# wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 12:49 AM EST

| | | |
|---|---|---|
| PDB ID | : | 7M0R |
| EMDB ID | : | EMD-23613 |
| Title | : | Cryo-EM structure of the Sema3A/PlexinA4/Neuropilin 1 complex |
| Authors | : | Lu, D.; Shang, G.; He, X.; Bai, X.; Zhang, X. |
| Deposited on | : | 2021-03-11 |
| Resolution | : | 3.70 Å(reported) |

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

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

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

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

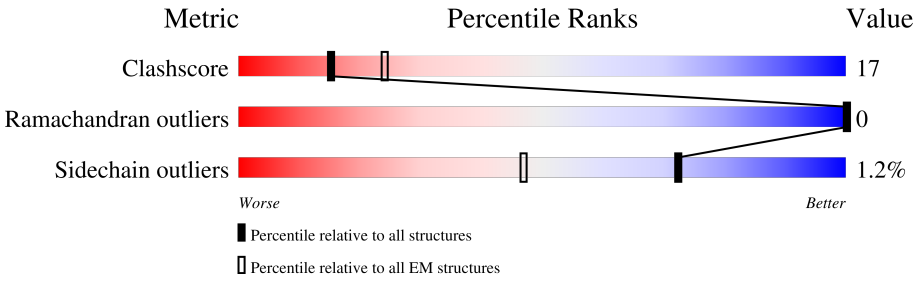
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.2 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | E | 567 | 22% 62% 19% 19% |
| 1 | F | 567 | 22% 62% 19% 19% |
| 2 | C | 614 | 7% 72% 23% . |
| 2 | D | 614 | 8% 72% 24% . |
| 3 | A | 1194 | 25% 60% 34% 5% |
| 3 | B | 1194 | 26% 60% 35% 5% |

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 30898 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 Neuropilin-1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | E | 458 | Total | C | N | O | S | 0 | 0 |
| | | | 2915 | 1823 | 514 | 566 | 12 | | |
| 1 | F | 458 | Total | C | N | O | S | 0 | 0 |
| | | | 2915 | 1823 | 514 | 566 | 12 | | |

- Molecule 2 is a protein called Semaphorin-3A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | C | 588 | Total | C | N | O | S | 0 | 0 |
| | | | 4492 | 2843 | 782 | 842 | 25 | | |
| 2 | D | 588 | Total | C | N | O | S | 0 | 0 |
| | | | 4492 | 2843 | 782 | 842 | 25 | | |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| C | 106 | LYS | ALA | engineered mutation | UNP O08665 |
| C | 475 | VAL | ILE | conflict | UNP O08665 |
| C | 551 | ALA | ARG | engineered mutation | UNP O08665 |
| C | 555 | ALA | ARG | engineered mutation | UNP O08665 |
| D | 106 | LYS | ALA | engineered mutation | UNP O08665 |
| D | 475 | VAL | ILE | conflict | UNP O08665 |
| D | 551 | ALA | ARG | engineered mutation | UNP O08665 |
| D | 555 | ALA | ARG | engineered mutation | UNP O08665 |

- Molecule 3 is a protein called Plexin-A4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | A | 1133 | Total | C | N | O | S | 0 | 0 |
| | | | 8040 | 5103 | 1362 | 1511 | 64 | | |
| 3 | B | 1133 | Total | C | N | O | S | 0 | 0 |
| | | | 8040 | 5103 | 1362 | 1511 | 64 | | |

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

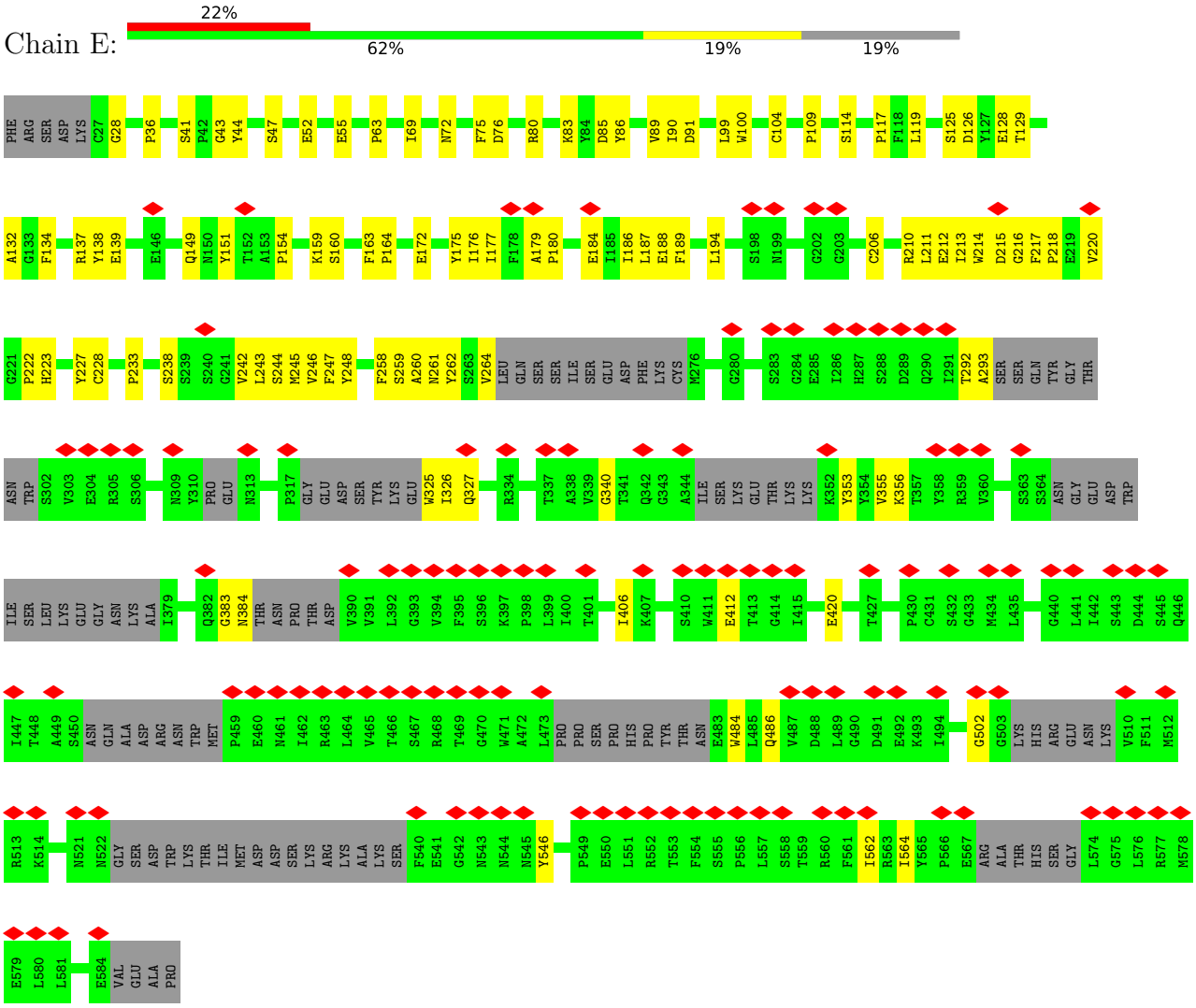
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 4 | E | 2 | Total Ca<br>2 2 | 0 |
| 4 | F | 2 | Total Ca<br>2 2 | 0 |

# 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.

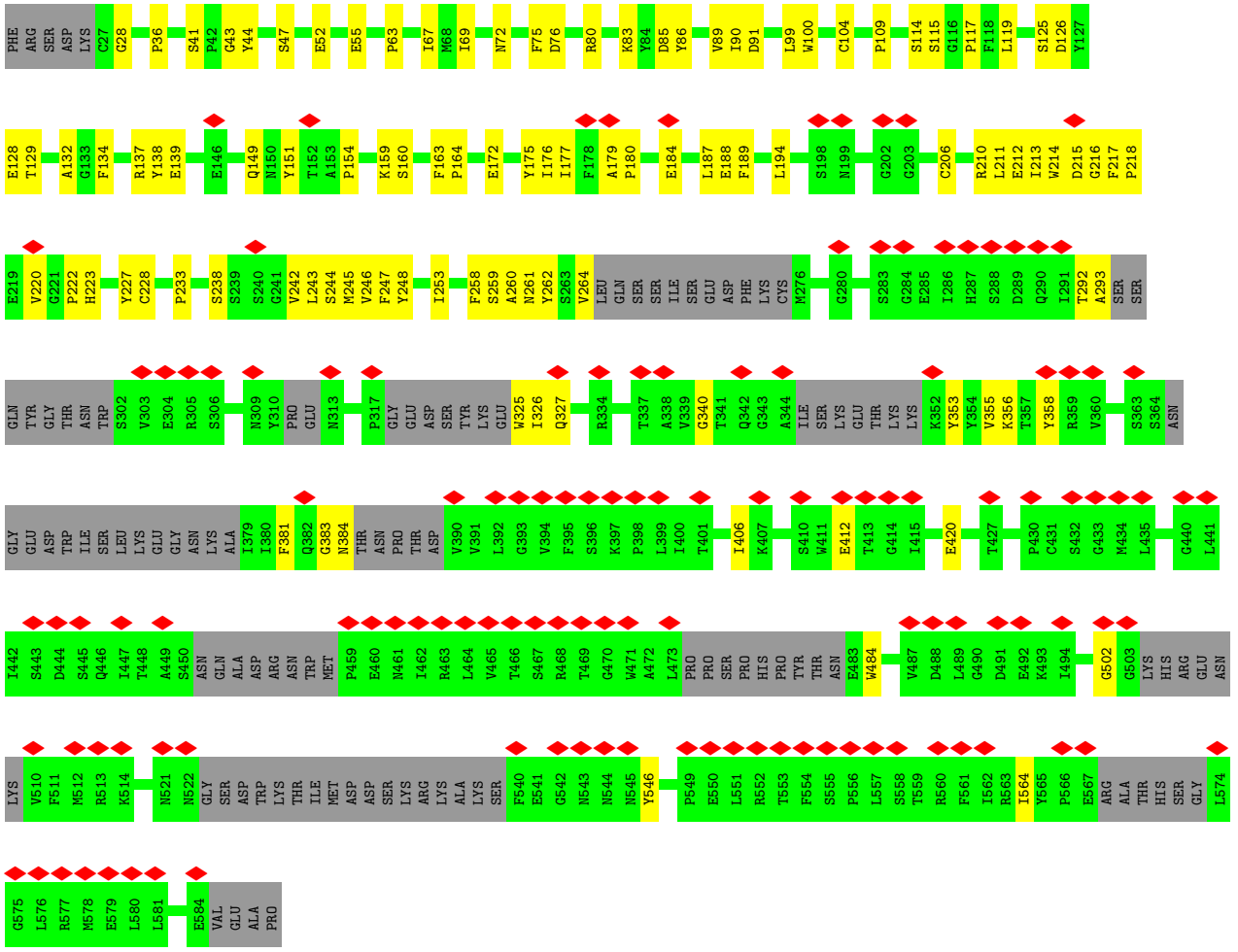
• Molecule 1: Neuropilin-1

Chain E:



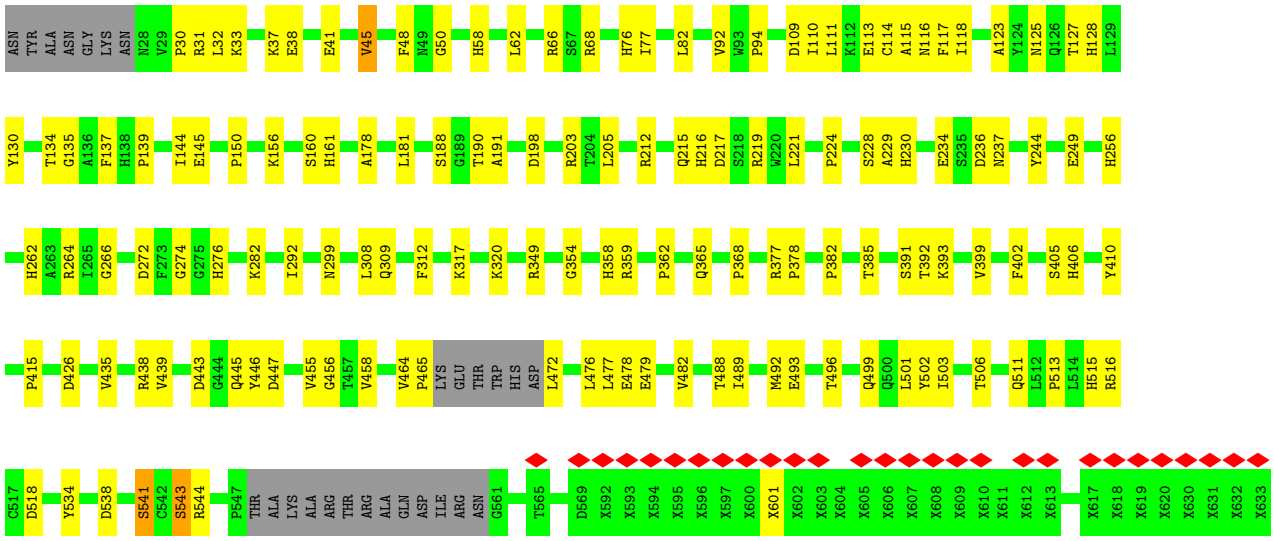

• Molecule 1: Neuropilin-1

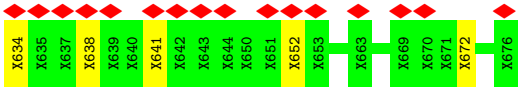
Chain F:



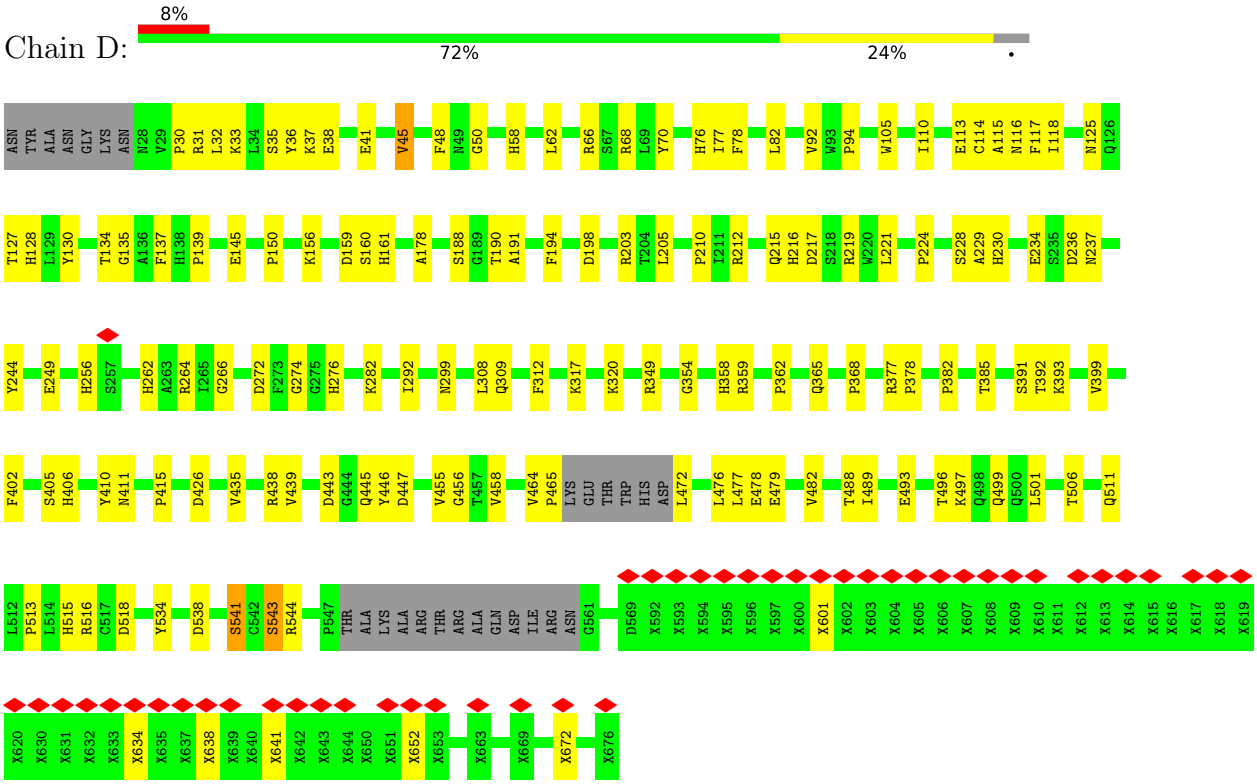
• Molecule 2: Semaphorin-3A

Chain C:

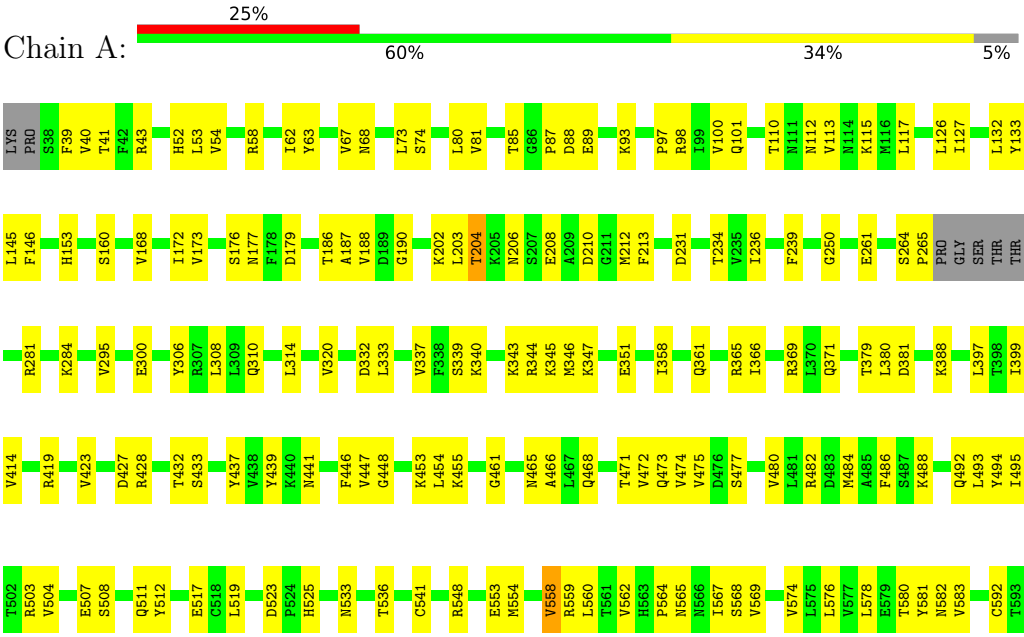



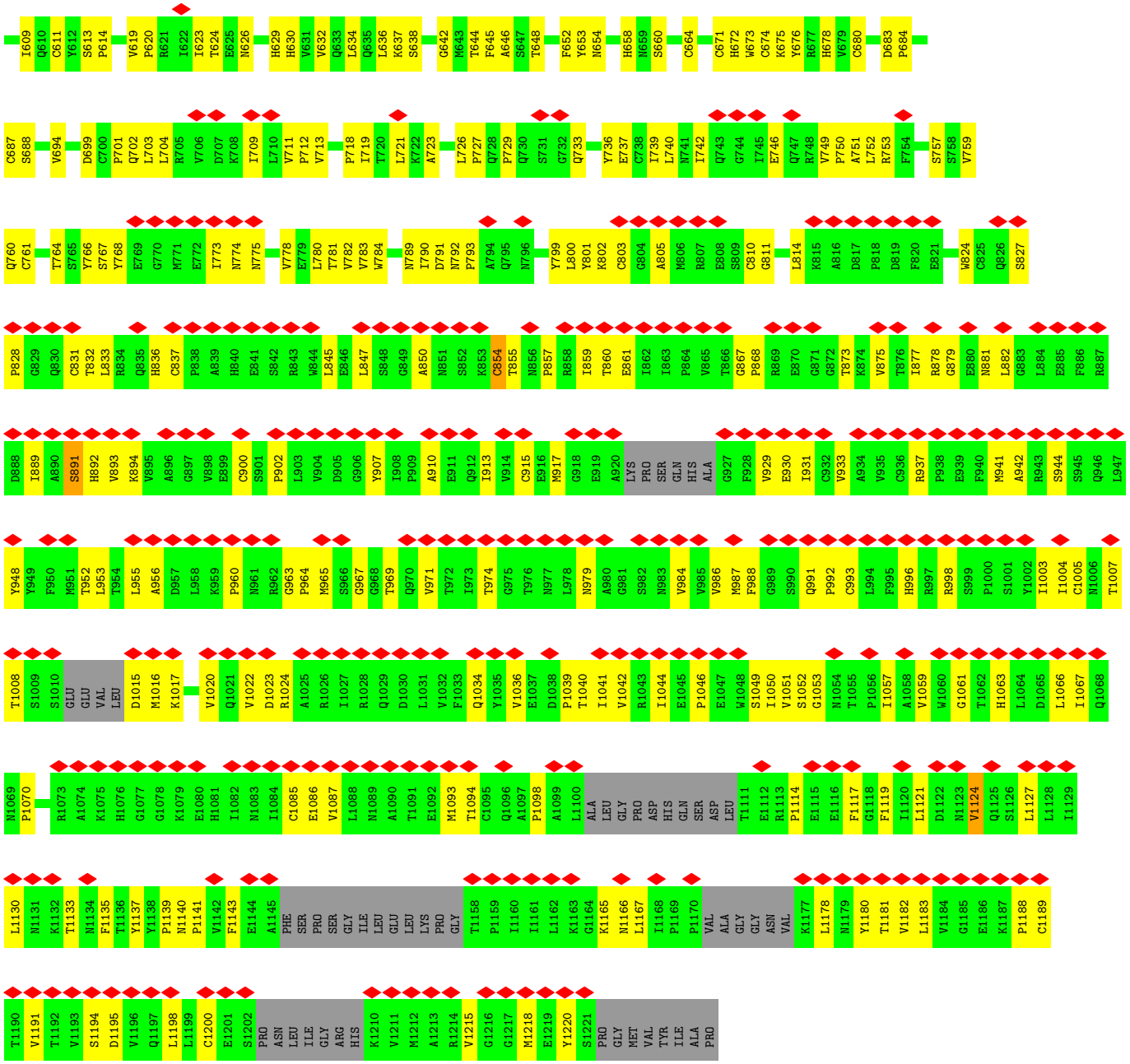


• Molecule 2: Semaphorin-3A



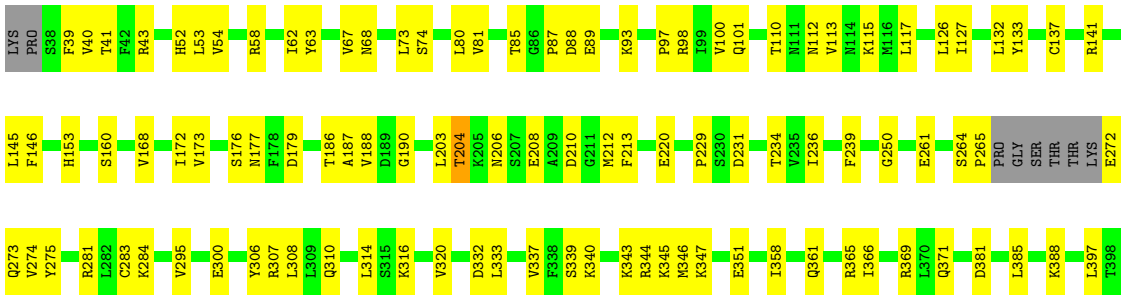
• Molecule 3: Plexin-A4

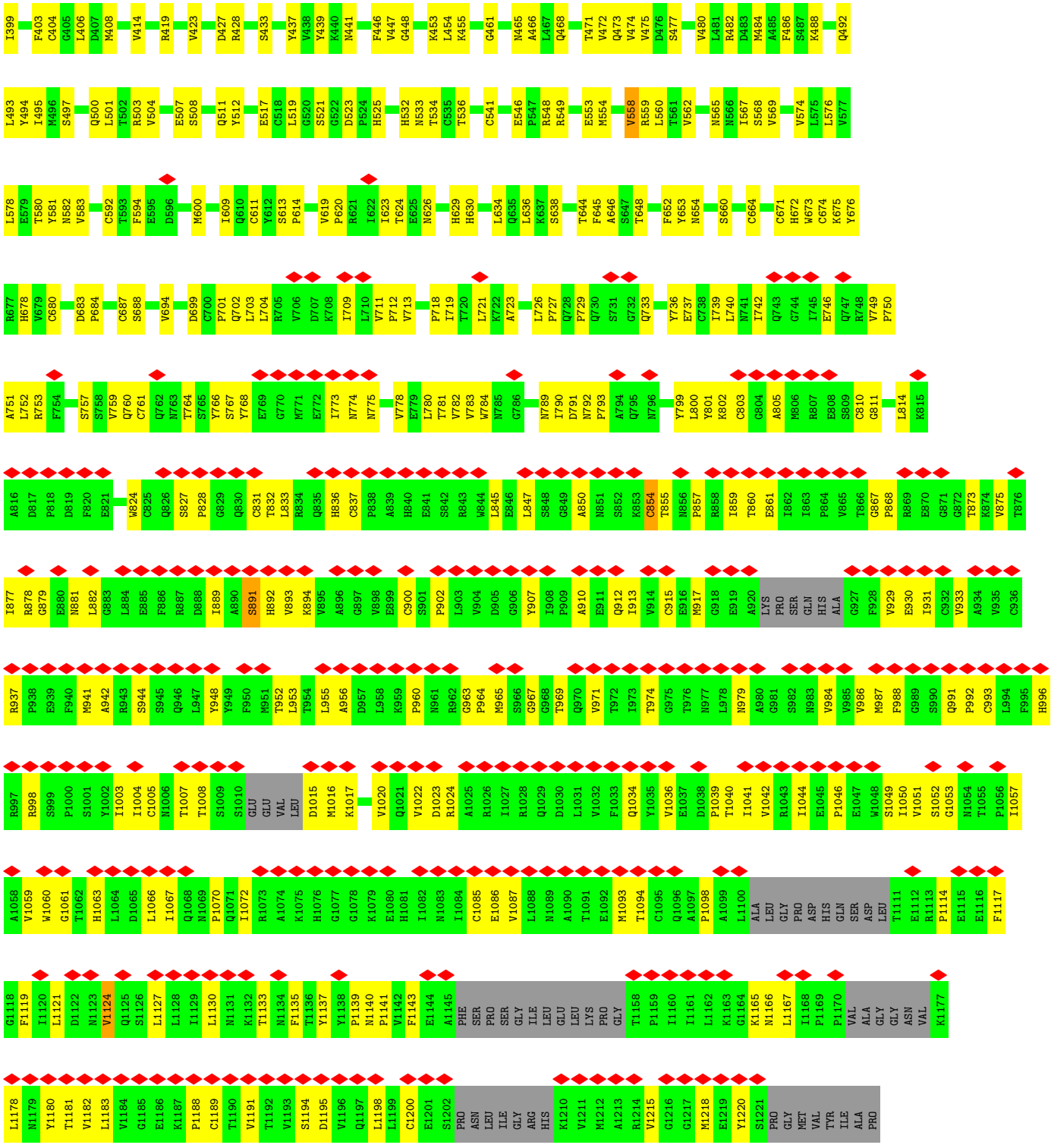




• Molecule 3: Plexin-A4

Chain B:


I399 F403 C404 G405 L406 D407 M408 V414 R419 V423 D427 R428 S433 Y437 V438 Y439 K440 N441 F446 V447 G448 K453 L454 K455 G461 N465 A466 L467 Q468 T471 V472 Q473 V474 V475 D476 S477 V480 L481 R482 D483 M484 A485 F486 S487 K488 Q492
L493 Y494 I495 M496 S497 Q500 L501 T502 R503 V504 E507 S508 Q511 Y512 E517 C518 L519 G520 S521 G522 D523 P524 H525 H532 N533 T534 C535 T536 C541 E546 P547 R548 R549 E553 M554 V558 R559 L560 T561 V562 N565 N566 I567 S568 V569 V574 L575 L576 V577
L578 E579 T580 Y581 N582 V583 C592 T593 F594 E595 D596 M600 I609 Q610 C611 Y612 S613 P614 V619 P620 R621 I622 I623 T624 E625 N626 H629 H630 L634 Q635 L636 K637 S638 T644 F645 A646 S647 T648 F652 Y653 N654 S660 C664 C671 H672 W673 C674 K675 Y676
R677 H678 V679 C680 D683 P684 C687 S688 V694 D699 C700 P701 Q702 L703 L704 R705 V706 D707 K708 I709 L710 V711 P712 V713 P718 I719 T720 L721 K722 A723 L726 P727 Q728 P729 Q730 S731 G732 Q733 Y736 E737 C738 I739 L740 N741 I742 Q743 G744 I745 E746 Q747 R748 V749 P750
A751 L752 R753 F754 S757 S758 V759 Q760 C761 Q762 N763 T764 S765 Y766 S767 Y768 E769 G770 M771 E772 I773 N774 N775 V778 E779 L780 T781 V782 V783 W784 N785 G786 N789 I790 D791 N792 P793 A794 Q795 N796 Y799 L800 Y801 K802 C803 C804 A805 M806 R807 E808 S809 C810 G811 L814 K815
A816 D817 P818 D819 F820 E821 W824 C825 Q826 S827 P828 G829 Q830 C831 T832 L833 R834 Q835 H836 C837 P838 A839 H840 E841 S842 R843 W844 L845 E846 L847 S848 G849 A850 N851 S852 K853 C854 T855 N856 P857 R858 I859 T860 E861 I862 I863 P864 V865 T866 G867 P868 R869 E870 G871 G872 T873 K874 V875 T876
I877 R878 G879 E880 N881 L882 G883 L884 E885 F886 R887 D888 I889 A890 S891 H892 V893 K894 V895 A896 G897 V898 E899 C900 S901 P902 L903 V904 D905 G906 Y907 I908 P909 A910 E911 Q912 I913 V914 C915 E916 M917 G918 E919 A920 LYS PRO SER GLN HIS ALA G927 F928 V929 E930 I931 C932 V933 A934 V935 C936
R937 P938 E939 F940 M941 A942 R943 S944 S945 Q946 L947 Y948 Y949 F950 M951 T952 L953 T954 L955 A956 D957 L958 K959 P960 N961 R962 G963 P964 M965 S966 G967 G968 T969 Q970 V971 T972 I973 T974 G975 T976 N977 L978 N979 A980 G981 S982 N983 V984 V985 V986 M987 F988 G989 S990 Q991 P992 C993 L994 F995 H996
R997 R998 S999 P1000 S1001 Y1002 I1003 I1004 C1005 N1006 T1007 T1008 S1009 S1010 GLU GLU VAL LEU D1015 M1016 K1017 V1020 Q1021 V1022 D1023 R1024 A1025 R1026 I1027 R1028 Q1029 D1030 L1031 V1032 F1033 Q1034 Y1035 V1036 E1037 D1038 P1039 T1040 I1041 V1042 R1043 I1044 E1045 P1046 E1047 W1048 S1049 I1050 V1051 S1052 G1053 N1054 T1055 P1056 I1057
A1058 V1059 W1060 G1061 T1062 H1063 L1064 D1065 L1066 I1067 Q1068 N1069 P1070 Q1071 I1072 R1073 A1074 K1075 H1076 G1077 G1078 K1079 E1080 H1081 I1082 N1083 I1084 C1085 E1086 V1087 L1088 N1089 A1090 T1091 E1092 M1093 T1094 C1095 Q1096 A1097 P1098 A1099 L1100 ALA LEU GLY PRO ASP HIS GLN SER ASP LEU T1111 E1112 R1113 P1114 E1115 E1116 F1117
G1118 F1119 I1120 L1121 D1122 N1123 V1124 Q1125 S1126 L1127 L1128 I1129 L1130 N1131 K1132 T1133 N1134 F1135 T1136 Y1137 Y1138 P1139 N1140 P1141 V1142 F1143 E1144 A1145 PHE SER PRO SER GLY ILE LEU GLU LEU LYS PRO GLY T1158 P1159 I1160 I1161 L1162 K1163 G1164 K1165 N1166 L1167 I1168 P1169 P1170 VAL ALA GLY GLY ASN VAL K1177
L1178 N1179 Y1180 T1181 V1182 L1183 V1184 G1185 E1186 K1187 P1188 C1189 T1190 V1191 T1192 V1193 S1194 D1195 V1196 Q1197 L1198 L1199 C1200 E1201 S1202 PRO ASN LEU ILE GLY ARG HIS K1210 V1211 M1212 A1213 R1214 V1215 G1216 G1217 M1218 E1219 Y1220 S1221 PRO GLY MET VAL TYR ILE ALA PRO

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C2 | Depositor |
| Number of particles used | 26741 | 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 ($e^-/Å^2$) | 50 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 0.048 | Depositor |
| Minimum map value | -0.016 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.002 | Depositor |
| Recommended contour level | 0.01 | Depositor |
| Map size (Å) | 302.40002, 302.40002, 302.40002 | wwPDB |
| Map dimensions | 280, 280, 280 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.08, 1.08, 1.08 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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

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 | E | 0.27 | 0/2965 | 0.46 | 0/4045 |
| 1 | F | 0.27 | 0/2965 | 0.46 | 0/4045 |
| 2 | C | 0.34 | 0/4281 | 0.45 | 1/5809 (0.0%) |
| 2 | D | 0.34 | 0/4281 | 0.46 | 1/5809 (0.0%) |
| 3 | A | 0.29 | 0/8211 | 0.47 | 0/11236 |
| 3 | B | 0.29 | 0/8211 | 0.47 | 0/11236 |
| All | All | 0.30 | 0/30914 | 0.47 | 2/42180 (0.0%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | C | 465 | PRO | N-CA-CB | 5.92 | 110.41 | 103.30 |
| 2 | D | 465 | PRO | N-CA-CB | 5.92 | 110.40 | 103.30 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | E | 2915 | 0 | 2144 | 70 | 0 |
| 1 | F | 2915 | 0 | 2144 | 72 | 0 |
| 2 | C | 4492 | 0 | 4067 | 91 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | D | 4492 | 0 | 4067 | 95 | 0 |
| 3 | A | 8040 | 0 | 7294 | 323 | 0 |
| 3 | B | 8040 | 0 | 7294 | 326 | 0 |
| 4 | E | 2 | 0 | 0 | 0 | 0 |
| 4 | F | 2 | 0 | 0 | 0 | 0 |
| All | All | 30898 | 0 | 27010 | 963 | 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 17.

The worst 5 of 963 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) |
|---|---|---|---|
| 3:A:986:VAL:HG23 | 3:A:993:CYS:HB3 | 1.54 | 0.90 |
| 3:B:986:VAL:HG23 | 3:B:993:CYS:HB3 | 1.54 | 0.89 |
| 3:B:857:PRO:HB2 | 3:B:942:ALA:HB2 | 1.57 | 0.86 |
| 1:E:353:TYR:HA | 1:E:412:GLU:O | 1.76 | 0.86 |
| 1:F:353:TYR:HA | 1:F:412:GLU:O | 1.76 | 0.85 |

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 | E | 432/567 (76%) | 418 (97%) | 14 (3%) | 0 | 100 | 100 |
| 1 | F | 432/567 (76%) | 418 (97%) | 14 (3%) | 0 | 100 | 100 |
| 2 | C | 517/614 (84%) | 497 (96%) | 20 (4%) | 0 | 100 | 100 |
| 2 | D | 517/614 (84%) | 498 (96%) | 19 (4%) | 0 | 100 | 100 |
| 3 | A | 1117/1194 (94%) | 1059 (95%) | 58 (5%) | 0 | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 3 | B | 1117/1194 (94%) | 1060 (95%) | 57 (5%) | 0 | 100 | 100 |
| All | All | 4132/4750 (87%) | 3950 (96%) | 182 (4%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | E | 193/496 (39%) | 193 (100%) | 0 | 100 | 100 |
| 1 | F | 193/496 (39%) | 193 (100%) | 0 | 100 | 100 |
| 2 | C | 458/482 (95%) | 451 (98%) | 7 (2%) | 65 | 81 |
| 2 | D | 458/482 (95%) | 451 (98%) | 7 (2%) | 65 | 81 |
| 3 | A | 793/1056 (75%) | 782 (99%) | 11 (1%) | 67 | 82 |
| 3 | B | 793/1056 (75%) | 782 (99%) | 11 (1%) | 67 | 82 |
| All | All | 2888/4068 (71%) | 2852 (99%) | 36 (1%) | 72 | 84 |

5 of 36 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | B | 558 | VAL |
| 3 | B | 1124 | VAL |
| 3 | B | 568 | SER |
| 3 | B | 854 | CYS |
| 2 | D | 541 | SER |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | D | 358 | HIS |
| 3 | A | 114 | ASN |
| 3 | B | 979 | ASN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | D | 365 | GLN |
| 2 | D | 445 | GLN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 2 | C | 6 |
| 2 | D | 6 |

The worst 5 of 12 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | C | 569:ASP | C | 592:UNK | N | 26.06 |
| 1 | D | 569:ASP | C | 592:UNK | N | 26.06 |
| 1 | C | 620:UNK | C | 630:UNK | N | 16.07 |
| 1 | D | 620:UNK | C | 630:UNK | N | 16.07 |
| 1 | C | 644:UNK | C | 650:UNK | N | 10.23 |

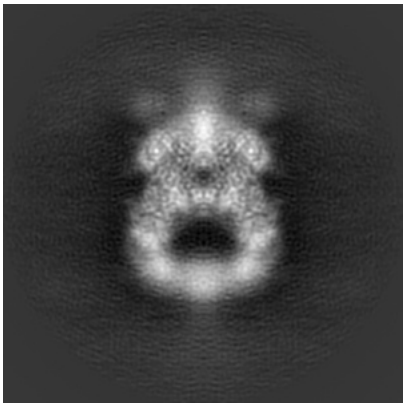
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23613. These allow visual inspection of the internal detail of the map and identification of artifacts.

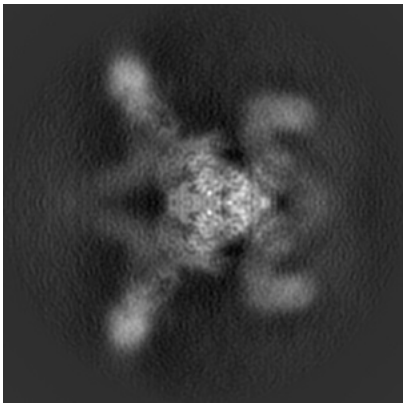
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

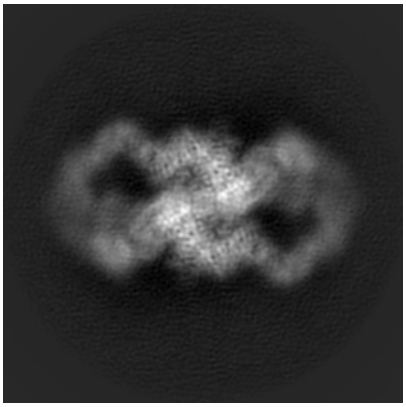
### 6.1.1 Primary map



X



Y

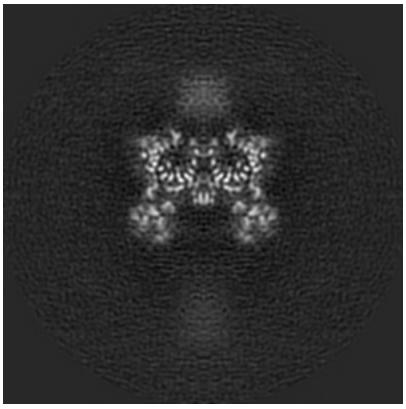


Z

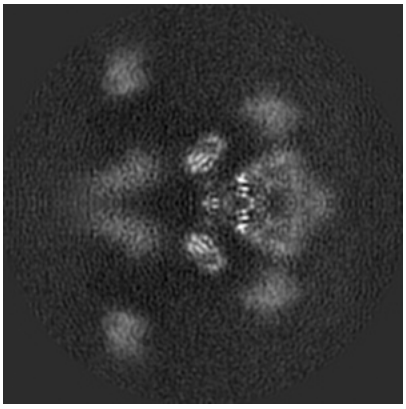
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

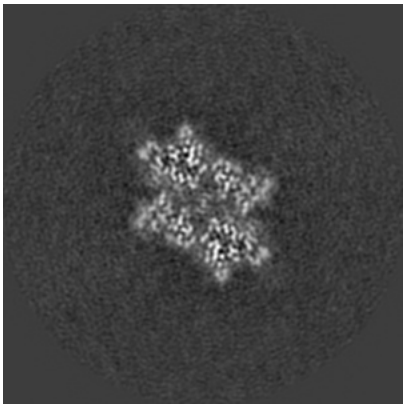
### 6.2.1 Primary map



X Index: 140



Y Index: 140

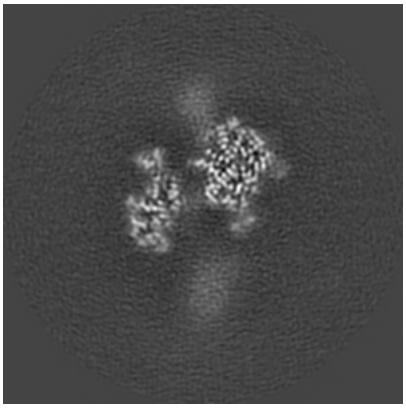


Z Index: 140

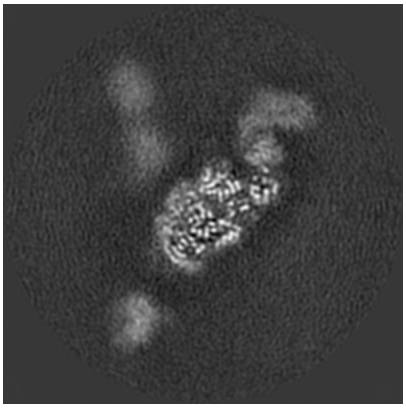
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

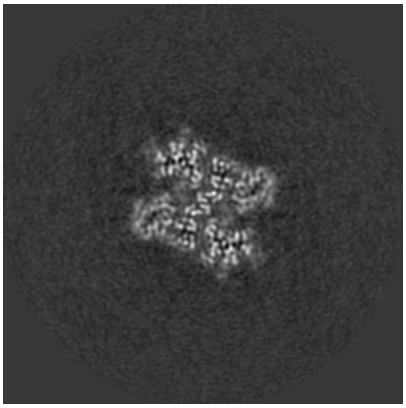
### 6.3.1 Primary map



X Index: 151



Y Index: 168

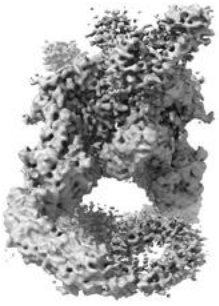


Z Index: 145

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

## 6.4 Orthogonal surface views (i)

### 6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

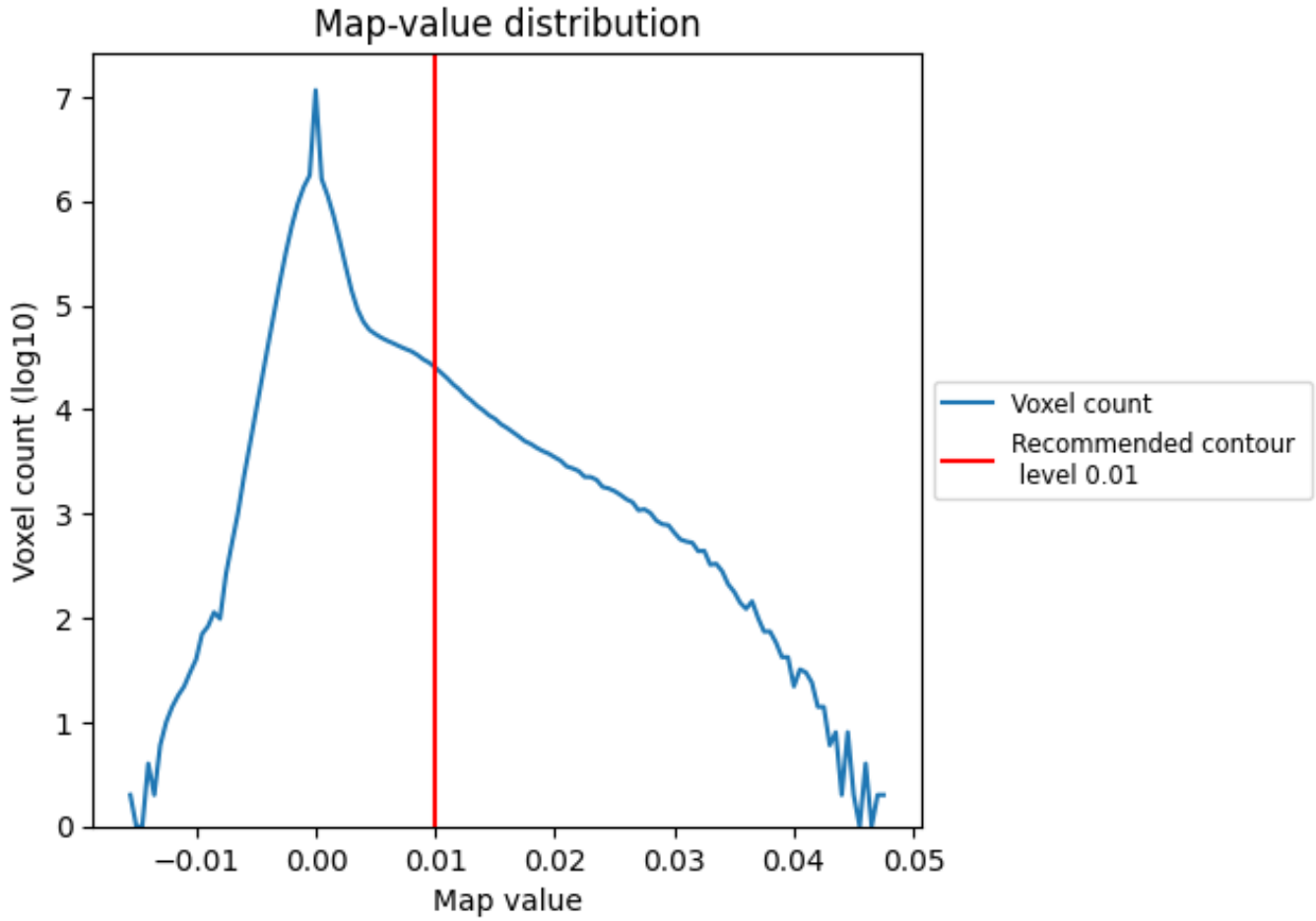
## 6.5 Mask visualisation (i)

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

# 7 Map analysis

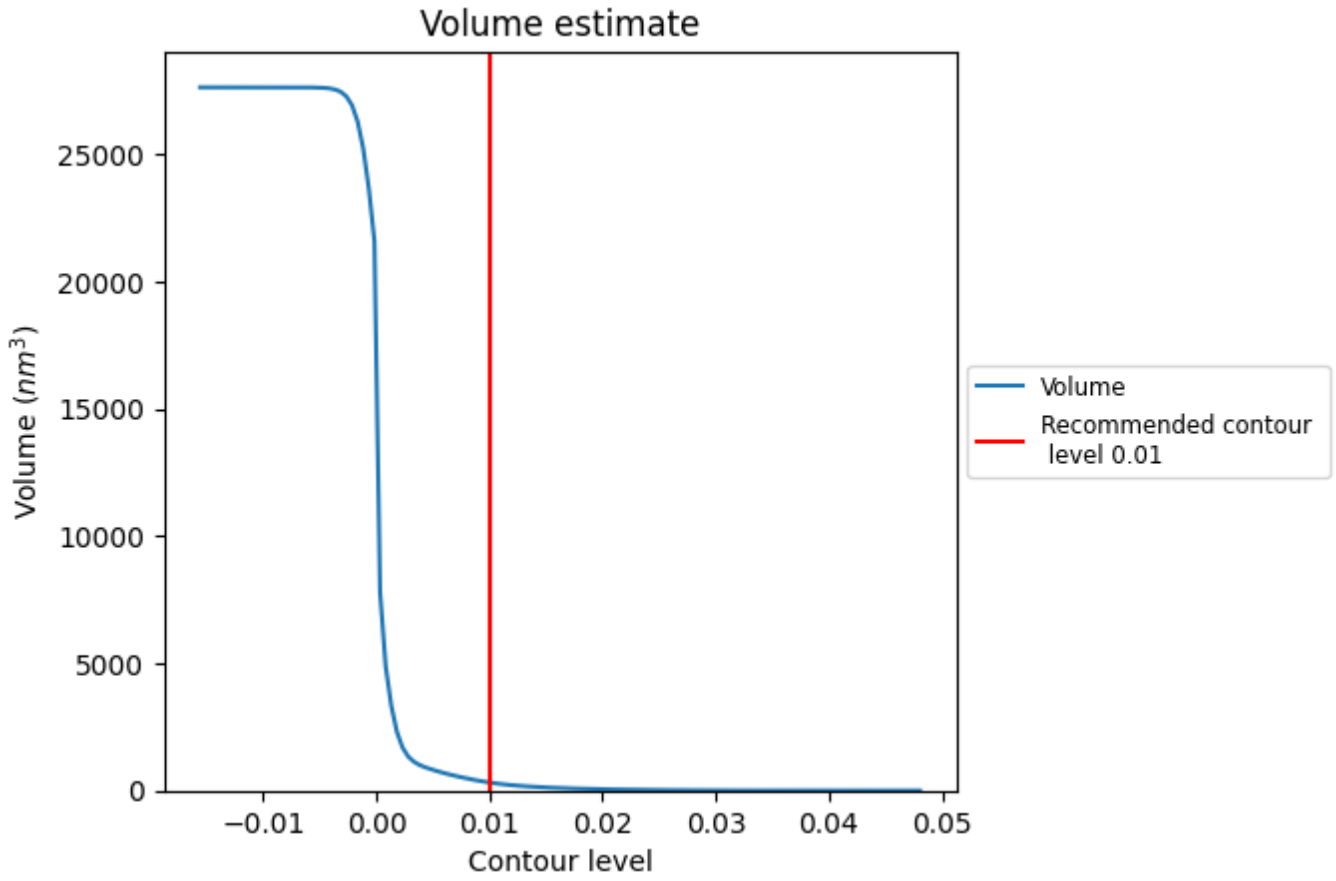
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

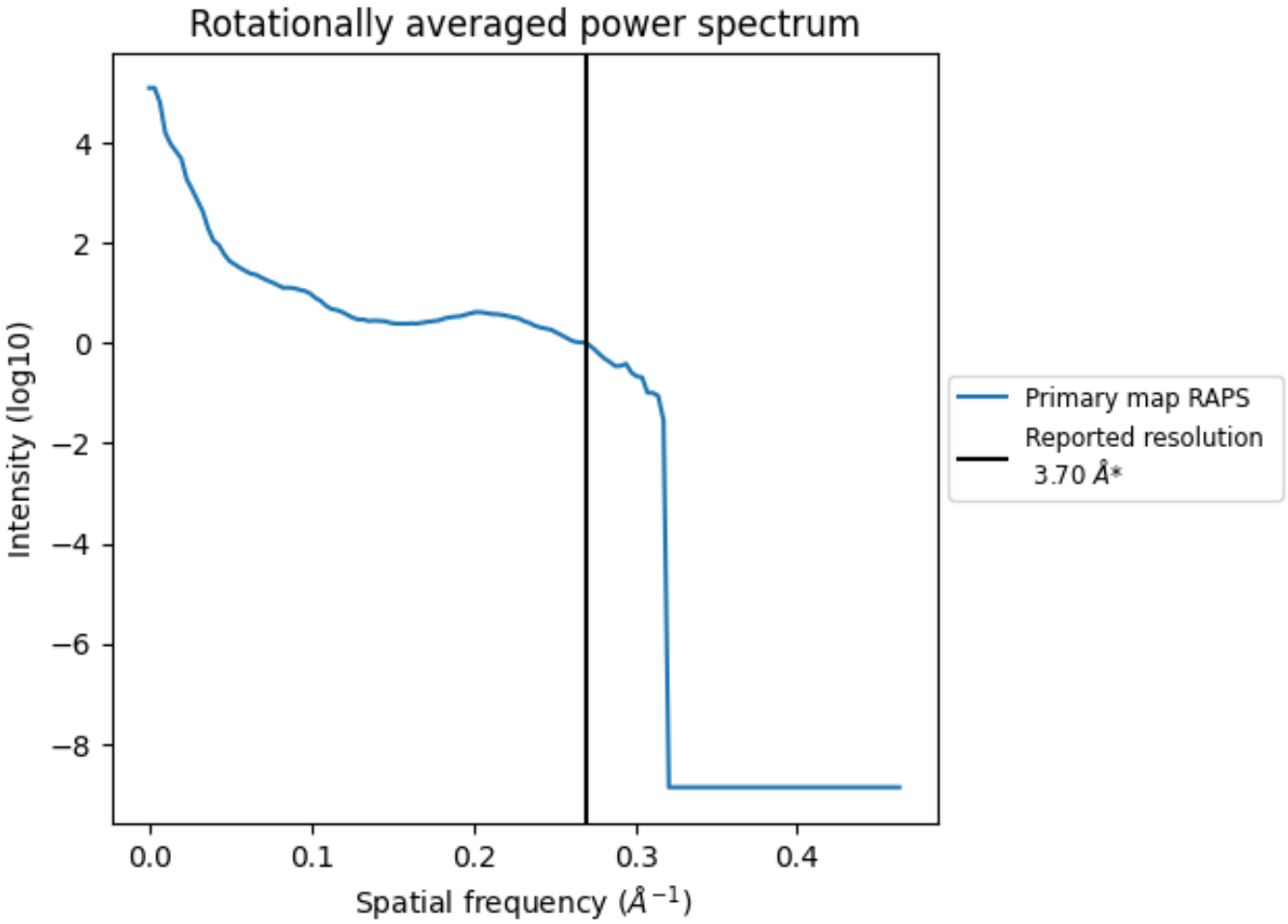
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 318 $nm^3$; this corresponds to an approximate mass of 287 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum (i)

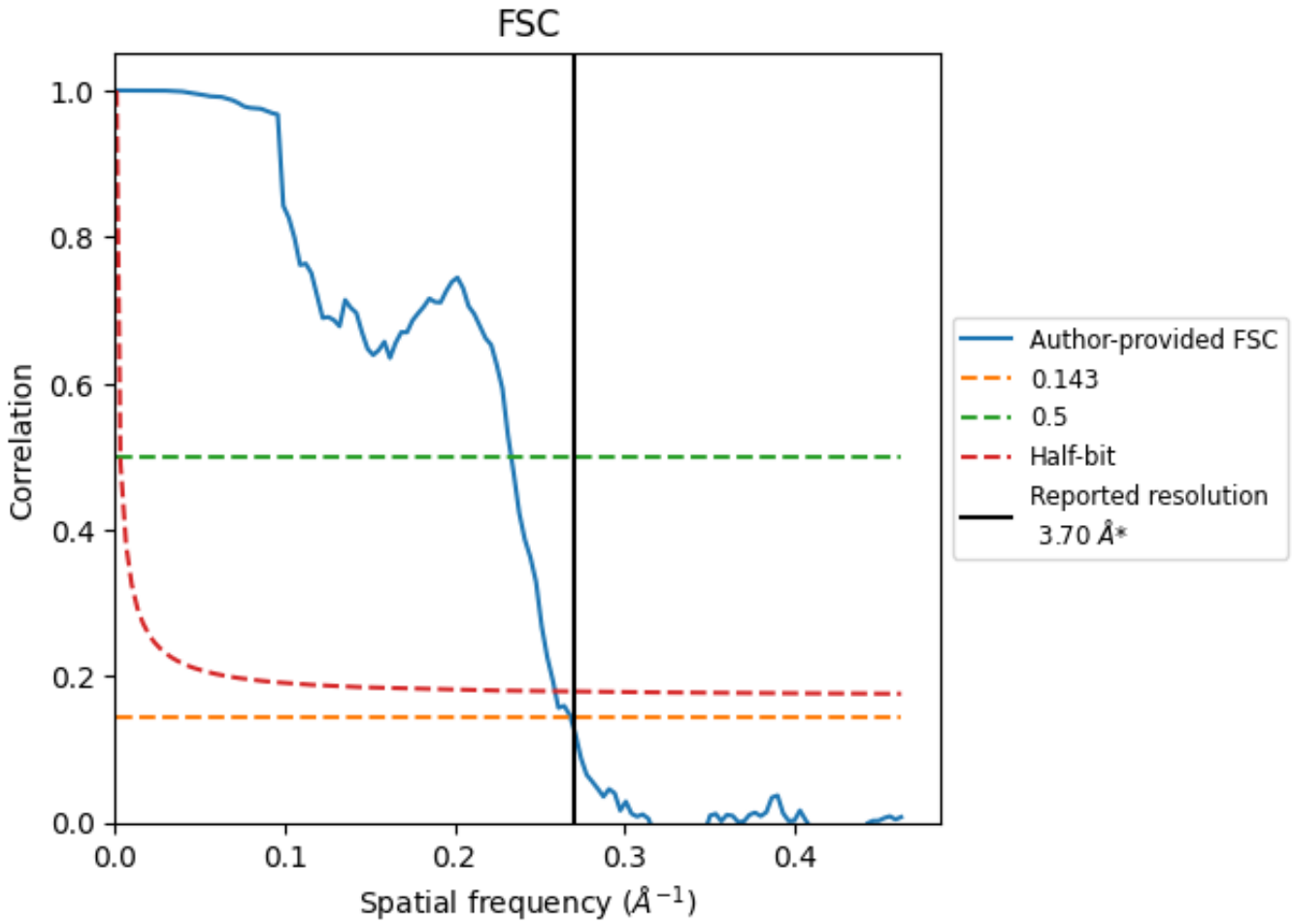



*Reported resolution corresponds to spatial frequency of 0.270 Å$^{-1}$

# 8 Fourier-Shell correlation

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 0.270 Å$^{-1}$

## 8.2 Resolution estimates (i)

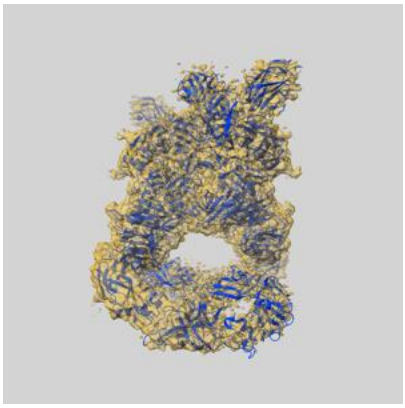
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.70 | - | - |
| Author-provided FSC curve | 3.73 | 4.29 | 3.86 |
| Unmasked-calculated* | - | - | - |

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

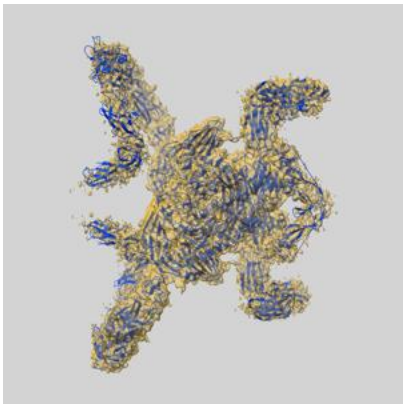
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23613 and PDB model 7M0R. Per-residue inclusion information can be found in section 3 on page 5.

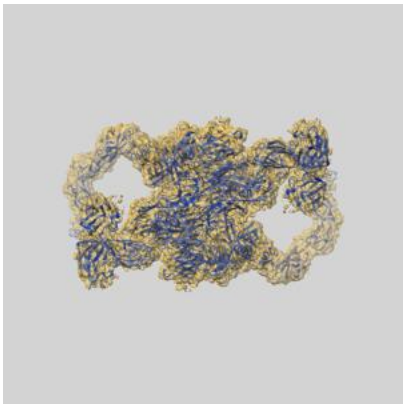
## 9.1 Map-model overlay



X



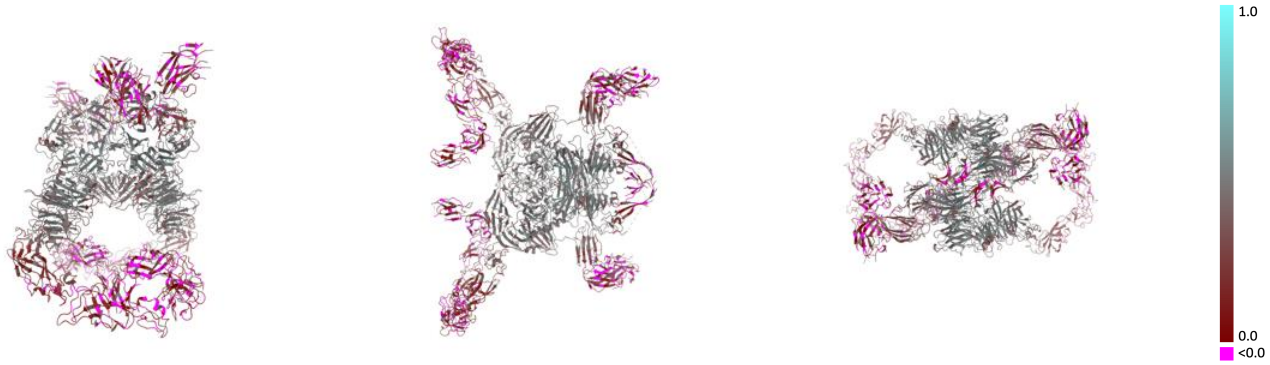
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

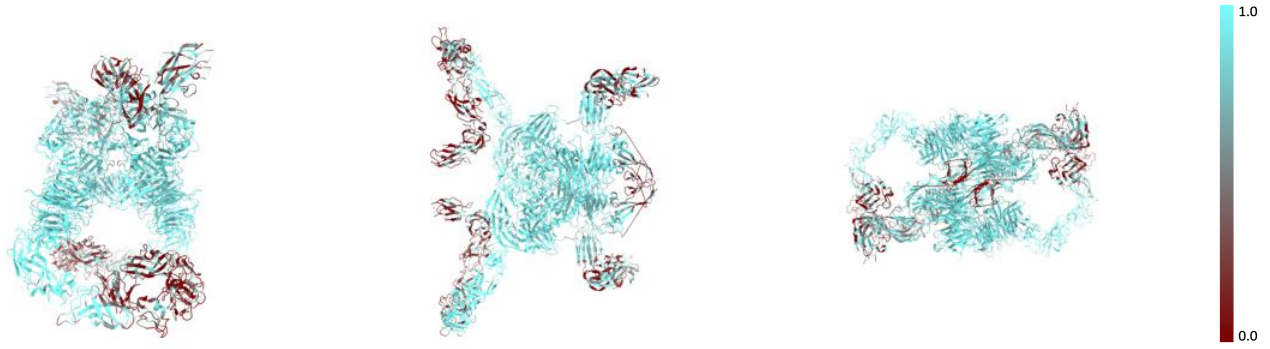
## 9.2 Q-score mapped to coordinate model




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.

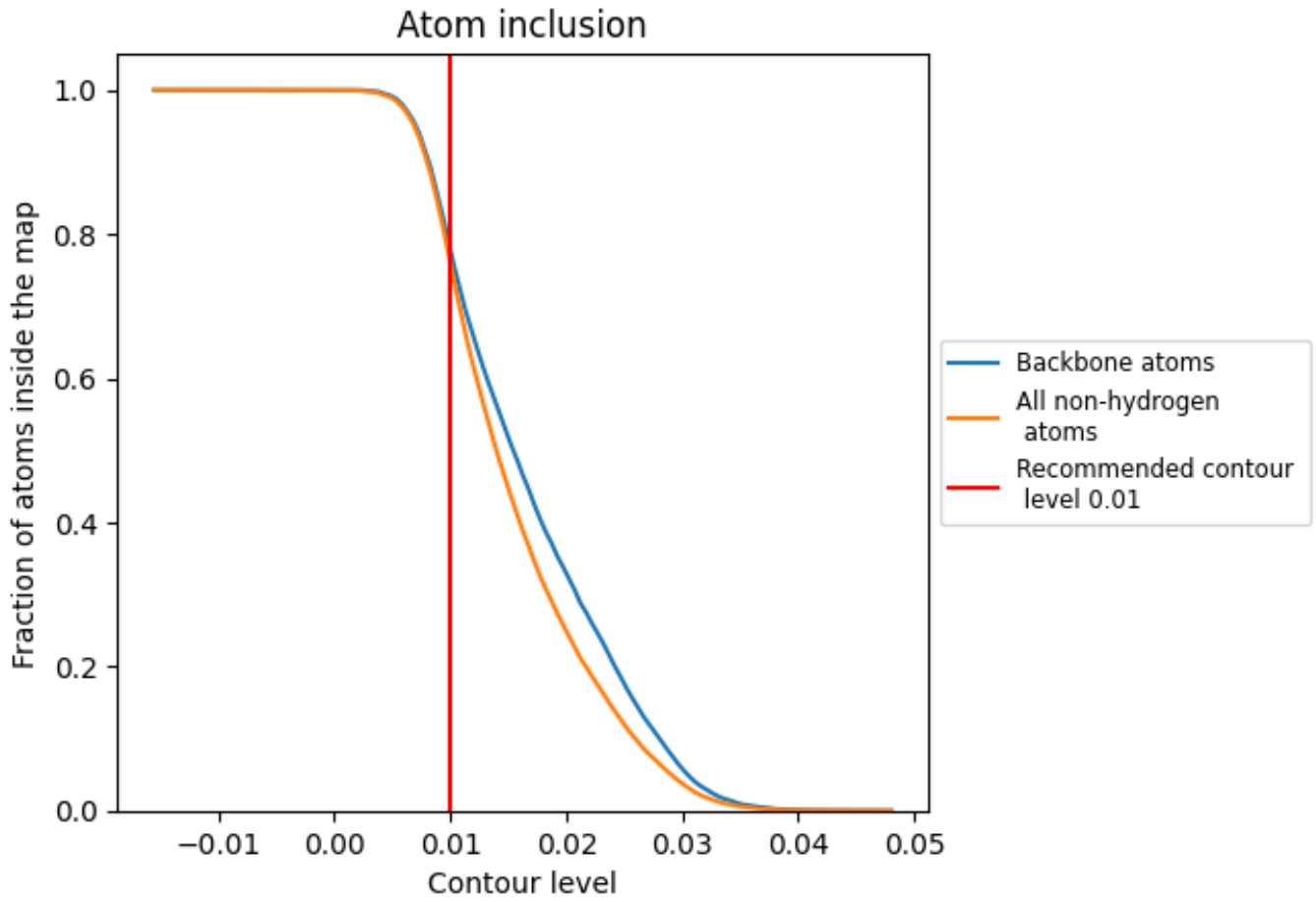
## 9.3 Atom inclusion mapped to coordinate model




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 (0.01).

## 9.4 Atom inclusion (i)




At the recommended contour level, 78% of all backbone atoms, 76% 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 (0.01) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7606 | 0.3300 |
| A | 0.7204 | 0.2870 |
| B | 0.7199 | 0.2870 |
| C | 0.8798 | 0.4390 |
| D | 0.8852 | 0.4460 |
| E | 0.6854 | 0.2780 |
| F | 0.6854 | 0.2780 |