# Full wwPDB EM Validation Report

Nov 28, 2022 – 08:21 AM EST

| | | |
|---|---|---|
| PDB ID | : | 7MWF |
| EMDB ID | : | EMD-22430 |
| Title | : | HUWE1 in map with focus on interface |
| Authors | : | Hunkeler, M.; Fischer, E.S. |
| Deposited on | : | 2021-05-16 |
| Resolution | : | 3.30 Å(reported) |

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

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

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

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

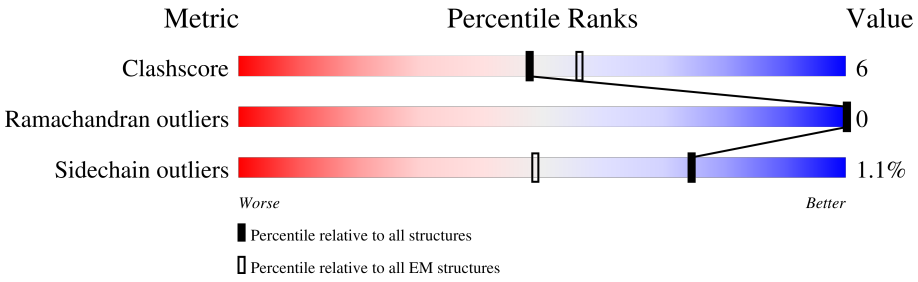
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | 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 3.30 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 | 4411 | 18% 46% 9% 45% |

# 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 38719 atoms, of which 19554 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 E3 ubiquitin-protein ligase HUWE1.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 1 | A | 2427 | 38719 | 12225 | 19554 | 3292 | 3528 | 120 | 0 | 0 |

There are 37 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | -36 | MET | - | expression tag | UNP Q7Z6Z7 |
| A | -35 | ASP | - | expression tag | UNP Q7Z6Z7 |
| A | -34 | TYR | - | expression tag | UNP Q7Z6Z7 |
| A | -33 | LYS | - | expression tag | UNP Q7Z6Z7 |
| A | -32 | ASP | - | expression tag | UNP Q7Z6Z7 |
| A | -31 | ASP | - | expression tag | UNP Q7Z6Z7 |
| A | -30 | ASP | - | expression tag | UNP Q7Z6Z7 |
| A | -29 | ASP | - | expression tag | UNP Q7Z6Z7 |
| A | -28 | LYS | - | expression tag | UNP Q7Z6Z7 |
| A | -27 | LEU | - | expression tag | UNP Q7Z6Z7 |
| A | -26 | ALA | - | expression tag | UNP Q7Z6Z7 |
| A | -25 | ALA | - | expression tag | UNP Q7Z6Z7 |
| A | -24 | ALA | - | expression tag | UNP Q7Z6Z7 |
| A | -23 | ASN | - | expression tag | UNP Q7Z6Z7 |
| A | -22 | SER | - | expression tag | UNP Q7Z6Z7 |
| A | -21 | SER | - | expression tag | UNP Q7Z6Z7 |
| A | -20 | ILE | - | expression tag | UNP Q7Z6Z7 |
| A | -19 | ASP | - | expression tag | UNP Q7Z6Z7 |
| A | -18 | LEU | - | expression tag | UNP Q7Z6Z7 |
| A | -17 | ILE | - | expression tag | UNP Q7Z6Z7 |
| A | -16 | SER | - | expression tag | UNP Q7Z6Z7 |
| A | -15 | THR | - | expression tag | UNP Q7Z6Z7 |
| A | -14 | SER | - | expression tag | UNP Q7Z6Z7 |
| A | -13 | LEU | - | expression tag | UNP Q7Z6Z7 |
| A | -12 | TYR | - | expression tag | UNP Q7Z6Z7 |
| A | -11 | LYS | - | expression tag | UNP Q7Z6Z7 |
| A | -10 | LYS | - | expression tag | UNP Q7Z6Z7 |
| A | -9 | ALA | - | expression tag | UNP Q7Z6Z7 |

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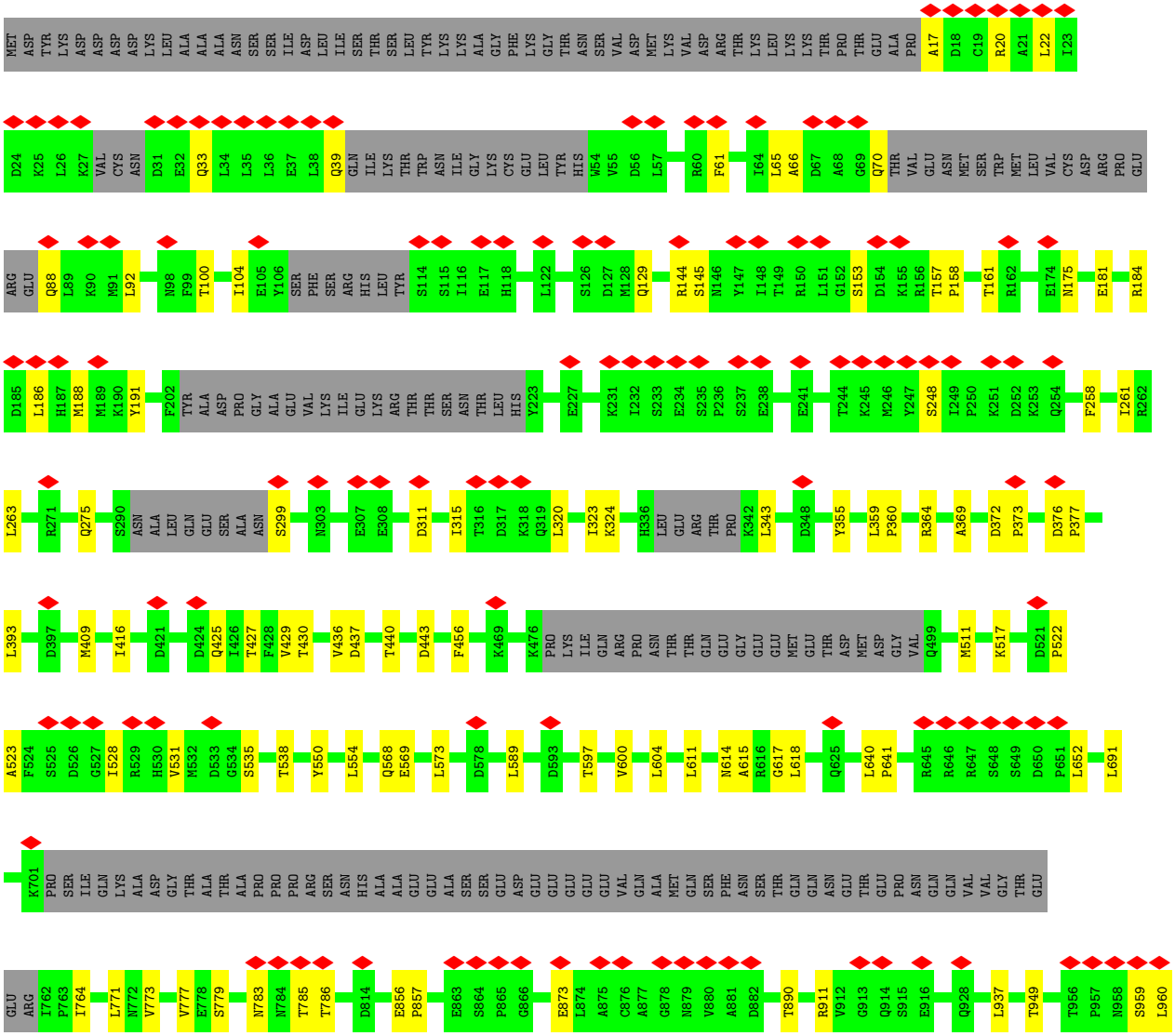
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | -8 | GLY | - | expression tag | UNP Q7Z6Z7 |
| A | -7 | PHE | - | expression tag | UNP Q7Z6Z7 |
| A | -6 | LYS | - | expression tag | UNP Q7Z6Z7 |
| A | -5 | GLY | - | expression tag | UNP Q7Z6Z7 |
| A | -4 | THR | - | expression tag | UNP Q7Z6Z7 |
| A | -3 | ASN | - | expression tag | UNP Q7Z6Z7 |
| A | -2 | SER | - | expression tag | UNP Q7Z6Z7 |
| A | -1 | VAL | - | expression tag | UNP Q7Z6Z7 |
| A | 0 | ASP | - | expression tag | UNP Q7Z6Z7 |

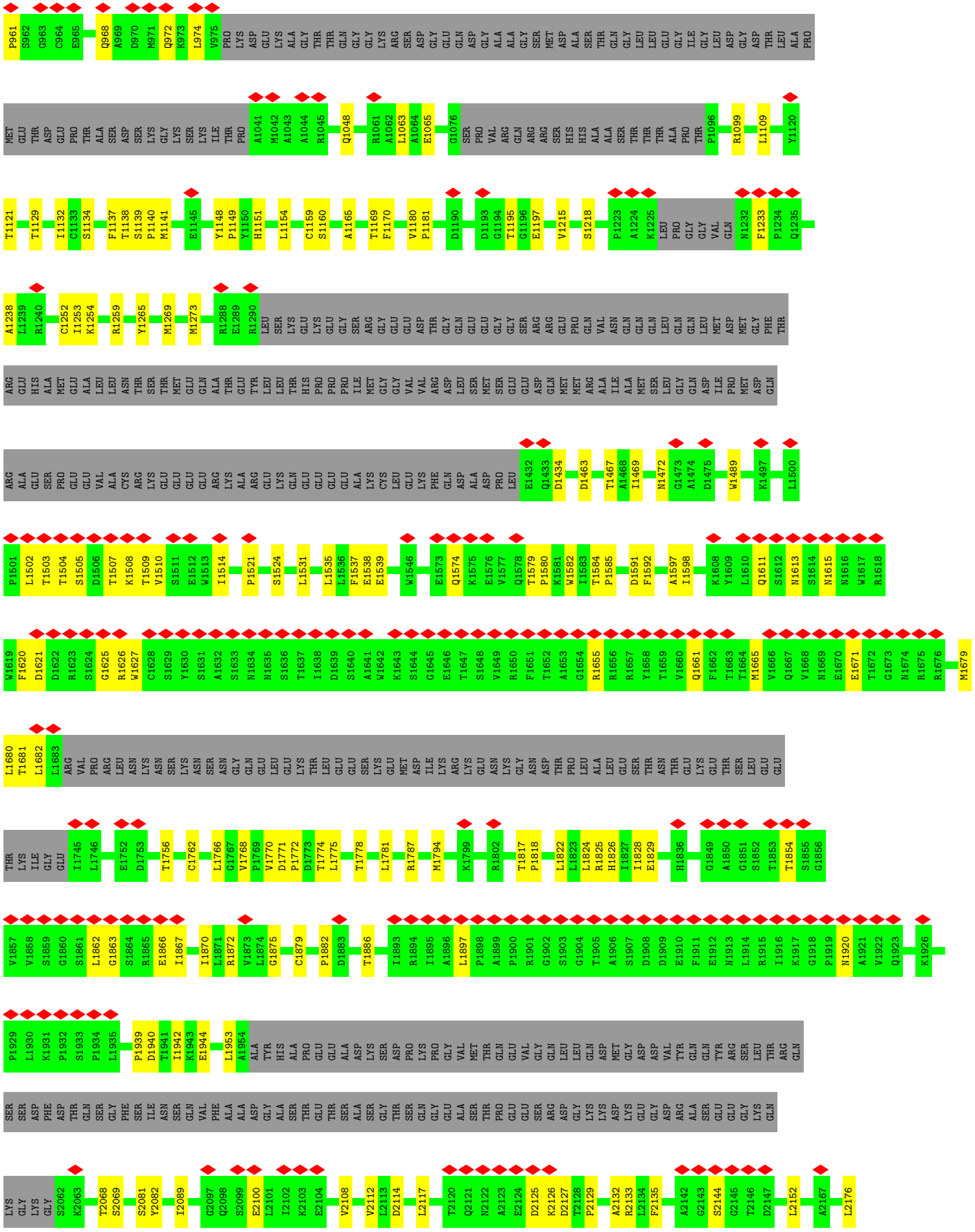
# 3 Residue-property plots (i)

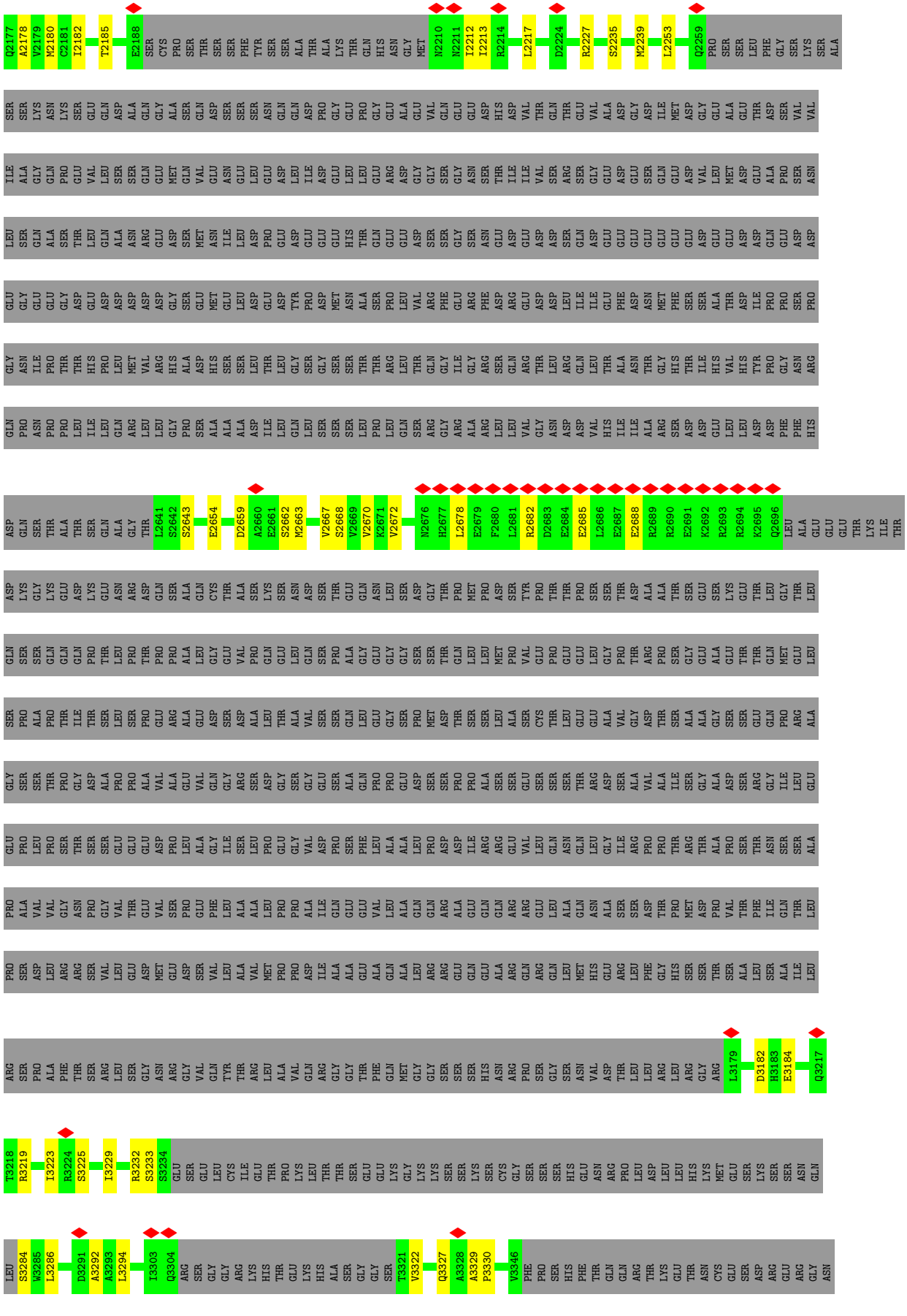
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

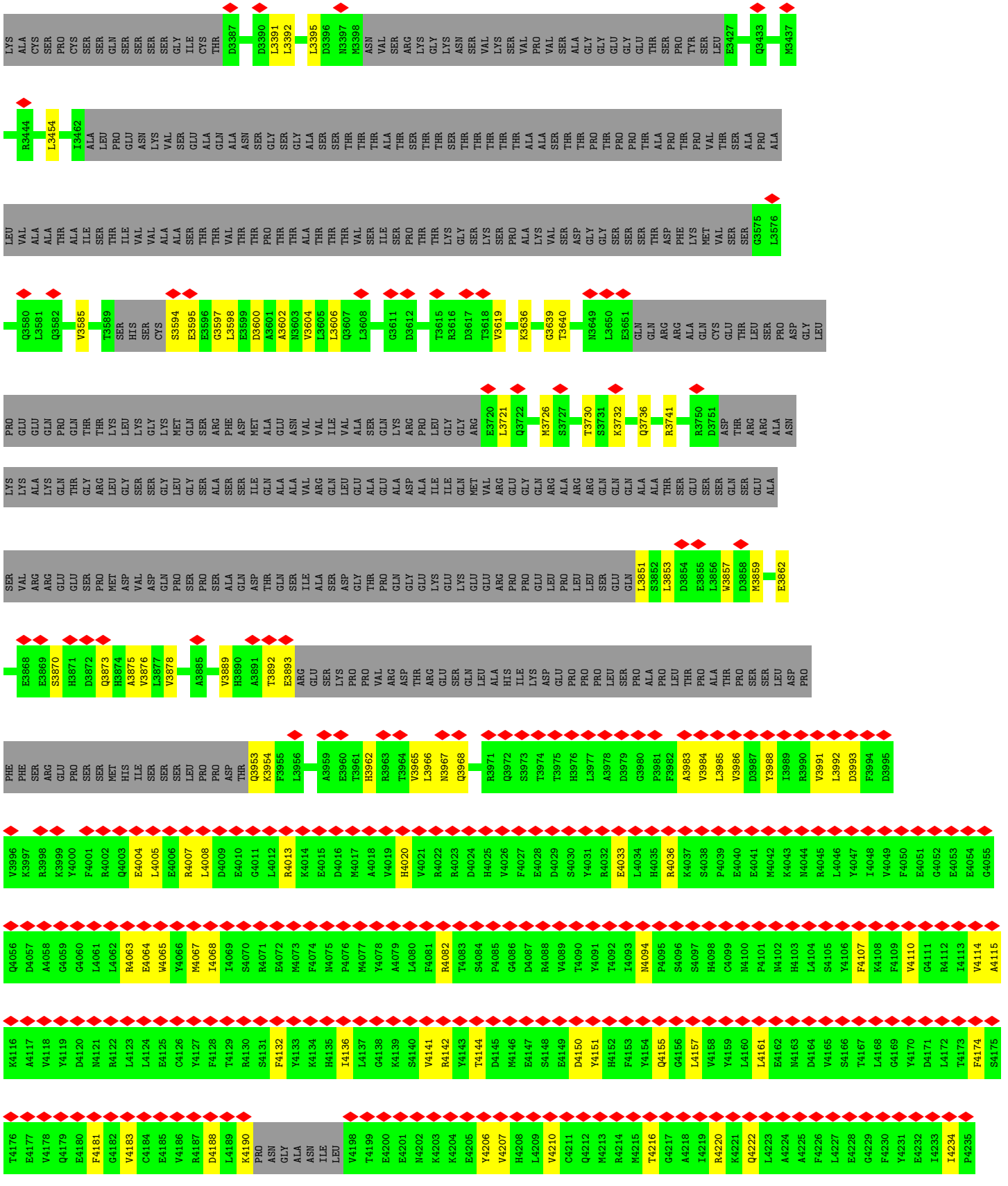
- Molecule 1: E3 ubiquitin-protein ligase HUWE1

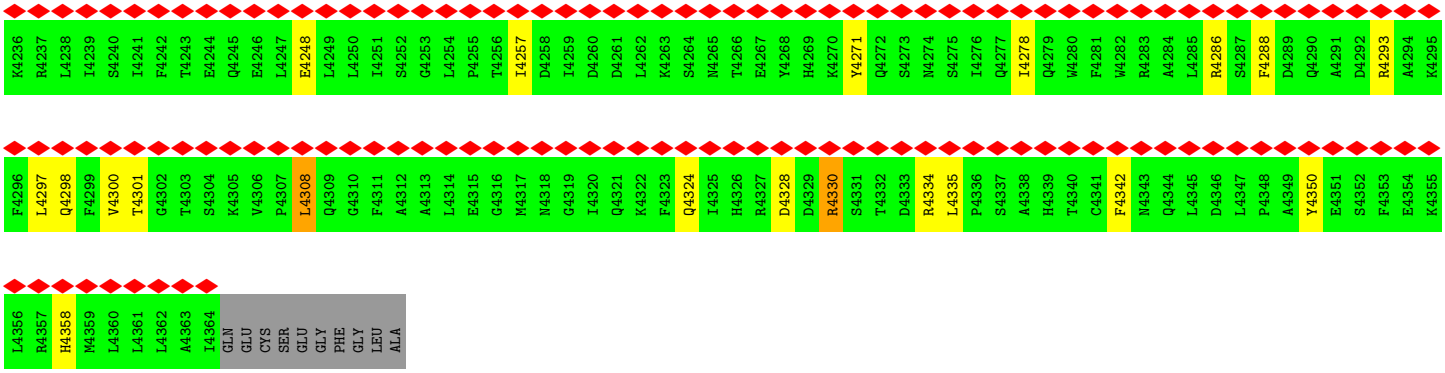
Chain A:




Q2177 A2178 V2179 M2180 C2181 I2182 T2185 E2188 N2210 N2211 I2212 I2213 R2214 L2217 D2224 R2227 S2235 M2239 L2253 Q2259
L2641 S2642 S2643 E2654 D2659 A2660 E2661 S2662 M2663 V2667 S2668 V2669 V2670 K2671 V2672 N2676 H2677 L2678 E2679 F2680 L2681 R2682 D2683 E2684 E2685 L2686 E2687 E2688 R2689 R2690 E2691 K2692 R2693 R2694 K2695 Q2696
L3179 D3182 H3183 E3184 Q3217
T3218 R3219 I3223 R3224 S3225 I3229 R3232 S3233 S3234
L3284 W3285 L3286 D3291 A3292 A3293 L3294 I3303 Q3304 T3321 V3322 Q3327 A3328 A3329 P3330 V3346




K4236 R4237 L4238 I4239 S4240 I4241 F4242 T4243 E4244 Q4245 E4246 L4247 E4248 L4249 L4250 I4251 S4252 G4253 L4254 P4255 T4256 I4257 D4258 I4259 D4260 D4261 L4262 K4263 S4264 N4265 T4266 E4267 Y4268 H4269 K4270 Y4271 Q4272 S4273 M4274 S4275 I4276 Q4277 I4278 Q4279 W4280 F4281 W4282 R4283 A4284 L4285 R4286 S4287 F4288 D4289 Q4290 A4291 D4292 R4293 A4294 K4295
F4296 L4297 Q4298 F4299 V4300 T4301 G4302 T4303 S4304 K4305 V4306 P4307 L4308 Q4309 G4310 F4311 A4312 A4313 L4314 E4315 G4316 M4317 N4318 G4319 I4320 Q4321 K4322 F4323 Q4324 I4325 H4326 R4327 D4328 D4329 R4330 S4331 T4332 D4333 R4334 L4335 P4336 S4337 A4338 H4339 T4340 C4341 F4342 N4343 Q4344 L4345 D4346 L4347 P4348 A4349 Y4350 E4351 S4352 F4353 E4354 K4355
L4356 R4357 H4358 M4359 L4360 L4361 L4362 A4363 I4364 GLN GLU CYS SER GLU GLY PHE GLY LEU ALA

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 125477 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION; standard correction in Relion | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 45.68 | Depositor |
| Minimum defocus (nm) | -800 | Depositor |
| Maximum defocus (nm) | -2500 | Depositor |
| Magnification | 105000 | Depositor |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 0.139 | Depositor |
| Minimum map value | -0.070 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.003 | Depositor |
| Recommended contour level | 0.024 | Depositor |
| Map size (Å) | 300.3, 300.3, 300.3 | wwPDB |
| Map dimensions | 364, 364, 364 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.825, 0.825, 0.825 | 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 | 0.32 | 0/19509 | 0.53 | 0/26411 |

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 | 19165 | 19554 | 19539 | 242 | 0 |
| All | All | 19165 | 19554 | 19539 | 242 | 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 6.

All (242) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2227:ARG:NH2 | 1:A:3184:GLU:OE1 | 2.12 | 0.82 |
| 1:A:568:GLN:O | 1:A:4063:ARG:NH2 | 2.18 | 0.77 |
| 1:A:1109:LEU:HD22 | 1:A:1138:THR:HG22 | 1.69 | 0.75 |
| 1:A:1825:ARG:NH1 | 1:A:2081:SER:OG | 2.20 | 0.75 |
| 1:A:1134:SER:O | 1:A:1138:THR:HG23 | 1.87 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:4248:GLU:OE1 | 1:A:4298:GLN:NE2 | 2.21 | 0.72 |
| 1:A:1510:VAL:O | 1:A:1514:ILE:HG23 | 1.91 | 0.70 |
| 1:A:4328:ASP:OD2 | 1:A:4330:ARG:NE | 2.25 | 0.70 |
| 1:A:4286:ARG:O | 1:A:4293:ARG:NH2 | 2.25 | 0.69 |
| 1:A:569:GLU:OE1 | 1:A:4063:ARG:NH1 | 2.25 | 0.68 |
| 1:A:2663:MET:O | 1:A:2667:VAL:HG23 | 1.94 | 0.68 |
| 1:A:66:ALA:O | 1:A:70:GLN:NE2 | 2.27 | 0.66 |
| 1:A:652:LEU:HB3 | 1:A:771:LEU:HD21 | 1.77 | 0.65 |
| 1:A:1826:HIS:NE2 | 1:A:2654:GLU:OE2 | 2.29 | 0.65 |
| 1:A:1579:THR:OG1 | 1:A:1770:VAL:O | 2.16 | 0.64 |
| 1:A:1507:THR:O | 1:A:1509:THR:HG23 | 1.97 | 0.63 |
| 1:A:1829:GLU:OE2 | 1:A:2082:TYR:OH | 2.15 | 0.63 |
| 1:A:4082:ARG:NH1 | 1:A:4094:ASN:OD1 | 2.31 | 0.63 |
| 1:A:2069:SER:OG | 1:A:2125:ASP:OD2 | 2.07 | 0.63 |
| 1:A:1655:ARG:HE | 1:A:1655:ARG:HA | 1.65 | 0.61 |
| 1:A:1504:THR:O | 1:A:1505:SER:OG | 2.12 | 0.61 |
| 1:A:3851:LEU:HD13 | 1:A:3851:LEU:O | 2.01 | 0.61 |
| 1:A:1671:GLU:N | 1:A:1671:GLU:OE2 | 2.34 | 0.60 |
| 1:A:4161:LEU:HD21 | 1:A:4207:VAL:HG21 | 1.84 | 0.60 |
| 1:A:1539:GLU:OE2 | 1:A:1539:GLU:N | 2.35 | 0.59 |
| 1:A:1822:LEU:O | 1:A:1826:HIS:ND1 | 2.36 | 0.59 |
| 1:A:157:THR:OG1 | 1:A:158:PRO:HD3 | 2.03 | 0.58 |
| 1:A:3292:ALA:HB1 | 1:A:3327:GLN:HB3 | 1.86 | 0.58 |
| 1:A:355:TYR:O | 1:A:364:ARG:NH2 | 2.37 | 0.57 |
| 1:A:1817:THR:OG1 | 1:A:1818:PRO:HD3 | 2.03 | 0.57 |
| 1:A:785:THR:HG22 | 1:A:785:THR:O | 2.03 | 0.57 |
| 1:A:4324:GLN:NE2 | 1:A:4342:PHE:O | 2.37 | 0.57 |
| 1:A:1165:ALA:O | 1:A:1169:THR:HG23 | 2.06 | 0.56 |
| 1:A:1897:LEU:HD21 | 1:A:2682:ARG:HG2 | 1.87 | 0.55 |
| 1:A:100:THR:HG22 | 1:A:104:ILE:HD13 | 1.89 | 0.55 |
| 1:A:3639:GLY:N | 1:A:3859:MET:HE1 | 2.21 | 0.55 |
| 1:A:4174:PHE:CD2 | 1:A:4190:LYS:HG2 | 2.42 | 0.54 |
| 1:A:425:GLN:O | 1:A:429:VAL:HG23 | 2.07 | 0.54 |
| 1:A:4115:ALA:HB1 | 1:A:4234:ILE:HG12 | 1.90 | 0.54 |
| 1:A:3721:LEU:HD12 | 1:A:3875:ALA:HB1 | 1.89 | 0.54 |
| 1:A:786:THR:HG22 | 1:A:786:THR:O | 2.07 | 0.53 |
| 1:A:1510:VAL:HG12 | 1:A:1574:GLN:OE1 | 2.08 | 0.53 |
| 1:A:3726:MET:O | 1:A:3730:THR:HG23 | 2.08 | 0.53 |
| 1:A:175:ASN:ND2 | 1:A:3327:GLN:OE1 | 2.43 | 0.52 |
| 1:A:1132:ILE:HD12 | 1:A:1197:GLU:HG2 | 1.92 | 0.52 |
| 1:A:1762:CYS:SG | 1:A:1778:THR:OG1 | 2.67 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3873:GLN:OE1 | 1:A:3968:GLN:NE2 | 2.33 | 0.51 |
| 1:A:181:GLU:OE1 | 1:A:184:ARG:NH2 | 2.37 | 0.51 |
| 1:A:263:LEU:CD2 | 1:A:3294:LEU:HD21 | 2.41 | 0.51 |
| 1:A:1655:ARG:HA | 1:A:1655:ARG:NE | 2.25 | 0.51 |
| 1:A:1766:LEU:HD23 | 1:A:1775:LEU:HD22 | 1.92 | 0.50 |
| 1:A:4300:VAL:HG23 | 1:A:4301:THR:HG23 | 1.93 | 0.50 |
| 1:A:1626:ARG:NH1 | 1:A:1920:ASN:OD1 | 2.44 | 0.50 |
| 1:A:550:TYR:HB3 | 1:A:554:LEU:HD23 | 1.94 | 0.50 |
| 1:A:1151:HIS:NE2 | 1:A:1218:SER:OG | 2.45 | 0.50 |
| 1:A:2117:LEU:HG | 1:A:2178:ALA:HB1 | 1.93 | 0.50 |
| 1:A:1768:VAL:HG23 | 1:A:1768:VAL:O | 2.11 | 0.50 |
| 1:A:359:LEU:HB3 | 1:A:360:PRO:HD3 | 1.93 | 0.50 |
| 1:A:2126:LYS:HG3 | 1:A:2127:ASP:OD1 | 2.12 | 0.50 |
| 1:A:22:LEU:HD22 | 1:A:39:GLN:NE2 | 2.27 | 0.50 |
| 1:A:522:PRO:O | 1:A:523:ALA:HB3 | 2.12 | 0.50 |
| 1:A:372:ASP:OD1 | 1:A:373:PRO:HD2 | 2.13 | 0.49 |
| 1:A:1882:PRO:O | 1:A:1886:THR:HG23 | 2.13 | 0.49 |
| 1:A:184:ARG:O | 1:A:186:LEU:HD23 | 2.12 | 0.49 |
| 1:A:1597:ALA:O | 1:A:1598:ILE:C | 2.50 | 0.49 |
| 1:A:2100:GLU:OE1 | 1:A:2100:GLU:N | 2.43 | 0.49 |
| 1:A:611:LEU:O | 1:A:617:GLY:HA3 | 2.13 | 0.49 |
| 1:A:1584:THR:HG22 | 1:A:1774:THR:HA | 1.95 | 0.49 |
| 1:A:1771:ASP:OD1 | 1:A:1772:PRO:HD2 | 2.13 | 0.48 |
| 1:A:3233:SER:OG | 1:A:3329:ALA:HB1 | 2.13 | 0.48 |
| 1:A:1770:VAL:HG23 | 1:A:1771:ASP:H | 1.77 | 0.48 |
| 1:A:3985:LEU:HD11 | 1:A:3992:LEU:HD21 | 1.95 | 0.48 |
| 1:A:1615:ASN:HB3 | 1:A:1680:LEU:HD21 | 1.95 | 0.48 |
| 1:A:1661:GLN:O | 1:A:1665:MET:N | 2.46 | 0.48 |
| 1:A:4150:ASP:OD2 | 1:A:4150:ASP:N | 2.47 | 0.48 |
| 1:A:1265:TYR:O | 1:A:1269:MET:SD | 2.72 | 0.48 |
| 1:A:1862:LEU:O | 1:A:1866:GLU:OE2 | 2.32 | 0.48 |
| 1:A:2176:LEU:O | 1:A:2180:MET:HG2 | 2.14 | 0.47 |
| 1:A:437:ASP:OD1 | 1:A:517:LYS:HE2 | 2.14 | 0.47 |
| 1:A:61:PHE:O | 1:A:65:LEU:HG | 2.14 | 0.47 |
| 1:A:1775:LEU:HA | 1:A:1778:THR:HG22 | 1.96 | 0.47 |
| 1:A:4330:ARG:HD3 | 1:A:4330:ARG:N | 2.30 | 0.47 |
| 1:A:911:ARG:NH2 | 1:A:1065:GLU:OE1 | 2.47 | 0.47 |
| 1:A:1502:LEU:HD13 | 1:A:1507:THR:CG2 | 2.44 | 0.47 |
| 1:A:1897:LEU:HD12 | 1:A:2685:GLU:OE2 | 2.13 | 0.47 |
| 1:A:416:ILE:O | 1:A:416:ILE:HG22 | 2.14 | 0.47 |
| 1:A:1170:PHE:CE1 | 1:A:1252:CYS:HB3 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3983:ALA:O | 1:A:3986:VAL:HG13 | 2.14 | 0.47 |
| 1:A:4288:PHE:O | 1:A:4293:ARG:NE | 2.47 | 0.46 |
| 1:A:3286:LEU:HD11 | 1:A:3392:LEU:CD1 | 2.45 | 0.46 |
| 1:A:4142:ARG:HG2 | 1:A:4142:ARG:HH11 | 1.79 | 0.46 |
| 1:A:129:GLN:NE2 | 1:A:275:GLN:OE1 | 2.47 | 0.46 |
| 1:A:1591:ASP:OD1 | 1:A:1781:LEU:HA | 2.15 | 0.46 |
| 1:A:4216:THR:O | 1:A:4220:ARG:N | 2.49 | 0.46 |
| 1:A:1875:GLY:HA2 | 1:A:2667:VAL:HG22 | 1.97 | 0.46 |
| 1:A:573:LEU:HD23 | 1:A:614:ASN:HB2 | 1.98 | 0.46 |
| 1:A:2212:ILE:HG13 | 1:A:2213:ILE:N | 2.30 | 0.46 |
| 1:A:4005:LEU:O | 1:A:4008:LEU:HG | 2.16 | 0.46 |
| 1:A:4271:TYR:CG | 1:A:4278:ILE:HD11 | 2.51 | 0.46 |
| 1:A:258:PHE:HA | 1:A:261:ILE:HG22 | 1.97 | 0.46 |
| 1:A:1159:CYS:SG | 1:A:1160:SER:N | 2.89 | 0.46 |
| 1:A:1866:GLU:OE2 | 1:A:1866:GLU:N | 2.48 | 0.46 |
| 1:A:1940:ASP:O | 1:A:1944:GLU:HG3 | 2.16 | 0.46 |
| 1:A:3594:SER:O | 1:A:3597:GLY:N | 2.49 | 0.46 |
| 1:A:856:GLU:N | 1:A:857:PRO:HD2 | 2.31 | 0.45 |
| 1:A:1254:LYS:O | 1:A:1259:ARG:NH1 | 2.50 | 0.45 |
| 1:A:535:SER:O | 1:A:538:THR:OG1 | 2.24 | 0.45 |
| 1:A:960:LEU:N | 1:A:961:PRO:HD2 | 2.31 | 0.45 |
| 1:A:1886:THR:HG22 | 1:A:2670:VAL:HG13 | 1.97 | 0.45 |
| 1:A:3219:ARG:HG2 | 1:A:3223:ILE:HD12 | 1.98 | 0.45 |
| 1:A:3967:ASN:OD1 | 1:A:3993:ASP:N | 2.43 | 0.45 |
| 1:A:3636:LYS:O | 1:A:3640:THR:HG23 | 2.16 | 0.45 |
| 1:A:4132:PHE:CE2 | 1:A:4136:ILE:HD11 | 2.52 | 0.45 |
| 1:A:1253:ILE:HG23 | 1:A:1273:MET:HG3 | 1.98 | 0.45 |
| 1:A:181:GLU:O | 1:A:191:TYR:OH | 2.21 | 0.45 |
| 1:A:937:LEU:HD22 | 1:A:1063:LEU:HD21 | 1.99 | 0.45 |
| 1:A:972:GLN:HA | 1:A:972:GLN:OE1 | 2.17 | 0.45 |
| 1:A:4141:VAL:HG22 | 1:A:4142:ARG:N | 2.32 | 0.45 |
| 1:A:1879:CYS:SG | 1:A:2663:MET:HA | 2.57 | 0.45 |
| 1:A:1939:PRO:HD2 | 1:A:1942:ILE:HD12 | 1.99 | 0.45 |
| 1:A:144:ARG:HD2 | 1:A:145:SER:HB2 | 1.98 | 0.45 |
| 1:A:188:MET:HA | 1:A:188:MET:HE3 | 1.99 | 0.45 |
| 1:A:974:LEU:HD11 | 1:A:1048:GLN:HB2 | 1.99 | 0.45 |
| 1:A:968:GLN:O | 1:A:972:GLN:HG2 | 2.17 | 0.45 |
| 1:A:3736:GLN:NE2 | 1:A:3878:VAL:O | 2.37 | 0.45 |
| 1:A:3853:LEU:O | 1:A:3857:TRP:CD1 | 2.70 | 0.45 |
| 1:A:4064:GLU:OE1 | 1:A:4067:MET:HE3 | 2.17 | 0.45 |
| 1:A:4174:PHE:CZ | 1:A:4206:TYR:HB2 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2117:LEU:O | 1:A:2129:PRO:HB3 | 2.18 | 0.44 |
| 1:A:2152:LEU:HD13 | 1:A:2152:LEU:C | 2.37 | 0.44 |
| 1:A:88:GLN:O | 1:A:92:LEU:HD13 | 2.18 | 0.44 |
| 1:A:311:ASP:O | 1:A:315:ILE:HG12 | 2.17 | 0.44 |
| 1:A:3602:ALA:O | 1:A:3606:LEU:HG | 2.16 | 0.44 |
| 1:A:2659:ASP:OD1 | 1:A:2659:ASP:N | 2.51 | 0.44 |
| 1:A:456:PHE:CD1 | 1:A:511:MET:HG3 | 2.52 | 0.44 |
| 1:A:1137:PHE:CZ | 1:A:1141:MET:SD | 3.10 | 0.44 |
| 1:A:1180:VAL:HG12 | 1:A:1181:PRO:O | 2.17 | 0.44 |
| 1:A:1132:ILE:CD1 | 1:A:1197:GLU:HG2 | 2.47 | 0.44 |
| 1:A:1215:VAL:HG12 | 1:A:1238:ALA:HB1 | 2.00 | 0.44 |
| 1:A:1621:ASP:O | 1:A:1625:GLY:N | 2.50 | 0.44 |
| 1:A:4308:LEU:HD12 | 1:A:4308:LEU:H | 1.83 | 0.44 |
| 1:A:3966:LEU:HD21 | 1:A:3985:LEU:HD21 | 1.98 | 0.44 |
| 1:A:1620:PHE:HZ | 1:A:1863:GLY:HA2 | 1.84 | 0.43 |
| 1:A:33:GLN:OE1 | 1:A:92:LEU:HD11 | 2.18 | 0.43 |
| 1:A:2108:VAL:O | 1:A:2112:VAL:HG23 | 2.18 | 0.43 |
| 1:A:3454:LEU:HD11 | 1:A:3585:VAL:HG11 | 1.99 | 0.43 |
| 1:A:1826:HIS:CE1 | 1:A:2654:GLU:OE2 | 2.72 | 0.43 |
| 1:A:2668:SER:O | 1:A:2672:VAL:HG23 | 2.19 | 0.43 |
| 1:A:1469:ILE:O | 1:A:1472:ASN:O | 2.37 | 0.43 |
| 1:A:1521:PRO:O | 1:A:1524:SER:OG | 2.25 | 0.43 |
| 1:A:4142:ARG:NE | 1:A:4144:THR:OG1 | 2.52 | 0.43 |
| 1:A:1867:ILE:CD1 | 1:A:2678:LEU:HD12 | 2.48 | 0.43 |
| 1:A:440:THR:HA | 1:A:443:ASP:O | 2.19 | 0.42 |
| 1:A:1682:LEU:HD12 | 1:A:1682:LEU:N | 2.33 | 0.42 |
| 1:A:3225:SER:O | 1:A:3229:ILE:HG13 | 2.19 | 0.42 |
| 1:A:3851:LEU:HD12 | 1:A:3889:VAL:HG21 | 1.99 | 0.42 |
| 1:A:691:LEU:HD13 | 1:A:764:ILE:HD11 | 2.00 | 0.42 |
| 1:A:1770:VAL:HG23 | 1:A:1774:THR:HB | 2.01 | 0.42 |
| 1:A:2688:GLU:OE2 | 1:A:2688:GLU:HA | 2.19 | 0.42 |
| 1:A:3876:VAL:HG21 | 1:A:3965:VAL:CG1 | 2.49 | 0.42 |
| 1:A:409:MET:SD | 1:A:436:VAL:HG13 | 2.59 | 0.42 |
| 1:A:427:THR:O | 1:A:430:THR:HG22 | 2.20 | 0.42 |
| 1:A:1195:THR:HG22 | 1:A:1195:THR:O | 2.18 | 0.42 |
| 1:A:3598:LEU:HD13 | 1:A:3741:ARG:HD2 | 2.01 | 0.42 |
| 1:A:3600:ASP:O | 1:A:3604:VAL:HG23 | 2.19 | 0.42 |
| 1:A:3988:TYR:O | 1:A:3991:VAL:HG22 | 2.18 | 0.42 |
| 1:A:4151:TYR:O | 1:A:4155:GLN:HG3 | 2.20 | 0.42 |
| 1:A:528:ILE:HD12 | 1:A:531:VAL:HG21 | 2.01 | 0.42 |
| 1:A:1584:THR:OG1 | 1:A:1585:PRO:HD3 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1508:LYS:O | 1:A:1509:THR:OG1 | 2.27 | 0.42 |
| 1:A:1824:LEU:O | 1:A:1828:ILE:HG12 | 2.18 | 0.42 |
| 1:A:1828:ILE:HD13 | 1:A:1942:ILE:HG23 | 2.01 | 0.42 |
| 1:A:3953:GLN:HG2 | 1:A:3954:LYS:H | 1.85 | 0.42 |
| 1:A:773:VAL:O | 1:A:777:VAL:HG23 | 2.19 | 0.42 |
| 1:A:1611:GLN:HE21 | 1:A:1613:ASN:H | 1.68 | 0.42 |
| 1:A:1627:TRP:CZ3 | 1:A:1679:MET:HB3 | 2.55 | 0.42 |
| 1:A:3876:VAL:HG21 | 1:A:3965:VAL:HG13 | 2.01 | 0.42 |
| 1:A:528:ILE:HD12 | 1:A:531:VAL:CG2 | 2.50 | 0.42 |
| 1:A:3391:LEU:O | 1:A:3395:LEU:HG | 2.20 | 0.42 |
| 1:A:3962:HIS:O | 1:A:3965:VAL:N | 2.52 | 0.42 |
| 1:A:1139:SER:HB3 | 1:A:1140:PRO:HD3 | 2.02 | 0.42 |
| 1:A:1854:THR:HG21 | 1:A:1872:ARG:HH12 | 1.85 | 0.42 |
| 1:A:1953:LEU:HA | 1:A:2068:THR:HG22 | 2.02 | 0.42 |
| 1:A:4110:VAL:O | 1:A:4114:VAL:HG23 | 2.20 | 0.42 |
| 1:A:248:SER:O | 1:A:248:SER:OG | 2.36 | 0.41 |
| 1:A:376:ASP:HA | 1:A:377:PRO:HD3 | 1.87 | 0.41 |
| 1:A:1680:LEU:HD23 | 1:A:1681:THR:N | 2.35 | 0.41 |
| 1:A:4065:TRP:O | 1:A:4068:ILE:HG13 | 2.20 | 0.41 |
| 1:A:2133:ARG:HG3 | 1:A:2182:ILE:HD12 | 2.03 | 0.41 |
| 1:A:4188:ASP:OD2 | 1:A:4188:ASP:N | 2.52 | 0.41 |
| 1:A:369:ALA:HB1 | 1:A:376:ASP:O | 2.20 | 0.41 |
| 1:A:589:LEU:HD22 | 1:A:604:LEU:CD2 | 2.50 | 0.41 |
| 1:A:1756:THR:HG22 | 1:A:1794:MET:CE | 2.50 | 0.41 |
| 1:A:4020:HIS:O | 1:A:4033:GLU:OE1 | 2.38 | 0.41 |
| 1:A:153:SER:O | 1:A:153:SER:OG | 2.38 | 0.41 |
| 1:A:614:ASN:O | 1:A:615:ALA:HB3 | 2.21 | 0.41 |
| 1:A:779:SER:O | 1:A:783:ASN:HB2 | 2.21 | 0.41 |
| 1:A:949:THR:HG21 | 1:A:1129:THR:HG23 | 2.02 | 0.41 |
| 1:A:2112:VAL:CG1 | 1:A:2132:ALA:HB1 | 2.50 | 0.41 |
| 1:A:4206:TYR:O | 1:A:4210:VAL:HG12 | 2.21 | 0.41 |
| 1:A:1538:GLU:HA | 1:A:1592:PHE:CZ | 2.56 | 0.41 |
| 1:A:1611:GLN:O | 1:A:1615:ASN:ND2 | 2.54 | 0.41 |
| 1:A:1463:ASP:O | 1:A:1467:THR:HG23 | 2.21 | 0.41 |
| 1:A:1787:ARG:HD3 | 1:A:2654:GLU:OE2 | 2.20 | 0.41 |
| 1:A:640:LEU:N | 1:A:641:PRO:HD2 | 2.36 | 0.41 |
| 1:A:1148:TYR:CD1 | 1:A:1218:SER:HA | 2.56 | 0.41 |
| 1:A:320:LEU:O | 1:A:323:ILE:N | 2.53 | 0.41 |
| 1:A:1535:LEU:O | 1:A:1539:GLU:OE2 | 2.39 | 0.41 |
| 1:A:2089:ILE:HG21 | 1:A:2135:PHE:HZ | 1.86 | 0.41 |
| 1:A:3232:ARG:NH1 | 1:A:3322:VAL:O | 2.46 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3329:ALA:HB3 | 1:A:3330:PRO:HD3 | 2.03 | 0.41 |
| 1:A:315:ILE:O | 1:A:324:LYS:NZ | 2.47 | 0.41 |
| 1:A:618:LEU:HD23 | 1:A:618:LEU:O | 2.20 | 0.41 |
| 1:A:1580:PRO:HB3 | 1:A:1582:TRP:NE1 | 2.36 | 0.41 |
| 1:A:1770:VAL:HG23 | 1:A:1771:ASP:N | 2.36 | 0.41 |
| 1:A:4157:LEU:O | 1:A:4161:LEU:HG | 2.21 | 0.41 |
| 1:A:4330:ARG:HD3 | 1:A:4330:ARG:H | 1.85 | 0.41 |
| 1:A:4334:ARG:O | 1:A:4350:TYR:OH | 2.31 | 0.41 |
| 1:A:343:LEU:HD11 | 1:A:393:LEU:HD12 | 2.03 | 0.41 |
| 1:A:873:GLU:OE2 | 1:A:890:THR:HA | 2.21 | 0.41 |
| 1:A:2217:LEU:HD21 | 1:A:2253:LEU:HD21 | 2.03 | 0.41 |
| 1:A:4004:GLU:OE1 | 1:A:4007:ARG:NE | 2.53 | 0.41 |
| 1:A:4334:ARG:HD3 | 1:A:4335:LEU:O | 2.21 | 0.41 |
| 1:A:1434:ASP:N | 1:A:1434:ASP:OD2 | 2.54 | 0.40 |
| 1:A:4181:PHE:N | 1:A:4181:PHE:CD1 | 2.87 | 0.40 |
| 1:A:974:LEU:C | 1:A:974:LEU:HD13 | 2.42 | 0.40 |
| 1:A:3892:THR:O | 1:A:3893:GLU:C | 2.60 | 0.40 |
| 1:A:4257:ILE:HD11 | 1:A:4297:LEU:HD22 | 2.03 | 0.40 |
| 1:A:17:ALA:O | 1:A:20:ARG:N | 2.54 | 0.40 |
| 1:A:1149:PRO:CB | 1:A:1154:LEU:HD11 | 2.52 | 0.40 |
| 1:A:3182:ASP:OD1 | 1:A:3182:ASP:N | 2.49 | 0.40 |
| 1:A:3595:GLU:HA | 1:A:3598:LEU:HG | 2.03 | 0.40 |
| 1:A:597:THR:CG2 | 1:A:600:VAL:HG23 | 2.52 | 0.40 |
| 1:A:974:LEU:HD11 | 1:A:1048:GLN:HG3 | 2.03 | 0.40 |
| 1:A:1099:ARG:HH22 | 1:A:1233:PHE:HB3 | 1.86 | 0.40 |
| 1:A:1503:THR:HG23 | 1:A:1504:THR:HG23 | 2.03 | 0.40 |
| 1:A:4107:PHE:CE1 | 1:A:4222:GLN:HG2 | 2.56 | 0.40 |
| 1:A:4107:PHE:HA | 1:A:4110:VAL:HG12 | 2.02 | 0.40 |
| 1:A:157:THR:O | 1:A:161:THR:HG23 | 2.22 | 0.40 |
| 1:A:1531:LEU:HD23 | 1:A:1531:LEU:O | 2.21 | 0.40 |
| 1:A:3859:MET:HA | 1:A:3862:GLU:HG2 | 2.02 | 0.40 |
| 1:A:4207:VAL:HA | 1:A:4210:VAL:HG12 | 2.03 | 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 | 2369/4411 (54%) | 2310 (98%) | 59 (2%) | 0 | 100 100 |

There are no Ramachandran outliers to report.

### 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 | 2149/3839 (56%) | 2125 (99%) | 24 (1%) | 73 85 |

All (24) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 299 | SER |
| 1 | A | 959 | SER |
| 1 | A | 1121 | THR |
| 1 | A | 1489 | TRP |
| 1 | A | 1537 | PHE |
| 1 | A | 1870 | ILE |
| 1 | A | 2114 | ASP |
| 1 | A | 2144 | SER |
| 1 | A | 2185 | THR |
| 1 | A | 2235 | SER |
| 1 | A | 2239 | MET |
| 1 | A | 2643 | SER |
| 1 | A | 2662 | SER |
| 1 | A | 3284 | SER |
| 1 | A | 3619 | VAL |
| 1 | A | 3732 | LYS |
| 1 | A | 3870 | SER |
| 1 | A | 3984 | VAL |
| 1 | A | 4013 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 4036 | ARG |
| 1 | A | 4183 | VAL |
| 1 | A | 4308 | LEU |
| 1 | A | 4330 | ARG |
| 1 | A | 4358 | HIS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 118 | HIS |
| 1 | A | 1258 | ASN |
| 1 | A | 1569 | GLN |
| 1 | A | 1611 | GLN |
| 1 | A | 4269 | HIS |

#### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates

There are no monosaccharides in this entry.

### 5.6 Ligand geometry

There are no ligands in this entry.

### 5.7 Other polymers

There are no such residues in this entry.

### 5.8 Polymer linkage issues

There are no chain breaks in this entry.

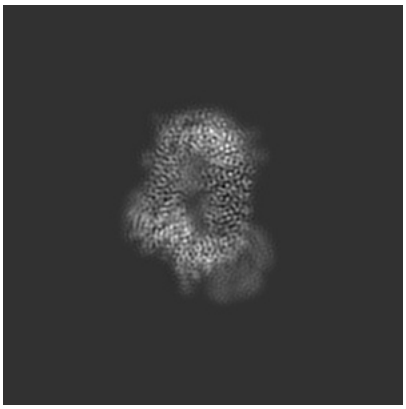
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22430. These allow visual inspection of the internal detail of the map and identification of artifacts.

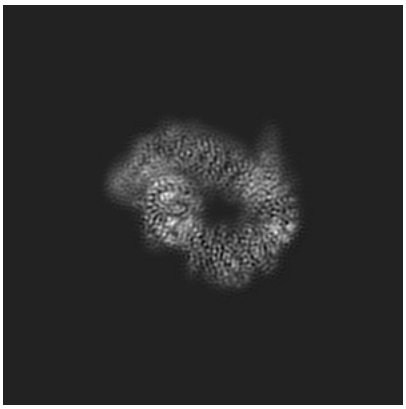
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

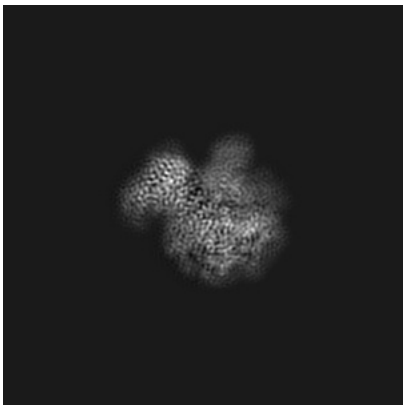
### 6.1.1 Primary map



X

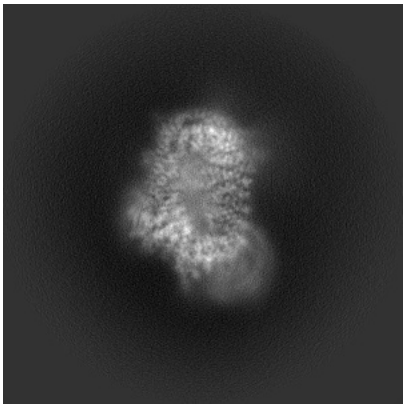


Y

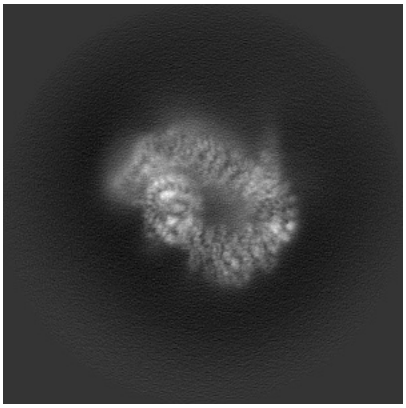


Z

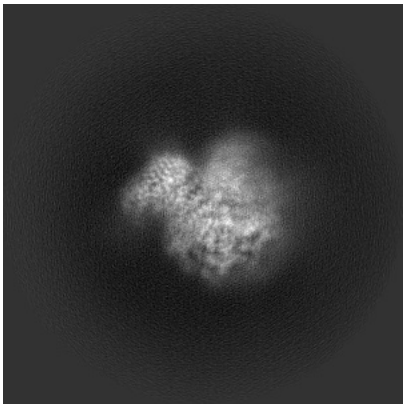
### 6.1.2 Raw map



X



Y

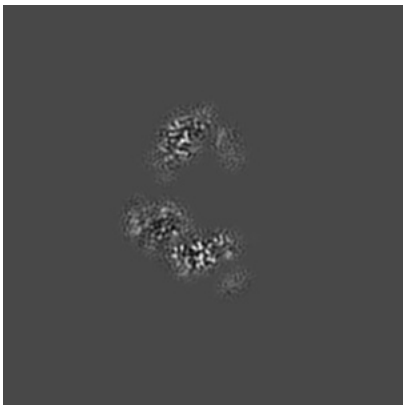


Z

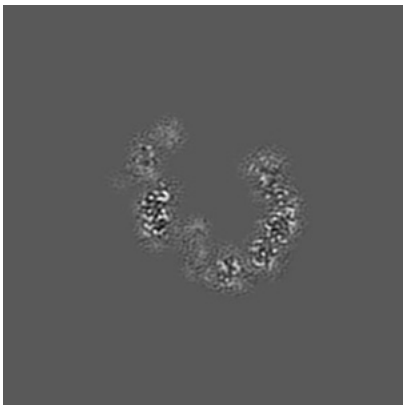
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

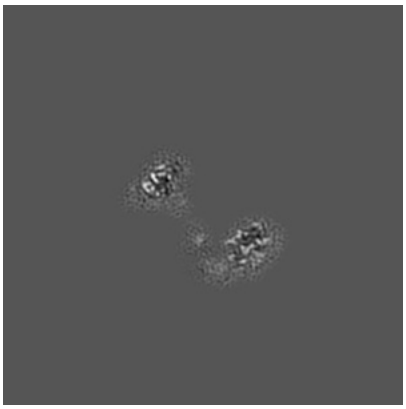
### 6.2.1 Primary map



X Index: 182

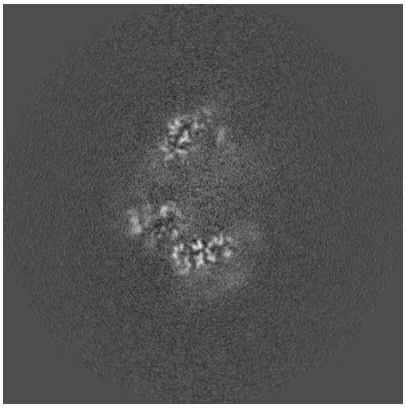


Y Index: 182

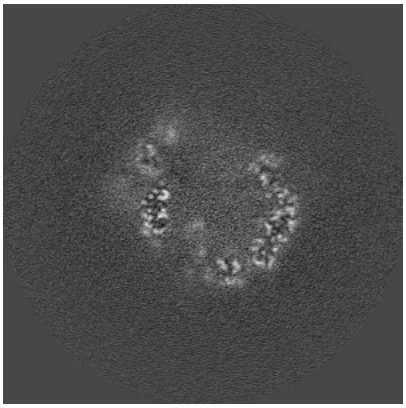


Z Index: 182

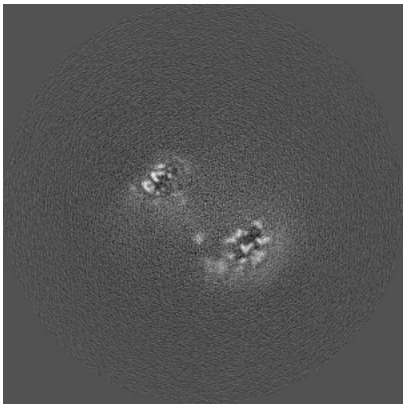
### 6.2.2 Raw map



X Index: 182



Y Index: 182

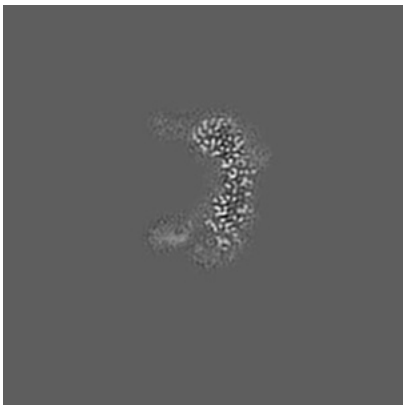


Z Index: 182

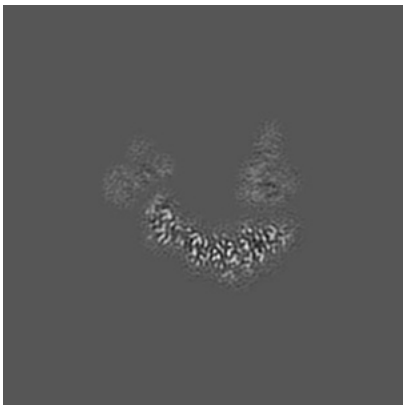
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

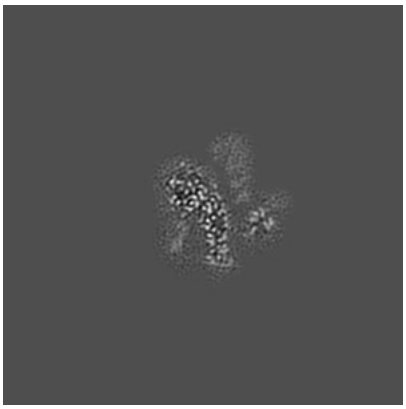
### 6.3.1 Primary map



X Index: 149

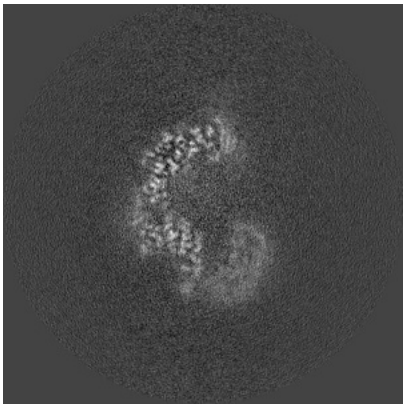


Y Index: 202

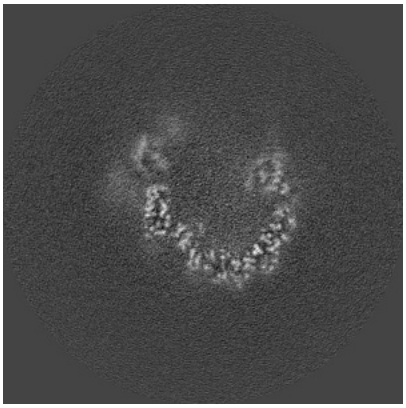


Z Index: 145

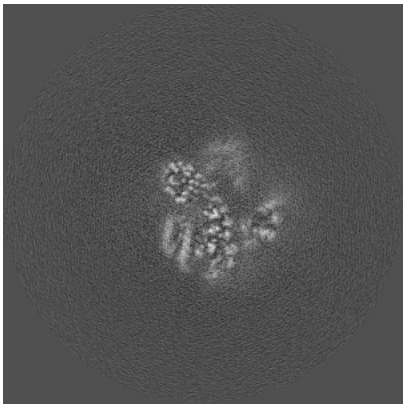
### 6.3.2 Raw map



X Index: 203



Y Index: 189



Z Index: 152

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

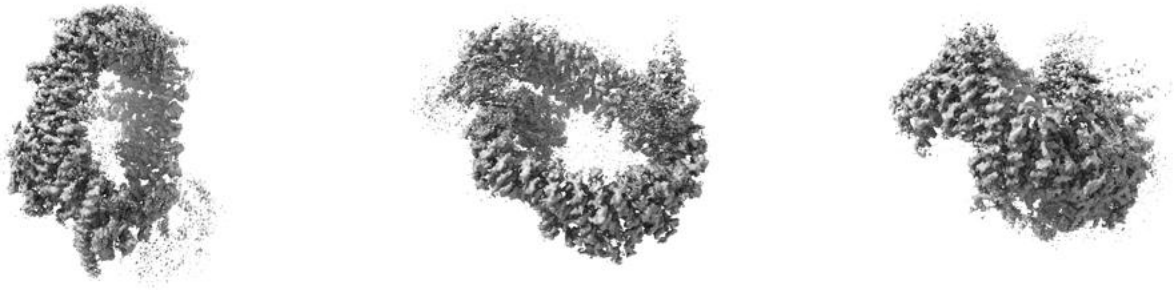
## 6.4 Orthogonal surface views (i)

### 6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.024. 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.

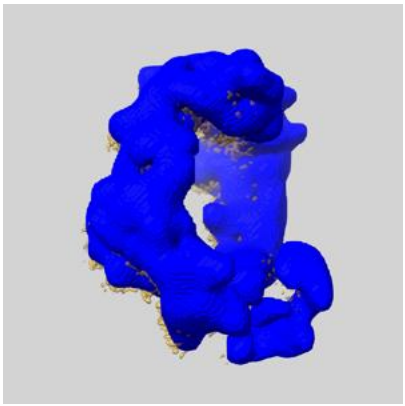
## 6.5 Mask visualisation (i)

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

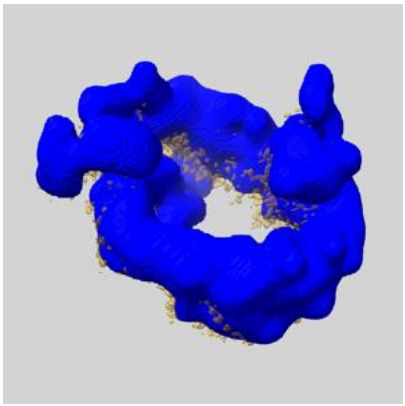
A mask typically either:

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

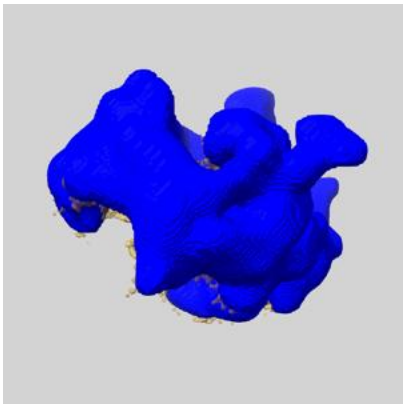
### 6.5.1 emd_22430_msk_1.map (i)



X



Y

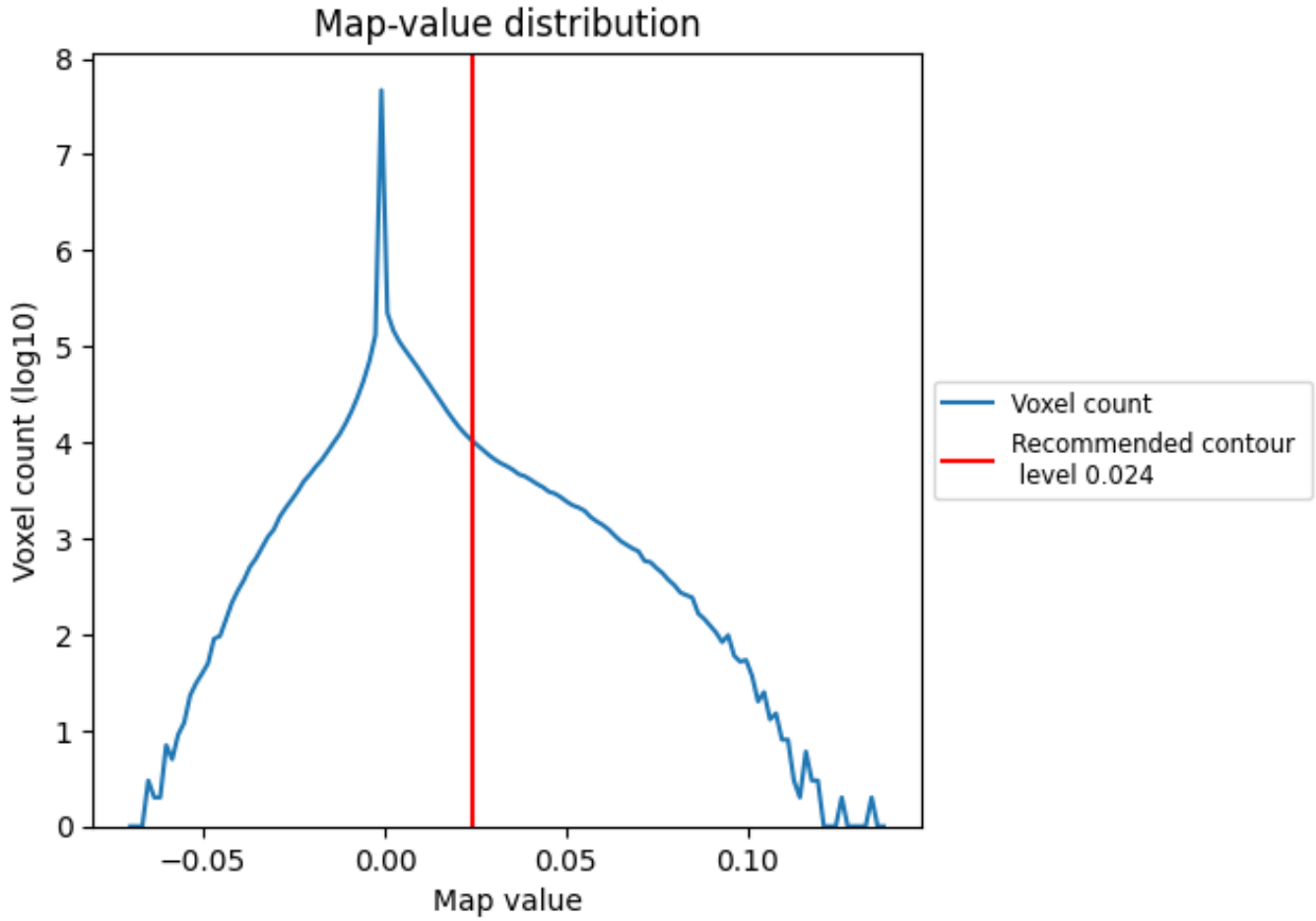


Z

# 7 Map analysis

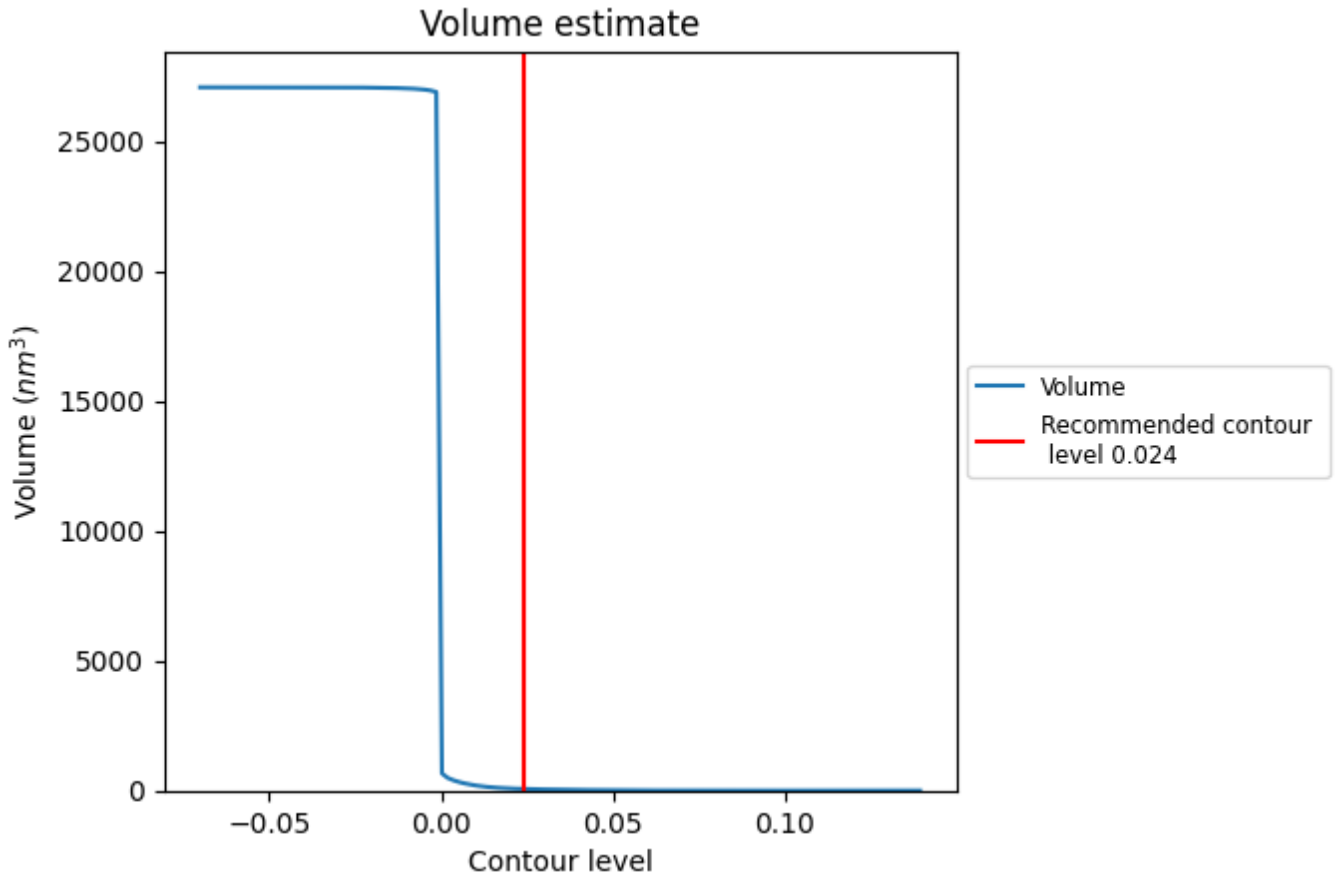
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

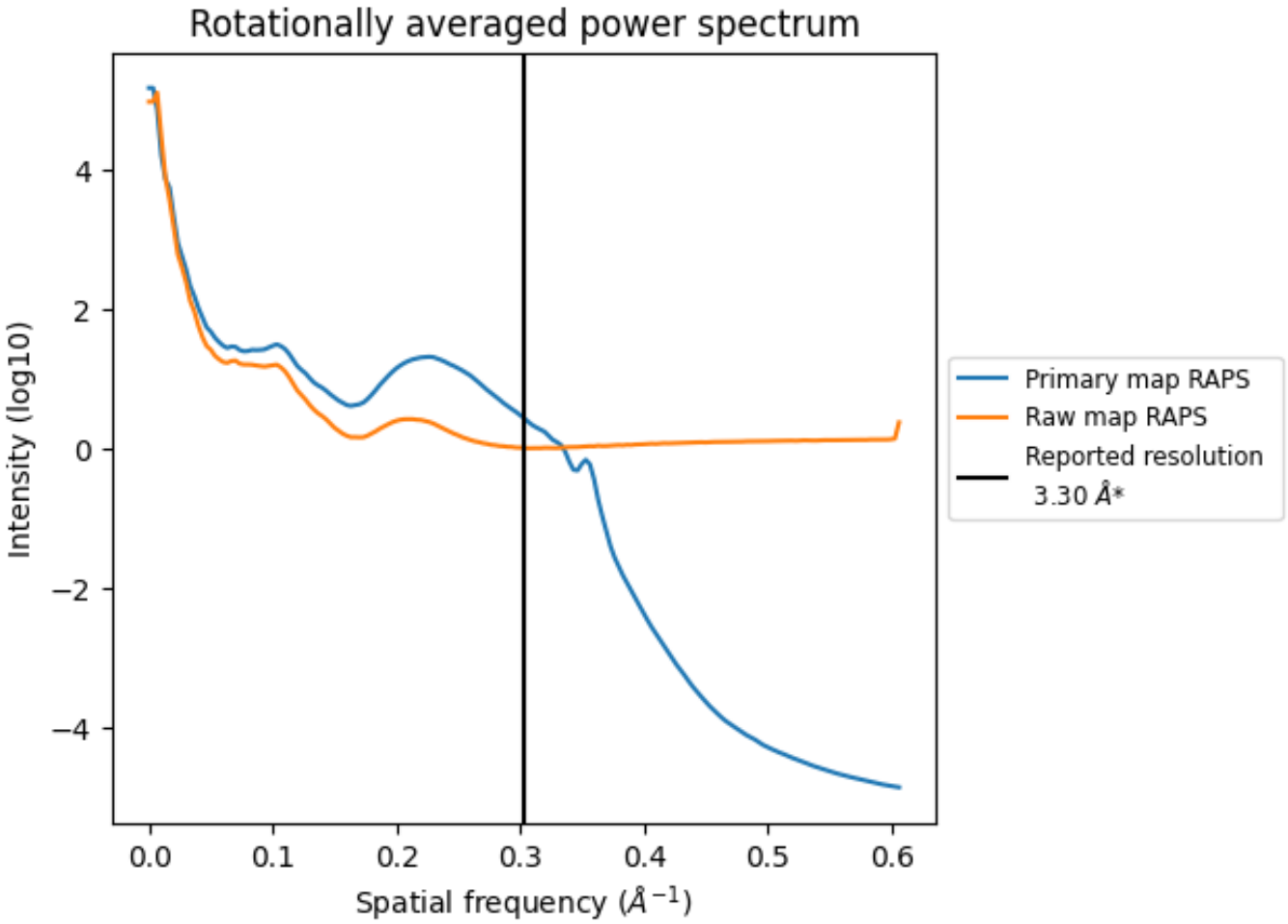
## 7.2 Volume estimate




The volume at the recommended contour level is 62 $nm^3$; this corresponds to an approximate mass of 56 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)

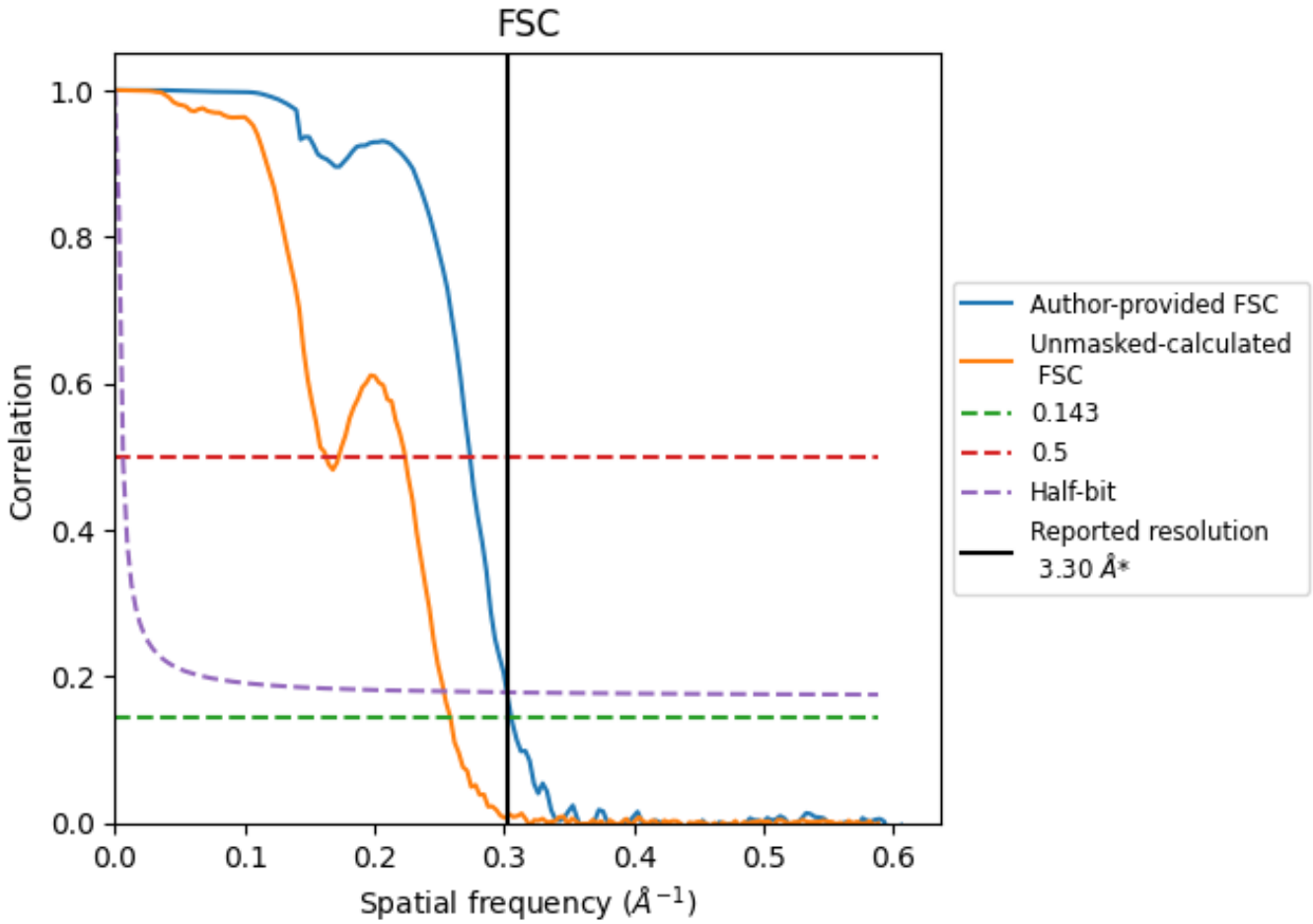



*Reported resolution corresponds to spatial frequency of 0.303 Å$^{-1}$

# 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 0.303 Å$^{-1}$

## 8.2 Resolution estimates (i)

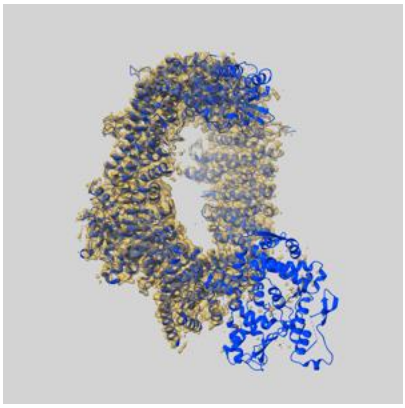
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.30 | - | - |
| Author-provided FSC curve | 3.27 | 3.65 | 3.31 |
| Unmasked-calculated* | 3.87 | 6.14 | 3.94 |

*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 3.87 differs from the reported value 3.3 by more than 10 %

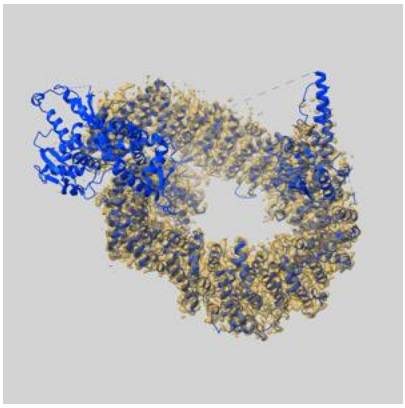
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22430 and PDB model 7MWF. Per-residue inclusion information can be found in section 3 on page 5.

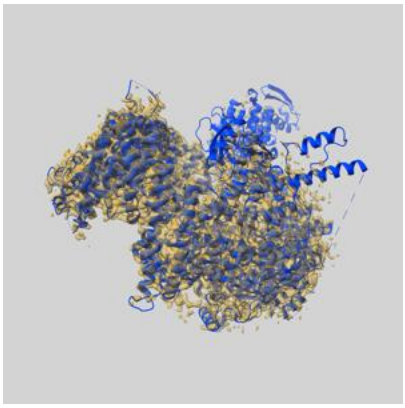
## 9.1 Map-model overlay



X



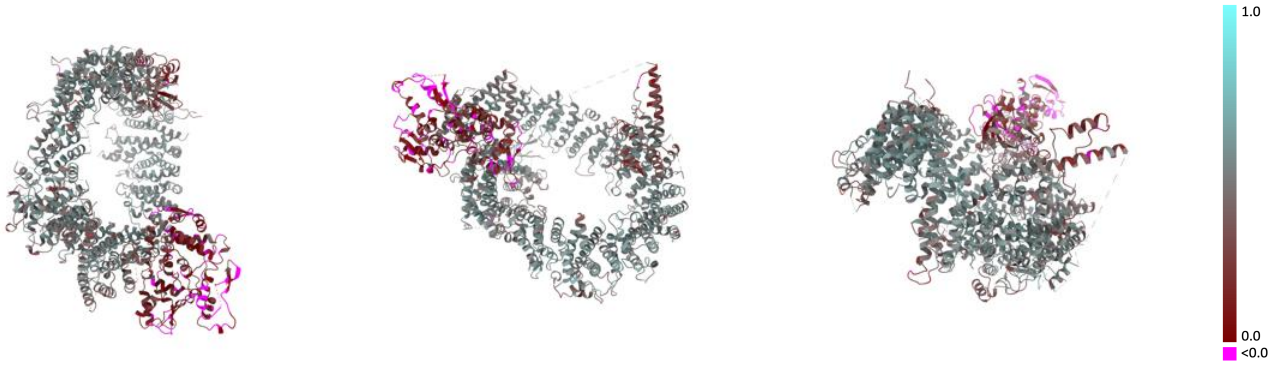
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.024 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.

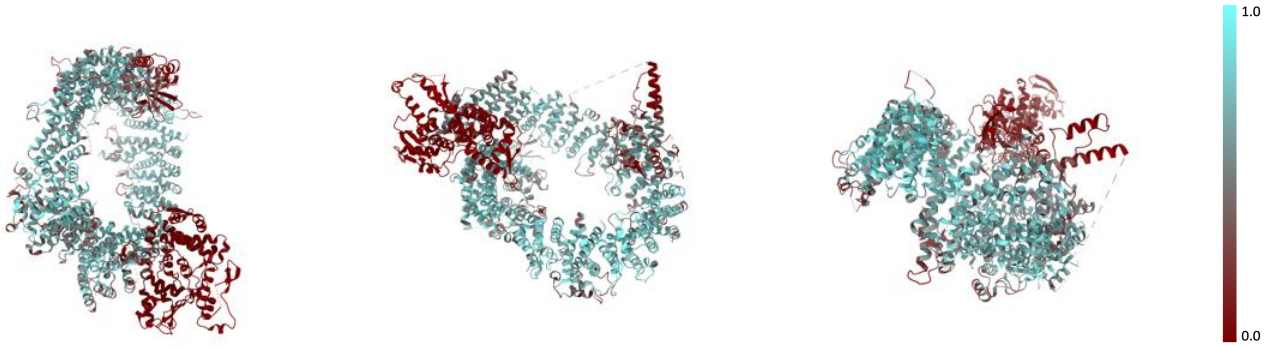
## 9.2 Q-score mapped to coordinate model (i)




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.

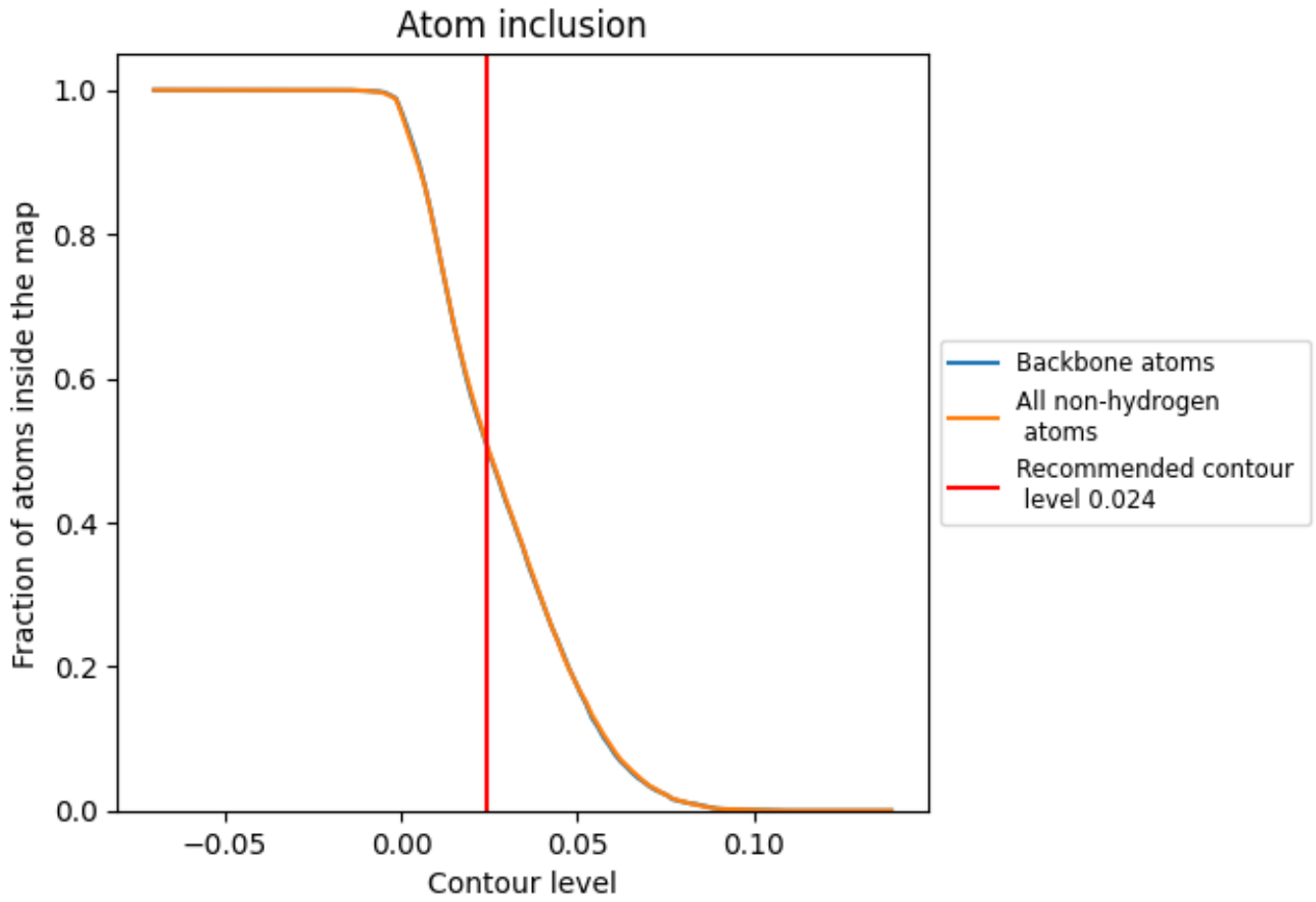
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.024).

## 9.4 Atom inclusion (i)




At the recommended contour level, 51% of all backbone atoms, 51% 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 (0.024) and Q-score for the entire model and for each chain.


| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.5130 | 0.4230 |
| A | 0.5135 | 0.4230 |