# Full wwPDB EM Validation Report (i)

Sep 2, 2026 – 09:00 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 36RO / pdb_000036ro |
| EMDB ID | : | EMD-77809 |
| Title | : | Cryo-EM structure of Pyrococcus furiosus RNA polymerase without stalk (no Rpo4/Rpo7) |
| Authors | : | Fordjour, G.N.R.; Armache, J.-P.; Murakami, K.S. |
| Deposited on | : | 2026-06-29 |
| Resolution | : | 4.56 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.

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

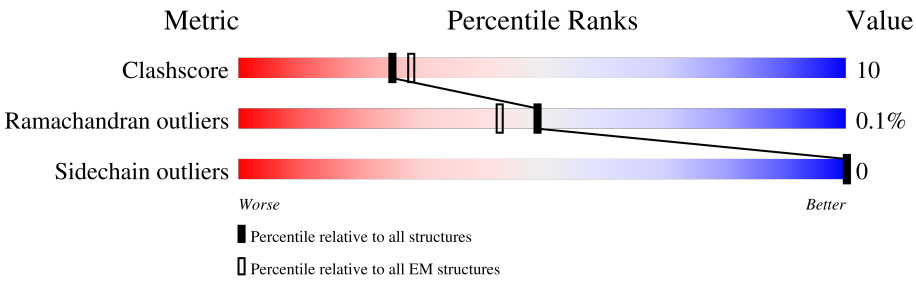
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev133 |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.50 |

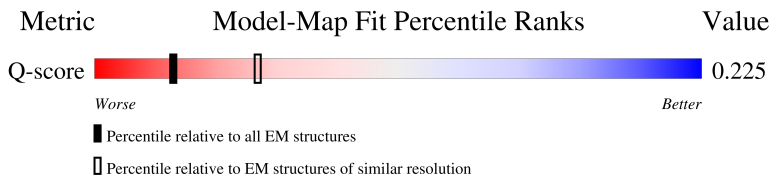
# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.56 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) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 2435 ( 4.06 - 5.06 ) |

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 | 907 | 75% 25% |
| 2 | B | 1117 | 69% 27% |
| 3 | C | 397 | 70% 27% |
| 4 | D | 275 | 69% 25% 6% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 5 | L | 95 | 68% 31% • |
| 6 | H | 82 | 78% 15% 7% |
| 7 | N | 65 | 78% 22% |
| 8 | K | 57 | 72% 25% • |
| 9 | P | 49 | 78% 20% • |

# 2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 23712 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 DNA-directed RNA polymerase subunit Rpo1N.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 901 | 7197 | 4541 | 1282 | 1335 | 39 | 0 | 0 |

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | B | 1076 | 8637 | 5474 | 1533 | 1596 | 34 | 0 | 0 |

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit Rpo1C.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | C | 388 | 3041 | 1921 | 525 | 585 | 10 | 0 | 0 |

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit Rpo3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | D | 258 | 2086 | 1358 | 330 | 396 | 2 | 0 | 0 |

There are 14 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | 262 | TRP | - | expression tag | UNP Q8U0E4 |
| D | 263 | SER | - | expression tag | UNP Q8U0E4 |
| D | 264 | HIS | - | expression tag | UNP Q8U0E4 |
| D | 265 | PRO | - | expression tag | UNP Q8U0E4 |
| D | 266 | GLN | - | expression tag | UNP Q8U0E4 |
| D | 267 | PHE | - | expression tag | UNP Q8U0E4 |
| D | 268 | GLU | - | expression tag | UNP Q8U0E4 |
| D | 269 | LYS | - | expression tag | UNP Q8U0E4 |
| D | 270 | HIS | - | expression tag | UNP Q8U0E4 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | 271 | HIS | - | expression tag | UNP Q8U0E4 |
| D | 272 | HIS | - | expression tag | UNP Q8U0E4 |
| D | 273 | HIS | - | expression tag | UNP Q8U0E4 |
| D | 274 | HIS | - | expression tag | UNP Q8U0E4 |
| D | 275 | HIS | - | expression tag | UNP Q8U0E4 |

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit Rpo11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | L | 94 | 777 | 500 | 129 | 146 | 2 | 0 | 0 |

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit Rpo5.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 6 | H | 76 | 609 | 398 | 100 | 111 | 0 | 0 |

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit Rpo10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 7 | N | 65 | 543 | 345 | 94 | 97 | 7 | 0 | 0 |

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit Rpo6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 8 | K | 55 | 424 | 281 | 71 | 71 | 1 | 0 | 0 |

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit Rpo12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 9 | P | 48 | 393 | 251 | 75 | 63 | 4 | 0 | 0 |

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Zn | |
| 10 | A | 2 | 2 | 2 | 0 |

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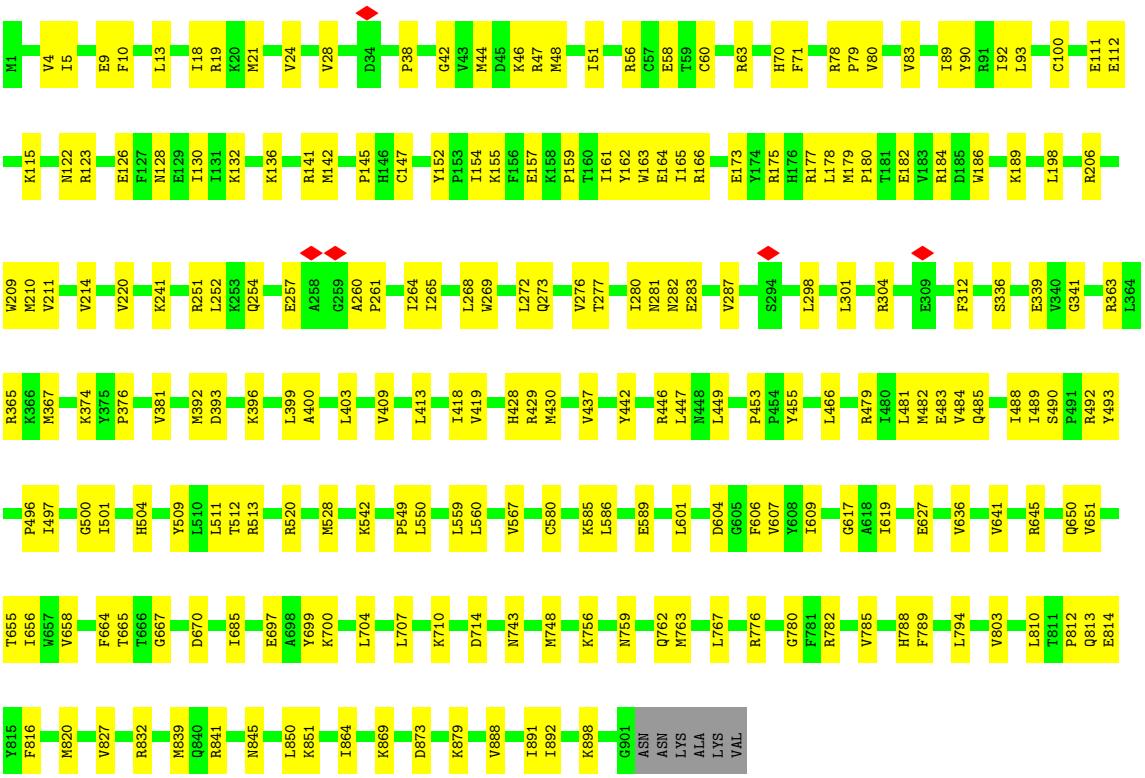
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Zn | |
| 10 | B | 1 | 1 | 1 | 0 |
| | | | Total | Zn | |
| 10 | N | 1 | 1 | 1 | 0 |
| | | | Total | Zn | |
| 10 | P | 1 | 1 | 1 | 0 |

# 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.

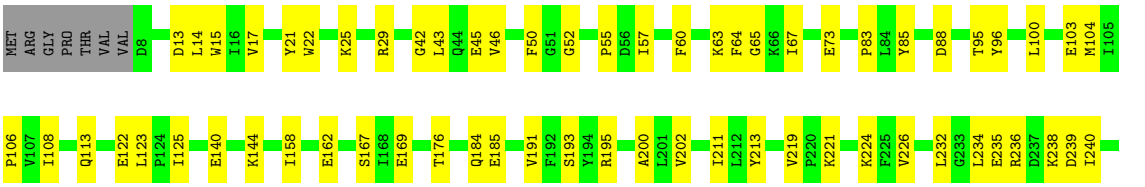
• Molecule 1: DNA-directed RNA polymerase subunit Rpo1N

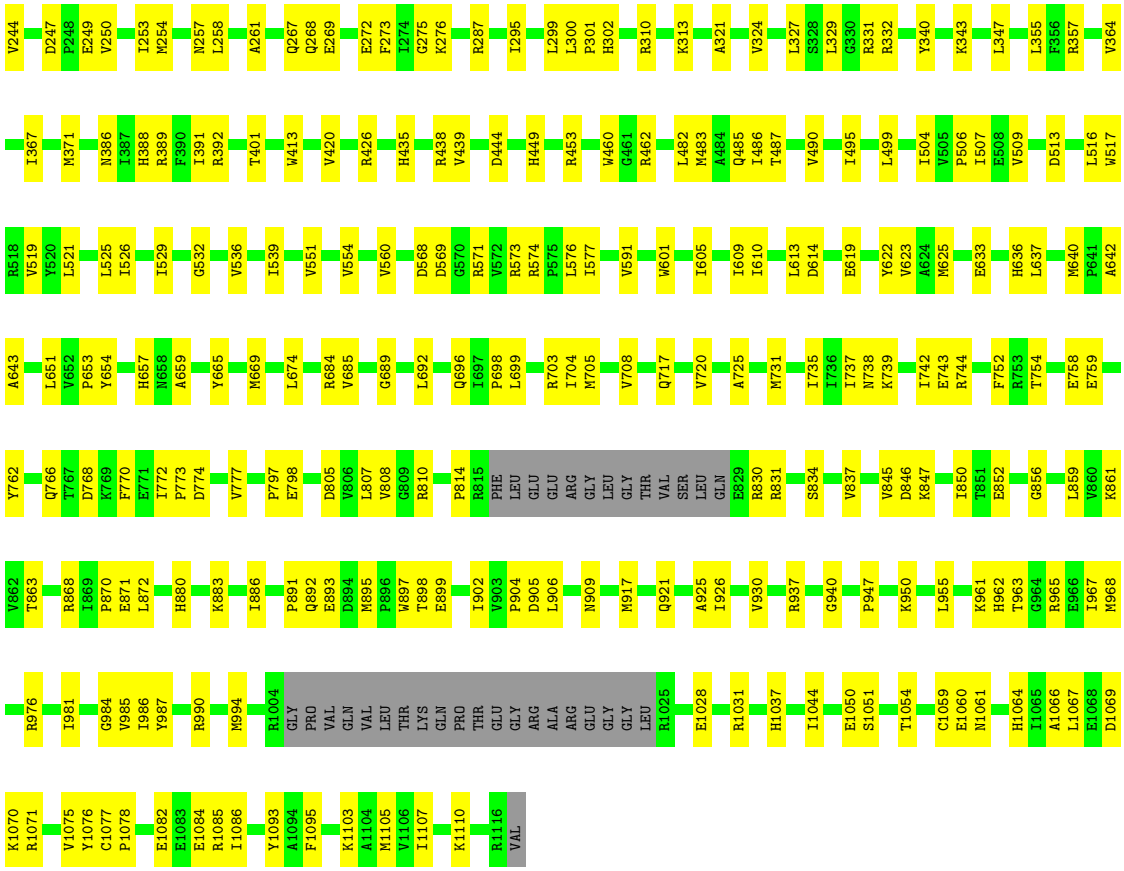
Chain A:




• Molecule 2: DNA-directed RNA polymerase subunit beta

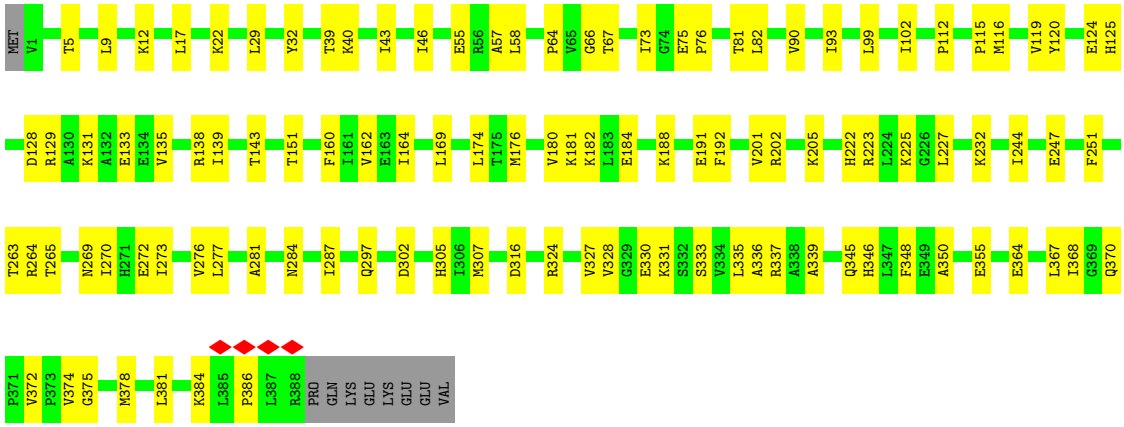
Chain B:





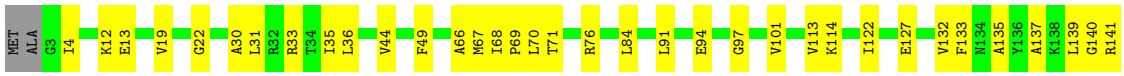

- Molecule 3: DNA-directed RNA polymerase subunit Rpo1C

Chain C:




- Molecule 4: DNA-directed RNA polymerase subunit Rpo3

Chain D:



G142 K143 D144 H145 W148 Q149 F152 V153 Y154 Y155 K156 Y157 V161 H162 I163 I167 L176 K179 L182 V191 L192 V193 K197 P198 P202 K203 D204 F205 E209 E212 I213 I223 V226 L232 E235 E236 I237 I240 A241 L242 K243 I244

L259 T260 SER TRP SER HIS PRO GLN PHE GLU LYS HIS HIS HIS HIS HIS HIS

- Molecule 5: DNA-directed RNA polymerase subunit Rpo11

Chain L: 68% 31%

M1 K2 I3 E14 F15 Y16 L17 T23 T31 L32 R33 K39 A42 H47 P48 I49 T50 M51 A52 R53 K54 P55 R56 F57 R58 D62 T66 E69 A74 I78 E84 V85 A88 W89 E90 K91 K94 SER

- Molecule 6: DNA-directed RNA polymerase subunit Rpo5

Chain H: 78% 15% 7%

MET ALA GLY LYS LYS E6 I9 H12 V13 L14 V15 L21 S22 E23 E24 E25 K26 K27 Q39 Q42 V60 E81 ASP

- Molecule 7: DNA-directed RNA polymerase subunit Rpo10

Chain N: 78% 22%

M1 R6 I14 G15 P31 V34 R42 Y43 L49 L55 I56 I59 M60 V64 Y65

- Molecule 8: DNA-directed RNA polymerase subunit Rpo6

Chain K: 72% 25%

MET F2 R11 I12 I13 G14 L18 V26 L27 I28 D29 V30 P31 I34 T35 E38 I41 R55 P56 SER

- Molecule 9: DNA-directed RNA polymerase subunit Rpo12

Chain P: 78% 20%

MET V2 Y6 V15 L25 R26 C27 P28 Y29 C30 L35 P38 R39 P40 A48 I49

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 61865 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TALOS ARCTICA | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/Å^2$) | 50 | Depositor |
| Minimum defocus (nm) | 800 | Depositor |
| Maximum defocus (nm) | 2200 | Depositor |
| Magnification | Not provided | |
| Image detector | FEI FALCON IV (4k x 4k) | Depositor |
| Maximum map value | 0.696 | Depositor |
| Minimum map value | -0.175 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 0.027 | Depositor |
| Recommended contour level | 0.15 | Depositor |
| Map size (Å) | 377.6, 377.6, 377.6 | wwPDB |
| Map dimensions | 400, 400, 400 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.944, 0.944, 0.944 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

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 | 0.15 | 0/7338 | 0.40 | 0/9907 |
| 2 | B | 0.15 | 0/8811 | 0.38 | 0/11905 |
| 3 | C | 0.14 | 0/3081 | 0.38 | 0/4156 |
| 4 | D | 0.15 | 0/2133 | 0.35 | 0/2894 |
| 5 | L | 0.16 | 0/792 | 0.41 | 0/1067 |
| 6 | H | 0.17 | 0/622 | 0.44 | 0/841 |
| 7 | N | 0.16 | 0/553 | 0.39 | 0/740 |
| 8 | K | 0.19 | 0/433 | 0.47 | 0/588 |
| 9 | P | 0.16 | 0/400 | 0.46 | 0/534 |
| All | All | 0.15 | 0/24163 | 0.39 | 0/32632 |

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 (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 | 7197 | 0 | 7263 | 164 | 0 |
| 2 | B | 8637 | 0 | 8708 | 213 | 0 |
| 3 | C | 3041 | 0 | 3151 | 79 | 0 |
| 4 | D | 2086 | 0 | 2109 | 48 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 5 | L | 777 | 0 | 788 | 21 | 0 |
| 6 | H | 609 | 0 | 634 | 12 | 0 |
| 7 | N | 543 | 0 | 541 | 10 | 0 |
| 8 | K | 424 | 0 | 460 | 9 | 0 |
| 9 | P | 393 | 0 | 423 | 7 | 0 |
| 10 | A | 2 | 0 | 0 | 0 | 0 |
| 10 | B | 1 | 0 | 0 | 0 | 0 |
| 10 | N | 1 | 0 | 0 | 0 | 0 |
| 10 | P | 1 | 0 | 0 | 0 | 0 |
| All | All | 23712 | 0 | 24077 | 495 | 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 10.

All (495) 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:60:CYS:SG | 1:A:70:HIS:CE1 | 2.67 | 0.87 |
| 2:B:669:MET:HE3 | 2:B:883:LYS:HB3 | 1.64 | 0.79 |
| 1:A:10:PHE:HB3 | 2:B:1107:ILE:HD11 | 1.67 | 0.76 |
| 1:A:892:ILE:HD13 | 3:C:46:ILE:HG12 | 1.69 | 0.74 |
| 2:B:893:GLU:HB2 | 4:D:33:ARG:HG3 | 1.70 | 0.74 |
| 2:B:106:PRO:HG2 | 2:B:113:GLN:HB2 | 1.70 | 0.72 |
| 2:B:504:ILE:HG12 | 2:B:529:ILE:HD11 | 1.72 | 0.71 |
| 3:C:174:LEU:HD21 | 3:C:225:LYS:HE2 | 1.72 | 0.71 |
| 1:A:157:GLU:HB3 | 1:A:161:ILE:HB | 1.72 | 0.71 |
| 1:A:312:PHE:HB3 | 3:C:339:ALA:HA | 1.72 | 0.71 |
| 3:C:333:SER:HB3 | 3:C:336:ALA:HB3 | 1.70 | 0.71 |
| 2:B:868:ARG:HH11 | 2:B:994:MET:HG3 | 1.57 | 0.70 |
| 1:A:832:ARG:HH21 | 3:C:82:LEU:H | 1.41 | 0.68 |
| 2:B:814:PRO:HA | 2:B:831:ARG:HG3 | 1.76 | 0.68 |
| 4:D:153:VAL:HG12 | 4:D:226:VAL:HA | 1.75 | 0.67 |
| 5:L:31:THR:HG23 | 5:L:74:ALA:HB1 | 1.74 | 0.67 |
| 9:P:27:CYS:HB3 | 9:P:30:CYS:SG | 2.35 | 0.66 |
| 2:B:43:LEU:HB3 | 2:B:67:ILE:HG12 | 1.78 | 0.66 |
| 1:A:670:ASP:HA | 1:A:743:ASN:HD21 | 1.59 | 0.66 |
| 1:A:667:GLY:H | 2:B:965:ARG:HH21 | 1.44 | 0.66 |
| 1:A:5:ILE:HD12 | 3:C:370:GLN:HE21 | 1.60 | 0.65 |
| 1:A:60:CYS:HA | 2:B:1069:ASP:HA | 1.77 | 0.65 |
| 1:A:707:LEU:HD13 | 3:C:90:VAL:HG21 | 1.78 | 0.65 |
| 4:D:19:VAL:HG22 | 4:D:223:ILE:HG12 | 1.79 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:839:MET:HE1 | 3:C:102:ILE:HG22 | 1.79 | 0.65 |
| 4:D:91:LEU:HB2 | 4:D:135:ALA:HB3 | 1.79 | 0.65 |
| 1:A:56:ARG:HE | 1:A:63:ARG:HE | 1.44 | 0.64 |
| 4:D:209:GLU:HA | 4:D:213:ILE:HB | 1.78 | 0.64 |
| 3:C:324:ARG:HA | 3:C:328:VAL:HB | 1.80 | 0.64 |
| 8:K:2:PHE:HE1 | 8:K:55:ARG:HE | 1.46 | 0.64 |
| 2:B:14:LEU:HD11 | 2:B:577:ILE:HD11 | 1.80 | 0.64 |
| 2:B:65:GLY:HA3 | 2:B:103:GLU:HG2 | 1.80 | 0.64 |
| 1:A:4:VAL:HA | 3:C:370:GLN:HE22 | 1.64 | 0.63 |
| 5:L:14:GLU:HA | 5:L:58:ARG:HA | 1.80 | 0.63 |
| 1:A:381:VAL:HG23 | 1:A:409:VAL:HG22 | 1.81 | 0.62 |
| 2:B:925:ALA:HB1 | 2:B:984:GLY:HA3 | 1.80 | 0.62 |
| 1:A:111:GLU:HG3 | 1:A:115:LYS:HZ3 | 1.65 | 0.62 |
| 3:C:128:ASP:HB3 | 3:C:131:LYS:HB2 | 1.82 | 0.62 |
| 4:D:71:THR:HG22 | 4:D:114:LYS:H | 1.65 | 0.62 |
| 1:A:260:ALA:HB1 | 1:A:264:ILE:HD11 | 1.82 | 0.61 |
| 3:C:337:ARG:HH12 | 3:C:346:HIS:HB2 | 1.65 | 0.61 |
| 1:A:374:LYS:HG3 | 1:A:376:PRO:HD2 | 1.82 | 0.61 |
| 2:B:1064:HIS:CG | 2:B:1077:CYS:SG | 2.94 | 0.61 |
| 1:A:586:LEU:HD22 | 1:A:601:LEU:HD12 | 1.83 | 0.61 |
| 2:B:310:ARG:HA | 2:B:313:LYS:HE2 | 1.83 | 0.61 |
| 2:B:705:MET:HA | 2:B:708:VAL:HG12 | 1.83 | 0.61 |
| 2:B:1075:VAL:HG23 | 2:B:1086:ILE:HD13 | 1.82 | 0.61 |
| 1:A:560:LEU:HD11 | 1:A:650:GLN:HB3 | 1.82 | 0.61 |
| 1:A:520:ARG:HB2 | 1:A:549:PRO:HG2 | 1.83 | 0.60 |
| 2:B:232:LEU:HD22 | 2:B:295:ILE:HD11 | 1.82 | 0.60 |
| 1:A:485:GLN:HB3 | 1:A:641:VAL:HG12 | 1.83 | 0.60 |
| 2:B:696:GLN:HB3 | 2:B:717:GLN:HA | 1.82 | 0.60 |
| 7:N:14:ILE:HD11 | 7:N:49:LEU:HG | 1.84 | 0.60 |
| 2:B:57:ILE:HG21 | 2:B:60:PHE:HB3 | 1.83 | 0.60 |
| 5:L:33:ARG:HH21 | 5:L:42:ALA:HA | 1.65 | 0.59 |
| 2:B:55:PRO:HB3 | 2:B:371:MET:HE3 | 1.83 | 0.59 |
| 3:C:328:VAL:HA | 3:C:331:LYS:HD3 | 1.83 | 0.59 |
| 4:D:140:GLY:HA3 | 4:D:148:TRP:CE2 | 2.38 | 0.59 |
| 1:A:252:LEU:HD21 | 1:A:269:TRP:HA | 1.83 | 0.59 |
| 1:A:38:PRO:HB3 | 1:A:44:MET:HG3 | 1.82 | 0.59 |
| 1:A:393:ASP:HA | 1:A:396:LYS:HD2 | 1.85 | 0.59 |
| 1:A:60:CYS:SG | 1:A:70:HIS:HE1 | 2.17 | 0.59 |
| 1:A:418:ILE:HG13 | 1:A:479:ARG:HB2 | 1.85 | 0.59 |
| 2:B:386:ASN:HB3 | 2:B:389:ARG:HG2 | 1.85 | 0.59 |
| 3:C:29:LEU:HD21 | 3:C:43:ILE:HD12 | 1.84 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:143:THR:HB | 3:C:223:ARG:HH12 | 1.68 | 0.58 |
| 2:B:499:LEU:HB3 | 2:B:504:ILE:HD12 | 1.85 | 0.58 |
| 4:D:176:LEU:HD12 | 4:D:179:LYS:HE3 | 1.85 | 0.58 |
| 1:A:419:VAL:HG11 | 1:A:466:LEU:HD12 | 1.86 | 0.58 |
| 1:A:260:ALA:HB3 | 1:A:265:ILE:HD11 | 1.85 | 0.58 |
| 3:C:372:VAL:HG12 | 3:C:374:VAL:H | 1.69 | 0.57 |
| 1:A:879:LYS:HD3 | 3:C:57:ALA:HA | 1.85 | 0.57 |
| 2:B:774:ASP:HB3 | 2:B:777:VAL:HG13 | 1.87 | 0.57 |
| 4:D:66:ALA:HB2 | 9:P:48:ALA:HB1 | 1.85 | 0.57 |
| 2:B:623:VAL:HG22 | 2:B:636:HIS:HB2 | 1.86 | 0.57 |
| 6:H:21:LEU:HB2 | 6:H:26:LYS:HZ3 | 1.68 | 0.57 |
| 2:B:355:LEU:HD22 | 2:B:413:TRP:HZ3 | 1.69 | 0.57 |
| 1:A:154:ILE:HG23 | 1:A:164:GLU:HB3 | 1.86 | 0.56 |
| 1:A:162:TYR:H | 1:A:177:ARG:HH12 | 1.53 | 0.56 |
| 2:B:104:MET:HG3 | 2:B:391:ILE:HG21 | 1.86 | 0.56 |
| 2:B:234:LEU:HD21 | 2:B:239:ASP:HB2 | 1.87 | 0.56 |
| 3:C:125:HIS:CD2 | 3:C:131:LYS:HB3 | 2.40 | 0.56 |
| 1:A:186:TRP:HA | 1:A:189:LYS:HE3 | 1.87 | 0.56 |
| 5:L:51:MET:HE3 | 5:L:54:LYS:HG2 | 1.88 | 0.56 |
| 2:B:247:ASP:HB3 | 2:B:250:VAL:HG22 | 1.87 | 0.56 |
| 3:C:112:PRO:HG2 | 3:C:115:PRO:HB3 | 1.86 | 0.56 |
| 6:H:9:ILE:HG22 | 6:H:15:VAL:HG11 | 1.87 | 0.56 |
| 4:D:70:LEU:HD12 | 4:D:113:VAL:HG12 | 1.87 | 0.56 |
| 1:A:157:GLU:HB2 | 1:A:163:TRP:HD1 | 1.70 | 0.56 |
| 2:B:805:ASP:H | 2:B:837:VAL:HG12 | 1.71 | 0.55 |
| 2:B:739:LYS:HA | 2:B:742:ILE:HD12 | 1.88 | 0.55 |
| 1:A:60:CYS:HB3 | 2:B:1067:LEU:HG | 1.88 | 0.55 |
| 8:K:31:PRO:HD2 | 8:K:34:ILE:HD13 | 1.87 | 0.55 |
| 3:C:375:GLY:H | 3:C:378:MET:HE1 | 1.72 | 0.55 |
| 2:B:772:ILE:HD12 | 2:B:773:PRO:HD2 | 1.89 | 0.55 |
| 2:B:797:PRO:HD2 | 9:P:40:PRO:HD3 | 1.88 | 0.55 |
| 3:C:182:LYS:HG3 | 3:C:222:HIS:HE1 | 1.72 | 0.55 |
| 2:B:340:TYR:HA | 2:B:343:LYS:HB3 | 1.88 | 0.55 |
| 2:B:738:ASN:HD21 | 2:B:892:GLN:HA | 1.72 | 0.55 |
| 2:B:898:THR:HG22 | 2:B:902:ILE:H | 1.72 | 0.55 |
| 3:C:335:LEU:HB3 | 3:C:367:LEU:HD21 | 1.87 | 0.55 |
| 1:A:851:LYS:HD3 | 3:C:374:VAL:HG22 | 1.88 | 0.54 |
| 2:B:893:GLU:HA | 4:D:36:LEU:HD23 | 1.89 | 0.54 |
| 1:A:453:PRO:HG3 | 1:A:501:ILE:HD11 | 1.90 | 0.54 |
| 4:D:167:ILE:HD11 | 4:D:212:GLU:HB3 | 1.88 | 0.54 |
| 4:D:12:LYS:HG3 | 4:D:13:GLU:H | 1.71 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:119:VAL:HB | 3:C:244:ILE:HB | 1.89 | 0.54 |
| 2:B:810:ARG:HB3 | 2:B:834:SER:HA | 1.89 | 0.54 |
| 1:A:428:HIS:HB3 | 3:C:75:GLU:HB2 | 1.90 | 0.54 |
| 1:A:607:VAL:HA | 1:A:617:GLY:HA3 | 1.90 | 0.54 |
| 2:B:273:PHE:HA | 2:B:276:LYS:HE2 | 1.89 | 0.54 |
| 3:C:64:PRO:HB2 | 3:C:67:THR:HG22 | 1.90 | 0.54 |
| 1:A:92:ILE:HG12 | 1:A:198:LEU:HD12 | 1.90 | 0.54 |
| 1:A:301:LEU:HA | 1:A:304:ARG:HG2 | 1.89 | 0.54 |
| 2:B:519:VAL:HG13 | 2:B:526:ILE:HB | 1.90 | 0.54 |
| 1:A:604:ASP:HA | 1:A:617:GLY:HA2 | 1.90 | 0.54 |
| 3:C:316:ASP:HA | 6:H:42:GLN:H | 1.73 | 0.54 |
| 1:A:165:ILE:HG22 | 1:A:173:GLU:HG3 | 1.89 | 0.53 |
| 1:A:381:VAL:HG11 | 1:A:399:LEU:HD22 | 1.89 | 0.53 |
| 2:B:235:GLU:HG2 | 2:B:267:GLN:HA | 1.90 | 0.53 |
| 2:B:968:MET:HG3 | 2:B:981:ILE:HD11 | 1.90 | 0.53 |
| 1:A:891:ILE:HG23 | 3:C:46:ILE:HD11 | 1.89 | 0.53 |
| 5:L:15:PHE:HB3 | 5:L:57:PHE:HB2 | 1.90 | 0.53 |
| 1:A:485:GLN:HG2 | 1:A:645:ARG:HB2 | 1.88 | 0.53 |
| 1:A:762:GLN:HE22 | 1:A:767:LEU:HG | 1.74 | 0.53 |
| 2:B:720:VAL:HG23 | 2:B:904:PRO:HA | 1.90 | 0.53 |
| 2:B:899:GLU:HB2 | 2:B:967:ILE:HG13 | 1.89 | 0.53 |
| 3:C:120:TYR:HB3 | 3:C:264:ARG:HH21 | 1.71 | 0.53 |
| 2:B:735:ILE:HB | 2:B:906:LEU:HD11 | 1.89 | 0.53 |
| 1:A:165:ILE:HG12 | 1:A:175:ARG:HG2 | 1.90 | 0.53 |
| 4:D:84:LEU:HD21 | 4:D:141:ARG:HG2 | 1.91 | 0.53 |
| 3:C:93:ILE:HD11 | 3:C:116:MET:HE2 | 1.90 | 0.53 |
| 1:A:100:CYS:HB3 | 1:A:147:CYS:SG | 2.49 | 0.53 |
| 3:C:169:LEU:HD11 | 3:C:176:MET:HE3 | 1.90 | 0.53 |
| 2:B:737:ILE:HG22 | 2:B:906:LEU:HD13 | 1.91 | 0.52 |
| 9:P:6:TYR:HA | 9:P:38:PRO:HD3 | 1.92 | 0.52 |
| 1:A:446:ARG:HH12 | 5:L:49:ILE:HG21 | 1.75 | 0.52 |
| 4:D:49:PHE:HA | 4:D:133:PHE:HB3 | 1.91 | 0.52 |
| 3:C:350:ALA:HB1 | 3:C:355:GLU:HG2 | 1.92 | 0.52 |
| 1:A:51:ILE:HG23 | 1:A:220:VAL:HG13 | 1.92 | 0.52 |
| 2:B:295:ILE:HG13 | 2:B:299:LEU:HD13 | 1.91 | 0.52 |
| 2:B:759:GLU:HB2 | 2:B:768:ASP:HB2 | 1.92 | 0.52 |
| 3:C:139:ILE:HA | 3:C:227:LEU:HD23 | 1.90 | 0.52 |
| 2:B:659:ALA:HB2 | 2:B:917:MET:HB2 | 1.92 | 0.52 |
| 4:D:202:PRO:HG2 | 4:D:205:PHE:HD2 | 1.75 | 0.52 |
| 2:B:762:TYR:HB2 | 2:B:766:GLN:HG2 | 1.91 | 0.52 |
| 2:B:735:ILE:HG13 | 2:B:886:ILE:HG22 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:56:ARG:NE | 1:A:63:ARG:HE | 2.08 | 0.51 |
| 2:B:13:ASP:HB3 | 2:B:591:VAL:HG11 | 1.91 | 0.51 |
| 4:D:161:VAL:HB | 4:D:193:VAL:HB | 1.92 | 0.51 |
| 2:B:1059:CYS:HA | 2:B:1086:ILE:HA | 1.92 | 0.51 |
| 3:C:135:VAL:HG12 | 3:C:138:ARG:HH21 | 1.74 | 0.51 |
| 2:B:211:ILE:HD13 | 2:B:257:ASN:HD22 | 1.76 | 0.51 |
| 2:B:758:GLU:N | 2:B:810:ARG:HH22 | 2.07 | 0.51 |
| 2:B:976:ARG:HH21 | 4:D:157:TYR:HB2 | 1.75 | 0.51 |
| 4:D:69:PRO:HB3 | 7:N:6:ARG:HH21 | 1.76 | 0.51 |
| 2:B:665:TYR:HB3 | 2:B:669:MET:HE1 | 1.92 | 0.51 |
| 4:D:242:LEU:HD21 | 5:L:85:VAL:HG12 | 1.92 | 0.51 |
| 1:A:19:ARG:HB2 | 1:A:214:VAL:HG21 | 1.93 | 0.51 |
| 1:A:141:ARG:HD3 | 1:A:145:PRO:HD3 | 1.92 | 0.51 |
| 1:A:812:PRO:HG3 | 2:B:625:MET:HE2 | 1.92 | 0.51 |
| 2:B:846:ASP:HB3 | 2:B:863:THR:HB | 1.92 | 0.51 |
| 8:K:13:ILE:HG12 | 8:K:41:ILE:HD13 | 1.93 | 0.51 |
| 1:A:816:PHE:O | 1:A:820:MET:HG3 | 2.11 | 0.51 |
| 2:B:485:GLN:HE22 | 2:B:573:ARG:HH21 | 1.58 | 0.51 |
| 2:B:60:PHE:HB2 | 2:B:108:ILE:HD13 | 1.92 | 0.51 |
| 2:B:640:MET:HG3 | 2:B:642:ALA:H | 1.76 | 0.51 |
| 1:A:89:ILE:HG13 | 1:A:210:MET:HE2 | 1.93 | 0.50 |
| 3:C:281:ALA:HB2 | 6:H:15:VAL:HG22 | 1.93 | 0.50 |
| 1:A:365:ARG:HD3 | 1:A:400:ALA:HB1 | 1.92 | 0.50 |
| 2:B:814:PRO:HD3 | 2:B:830:ARG:HA | 1.92 | 0.50 |
| 3:C:284:ASN:HB3 | 6:H:14:LEU:HD22 | 1.92 | 0.50 |
| 1:A:152:TYR:CD2 | 1:A:166:ARG:HG2 | 2.47 | 0.50 |
| 2:B:14:LEU:HA | 2:B:17:VAL:HG22 | 1.92 | 0.50 |
| 1:A:179:MET:HB2 | 1:A:182:GLU:HG2 | 1.93 | 0.50 |
| 2:B:95:THR:HG22 | 2:B:158:ILE:HA | 1.93 | 0.50 |
| 4:D:143:LYS:HG2 | 5:L:53:ARG:HH22 | 1.75 | 0.50 |
| 1:A:80:VAL:HA | 1:A:273:GLN:HE22 | 1.76 | 0.50 |
| 1:A:482:MET:HE1 | 2:B:1037:HIS:CE1 | 2.46 | 0.50 |
| 2:B:321:ALA:HA | 2:B:324:VAL:HG12 | 1.93 | 0.50 |
| 2:B:897:TRP:CD1 | 4:D:154:TYR:HB2 | 2.47 | 0.50 |
| 4:D:30:ALA:HA | 5:L:23:THR:HG23 | 1.94 | 0.50 |
| 2:B:22:TRP:HH2 | 2:B:482:LEU:HD22 | 1.77 | 0.50 |
| 2:B:269:GLU:HA | 2:B:272:GLU:HB2 | 1.93 | 0.50 |
| 2:B:568:ASP:H | 2:B:571:ARG:HH21 | 1.60 | 0.49 |
| 2:B:754:THR:HG22 | 2:B:863:THR:HG23 | 1.94 | 0.49 |
| 2:B:850:ILE:HG13 | 9:P:35:LEU:HB3 | 1.94 | 0.49 |
| 3:C:119:VAL:HA | 3:C:265:THR:HG23 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:52:GLY:HA2 | 2:B:63:LYS:HA | 1.93 | 0.49 |
| 3:C:164:ILE:HB | 3:C:176:MET:HE2 | 1.94 | 0.49 |
| 8:K:35:THR:HB | 8:K:38:GLU:HG3 | 1.95 | 0.49 |
| 2:B:539:ILE:HG23 | 2:B:554:VAL:HG11 | 1.93 | 0.49 |
| 2:B:743:GLU:HB2 | 4:D:145:HIS:CE1 | 2.48 | 0.49 |
| 2:B:930:VAL:HG23 | 2:B:955:LEU:HD12 | 1.94 | 0.49 |
| 1:A:665:THR:HG21 | 2:B:981:ILE:HA | 1.95 | 0.49 |
| 2:B:140:GLU:HG3 | 2:B:144:LYS:HZ2 | 1.78 | 0.49 |
| 3:C:384:LYS:HG3 | 3:C:386:PRO:HD2 | 1.95 | 0.49 |
| 6:H:23:GLU:HA | 6:H:26:LYS:HD2 | 1.94 | 0.49 |
| 1:A:756:LYS:H | 1:A:759:ASN:HB2 | 1.78 | 0.49 |
| 4:D:44:VAL:HA | 4:D:137:ALA:HA | 1.95 | 0.49 |
| 1:A:282:ASN:HD21 | 1:A:298:LEU:HB2 | 1.78 | 0.49 |
| 1:A:449:LEU:HD13 | 2:B:731:MET:HG3 | 1.94 | 0.49 |
| 1:A:812:PRO:HB2 | 2:B:460:TRP:HH2 | 1.77 | 0.49 |
| 2:B:576:LEU:HD12 | 2:B:613:LEU:HD12 | 1.94 | 0.49 |
| 2:B:1060:GLU:HG2 | 2:B:1085:ARG:HB3 | 1.95 | 0.49 |
| 1:A:155:LYS:H | 1:A:164:GLU:HA | 1.77 | 0.49 |
| 1:A:184:ARG:HH21 | 1:A:211:VAL:HB | 1.78 | 0.48 |
| 4:D:4:ILE:HG22 | 4:D:22:GLY:HA3 | 1.95 | 0.48 |
| 6:H:21:LEU:HD13 | 6:H:60:VAL:HG12 | 1.95 | 0.48 |
| 1:A:782:ARG:HH21 | 2:B:619:GLU:HG3 | 1.79 | 0.48 |
| 2:B:46:VAL:HG23 | 2:B:357:ARG:HG2 | 1.95 | 0.48 |
| 2:B:96:TYR:HD1 | 2:B:125:ILE:HB | 1.76 | 0.48 |
| 2:B:685:VAL:HG23 | 2:B:754:THR:HG21 | 1.95 | 0.48 |
| 4:D:31:LEU:O | 4:D:35:ILE:HG12 | 2.13 | 0.48 |
| 4:D:152:PHE:HD2 | 7:N:42:ARG:HH12 | 1.60 | 0.48 |
| 2:B:224:LYS:HE2 | 2:B:261:ALA:HA | 1.95 | 0.48 |
| 7:N:31:PRO:HA | 7:N:34:VAL:HG12 | 1.94 | 0.48 |
| 1:A:21:MET:HE1 | 1:A:71:PHE:HD2 | 1.77 | 0.48 |
| 1:A:699:TYR:HB2 | 1:A:704:LEU:HD22 | 1.95 | 0.48 |
| 1:A:710:LYS:HB3 | 1:A:714:ASP:HB2 | 1.95 | 0.48 |
| 2:B:495:ILE:HG22 | 2:B:521:LEU:HD11 | 1.96 | 0.48 |
| 3:C:55:GLU:HA | 3:C:58:LEU:HD12 | 1.96 | 0.48 |
| 2:B:720:VAL:HG23 | 2:B:905:ASP:H | 1.79 | 0.48 |
| 2:B:852:GLU:HB3 | 2:B:856:GLY:HA2 | 1.96 | 0.48 |
| 3:C:129:ARG:HE | 3:C:133:GLU:HG2 | 1.78 | 0.48 |
| 2:B:193:SER:H | 2:B:200:ALA:HB3 | 1.79 | 0.48 |
| 1:A:251:ARG:HG2 | 1:A:268:LEU:HD21 | 1.96 | 0.47 |
| 2:B:15:TRP:HH2 | 2:B:704:ILE:HA | 1.79 | 0.47 |
| 1:A:206:ARG:HB3 | 1:A:209:TRP:CD2 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:167:SER:HB2 | 2:B:439:VAL:HG22 | 1.95 | 0.47 |
| 2:B:300:LEU:HD22 | 2:B:302:HIS:HE1 | 1.79 | 0.47 |
| 3:C:93:ILE:HA | 3:C:232:LYS:HZ2 | 1.78 | 0.47 |
| 1:A:162:TYR:H | 1:A:177:ARG:NH1 | 2.11 | 0.47 |
| 2:B:1075:VAL:HG21 | 2:B:1086:ILE:HG21 | 1.96 | 0.47 |
| 1:A:336:SER:HB3 | 1:A:339:GLU:HG3 | 1.96 | 0.47 |
| 2:B:720:VAL:HG12 | 2:B:985:VAL:HG22 | 1.97 | 0.47 |
| 2:B:744:ARG:HA | 4:D:67:MET:HE3 | 1.95 | 0.47 |
| 4:D:156:LYS:HD3 | 4:D:223:ILE:HD12 | 1.96 | 0.47 |
| 4:D:182:LEU:HD11 | 4:D:197:LYS:HB2 | 1.96 | 0.47 |
| 1:A:21:MET:HG2 | 2:B:1078:PRO:HG2 | 1.95 | 0.47 |
| 2:B:25:LYS:HD3 | 2:B:29:ARG:HG2 | 1.96 | 0.47 |
| 2:B:807:LEU:HD11 | 2:B:837:VAL:HB | 1.96 | 0.47 |
| 3:C:368:ILE:HG23 | 3:C:370:GLN:H | 1.79 | 0.47 |
| 1:A:827:VAL:HG21 | 2:B:453:ARG:HB3 | 1.97 | 0.47 |
| 2:B:21:TYR:HB2 | 2:B:601:TRP:CE3 | 2.50 | 0.47 |
| 3:C:17:LEU:HB2 | 3:C:22:LYS:HZ3 | 1.80 | 0.47 |
| 5:L:66:THR:HB | 5:L:69:GLU:OE1 | 2.15 | 0.47 |
| 1:A:79:PRO:HB2 | 1:A:180:PRO:HB2 | 1.95 | 0.47 |
| 1:A:484:VAL:O | 1:A:488:ILE:HG23 | 2.15 | 0.47 |
| 1:A:512:THR:HG21 | 1:A:619:ILE:HG13 | 1.96 | 0.47 |
| 2:B:490:VAL:HG21 | 2:B:551:VAL:HG21 | 1.97 | 0.47 |
| 3:C:160:PHE:HB3 | 3:C:201:VAL:HG23 | 1.96 | 0.47 |
| 5:L:17:LEU:HD22 | 5:L:55:PRO:HG2 | 1.96 | 0.47 |
| 2:B:22:TRP:HZ2 | 2:B:482:LEU:HB3 | 1.80 | 0.47 |
| 2:B:1085:ARG:HA | 2:B:1085:ARG:HD2 | 1.65 | 0.47 |
| 1:A:280:ILE:HD11 | 2:B:1105:MET:SD | 2.55 | 0.46 |
| 1:A:493:TYR:CE1 | 1:A:627:GLU:HG3 | 2.50 | 0.46 |
| 2:B:364:VAL:HA | 2:B:367:ILE:HD12 | 1.98 | 0.46 |
| 2:B:1054:THR:HB | 2:B:1093:TYR:CE1 | 2.49 | 0.46 |
| 3:C:345:GLN:HA | 3:C:348:PHE:HD2 | 1.80 | 0.46 |
| 2:B:244:VAL:HG21 | 2:B:254:MET:HG2 | 1.97 | 0.46 |
| 2:B:487:THR:HG23 | 2:B:569:ASP:HA | 1.97 | 0.46 |
| 2:B:622:TYR:HE2 | 2:B:633:GLU:HG3 | 1.81 | 0.46 |
| 3:C:39:THR:O | 3:C:43:ILE:HG12 | 2.15 | 0.46 |
| 3:C:263:THR:HA | 6:H:12:HIS:HA | 1.98 | 0.46 |
| 3:C:364:GLU:HA | 3:C:367:LEU:HG | 1.96 | 0.46 |
| 1:A:24:VAL:HB | 1:A:47:ARG:HB2 | 1.98 | 0.46 |
| 1:A:483:GLU:OE1 | 1:A:485:GLN:HB2 | 2.16 | 0.46 |
| 2:B:926:ILE:HG23 | 2:B:955:LEU:HD13 | 1.96 | 0.46 |
| 2:B:1054:THR:HB | 2:B:1093:TYR:HE1 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1095:PHE:CD2 | 3:C:368:ILE:HG13 | 2.50 | 0.46 |
| 2:B:122:GLU:H | 2:B:401:THR:HG22 | 1.80 | 0.46 |
| 2:B:871:GLU:O | 2:B:886:ILE:HD11 | 2.15 | 0.46 |
| 2:B:176:THR:HA | 2:B:191:VAL:HB | 1.97 | 0.46 |
| 2:B:808:VAL:O | 2:B:834:SER:HB2 | 2.16 | 0.46 |
| 2:B:191:VAL:HG13 | 2:B:202:VAL:HG23 | 1.97 | 0.46 |
| 3:C:302:ASP:HB3 | 3:C:305:HIS:CD2 | 2.50 | 0.46 |
| 1:A:780:GLY:HA3 | 1:A:785:VAL:HA | 1.97 | 0.46 |
| 2:B:15:TRP:CZ2 | 2:B:703:ARG:HG3 | 2.50 | 0.46 |
| 2:B:483:MET:HE2 | 2:B:574:ARG:HB2 | 1.97 | 0.46 |
| 5:L:31:THR:HG21 | 5:L:78:ILE:HD11 | 1.97 | 0.46 |
| 2:B:426:ARG:HG3 | 2:B:684:ARG:HH21 | 1.81 | 0.46 |
| 2:B:327:LEU:HD21 | 2:B:332:ARG:HD2 | 1.98 | 0.45 |
| 7:N:56:ILE:O | 7:N:60:MET:HG2 | 2.16 | 0.45 |
| 2:B:609:ILE:HG22 | 2:B:610:ILE:HG12 | 1.98 | 0.45 |
| 2:B:100:LEU:HD12 | 2:B:123:LEU:HD22 | 1.98 | 0.45 |
| 2:B:1059:CYS:HB2 | 2:B:1064:HIS:HE2 | 1.81 | 0.45 |
| 5:L:90:GLU:O | 5:L:94:LYS:HG2 | 2.17 | 0.45 |
| 1:A:396:LYS:HA | 1:A:399:LEU:HD12 | 1.97 | 0.45 |
| 1:A:664:PHE:CZ | 1:A:748:MET:HE3 | 2.51 | 0.45 |
| 2:B:770:PHE:HE1 | 2:B:810:ARG:HE | 1.64 | 0.45 |
| 5:L:39:LYS:HE2 | 5:L:62:ASP:HA | 1.98 | 0.45 |
| 2:B:219:VAL:HG22 | 2:B:221:LYS:H | 1.81 | 0.45 |
| 5:L:47:HIS:CE1 | 5:L:49:ILE:HD13 | 2.52 | 0.45 |
| 2:B:236:ARG:O | 2:B:240:ILE:HG13 | 2.17 | 0.45 |
| 2:B:947:PRO:HG2 | 2:B:950:LYS:HB3 | 1.99 | 0.45 |
| 6:H:24:GLU:HA | 6:H:27:LYS:HG2 | 1.99 | 0.45 |
| 8:K:34:ILE:HB | 8:K:38:GLU:OE2 | 2.17 | 0.45 |
| 1:A:122:ASN:HB2 | 1:A:123:ARG:HH11 | 1.81 | 0.45 |
| 1:A:789:PHE:HZ | 1:A:813:GLN:HG2 | 1.82 | 0.45 |
| 2:B:73:GLU:HG3 | 2:B:83:PRO:HA | 1.99 | 0.45 |
| 8:K:26:VAL:HG12 | 8:K:28:ILE:H | 1.81 | 0.45 |
| 9:P:15:VAL:HG21 | 9:P:28:PRO:HD2 | 1.98 | 0.45 |
| 1:A:542:LYS:HG2 | 1:A:550:LEU:HD12 | 1.99 | 0.45 |
| 2:B:921:GLN:HE21 | 2:B:986:ILE:HD12 | 1.82 | 0.45 |
| 3:C:180:VAL:HG13 | 3:C:192:PHE:HD2 | 1.82 | 0.45 |
| 1:A:841:ARG:HH12 | 1:A:845:ASN:HB2 | 1.82 | 0.45 |
| 1:A:892:ILE:HG21 | 3:C:32:TYR:CD2 | 2.52 | 0.45 |
| 2:B:1066:ALA:HB1 | 2:B:1075:VAL:HB | 1.98 | 0.45 |
| 3:C:287:ILE:HD11 | 3:C:307:MET:HA | 1.98 | 0.45 |
| 2:B:653:PRO:HG2 | 2:B:880:HIS:CE1 | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:273:ILE:HD11 | 3:C:277:LEU:HD12 | 1.98 | 0.44 |
| 2:B:685:VAL:HG21 | 2:B:861:LYS:HD3 | 1.99 | 0.44 |
| 2:B:895:MET:HE2 | 2:B:904:PRO:HD2 | 1.99 | 0.44 |
| 4:D:156:LYS:HG2 | 4:D:223:ILE:HB | 2.00 | 0.44 |
| 1:A:269:TRP:O | 1:A:273:GLN:HG2 | 2.18 | 0.44 |
| 2:B:236:ARG:HH12 | 2:B:238:LYS:HB3 | 1.82 | 0.44 |
| 2:B:506:PRO:HG2 | 2:B:509:VAL:HG23 | 1.98 | 0.44 |
| 3:C:270:ILE:HA | 3:C:273:ILE:HG22 | 2.00 | 0.44 |
| 7:N:55:LEU:O | 7:N:59:ILE:HG12 | 2.17 | 0.44 |
| 1:A:381:VAL:HG21 | 1:A:403:LEU:HD21 | 1.99 | 0.44 |
| 1:A:446:ARG:HH22 | 5:L:49:ILE:HG21 | 1.81 | 0.44 |
| 1:A:447:LEU:HD11 | 1:A:455:TYR:HE2 | 1.82 | 0.44 |
| 1:A:656:ILE:HD12 | 1:A:656:ILE:HA | 1.89 | 0.44 |
| 2:B:22:TRP:CZ2 | 2:B:482:LEU:HB3 | 2.52 | 0.44 |
| 2:B:651:LEU:HD12 | 2:B:705:MET:HE3 | 1.98 | 0.44 |
| 3:C:205:LYS:HD2 | 3:C:205:LYS:HA | 1.76 | 0.44 |
| 1:A:162:TYR:HB2 | 1:A:178:LEU:HB2 | 2.00 | 0.44 |
| 1:A:429:ARG:HG2 | 2:B:1037:HIS:NE2 | 2.32 | 0.44 |
| 1:A:788:HIS:HD1 | 2:B:623:VAL:HB | 1.82 | 0.44 |
| 2:B:674:LEU:HD23 | 2:B:692:LEU:HB2 | 1.99 | 0.44 |
| 3:C:124:GLU:HG3 | 3:C:131:LYS:HZ1 | 1.82 | 0.44 |
| 3:C:181:LYS:O | 3:C:184:GLU:HG2 | 2.16 | 0.44 |
| 3:C:251:PHE:CD2 | 3:C:276:VAL:HG21 | 2.53 | 0.44 |
| 1:A:898:LYS:HB2 | 1:A:898:LYS:HE3 | 1.73 | 0.44 |
| 1:A:71:PHE:HE2 | 2:B:1103:LYS:HD3 | 1.82 | 0.44 |
| 1:A:489:ILE:HA | 1:A:496:PRO:HA | 2.00 | 0.44 |
| 4:D:36:LEU:HA | 4:D:149:GLN:HE22 | 1.81 | 0.44 |
| 1:A:112:GLU:HA | 1:A:115:LYS:HE2 | 2.00 | 0.44 |
| 2:B:517:TRP:CD1 | 2:B:532:GLY:H | 2.35 | 0.44 |
| 2:B:536:VAL:HG23 | 2:B:554:VAL:HG22 | 2.00 | 0.44 |
| 2:B:654:TYR:CZ | 2:B:940:GLY:HA2 | 2.53 | 0.44 |
| 3:C:82:LEU:HD12 | 3:C:99:LEU:HD23 | 1.99 | 0.44 |
| 3:C:302:ASP:HB3 | 3:C:305:HIS:HD2 | 1.82 | 0.44 |
| 1:A:341:GLY:HA3 | 1:A:446:ARG:HB2 | 2.00 | 0.44 |
| 1:A:655:THR:HA | 1:A:658:VAL:HG12 | 2.00 | 0.44 |
| 1:A:685:ILE:HD13 | 1:A:803:VAL:HG13 | 2.00 | 0.44 |
| 1:A:888:VAL:HA | 1:A:891:ILE:HG22 | 1.99 | 0.44 |
| 2:B:483:MET:HB3 | 2:B:643:ALA:HB1 | 2.00 | 0.44 |
| 2:B:1064:HIS:HE1 | 2:B:1084:GLU:HG3 | 1.83 | 0.44 |
| 3:C:5:THR:HG22 | 3:C:40:LYS:HZ1 | 1.83 | 0.44 |
| 1:A:428:HIS:CE1 | 1:A:430:MET:HB2 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:232:LEU:HB2 | 4:D:237:ILE:HD11 | 2.00 | 0.43 |
| 8:K:14:GLY:O | 8:K:18:LEU:HD23 | 2.18 | 0.43 |
| 2:B:57:ILE:HG13 | 2:B:60:PHE:HD2 | 1.84 | 0.43 |
| 2:B:961:LYS:HG3 | 2:B:963:THR:H | 1.82 | 0.43 |
| 1:A:492:ARG:HD2 | 3:C:76:PRO:HG3 | 2.01 | 0.43 |
| 2:B:42:GLY:HA2 | 2:B:45:GLU:HG2 | 2.00 | 0.43 |
| 2:B:513:ASP:HB2 | 2:B:516:LEU:HB2 | 2.01 | 0.43 |
| 2:B:899:GLU:HG3 | 4:D:198:PRO:HB3 | 2.00 | 0.43 |
| 3:C:81:THR:H | 3:C:297:GLN:NE2 | 2.16 | 0.43 |
| 5:L:88:ALA:HA | 5:L:91:LYS:NZ | 2.33 | 0.43 |
| 9:P:25:LEU:HD21 | 9:P:35:LEU:HB2 | 2.00 | 0.43 |
| 2:B:268:GLN:HG3 | 2:B:269:GLU:H | 1.82 | 0.43 |
| 2:B:367:ILE:O | 2:B:371:MET:HG2 | 2.17 | 0.43 |
| 1:A:763:MET:HB3 | 2:B:917:MET:SD | 2.58 | 0.43 |
| 4:D:35:ILE:HD12 | 4:D:237:ILE:HG22 | 2.01 | 0.43 |
| 3:C:9:LEU:HA | 3:C:12:LYS:HG2 | 2.00 | 0.43 |
| 4:D:4:ILE:HD11 | 5:L:84:GLU:HB3 | 2.01 | 0.43 |
| 6:H:26:LYS:HG2 | 6:H:60:VAL:HB | 2.00 | 0.43 |
| 1:A:363:ARG:O | 1:A:367:MET:HG2 | 2.18 | 0.43 |
| 1:A:699:TYR:HA | 1:A:704:LEU:HB2 | 2.00 | 0.43 |
| 4:D:101:VAL:HG13 | 4:D:122:ILE:HB | 1.99 | 0.43 |
| 1:A:136:LYS:HA | 1:A:136:LYS:HD3 | 1.82 | 0.43 |
| 1:A:142:MET:HE3 | 1:A:142:MET:O | 2.19 | 0.43 |
| 2:B:704:ILE:HD12 | 2:B:704:ILE:H | 1.83 | 0.43 |
| 4:D:259:LEU:HD22 | 5:L:3:ILE:HG21 | 2.00 | 0.43 |
| 1:A:254:GLN:HA | 1:A:257:GLU:HG2 | 1.99 | 0.43 |
| 1:A:850:LEU:HB2 | 3:C:66:GLY:HA3 | 2.00 | 0.43 |
| 2:B:699:LEU:HA | 2:B:937:ARG:HG2 | 2.00 | 0.43 |
| 3:C:191:GLU:HG2 | 3:C:202:ARG:HB2 | 2.00 | 0.43 |
| 4:D:68:ILE:HD12 | 4:D:69:PRO:HD2 | 2.01 | 0.43 |
| 1:A:78:ARG:HG3 | 1:A:252:LEU:HD23 | 2.01 | 0.43 |
| 1:A:252:LEU:HD22 | 1:A:272:LEU:HD22 | 2.01 | 0.43 |
| 1:A:762:GLN:NE2 | 1:A:767:LEU:HG | 2.34 | 0.43 |
| 1:A:24:VAL:HG11 | 1:A:48:MET:HB2 | 2.00 | 0.42 |
| 1:A:241:LYS:HD2 | 1:A:241:LYS:HA | 1.77 | 0.42 |
| 1:A:667:GLY:H | 2:B:965:ARG:NH2 | 2.14 | 0.42 |
| 2:B:85:TYR:HB2 | 2:B:88:ASP:CG | 2.44 | 0.42 |
| 2:B:689:GLY:HA3 | 2:B:752:PHE:HB2 | 2.00 | 0.42 |
| 3:C:251:PHE:HD2 | 3:C:276:VAL:HG21 | 1.84 | 0.42 |
| 1:A:90:TYR:HE1 | 1:A:154:ILE:HG22 | 1.84 | 0.42 |
| 1:A:485:GLN:HB2 | 1:A:485:GLN:HE21 | 1.62 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:500:GLY:HA3 | 1:A:504:HIS:HB2 | 2.02 | 0.42 |
| 2:B:50:PHE:HB3 | 2:B:64:PHE:CE2 | 2.54 | 0.42 |
| 2:B:1064:HIS:HA | 2:B:1103:LYS:HZ1 | 1.84 | 0.42 |
| 8:K:30:VAL:HB | 8:K:34:ILE:HD11 | 2.01 | 0.42 |
| 1:A:78:ARG:HB3 | 1:A:269:TRP:CE2 | 2.54 | 0.42 |
| 2:B:847:LYS:HE3 | 7:N:64:VAL:HG22 | 2.00 | 0.42 |
| 1:A:281:ASN:OD1 | 1:A:283:GLU:HG3 | 2.20 | 0.42 |
| 1:A:490:SER:HB3 | 1:A:497:ILE:HB | 2.01 | 0.42 |
| 1:A:580:CYS:HB2 | 1:A:606:PHE:HB2 | 2.02 | 0.42 |
| 2:B:226:VAL:HG21 | 2:B:258:LEU:HA | 2.01 | 0.42 |
| 2:B:329:LEU:HB3 | 2:B:331:ARG:NH1 | 2.34 | 0.42 |
| 2:B:698:PRO:HG3 | 2:B:987:TYR:CZ | 2.54 | 0.42 |
| 4:D:94:GLU:HG3 | 4:D:132:VAL:HG13 | 2.02 | 0.42 |
| 1:A:126:GLU:O | 1:A:130:ILE:HG12 | 2.19 | 0.42 |
| 1:A:261:PRO:O | 1:A:265:ILE:HG12 | 2.19 | 0.42 |
| 2:B:272:GLU:HB3 | 2:B:276:LYS:NZ | 2.35 | 0.42 |
| 2:B:870:PRO:HG3 | 2:B:990:ARG:HH12 | 1.84 | 0.42 |
| 3:C:151:THR:HA | 3:C:162:VAL:HA | 2.02 | 0.42 |
| 2:B:507:ILE:HG12 | 2:B:525:LEU:HD21 | 2.01 | 0.42 |
| 3:C:73:ILE:HD12 | 3:C:73:ILE:HA | 1.91 | 0.42 |
| 1:A:83:VAL:HG11 | 1:A:277:THR:HG23 | 2.02 | 0.42 |
| 1:A:89:ILE:HG21 | 1:A:210:MET:HE2 | 2.00 | 0.42 |
| 1:A:481:LEU:HD21 | 2:B:1037:HIS:HB3 | 2.02 | 0.42 |
| 2:B:642:ALA:HB1 | 2:B:704:ILE:HD11 | 2.02 | 0.42 |
| 2:B:725:ALA:HA | 2:B:909:ASN:OD1 | 2.19 | 0.42 |
| 2:B:798:GLU:N | 2:B:845:VAL:HB | 2.35 | 0.42 |
| 6:H:26:LYS:HZ2 | 6:H:60:VAL:H | 1.67 | 0.42 |
| 2:B:195:ARG:HB2 | 2:B:301:PRO:HB2 | 2.00 | 0.42 |
| 2:B:332:ARG:HH22 | 2:B:560:VAL:HG11 | 1.85 | 0.42 |
| 2:B:739:LYS:HB3 | 2:B:891:PRO:HA | 2.02 | 0.42 |
| 4:D:163:ILE:HB | 4:D:191:VAL:HG13 | 2.02 | 0.42 |
| 4:D:240:ILE:O | 4:D:244:ILE:HG12 | 2.20 | 0.42 |
| 1:A:70:HIS:CE1 | 2:B:1067:LEU:HD11 | 2.55 | 0.42 |
| 1:A:489:ILE:HD11 | 1:A:636:VAL:HG21 | 2.02 | 0.42 |
| 1:A:776:ARG:HH22 | 1:A:794:LEU:HB3 | 1.84 | 0.42 |
| 2:B:577:ILE:HB | 2:B:637:LEU:HB3 | 2.01 | 0.42 |
| 3:C:384:LYS:HA | 3:C:384:LYS:HD2 | 1.81 | 0.42 |
| 4:D:163:ILE:HA | 4:D:213:ILE:HD12 | 2.00 | 0.42 |
| 1:A:56:ARG:HH11 | 2:B:1070:LYS:HD3 | 1.85 | 0.41 |
| 2:B:601:TRP:O | 2:B:605:ILE:HG12 | 2.20 | 0.41 |
| 1:A:442:TYR:CG | 2:B:872:LEU:HD13 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:869:LYS:HE3 | 1:A:873:ASP:HA | 2.00 | 0.41 |
| 2:B:435:HIS:HD2 | 2:B:438:ARG:HD2 | 1.85 | 0.41 |
| 2:B:1044:ILE:HD12 | 2:B:1044:ILE:HA | 1.89 | 0.41 |
| 4:D:235:GLU:HA | 5:L:89:TRP:HZ2 | 1.84 | 0.41 |
| 1:A:277:THR:HA | 1:A:280:ILE:HG22 | 2.03 | 0.41 |
| 1:A:697:GLU:HA | 1:A:700:LYS:HG2 | 2.02 | 0.41 |
| 2:B:140:GLU:HG3 | 2:B:144:LYS:NZ | 2.35 | 0.41 |
| 3:C:269:ASN:HB3 | 3:C:272:GLU:HB3 | 2.02 | 0.41 |
| 4:D:84:LEU:HD23 | 4:D:139:LEU:HB3 | 2.02 | 0.41 |
| 7:N:1:MET:N | 7:N:1:MET:HE2 | 2.35 | 0.41 |
| 2:B:654:TYR:HB3 | 2:B:657:HIS:ND1 | 2.36 | 0.41 |
| 2:B:413:TRP:CD1 | 2:B:420:VAL:HG21 | 2.56 | 0.41 |
| 2:B:1070:LYS:HG3 | 2:B:1071:ARG:HD3 | 2.01 | 0.41 |
| 2:B:1076:TYR:HB3 | 2:B:1082:GLU:HG2 | 2.02 | 0.41 |
| 3:C:176:MET:O | 3:C:180:VAL:HG23 | 2.21 | 0.41 |
| 3:C:188:LYS:HE2 | 3:C:188:LYS:HB2 | 1.90 | 0.41 |
| 2:B:213:TYR:CZ | 2:B:224:LYS:HG2 | 2.55 | 0.41 |
| 2:B:388:HIS:C | 2:B:392:ARG:HE | 2.28 | 0.41 |
| 3:C:116:MET:HA | 3:C:247:GLU:HA | 2.02 | 0.41 |
| 1:A:651:VAL:O | 1:A:655:THR:HG22 | 2.21 | 0.41 |
| 2:B:891:PRO:HB2 | 2:B:893:GLU:CD | 2.46 | 0.41 |
| 1:A:511:LEU:HB2 | 1:A:658:VAL:HG11 | 2.03 | 0.41 |
| 2:B:674:LEU:HB3 | 2:B:990:ARG:HB3 | 2.02 | 0.41 |
| 2:B:902:ILE:HG13 | 7:N:43:TYR:CZ | 2.55 | 0.41 |
| 1:A:13:LEU:HD13 | 1:A:18:ILE:HD13 | 2.02 | 0.41 |
| 1:A:80:VAL:HG11 | 1:A:276:VAL:HG11 | 2.02 | 0.41 |
| 1:A:93:LEU:HD11 | 1:A:154:ILE:HG21 | 2.03 | 0.41 |
| 1:A:277:THR:HG21 | 1:A:287:VAL:HG21 | 2.03 | 0.41 |
| 1:A:509:TYR:O | 1:A:513:ARG:HB2 | 2.20 | 0.41 |
| 2:B:184:GLN:O | 2:B:185:GLU:HG3 | 2.20 | 0.41 |
| 2:B:275:GLY:HA3 | 2:B:287:ARG:HB3 | 2.03 | 0.41 |
| 2:B:758:GLU:HB3 | 2:B:859:LEU:HD13 | 2.03 | 0.41 |
| 2:B:1064:HIS:CE1 | 2:B:1084:GLU:HG3 | 2.56 | 0.41 |
| 3:C:327:VAL:HA | 3:C:330:GLU:HG2 | 2.02 | 0.41 |
| 3:C:381:LEU:HD21 | 8:K:11:ARG:HG3 | 2.03 | 0.41 |
| 1:A:567:VAL:H | 1:A:609:ILE:HG23 | 1.86 | 0.41 |
| 1:A:810:LEU:HD12 | 1:A:814:GLU:HB3 | 2.02 | 0.41 |
| 2:B:413:TRP:NE1 | 2:B:420:VAL:HG21 | 2.36 | 0.41 |
| 2:B:444:ASP:H | 2:B:449:HIS:HE1 | 1.68 | 0.41 |
| 1:A:28:VAL:O | 1:A:42:GLY:HA2 | 2.20 | 0.40 |
| 2:B:347:LEU:HD11 | 2:B:486:ILE:HG21 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:413:LEU:HG | 1:A:437:VAL:HG11 | 2.03 | 0.40 |
| 1:A:528:MET:HE1 | 5:L:58:ARG:HB3 | 2.02 | 0.40 |
| 2:B:962:HIS:CE1 | 4:D:203:LYS:HG3 | 2.56 | 0.40 |
| 1:A:9:GLU:O | 2:B:1110:LYS:HB3 | 2.21 | 0.40 |
| 1:A:128:ASN:HB3 | 1:A:132:LYS:HZ1 | 1.85 | 0.40 |
| 1:A:803:VAL:H | 1:A:814:GLU:CD | 2.30 | 0.40 |
| 1:A:864:ILE:HD12 | 6:H:39:GLN:HA | 2.03 | 0.40 |
| 2:B:169:GLU:HG3 | 2:B:343:LYS:HD3 | 2.03 | 0.40 |
| 2:B:249:GLU:O | 2:B:253:ILE:HG12 | 2.22 | 0.40 |
| 2:B:1050:GLU:HG3 | 2:B:1051:SER:H | 1.86 | 0.40 |
| 4:D:97:GLY:HA2 | 4:D:127:GLU:HA | 2.02 | 0.40 |
| 1:A:585:LYS:O | 1:A:589:GLU:HG2 | 2.22 | 0.40 |
| 2:B:15:TRP:CH2 | 2:B:703:ARG:HG3 | 2.56 | 0.40 |
| 3:C:305:HIS:CD2 | 3:C:305:HIS:H | 2.37 | 0.40 |
| 7:N:14:ILE:HG23 | 7:N:15:GLY:H | 1.86 | 0.40 |
| 1:A:46:LYS:HB2 | 1:A:58:GLU:HG2 | 2.04 | 0.40 |
| 1:A:559:LEU:HD23 | 1:A:559:LEU:HA | 1.89 | 0.40 |
| 2:B:162:GLU:CD | 2:B:684:ARG:HH22 | 2.30 | 0.40 |
| 2:B:462:ARG:HH22 | 2:B:614:ASP:C | 2.30 | 0.40 |
| 2:B:1028:GLU:HB2 | 2:B:1031:ARG:NH2 | 2.37 | 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 | 899/907 (99%) | 845 (94%) | 52 (6%) | 2 (0%) | 43 77 |
| 2 | B | 1070/1117 (96%) | 1025 (96%) | 44 (4%) | 1 (0%) | 48 83 |
| 3 | C | 386/397 (97%) | 367 (95%) | 19 (5%) | 0 | 100 100 |
| 4 | D | 256/275 (93%) | 243 (95%) | 12 (5%) | 1 (0%) | 30 67 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 5 | L | 92/95 (97%) | 84 (91%) | 8 (9%) | 0 | 100 | 100 |
| 6 | H | 74/82 (90%) | 70 (95%) | 4 (5%) | 0 | 100 | 100 |
| 7 | N | 63/65 (97%) | 60 (95%) | 3 (5%) | 0 | 100 | 100 |
| 8 | K | 53/57 (93%) | 51 (96%) | 2 (4%) | 0 | 100 | 100 |
| 9 | P | 46/49 (94%) | 45 (98%) | 1 (2%) | 0 | 100 | 100 |
| All | All | 2939/3044 (97%) | 2790 (95%) | 145 (5%) | 4 (0%) | 49 | 83 |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 1061 | ASN |
| 1 | A | 392 | MET |
| 4 | D | 76 | ARG |
| 1 | A | 159 | PRO |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 777/782 (99%) | 777 (100%) | 0 | 100 | 100 |
| 2 | B | 929/962 (97%) | 929 (100%) | 0 | 100 | 100 |
| 3 | C | 336/345 (97%) | 336 (100%) | 0 | 100 | 100 |
| 4 | D | 230/246 (94%) | 230 (100%) | 0 | 100 | 100 |
| 5 | L | 83/84 (99%) | 83 (100%) | 0 | 100 | 100 |
| 6 | H | 66/70 (94%) | 66 (100%) | 0 | 100 | 100 |
| 7 | N | 60/60 (100%) | 60 (100%) | 0 | 100 | 100 |
| 8 | K | 45/47 (96%) | 45 (100%) | 0 | 100 | 100 |
| 9 | P | 44/45 (98%) | 44 (100%) | 0 | 100 | 100 |
| All | All | 2570/2641 (97%) | 2570 (100%) | 0 | 100 | 100 |

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 255 | ASN |
| 1 | A | 262 | GLN |
| 1 | A | 282 | ASN |
| 1 | A | 428 | HIS |
| 1 | A | 804 | ASN |
| 1 | A | 867 | GLN |
| 2 | B | 257 | ASN |
| 2 | B | 267 | GLN |
| 2 | B | 302 | HIS |
| 2 | B | 376 | GLN |
| 2 | B | 393 | ASN |
| 2 | B | 449 | HIS |
| 2 | B | 581 | ASN |
| 2 | B | 592 | GLN |
| 2 | B | 727 | GLN |
| 2 | B | 880 | HIS |
| 2 | B | 892 | GLN |
| 2 | B | 921 | GLN |
| 2 | B | 1000 | HIS |
| 3 | C | 86 | HIS |
| 3 | C | 305 | HIS |
| 3 | C | 360 | ASN |
| 3 | C | 370 | GLN |
| 4 | D | 149 | GLN |
| 5 | L | 22 | HIS |
| 5 | L | 47 | HIS |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

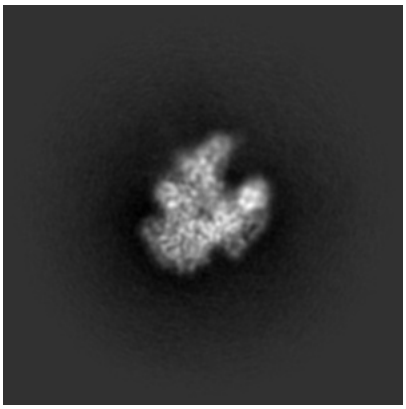
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-77809. These allow visual inspection of the internal detail of the map and identification of artifacts.

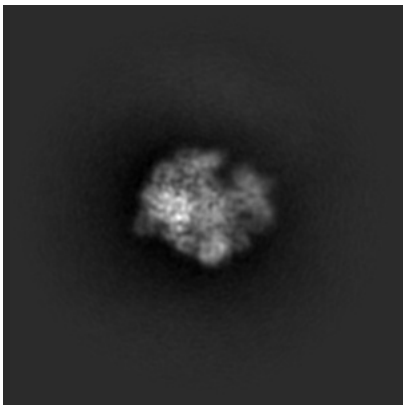
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections (i)

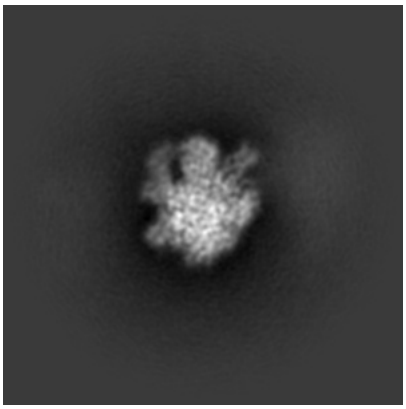
### 6.1.1 Primary map



X

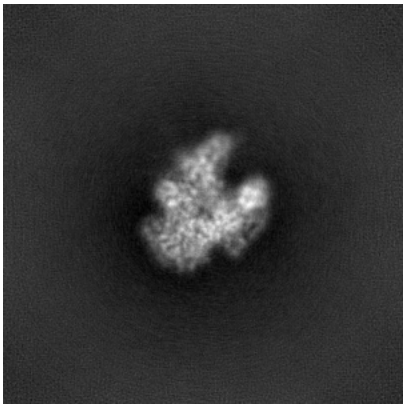


Y

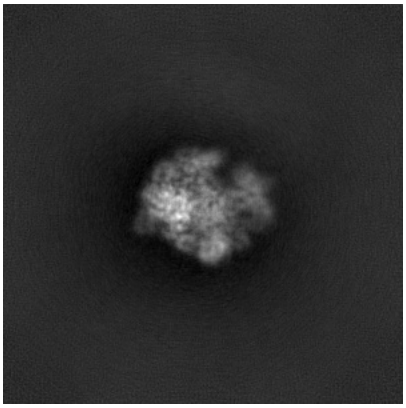


Z

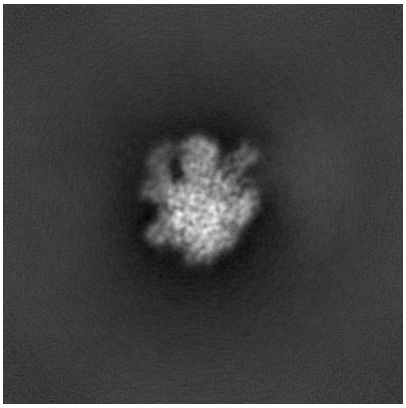
### 6.1.2 Raw map



X



Y

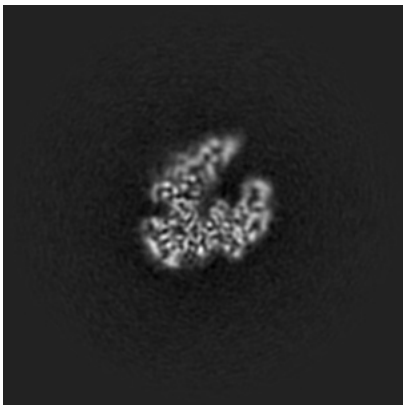


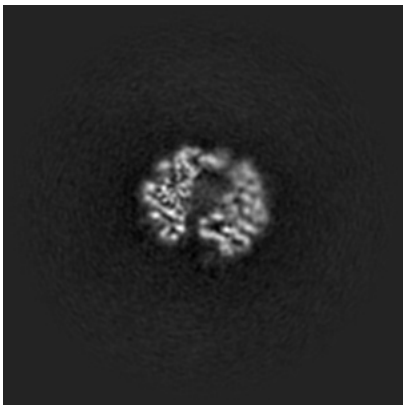
Z

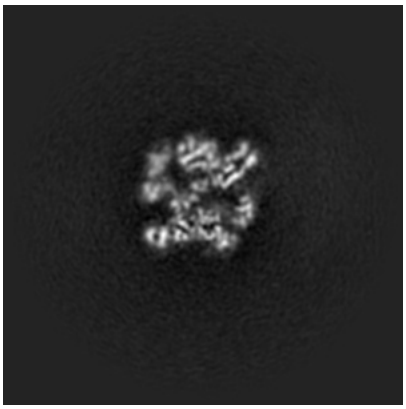
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

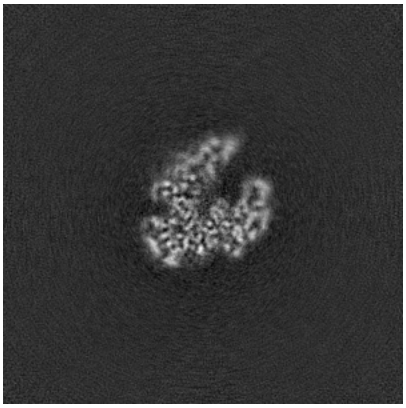
### 6.2.1 Primary map

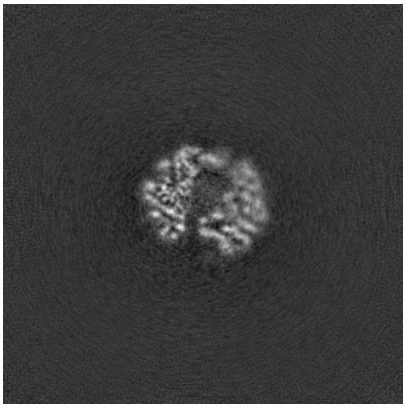

X Index: 200

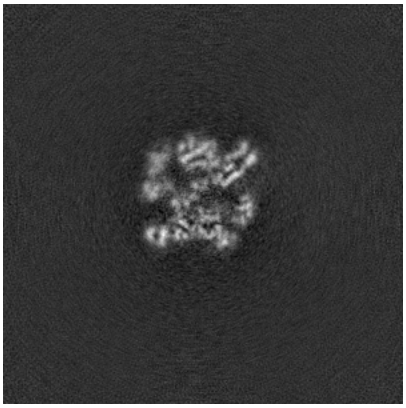

Y Index: 200


Z Index: 200

### 6.2.2 Raw map


X Index: 200

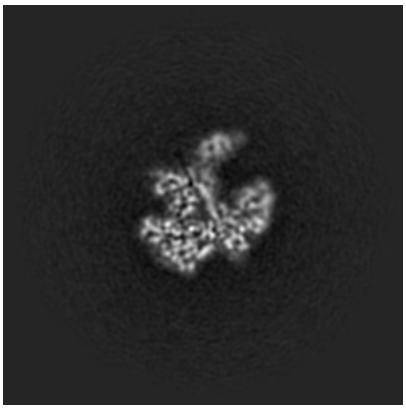

Y Index: 200

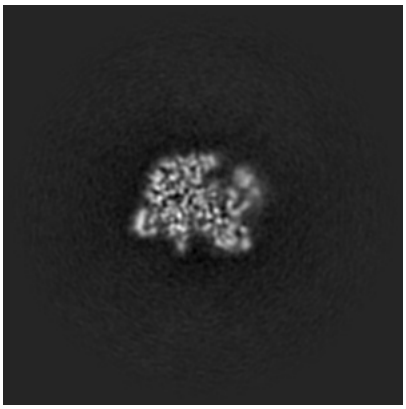

Z Index: 200

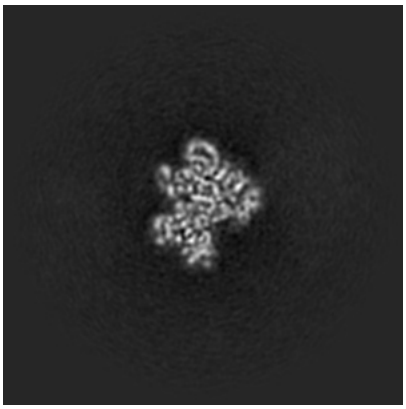
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

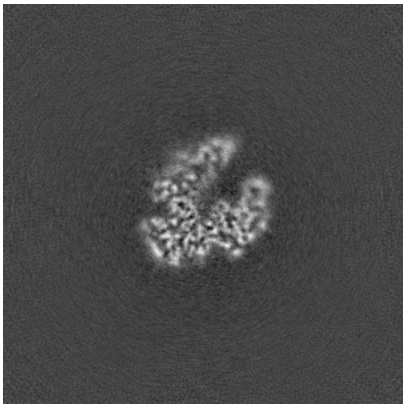
### 6.3.1 Primary map

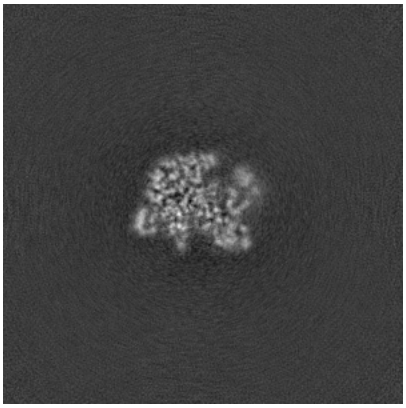

X Index: 189

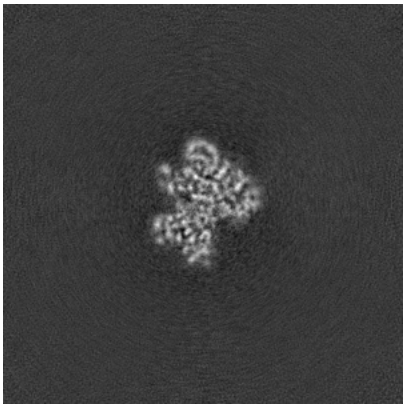

Y Index: 188


Z Index: 180

### 6.3.2 Raw map


X Index: 202


Y Index: 188

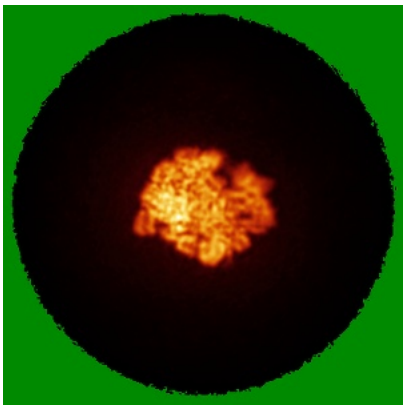

Z Index: 181

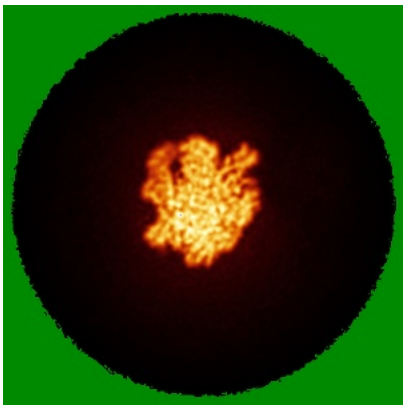
The images above show the largest variance slices of the map in three orthogonal directions.

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

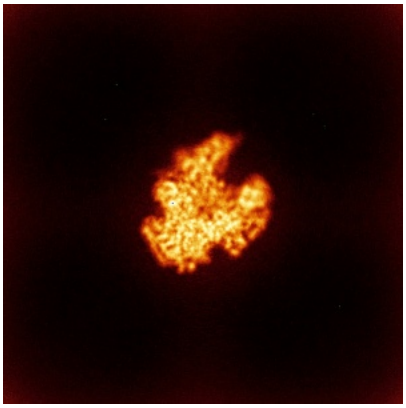
### 6.4.1 Primary map

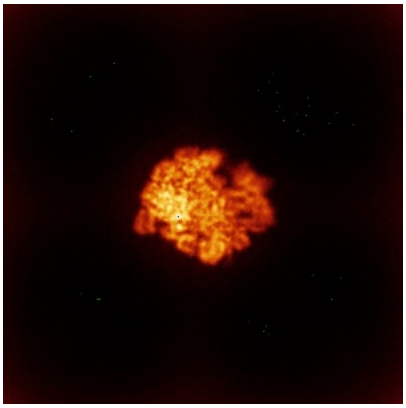
X

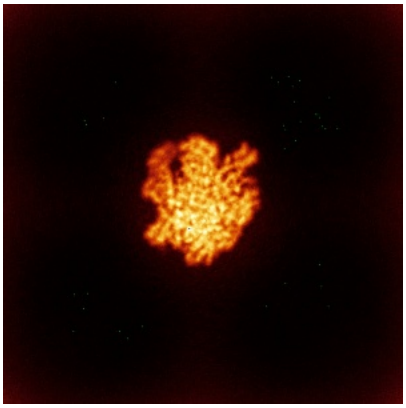

Y


Z

### 6.4.2 Raw map


X

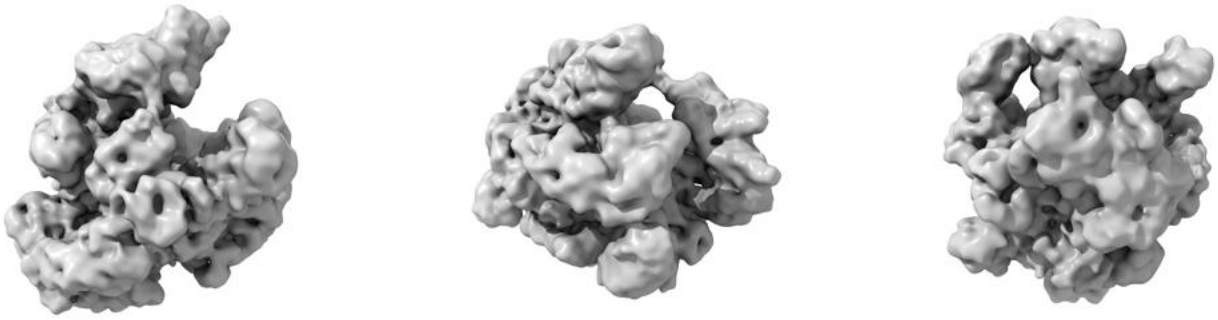

Y


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 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 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.

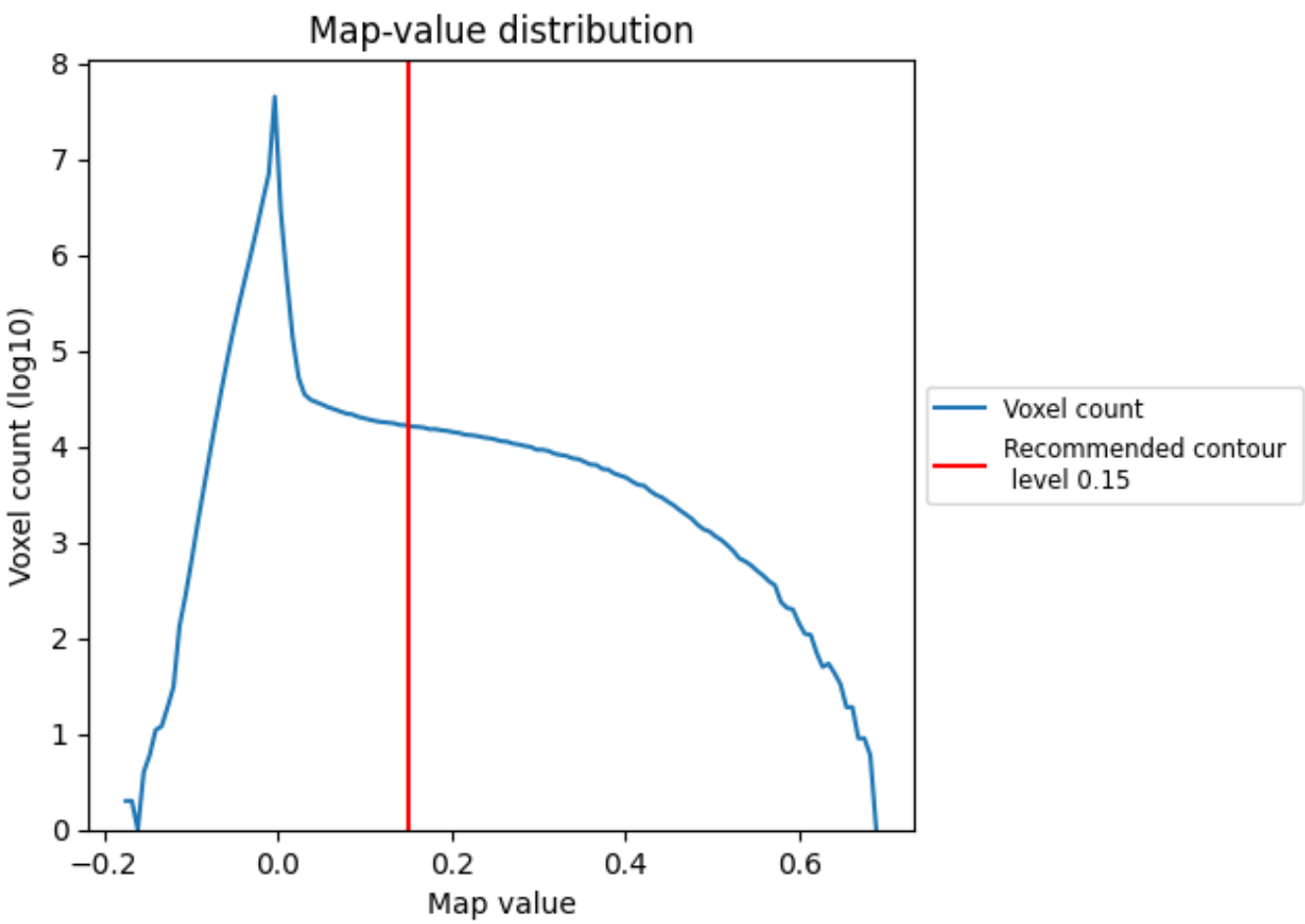
## 6.6 Mask visualisation (i)

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

# 7 Map analysis (i)

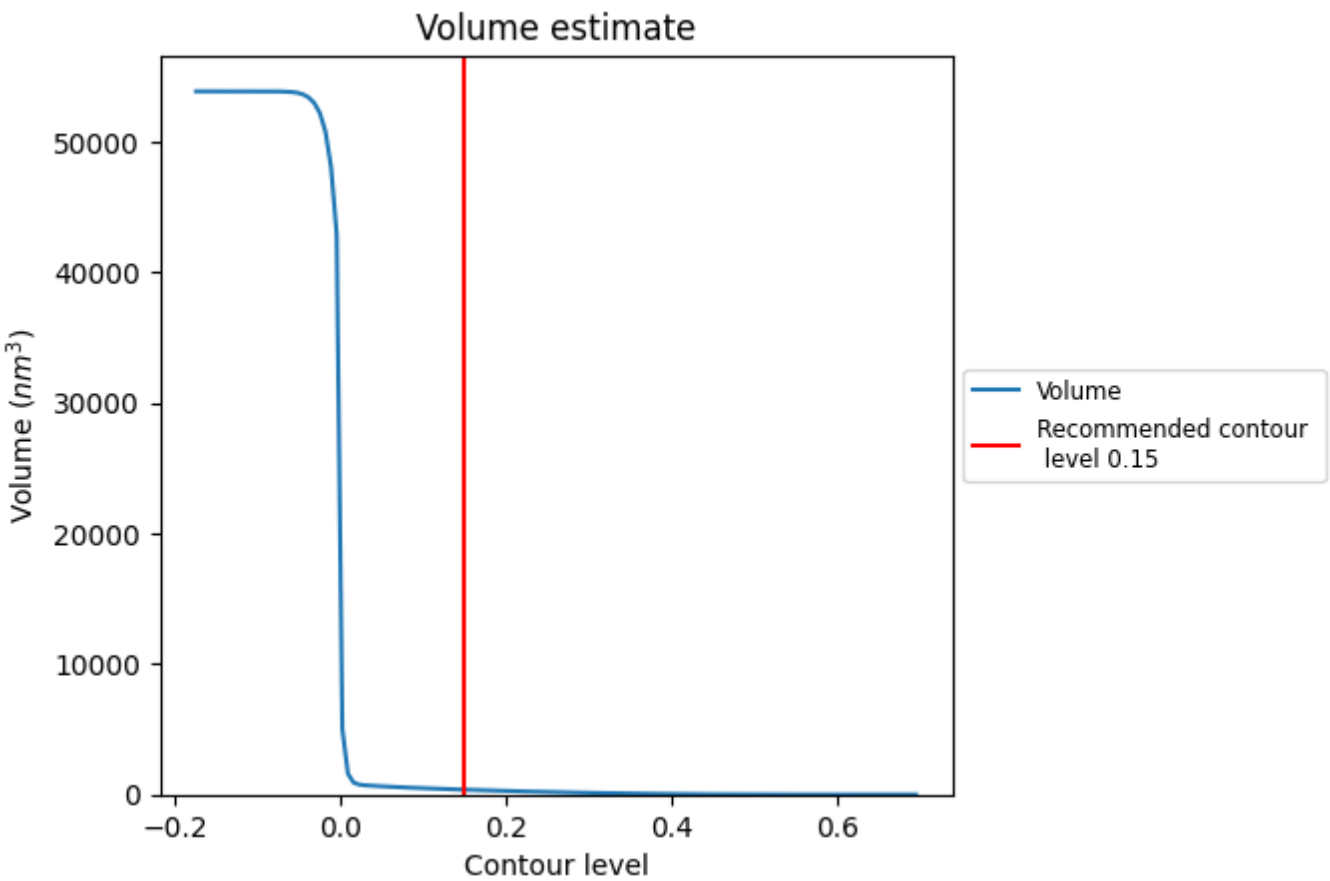
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)




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

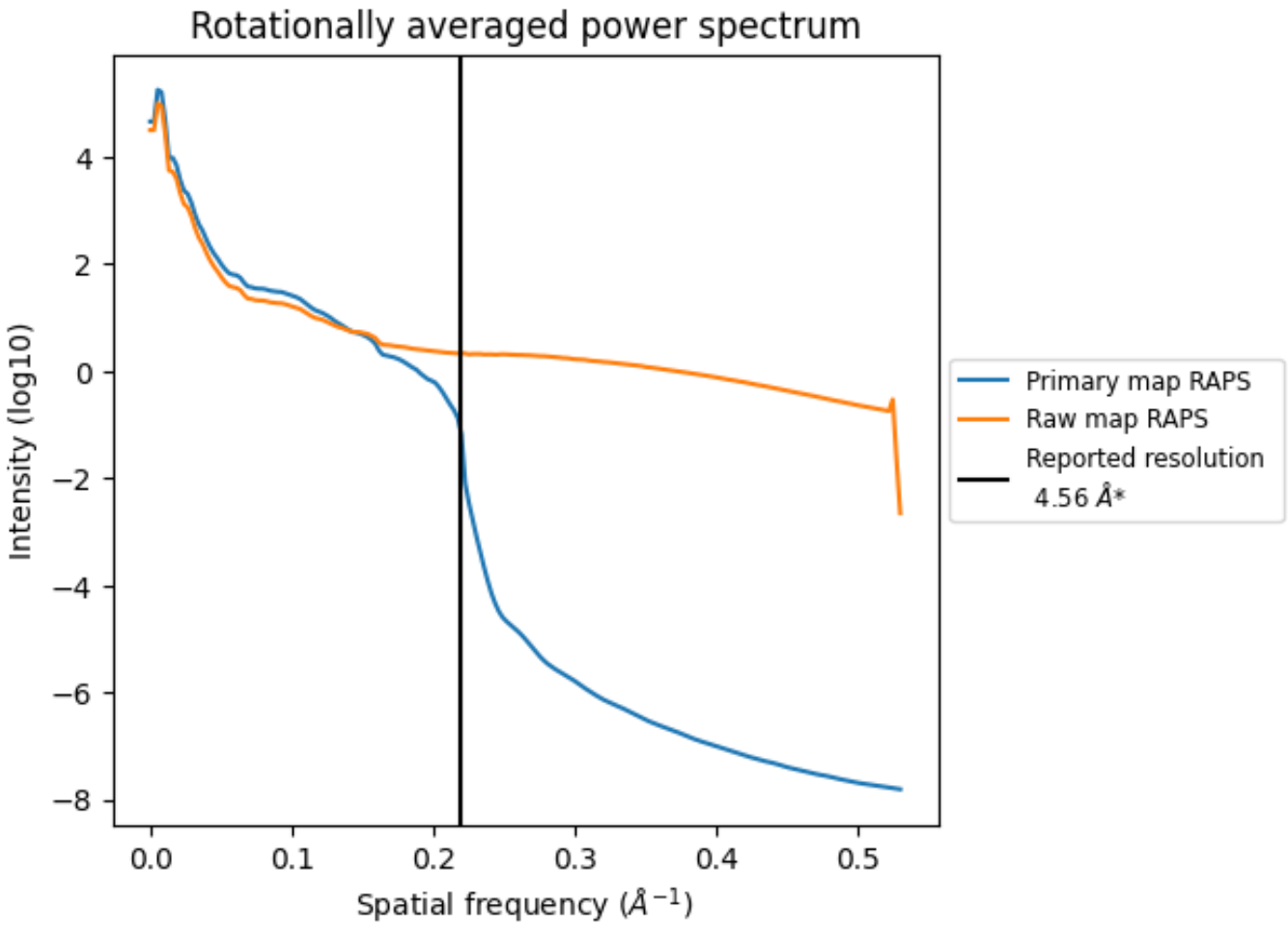
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 374 $nm^3$; this corresponds to an approximate mass of 337 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)

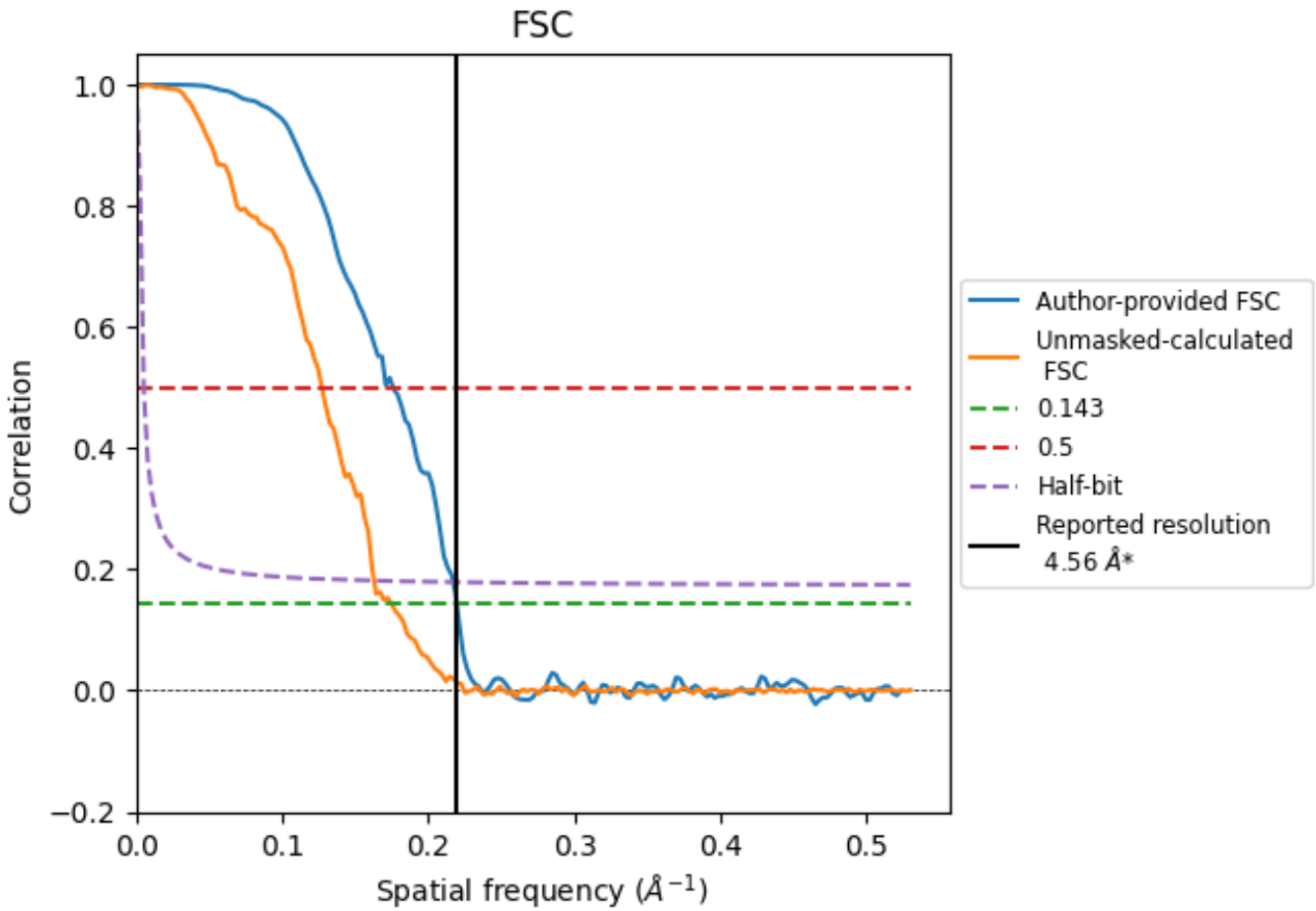



*Reported resolution corresponds to spatial frequency of 0.219 Å$^{-1}$

# 8 Fourier-Shell correlation (i)

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 (i)




*Reported resolution corresponds to spatial frequency of 0.219 Å$^{-1}$

## 8.2 Resolution estimates (i)

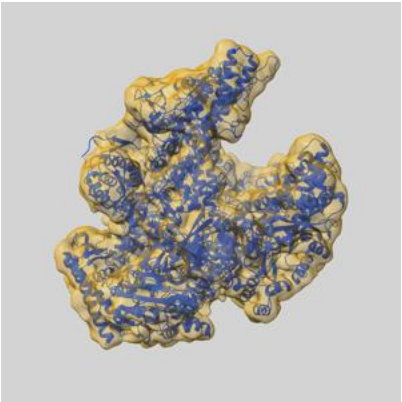
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 4.56 | - | - |
| Author-provided FSC curve | 4.56 | 5.69 | 4.61 |
| Unmasked-calculated* | 5.72 | 7.87 | 6.14 |

*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 5.72 differs from the reported value 4.56 by more than 10 %

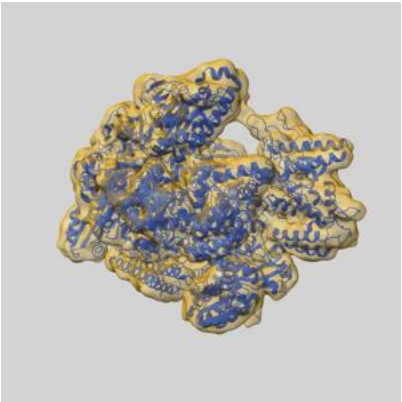
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-77809 and PDB model 36RO. Per-residue inclusion information can be found in section 3 on page 7.

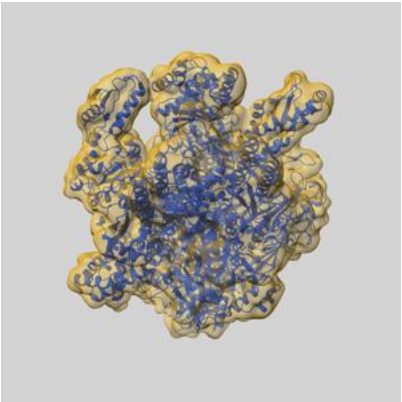
## 9.1 Map-model overlay (i)



X



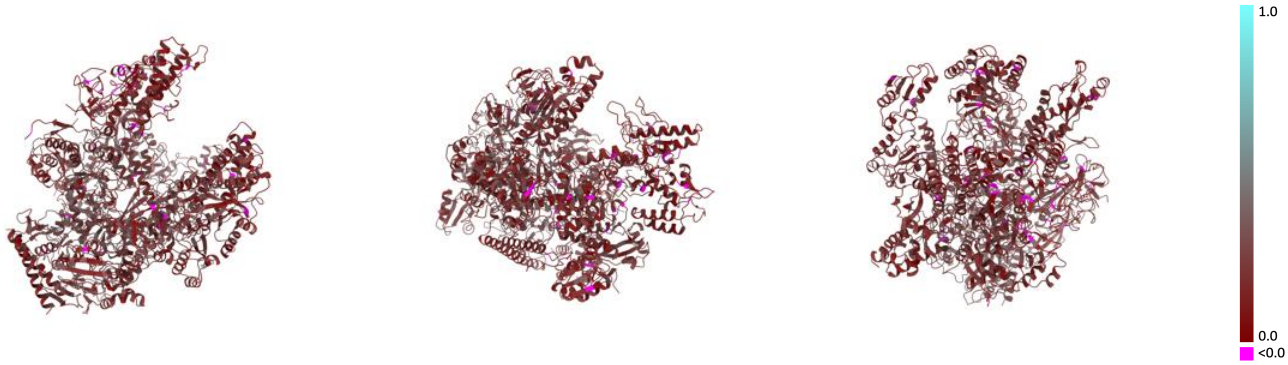
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

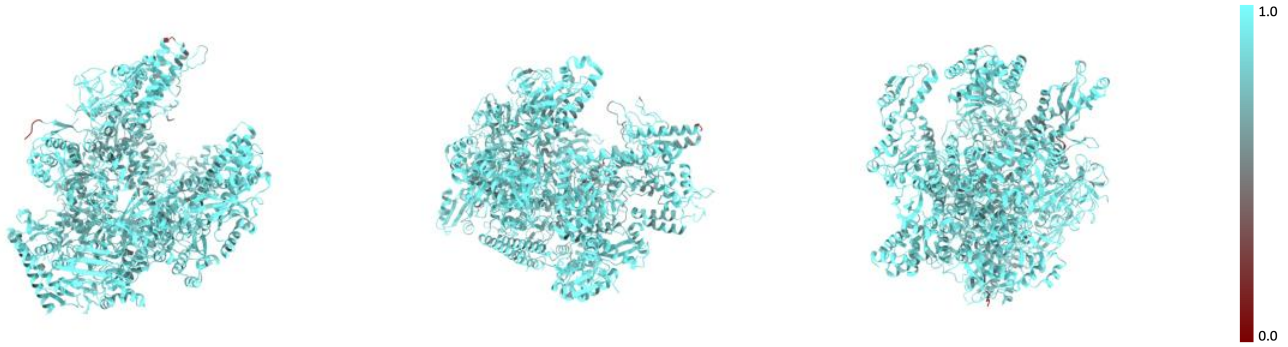
## 9.2 Q-score mapped to coordinate model (i)




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.

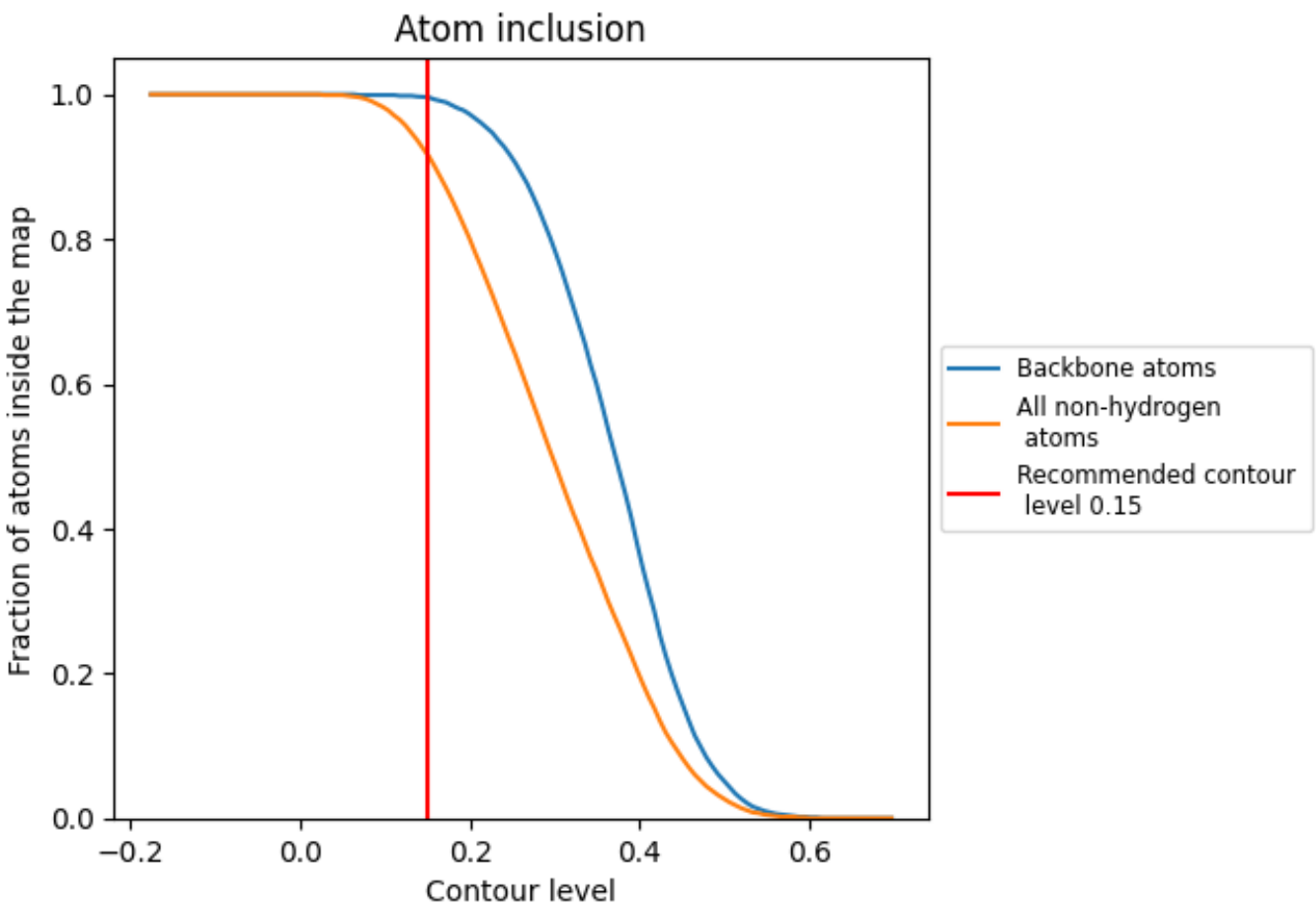
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.15).

## 9.4 Atom inclusion (i)




At the recommended contour level, 100% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.9170 | 0.2250 |
| A | 0.9160 | 0.2170 |
| B | 0.9160 | 0.2300 |
| C | 0.8950 | 0.1970 |
| D | 0.9350 | 0.2510 |
| H | 0.9620 | 0.2410 |
| K | 0.9420 | 0.2430 |
| L | 0.9250 | 0.2380 |
| N | 0.9370 | 0.2420 |
| P | 0.9070 | 0.2430 |