# Full wwPDB EM Validation Report ⓘ

Nov 13, 2023 – 03:18 am GMT

| | | |
|---|---|---|
| PDB ID | : | 8PC1 |
| EMDB ID | : | EMD-17593 |
| Title | : | Sub-tomogram average of the closed conformation of the Nap adhesion complex from the human pathogen Mycoplasma genitalium. |
| Authors | : | Sprankel, L.; Scheffer, M.P.; Frangakis, A.S. |
| Deposited on | : | 2023-06-09 |
| Resolution | : | 18.00 Å(reported) |
| Based on initial models | : | 6R3T, 6RUT |

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

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

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

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

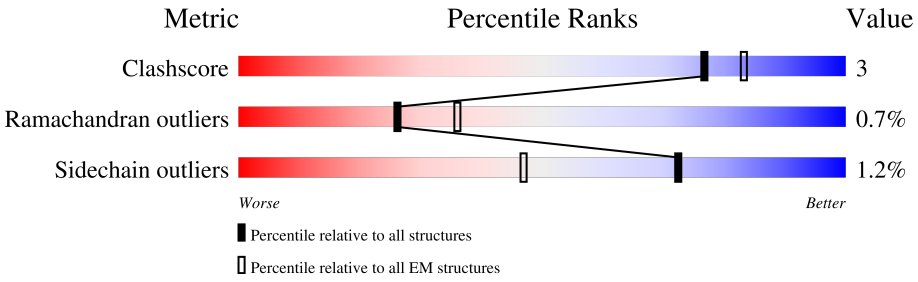
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev70 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 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 18.00 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 | B | 1444 | 12% 85% · 11% |
| 2 | A | 1053 | 9% 64% 20% · 14% |

# 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 33447 atoms, of which 16454 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 Adhesin P1.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 1 | B | 1285 | 19786 | 6365 | 9737 | 1699 | 1971 | 14 | 0 | 0 |

- Molecule 2 is a protein called Mgp-operon protein 3.

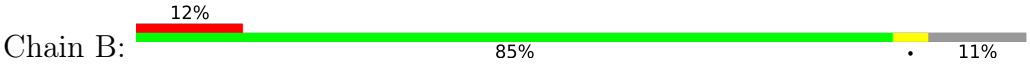
| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 2 | A | 902 | 13661 | 4350 | 6717 | 1165 | 1423 | 6 | 0 | 0 |

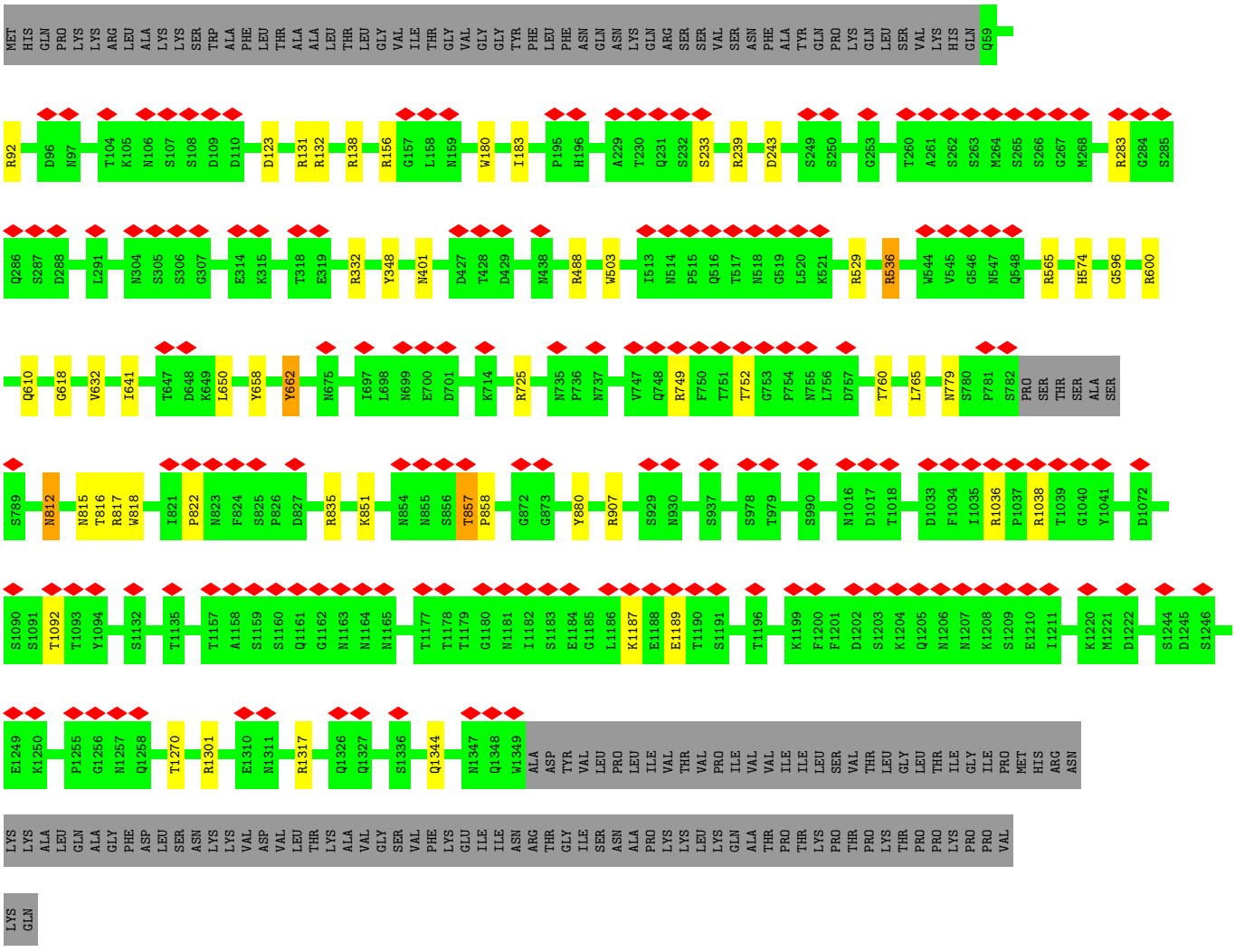
# 3 Residue-property plots (i)

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: Adhesin P1

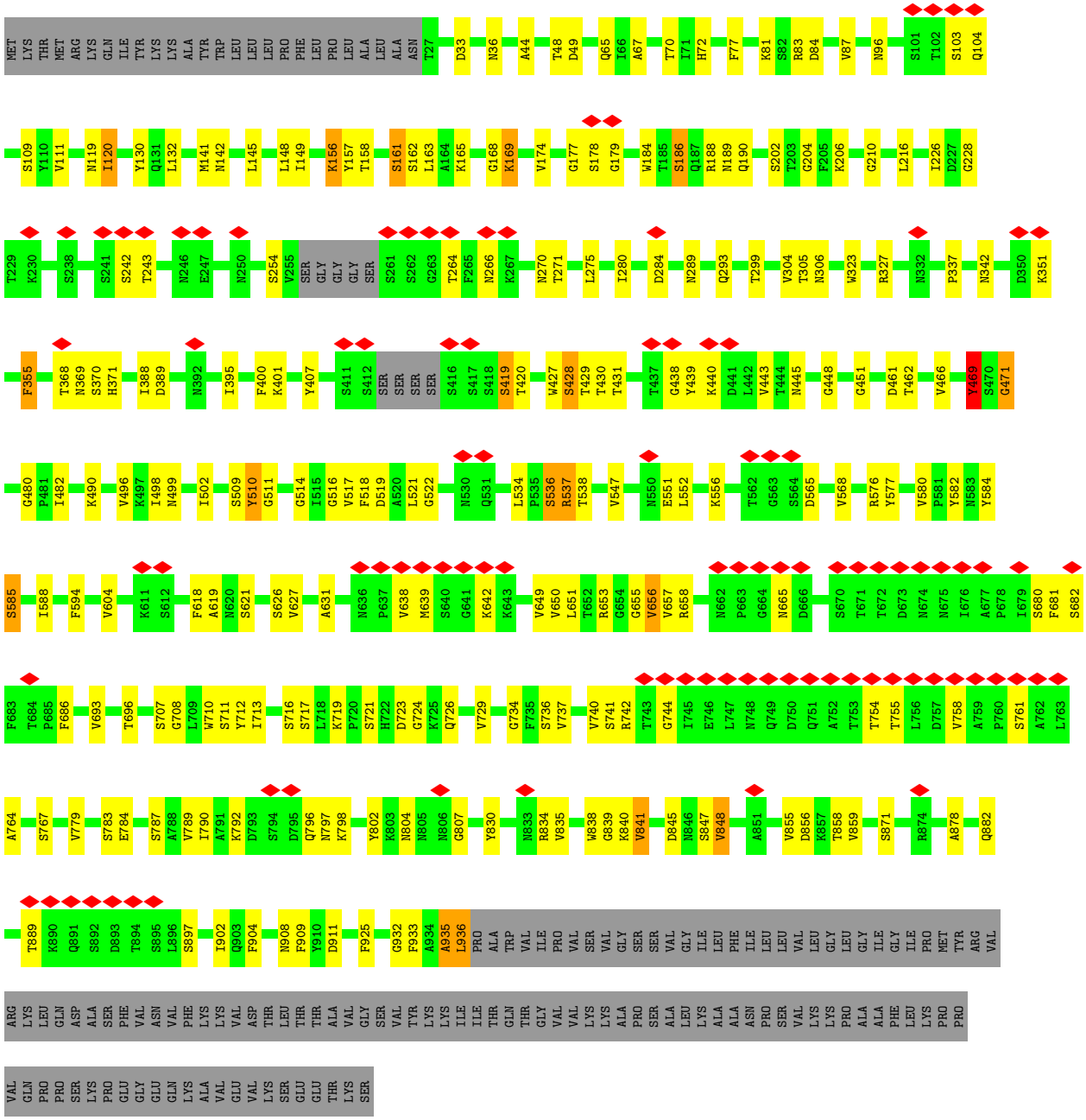
Chain B:




• Molecule 2: Mgp-operon protein 3

Chain A:


MET LYS THR MET ARG LYS GLN ILE TYR LYS LYS ALA TYR TRP LEU LEU LEU PRO PHE LEU PRO LEU ALA LEU ALA ASN T27 D33 N36 A44 T48 D49 Q65 I66 A67 T70 I71 H72 F77 K81 S82 R83 D84 V87 N96 S101 T102 S103 Q104
S109 Y110 V111 N119 I120 Y130 Q131 L132 M141 N142 L145 L148 I149 K156 Y157 T158 S161 S162 L163 A164 K165 G168 K169 V174 G177 S178 G179 W184 T185 S186 Q187 R188 N189 Q190 S202 T203 G204 F205 K206 G210 L216 I226 D227 G228
T229 K230 S238 S241 S242 T243 N246 E247 N250 S254 V255 SER GLY GLY SER S261 S262 G263 T264 F265 N266 K267 N270 T271 L275 I280 D284 N289 Q293 T299 V304 T305 N306 W323 R327 N332 P337 N342 D350 K351
F355 T368 N369 S370 H371 I388 D389 N392 I395 F400 K401 Y407 S411 S412 SER SER SER SER S416 S417 S418 S419 T420 W427 S428 T429 T430 T431 T437 G438 Y439 K440 D441 L442 V443 T444 N445 G448 G451 D461 T462 V466 Y468 S470 G471
G480 P481 I482 K490 V496 K497 I498 N499 I502 S509 Y510 G511 G514 I515 G516 V517 F518 D519 A520 L521 G522 N530 Q531 L534 P535 S536 R537 T538 V547 N550 E551 L552 K556 T562 G563 S564 D565 V568 R576 Y577 V580 P581 Y582 N583 Y584
S585 I588 F594 V604 K611 S612 F618 A619 N620 S621 S626 V627 A631 N636 P637 V638 M639 S640 G641 K642 K643 V649 V650 L651 T652 R653 G654 G655 V656 V657 R658 N662 P663 G664 N665 D666 S670 T671 T672 D673 N674 N675 I676 A677 P678 I679 S680 F681 S682
F683 T684 P685 F686 V693 T696 S707 G708 L709 W710 S711 Y712 I713 S716 S717 L718 K719 P720 S721 H722 D723 G724 K725 Q726 V729 G734 F735 S736 V737 V740 S741 R742 T743 G744 I745 E746 L747 N748 Q749 D750 Q751 A752 T753 T754 T755 L756 D757 V758 A759 P760 S761 A762 L763
A764 S767 V779 S783 E784 S787 A788 V789 I790 A791 K792 D793 S794 D795 Q796 N797 K798 Y802 K803 N804 N805 N806 G807 Y830 N833 R834 V835 W838 G839 K840 V841 D845 N846 S847 V848 A851 V855 D856 K857 T858 V859 S871 R874 A878 Q882
T889 K890 Q891 S892 D893 T894 S895 L896 S897 I902 Q903 F904 N908 F909 Y910 D911 F925 G932 F933 A934 A935 L936 PRO ALA TRP VAL ILE PRO VAL SER VAL GLY SER SER VAL GLY ILE LEU PHE ILE LEU LEU VAL LEU GLY LEU GLY ILE GLY ILE PRO MET TYR ARG VAL
ARG LYS LEU GLN ASP ALA SER PHE VAL ASN VAL PHE LYS LYS VAL ASP THR LEU THR THR ALA VAL GLY SER VAL TYR LYS LYS ILE ILE THR GLN THR GLY VAL VAL LYS LYS ALA PRO SER ALA LEU LYS ALA ALA ASN PRO SER VAL LYS LYS PRO ALA ALA PHE LEU LYS PRO PRO
VAL GLN PRO PRO SER LYS PRO GLU GLY GLU GLN LYS ALA VAL GLU VAL LYS SER GLU GLU THR LYS SER

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SUBTOMOGRAM AVERAGING | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of subtomograms used | 13870 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 120 | Depositor |
| Minimum defocus (nm) | 2000 | Depositor |
| Maximum defocus (nm) | 4000 | Depositor |
| Magnification | 105000 | Depositor |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.001 | Depositor |
| Minimum map value | -0.001 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.000 | Depositor |
| Recommended contour level | 0.000145 | Depositor |
| Map size (Å) | 332.8, 332.8, 332.8 | wwPDB |
| Map dimensions | 64, 64, 64 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 5.2, 5.2, 5.2 | 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 | B | 0.71 | 0/10303 | 0.97 | 20/14029 (0.1%) |
| 2 | A | 2.65 | 138/7088 (1.9%) | 1.47 | 31/9641 (0.3%) |
| All | All | 1.78 | 138/17391 (0.8%) | 1.20 | 51/23670 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | B | 0 | 2 |
| 2 | A | 0 | 1 |
| All | All | 0 | 3 |

All (138) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | A | 936 | LEU | CB-CG | 105.55 | 4.58 | 1.52 |
| 2 | A | 936 | LEU | CA-CB | 98.42 | 3.80 | 1.53 |
| 2 | A | 936 | LEU | CG-CD2 | 69.15 | 4.07 | 1.51 |
| 2 | A | 936 | LEU | CG-CD1 | 65.89 | 3.95 | 1.51 |
| 2 | A | 936 | LEU | N-CA | 50.53 | 2.47 | 1.46 |
| 2 | A | 935 | ALA | C-N | 23.86 | 1.89 | 1.34 |
| 2 | A | 936 | LEU | CA-C | 22.35 | 2.11 | 1.52 |
| 2 | A | 653 | ARG | CZ-NH2 | -7.56 | 1.23 | 1.33 |
| 2 | A | 834 | ARG | CZ-NH2 | -7.55 | 1.23 | 1.33 |
| 2 | A | 576 | ARG | CZ-NH2 | -7.50 | 1.23 | 1.33 |
| 2 | A | 537 | ARG | CZ-NH2 | -7.46 | 1.23 | 1.33 |
| 2 | A | 658 | ARG | CZ-NH2 | -7.45 | 1.23 | 1.33 |
| 2 | A | 188 | ARG | CZ-NH2 | -7.44 | 1.23 | 1.33 |
| 2 | A | 742 | ARG | CZ-NH2 | -7.40 | 1.23 | 1.33 |
| 2 | A | 537 | ARG | CZ-NH1 | -7.18 | 1.23 | 1.33 |
| 2 | A | 742 | ARG | CZ-NH1 | -7.05 | 1.23 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | A | 653 | ARG | CZ-NH1 | -7.00 | 1.24 | 1.33 |
| 2 | A | 188 | ARG | CZ-NH1 | -6.99 | 1.24 | 1.33 |
| 2 | A | 658 | ARG | CZ-NH1 | -6.94 | 1.24 | 1.33 |
| 2 | A | 576 | ARG | CZ-NH1 | -6.91 | 1.24 | 1.33 |
| 2 | A | 834 | ARG | CZ-NH1 | -6.90 | 1.24 | 1.33 |
| 2 | A | 712 | TYR | CD1-CE1 | -6.42 | 1.29 | 1.39 |
| 2 | A | 656 | VAL | CB-CG1 | -6.25 | 1.39 | 1.52 |
| 2 | A | 737 | VAL | CB-CG1 | -6.14 | 1.40 | 1.52 |
| 2 | A | 510 | TYR | CD1-CE1 | -6.01 | 1.30 | 1.39 |
| 2 | A | 439 | TYR | CD1-CE1 | -5.98 | 1.30 | 1.39 |
| 2 | A | 712 | TYR | CD2-CE2 | -5.92 | 1.30 | 1.39 |
| 2 | A | 577 | TYR | CD2-CE2 | -5.76 | 1.30 | 1.39 |
| 2 | A | 802 | TYR | CD1-CE1 | -5.76 | 1.30 | 1.39 |
| 2 | A | 510 | TYR | CD2-CE2 | -5.74 | 1.30 | 1.39 |
| 2 | A | 157 | TYR | CD1-CE1 | -5.72 | 1.30 | 1.39 |
| 2 | A | 439 | TYR | CD2-CE2 | -5.71 | 1.30 | 1.39 |
| 2 | A | 480 | GLY | N-CA | -5.68 | 1.37 | 1.46 |
| 2 | A | 802 | TYR | CD2-CE2 | -5.67 | 1.30 | 1.39 |
| 2 | A | 577 | TYR | CD1-CE1 | -5.65 | 1.30 | 1.39 |
| 2 | A | 168 | GLY | N-CA | -5.64 | 1.37 | 1.46 |
| 2 | A | 471 | GLY | N-CA | -5.63 | 1.37 | 1.46 |
| 2 | A | 839 | GLY | N-CA | -5.59 | 1.37 | 1.46 |
| 2 | A | 204 | GLY | N-CA | -5.57 | 1.37 | 1.46 |
| 2 | A | 177 | GLY | N-CA | -5.56 | 1.37 | 1.46 |
| 2 | A | 157 | TYR | CD2-CE2 | -5.55 | 1.31 | 1.39 |
| 2 | A | 228 | GLY | N-CA | -5.54 | 1.37 | 1.46 |
| 2 | A | 830 | TYR | CD1-CE1 | -5.49 | 1.31 | 1.39 |
| 2 | A | 650 | VAL | CB-CG2 | -5.49 | 1.41 | 1.52 |
| 2 | A | 807 | GLY | N-CA | -5.47 | 1.37 | 1.46 |
| 2 | A | 210 | GLY | N-CA | -5.46 | 1.37 | 1.46 |
| 2 | A | 517 | VAL | CB-CG2 | -5.45 | 1.41 | 1.52 |
| 2 | A | 451 | GLY | N-CA | -5.45 | 1.37 | 1.46 |
| 2 | A | 511 | GLY | N-CA | -5.44 | 1.37 | 1.46 |
| 2 | A | 744 | GLY | N-CA | -5.44 | 1.37 | 1.46 |
| 2 | A | 428 | SER | CB-OG | -5.43 | 1.35 | 1.42 |
| 2 | A | 767 | SER | CB-OG | -5.42 | 1.35 | 1.42 |
| 2 | A | 708 | GLY | N-CA | -5.42 | 1.38 | 1.46 |
| 2 | A | 657 | VAL | CB-CG1 | -5.40 | 1.41 | 1.52 |
| 2 | A | 734 | GLY | N-CA | -5.38 | 1.38 | 1.46 |
| 2 | A | 174 | VAL | CB-CG2 | -5.37 | 1.41 | 1.52 |
| 2 | A | 830 | TYR | CD2-CE2 | -5.37 | 1.31 | 1.39 |
| 2 | A | 466 | VAL | CB-CG2 | -5.37 | 1.41 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | A | 522 | GLY | N-CA | -5.36 | 1.38 | 1.46 |
| 2 | A | 649 | VAL | CB-CG2 | -5.36 | 1.41 | 1.52 |
| 2 | A | 174 | VAL | CB-CG1 | -5.36 | 1.41 | 1.52 |
| 2 | A | 438 | GLY | N-CA | -5.35 | 1.38 | 1.46 |
| 2 | A | 514 | GLY | N-CA | -5.34 | 1.38 | 1.46 |
| 2 | A | 516 | GLY | N-CA | -5.33 | 1.38 | 1.46 |
| 2 | A | 466 | VAL | CB-CG1 | -5.33 | 1.41 | 1.52 |
| 2 | A | 693 | VAL | CB-CG1 | -5.33 | 1.41 | 1.52 |
| 2 | A | 621 | SER | CB-OG | -5.32 | 1.35 | 1.42 |
| 2 | A | 710 | TRP | CD1-NE1 | -5.32 | 1.28 | 1.38 |
| 2 | A | 789 | VAL | CB-CG2 | -5.32 | 1.41 | 1.52 |
| 2 | A | 626 | SER | CB-OG | -5.31 | 1.35 | 1.42 |
| 2 | A | 737 | VAL | CB-CG2 | -5.31 | 1.41 | 1.52 |
| 2 | A | 655 | GLY | N-CA | -5.28 | 1.38 | 1.46 |
| 2 | A | 184 | TRP | CD1-NE1 | -5.27 | 1.28 | 1.38 |
| 2 | A | 427 | TRP | CD1-NE1 | -5.27 | 1.28 | 1.38 |
| 2 | A | 536 | SER | CB-OG | -5.27 | 1.35 | 1.42 |
| 2 | A | 585 | SER | CB-OG | -5.27 | 1.35 | 1.42 |
| 2 | A | 657 | VAL | CB-CG2 | -5.27 | 1.41 | 1.52 |
| 2 | A | 783 | SER | CB-OG | -5.27 | 1.35 | 1.42 |
| 2 | A | 721 | SER | CB-OG | -5.27 | 1.35 | 1.42 |
| 2 | A | 740 | VAL | CB-CG1 | -5.26 | 1.41 | 1.52 |
| 2 | A | 162 | SER | CB-OG | -5.25 | 1.35 | 1.42 |
| 2 | A | 717 | SER | CB-OG | -5.25 | 1.35 | 1.42 |
| 2 | A | 443 | VAL | CB-CG1 | -5.25 | 1.41 | 1.52 |
| 2 | A | 711 | SER | CB-OG | -5.24 | 1.35 | 1.42 |
| 2 | A | 682 | SER | CB-OG | -5.23 | 1.35 | 1.42 |
| 2 | A | 716 | SER | CB-OG | -5.22 | 1.35 | 1.42 |
| 2 | A | 161 | SER | CB-OG | -5.21 | 1.35 | 1.42 |
| 2 | A | 443 | VAL | CB-CG2 | -5.20 | 1.42 | 1.52 |
| 2 | A | 758 | VAL | CB-CG2 | -5.20 | 1.42 | 1.52 |
| 2 | A | 186 | SER | CB-OG | -5.19 | 1.35 | 1.42 |
| 2 | A | 179 | GLY | N-CA | -5.19 | 1.38 | 1.46 |
| 2 | A | 656 | VAL | CB-CG2 | -5.18 | 1.42 | 1.52 |
| 2 | A | 202 | SER | CB-OG | -5.17 | 1.35 | 1.42 |
| 2 | A | 740 | VAL | CB-CG2 | -5.17 | 1.42 | 1.52 |
| 2 | A | 627 | VAL | CB-CG2 | -5.16 | 1.42 | 1.52 |
| 2 | A | 517 | VAL | CB-CG1 | -5.16 | 1.42 | 1.52 |
| 2 | A | 741 | SER | CB-OG | -5.16 | 1.35 | 1.42 |
| 2 | A | 448 | GLY | N-CA | -5.15 | 1.38 | 1.46 |
| 2 | A | 707 | SER | CB-OG | -5.15 | 1.35 | 1.42 |
| 2 | A | 580 | VAL | CB-CG2 | -5.15 | 1.42 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | A | 848 | VAL | CB-CG2 | -5.15 | 1.42 | 1.52 |
| 2 | A | 680 | SER | CB-OG | -5.14 | 1.35 | 1.42 |
| 2 | A | 650 | VAL | CB-CG1 | -5.14 | 1.42 | 1.52 |
| 2 | A | 787 | SER | CB-OG | -5.14 | 1.35 | 1.42 |
| 2 | A | 789 | VAL | CB-CG1 | -5.14 | 1.42 | 1.52 |
| 2 | A | 838 | TRP | CD1-NE1 | -5.14 | 1.29 | 1.38 |
| 2 | A | 693 | VAL | CB-CG2 | -5.14 | 1.42 | 1.52 |
| 2 | A | 178 | SER | CB-OG | -5.14 | 1.35 | 1.42 |
| 2 | A | 580 | VAL | CB-CG1 | -5.13 | 1.42 | 1.52 |
| 2 | A | 761 | SER | CB-OG | -5.12 | 1.35 | 1.42 |
| 2 | A | 627 | VAL | CB-CG1 | -5.12 | 1.42 | 1.52 |
| 2 | A | 871 | SER | CB-OG | -5.12 | 1.35 | 1.42 |
| 2 | A | 638 | VAL | CB-CG1 | -5.12 | 1.42 | 1.52 |
| 2 | A | 156 | LYS | CE-NZ | -5.11 | 1.36 | 1.49 |
| 2 | A | 736 | SER | CB-OG | -5.11 | 1.35 | 1.42 |
| 2 | A | 165 | LYS | CE-NZ | -5.10 | 1.36 | 1.49 |
| 2 | A | 509 | SER | CB-OG | -5.10 | 1.35 | 1.42 |
| 2 | A | 719 | LYS | CE-NZ | -5.09 | 1.36 | 1.49 |
| 2 | A | 729 | VAL | CB-CG2 | -5.09 | 1.42 | 1.52 |
| 2 | A | 649 | VAL | CB-CG1 | -5.08 | 1.42 | 1.52 |
| 2 | A | 758 | VAL | CB-CG1 | -5.07 | 1.42 | 1.52 |
| 2 | A | 855 | VAL | CB-CG1 | -5.07 | 1.42 | 1.52 |
| 2 | A | 932 | GLY | N-CA | -5.07 | 1.38 | 1.46 |
| 2 | A | 638 | VAL | CB-CG2 | -5.06 | 1.42 | 1.52 |
| 2 | A | 847 | SER | CB-OG | -5.06 | 1.35 | 1.42 |
| 2 | A | 642 | LYS | CE-NZ | -5.06 | 1.36 | 1.49 |
| 2 | A | 855 | VAL | CB-CG2 | -5.05 | 1.42 | 1.52 |
| 2 | A | 440 | LYS | CE-NZ | -5.05 | 1.36 | 1.49 |
| 2 | A | 419 | SER | CB-OG | -5.04 | 1.35 | 1.42 |
| 2 | A | 840 | LYS | CE-NZ | -5.03 | 1.36 | 1.49 |
| 2 | A | 841 | VAL | CB-CG2 | -5.03 | 1.42 | 1.52 |
| 2 | A | 859 | VAL | CB-CG2 | -5.03 | 1.42 | 1.52 |
| 2 | A | 206 | LYS | CE-NZ | -5.03 | 1.36 | 1.49 |
| 2 | A | 169 | LYS | CE-NZ | -5.02 | 1.36 | 1.49 |
| 2 | A | 792 | LYS | CE-NZ | -5.01 | 1.36 | 1.49 |
| 2 | A | 835 | VAL | CB-CG2 | -5.01 | 1.42 | 1.52 |
| 2 | A | 848 | VAL | CB-CG1 | -5.00 | 1.42 | 1.52 |
| 2 | A | 798 | LYS | CE-NZ | -5.00 | 1.36 | 1.49 |

All (51) bond angle outliers are listed below:

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | A | 936 | LEU | CB-CG-CD1 | -41.45 | 40.54 | 111.00 |
| 2 | A | 936 | LEU | CA-CB-CG | -31.74 | 42.30 | 115.30 |
| 2 | A | 936 | LEU | CB-CG-CD2 | -29.88 | 60.21 | 111.00 |
| 2 | A | 936 | LEU | CB-CA-C | -24.94 | 62.82 | 110.20 |
| 2 | A | 935 | ALA | C-N-CA | -23.64 | 62.59 | 121.70 |
| 2 | A | 936 | LEU | N-CA-CB | -21.57 | 67.26 | 110.40 |
| 2 | A | 936 | LEU | CD1-CG-CD2 | -14.08 | 68.25 | 110.50 |
| 2 | A | 936 | LEU | N-CA-C | -12.33 | 77.72 | 111.00 |
| 2 | A | 935 | ALA | O-C-N | 12.27 | 142.34 | 122.70 |
| 2 | A | 469 | TYR | CB-CG-CD1 | -9.69 | 115.19 | 121.00 |
| 2 | A | 935 | ALA | CA-C-N | -9.24 | 96.87 | 117.20 |
| 1 | B | 488 | ARG | NE-CZ-NH2 | 8.00 | 124.30 | 120.30 |
| 2 | A | 469 | TYR | CB-CG-CD2 | 7.66 | 125.60 | 121.00 |
| 1 | B | 907 | ARG | NE-CZ-NH2 | 7.54 | 124.07 | 120.30 |
| 2 | A | 157 | TYR | CB-CG-CD2 | 7.01 | 125.20 | 121.00 |
| 2 | A | 518 | PHE | CB-CG-CD2 | 6.92 | 125.65 | 120.80 |
| 2 | A | 577 | TYR | CB-CG-CD2 | 6.83 | 125.10 | 121.00 |
| 1 | B | 565 | ARG | NE-CZ-NH2 | 6.81 | 123.70 | 120.30 |
| 2 | A | 658 | ARG | CD-NE-CZ | 6.67 | 132.93 | 123.60 |
| 2 | A | 188 | ARG | CD-NE-CZ | 6.59 | 132.83 | 123.60 |
| 2 | A | 537 | ARG | CD-NE-CZ | 6.54 | 132.76 | 123.60 |
| 1 | B | 536 | ARG | NE-CZ-NH2 | 6.53 | 123.57 | 120.30 |
| 1 | B | 835 | ARG | NE-CZ-NH2 | 6.52 | 123.56 | 120.30 |
| 1 | B | 239 | ARG | NE-CZ-NH2 | 6.47 | 123.54 | 120.30 |
| 2 | A | 618 | PHE | CB-CG-CD2 | 6.45 | 125.31 | 120.80 |
| 1 | B | 138 | ARG | NE-CZ-NH2 | 6.42 | 123.51 | 120.30 |
| 2 | A | 653 | ARG | CD-NE-CZ | 6.40 | 132.56 | 123.60 |
| 2 | A | 686 | PHE | CB-CG-CD2 | -6.40 | 116.32 | 120.80 |
| 1 | B | 132 | ARG | NE-CZ-NH2 | 6.37 | 123.48 | 120.30 |
| 1 | B | 1038 | ARG | NE-CZ-NH2 | 6.22 | 123.41 | 120.30 |
| 1 | B | 529 | ARG | NE-CZ-NH2 | 6.14 | 123.37 | 120.30 |
| 2 | A | 639 | MET | CA-CB-CG | 6.14 | 123.73 | 113.30 |
| 2 | A | 355 | PHE | CB-CG-CD2 | 6.04 | 125.03 | 120.80 |
| 1 | B | 1317 | ARG | NE-CZ-NH2 | 5.84 | 123.22 | 120.30 |
| 2 | A | 400 | PHE | CB-CG-CD2 | 5.73 | 124.81 | 120.80 |
| 1 | B | 283 | ARG | NE-CZ-NH2 | 5.69 | 123.15 | 120.30 |
| 1 | B | 662 | TYR | CB-CG-CD2 | -5.65 | 117.61 | 121.00 |
| 1 | B | 749 | ARG | NE-CZ-NH2 | 5.64 | 123.12 | 120.30 |
| 2 | A | 712 | TYR | CB-CG-CD2 | 5.62 | 124.37 | 121.00 |
| 1 | B | 156 | ARG | NE-CZ-NH2 | 5.61 | 123.11 | 120.30 |
| 2 | A | 904 | PHE | CB-CG-CD2 | 5.59 | 124.71 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | A | 830 | TYR | CB-CG-CD2 | 5.50 | 124.30 | 121.00 |
| 1 | B | 92 | ARG | NE-CZ-NH2 | 5.43 | 123.02 | 120.30 |
| 1 | B | 907 | ARG | NE-CZ-NH1 | -5.40 | 117.60 | 120.30 |
| 2 | A | 802 | TYR | CB-CG-CD2 | 5.40 | 124.24 | 121.00 |
| 1 | B | 1036 | ARG | NE-CZ-NH2 | 5.33 | 122.97 | 120.30 |
| 1 | B | 600 | ARG | NE-CZ-NH2 | 5.28 | 122.94 | 120.30 |
| 2 | A | 681 | PHE | CB-CG-CD2 | 5.12 | 124.38 | 120.80 |
| 1 | B | 332 | ARG | NE-CZ-NH2 | 5.11 | 122.86 | 120.30 |
| 2 | A | 933 | PHE | CB-CG-CD2 | 5.07 | 124.35 | 120.80 |
| 2 | A | 188 | ARG | CG-CD-NE | 5.02 | 122.35 | 111.80 |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | A | 584 | TYR | Sidechain |
| 1 | B | 348 | TYR | Sidechain |
| 1 | B | 880 | TYR | Sidechain |

## 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 | B | 10049 | 9737 | 9727 | 3 | 0 |
| 2 | A | 6944 | 6717 | 6713 | 98 | 0 |
| All | All | 16993 | 16454 | 16440 | 101 | 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 3.

All (101) 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) |
|---|---|---|---|
| 2:A:935:ALA:C | 2:A:936:LEU:N | 1.88 | 1.26 |
| 2:A:936:LEU:CA | 2:A:936:LEU:C | 2.11 | 1.19 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:935:ALA:C | 2:A:936:LEU:CA | 2.32 | 0.98 |
| 2:A:856:ASP:O | 2:A:936:LEU:HD12 | 1.71 | 0.91 |
| 2:A:429:THR:HG1 | 2:A:538:THR:HG1 | 1.24 | 0.83 |
| 2:A:428:SER:OG | 2:A:519:ASP:OD2 | 1.96 | 0.81 |
| 2:A:935:ALA:O | 2:A:936:LEU:CA | 2.28 | 0.81 |
| 2:A:858:THR:OG1 | 2:A:936:LEU:HB2 | 1.84 | 0.78 |
| 2:A:936:LEU:N | 2:A:936:LEU:CA | 2.47 | 0.77 |
| 2:A:264:THR:OG1 | 2:A:266:ASN:OD1 | 2.04 | 0.71 |
| 2:A:130:TYR:OH | 2:A:327:ARG:O | 2.08 | 0.70 |
| 2:A:856:ASP:O | 2:A:936:LEU:CD1 | 2.40 | 0.69 |
| 2:A:430:THR:OG1 | 2:A:519:ASP:OD1 | 2.10 | 0.69 |
| 2:A:935:ALA:CA | 2:A:936:LEU:N | 2.55 | 0.69 |
| 2:A:889:THR:OG1 | 2:A:897:SER:OG | 2.05 | 0.68 |
| 2:A:148:LEU:HD23 | 2:A:149:ILE:N | 2.09 | 0.67 |
| 2:A:889:THR:O | 2:A:897:SER:N | 2.31 | 0.63 |
| 2:A:445:ASN:O | 2:A:537:ARG:NH2 | 2.31 | 0.63 |
| 2:A:723:ASP:OD1 | 2:A:724:GLY:N | 2.31 | 0.62 |
| 2:A:270:ASN:O | 2:A:726:GLN:NE2 | 2.33 | 0.60 |
| 2:A:889:THR:OG1 | 2:A:897:SER:O | 2.17 | 0.59 |
| 2:A:784:GLU:O | 2:A:804:ASN:ND2 | 2.35 | 0.58 |
| 2:A:65:GLN:OE1 | 2:A:83:ARG:NE | 2.37 | 0.58 |
| 2:A:169:LYS:NZ | 2:A:419:SER:O | 2.36 | 0.58 |
| 2:A:420:THR:HG22 | 2:A:420:THR:O | 2.04 | 0.57 |
| 2:A:889:THR:N | 2:A:897:SER:O | 2.33 | 0.56 |
| 2:A:145:LEU:HD23 | 2:A:216:LEU:HD13 | 1.89 | 0.55 |
| 2:A:370:SER:OG | 2:A:498:ILE:N | 2.39 | 0.55 |
| 2:A:163:LEU:HD12 | 2:A:510:TYR:CE1 | 2.42 | 0.55 |
| 2:A:87:VAL:O | 2:A:289:ASN:ND2 | 2.37 | 0.54 |
| 2:A:163:LEU:HD12 | 2:A:510:TYR:HE1 | 1.71 | 0.54 |
| 2:A:908:ASN:OD1 | 2:A:909:PHE:N | 2.40 | 0.54 |
| 2:A:588:ILE:HD11 | 2:A:604:VAL:HG13 | 1.89 | 0.54 |
| 2:A:156:LYS:HG3 | 2:A:696:THR:HG21 | 1.89 | 0.53 |
| 2:A:431:THR:HB | 2:A:534:LEU:HD12 | 1.91 | 0.53 |
| 2:A:521:LEU:HD12 | 2:A:582:TYR:HA | 1.91 | 0.53 |
| 2:A:280:ILE:HG23 | 2:A:293:GLN:CD | 2.30 | 0.52 |
| 2:A:109:SER:O | 2:A:132:LEU:HD12 | 2.09 | 0.52 |
| 2:A:878:ALA:N | 2:A:882:GLN:OE1 | 2.40 | 0.52 |
| 2:A:389:ASP:OD2 | 2:A:631:ALA:N | 2.42 | 0.52 |
| 2:A:323:TRP:CD1 | 2:A:337:PRO:HB3 | 2.45 | 0.51 |
| 2:A:186:SER:O | 2:A:189:ASN:ND2 | 2.43 | 0.51 |
| 2:A:521:LEU:HD11 | 2:A:585:SER:OG | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:935:ALA:N | 2:A:936:LEU:N | 2.59 | 0.51 |
| 2:A:754:THR:HG23 | 2:A:755:THR:HG23 | 1.92 | 0.50 |
| 2:A:148:LEU:HD21 | 2:A:502:ILE:HG12 | 1.93 | 0.50 |
| 2:A:141:MET:O | 2:A:145:LEU:HD13 | 2.12 | 0.50 |
| 2:A:401:LYS:NZ | 2:A:538:THR:O | 2.43 | 0.49 |
| 2:A:395:ILE:HD12 | 2:A:552:LEU:HD11 | 1.93 | 0.49 |
| 2:A:161:SER:OG | 2:A:226:ILE:O | 2.15 | 0.49 |
| 2:A:254:SER:OG | 2:A:270:ASN:ND2 | 2.38 | 0.49 |
| 2:A:77:PHE:CD2 | 2:A:304:VAL:HG11 | 2.48 | 0.48 |
| 2:A:271:THR:O | 2:A:275:LEU:HD23 | 2.14 | 0.48 |
| 2:A:490:LYS:N | 2:A:490:LYS:HD3 | 2.29 | 0.48 |
| 2:A:556:LYS:O | 2:A:556:LYS:HD2 | 2.14 | 0.47 |
| 2:A:656:VAL:HG11 | 2:A:764:ALA:HB2 | 1.96 | 0.47 |
| 2:A:471:GLY:O | 2:A:482:ILE:N | 2.47 | 0.47 |
| 2:A:33:ASP:OD1 | 2:A:36:ASN:N | 2.47 | 0.46 |
| 2:A:48:THR:O | 2:A:49:ASP:OD1 | 2.34 | 0.46 |
| 2:A:305:THR:HG22 | 2:A:306:ASN:N | 2.31 | 0.46 |
| 2:A:119:ASN:C | 2:A:120:ILE:HD12 | 2.37 | 0.45 |
| 1:B:180:TRP:HA | 1:B:183:ILE:HG22 | 1.97 | 0.45 |
| 2:A:369:ASN:O | 2:A:371:HIS:N | 2.48 | 0.45 |
| 2:A:651:LEU:HD23 | 2:A:656:VAL:HG12 | 1.98 | 0.45 |
| 2:A:72:HIS:HB2 | 2:A:304:VAL:HG21 | 1.98 | 0.45 |
| 2:A:902:ILE:HD13 | 2:A:925:PHE:CE2 | 2.51 | 0.45 |
| 2:A:119:ASN:O | 2:A:120:ILE:HB | 2.17 | 0.45 |
| 2:A:189:ASN:OD1 | 2:A:190:GLN:N | 2.50 | 0.44 |
| 2:A:242:SER:OG | 2:A:243:THR:N | 2.50 | 0.44 |
| 2:A:665:ASN:O | 2:A:665:ASN:OD1 | 2.36 | 0.44 |
| 2:A:67:ALA:HB2 | 2:A:81:LYS:HD2 | 1.99 | 0.44 |
| 2:A:388:ILE:HD11 | 2:A:395:ILE:CG2 | 2.48 | 0.44 |
| 2:A:536:SER:O | 2:A:536:SER:OG | 2.35 | 0.44 |
| 2:A:902:ILE:HD13 | 2:A:925:PHE:CZ | 2.53 | 0.43 |
| 2:A:395:ILE:HD12 | 2:A:552:LEU:CD1 | 2.48 | 0.43 |
| 2:A:713:ILE:HD11 | 2:A:779:VAL:HG11 | 2.01 | 0.43 |
| 2:A:342:ASN:O | 2:A:568:VAL:N | 2.43 | 0.43 |
| 2:A:496:VAL:O | 2:A:496:VAL:HG13 | 2.19 | 0.43 |
| 2:A:132:LEU:HD23 | 2:A:323:TRP:CB | 2.49 | 0.42 |
| 2:A:547:VAL:HG23 | 2:A:551:GLU:HG3 | 2.01 | 0.42 |
| 2:A:796:GLN:OE1 | 2:A:797:ASN:N | 2.53 | 0.42 |
| 2:A:911:ASP:OD1 | 2:A:911:ASP:N | 2.53 | 0.42 |
| 1:B:857:THR:HB | 1:B:858:PRO:CD | 2.50 | 0.42 |
| 2:A:407:TYR:N | 2:A:499:ASN:O | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:103:SER:O | 2:A:104:GLN:HG3 | 2.20 | 0.41 |
| 2:A:368:THR:HG23 | 2:A:369:ASN:N | 2.35 | 0.41 |
| 2:A:845:ASP:O | 2:A:848:VAL:HG12 | 2.19 | 0.41 |
| 2:A:96:ASN:ND2 | 2:A:142:ASN:OD1 | 2.53 | 0.41 |
| 2:A:158:THR:O | 2:A:619:ALA:HB3 | 2.19 | 0.41 |
| 2:A:342:ASN:ND2 | 2:A:565:ASP:OD1 | 2.54 | 0.41 |
| 2:A:469:TYR:CD1 | 2:A:469:TYR:N | 2.88 | 0.41 |
| 2:A:841:VAL:O | 2:A:841:VAL:HG13 | 2.19 | 0.41 |
| 2:A:275:LEU:HD13 | 2:A:280:ILE:HD13 | 2.03 | 0.41 |
| 2:A:462:THR:HB | 2:A:594:PHE:CE2 | 2.55 | 0.41 |
| 2:A:111:VAL:HG13 | 2:A:132:LEU:HD11 | 2.03 | 0.41 |
| 2:A:70:THR:HG21 | 2:A:304:VAL:HG13 | 2.02 | 0.40 |
| 2:A:299:THR:HA | 2:A:323:TRP:HZ3 | 1.87 | 0.40 |
| 1:B:574:HIS:CE1 | 1:B:596:GLY:HA3 | 2.56 | 0.40 |
| 2:A:84:ASP:O | 2:A:84:ASP:OD1 | 2.40 | 0.40 |
| 2:A:44:ALA:HB1 | 2:A:790:ILE:HD11 | 2.02 | 0.40 |
| 2:A:351:LYS:HG3 | 2:A:355:PHE:CE2 | 2.56 | 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 | B | 1281/1444 (89%) | 1187 (93%) | 81 (6%) | 13 (1%) | 15 | 55 |
| 2 | A | 896/1053 (85%) | 842 (94%) | 52 (6%) | 2 (0%) | 47 | 81 |
| All | All | 2177/2497 (87%) | 2029 (93%) | 133 (6%) | 15 (1%) | 26 | 63 |

All (15) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 1092 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 779 | ASN |
| 1 | B | 812 | ASN |
| 1 | B | 233 | SER |
| 1 | B | 815 | ASN |
| 1 | B | 817 | ARG |
| 1 | B | 1187 | LYS |
| 2 | A | 120 | ILE |
| 1 | B | 818 | TRP |
| 1 | B | 822 | PRO |
| 1 | B | 857 | THR |
| 1 | B | 1189 | GLU |
| 2 | A | 284 | ASP |
| 1 | B | 641 | ILE |
| 1 | B | 618 | GLY |

### 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 | B | 1122/1267 (89%) | 1101 (98%) | 21 (2%) | 57 75 |
| 2 | A | 787/914 (86%) | 785 (100%) | 2 (0%) | 92 95 |
| All | All | 1909/2181 (88%) | 1886 (99%) | 23 (1%) | 72 83 |

All (23) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 123 | ASP |
| 1 | B | 131 | ARG |
| 1 | B | 243 | ASP |
| 1 | B | 401 | ASN |
| 1 | B | 503 | TRP |
| 1 | B | 536 | ARG |
| 1 | B | 610 | GLN |
| 1 | B | 632 | VAL |
| 1 | B | 650 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 658 | TYR |
| 1 | B | 662 | TYR |
| 1 | B | 725 | ARG |
| 1 | B | 752 | THR |
| 1 | B | 760 | THR |
| 1 | B | 765 | LEU |
| 1 | B | 812 | ASN |
| 1 | B | 816 | THR |
| 1 | B | 851 | LYS |
| 1 | B | 1270 | THR |
| 1 | B | 1301 | ARG |
| 1 | B | 1344 | GLN |
| 2 | A | 461 | ASP |
| 2 | A | 469 | TYR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 574 | HIS |
| 1 | B | 908 | ASN |
| 2 | A | 96 | ASN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 2 | A | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | A | 935:ALA | C | 936:LEU | N | 1.88 |

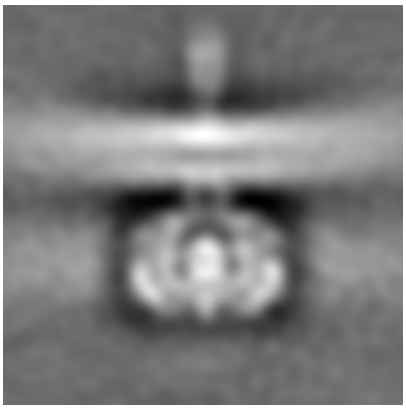
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17593. These allow visual inspection of the internal detail of the map and identification of artifacts.

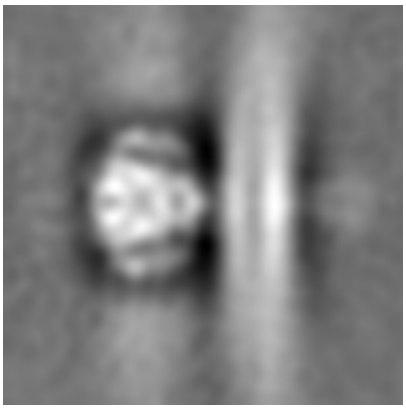
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

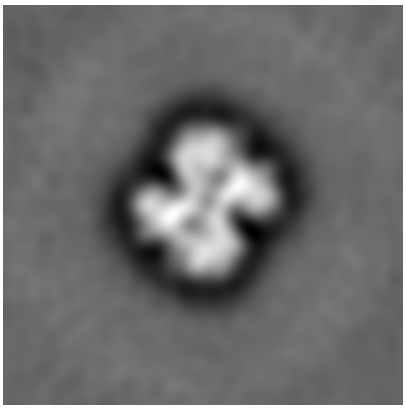
### 6.1.1 Primary map



X

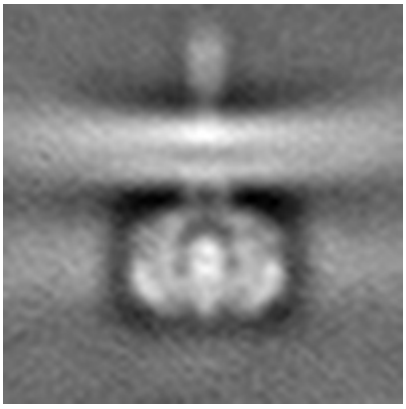


Y

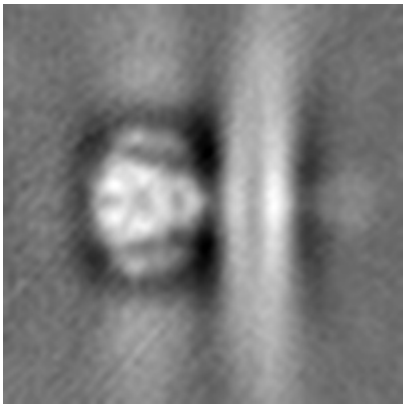


Z

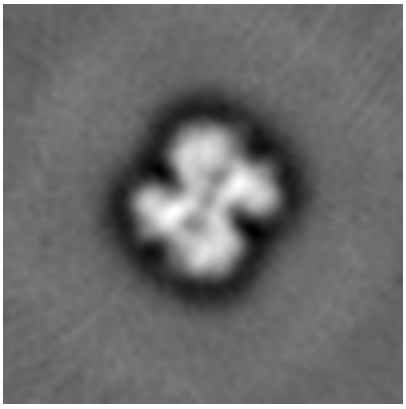
### 6.1.2 Raw map



X



Y

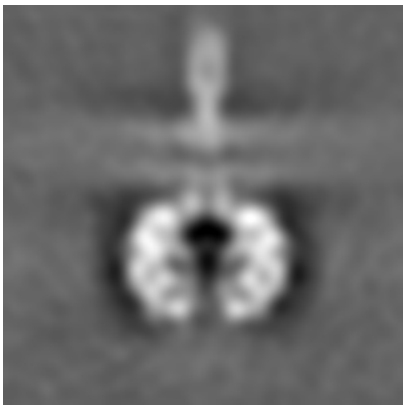


Z

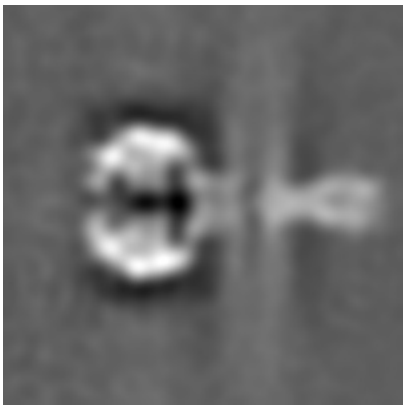
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

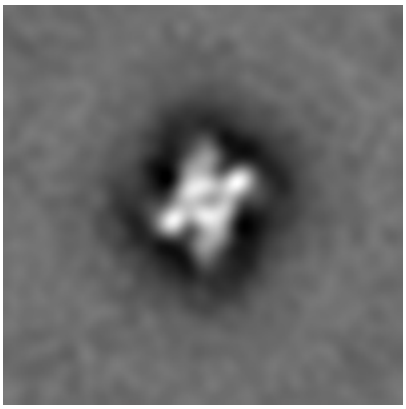
### 6.2.1 Primary map



X Index: 32

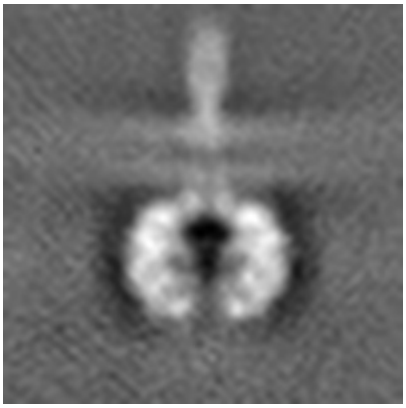


Y Index: 32

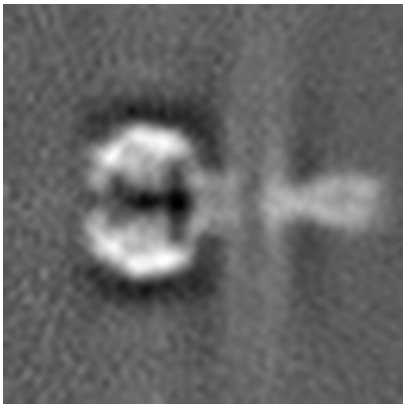


Z Index: 32

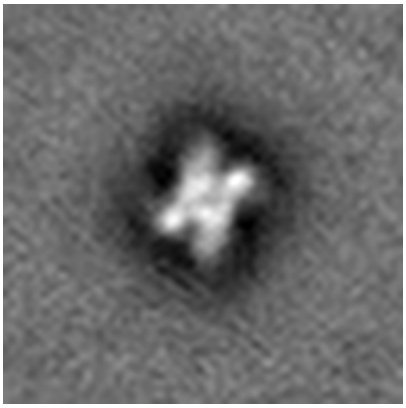
### 6.2.2 Raw map



X Index: 32



Y Index: 32

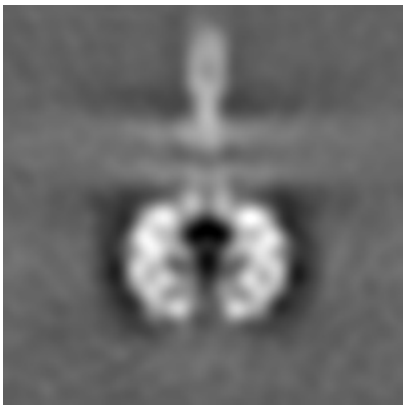


Z Index: 32

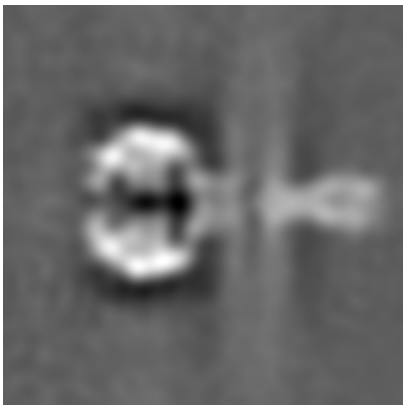
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

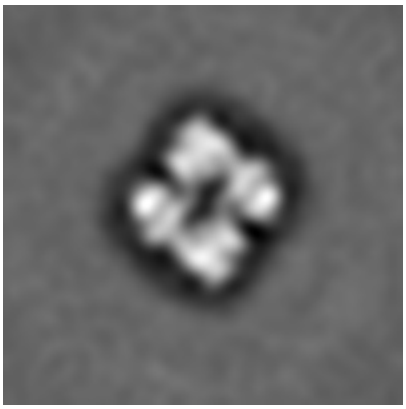
### 6.3.1 Primary map



X Index: 32

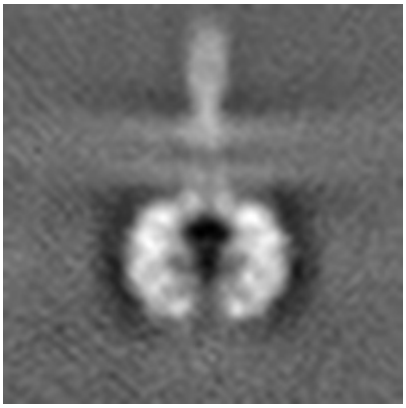


Y Index: 32

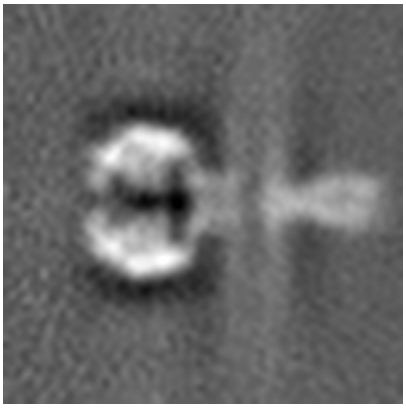


Z Index: 25

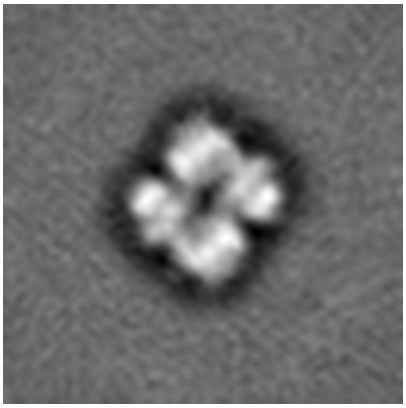
### 6.3.2 Raw map



X Index: 32



Y Index: 32

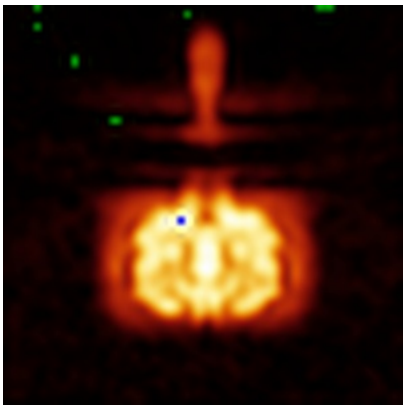


Z Index: 24

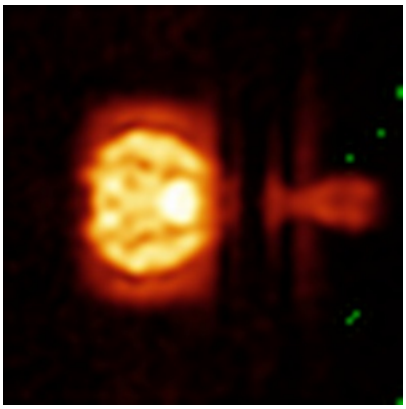
The images above show the largest variance slices of the map in three orthogonal directions.

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

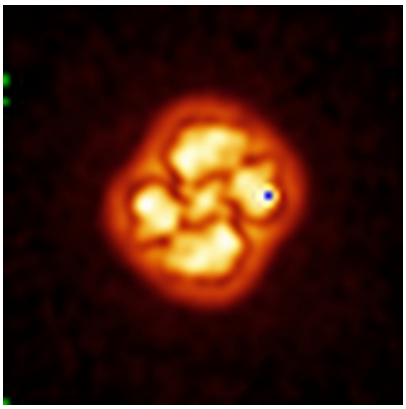
### 6.4.1 Primary map



X

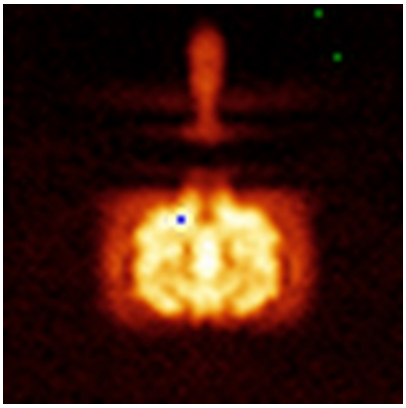


Y

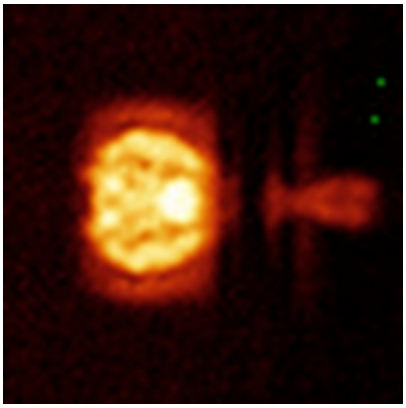


Z

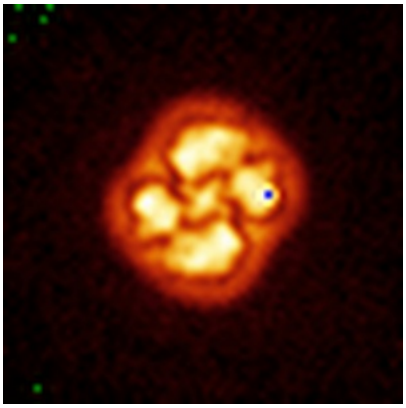
### 6.4.2 Raw map



X



Y

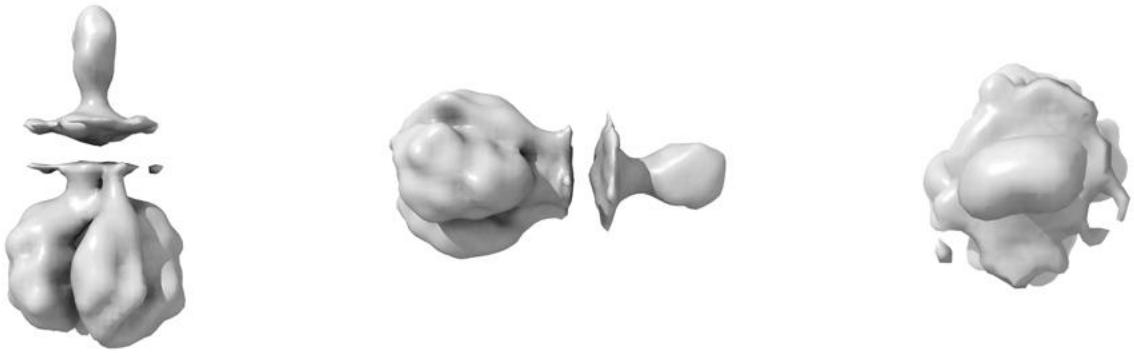


Z

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)

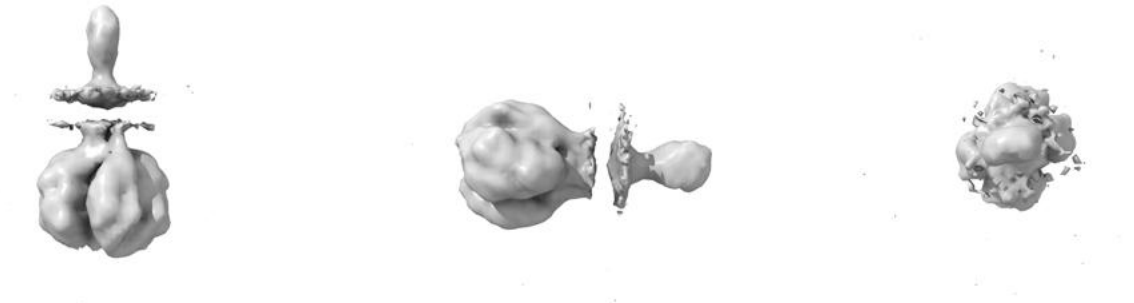
### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.000145. 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.

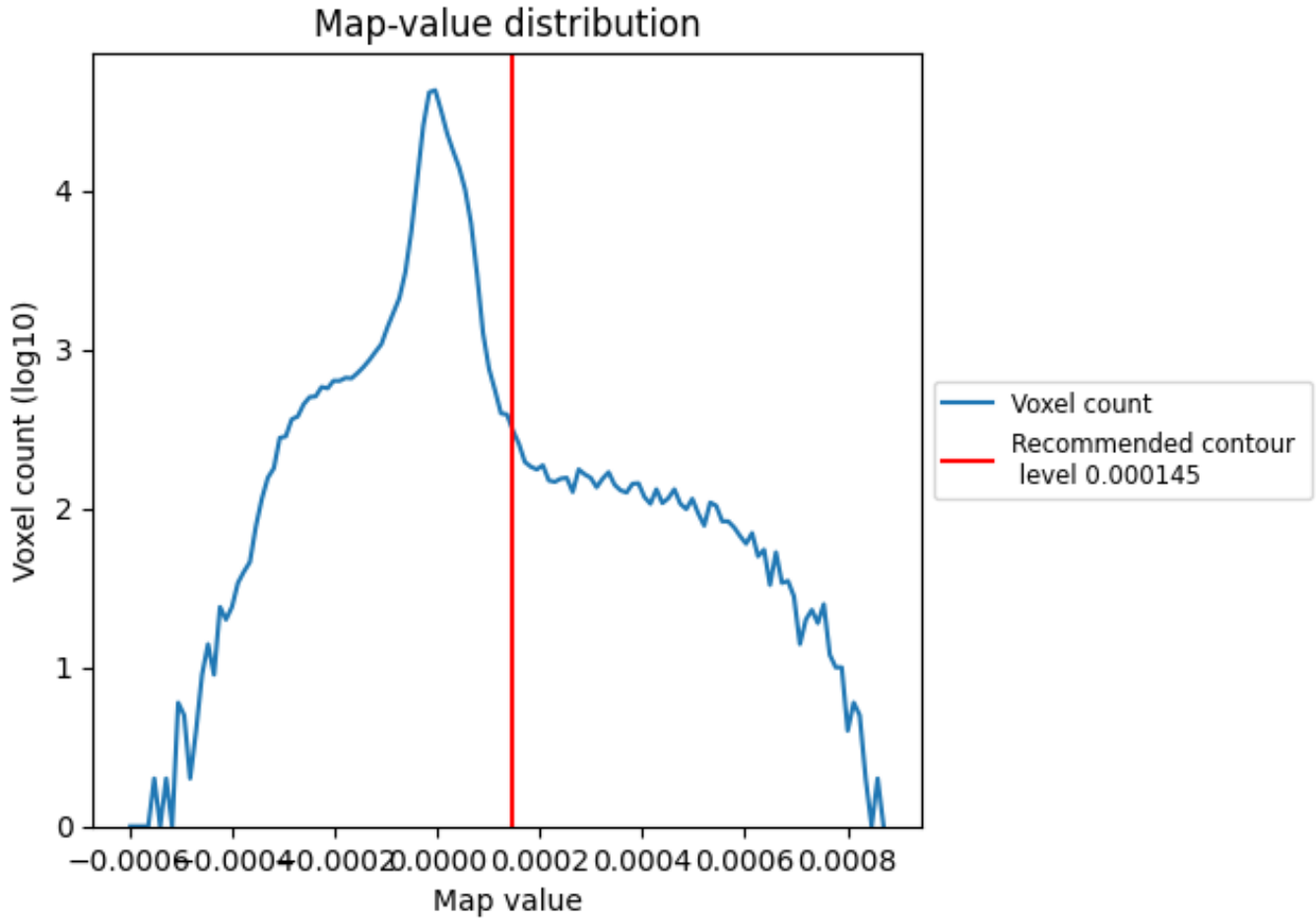
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

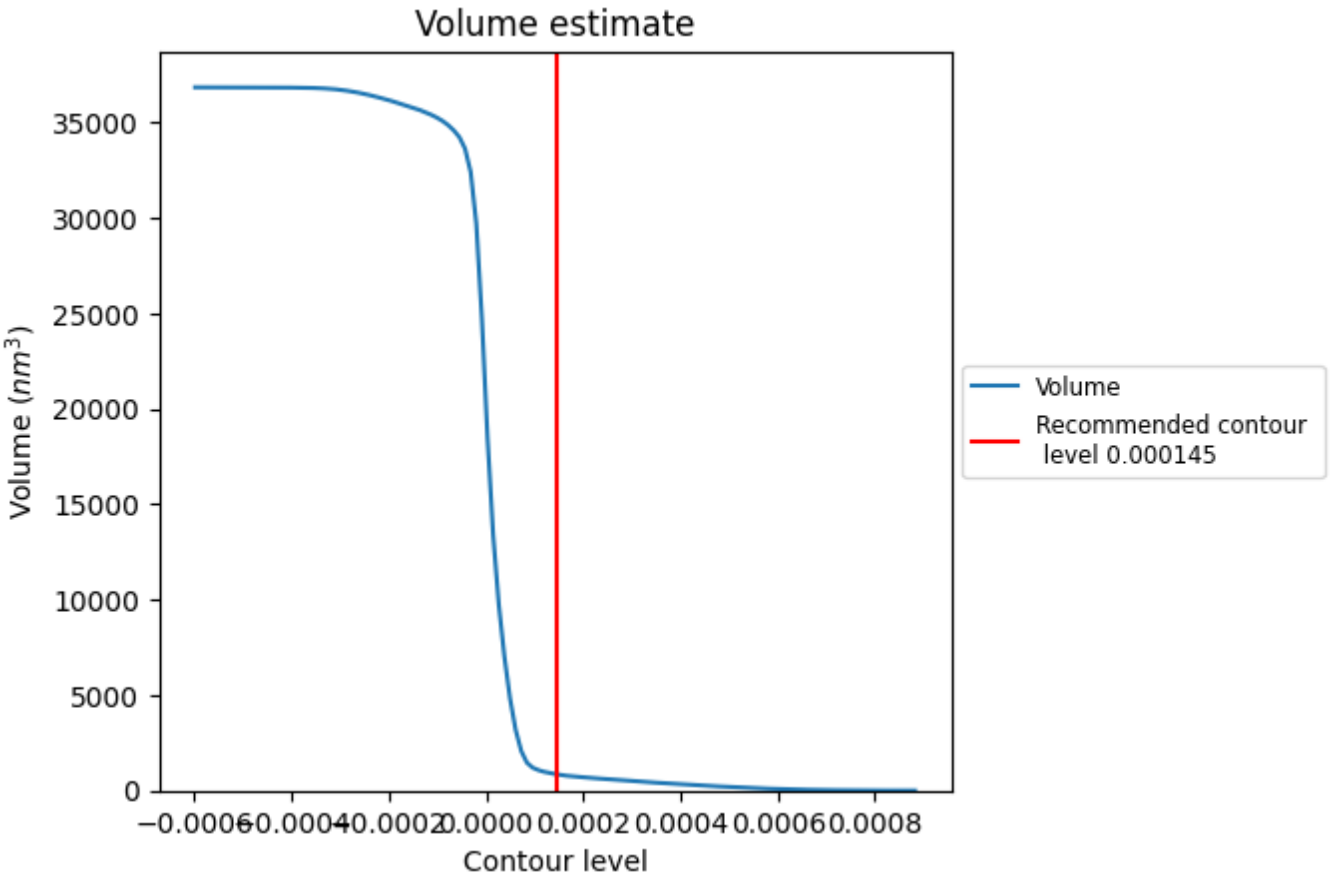
This section contains the results of statistical analysis of the map.

## 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.

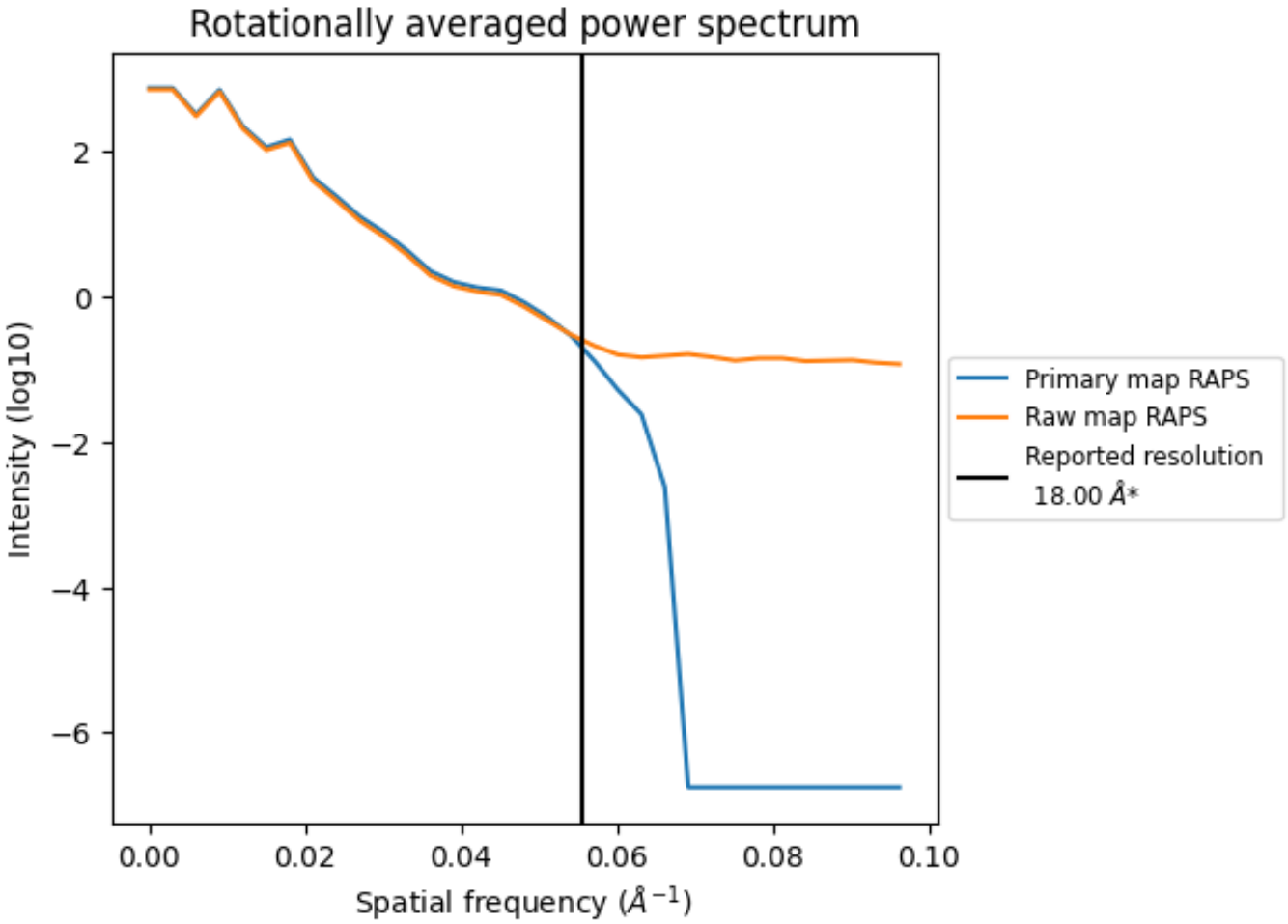
## 7.2 Volume estimate




The volume at the recommended contour level is 852 $nm^3$; this corresponds to an approximate mass of 770 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)

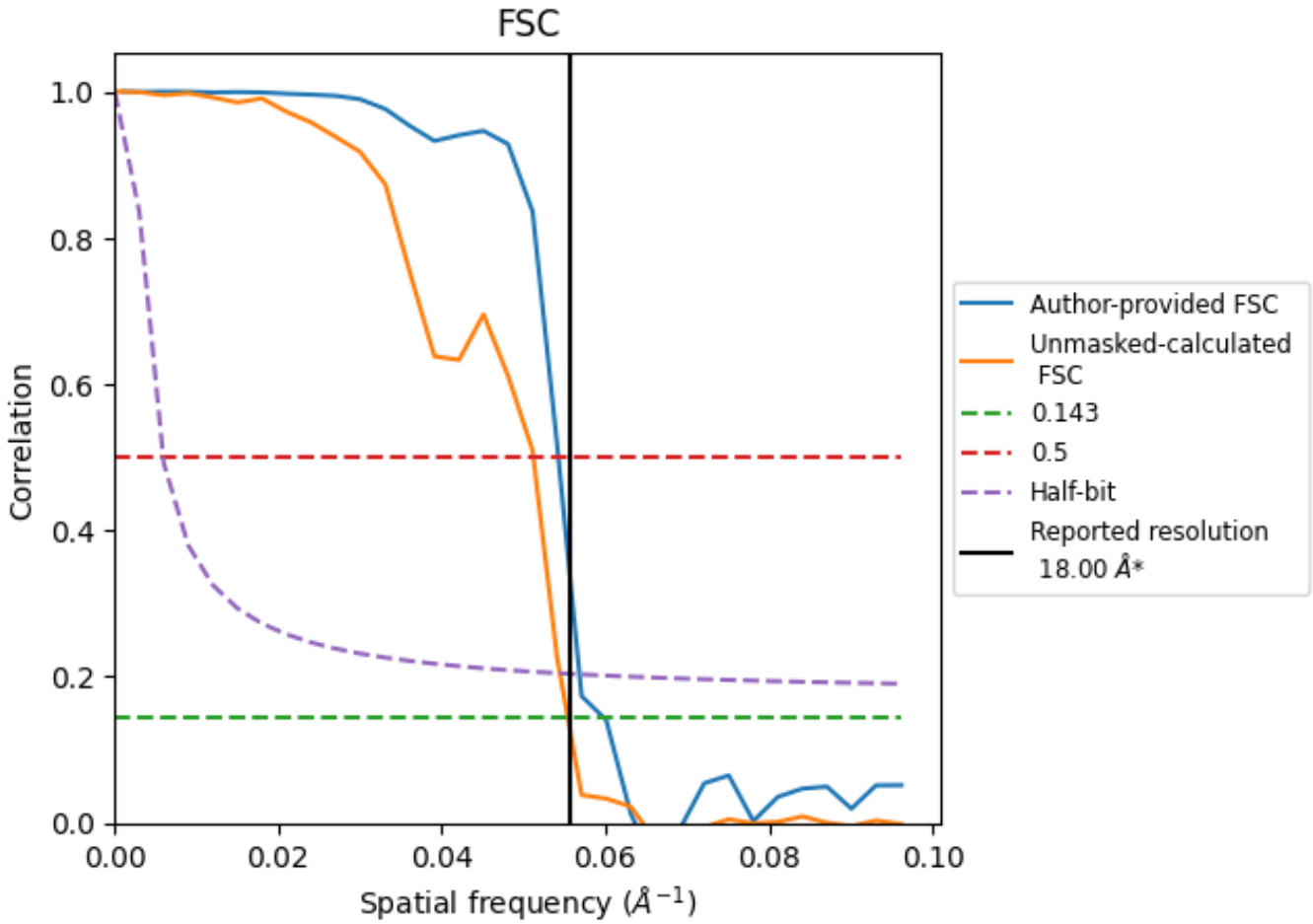



*Reported resolution corresponds to spatial frequency of 0.056 Å$^{-1}$

# 8 Fourier-Shell correlation

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

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.056 Å$^{-1}$

## 8.2 Resolution estimates (i)

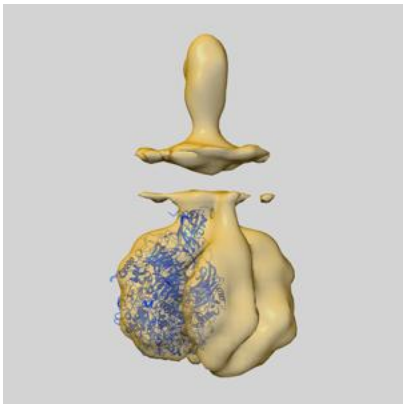
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 18.00 | - | - |
| Author-provided FSC curve | 16.69 | 18.45 | 17.61 |
| Unmasked-calculated* | 18.05 | 19.53 | 18.38 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

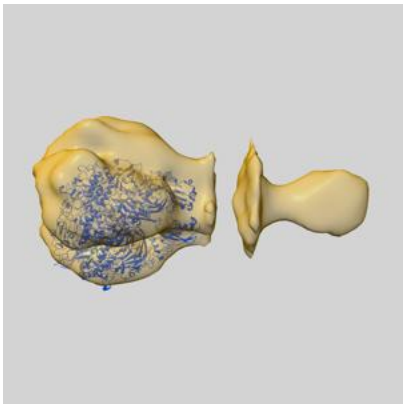
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17593 and PDB model 8PC1. Per-residue inclusion information can be found in section 3 on page 4.

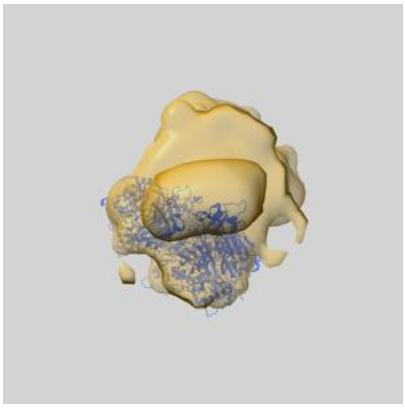
## 9.1 Map-model overlay



X



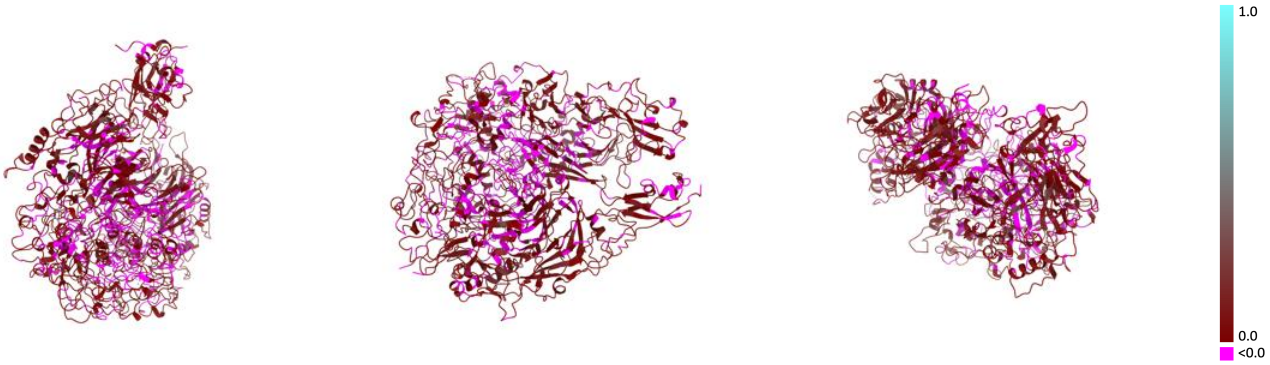
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.000145 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.

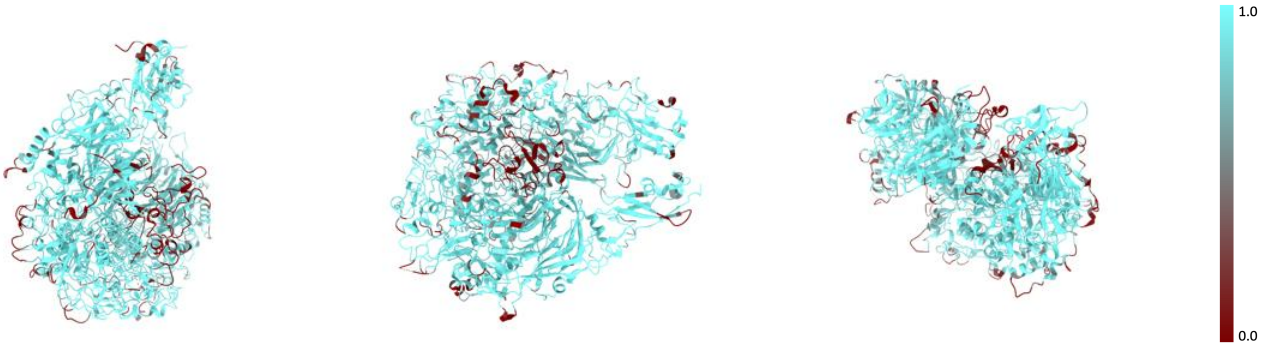
## 9.2 Q-score mapped to coordinate model




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.

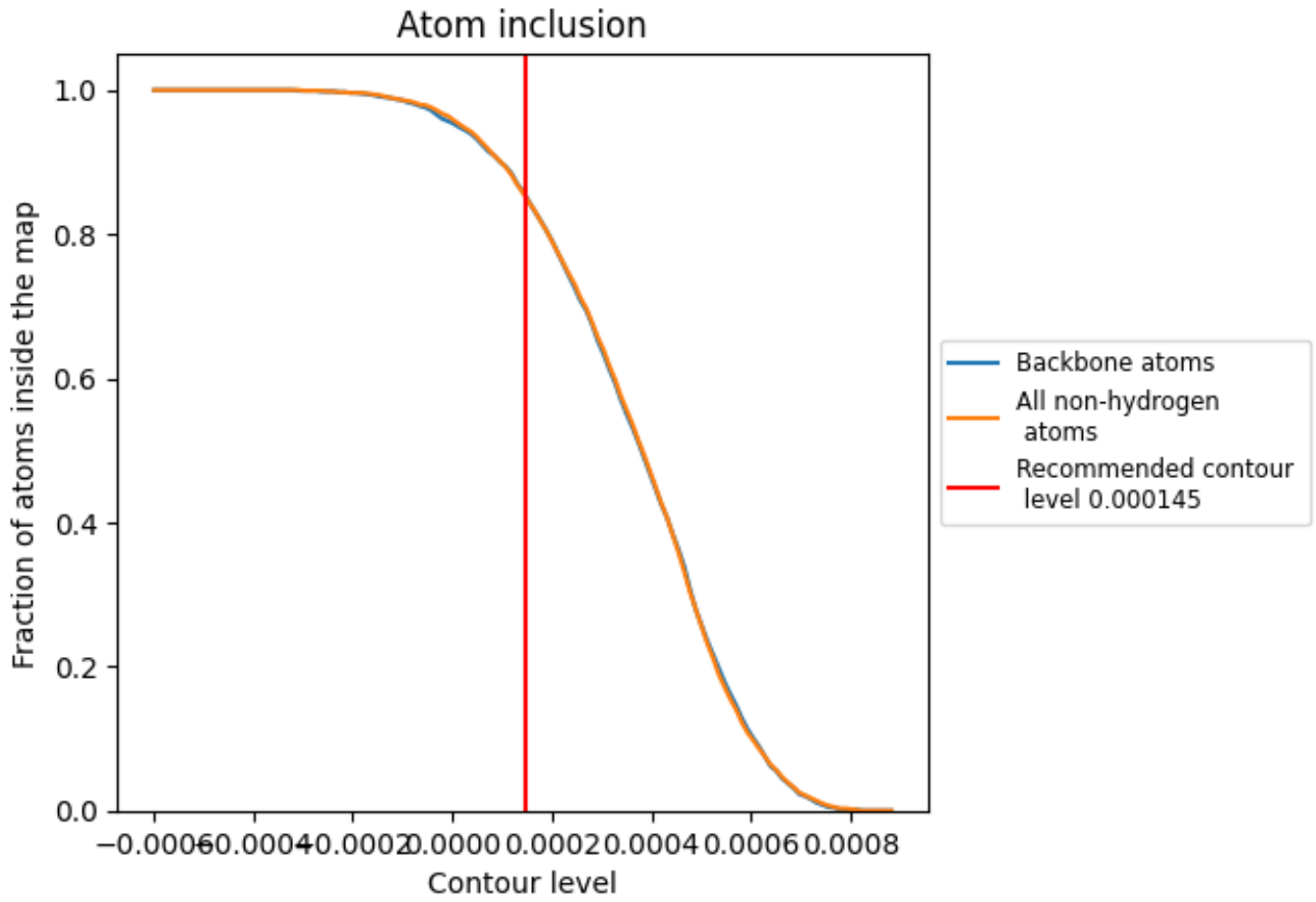
## 9.3 Atom inclusion mapped to coordinate model




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 (0.000145).

## 9.4 Atom inclusion (i)




At the recommended contour level, 86% of all backbone atoms, 85% 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 (0.000145) and Q-score for the entire model and for each chain.


| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8540 | 0.0450 |
| A | 0.8720 | 0.0480 |
| B | 0.8450 | 0.0430 |