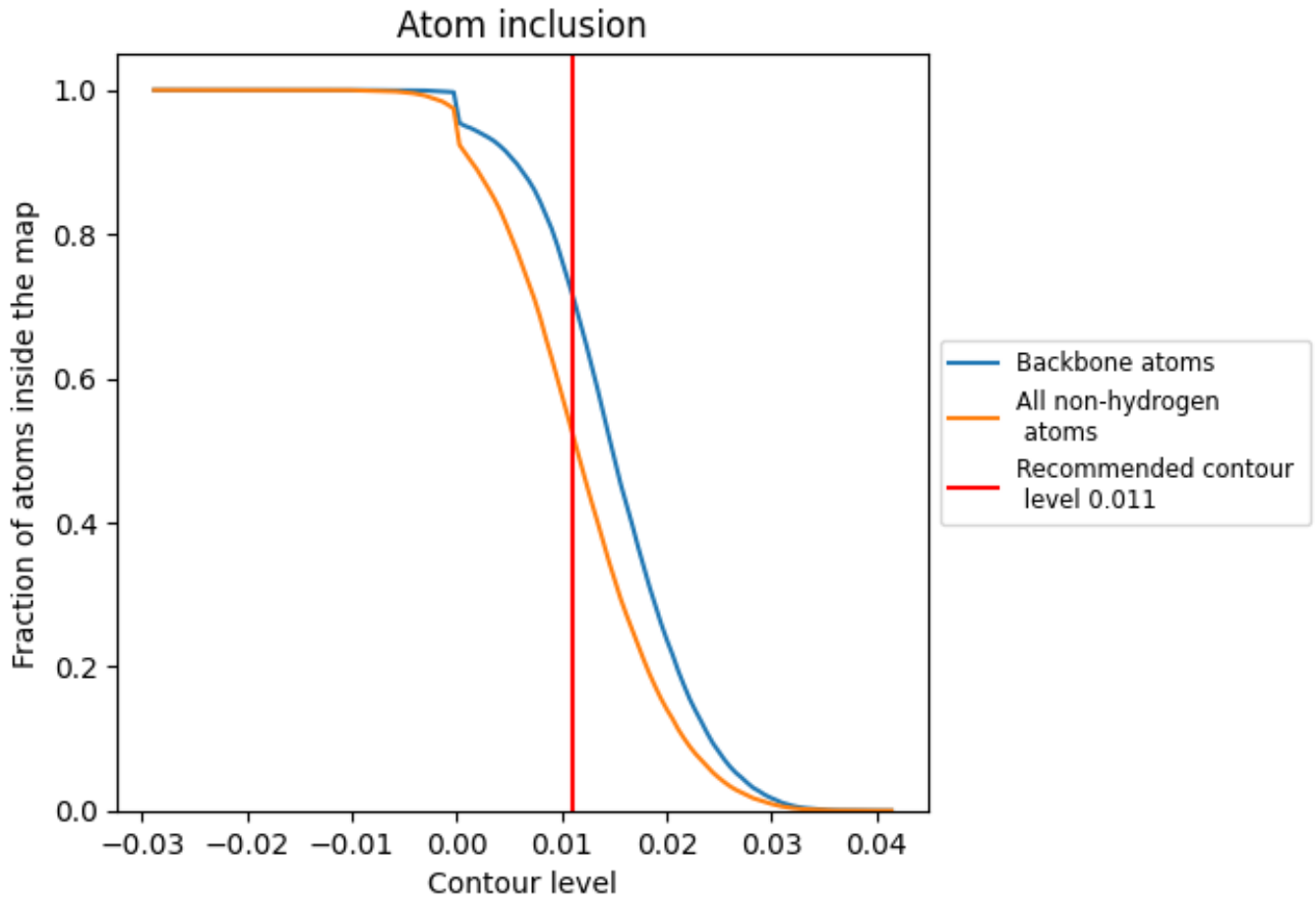
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.011).

## 9.4 Atom inclusion (i)




At the recommended contour level, 72% of all backbone atoms, 53% 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 (0.011) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.5253 | 0.1690 |
| A | 0.5760 | 0.2050 |
| B | 0.4766 | 0.1300 |
| C | 0.5201 | 0.1530 |
| D | 0.5676 | 0.2240 |
| E | 0.7647 | 0.1670 |
| F | 0.7059 | 0.1190 |
| G | 0.7059 | 0.0980 |
| H | 0.8118 | 0.1370 |
| I | 0.4258 | 0.1060 |
| J | 0.4200 | 0.1040 |