# Full wwPDB EM Validation Report

Mar 20, 2024 – 04:38 AM JST

| | | |
|---|---|---|
| PDB ID | : | 6LAR |
| EMDB ID | : | EMD-0862 |
| Title | : | Structure of ESX-3 complex |
| Authors | : | Wang, S.H.; Zhou, K.X.; Li, J.; Rao, Z.H. |
| Deposited on | : | 2019-11-13 |
| Resolution | : | 3.70 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 (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:

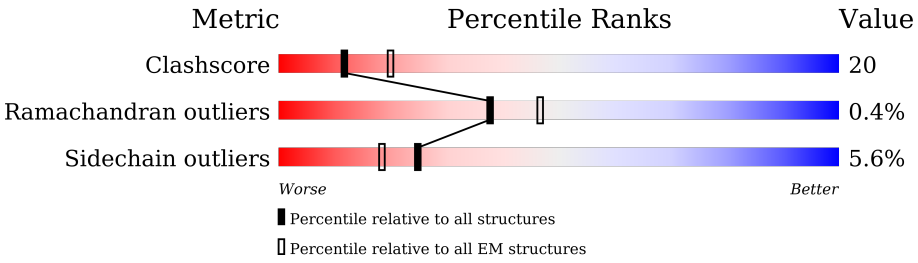
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev70 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 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 | 518 | 9% 5% 84% |
| 1 | I | 518 | 8% 89% |
| 2 | B | 475 | 11% 63% 27% 10% |
| 2 | C | 475 | 23% 71% 22% 7% |
| 2 | E | 475 | 6% 57% 29% 10% |
| 2 | H | 475 | 13% 64% 29% 7% |
| 3 | F | 449 | 11% 38% 35% 25% |
| 3 | J | 449 | 9% 34% 36% 28% |

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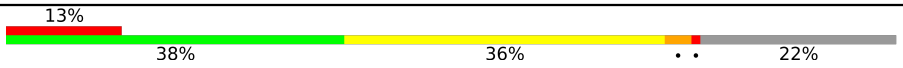
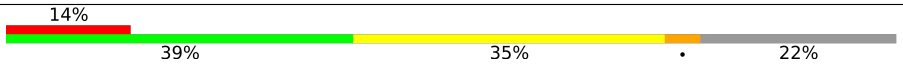
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | D | 309 |   |
| 4 | G | 309 |   |

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 22448 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 ESX-3 secretion system ATPase EccB3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 81 | Total | C | N | O | S | 0 | 0 |
| | | | 642 | 402 | 127 | 110 | 3 | | |
| 1 | I | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 461 | 297 | 87 | 74 | 3 | | |

- Molecule 2 is a protein called ESX-3 secretion system protein EccD3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 427 | Total | C | N | O | S | 0 | 0 |
| | | | 3055 | 1986 | 527 | 534 | 8 | | |
| 2 | C | 442 | Total | C | N | O | S | 0 | 0 |
| | | | 3168 | 2063 | 548 | 549 | 8 | | |
| 2 | E | 427 | Total | C | N | O | S | 0 | 0 |
| | | | 3055 | 1986 | 527 | 534 | 8 | | |
| 2 | H | 442 | Total | C | N | O | S | 0 | 0 |
| | | | 3168 | 2063 | 548 | 549 | 8 | | |

- Molecule 3 is a protein called ESX-3 secretion system protein EccC3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | F | 336 | Total | C | N | O | S | 0 | 0 |
| | | | 2667 | 1671 | 501 | 491 | 4 | | |
| 3 | J | 324 | Total | C | N | O | S | 0 | 0 |
| | | | 2574 | 1608 | 483 | 479 | 4 | | |

There are 36 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| F | 432 | HIS | - | expression tag | UNP A0QQ40 |
| F | 433 | LEU | - | expression tag | UNP A0QQ40 |
| F | 434 | GLY | - | expression tag | UNP A0QQ40 |
| F | 435 | GLY | - | expression tag | UNP A0QQ40 |
| F | 436 | ILE | - | expression tag | UNP A0QQ40 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| F | 437 | LYS | - | expression tag | UNP A0QQ40 |
| F | 438 | ALA | - | expression tag | UNP A0QQ40 |
| F | 439 | PHE | - | expression tag | UNP A0QQ40 |
| F | 440 | HIS | - | expression tag | UNP A0QQ40 |
| F | 441 | HIS | - | expression tag | UNP A0QQ40 |
| F | 442 | HIS | - | expression tag | UNP A0QQ40 |
| F | 443 | HIS | - | expression tag | UNP A0QQ40 |
| F | 444 | HIS | - | expression tag | UNP A0QQ40 |
| F | 445 | HIS | - | expression tag | UNP A0QQ40 |
| F | 446 | HIS | - | expression tag | UNP A0QQ40 |
| F | 447 | HIS | - | expression tag | UNP A0QQ40 |
| F | 448 | HIS | - | expression tag | UNP A0QQ40 |
| F | 449 | HIS | - | expression tag | UNP A0QQ40 |
| J | 432 | HIS | - | expression tag | UNP A0QQ40 |
| J | 433 | LEU | - | expression tag | UNP A0QQ40 |
| J | 434 | GLY | - | expression tag | UNP A0QQ40 |
| J | 435 | GLY | - | expression tag | UNP A0QQ40 |
| J | 436 | ILE | - | expression tag | UNP A0QQ40 |
| J | 437 | LYS | - | expression tag | UNP A0QQ40 |
| J | 438 | ALA | - | expression tag | UNP A0QQ40 |
| J | 439 | PHE | - | expression tag | UNP A0QQ40 |
| J | 440 | HIS | - | expression tag | UNP A0QQ40 |
| J | 441 | HIS | - | expression tag | UNP A0QQ40 |
| J | 442 | HIS | - | expression tag | UNP A0QQ40 |
| J | 443 | HIS | - | expression tag | UNP A0QQ40 |
| J | 444 | HIS | - | expression tag | UNP A0QQ40 |
| J | 445 | HIS | - | expression tag | UNP A0QQ40 |
| J | 446 | HIS | - | expression tag | UNP A0QQ40 |
| J | 447 | HIS | - | expression tag | UNP A0QQ40 |
| J | 448 | HIS | - | expression tag | UNP A0QQ40 |
| J | 449 | HIS | - | expression tag | UNP A0QQ40 |

- Molecule 4 is a protein called ESX-3 secretion system protein EccE3.

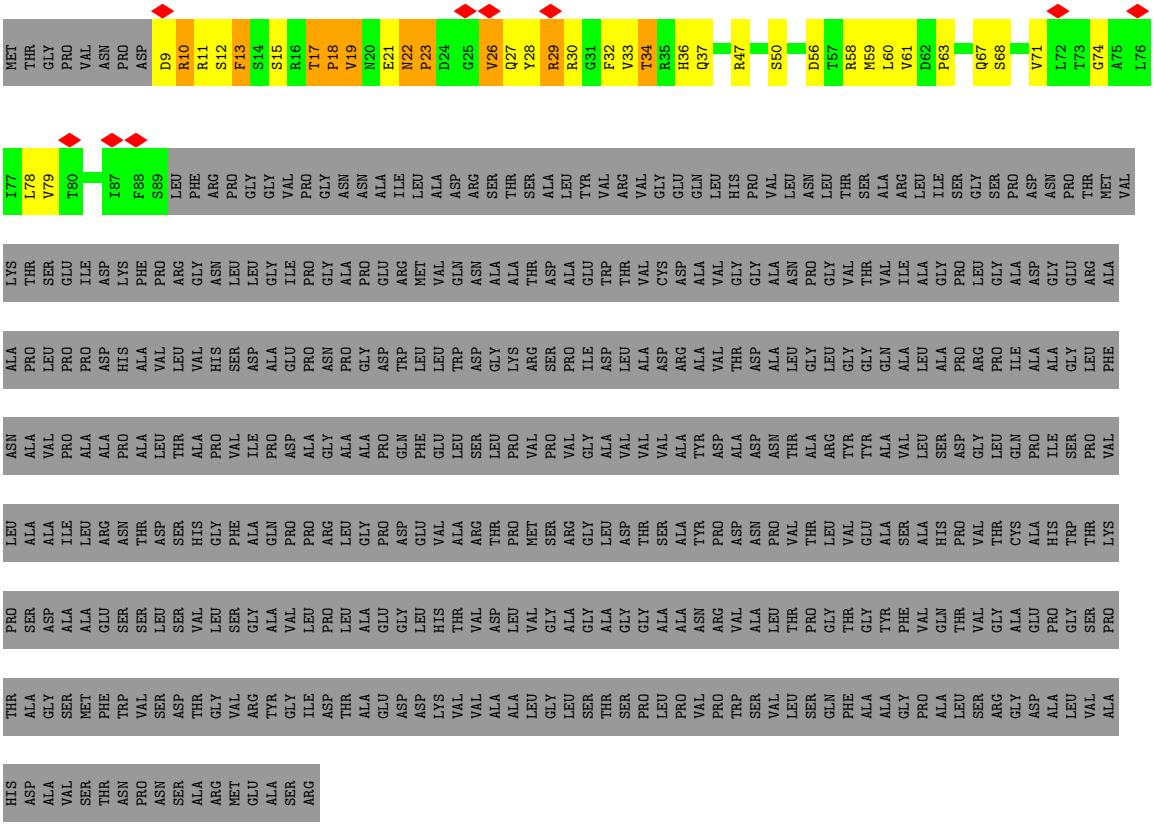
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | G | 241 | Total | C | N | O | S | 0 | 0 |
| | | | 1829 | 1160 | 336 | 328 | 5 | | |
| 4 | D | 241 | Total | C | N | O | S | 0 | 0 |
| | | | 1829 | 1160 | 336 | 328 | 5 | | |

# 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.

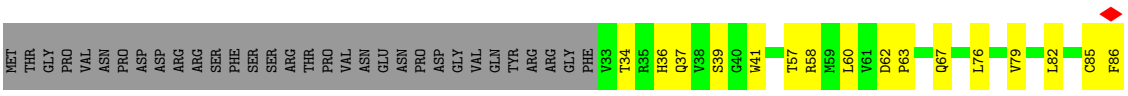
• Molecule 1: ESX-3 secretion system ATPase EccB3

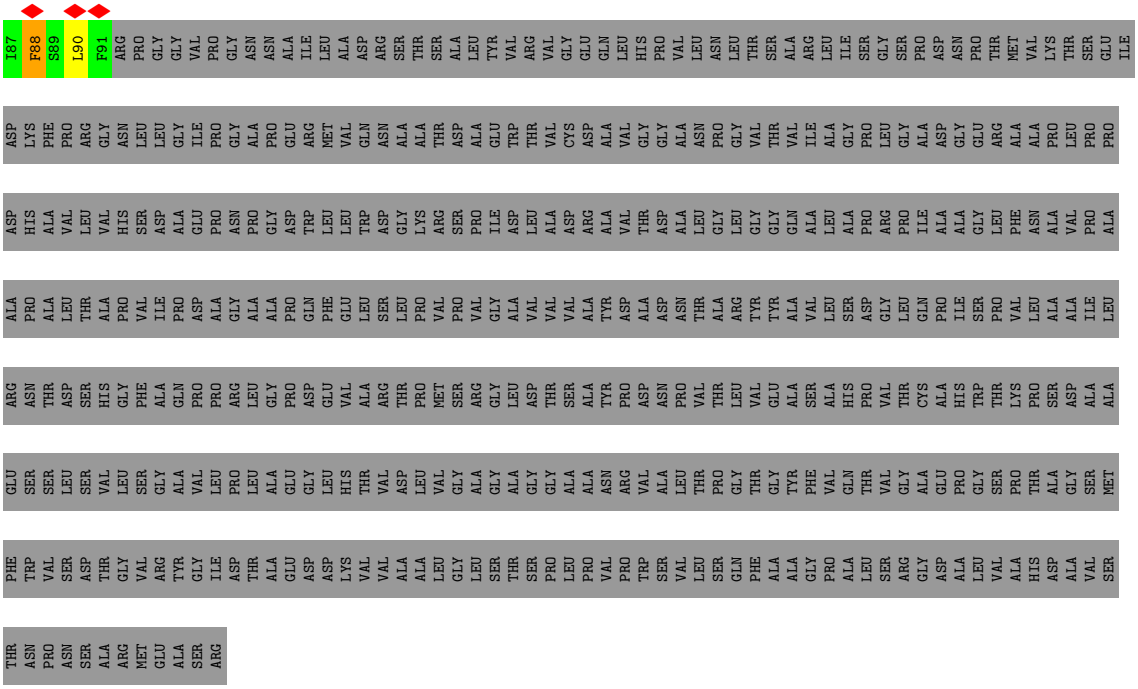
Chain A:


• Molecule 1: ESX-3 secretion system ATPase EccB3

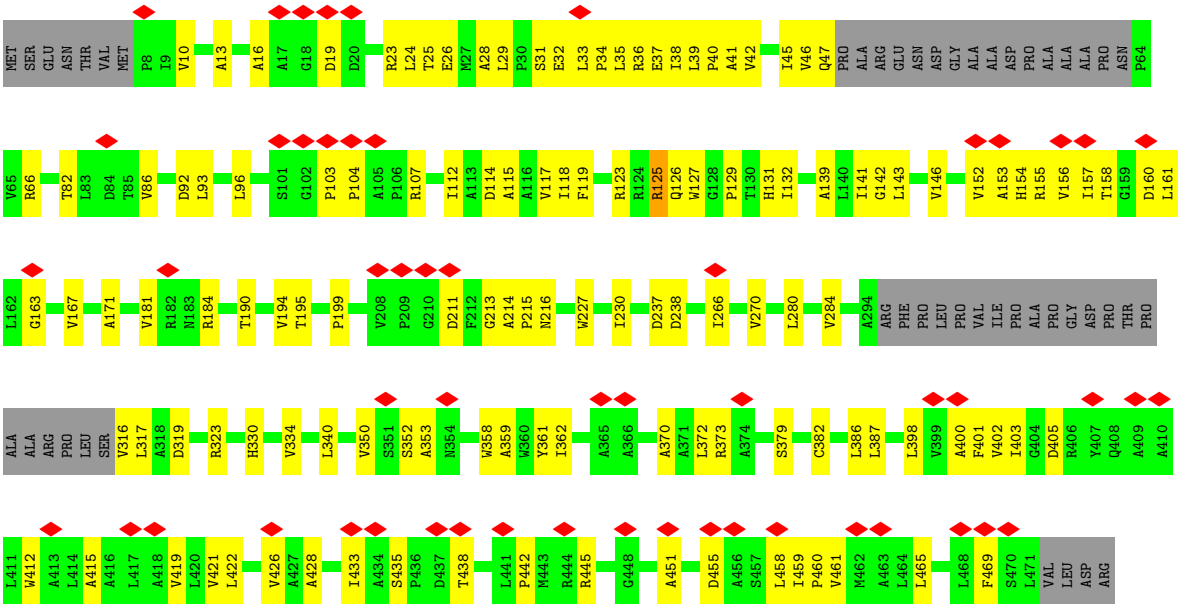
Chain I:



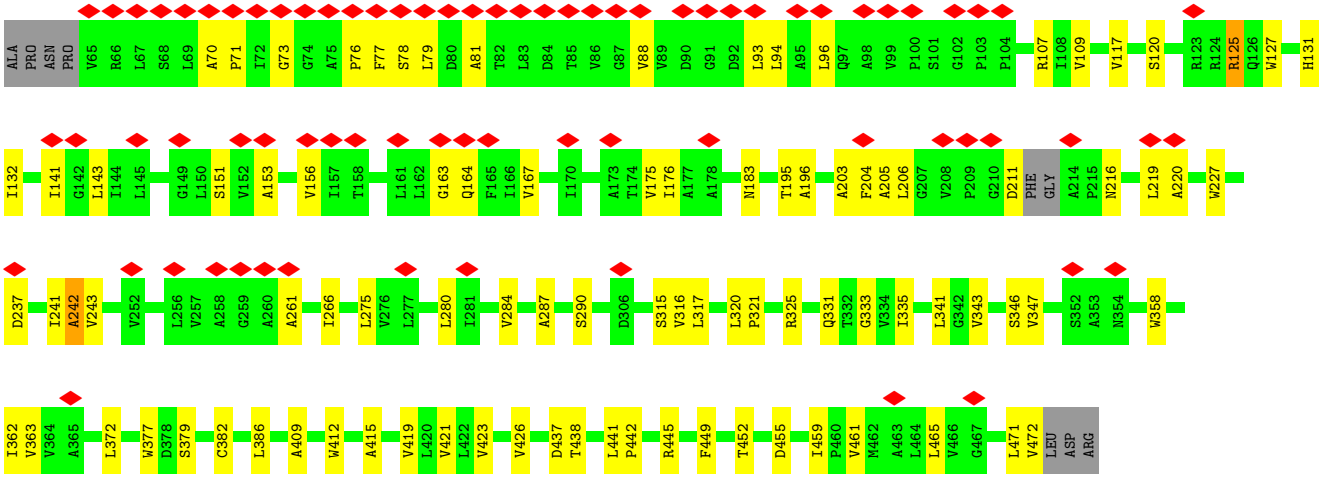
• Molecule 2: ESX-3 secretion system protein EccD3

Chain B:

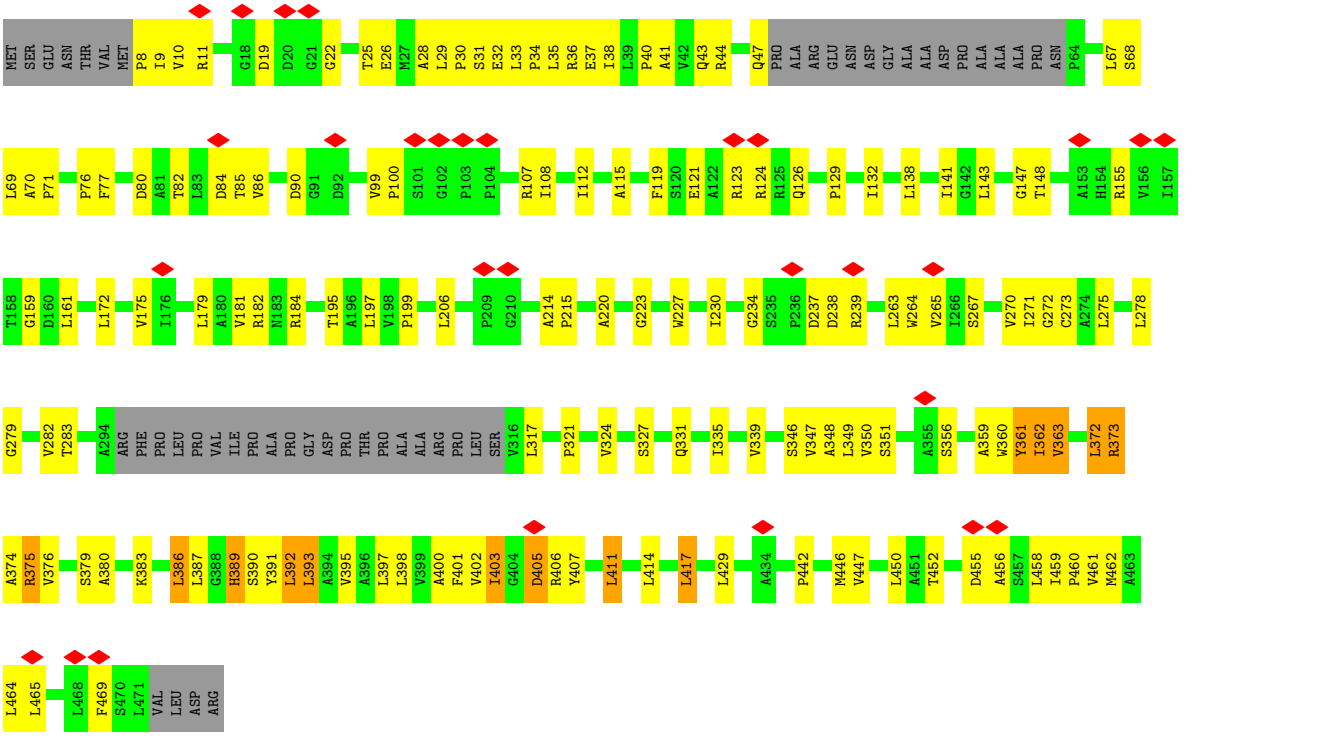
• Molecule 2: ESX-3 secretion system protein EccD3

Chain C:

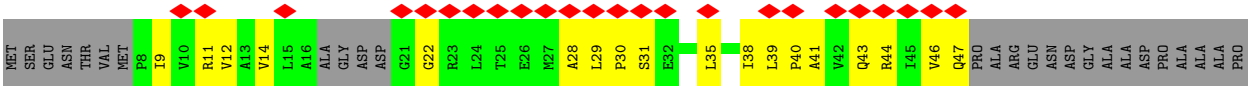
• Molecule 2: ESX-3 secretion system protein EccD3

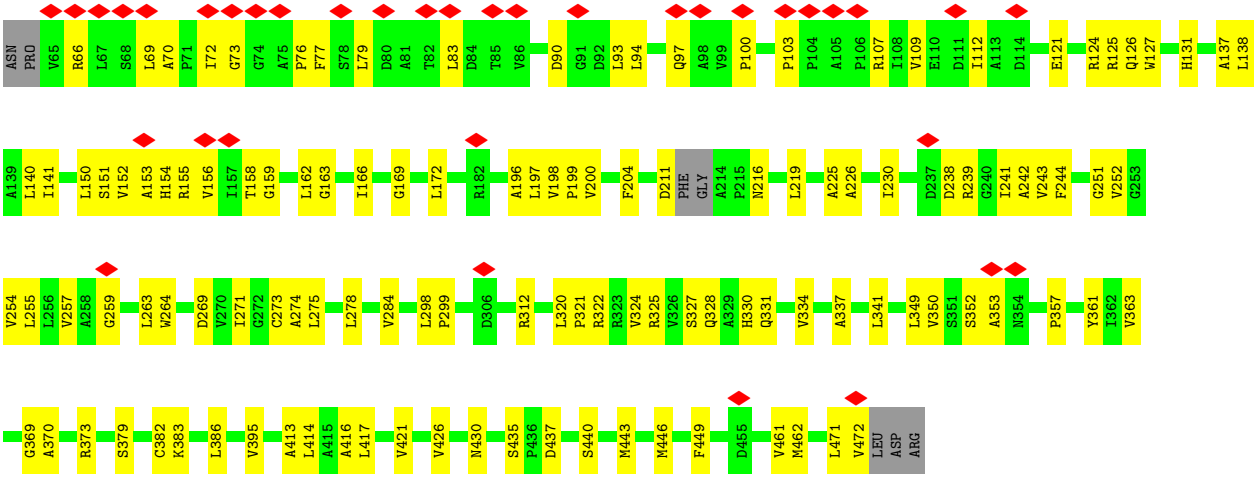
Chain E:

• Molecule 2: ESX-3 secretion system protein EccD3

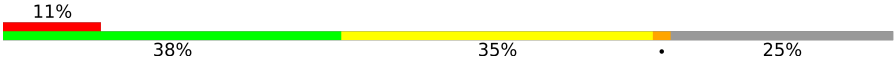
Chain H:

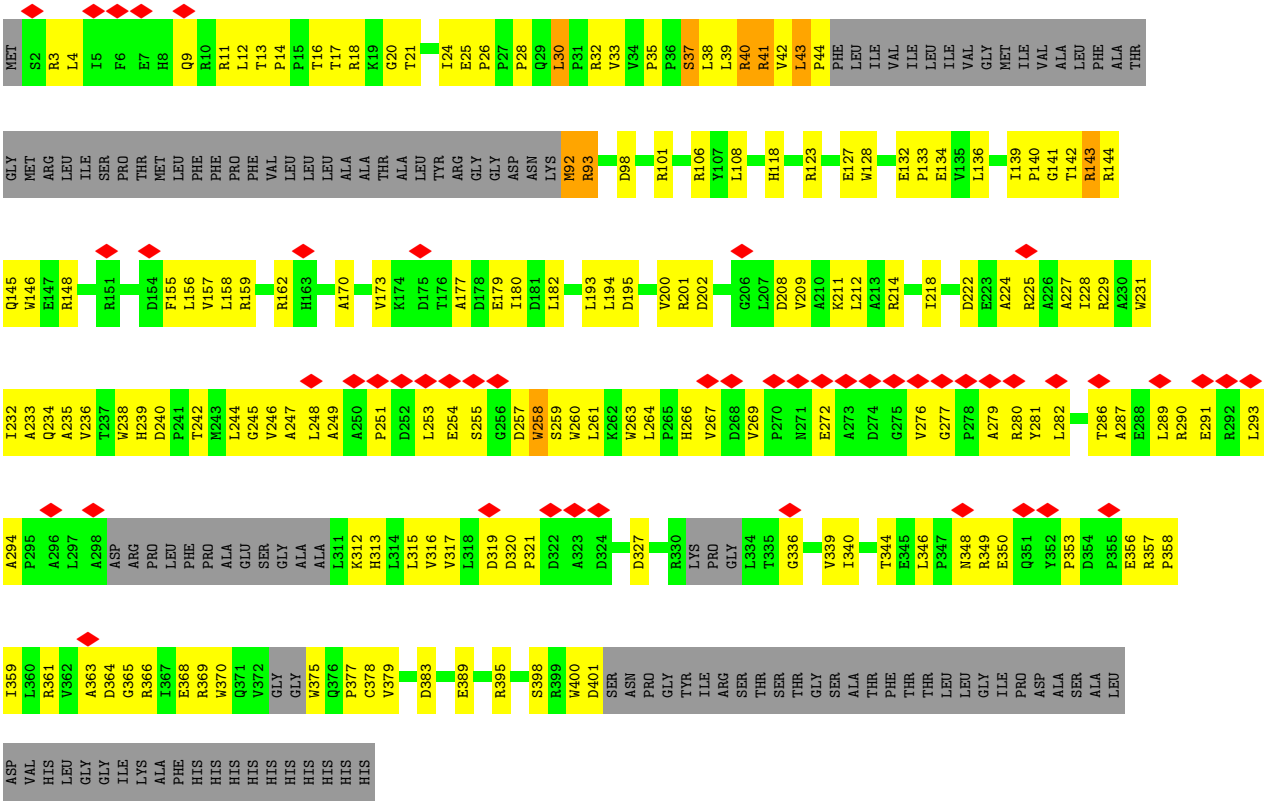





• Molecule 3: ESX-3 secretion system protein EccC3

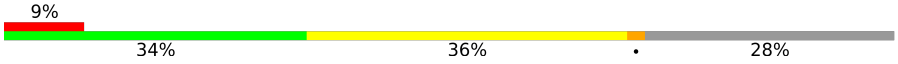
Chain F:

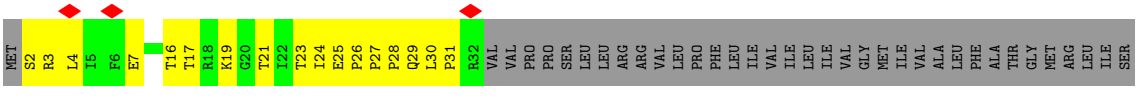


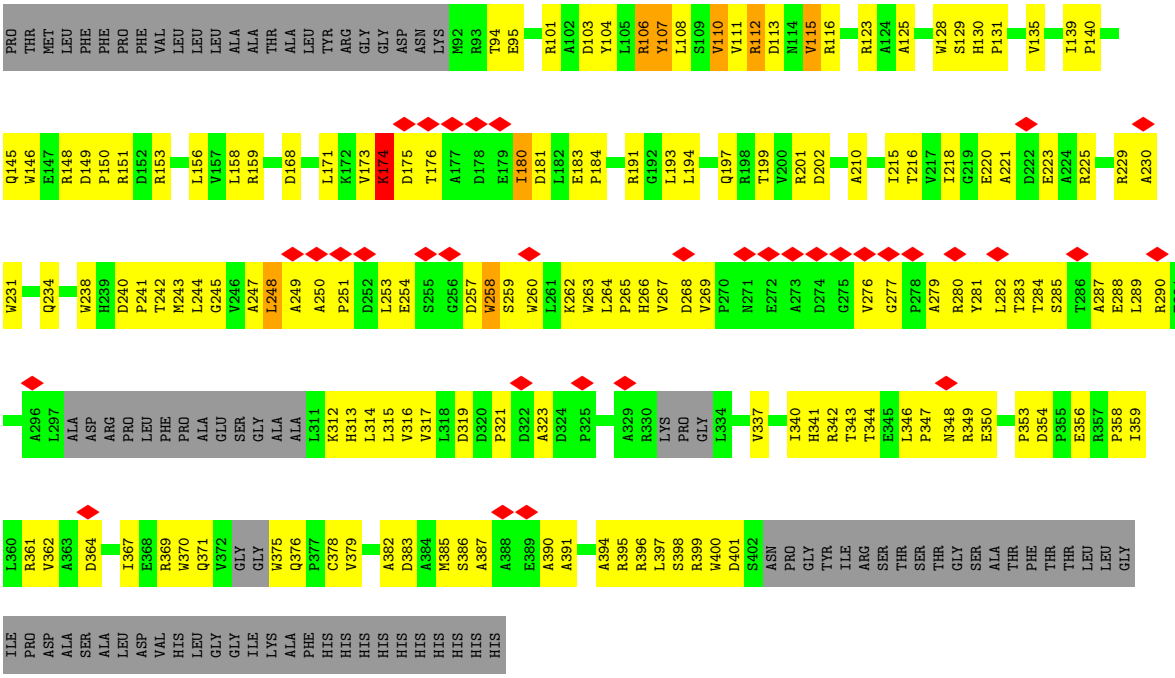



• Molecule 3: ESX-3 secretion system protein EccC3

Chain J:

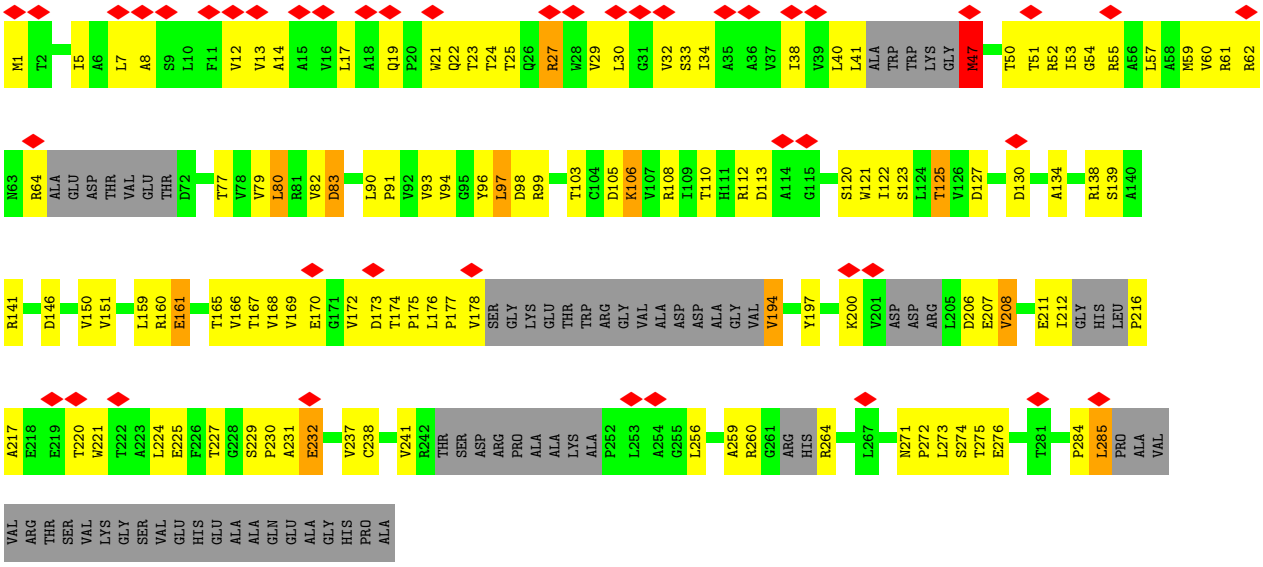




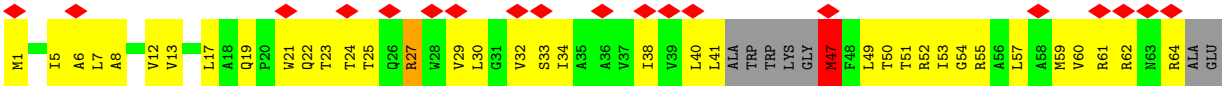
• Molecule 4: ESX-3 secretion system protein EccE3

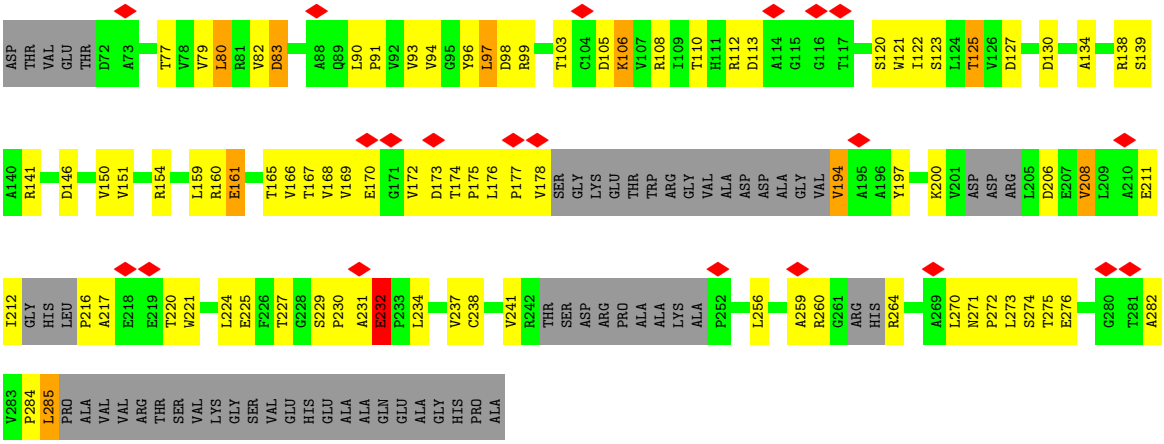
Chain G:

• Molecule 4: ESX-3 secretion system protein EccE3

Chain D:


ASP THR VAL GLU THR D72 A73 T77 V78 V79 L80 R81 V82 D83 A88 Q89 L90 P91 V92 V93 V94 G95 Y96 L97 D98 R99 T103 C104 D105 K106 V107 R108 I109 T110 H111 R112 D113 A114 G115 G116 T117 S120 W121 I122 S123 L124 T125 V126 D127 D130 A134 R138 S139
A140 R141 D146 V150 V151 R154 L159 R160 E161 T165 V166 T167 V168 V169 E170 G171 V172 D173 T174 P175 L176 P177 V178 SER GLY LYS GLU THR TRP ARG GLY VAL ALA ASP ASP ALA GLY VAL V194 A195 A196 Y197 K200 V201 ASP ASP ARG L205 D206 E207 V208 L209 A210 E211
I212 GLY HIS LEU P216 A217 E218 E219 T220 W221 L224 E225 F226 T227 G228 S229 P230 A231 E232 P233 L234 V237 C238 V241 R242 THR SER ASP ARG PRO ALA ALA LYS ALA P252 L256 A259 R260 G261 ARG HIS R264 A269 L270 N271 P272 L273 S274 T275 E276 G280 T281 A282
V283 P284 L285 PRO ALA ALA VAL VAL ARG THR SER VAL LYS GLY SER VAL GLU HIS GLU ALA ALA GLN GLU ALA GLY HIS PRO ALA

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 215839 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 50 | Depositor |
| Minimum defocus (nm) | 1500 | Depositor |
| Maximum defocus (nm) | 2500 | Depositor |
| Magnification | 29000 | Depositor |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 0.173 | Depositor |
| Minimum map value | -0.113 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.004 | Depositor |
| Recommended contour level | 0.03 | Depositor |
| Map size (Å) | 360.8, 360.8, 360.8 | wwPDB |
| Map dimensions | 440, 440, 440 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.82, 0.82, 0.82 | 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 | 0.52 | 0/654 | 0.56 | 0/883 |
| 1 | I | 0.42 | 0/469 | 0.50 | 0/634 |
| 2 | B | 0.34 | 0/3111 | 0.52 | 0/4271 |
| 2 | C | 0.36 | 0/3229 | 0.51 | 0/4438 |
| 2 | E | 0.40 | 0/3111 | 0.52 | 0/4271 |
| 2 | H | 0.41 | 0/3229 | 0.52 | 0/4438 |
| 3 | F | 0.38 | 0/2727 | 0.54 | 0/3727 |
| 3 | J | 0.40 | 0/2631 | 0.57 | 1/3593 (0.0%) |
| 4 | D | 0.35 | 0/1855 | 0.56 | 2/2531 (0.1%) |
| 4 | G | 0.35 | 0/1855 | 0.56 | 2/2531 (0.1%) |
| All | All | 0.38 | 0/22871 | 0.53 | 5/31317 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 3 | J | 0 | 1 |

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | G | 232 | GLU | CA-CB-CG | 7.09 | 129.01 | 113.40 |
| 4 | D | 232 | GLU | CA-CB-CG | 7.07 | 128.94 | 113.40 |
| 3 | J | 248 | LEU | CA-CB-CG | 5.40 | 127.73 | 115.30 |
| 4 | D | 47 | MET | CA-CB-CG | 5.40 | 122.47 | 113.30 |
| 4 | G | 47 | MET | CA-CB-CG | 5.38 | 122.45 | 113.30 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 3 | J | 323 | ALA | Peptide |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 642 | 0 | 653 | 56 | 0 |
| 1 | I | 461 | 0 | 487 | 16 | 0 |
| 2 | B | 3055 | 0 | 3235 | 95 | 0 |
| 2 | C | 3168 | 0 | 3367 | 75 | 0 |
| 2 | E | 3055 | 0 | 3235 | 151 | 0 |
| 2 | H | 3168 | 0 | 3367 | 100 | 0 |
| 3 | F | 2667 | 0 | 2661 | 143 | 0 |
| 3 | J | 2574 | 0 | 2549 | 197 | 0 |
| 4 | D | 1829 | 0 | 1907 | 83 | 0 |
| 4 | G | 1829 | 0 | 1907 | 74 | 0 |
| All | All | 22448 | 0 | 23368 | 903 | 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 20.

All (903) 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:13:PHE:CE2 | 3:J:104:TYR:HD1 | 1.39 | 1.39 |
| 2:E:346:SER:OG | 2:E:363:VAL:HG12 | 1.20 | 1.33 |
| 2:E:346:SER:OG | 2:E:363:VAL:CG1 | 1.86 | 1.24 |
| 1:A:13:PHE:CE2 | 3:J:104:TYR:CD1 | 2.30 | 1.18 |
| 2:E:107:ARG:NE | 3:J:116:ARG:HH21 | 1.39 | 1.17 |
| 3:J:26:PRO:HG3 | 3:J:175:ASP:HB3 | 1.16 | 1.13 |
| 1:A:22:ASN:HB2 | 1:A:23:PRO:CD | 1.79 | 1.11 |
| 2:E:107:ARG:HE | 3:J:116:ARG:NH2 | 1.47 | 1.10 |
| 1:A:18:PRO:HD2 | 3:J:110:VAL:HG11 | 1.31 | 1.07 |
| 1:A:13:PHE:CD2 | 3:J:104:TYR:HD1 | 1.73 | 1.06 |
| 2:E:107:ARG:NE | 3:J:116:ARG:NH2 | 2.01 | 1.04 |
| 2:E:414:LEU:HD12 | 2:H:150:LEU:CD2 | 1.87 | 1.03 |
| 1:A:18:PRO:HG2 | 3:J:110:VAL:CG1 | 1.91 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:13:PHE:HE2 | 3:J:104:TYR:HA | 1.26 | 0.99 |
| 1:A:18:PRO:CD | 3:J:110:VAL:HG11 | 1.93 | 0.99 |
| 3:J:26:PRO:HG3 | 3:J:175:ASP:CB | 1.94 | 0.98 |
| 2:E:414:LEU:HD12 | 2:H:150:LEU:HD23 | 1.46 | 0.96 |
| 1:A:22:ASN:HB2 | 1:A:23:PRO:HD2 | 1.46 | 0.95 |
| 1:A:29:ARG:HG2 | 1:A:29:ARG:HH11 | 1.29 | 0.94 |
| 2:E:350:VAL:HG11 | 2:E:360:TRP:CZ3 | 2.03 | 0.94 |
| 2:E:107:ARG:CD | 3:J:116:ARG:NH2 | 2.32 | 0.93 |
| 1:A:13:PHE:CD2 | 3:J:104:TYR:CD1 | 2.53 | 0.93 |
| 3:J:371:GLN:HB3 | 3:J:376:GLN:HE21 | 1.32 | 0.92 |
| 2:E:346:SER:HG | 2:E:363:VAL:HG12 | 0.92 | 0.92 |
| 1:A:18:PRO:CG | 3:J:110:VAL:CG1 | 2.48 | 0.91 |
| 3:J:264:LEU:HB2 | 3:J:267:VAL:HG23 | 1.53 | 0.91 |
| 2:C:379:SER:HG | 2:C:382:CYS:HG | 0.93 | 0.91 |
| 3:F:35:PRO:HG2 | 3:J:95:GLU:CB | 2.02 | 0.89 |
| 3:F:248:LEU:HD11 | 3:F:258:TRP:HB3 | 1.54 | 0.89 |
| 2:E:107:ARG:HD3 | 3:J:116:ARG:NH2 | 1.89 | 0.88 |
| 3:F:35:PRO:HG2 | 3:J:95:GLU:HB2 | 1.56 | 0.87 |
| 3:J:26:PRO:CG | 3:J:175:ASP:HB3 | 2.04 | 0.87 |
| 3:J:341:HIS:NE2 | 3:J:343:THR:OG1 | 2.08 | 0.87 |
| 2:E:107:ARG:CD | 3:J:116:ARG:HH21 | 1.89 | 0.85 |
| 3:F:127:GLU:OE1 | 3:F:162:ARG:NH1 | 2.10 | 0.85 |
| 3:F:38:LEU:HA | 3:F:41:ARG:HG2 | 1.59 | 0.84 |
| 2:E:414:LEU:CD1 | 2:H:150:LEU:HD23 | 2.08 | 0.84 |
| 2:E:414:LEU:O | 2:E:414:LEU:HD23 | 1.79 | 0.83 |
| 1:A:22:ASN:HB2 | 1:A:23:PRO:HD3 | 1.61 | 0.83 |
| 3:F:43:LEU:H | 3:F:44:PRO:HD2 | 1.44 | 0.82 |
| 2:H:298:LEU:O | 2:H:312:ARG:NH1 | 2.12 | 0.82 |
| 1:A:18:PRO:CG | 3:J:110:VAL:HG11 | 2.09 | 0.82 |
| 1:A:13:PHE:CE2 | 3:J:104:TYR:HA | 2.14 | 0.82 |
| 4:D:108:ARG:HB3 | 4:D:123:SER:HB2 | 1.62 | 0.82 |
| 3:J:264:LEU:HD21 | 3:J:394:ALA:HA | 1.62 | 0.82 |
| 2:E:107:ARG:HE | 3:J:116:ARG:HH21 | 0.84 | 0.81 |
| 4:G:108:ARG:HB3 | 4:G:123:SER:HB2 | 1.62 | 0.81 |
| 2:E:82:THR:HG23 | 2:E:84:ASP:H | 1.47 | 0.80 |
| 3:J:251:PRO:HA | 3:J:284:THR:HG23 | 1.64 | 0.79 |
| 4:G:194:VAL:N | 4:G:241:VAL:O | 2.16 | 0.79 |
| 3:J:3:ARG:NH2 | 3:J:263:TRP:O | 2.15 | 0.79 |
| 2:E:143:LEU:HD22 | 2:H:421:VAL:HG11 | 1.64 | 0.79 |
| 3:J:262:LYS:HD2 | 3:J:280:ARG:HG2 | 1.65 | 0.79 |
| 4:D:194:VAL:N | 4:D:241:VAL:O | 2.16 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:J:229:ARG:HH21 | 3:J:386:SER:HA | 1.48 | 0.78 |
| 1:A:13:PHE:HE2 | 3:J:104:TYR:HD1 | 1.29 | 0.78 |
| 2:E:392:LEU:HD12 | 2:E:392:LEU:O | 1.84 | 0.78 |
| 3:J:26:PRO:CG | 3:J:175:ASP:CB | 2.61 | 0.78 |
| 1:A:22:ASN:CB | 1:A:23:PRO:CD | 2.60 | 0.78 |
| 2:E:11:ARG:N | 2:E:90:ASP:OD1 | 2.16 | 0.77 |
| 2:E:335:ILE:HG21 | 2:E:386:LEU:CD2 | 2.14 | 0.77 |
| 3:F:254:GLU:HA | 3:F:259:SER:HB3 | 1.65 | 0.77 |
| 2:H:379:SER:OG | 2:H:382:CYS:SG | 2.43 | 0.77 |
| 2:C:331:GLN:NE2 | 2:C:382:CYS:SG | 2.58 | 0.77 |
| 2:E:414:LEU:HD12 | 2:H:150:LEU:HD22 | 1.66 | 0.77 |
| 2:E:335:ILE:HG21 | 2:E:386:LEU:HD23 | 1.67 | 0.76 |
| 2:B:153:ALA:HA | 2:B:156:VAL:HG22 | 1.68 | 0.76 |
| 3:F:43:LEU:N | 3:F:44:PRO:HD2 | 2.00 | 0.75 |
| 4:G:17:LEU:HD12 | 4:G:19:GLN:HE22 | 1.51 | 0.75 |
| 3:J:229:ARG:NE | 3:J:385:MET:O | 2.20 | 0.74 |
| 1:A:58:ARG:O | 3:F:106:ARG:NH1 | 2.19 | 0.74 |
| 2:E:335:ILE:CG2 | 2:E:386:LEU:HD23 | 2.16 | 0.74 |
| 3:J:314:LEU:HB2 | 3:J:337:VAL:HG22 | 1.69 | 0.74 |
| 4:D:17:LEU:HD12 | 4:D:19:GLN:HE22 | 1.51 | 0.74 |
| 2:B:154:HIS:CE1 | 2:B:160:ASP:HB3 | 2.23 | 0.74 |
| 3:J:243:MET:SD | 3:J:312:LYS:NZ | 2.59 | 0.73 |
| 1:A:13:PHE:HE2 | 3:J:104:TYR:CD1 | 2.03 | 0.73 |
| 3:J:94:THR:OG1 | 3:J:95:GLU:OE2 | 2.04 | 0.73 |
| 3:F:313:HIS:NE2 | 3:F:336:GLY:O | 2.22 | 0.73 |
| 2:E:155:ARG:O | 2:E:155:ARG:NH1 | 2.20 | 0.72 |
| 2:E:346:SER:OG | 2:E:363:VAL:HG11 | 1.89 | 0.72 |
| 2:B:107:ARG:HH22 | 2:B:118:ILE:HG21 | 1.54 | 0.72 |
| 3:J:369:ARG:NE | 3:J:378:CYS:SG | 2.62 | 0.72 |
| 2:C:358:TRP:HB2 | 2:C:465:LEU:HD13 | 1.71 | 0.72 |
| 2:B:36:ARG:NE | 3:F:389:GLU:OE1 | 2.23 | 0.71 |
| 2:E:26:GLU:OE1 | 4:D:154:ARG:NH1 | 2.22 | 0.71 |
| 2:E:350:VAL:CG1 | 2:E:360:TRP:CH2 | 2.73 | 0.71 |
| 3:J:112:ARG:HG3 | 3:J:112:ARG:HH11 | 1.53 | 0.71 |
| 1:A:29:ARG:HG2 | 1:A:29:ARG:NH1 | 1.97 | 0.70 |
| 3:J:248:LEU:HD21 | 3:J:258:TRP:HB3 | 1.74 | 0.70 |
| 2:C:11:ARG:HD3 | 3:F:276:VAL:HB | 1.73 | 0.70 |
| 3:J:341:HIS:HE2 | 3:J:343:THR:HG1 | 1.28 | 0.70 |
| 4:D:59:MET:SD | 4:D:62:ARG:NH1 | 2.59 | 0.70 |
| 4:G:59:MET:SD | 4:G:62:ARG:NH1 | 2.59 | 0.70 |
| 2:E:99:VAL:HG22 | 2:E:100:PRO:HD2 | 1.72 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:211:ASP:OD1 | 2:H:216:ASN:ND2 | 2.25 | 0.70 |
| 3:F:98:ASP:OD1 | 3:F:101:ARG:NH1 | 2.24 | 0.70 |
| 3:J:371:GLN:HB3 | 3:J:376:GLN:NE2 | 2.06 | 0.70 |
| 2:B:157:ILE:HG23 | 2:B:158:THR:HG23 | 1.73 | 0.70 |
| 2:B:155:ARG:NH1 | 2:B:160:ASP:O | 2.24 | 0.70 |
| 2:E:29:LEU:HD13 | 2:E:38:ILE:HD12 | 1.72 | 0.69 |
| 2:E:393:LEU:O | 2:E:393:LEU:HD12 | 1.92 | 0.69 |
| 3:F:264:LEU:HD11 | 3:F:266:HIS:HB2 | 1.74 | 0.69 |
| 3:J:254:GLU:HA | 3:J:259:SER:HB2 | 1.73 | 0.69 |
| 3:F:370:TRP:HA | 3:F:375:TRP:HE1 | 1.56 | 0.69 |
| 1:A:18:PRO:HG2 | 3:J:110:VAL:HG11 | 1.71 | 0.69 |
| 3:J:24:ILE:HD13 | 3:J:24:ILE:N | 2.06 | 0.69 |
| 3:F:43:LEU:H | 3:F:44:PRO:CD | 2.05 | 0.69 |
| 2:E:182:ARG:NH1 | 2:E:234:GLY:O | 2.25 | 0.69 |
| 3:J:253:LEU:HG | 3:J:254:GLU:HG3 | 1.74 | 0.68 |
| 3:F:225:ARG:HA | 3:F:228:ILE:HD12 | 1.75 | 0.68 |
| 1:A:22:ASN:ND2 | 3:J:113:ASP:O | 2.26 | 0.68 |
| 2:C:205:ALA:HB2 | 2:C:220:ALA:HB2 | 1.75 | 0.68 |
| 2:B:372:LEU:HD23 | 2:B:451:ALA:HB2 | 1.76 | 0.68 |
| 3:F:158:LEU:HD23 | 3:F:231:TRP:HB2 | 1.76 | 0.68 |
| 3:F:41:ARG:O | 3:F:41:ARG:HG3 | 1.94 | 0.67 |
| 3:F:363:ALA:HB3 | 3:F:366:ARG:HB2 | 1.74 | 0.67 |
| 1:A:18:PRO:HG2 | 3:J:110:VAL:HG13 | 1.76 | 0.67 |
| 2:H:241:ILE:HG13 | 2:H:243:VAL:HG12 | 1.75 | 0.67 |
| 2:B:421:VAL:HG21 | 2:C:143:LEU:HD13 | 1.77 | 0.67 |
| 2:C:71:PRO:HD3 | 2:C:77:PHE:CZ | 2.30 | 0.67 |
| 3:F:9:GLN:HG2 | 3:F:143:ARG:HE | 1.61 | 0.66 |
| 2:E:414:LEU:CD1 | 2:H:150:LEU:CD2 | 2.67 | 0.66 |
| 2:H:35:LEU:HB2 | 2:H:79:LEU:HD12 | 1.77 | 0.65 |
| 3:F:43:LEU:N | 3:F:44:PRO:CD | 2.59 | 0.65 |
| 3:F:212:LEU:HD12 | 3:F:358:PRO:HD3 | 1.77 | 0.65 |
| 4:D:60:VAL:O | 4:D:64:ARG:NH2 | 2.29 | 0.65 |
| 3:F:225:ARG:NH1 | 3:F:257:ASP:OD2 | 2.30 | 0.65 |
| 4:G:60:VAL:O | 4:G:64:ARG:NH2 | 2.29 | 0.65 |
| 2:E:350:VAL:HG11 | 2:E:360:TRP:CH2 | 2.32 | 0.65 |
| 2:H:121:GLU:OE1 | 2:H:124:ARG:NH2 | 2.28 | 0.65 |
| 3:F:253:LEU:HG | 3:F:254:GLU:HG2 | 1.79 | 0.65 |
| 1:A:18:PRO:CD | 3:J:110:VAL:CG1 | 2.73 | 0.64 |
| 3:F:353:PRO:HG3 | 3:F:370:TRP:CD1 | 2.31 | 0.64 |
| 2:E:22:GLY:N | 2:H:112:ILE:O | 2.29 | 0.64 |
| 3:F:11:ARG:NH1 | 3:F:12:LEU:O | 2.30 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:440:SER:HG | 2:H:443:MET:H | 1.44 | 0.64 |
| 3:F:142:THR:HG22 | 3:F:143:ARG:H | 1.62 | 0.64 |
| 2:H:155:ARG:HA | 2:H:158:THR:O | 1.98 | 0.64 |
| 3:J:243:MET:HA | 3:J:312:LYS:HD2 | 1.77 | 0.64 |
| 2:B:92:ASP:OD1 | 2:B:93:LEU:N | 2.31 | 0.64 |
| 2:B:160:ASP:OD1 | 2:B:161:LEU:N | 2.29 | 0.64 |
| 2:B:123:ARG:HG3 | 2:B:125:ARG:HB3 | 1.80 | 0.64 |
| 2:C:141:ILE:HD12 | 2:C:195:THR:HG21 | 1.80 | 0.64 |
| 4:G:161:GLU:OE1 | 4:G:161:GLU:HA | 1.98 | 0.63 |
| 4:G:54:GLY:HA2 | 4:G:57:LEU:HD12 | 1.80 | 0.63 |
| 4:D:174:THR:OG1 | 4:D:176:LEU:O | 2.16 | 0.63 |
| 4:D:220:THR:HA | 4:D:241:VAL:HG12 | 1.80 | 0.63 |
| 2:B:379:SER:OG | 2:B:382:CYS:SG | 2.52 | 0.63 |
| 3:F:258:TRP:NE1 | 3:F:319:ASP:OD2 | 2.31 | 0.63 |
| 3:F:350:GLU:HB3 | 3:F:370:TRP:HE1 | 1.63 | 0.63 |
| 3:J:248:LEU:HD23 | 3:J:282:LEU:HG | 1.80 | 0.63 |
| 2:C:409:ALA:HA | 2:C:412:TRP:HD1 | 1.61 | 0.63 |
| 3:F:261:LEU:HD22 | 3:F:264:LEU:HD22 | 1.81 | 0.63 |
| 4:D:161:GLU:HA | 4:D:161:GLU:OE1 | 1.99 | 0.63 |
| 3:J:115:VAL:HG21 | 3:J:171:LEU:HD11 | 1.81 | 0.62 |
| 3:J:230:ALA:HA | 3:J:385:MET:HB2 | 1.81 | 0.62 |
| 4:D:54:GLY:HA2 | 4:D:57:LEU:HD12 | 1.80 | 0.62 |
| 2:E:141:ILE:HD12 | 2:E:195:THR:HG21 | 1.81 | 0.62 |
| 2:B:114:ASP:HA | 2:B:117:VAL:HG12 | 1.81 | 0.62 |
| 4:G:174:THR:OG1 | 4:G:176:LEU:O | 2.16 | 0.62 |
| 4:G:220:THR:HA | 4:G:241:VAL:HG12 | 1.81 | 0.62 |
| 3:J:341:HIS:CD2 | 3:J:343:THR:HG1 | 2.16 | 0.62 |
| 2:C:73:GLY:O | 2:C:107:ARG:NH1 | 2.32 | 0.62 |
| 3:F:247:ALA:HB3 | 3:F:316:VAL:HG12 | 1.82 | 0.62 |
| 3:J:112:ARG:HH11 | 3:J:112:ARG:CG | 2.13 | 0.62 |
| 3:J:159:ARG:N | 3:J:234:GLN:OE1 | 2.30 | 0.62 |
| 2:E:392:LEU:HD12 | 2:E:392:LEU:C | 2.20 | 0.62 |
| 3:F:370:TRP:HA | 3:F:375:TRP:NE1 | 2.13 | 0.62 |
| 2:E:324:VAL:O | 2:E:327:SER:OG | 2.16 | 0.62 |
| 2:E:275:LEU:O | 2:E:279:GLY:N | 2.28 | 0.62 |
| 2:E:373:ARG:O | 2:E:376:VAL:HG12 | 1.99 | 0.62 |
| 3:J:343:THR:HG22 | 3:J:344:THR:H | 1.65 | 0.61 |
| 3:J:262:LYS:HD3 | 3:J:282:LEU:HD13 | 1.81 | 0.61 |
| 1:A:22:ASN:CB | 1:A:23:PRO:HD2 | 2.26 | 0.61 |
| 2:E:70:ALA:HB2 | 2:E:76:PRO:HA | 1.83 | 0.61 |
| 1:I:62:ASP:OD1 | 1:I:62:ASP:N | 2.32 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:35:PRO:HG2 | 3:J:95:GLU:HB3 | 1.81 | 0.61 |
| 4:G:47:MET:O | 4:G:47:MET:HG3 | 2.00 | 0.61 |
| 3:J:260:TRP:CE3 | 3:J:391:ALA:HA | 2.35 | 0.61 |
| 2:B:37:GLU:HB2 | 2:C:93:LEU:HD21 | 1.82 | 0.61 |
| 2:H:275:LEU:O | 2:H:278:LEU:N | 2.34 | 0.60 |
| 3:F:42:VAL:HG13 | 3:F:42:VAL:O | 2.01 | 0.60 |
| 3:J:317:VAL:HG12 | 3:J:340:ILE:HD13 | 1.82 | 0.60 |
| 1:A:26:VAL:HG22 | 1:A:26:VAL:O | 2.01 | 0.60 |
| 3:F:290:ARG:O | 3:F:294:ALA:N | 2.35 | 0.60 |
| 2:B:139:ALA:HB1 | 2:C:421:VAL:HG12 | 1.83 | 0.60 |
| 2:B:361:TYR:HE2 | 2:B:461:VAL:HG11 | 1.67 | 0.60 |
| 2:H:73:GLY:O | 2:H:107:ARG:NH2 | 2.34 | 0.60 |
| 2:H:263:LEU:HB2 | 2:H:264:TRP:CE3 | 2.36 | 0.60 |
| 2:H:46:VAL:HG13 | 2:H:47:GLN:HG2 | 1.84 | 0.60 |
| 1:I:34:THR:HG23 | 1:I:37:GLN:H | 1.66 | 0.60 |
| 4:D:47:MET:HG3 | 4:D:47:MET:O | 2.00 | 0.60 |
| 3:J:353:PRO:HG3 | 3:J:370:TRP:HD1 | 1.67 | 0.59 |
| 4:G:22:GLN:O | 4:G:23:THR:OG1 | 2.19 | 0.59 |
| 2:H:9:ILE:HD11 | 2:H:28:ALA:HB1 | 1.83 | 0.59 |
| 3:F:359:ILE:HB | 3:F:370:TRP:HB3 | 1.82 | 0.59 |
| 2:E:350:VAL:HG11 | 2:E:360:TRP:CE3 | 2.37 | 0.59 |
| 3:J:257:ASP:O | 3:J:259:SER:N | 2.35 | 0.59 |
| 2:B:66:ARG:NH2 | 3:F:389:GLU:OE2 | 2.25 | 0.59 |
| 3:J:399:ARG:HB2 | 3:J:400:TRP:CE3 | 2.37 | 0.59 |
| 2:B:155:ARG:NH1 | 2:B:160:ASP:H | 2.00 | 0.59 |
| 3:J:276:VAL:HG13 | 3:J:280:ARG:HD2 | 1.84 | 0.59 |
| 3:J:387:ALA:HA | 3:J:390:ALA:HB3 | 1.83 | 0.59 |
| 2:H:169:GLY:HA2 | 2:H:172:LEU:HD12 | 1.85 | 0.59 |
| 2:H:395:VAL:HG22 | 2:H:417:LEU:HD21 | 1.85 | 0.59 |
| 3:J:218:ILE:HG21 | 3:J:346:LEU:HG | 1.85 | 0.59 |
| 2:C:167:VAL:HG12 | 2:C:203:ALA:HB2 | 1.83 | 0.59 |
| 4:G:208:VAL:O | 4:G:212:ILE:HD12 | 2.03 | 0.59 |
| 4:D:208:VAL:O | 4:D:212:ILE:HD12 | 2.03 | 0.59 |
| 1:A:32:PHE:CE1 | 1:I:63:PRO:HG3 | 2.38 | 0.58 |
| 3:F:11:ARG:HH12 | 3:F:13:THR:HA | 1.68 | 0.58 |
| 2:E:41:ALA:HA | 2:E:44:ARG:HE | 1.68 | 0.58 |
| 1:A:58:ARG:HB3 | 3:F:106:ARG:HH11 | 1.69 | 0.58 |
| 3:J:260:TRP:CE2 | 3:J:390:ALA:HB1 | 2.38 | 0.58 |
| 2:E:350:VAL:HG21 | 2:E:363:VAL:HG21 | 1.84 | 0.58 |
| 4:D:91:PRO:HA | 4:D:94:VAL:HG12 | 1.86 | 0.58 |
| 2:E:11:ARG:HG2 | 2:E:28:ALA:HB2 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:J:3:ARG:HH21 | 3:J:398:SER:HA | 1.69 | 0.58 |
| 2:C:211:ASP:O | 2:C:216:ASN:ND2 | 2.36 | 0.58 |
| 2:C:287:ALA:O | 2:C:290:SER:OG | 2.18 | 0.58 |
| 2:C:335:ILE:HD11 | 2:C:377:TRP:CE2 | 2.39 | 0.58 |
| 2:C:196:ALA:HB3 | 2:C:227:TRP:HE1 | 1.69 | 0.58 |
| 1:A:18:PRO:CG | 3:J:110:VAL:HG12 | 2.34 | 0.58 |
| 2:H:322:ARG:HA | 2:H:325:ARG:HH11 | 1.69 | 0.57 |
| 3:J:215:ILE:HB | 3:J:340:ILE:HG13 | 1.85 | 0.57 |
| 2:E:238:ASP:OD1 | 2:E:239:ARG:N | 2.32 | 0.57 |
| 4:G:79:VAL:HG23 | 4:G:169:VAL:HG23 | 1.87 | 0.57 |
| 4:D:22:GLN:O | 4:D:23:THR:OG1 | 2.20 | 0.57 |
| 2:B:29:LEU:HD13 | 2:B:38:ILE:HG21 | 1.84 | 0.57 |
| 3:J:247:ALA:HB3 | 3:J:316:VAL:HA | 1.87 | 0.57 |
| 4:D:79:VAL:HG23 | 4:D:169:VAL:HG23 | 1.86 | 0.57 |
| 3:F:14:PRO:HG3 | 3:F:128:TRP:CD1 | 2.40 | 0.57 |
| 4:G:91:PRO:HA | 4:G:94:VAL:HG12 | 1.86 | 0.57 |
| 3:J:145:GLN:HG3 | 3:J:146:TRP:H | 1.69 | 0.57 |
| 4:D:82:VAL:O | 4:D:120:SER:OG | 2.20 | 0.57 |
| 4:G:259:ALA:O | 4:G:264:ARG:NH2 | 2.38 | 0.57 |
| 3:F:208:ASP:OD2 | 3:F:211:LYS:NZ | 2.37 | 0.57 |
| 4:G:82:VAL:O | 4:G:120:SER:OG | 2.20 | 0.57 |
| 2:H:151:SER:OG | 2:H:163:GLY:O | 2.23 | 0.57 |
| 2:E:10:VAL:O | 2:E:29:LEU:N | 2.34 | 0.56 |
| 2:H:40:PRO:HA | 2:H:43:GLN:HB2 | 1.87 | 0.56 |
| 2:C:241:ILE:HG13 | 2:C:243:VAL:HG12 | 1.86 | 0.56 |
| 2:E:11:ARG:HA | 2:E:28:ALA:HA | 1.86 | 0.56 |
| 3:J:244:LEU:HD11 | 3:J:315:LEU:HD23 | 1.87 | 0.56 |
| 3:F:218:ILE:HD13 | 3:F:359:ILE:HG23 | 1.87 | 0.56 |
| 3:F:257:ASP:O | 3:F:259:SER:N | 2.38 | 0.56 |
| 4:G:105:ASP:OD2 | 4:G:127:ASP:N | 2.39 | 0.56 |
| 2:E:401:PHE:HB3 | 2:E:406:ARG:HB3 | 1.86 | 0.56 |
| 2:H:331:GLN:NE2 | 2:H:382:CYS:SG | 2.78 | 0.56 |
| 3:J:283:THR:OG1 | 3:J:284:THR:N | 2.39 | 0.56 |
| 3:J:361:ARG:HH21 | 3:J:375:TRP:HZ3 | 1.53 | 0.56 |
| 4:D:259:ALA:O | 4:D:264:ARG:NH2 | 2.38 | 0.56 |
| 1:A:50:SER:OG | 1:A:50:SER:O | 2.23 | 0.56 |
| 3:F:229:ARG:HG2 | 3:F:260:TRP:CZ2 | 2.40 | 0.56 |
| 4:G:97:LEU:HD11 | 4:G:227:THR:HA | 1.88 | 0.56 |
| 1:A:13:PHE:CZ | 3:J:107:TYR:CD2 | 2.94 | 0.56 |
| 2:C:442:PRO:HA | 2:C:445:ARG:HD3 | 1.88 | 0.56 |
| 2:E:347:VAL:O | 2:E:351:SER:HB3 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:352:SER:OG | 2:B:353:ALA:N | 2.39 | 0.56 |
| 2:E:37:GLU:OE2 | 3:J:395:ARG:NH1 | 2.39 | 0.56 |
| 2:E:350:VAL:CG1 | 2:E:360:TRP:CZ3 | 2.84 | 0.56 |
| 2:H:327:SER:OG | 2:H:328:GLN:N | 2.38 | 0.56 |
| 3:J:26:PRO:CG | 3:J:175:ASP:HB2 | 2.35 | 0.56 |
| 4:D:105:ASP:OD2 | 4:D:127:ASP:N | 2.39 | 0.56 |
| 3:F:263:TRP:HB3 | 3:F:398:SER:HB3 | 1.86 | 0.56 |
| 4:G:50:THR:HA | 4:G:53:ILE:HD12 | 1.88 | 0.56 |
| 2:E:335:ILE:CG2 | 2:E:386:LEU:CD2 | 2.81 | 0.56 |
| 4:D:50:THR:HA | 4:D:53:ILE:HD12 | 1.88 | 0.56 |
| 4:D:83:ASP:N | 4:D:83:ASP:OD1 | 2.37 | 0.56 |
| 3:F:224:ALA:O | 3:F:228:ILE:HG13 | 2.06 | 0.56 |
| 2:H:39:LEU:HG | 2:H:40:PRO:HD3 | 1.88 | 0.56 |
| 2:B:35:LEU:O | 2:B:39:LEU:HD23 | 2.06 | 0.56 |
| 2:E:398:LEU:C | 2:E:398:LEU:HD23 | 2.27 | 0.55 |
| 3:J:27:PRO:CB | 3:J:28:PRO:HD2 | 2.36 | 0.55 |
| 2:H:151:SER:O | 2:H:154:HIS:HB3 | 2.06 | 0.55 |
| 3:J:220:GLU:O | 3:J:342:ARG:NH2 | 2.39 | 0.55 |
| 2:C:321:PRO:HB2 | 2:C:325:ARG:HH12 | 1.71 | 0.55 |
| 3:F:370:TRP:HE3 | 3:F:375:TRP:NE1 | 2.03 | 0.55 |
| 1:A:33:VAL:HG23 | 1:A:33:VAL:O | 2.06 | 0.55 |
| 2:E:82:THR:O | 2:E:86:VAL:HG12 | 2.06 | 0.55 |
| 2:H:440:SER:OG | 2:H:443:MET:N | 2.21 | 0.55 |
| 2:B:23:ARG:HH11 | 2:C:109:VAL:HG11 | 1.72 | 0.55 |
| 4:G:146:ASP:O | 4:G:150:VAL:HG23 | 2.07 | 0.55 |
| 3:J:130:HIS:O | 3:J:159:ARG:NE | 2.39 | 0.55 |
| 3:J:131:PRO:HB2 | 3:J:135:VAL:HB | 1.88 | 0.55 |
| 3:J:258:TRP:HE1 | 3:J:319:ASP:HB2 | 1.71 | 0.55 |
| 4:D:110:THR:HG1 | 4:D:121:TRP:HD1 | 1.54 | 0.55 |
| 2:B:227:TRP:HA | 2:B:230:ILE:HD12 | 1.87 | 0.55 |
| 3:J:158:LEU:HD23 | 3:J:231:TRP:CD1 | 2.42 | 0.55 |
| 2:B:155:ARG:HH11 | 2:B:160:ASP:H | 1.55 | 0.55 |
| 4:G:83:ASP:OD1 | 4:G:83:ASP:N | 2.37 | 0.55 |
| 2:E:126:GLN:CD | 2:E:126:GLN:H | 2.09 | 0.55 |
| 2:E:356:SER:HB3 | 2:E:359:ALA:HB2 | 1.88 | 0.55 |
| 3:F:146:TRP:CH2 | 3:F:266:HIS:HE1 | 2.25 | 0.55 |
| 3:J:245:GLY:O | 3:J:314:LEU:HA | 2.07 | 0.55 |
| 2:B:330:HIS:O | 2:B:334:VAL:HG23 | 2.07 | 0.54 |
| 2:H:471:LEU:HD23 | 2:H:472:VAL:HG23 | 1.89 | 0.54 |
| 3:J:129:SER:O | 3:J:130:HIS:ND1 | 2.39 | 0.54 |
| 3:J:158:LEU:HD23 | 3:J:231:TRP:HD1 | 1.72 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:19:ASP:OD1 | 2:B:19:ASP:N | 2.36 | 0.54 |
| 2:C:153:ALA:HA | 2:C:156:VAL:HG12 | 1.89 | 0.54 |
| 4:G:113:ASP:HB3 | 4:G:220:THR:HB | 1.89 | 0.54 |
| 4:D:113:ASP:HB3 | 4:D:220:THR:HB | 1.89 | 0.54 |
| 4:D:146:ASP:O | 4:D:150:VAL:HG23 | 2.07 | 0.54 |
| 3:F:3:ARG:HD2 | 3:F:401:ASP:HB2 | 1.90 | 0.54 |
| 4:D:97:LEU:HD11 | 4:D:227:THR:HA | 1.88 | 0.54 |
| 4:D:106:LYS:HE3 | 4:D:125:THR:HG21 | 1.90 | 0.54 |
| 2:B:125:ARG:NH1 | 2:B:126:GLN:OE1 | 2.39 | 0.54 |
| 2:B:350:VAL:HG22 | 2:B:359:ALA:HB1 | 1.89 | 0.54 |
| 3:F:247:ALA:HB2 | 3:F:293:LEU:HD21 | 1.88 | 0.54 |
| 2:E:227:TRP:HA | 2:E:230:ILE:HD12 | 1.90 | 0.54 |
| 3:J:174:LYS:HD2 | 3:J:174:LYS:O | 2.08 | 0.54 |
| 2:C:261:ALA:HA | 2:C:266:ILE:HG13 | 1.90 | 0.54 |
| 4:G:108:ARG:HA | 4:G:225:GLU:HA | 1.89 | 0.54 |
| 2:E:35:LEU:HD11 | 2:E:69:LEU:HD12 | 1.87 | 0.54 |
| 2:E:270:VAL:HA | 2:E:273:CYS:SG | 2.48 | 0.54 |
| 3:J:247:ALA:HB1 | 3:J:289:LEU:HD11 | 1.89 | 0.54 |
| 4:D:172:VAL:HG13 | 4:D:173:ASP:H | 1.73 | 0.54 |
| 2:C:164:GLN:NE2 | 2:C:206:LEU:O | 2.41 | 0.54 |
| 3:F:139:ILE:HD11 | 3:F:144:ARG:HB2 | 1.88 | 0.54 |
| 3:F:370:TRP:HE3 | 3:F:375:TRP:HE1 | 1.54 | 0.54 |
| 2:E:349:LEU:HD23 | 2:E:362:ILE:HG21 | 1.89 | 0.54 |
| 3:J:221:ALA:HA | 3:J:342:ARG:HH22 | 1.73 | 0.54 |
| 1:A:29:ARG:O | 1:A:29:ARG:HD3 | 2.07 | 0.53 |
| 2:B:35:LEU:HD12 | 2:B:35:LEU:H | 1.74 | 0.53 |
| 2:B:459:ILE:HD12 | 2:B:459:ILE:H | 1.72 | 0.53 |
| 3:F:229:ARG:HG2 | 3:F:260:TRP:HZ2 | 1.73 | 0.53 |
| 4:G:106:LYS:HE3 | 4:G:125:THR:HG21 | 1.90 | 0.53 |
| 4:G:172:VAL:HG13 | 4:G:173:ASP:H | 1.73 | 0.53 |
| 2:E:271:ILE:HD12 | 2:E:271:ILE:H | 1.73 | 0.53 |
| 3:J:104:TYR:O | 3:J:107:TYR:N | 2.33 | 0.53 |
| 2:B:33:LEU:N | 2:B:82:THR:OG1 | 2.42 | 0.53 |
| 2:B:154:HIS:HE1 | 2:B:160:ASP:HB3 | 1.70 | 0.53 |
| 3:F:133:PRO:HA | 3:F:136:LEU:HD22 | 1.90 | 0.53 |
| 2:E:442:PRO:O | 2:E:446:MET:N | 2.26 | 0.53 |
| 3:F:240:ASP:HB3 | 3:F:242:THR:HG22 | 1.90 | 0.53 |
| 3:J:156:LEU:HB2 | 3:J:210:ALA:HB2 | 1.90 | 0.53 |
| 4:D:108:ARG:HA | 4:D:225:GLU:HA | 1.89 | 0.53 |
| 4:D:224:LEU:HD12 | 4:D:225:GLU:H | 1.74 | 0.53 |
| 3:F:159:ARG:NE | 3:F:383:ASP:OD2 | 2.35 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:227:ALA:HB1 | 3:F:231:TRP:CZ3 | 2.42 | 0.53 |
| 4:G:224:LEU:HD12 | 4:G:225:GLU:H | 1.74 | 0.53 |
| 3:J:149:ASP:HB2 | 3:J:150:PRO:HD2 | 1.91 | 0.53 |
| 2:B:266:ILE:H | 2:B:266:ILE:HD12 | 1.73 | 0.53 |
| 2:E:458:LEU:O | 2:E:462:MET:N | 2.36 | 0.53 |
| 3:F:214:ARG:HB3 | 3:F:357:ARG:HG2 | 1.90 | 0.53 |
| 2:B:171:ALA:HB2 | 2:B:199:PRO:HB2 | 1.91 | 0.53 |
| 3:F:108:LEU:HD11 | 3:F:193:LEU:HD13 | 1.91 | 0.53 |
| 2:H:155:ARG:HH11 | 2:H:159:GLY:HA3 | 1.74 | 0.53 |
| 3:J:348:ASN:OD1 | 3:J:349:ARG:N | 2.40 | 0.53 |
| 3:F:368:GLU:HG2 | 3:F:377:PRO:HA | 1.91 | 0.53 |
| 3:J:3:ARG:HB3 | 3:J:401:ASP:HB2 | 1.91 | 0.53 |
| 3:J:264:LEU:HD22 | 3:J:397:LEU:HD23 | 1.90 | 0.53 |
| 2:B:317:LEU:H | 2:B:317:LEU:HD23 | 1.74 | 0.52 |
| 2:H:11:ARG:HA | 2:H:28:ALA:HA | 1.89 | 0.52 |
| 2:H:70:ALA:HB2 | 2:H:76:PRO:HA | 1.91 | 0.52 |
| 2:C:362:ILE:HD11 | 2:C:461:VAL:HG23 | 1.90 | 0.52 |
| 2:E:359:ALA:N | 2:E:465:LEU:HD11 | 2.25 | 0.52 |
| 2:E:374:ALA:HB2 | 2:E:386:LEU:HD12 | 1.92 | 0.52 |
| 2:H:273:CYS:HB3 | 2:H:462:MET:SD | 2.49 | 0.52 |
| 1:I:57:THR:O | 1:I:57:THR:OG1 | 2.28 | 0.52 |
| 2:B:163:GLY:O | 2:B:167:VAL:HG23 | 2.09 | 0.52 |
| 2:C:415:ALA:O | 2:C:419:VAL:HG23 | 2.09 | 0.52 |
| 2:B:181:VAL:HA | 2:B:184:ARG:HD2 | 1.91 | 0.52 |
| 1:A:11:ARG:HD2 | 3:J:29:GLN:HG3 | 1.92 | 0.52 |
| 2:C:70:ALA:HB2 | 2:C:76:PRO:HA | 1.91 | 0.52 |
| 3:F:361:ARG:HH12 | 3:F:363:ALA:HB2 | 1.74 | 0.52 |
| 3:F:136:LEU:O | 3:F:139:ILE:HG22 | 2.10 | 0.52 |
| 2:E:82:THR:HG23 | 2:E:85:THR:H | 1.75 | 0.52 |
| 2:H:153:ALA:O | 2:H:156:VAL:HG12 | 2.10 | 0.52 |
| 2:C:237:ASP:N | 2:C:237:ASP:OD1 | 2.41 | 0.52 |
| 4:G:61:ARG:HA | 4:G:64:ARG:NH1 | 2.25 | 0.51 |
| 2:C:13:ALA:HB2 | 3:F:395:ARG:HD3 | 1.91 | 0.51 |
| 4:G:77:THR:OG1 | 4:G:275:THR:HG22 | 2.10 | 0.51 |
| 2:E:391:TYR:CE1 | 2:E:417:LEU:CD2 | 2.94 | 0.51 |
| 4:D:77:THR:OG1 | 4:D:275:THR:HG22 | 2.10 | 0.51 |
| 2:E:30:PRO:HG3 | 2:H:72:ILE:HD12 | 1.91 | 0.51 |
| 3:J:123:ARG:NH1 | 3:J:202:ASP:O | 2.44 | 0.51 |
| 4:G:110:THR:HG1 | 4:G:121:TRP:HD1 | 1.59 | 0.51 |
| 1:A:63:PRO:O | 1:A:67:GLN:HG2 | 2.11 | 0.51 |
| 2:B:190:THR:O | 2:B:194:VAL:HG23 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:177:ALA:HB1 | 3:F:180:ILE:HG13 | 1.91 | 0.51 |
| 3:F:234:GLN:O | 3:F:238:TRP:HD1 | 1.94 | 0.51 |
| 1:A:10:ARG:HE | 3:J:31:PRO:HB3 | 1.75 | 0.51 |
| 3:J:260:TRP:CZ3 | 3:J:394:ALA:HB2 | 2.46 | 0.51 |
| 1:I:39:SER:O | 3:J:101:ARG:NH1 | 2.38 | 0.51 |
| 3:J:199:THR:OG1 | 3:J:201:ARG:NH2 | 2.44 | 0.51 |
| 2:H:198:VAL:HG13 | 2:H:199:PRO:HD3 | 1.92 | 0.50 |
| 4:D:61:ARG:HA | 4:D:64:ARG:NH1 | 2.25 | 0.50 |
| 3:F:11:ARG:HH22 | 3:F:14:PRO:HD2 | 1.76 | 0.50 |
| 3:F:244:LEU:N | 3:F:312:LYS:HZ3 | 2.09 | 0.50 |
| 3:F:251:PRO:HD3 | 3:F:320:ASP:OD1 | 2.12 | 0.50 |
| 3:J:361:ARG:NH2 | 3:J:375:TRP:HZ3 | 2.08 | 0.50 |
| 2:B:46:VAL:HG23 | 2:B:47:GLN:HG2 | 1.93 | 0.50 |
| 2:E:82:THR:CG2 | 2:E:85:THR:H | 2.24 | 0.50 |
| 2:C:41:ALA:HA | 2:C:44:ARG:NH2 | 2.27 | 0.50 |
| 2:E:350:VAL:CG1 | 2:E:360:TRP:CZ2 | 2.93 | 0.50 |
| 2:E:43:GLN:HE21 | 2:E:67:LEU:HD12 | 1.76 | 0.50 |
| 3:J:173:VAL:HG12 | 3:J:173:VAL:O | 2.11 | 0.50 |
| 3:J:359:ILE:HB | 3:J:370:TRP:HB3 | 1.93 | 0.50 |
| 2:B:152:VAL:O | 2:B:156:VAL:HG13 | 2.10 | 0.50 |
| 3:J:241:PRO:HA | 3:J:266:HIS:CE1 | 2.47 | 0.50 |
| 4:D:34:ILE:O | 4:D:38:ILE:HG12 | 2.12 | 0.50 |
| 3:F:139:ILE:N | 3:F:140:PRO:HD2 | 2.27 | 0.50 |
| 2:E:237:ASP:N | 2:E:237:ASP:OD1 | 2.44 | 0.50 |
| 3:J:264:LEU:HB2 | 3:J:267:VAL:CG2 | 2.35 | 0.50 |
| 2:B:13:ALA:HB1 | 2:B:24:LEU:HD11 | 1.94 | 0.50 |
| 2:B:455:ASP:N | 2:B:455:ASP:OD1 | 2.45 | 0.50 |
| 3:F:30:LEU:HD22 | 3:F:30:LEU:O | 2.12 | 0.50 |
| 3:F:248:LEU:HD23 | 3:F:249:ALA:N | 2.27 | 0.50 |
| 2:B:34:PRO:O | 2:B:37:GLU:HG2 | 2.12 | 0.49 |
| 3:F:317:VAL:HG12 | 3:F:340:ILE:HD13 | 1.94 | 0.49 |
| 2:B:127:TRP:O | 2:B:131:HIS:HD2 | 1.95 | 0.49 |
| 2:E:452:THR:HA | 2:E:455:ASP:OD2 | 2.12 | 0.49 |
| 2:C:471:LEU:HD23 | 2:C:472:VAL:HG23 | 1.95 | 0.49 |
| 3:J:21:THR:O | 3:J:21:THR:OG1 | 2.26 | 0.49 |
| 3:J:146:TRP:CE3 | 3:J:241:PRO:HD2 | 2.46 | 0.49 |
| 3:J:370:TRP:HA | 3:J:375:TRP:HE1 | 1.76 | 0.49 |
| 2:C:242:ALA:HB1 | 2:C:333:GLY:HA2 | 1.93 | 0.49 |
| 3:J:193:LEU:HD12 | 3:J:197:GLN:HG3 | 1.94 | 0.49 |
| 2:B:400:ALA:HA | 2:B:403:ILE:HG22 | 1.94 | 0.49 |
| 4:G:97:LEU:HB3 | 4:G:230:PRO:HD3 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:107:ARG:HD3 | 3:J:116:ARG:CZ | 2.42 | 0.49 |
| 3:J:148:ARG:HD2 | 3:J:238:TRP:HB3 | 1.93 | 0.49 |
| 4:D:206:ASP:OD1 | 4:D:206:ASP:N | 2.46 | 0.49 |
| 2:H:383:LYS:O | 2:H:386:LEU:N | 2.40 | 0.49 |
| 3:J:288:GLU:HG3 | 3:J:292:ARG:HH21 | 1.77 | 0.49 |
| 1:A:32:PHE:CZ | 1:I:63:PRO:HG2 | 2.48 | 0.49 |
| 4:G:34:ILE:O | 4:G:38:ILE:HG12 | 2.12 | 0.49 |
| 2:E:327:SER:O | 2:E:331:GLN:HG3 | 2.13 | 0.49 |
| 2:E:414:LEU:HD23 | 2:E:414:LEU:C | 2.32 | 0.49 |
| 3:J:230:ALA:HA | 3:J:385:MET:CB | 2.42 | 0.49 |
| 2:B:433:ILE:HD12 | 2:B:433:ILE:H | 1.77 | 0.49 |
| 3:F:369:ARG:NH2 | 3:F:378:CYS:SG | 2.86 | 0.49 |
| 2:E:265:VAL:HG22 | 2:E:267:SER:N | 2.28 | 0.49 |
| 3:F:277:GLY:HA3 | 3:F:280:ARG:HG3 | 1.95 | 0.49 |
| 2:E:34:PRO:HB2 | 2:E:36:ARG:HG2 | 1.94 | 0.49 |
| 3:F:132:GLU:OE2 | 3:F:134:GLU:HG2 | 2.13 | 0.48 |
| 3:F:247:ALA:HB1 | 3:F:289:LEU:HD21 | 1.93 | 0.48 |
| 2:B:25:THR:OG1 | 2:C:109:VAL:HG12 | 2.13 | 0.48 |
| 1:I:58:ARG:HA | 3:J:106:ARG:HG3 | 1.94 | 0.48 |
| 3:J:27:PRO:CB | 3:J:28:PRO:CD | 2.92 | 0.48 |
| 3:J:249:ALA:HB2 | 3:J:289:LEU:HB3 | 1.95 | 0.48 |
| 2:H:162:LEU:O | 2:H:166:ILE:HG12 | 2.13 | 0.48 |
| 3:J:267:VAL:O | 3:J:279:ALA:HB3 | 2.13 | 0.48 |
| 3:F:195:ASP:OD1 | 3:F:195:ASP:N | 2.47 | 0.48 |
| 3:F:248:LEU:HD12 | 3:F:261:LEU:HD12 | 1.96 | 0.48 |
| 4:D:208:VAL:O | 4:D:211:GLU:N | 2.46 | 0.48 |
| 2:B:398:LEU:O | 2:B:402:VAL:HG23 | 2.13 | 0.48 |
| 3:F:21:THR:HA | 3:F:170:ALA:HB3 | 1.94 | 0.48 |
| 3:F:255:SER:O | 3:F:255:SER:OG | 2.25 | 0.48 |
| 4:D:97:LEU:HB3 | 4:D:230:PRO:HD3 | 1.94 | 0.48 |
| 2:B:428:ALA:HB2 | 2:C:132:ILE:HG22 | 1.95 | 0.48 |
| 2:B:435:SER:HB2 | 2:B:438:THR:HG22 | 1.96 | 0.48 |
| 2:E:464:LEU:HD23 | 2:E:469:PHE:HE1 | 1.77 | 0.48 |
| 1:I:76:LEU:HA | 1:I:79:VAL:HG22 | 1.96 | 0.48 |
| 3:J:112:ARG:CG | 3:J:112:ARG:NH1 | 2.73 | 0.48 |
| 2:B:280:LEU:O | 2:B:284:VAL:HG22 | 2.13 | 0.48 |
| 2:E:25:THR:HG22 | 2:H:109:VAL:HB | 1.95 | 0.48 |
| 3:J:314:LEU:HD13 | 3:J:337:VAL:HG22 | 1.95 | 0.48 |
| 4:G:79:VAL:HA | 4:G:122:ILE:O | 2.13 | 0.48 |
| 2:H:138:LEU:HA | 2:H:141:ILE:HD12 | 1.96 | 0.48 |
| 2:C:320:LEU:N | 2:C:321:PRO:HD2 | 2.28 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:G:284:PRO:O | 4:G:285:LEU:HD23 | 2.14 | 0.47 |
| 3:J:276:VAL:HG13 | 3:J:277:GLY:H | 1.79 | 0.47 |
| 2:H:126:GLN:HG3 | 2:H:127:TRP:H | 1.79 | 0.47 |
| 2:B:213:GLY:HA3 | 2:B:216:ASN:ND2 | 2.29 | 0.47 |
| 2:C:423:VAL:HA | 2:C:426:VAL:HG12 | 1.95 | 0.47 |
| 3:F:16:THR:OG1 | 3:F:17:THR:N | 2.48 | 0.47 |
| 2:E:459:ILE:N | 2:E:460:PRO:HD2 | 2.29 | 0.47 |
| 2:H:76:PRO:HG2 | 2:H:100:PRO:HD3 | 1.97 | 0.47 |
| 3:J:250:ALA:O | 3:J:284:THR:HA | 2.14 | 0.47 |
| 3:J:260:TRP:CZ2 | 3:J:390:ALA:HB1 | 2.49 | 0.47 |
| 1:A:15:SER:OG | 3:J:103:ASP:OD2 | 2.28 | 0.47 |
| 3:J:145:GLN:HG3 | 3:J:146:TRP:N | 2.29 | 0.47 |
| 2:B:33:LEU:HB3 | 2:B:37:GLU:OE2 | 2.14 | 0.47 |
| 3:F:316:VAL:HG23 | 3:F:339:VAL:HG23 | 1.95 | 0.47 |
| 3:F:366:ARG:HB3 | 3:F:368:GLU:HG3 | 1.96 | 0.47 |
| 2:H:426:VAL:O | 2:H:430:ASN:HB3 | 2.15 | 0.47 |
| 3:J:225:ARG:HB3 | 3:J:258:TRP:CZ2 | 2.49 | 0.47 |
| 2:B:359:ALA:HA | 2:B:362:ILE:HG22 | 1.97 | 0.47 |
| 2:C:117:VAL:O | 2:C:120:SER:OG | 2.27 | 0.47 |
| 2:H:70:ALA:O | 2:H:94:LEU:HA | 2.15 | 0.47 |
| 2:H:239:ARG:C | 2:H:241:ILE:H | 2.18 | 0.47 |
| 2:H:320:LEU:N | 2:H:321:PRO:HD2 | 2.30 | 0.47 |
| 3:J:146:TRP:HB3 | 3:J:240:ASP:N | 2.30 | 0.47 |
| 3:J:240:ASP:HB2 | 3:J:242:THR:HG22 | 1.97 | 0.47 |
| 4:D:17:LEU:HA | 4:D:19:GLN:HE22 | 1.79 | 0.47 |
| 4:D:79:VAL:HA | 4:D:122:ILE:O | 2.13 | 0.47 |
| 1:A:60:LEU:HD23 | 1:A:60:LEU:HA | 1.75 | 0.47 |
| 2:C:125:ARG:H | 2:C:125:ARG:HD3 | 1.80 | 0.47 |
| 4:G:197:TYR:CD1 | 4:G:256:LEU:HB3 | 2.50 | 0.47 |
| 4:G:208:VAL:O | 4:G:211:GLU:N | 2.46 | 0.47 |
| 2:B:211:ASP:C | 2:B:213:GLY:H | 2.19 | 0.47 |
| 2:B:280:LEU:HD11 | 2:B:373:ARG:HH22 | 1.80 | 0.47 |
| 2:H:369:GLY:O | 2:H:373:ARG:NE | 2.48 | 0.47 |
| 3:J:353:PRO:HG3 | 3:J:370:TRP:CD1 | 2.49 | 0.47 |
| 4:D:216:PRO:HB2 | 4:D:217:ALA:H | 1.57 | 0.47 |
| 4:D:284:PRO:O | 4:D:285:LEU:HD23 | 2.14 | 0.47 |
| 2:B:16:ALA:HB2 | 2:B:96:LEU:HD22 | 1.96 | 0.47 |
| 2:C:127:TRP:O | 2:C:131:HIS:HD2 | 1.98 | 0.47 |
| 2:E:147:GLY:HA2 | 2:H:414:LEU:HD11 | 1.97 | 0.47 |
| 2:E:317:LEU:HD23 | 2:E:317:LEU:H | 1.80 | 0.47 |
| 4:D:197:TYR:CD1 | 4:D:256:LEU:HB3 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:11:ARG:NH2 | 3:F:277:GLY:HA2 | 2.30 | 0.46 |
| 3:F:18:ARG:O | 3:F:20:GLY:N | 2.48 | 0.46 |
| 3:F:212:LEU:HD13 | 3:F:356:GLU:HA | 1.96 | 0.46 |
| 2:B:141:ILE:HD12 | 2:B:195:THR:HG21 | 1.95 | 0.46 |
| 2:B:415:ALA:O | 2:B:419:VAL:HG23 | 2.15 | 0.46 |
| 2:C:36:ARG:HH21 | 2:C:79:LEU:HB3 | 1.80 | 0.46 |
| 2:C:38:ILE:HA | 2:C:41:ALA:HB3 | 1.96 | 0.46 |
| 2:C:455:ASP:OD1 | 2:C:455:ASP:N | 2.47 | 0.46 |
| 4:G:22:GLN:OE1 | 4:G:23:THR:HG23 | 2.14 | 0.46 |
| 4:G:206:ASP:OD1 | 4:G:206:ASP:N | 2.46 | 0.46 |
| 2:E:155:ARG:NH1 | 2:E:159:GLY:HA2 | 2.30 | 0.46 |
| 2:E:181:VAL:HG13 | 2:E:184:ARG:HB2 | 1.95 | 0.46 |
| 1:I:86:PHE:O | 1:I:90:LEU:HG | 2.15 | 0.46 |
| 4:G:108:ARG:O | 4:G:123:SER:N | 2.48 | 0.46 |
| 1:I:36:HIS:CG | 3:J:30:LEU:HD11 | 2.51 | 0.46 |
| 1:A:56:ASP:OD2 | 1:A:58:ARG:NH2 | 2.49 | 0.46 |
| 2:B:37:GLU:O | 2:B:40:PRO:HD2 | 2.16 | 0.46 |
| 3:F:28:PRO:O | 3:F:182:LEU:HD12 | 2.15 | 0.46 |
| 2:H:126:GLN:CG | 2:H:127:TRP:H | 2.29 | 0.46 |
| 3:J:216:THR:OG1 | 3:J:358:PRO:O | 2.33 | 0.46 |
| 4:D:96:TYR:HD1 | 4:D:99:ARG:HD3 | 1.80 | 0.46 |
| 3:F:145:GLN:O | 3:F:238:TRP:HA | 2.16 | 0.46 |
| 3:F:321:PRO:CB | 3:F:344:THR:HG23 | 2.45 | 0.46 |
| 3:F:378:CYS:O | 3:F:379:VAL:HG23 | 2.16 | 0.46 |
| 3:J:399:ARG:HB2 | 3:J:400:TRP:CZ3 | 2.50 | 0.46 |
| 4:D:22:GLN:OE1 | 4:D:23:THR:HG23 | 2.14 | 0.46 |
| 2:B:82:THR:O | 2:B:86:VAL:HG12 | 2.15 | 0.46 |
| 2:C:40:PRO:HB2 | 2:C:44:ARG:NH1 | 2.31 | 0.46 |
| 1:A:68:SER:O | 1:A:71:VAL:HG12 | 2.16 | 0.46 |
| 2:C:409:ALA:HA | 2:C:412:TRP:CD1 | 2.48 | 0.46 |
| 3:F:157:VAL:HA | 3:F:208:ASP:HA | 1.97 | 0.46 |
| 3:F:287:ALA:O | 3:F:291:GLU:HG2 | 2.15 | 0.46 |
| 4:G:17:LEU:HA | 4:G:19:GLN:HE22 | 1.79 | 0.46 |
| 2:E:339:VAL:HG21 | 2:E:386:LEU:HA | 1.98 | 0.46 |
| 3:J:16:THR:OG1 | 3:J:17:THR:N | 2.49 | 0.46 |
| 3:J:125:ALA:O | 3:J:128:TRP:N | 2.47 | 0.46 |
| 3:J:262:LYS:HZ2 | 3:J:280:ARG:NE | 2.14 | 0.46 |
| 4:D:112:ARG:HG3 | 4:D:221:TRP:CE2 | 2.51 | 0.46 |
| 1:A:60:LEU:HG | 3:F:106:ARG:HH12 | 1.80 | 0.46 |
| 2:B:143:LEU:HD22 | 2:C:421:VAL:HG21 | 1.96 | 0.46 |
| 3:F:123:ARG:NH1 | 3:F:202:ASP:O | 2.44 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:361:TYR:CD1 | 2:E:361:TYR:C | 2.89 | 0.46 |
| 2:H:100:PRO:HB3 | 4:D:161:GLU:OE1 | 2.15 | 0.46 |
| 1:A:13:PHE:CD1 | 1:A:13:PHE:C | 2.87 | 0.46 |
| 2:C:78:SER:HB3 | 2:C:81:ALA:HB2 | 1.97 | 0.46 |
| 4:G:52:ARG:HA | 4:G:55:ARG:HB2 | 1.98 | 0.46 |
| 4:G:96:TYR:HD1 | 4:G:99:ARG:HD3 | 1.80 | 0.46 |
| 4:G:97:LEU:HD22 | 4:G:230:PRO:HD3 | 1.98 | 0.46 |
| 2:E:68:SER:OG | 2:E:69:LEU:N | 2.46 | 0.46 |
| 3:J:148:ARG:HB2 | 3:J:238:TRP:O | 2.16 | 0.46 |
| 3:J:248:LEU:C | 3:J:289:LEU:HD22 | 2.37 | 0.46 |
| 3:J:281:TYR:CE1 | 3:J:292:ARG:HB3 | 2.51 | 0.46 |
| 3:J:314:LEU:O | 3:J:337:VAL:HA | 2.15 | 0.46 |
| 2:B:280:LEU:HD11 | 2:B:373:ARG:NH2 | 2.31 | 0.46 |
| 3:F:141:GLY:HA2 | 3:F:400:TRP:CH2 | 2.51 | 0.46 |
| 2:E:391:TYR:CE1 | 2:E:417:LEU:HD21 | 2.50 | 0.46 |
| 2:H:137:ALA:O | 2:H:140:LEU:N | 2.49 | 0.46 |
| 3:J:146:TRP:HZ2 | 3:J:397:LEU:HD11 | 1.81 | 0.46 |
| 3:F:327:ASP:OD1 | 3:F:327:ASP:N | 2.47 | 0.45 |
| 4:G:112:ARG:HG3 | 4:G:221:TRP:CE2 | 2.51 | 0.45 |
| 2:E:8:PRO:HD2 | 2:H:97:GLN:HE22 | 1.81 | 0.45 |
| 4:D:77:THR:HG23 | 4:D:125:THR:HG22 | 1.98 | 0.45 |
| 1:A:74:GLY:HA3 | 2:C:459:ILE:HD12 | 1.98 | 0.45 |
| 4:G:77:THR:HG23 | 4:G:125:THR:HG22 | 1.98 | 0.45 |
| 1:A:36:HIS:CE1 | 3:F:30:LEU:HD21 | 2.51 | 0.45 |
| 2:E:112:ILE:HD12 | 2:E:112:ILE:H | 1.82 | 0.45 |
| 2:E:121:GLU:O | 2:E:123:ARG:N | 2.47 | 0.45 |
| 2:E:206:LEU:HD23 | 2:E:206:LEU:HA | 1.77 | 0.45 |
| 3:J:104:TYR:O | 3:J:107:TYR:HB3 | 2.16 | 0.45 |
| 4:G:8:ALA:HB2 | 4:G:40:LEU:HD22 | 1.98 | 0.45 |
| 2:E:405:ASP:N | 2:E:405:ASP:OD1 | 2.49 | 0.45 |
| 1:I:85:CYS:HA | 1:I:88:PHE:HB3 | 1.98 | 0.45 |
| 3:J:174:LYS:HB3 | 3:J:174:LYS:HE2 | 1.46 | 0.45 |
| 3:J:346:LEU:HD21 | 3:J:361:ARG:HG3 | 1.98 | 0.45 |
| 2:B:319:ASP:O | 2:B:323:ARG:HG3 | 2.17 | 0.45 |
| 2:E:19:ASP:OD1 | 2:E:19:ASP:N | 2.43 | 0.45 |
| 2:H:269:ASP:HA | 2:H:349:LEU:HD22 | 1.98 | 0.45 |
| 3:J:263:TRP:HB2 | 3:J:394:ALA:HB1 | 1.97 | 0.45 |
| 2:C:449:PHE:O | 2:C:452:THR:OG1 | 2.32 | 0.45 |
| 2:E:82:THR:HG23 | 2:E:84:ASP:N | 2.24 | 0.45 |
| 3:J:378:CYS:O | 3:J:379:VAL:HG23 | 2.17 | 0.45 |
| 2:C:275:LEU:HD23 | 2:C:275:LEU:HA | 1.77 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:24:ILE:O | 3:F:173:VAL:HG23 | 2.17 | 0.45 |
| 4:G:175:PRO:HB3 | 4:G:221:TRP:CD2 | 2.52 | 0.45 |
| 2:E:36:ARG:HH22 | 2:E:80:ASP:HA | 1.81 | 0.45 |
| 2:E:374:ALA:O | 2:E:376:VAL:N | 2.49 | 0.45 |
| 2:H:254:VAL:HA | 2:H:257:VAL:HG12 | 1.98 | 0.45 |
| 2:H:417:LEU:O | 2:H:421:VAL:HG12 | 2.17 | 0.45 |
| 4:D:175:PRO:HB3 | 4:D:221:TRP:CD2 | 2.52 | 0.45 |
| 4:G:197:TYR:CG | 4:G:256:LEU:HD23 | 2.52 | 0.45 |
| 2:E:429:LEU:HD23 | 2:E:429:LEU:HA | 1.77 | 0.45 |
| 2:H:204:PHE:HB3 | 2:H:219:LEU:HG | 1.99 | 0.45 |
| 4:D:197:TYR:CG | 4:D:256:LEU:HD23 | 2.52 | 0.45 |
| 1:A:13:PHE:HZ | 3:J:107:TYR:CD2 | 2.35 | 0.45 |
| 1:A:34:THR:HG23 | 1:A:37:GLN:HG3 | 1.99 | 0.45 |
| 2:B:280:LEU:HD12 | 2:B:280:LEU:HA | 1.74 | 0.45 |
| 3:F:232:ILE:HD11 | 3:F:246:VAL:HG21 | 1.98 | 0.45 |
| 3:F:246:VAL:O | 3:F:267:VAL:HG23 | 2.17 | 0.45 |
| 3:F:377:PRO:C | 3:F:379:VAL:H | 2.19 | 0.45 |
| 3:J:240:ASP:N | 3:J:240:ASP:OD1 | 2.49 | 0.45 |
| 4:D:52:ARG:HA | 4:D:55:ARG:HB2 | 1.98 | 0.45 |
| 2:E:361:TYR:CD1 | 2:E:361:TYR:O | 2.70 | 0.45 |
| 2:E:361:TYR:O | 2:E:361:TYR:CG | 2.70 | 0.45 |
| 3:J:264:LEU:CD2 | 3:J:397:LEU:HB3 | 2.47 | 0.45 |
| 2:C:343:VAL:O | 2:C:347:VAL:HG12 | 2.17 | 0.44 |
| 3:F:267:VAL:O | 3:F:279:ALA:HB3 | 2.17 | 0.44 |
| 2:E:71:PRO:HD3 | 2:E:77:PHE:CZ | 2.52 | 0.44 |
| 2:E:372:LEU:HD12 | 2:E:372:LEU:HA | 1.77 | 0.44 |
| 2:H:29:LEU:HD11 | 2:H:38:ILE:HD12 | 1.98 | 0.44 |
| 2:H:273:CYS:HB3 | 2:H:462:MET:HE3 | 1.99 | 0.44 |
| 3:J:276:VAL:HG13 | 3:J:277:GLY:N | 2.33 | 0.44 |
| 3:J:285:SER:HB2 | 3:J:288:GLU:HB2 | 1.99 | 0.44 |
| 4:D:19:GLN:CD | 4:D:19:GLN:H | 2.20 | 0.44 |
| 3:F:229:ARG:HA | 3:F:232:ILE:HG22 | 1.99 | 0.44 |
| 3:F:264:LEU:HD23 | 3:F:267:VAL:HB | 1.99 | 0.44 |
| 4:G:229:SER:O | 4:G:231:ALA:N | 2.50 | 0.44 |
| 2:B:370:ALA:HA | 2:B:373:ARG:NH1 | 2.32 | 0.44 |
| 3:F:37:SER:HB3 | 3:F:40:ARG:HE | 1.81 | 0.44 |
| 3:F:257:ASP:O | 3:F:259:SER:OG | 2.29 | 0.44 |
| 3:F:261:LEU:HD23 | 3:F:261:LEU:HA | 1.73 | 0.44 |
| 2:E:411:LEU:H | 2:E:411:LEU:HG | 1.57 | 0.44 |
| 2:H:14:VAL:HA | 2:H:94:LEU:O | 2.17 | 0.44 |
| 3:J:3:ARG:NH2 | 3:J:265:PRO:HD3 | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:J:139:ILE:N | 3:J:140:PRO:HD2 | 2.32 | 0.44 |
| 4:D:172:VAL:HG13 | 4:D:173:ASP:N | 2.32 | 0.44 |
| 3:F:25:GLU:CD | 3:F:26:PRO:HD2 | 2.38 | 0.44 |
| 3:F:286:THR:OG1 | 3:F:287:ALA:N | 2.50 | 0.44 |
| 4:G:19:GLN:H | 4:G:19:GLN:CD | 2.20 | 0.44 |
| 2:E:33:LEU:HD22 | 2:E:34:PRO:HD2 | 1.99 | 0.44 |
| 2:E:124:ARG:NH2 | 2:E:126:GLN:HB2 | 2.32 | 0.44 |
| 1:I:39:SER:C | 3:J:101:ARG:HH12 | 2.18 | 0.44 |
| 4:D:50:THR:O | 4:D:53:ILE:HB | 2.18 | 0.44 |
| 4:D:229:SER:O | 4:D:231:ALA:N | 2.50 | 0.44 |
| 2:E:36:ARG:HH12 | 2:E:80:ASP:HB2 | 1.82 | 0.44 |
| 3:J:223:GLU:OE1 | 3:J:362:VAL:HG12 | 2.17 | 0.44 |
| 4:D:8:ALA:HB2 | 4:D:40:LEU:HD22 | 1.98 | 0.44 |
| 4:D:97:LEU:HD22 | 4:D:230:PRO:HD3 | 1.98 | 0.44 |
| 2:B:442:PRO:HA | 2:B:445:ARG:HD3 | 1.99 | 0.44 |
| 2:B:458:LEU:HA | 2:B:461:VAL:HG12 | 1.98 | 0.44 |
| 4:G:134:ALA:HB1 | 4:G:138:ARG:HH12 | 1.83 | 0.44 |
| 4:G:175:PRO:HB3 | 4:G:221:TRP:CG | 2.53 | 0.44 |
| 2:E:391:TYR:CD1 | 2:E:417:LEU:HD21 | 2.52 | 0.44 |
| 2:H:12:VAL:HG21 | 2:H:94:LEU:HD12 | 1.98 | 0.44 |
| 2:H:29:LEU:HD11 | 2:H:38:ILE:HG23 | 2.00 | 0.44 |
| 2:H:252:VAL:O | 2:H:255:LEU:HB3 | 2.17 | 0.44 |
| 3:J:220:GLU:C | 3:J:342:ARG:HH22 | 2.20 | 0.44 |
| 2:C:14:VAL:HA | 2:C:94:LEU:O | 2.17 | 0.44 |
| 3:F:233:ALA:HA | 3:F:236:VAL:HG22 | 1.99 | 0.44 |
| 2:E:278:LEU:O | 2:E:282:VAL:HG23 | 2.17 | 0.44 |
| 2:E:348:ALA:O | 2:E:351:SER:OG | 2.29 | 0.44 |
| 2:H:259:GLY:O | 2:H:263:LEU:HG | 2.18 | 0.44 |
| 3:J:107:TYR:O | 3:J:107:TYR:CD1 | 2.70 | 0.44 |
| 2:C:315:SER:OG | 2:C:316:VAL:N | 2.51 | 0.44 |
| 4:G:260:ARG:HD2 | 4:G:260:ARG:HA | 1.79 | 0.44 |
| 1:I:79:VAL:O | 1:I:82:LEU:HB3 | 2.18 | 0.44 |
| 3:J:112:ARG:O | 3:J:112:ARG:HG2 | 2.16 | 0.44 |
| 4:D:108:ARG:O | 4:D:123:SER:N | 2.48 | 0.44 |
| 1:A:13:PHE:CZ | 3:J:107:TYR:HD2 | 2.36 | 0.44 |
| 2:B:422:LEU:O | 2:B:426:VAL:HG22 | 2.17 | 0.44 |
| 2:C:341:LEU:HD23 | 2:C:341:LEU:HA | 1.76 | 0.44 |
| 3:F:12:LEU:HD12 | 3:F:12:LEU:H | 1.82 | 0.44 |
| 3:F:202:ASP:OD1 | 3:F:202:ASP:N | 2.51 | 0.44 |
| 4:G:172:VAL:HG13 | 4:G:173:ASP:N | 2.33 | 0.44 |
| 2:H:196:ALA:O | 2:H:200:VAL:HG23 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:60:LEU:HD23 | 1:I:60:LEU:HA | 1.89 | 0.44 |
| 4:D:123:SER:OG | 4:D:272:PRO:HB3 | 2.18 | 0.44 |
| 1:A:30:ARG:HD2 | 1:A:30:ARG:HA | 1.66 | 0.43 |
| 2:B:31:SER:OG | 2:B:32:GLU:N | 2.51 | 0.43 |
| 3:F:280:ARG:NH2 | 3:F:282:LEU:HD11 | 2.33 | 0.43 |
| 3:J:354:ASP:HB3 | 3:J:356:GLU:O | 2.18 | 0.43 |
| 3:F:200:VAL:HG12 | 3:F:201:ARG:O | 2.18 | 0.43 |
| 3:F:245:GLY:O | 3:F:315:LEU:N | 2.51 | 0.43 |
| 3:J:7:GLU:N | 3:J:7:GLU:OE1 | 2.52 | 0.43 |
| 1:A:10:ARG:NH2 | 3:J:31:PRO:HG3 | 2.32 | 0.43 |
| 1:A:15:SER:OG | 3:F:32:ARG:NH2 | 2.50 | 0.43 |
| 2:C:40:PRO:HB2 | 2:C:44:ARG:HH11 | 1.83 | 0.43 |
| 2:C:441:LEU:N | 2:C:442:PRO:HD2 | 2.33 | 0.43 |
| 2:E:375:ARG:HA | 2:E:375:ARG:HD3 | 1.65 | 0.43 |
| 2:E:379:SER:OG | 2:E:380:ALA:N | 2.51 | 0.43 |
| 2:E:447:VAL:HA | 2:E:450:LEU:HB3 | 2.01 | 0.43 |
| 3:J:4:LEU:O | 3:J:401:ASP:N | 2.50 | 0.43 |
| 4:D:175:PRO:HB3 | 4:D:221:TRP:CG | 2.53 | 0.43 |
| 2:C:445:ARG:HB3 | 2:C:449:PHE:CZ | 2.52 | 0.43 |
| 3:F:247:ALA:O | 3:F:317:VAL:HG22 | 2.18 | 0.43 |
| 3:F:281:TYR:CD2 | 3:F:293:LEU:HD11 | 2.54 | 0.43 |
| 2:E:119:PHE:CE2 | 2:H:321:PRO:HD3 | 2.54 | 0.43 |
| 2:B:238:ASP:OD1 | 2:B:238:ASP:N | 2.46 | 0.43 |
| 2:E:155:ARG:HD2 | 2:E:155:ARG:HA | 1.63 | 0.43 |
| 2:E:179:LEU:HD23 | 2:E:182:ARG:HH21 | 1.84 | 0.43 |
| 2:H:103:PRO:HD3 | 4:D:160:ARG:HB3 | 2.00 | 0.43 |
| 3:J:149:ASP:OD2 | 3:J:151:ARG:NH1 | 2.52 | 0.43 |
| 3:J:281:TYR:OH | 3:J:293:LEU:HG | 2.18 | 0.43 |
| 3:J:321:PRO:HA | 3:J:342:ARG:O | 2.18 | 0.43 |
| 2:C:88:VAL:HG11 | 2:C:94:LEU:HD11 | 2.00 | 0.43 |
| 4:G:50:THR:O | 4:G:53:ILE:HB | 2.18 | 0.43 |
| 2:E:273:CYS:HB3 | 2:E:462:MET:SD | 2.59 | 0.43 |
| 2:H:9:ILE:HA | 2:H:30:PRO:HA | 2.01 | 0.43 |
| 2:H:446:MET:O | 2:H:449:PHE:N | 2.51 | 0.43 |
| 3:J:260:TRP:CE3 | 3:J:394:ALA:HB2 | 2.53 | 0.43 |
| 2:E:99:VAL:CG2 | 2:E:100:PRO:HD2 | 2.44 | 0.43 |
| 4:D:90:LEU:O | 4:D:93:VAL:HG12 | 2.18 | 0.43 |
| 2:C:346:SER:OG | 2:C:363:VAL:HG23 | 2.19 | 0.43 |
| 4:G:80:LEU:O | 4:G:121:TRP:HA | 2.19 | 0.43 |
| 2:E:115:ALA:O | 2:H:324:VAL:HG21 | 2.19 | 0.43 |
| 2:H:197:LEU:HA | 2:H:200:VAL:HB | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:435:SER:O | 2:H:435:SER:OG | 2.36 | 0.43 |
| 3:J:173:VAL:HG21 | 3:J:194:LEU:HD11 | 2.01 | 0.43 |
| 4:D:103:THR:HG23 | 4:D:103:THR:O | 2.18 | 0.43 |
| 2:B:39:LEU:HA | 2:B:42:VAL:HG22 | 2.00 | 0.43 |
| 2:B:129:PRO:HA | 2:B:132:ILE:HD12 | 2.00 | 0.43 |
| 2:C:183:ASN:OD1 | 2:C:183:ASN:N | 2.47 | 0.43 |
| 3:F:222:ASP:OD1 | 3:F:222:ASP:N | 2.52 | 0.43 |
| 3:F:269:VAL:CG2 | 3:F:272:GLU:HB3 | 2.48 | 0.43 |
| 2:E:43:GLN:O | 2:E:47:GLN:HB2 | 2.18 | 0.43 |
| 2:H:330:HIS:O | 2:H:334:VAL:HG23 | 2.19 | 0.43 |
| 3:J:4:LEU:N | 3:J:399:ARG:O | 2.51 | 0.43 |
| 4:G:90:LEU:O | 4:G:93:VAL:HG12 | 2.17 | 0.43 |
| 4:G:103:THR:HG23 | 4:G:103:THR:O | 2.18 | 0.43 |
| 2:H:35:LEU:HD12 | 2:H:79:LEU:HA | 2.01 | 0.43 |
| 2:H:93:LEU:HD21 | 3:J:395:ARG:HH11 | 1.84 | 0.43 |
| 2:H:352:SER:OG | 2:H:353:ALA:N | 2.52 | 0.43 |
| 3:J:191:ARG:HD3 | 3:J:191:ARG:HA | 1.79 | 0.43 |
| 4:D:80:LEU:O | 4:D:121:TRP:HA | 2.19 | 0.43 |
| 2:C:151:SER:HB3 | 2:C:163:GLY:O | 2.19 | 0.42 |
| 2:E:9:ILE:HG13 | 2:E:29:LEU:C | 2.39 | 0.42 |
| 2:E:393:LEU:HD12 | 2:E:393:LEU:C | 2.39 | 0.42 |
| 2:H:320:LEU:HD12 | 2:H:320:LEU:HA | 1.83 | 0.42 |
| 2:H:370:ALA:HA | 2:H:373:ARG:HG2 | 2.00 | 0.42 |
| 2:C:317:LEU:HD23 | 2:C:317:LEU:HA | 1.74 | 0.42 |
| 3:F:349:ARG:HD3 | 3:F:349:ARG:HA | 1.72 | 0.42 |
| 4:G:27:ARG:O | 4:G:30:LEU:HB3 | 2.20 | 0.42 |
| 3:J:3:ARG:HH21 | 3:J:398:SER:CA | 2.32 | 0.42 |
| 3:J:347:PRO:HB2 | 3:J:350:GLU:HB2 | 2.01 | 0.42 |
| 4:D:134:ALA:HB1 | 4:D:138:ARG:HH12 | 1.83 | 0.42 |
| 2:C:386:LEU:HD23 | 2:C:386:LEU:HA | 1.77 | 0.42 |
| 3:F:155:PHE:CD2 | 3:F:156:LEU:HG | 2.55 | 0.42 |
| 3:F:208:ASP:OD1 | 3:F:209:VAL:N | 2.52 | 0.42 |
| 4:G:123:SER:OG | 4:G:272:PRO:HB3 | 2.18 | 0.42 |
| 4:G:224:LEU:HD12 | 4:G:225:GLU:N | 2.35 | 0.42 |
| 2:E:361:TYR:HE1 | 2:E:461:VAL:HG21 | 1.85 | 0.42 |
| 4:D:139:SER:OG | 4:D:141:ARG:HG3 | 2.20 | 0.42 |
| 1:A:78:LEU:HD23 | 1:A:79:VAL:HG23 | 2.01 | 0.42 |
| 2:B:118:ILE:HD13 | 2:B:118:ILE:HA | 1.86 | 0.42 |
| 3:F:214:ARG:O | 3:F:357:ARG:HA | 2.20 | 0.42 |
| 3:F:348:ASN:O | 3:F:349:ARG:NH1 | 2.44 | 0.42 |
| 2:E:172:LEU:O | 2:E:175:VAL:HB | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:220:ALA:O | 2:E:223:GLY:N | 2.51 | 0.42 |
| 2:E:403:ILE:HD12 | 2:E:403:ILE:HA | 1.77 | 0.42 |
| 3:J:287:ALA:HB2 | 3:J:290:ARG:HH21 | 1.83 | 0.42 |
| 4:D:40:LEU:HD23 | 4:D:41:LEU:HD22 | 2.02 | 0.42 |
| 2:B:161:LEU:HD23 | 2:B:161:LEU:HA | 1.81 | 0.42 |
| 2:C:11:ARG:HA | 2:C:28:ALA:HA | 2.00 | 0.42 |
| 2:C:280:LEU:O | 2:C:284:VAL:HG22 | 2.18 | 0.42 |
| 2:C:372:LEU:HD13 | 2:C:372:LEU:HA | 1.90 | 0.42 |
| 3:F:194:LEU:HD23 | 3:F:194:LEU:HA | 1.87 | 0.42 |
| 3:F:264:LEU:O | 3:F:267:VAL:HG12 | 2.20 | 0.42 |
| 2:E:32:GLU:CD | 2:H:22:GLY:H | 2.22 | 0.42 |
| 2:E:129:PRO:HA | 2:E:132:ILE:HD12 | 2.00 | 0.42 |
| 2:H:31:SER:OG | 2:H:83:LEU:HB2 | 2.19 | 0.42 |
| 2:B:10:VAL:O | 2:B:28:ALA:HA | 2.20 | 0.42 |
| 2:B:340:LEU:HA | 2:B:340:LEU:HD23 | 1.75 | 0.42 |
| 2:H:284:VAL:HG23 | 1:I:67:GLN:HB3 | 2.02 | 0.42 |
| 3:J:364:ASP:OD1 | 3:J:364:ASP:N | 2.50 | 0.42 |
| 4:D:175:PRO:HA | 4:D:221:TRP:CD1 | 2.54 | 0.42 |
| 2:E:321:PRO:HA | 2:E:324:VAL:HG12 | 2.01 | 0.42 |
| 3:J:281:TYR:HE1 | 3:J:292:ARG:HB3 | 1.84 | 0.42 |
| 3:J:281:TYR:CZ | 3:J:293:LEU:HG | 2.55 | 0.42 |
| 1:A:47:ARG:HD2 | 1:A:59:MET:HG3 | 2.01 | 0.42 |
| 2:B:103:PRO:HA | 2:B:104:PRO:HD3 | 1.85 | 0.42 |
| 2:B:401:PHE:O | 2:B:405:ASP:N | 2.53 | 0.42 |
| 2:E:456:ALA:HB1 | 4:D:6:ALA:HB2 | 2.02 | 0.42 |
| 2:H:41:ALA:O | 2:H:44:ARG:HB3 | 2.20 | 0.42 |
| 3:J:112:ARG:NH1 | 3:J:112:ARG:HB2 | 2.35 | 0.42 |
| 2:B:41:ALA:O | 2:B:45:ILE:HG12 | 2.18 | 0.42 |
| 3:F:158:LEU:HD11 | 3:F:235:ALA:HB2 | 2.01 | 0.42 |
| 2:H:350:VAL:HG23 | 2:H:363:VAL:HG11 | 2.01 | 0.42 |
| 2:C:204:PHE:HB3 | 2:C:219:LEU:HG | 2.02 | 0.42 |
| 3:F:158:LEU:HB3 | 3:F:231:TRP:HB2 | 2.02 | 0.42 |
| 4:G:40:LEU:HD23 | 4:G:41:LEU:HD22 | 2.01 | 0.42 |
| 4:G:175:PRO:HD2 | 4:G:271:ASN:HB3 | 2.02 | 0.42 |
| 4:G:176:LEU:HG | 4:G:177:PRO:HD2 | 2.01 | 0.42 |
| 2:E:31:SER:HB2 | 2:E:84:ASP:OD1 | 2.20 | 0.42 |
| 2:E:40:PRO:HB3 | 3:J:396:ARG:NH1 | 2.35 | 0.42 |
| 2:H:69:LEU:HB2 | 2:H:77:PHE:HD2 | 1.84 | 0.42 |
| 2:B:214:ALA:HB3 | 2:B:215:PRO:HD3 | 2.02 | 0.41 |
| 2:C:24:LEU:HD11 | 3:F:395:ARG:NH2 | 2.34 | 0.41 |
| 3:F:245:GLY:N | 3:F:313:HIS:O | 2.38 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:F:246:VAL:HA | 3:F:315:LEU:O | 2.20 | 0.41 |
| 2:E:272:GLY:HA2 | 2:E:275:LEU:HB2 | 2.01 | 0.41 |
| 2:H:11:ARG:N | 2:H:90:ASP:OD1 | 2.53 | 0.41 |
| 2:H:66:ARG:HA | 2:H:66:ARG:NE | 2.35 | 0.41 |
| 2:H:127:TRP:O | 2:H:131:HIS:HD2 | 2.02 | 0.41 |
| 2:B:412:TRP:N | 2:B:412:TRP:CD1 | 2.88 | 0.41 |
| 4:G:139:SER:OG | 4:G:141:ARG:HG3 | 2.20 | 0.41 |
| 2:E:459:ILE:HG23 | 2:E:460:PRO:HD3 | 2.02 | 0.41 |
| 2:H:225:ALA:HB2 | 2:H:251:GLY:HA3 | 2.02 | 0.41 |
| 2:H:299:PRO:HG2 | 1:I:41:TRP:CZ3 | 2.55 | 0.41 |
| 3:J:244:LEU:HD12 | 3:J:313:HIS:O | 2.20 | 0.41 |
| 4:D:160:ARG:HG3 | 4:D:166:VAL:HG22 | 2.02 | 0.41 |
| 2:B:142:GLY:O | 2:B:146:VAL:HG12 | 2.20 | 0.41 |
| 3:F:346:LEU:HD23 | 3:F:346:LEU:H | 1.85 | 0.41 |
| 4:G:160:ARG:HG3 | 4:G:166:VAL:HG22 | 2.02 | 0.41 |
| 2:E:138:LEU:HD23 | 2:E:138:LEU:HA | 1.81 | 0.41 |
| 2:E:386:LEU:H | 2:E:386:LEU:HG | 1.45 | 0.41 |
| 2:H:152:VAL:O | 2:H:156:VAL:N | 2.52 | 0.41 |
| 3:J:19:LYS:HD2 | 3:J:168:ASP:OD2 | 2.21 | 0.41 |
| 4:D:27:ARG:O | 4:D:30:LEU:HB3 | 2.19 | 0.41 |
| 2:C:204:PHE:O | 2:C:219:LEU:HD23 | 2.20 | 0.41 |
| 4:G:175:PRO:HA | 4:G:221:TRP:CD1 | 2.55 | 0.41 |
| 4:G:216:PRO:HB2 | 4:G:217:ALA:H | 1.57 | 0.41 |
| 2:E:389:HIS:ND1 | 2:E:389:HIS:C | 2.73 | 0.41 |
| 2:H:357:PRO:O | 2:H:361:TYR:N | 2.53 | 0.41 |
| 3:J:148:ARG:CD | 3:J:238:TRP:HB3 | 2.50 | 0.41 |
| 3:J:149:ASP:OD2 | 3:J:151:ARG:NH2 | 2.53 | 0.41 |
| 3:J:264:LEU:HD23 | 3:J:264:LEU:HA | 1.68 | 0.41 |
| 2:B:112:ILE:HA | 2:B:115:ALA:HB3 | 2.02 | 0.41 |
| 2:B:316:VAL:HG22 | 2:B:317:LEU:H | 1.86 | 0.41 |
| 2:C:175:VAL:HG12 | 2:C:176:ILE:HD13 | 2.03 | 0.41 |
| 2:E:161:LEU:HD13 | 2:E:161:LEU:HA | 1.92 | 0.41 |
| 2:E:214:ALA:HB3 | 2:E:215:PRO:HD3 | 2.02 | 0.41 |
| 2:E:263:LEU:HD12 | 2:E:264:TRP:N | 2.35 | 0.41 |
| 2:H:435:SER:OG | 2:H:437:ASP:OD1 | 2.29 | 0.41 |
| 4:D:49:LEU:O | 4:D:53:ILE:HG13 | 2.20 | 0.41 |
| 4:D:97:LEU:CD2 | 4:D:230:PRO:HD3 | 2.51 | 0.41 |
| 4:D:176:LEU:HG | 4:D:177:PRO:HD2 | 2.01 | 0.41 |
| 2:B:123:ARG:CG | 2:B:125:ARG:HB3 | 2.49 | 0.41 |
| 3:F:253:LEU:O | 3:F:259:SER:N | 2.47 | 0.41 |
| 2:E:283:THR:HG21 | 2:E:373:ARG:HH11 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:361:TYR:HD2 | 2:H:461:VAL:HG11 | 1.84 | 0.41 |
| 3:J:262:LYS:HE2 | 3:J:282:LEU:HB2 | 2.02 | 0.41 |
| 2:B:26:GLU:H | 2:B:26:GLU:HG3 | 1.73 | 0.41 |
| 2:C:437:ASP:OD1 | 2:C:438:THR:N | 2.54 | 0.41 |
| 4:G:159:LEU:HD23 | 4:G:166:VAL:HG11 | 2.03 | 0.41 |
| 2:H:226:ALA:O | 2:H:230:ILE:HG13 | 2.20 | 0.41 |
| 4:D:108:ARG:HG3 | 4:D:225:GLU:HB2 | 2.02 | 0.41 |
| 2:B:469:PHE:CE1 | 4:G:14:ALA:HA | 2.56 | 0.41 |
| 2:C:16:ALA:HB3 | 2:C:21:GLY:O | 2.21 | 0.41 |
| 2:C:96:LEU:HD23 | 2:C:96:LEU:HA | 1.80 | 0.41 |
| 2:H:413:ALA:O | 2:H:416:ALA:N | 2.54 | 0.41 |
| 3:J:269:VAL:HG13 | 3:J:279:ALA:CB | 2.51 | 0.41 |
| 4:D:175:PRO:HD2 | 4:D:271:ASN:HB3 | 2.02 | 0.41 |
| 2:B:237:ASP:OD1 | 2:B:238:ASP:N | 2.52 | 0.41 |
| 2:B:266:ILE:HG22 | 2:B:270:VAL:HG11 | 2.02 | 0.41 |
| 2:B:373:ARG:HB2 | 2:B:386:LEU:HD13 | 2.03 | 0.41 |
| 2:C:79:LEU:HD12 | 2:C:79:LEU:HA | 1.97 | 0.41 |
| 3:F:93:ARG:H | 3:F:93:ARG:HD3 | 1.86 | 0.41 |
| 3:F:364:ASP:OD1 | 3:F:365:GLY:N | 2.52 | 0.41 |
| 4:G:173:ASP:HB2 | 4:G:221:TRP:HH2 | 1.86 | 0.41 |
| 4:G:207:GLU:N | 4:G:207:GLU:OE1 | 2.54 | 0.41 |
| 2:E:35:LEU:HD23 | 2:E:35:LEU:O | 2.21 | 0.41 |
| 2:E:181:VAL:HG12 | 2:E:181:VAL:O | 2.20 | 0.41 |
| 2:E:350:VAL:HG12 | 2:E:360:TRP:CH2 | 2.54 | 0.41 |
| 2:H:242:ALA:O | 2:H:244:PHE:N | 2.53 | 0.41 |
| 2:H:337:ALA:O | 2:H:341:LEU:HG | 2.20 | 0.41 |
| 3:J:107:TYR:CD1 | 3:J:107:TYR:C | 2.94 | 0.41 |
| 3:J:367:ILE:HG13 | 3:J:382:ALA:HB2 | 2.02 | 0.41 |
| 4:D:159:LEU:HD23 | 4:D:166:VAL:HG11 | 2.02 | 0.41 |
| 4:D:170:GLU:OE1 | 4:D:170:GLU:N | 2.54 | 0.41 |
| 4:D:175:PRO:HA | 4:D:221:TRP:NE1 | 2.36 | 0.41 |
| 4:D:270:LEU:HD12 | 4:D:270:LEU:HA | 1.96 | 0.41 |
| 1:A:9:ASP:HB3 | 1:A:10:ARG:H | 1.64 | 0.41 |
| 1:A:61:VAL:O | 1:A:63:PRO:HD3 | 2.21 | 0.41 |
| 3:F:18:ARG:HH21 | 3:F:118:HIS:CD2 | 2.39 | 0.41 |
| 2:E:36:ARG:NH2 | 2:E:80:ASP:HA | 2.36 | 0.41 |
| 3:J:2:SER:OG | 3:J:3:ARG:N | 2.54 | 0.41 |
| 3:J:146:TRP:CD2 | 3:J:241:PRO:HD2 | 2.56 | 0.41 |
| 3:J:268:ASP:OD1 | 3:J:268:ASP:N | 2.47 | 0.41 |
| 3:F:132:GLU:HA | 3:F:159:ARG:CZ | 2.52 | 0.40 |
| 4:G:170:GLU:N | 4:G:170:GLU:OE1 | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:148:THR:OG1 | 2:E:199:PRO:HB3 | 2.20 | 0.40 |
| 3:J:183:GLU:CD | 3:J:184:PRO:HD2 | 2.42 | 0.40 |
| 4:D:121:TRP:CE3 | 4:D:172:VAL:HG23 | 2.56 | 0.40 |
| 2:E:107:ARG:HG2 | 2:E:108:ILE:H | 1.85 | 0.40 |
| 2:E:197:LEU:HB3 | 2:E:227:TRP:HD1 | 1.86 | 0.40 |
| 2:H:238:ASP:CG | 2:H:239:ARG:H | 2.25 | 0.40 |
| 4:D:224:LEU:HD12 | 4:D:225:GLU:N | 2.35 | 0.40 |
| 2:B:119:PHE:HE2 | 2:C:321:PRO:HD3 | 1.87 | 0.40 |
| 3:F:92:MET:SD | 3:F:92:MET:O | 2.79 | 0.40 |
| 3:F:148:ARG:HD2 | 3:F:239:HIS:NE2 | 2.36 | 0.40 |
| 4:G:97:LEU:CD2 | 4:G:230:PRO:HD3 | 2.51 | 0.40 |
| 2:E:356:SER:HB3 | 2:E:359:ALA:CB | 2.51 | 0.40 |
| 2:E:374:ALA:C | 2:E:376:VAL:H | 2.25 | 0.40 |
| 2:E:397:LEU:O | 2:E:400:ALA:HB3 | 2.21 | 0.40 |
| 4:D:259:ALA:HB3 | 4:D:264:ARG:HD3 | 2.02 | 0.40 |
| 4:D:260:ARG:HD2 | 4:D:260:ARG:HA | 1.79 | 0.40 |
| 2:H:271:ILE:O | 2:H:274:ALA:HB3 | 2.22 | 0.40 |
| 3:J:383:ASP:OD1 | 3:J:383:ASP:N | 2.55 | 0.40 |
| 1:A:17:THR:O | 3:F:179:GLU:HB3 | 2.21 | 0.40 |
| 2:B:358:TRP:HB2 | 2:B:465:LEU:HD13 | 2.03 | 0.40 |
| 2:B:387:LEU:HD23 | 2:B:387:LEU:HA | 1.86 | 0.40 |
| 2:B:459:ILE:N | 2:B:460:PRO:HD2 | 2.36 | 0.40 |
| 3:F:4:LEU:HD12 | 3:F:400:TRP:CD1 | 2.56 | 0.40 |
| 4:G:108:ARG:HG3 | 4:G:225:GLU:HB2 | 2.03 | 0.40 |
| 3:J:180:ILE:HA | 3:J:180:ILE:HD12 | 1.69 | 0.40 |
| 3:J:262:LYS:NZ | 3:J:282:LEU:HB2 | 2.36 | 0.40 |
| 4:D:173:ASP:HB2 | 4:D:221:TRP:HH2 | 1.86 | 0.40 |
| 4:D:232:GLU:OE1 | 4:D:284:PRO:HB3 | 2.22 | 0.40 |
| 4:D:234:LEU:HB3 | 4:D:282:ALA:HB1 | 2.04 | 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 | 79/518 (15%) | 68 (86%) | 6 (8%) | 5 (6%) | 1 17 |
| 1 | I | 57/518 (11%) | 55 (96%) | 2 (4%) | 0 | 100 100 |
| 2 | B | 421/475 (89%) | 384 (91%) | 37 (9%) | 0 | 100 100 |
| 2 | C | 434/475 (91%) | 386 (89%) | 47 (11%) | 1 (0%) | 47 78 |
| 2 | E | 421/475 (89%) | 362 (86%) | 58 (14%) | 1 (0%) | 47 78 |
| 2 | H | 434/475 (91%) | 371 (86%) | 63 (14%) | 0 | 100 100 |
| 3 | F | 326/449 (73%) | 263 (81%) | 62 (19%) | 1 (0%) | 41 74 |
| 3 | J | 314/449 (70%) | 256 (82%) | 55 (18%) | 3 (1%) | 15 51 |
| 4 | D | 225/309 (73%) | 196 (87%) | 29 (13%) | 0 | 100 100 |
| 4 | G | 225/309 (73%) | 196 (87%) | 29 (13%) | 0 | 100 100 |
| All | All | 2936/4452 (66%) | 2537 (86%) | 388 (13%) | 11 (0%) | 38 69 |

All (11) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 22 | ASN |
| 1 | A | 18 | PRO |
| 1 | A | 26 | VAL |
| 3 | F | 258 | TRP |
| 2 | C | 242 | ALA |
| 2 | E | 375 | ARG |
| 3 | J | 258 | TRP |
| 3 | J | 181 | ASP |
| 3 | J | 174 | LYS |
| 1 | A | 23 | PRO |
| 1 | A | 19 | VAL |

### 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 | 70/398 (18%) | 60 (86%) | 10 (14%) | 3 19 |
| 1 | I | 50/398 (13%) | 49 (98%) | 1 (2%) | 55 74 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 2 | B | 305/342 (89%) | 304 (100%) | 1 (0%) | 92 96 |
| 2 | C | 319/342 (93%) | 318 (100%) | 1 (0%) | 92 96 |
| 2 | E | 305/342 (89%) | 286 (94%) | 19 (6%) | 18 49 |
| 2 | H | 319/342 (93%) | 318 (100%) | 1 (0%) | 92 96 |
| 3 | F | 281/369 (76%) | 271 (96%) | 10 (4%) | 35 63 |
| 3 | J | 270/369 (73%) | 257 (95%) | 13 (5%) | 25 56 |
| 4 | D | 192/241 (80%) | 155 (81%) | 37 (19%) | 1 9 |
| 4 | G | 192/241 (80%) | 155 (81%) | 37 (19%) | 1 9 |
| All | All | 2303/3384 (68%) | 2173 (94%) | 130 (6%) | 25 53 |

All (130) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 10 | ARG |
| 1 | A | 12 | SER |
| 1 | A | 13 | PHE |
| 1 | A | 17 | THR |
| 1 | A | 19 | VAL |
| 1 | A | 21 | GLU |
| 1 | A | 27 | GLN |
| 1 | A | 28 | TYR |
| 1 | A | 29 | ARG |
| 1 | A | 34 | THR |
| 2 | B | 125 | ARG |
| 2 | C | 125 | ARG |
| 3 | F | 30 | LEU |
| 3 | F | 33 | VAL |
| 3 | F | 37 | SER |
| 3 | F | 39 | LEU |
| 3 | F | 40 | ARG |
| 3 | F | 41 | ARG |
| 3 | F | 43 | LEU |
| 3 | F | 92 | MET |
| 3 | F | 93 | ARG |
| 3 | F | 143 | ARG |
| 4 | G | 1 | MET |
| 4 | G | 5 | ILE |
| 4 | G | 7 | LEU |
| 4 | G | 12 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | G | 13 | VAL |
| 4 | G | 21 | TRP |
| 4 | G | 24 | THR |
| 4 | G | 25 | THR |
| 4 | G | 27 | ARG |
| 4 | G | 29 | VAL |
| 4 | G | 32 | VAL |
| 4 | G | 33 | SER |
| 4 | G | 47 | MET |
| 4 | G | 51 | THR |
| 4 | G | 80 | LEU |
| 4 | G | 83 | ASP |
| 4 | G | 97 | LEU |
| 4 | G | 98 | ASP |
| 4 | G | 106 | LYS |
| 4 | G | 125 | THR |
| 4 | G | 130 | ASP |
| 4 | G | 151 | VAL |
| 4 | G | 161 | GLU |
| 4 | G | 165 | THR |
| 4 | G | 167 | THR |
| 4 | G | 168 | VAL |
| 4 | G | 178 | VAL |
| 4 | G | 194 | VAL |
| 4 | G | 200 | LYS |
| 4 | G | 208 | VAL |
| 4 | G | 232 | GLU |
| 4 | G | 237 | VAL |
| 4 | G | 238 | CYS |
| 4 | G | 273 | LEU |
| 4 | G | 274 | SER |
| 4 | G | 276 | GLU |
| 4 | G | 285 | LEU |
| 2 | E | 361 | TYR |
| 2 | E | 362 | ILE |
| 2 | E | 363 | VAL |
| 2 | E | 372 | LEU |
| 2 | E | 373 | ARG |
| 2 | E | 383 | LYS |
| 2 | E | 386 | LEU |
| 2 | E | 387 | LEU |
| 2 | E | 389 | HIS |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | E | 390 | SER |
| 2 | E | 392 | LEU |
| 2 | E | 393 | LEU |
| 2 | E | 395 | VAL |
| 2 | E | 402 | VAL |
| 2 | E | 403 | ILE |
| 2 | E | 405 | ASP |
| 2 | E | 407 | TYR |
| 2 | E | 411 | LEU |
| 2 | E | 417 | LEU |
| 2 | H | 125 | ARG |
| 1 | I | 88 | PHE |
| 3 | J | 23 | THR |
| 3 | J | 25 | GLU |
| 3 | J | 106 | ARG |
| 3 | J | 107 | TYR |
| 3 | J | 108 | LEU |
| 3 | J | 110 | VAL |
| 3 | J | 111 | VAL |
| 3 | J | 112 | ARG |
| 3 | J | 115 | VAL |
| 3 | J | 153 | ARG |
| 3 | J | 174 | LYS |
| 3 | J | 176 | THR |
| 3 | J | 180 | ILE |
| 4 | D | 1 | MET |
| 4 | D | 5 | ILE |
| 4 | D | 7 | LEU |
| 4 | D | 12 | VAL |
| 4 | D | 13 | VAL |
| 4 | D | 21 | TRP |
| 4 | D | 24 | THR |
| 4 | D | 25 | THR |
| 4 | D | 27 | ARG |
| 4 | D | 29 | VAL |
| 4 | D | 32 | VAL |
| 4 | D | 33 | SER |
| 4 | D | 47 | MET |
| 4 | D | 51 | THR |
| 4 | D | 80 | LEU |
| 4 | D | 83 | ASP |
| 4 | D | 97 | LEU |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | D | 98 | ASP |
| 4 | D | 106 | LYS |
| 4 | D | 125 | THR |
| 4 | D | 130 | ASP |
| 4 | D | 151 | VAL |
| 4 | D | 161 | GLU |
| 4 | D | 165 | THR |
| 4 | D | 167 | THR |
| 4 | D | 168 | VAL |
| 4 | D | 178 | VAL |
| 4 | D | 194 | VAL |
| 4 | D | 200 | LYS |
| 4 | D | 208 | VAL |
| 4 | D | 232 | GLU |
| 4 | D | 237 | VAL |
| 4 | D | 238 | CYS |
| 4 | D | 273 | LEU |
| 4 | D | 274 | SER |
| 4 | D | 276 | GLU |
| 4 | D | 285 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 131 | HIS |
| 2 | B | 154 | HIS |
| 2 | B | 288 | GLN |
| 2 | C | 126 | GLN |
| 2 | C | 131 | HIS |
| 2 | C | 164 | GLN |
| 2 | C | 331 | GLN |
| 3 | F | 122 | GLN |
| 3 | F | 376 | GLN |
| 4 | G | 19 | GLN |
| 2 | E | 43 | GLN |
| 2 | E | 131 | HIS |
| 2 | E | 216 | ASN |
| 2 | H | 97 | GLN |
| 2 | H | 131 | HIS |
| 2 | H | 216 | ASN |
| 3 | J | 187 | HIS |
| 3 | J | 271 | ASN |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | J | 371 | GLN |
| 3 | J | 376 | GLN |
| 4 | D | 19 | GLN |

### 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.

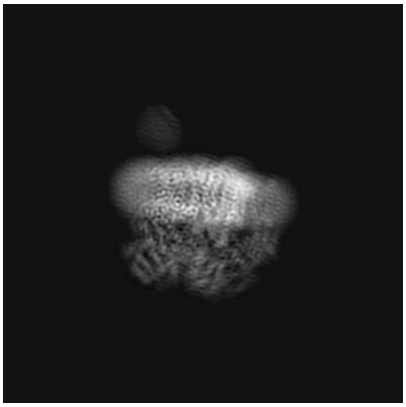
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0862. These allow visual inspection of the internal detail of the map and identification of artifacts.

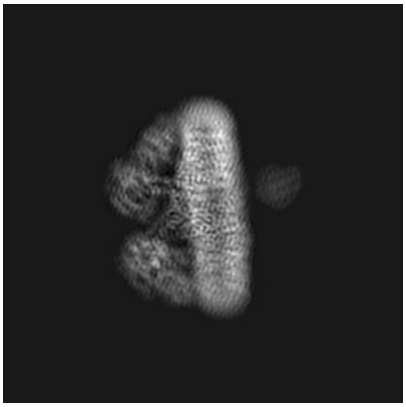
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

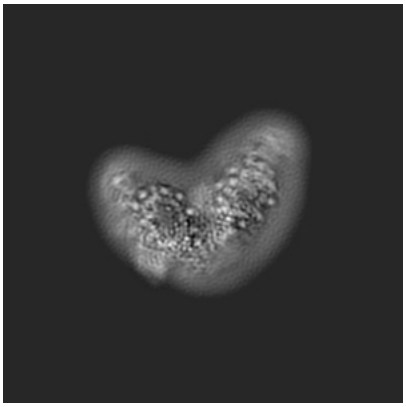
### 6.1.1 Primary map



X



Y

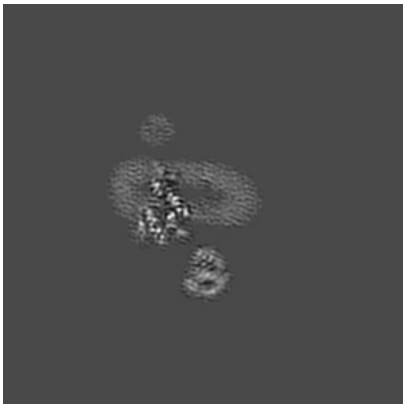


Z

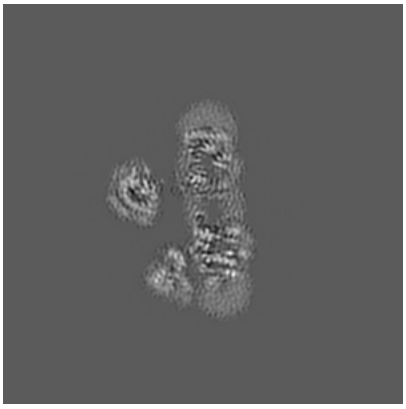
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

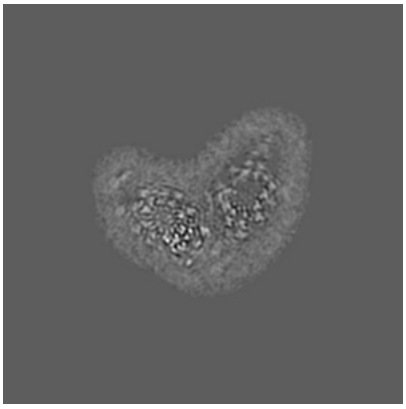
### 6.2.1 Primary map



X Index: 220



Y Index: 220

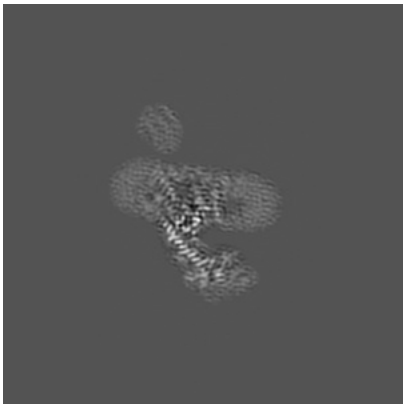


Z Index: 220

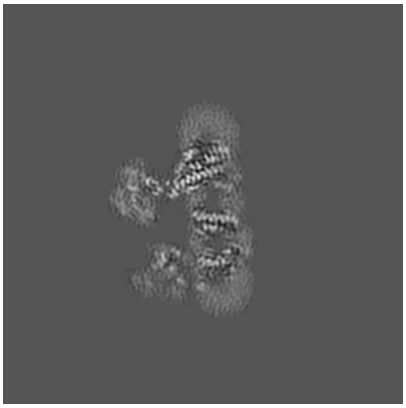
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

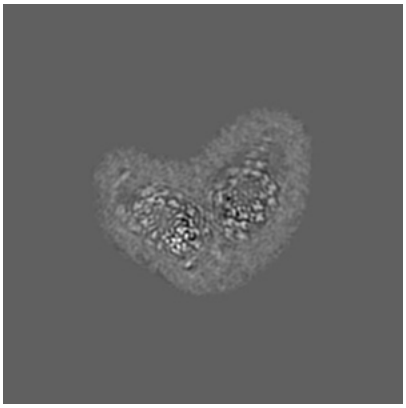
### 6.3.1 Primary map



X Index: 244



Y Index: 211

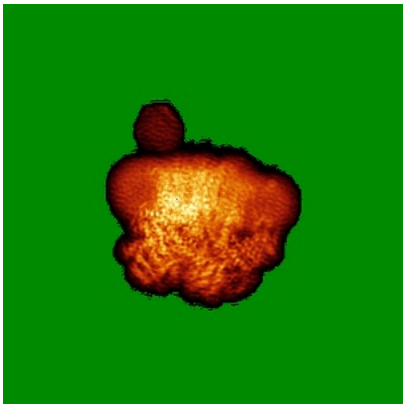


Z Index: 218

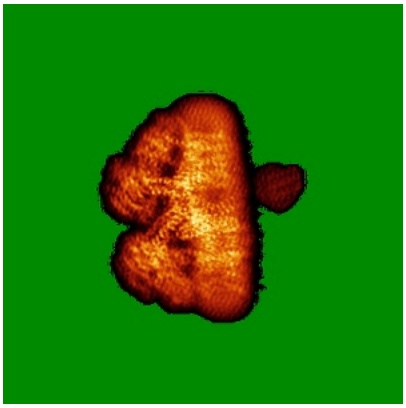
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) (i)

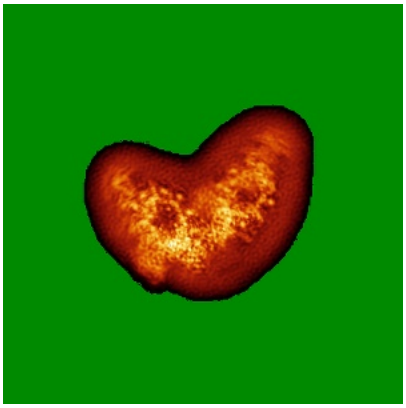
### 6.4.1 Primary map



X



Y

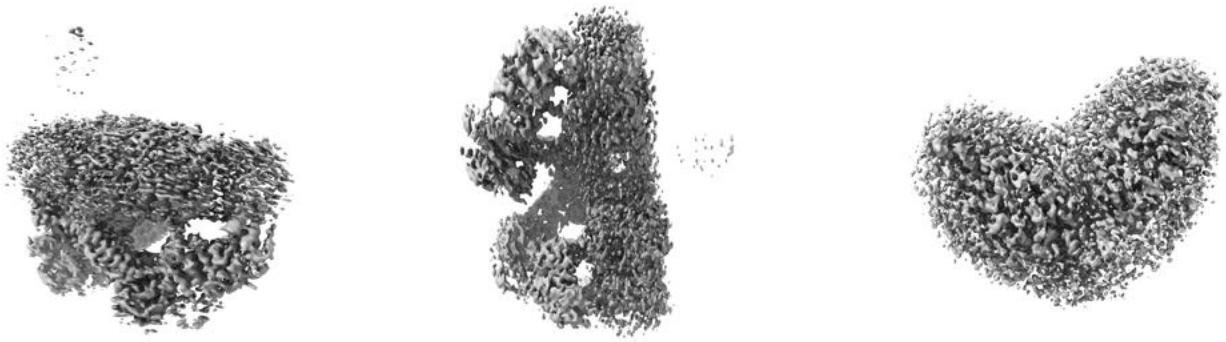


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

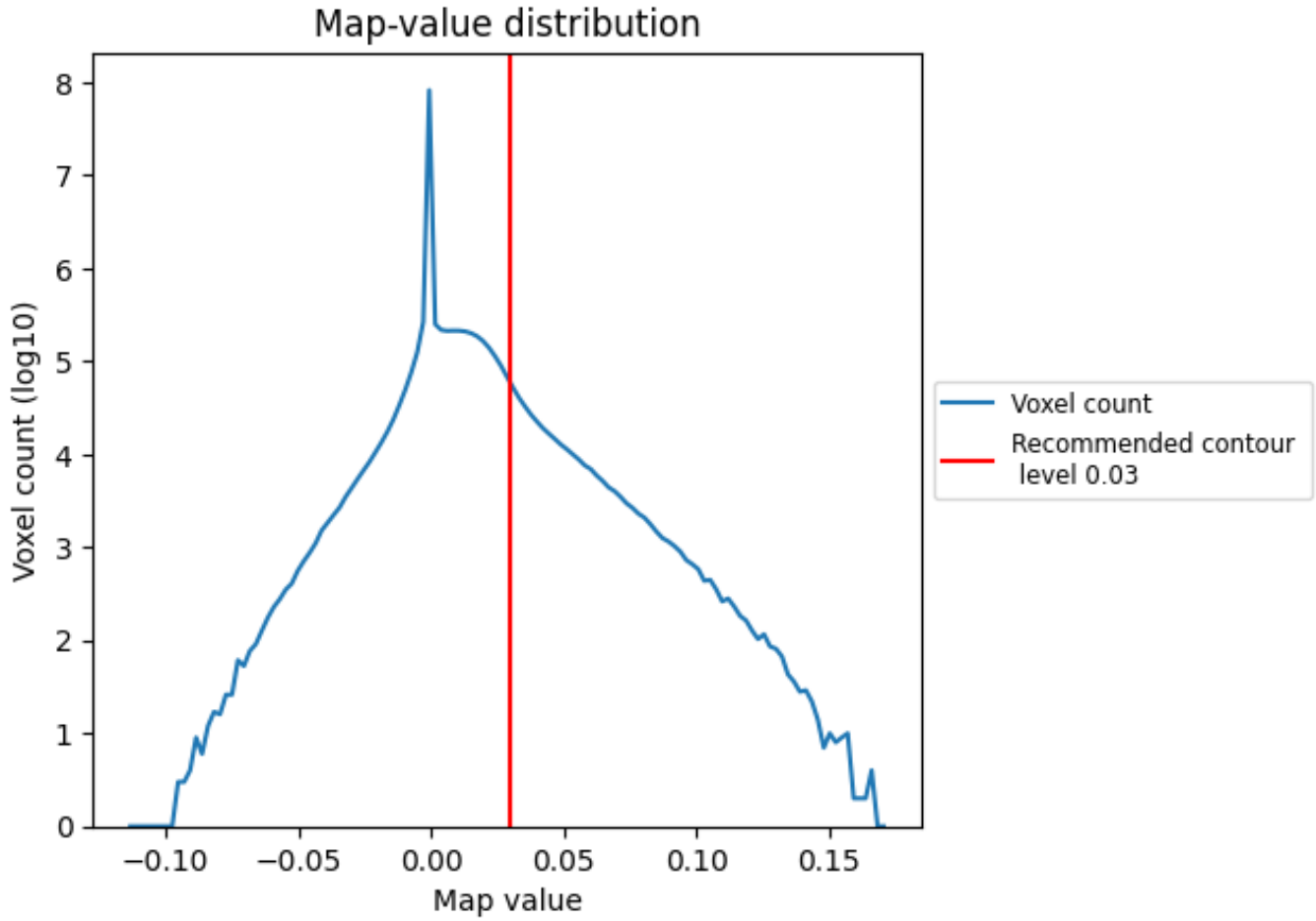
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

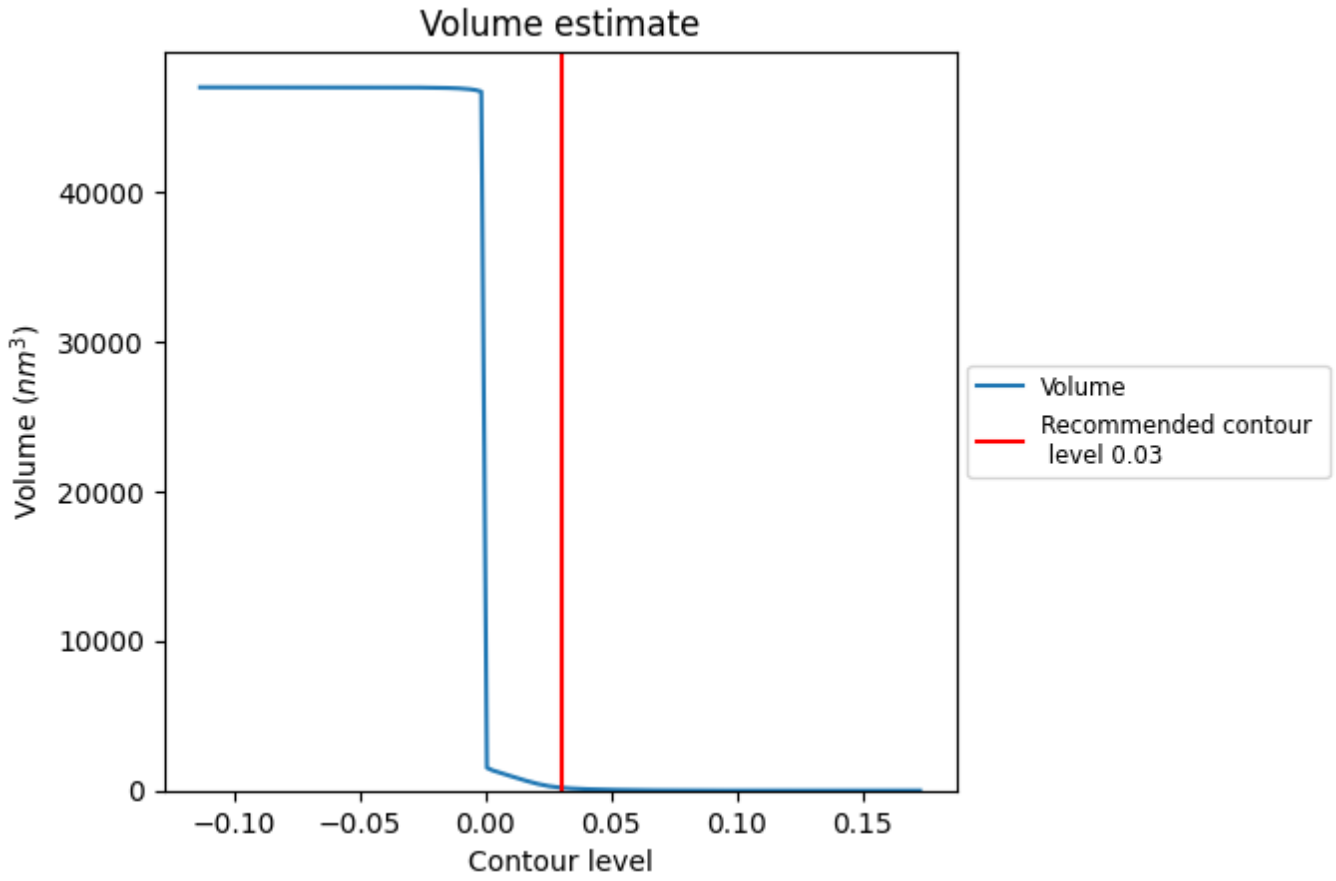
This section contains the results of statistical analysis of the map.

## 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.

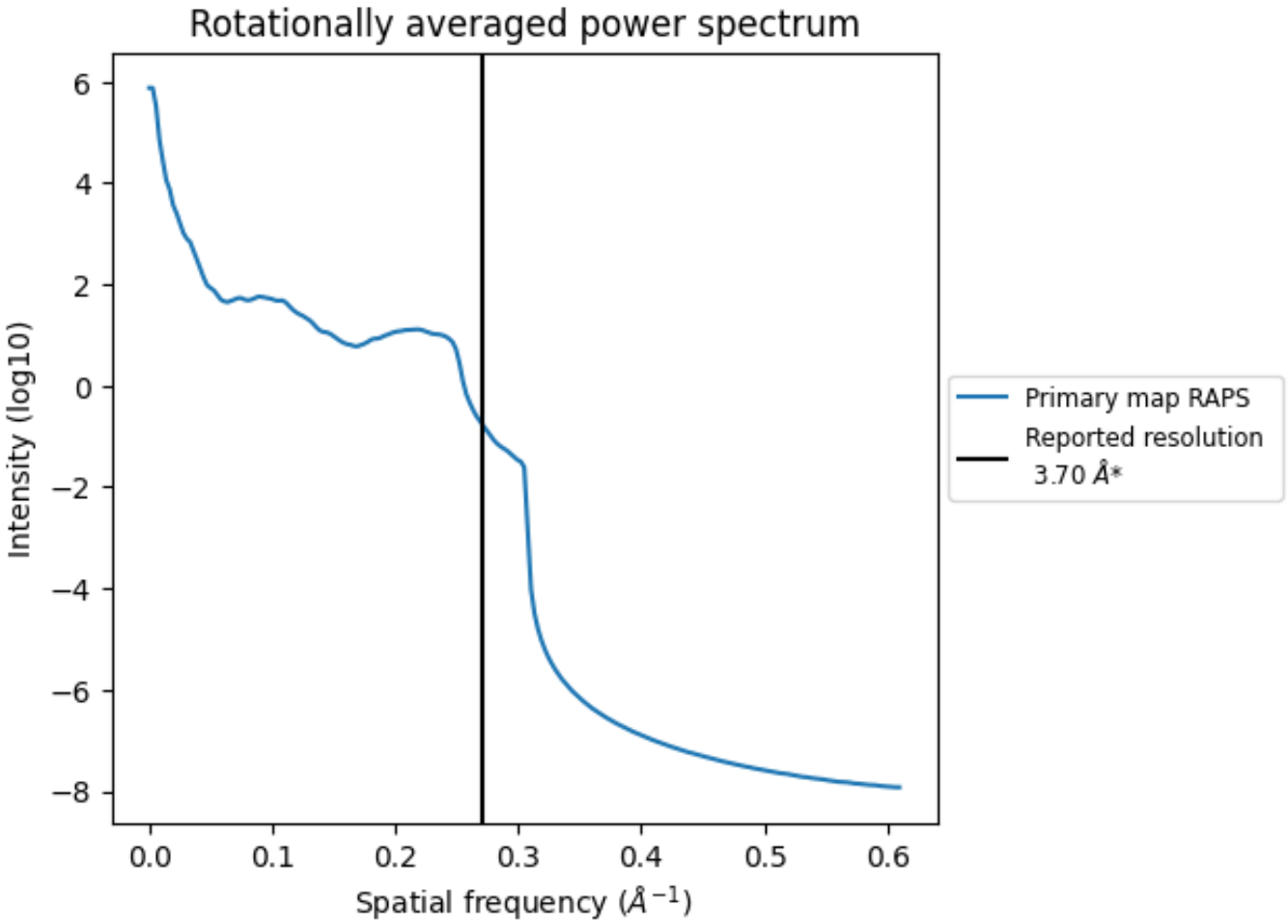
## 7.2 Volume estimate




The volume at the recommended contour level is 194 $nm^3$; this corresponds to an approximate mass of 175 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 0.270 Å$^{-1}$

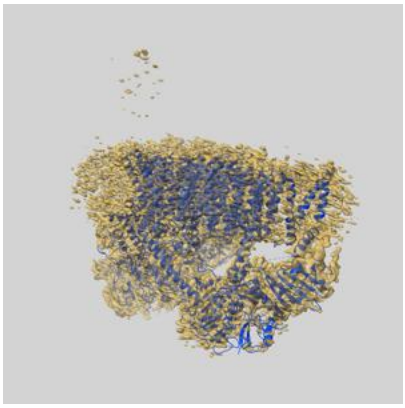
# 8 Fourier-Shell correlation (i)

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

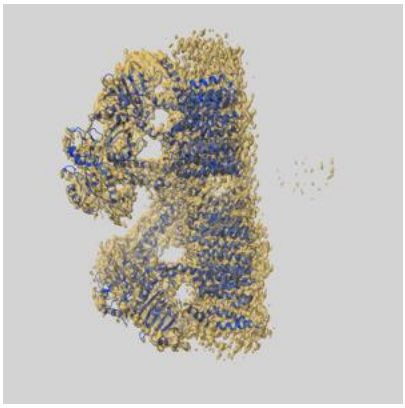
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0862 and PDB model 6LAR. Per-residue inclusion information can be found in section 3 on page 6.

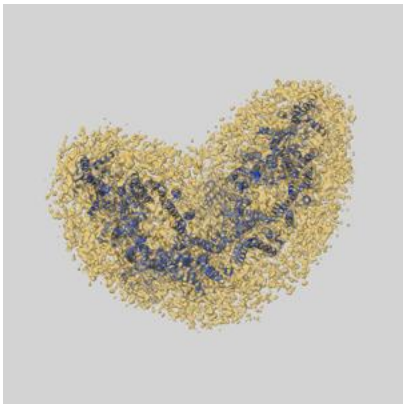
## 9.1 Map-model overlay



X



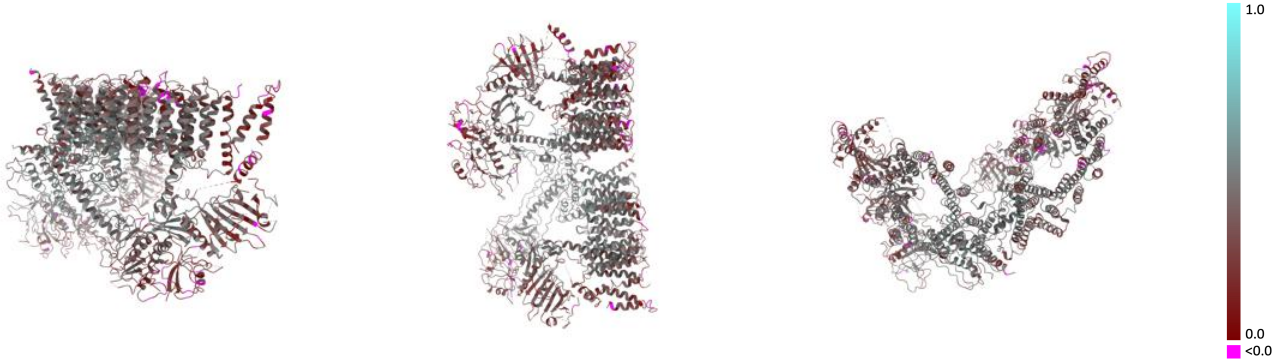
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

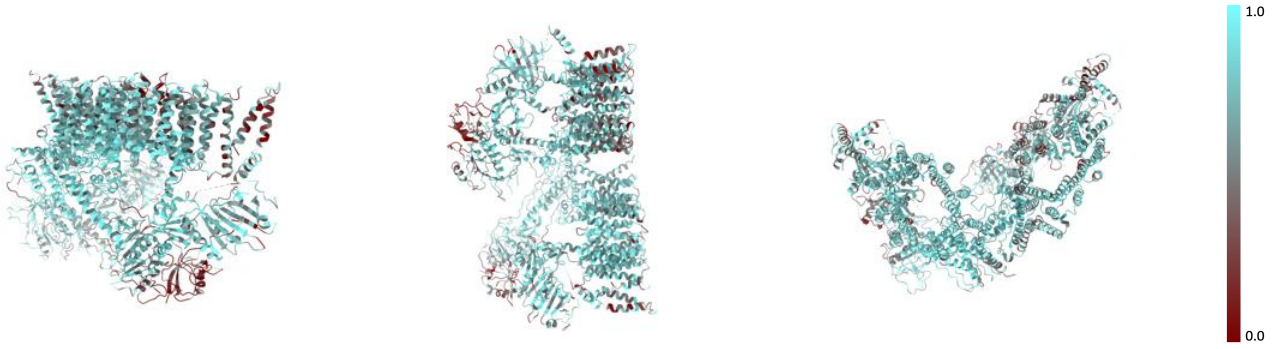
## 9.2 Q-score mapped to coordinate model




X Y Z

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

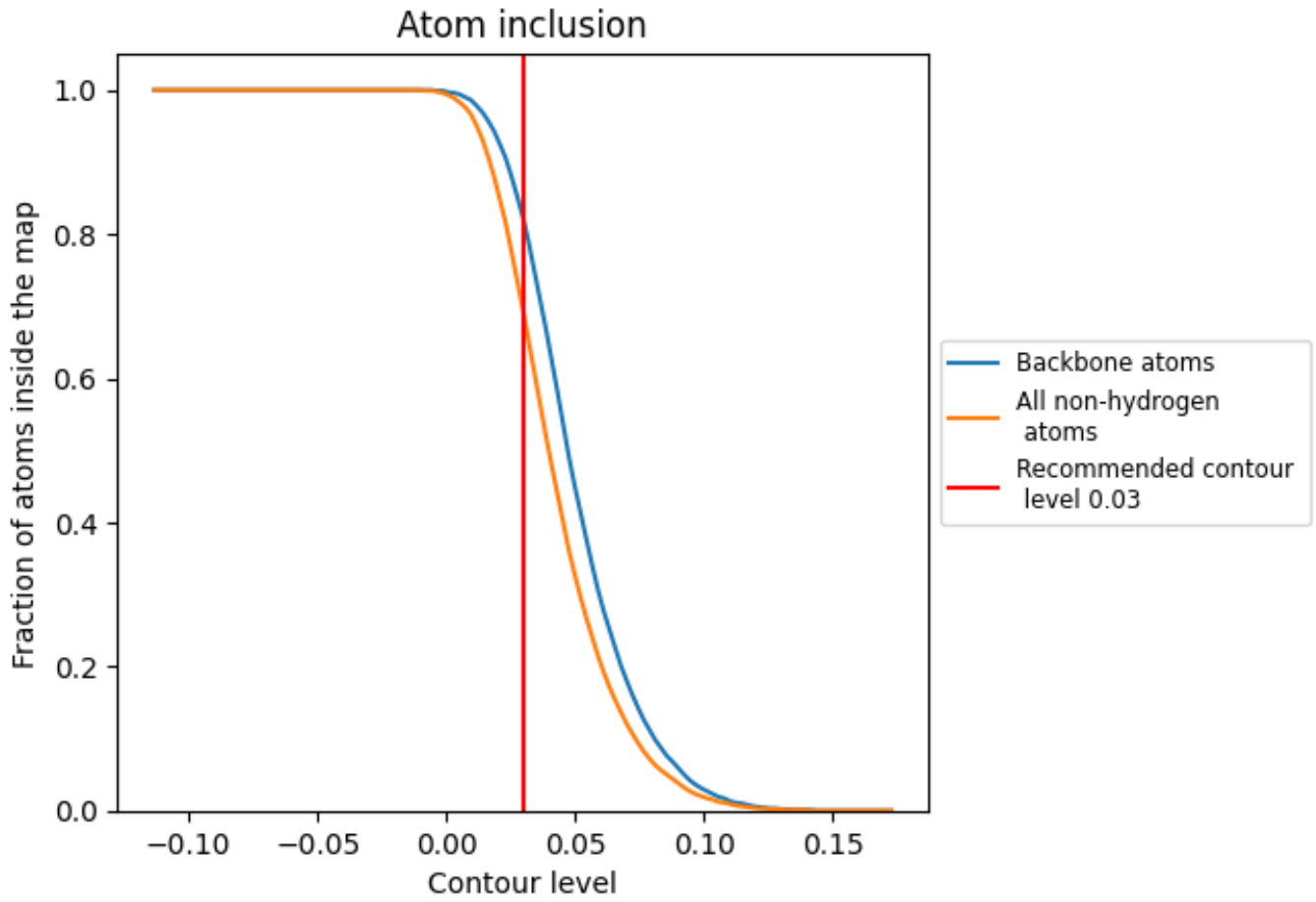
## 9.3 Atom inclusion mapped to coordinate model




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

## 9.4 Atom inclusion (i)




At the recommended contour level, 82% of all backbone atoms, 69% 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 (0.03) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.6900 | 0.3780 |
| A | 0.7760 | 0.4450 |
| B | 0.6820 | 0.3860 |
| C | 0.6040 | 0.3620 |
| D | 0.6540 | 0.3160 |
| E | 0.7410 | 0.4070 |
| F | 0.6870 | 0.3640 |
| G | 0.6310 | 0.3110 |
| H | 0.7220 | 0.4260 |
| I | 0.7890 | 0.4410 |
| J | 0.7360 | 0.3740 |