# wwPDB EM Validation Summary Report (i)

May 11, 2024 – 11:43 pm BST

| | | |
|---|---|---|
| PDB ID | : | 6R8Z |
| EMDB ID | : | EMD-4763 |
| Title | : | Cryo-EM structure of NCP_THF2(-1)-UV-DDB |
| Authors | : | Matsumoto, S.; Cavadini, S.; Bunker, R.D.; Thoma, N.H. |
| Deposited on | : | 2019-04-02 |
| Resolution | : | 3.90 Å(reported) |
| Based on initial models | : | 4E54, 4ZUX, 5Y0C, 3EI4 |

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:

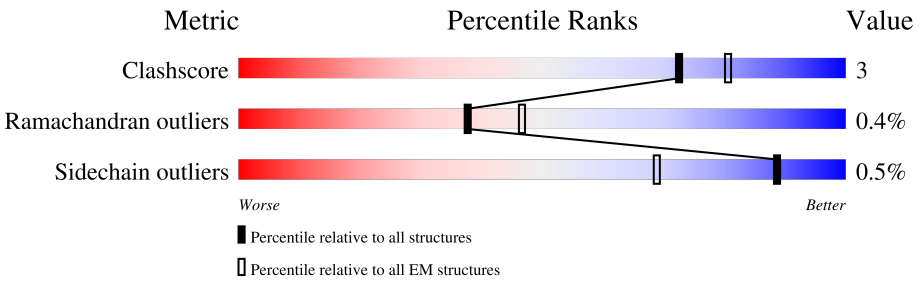
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev92 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.2 |

# 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 3.90 Å.

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




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

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 139 | 62% 11% 27% |
| 1 | E | 139 | 6% 64% 9% 27% |
| 2 | B | 106 | 6% 72% 8% 19% |
| 2 | F | 106 | 74% 23% |
| 3 | C | 133 | 8% 81% 7% 12% |
| 3 | G | 133 | 8% 81% 6% 12% |
| 4 | D | 129 | 68% 7% 25% |
| 4 | H | 129 | 65% 10% 25% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 5 | I | 145 | 87% 12% |
| 6 | J | 145 | 88% 12% |
| 7 | K | 1163 | 31% 62% 9% 29% |
| 8 | L | 431 | 7% 74% 8% 16% |

# 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 40831 atoms, of which 19214 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 Histone H3.1.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 1 | A | 101 | 1708 | 525 | 876 | 161 | 142 | 4 | 0 | 0 |
| 1 | E | 101 | 1708 | 525 | 876 | 161 | 142 | 4 | 0 | 0 |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | -2 | GLY | - | expression tag | UNP P68431 |
| A | -1 | SER | - | expression tag | UNP P68431 |
| A | 0 | HIS | - | expression tag | UNP P68431 |
| E | -2 | GLY | - | expression tag | UNP P68431 |
| E | -1 | SER | - | expression tag | UNP P68431 |
| E | 0 | HIS | - | expression tag | UNP P68431 |

- Molecule 2 is a protein called Histone H4.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 2 | B | 86 | 1434 | 436 | 740 | 140 | 117 | 1 | 0 | 0 |
| 2 | F | 82 | 1348 | 412 | 695 | 127 | 113 | 1 | 0 | 0 |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | -2 | GLY | - | expression tag | UNP P62805 |
| B | -1 | SER | - | expression tag | UNP P62805 |
| B | 0 | HIS | - | expression tag | UNP P62805 |
| F | -2 | GLY | - | expression tag | UNP P62805 |
| F | -1 | SER | - | expression tag | UNP P62805 |
| F | 0 | HIS | - | expression tag | UNP P62805 |

- Molecule 3 is a protein called Histone H2A type 1-B/E.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | | |
| 3 | C | 117 | 1878 | 571 | 969 | 181 | 157 | 0 | 0 |
| 3 | G | 117 | 1878 | 571 | 969 | 181 | 157 | 0 | 0 |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| C | -2 | GLY | - | expression tag | UNP P04908 |
| C | -1 | SER | - | expression tag | UNP P04908 |
| C | 0 | HIS | - | expression tag | UNP P04908 |
| G | -2 | GLY | - | expression tag | UNP P04908 |
| G | -1 | SER | - | expression tag | UNP P04908 |
| G | 0 | HIS | - | expression tag | UNP P04908 |

- Molecule 4 is a protein called Histone H2B type 1-J.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 4 | D | 97 | 1559 | 480 | 793 | 142 | 142 | 2 | 0 | 0 |
| 4 | H | 97 | 1560 | 480 | 794 | 142 | 142 | 2 | 0 | 0 |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | -2 | GLY | - | expression tag | UNP P06899 |
| D | -1 | SER | - | expression tag | UNP P06899 |
| D | 0 | HIS | - | expression tag | UNP P06899 |
| H | -2 | GLY | - | expression tag | UNP P06899 |
| H | -1 | SER | - | expression tag | UNP P06899 |
| H | 0 | HIS | - | expression tag | UNP P06899 |

- Molecule 5 is a DNA chain called Human alpha-satellite DNA (145-MER).

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | P | | |
| 5 | I | 145 | 4611 | 1421 | 1641 | 535 | 870 | 144 | 0 | 0 |

- Molecule 6 is a DNA chain called Human alpha-satellite DNA (145-MER) with abasic sites at positions 97-98.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | P | | |
| 6 | J | 145 | 4581 | 1410 | 1632 | 532 | 863 | 144 | 0 | 0 |

- Molecule 7 is a protein called DNA damage-binding protein 1.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 7 | K | 825 | 12900 | 4100 | 6422 | 1092 | 1250 | 36 | 0 | 0 |

There are 23 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| K | -22 | MET | - | initiating methionine | UNP Q16531 |
| K | -21 | ALA | - | expression tag | UNP Q16531 |
| K | -20 | SER | - | expression tag | UNP Q16531 |
| K | -19 | TRP | - | expression tag | UNP Q16531 |
| K | -18 | SER | - | expression tag | UNP Q16531 |
| K | -17 | HIS | - | expression tag | UNP Q16531 |
| K | -16 | PRO | - | expression tag | UNP Q16531 |
| K | -15 | GLN | - | expression tag | UNP Q16531 |
| K | -14 | PHE | - | expression tag | UNP Q16531 |
| K | -13 | GLU | - | expression tag | UNP Q16531 |
| K | -12 | LYS | - | expression tag | UNP Q16531 |
| K | -11 | VAL | - | expression tag | UNP Q16531 |
| K | -10 | ASP | - | expression tag | UNP Q16531 |
| K | -9 | GLU | - | expression tag | UNP Q16531 |
| K | -8 | ASN | - | expression tag | UNP Q16531 |
| K | -7 | LEU | - | expression tag | UNP Q16531 |
| K | -6 | TYR | - | expression tag | UNP Q16531 |
| K | -5 | PHE | - | expression tag | UNP Q16531 |
| K | -4 | GLN | - | expression tag | UNP Q16531 |
| K | -3 | GLY | - | expression tag | UNP Q16531 |
| K | -2 | GLY | - | expression tag | UNP Q16531 |
| K | -1 | GLY | - | expression tag | UNP Q16531 |
| K | 0 | ARG | - | expression tag | UNP Q16531 |

- Molecule 8 is a protein called DNA damage-binding protein 2.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 8 | L | 361 | 5666 | 1815 | 2807 | 515 | 513 | 16 | 0 | 0 |

There are 4 discrepancies between the modelled and reference sequences:

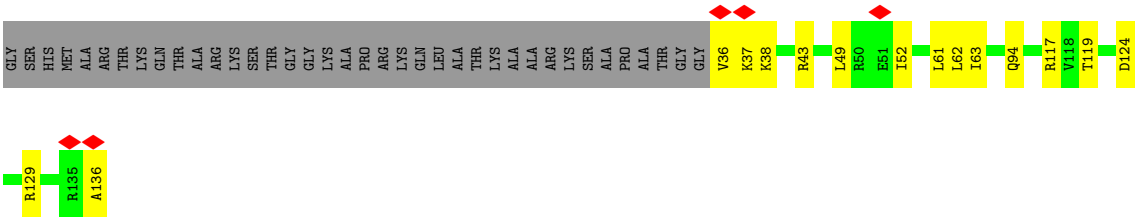
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| L | -3 | GLY | - | expression tag | UNP Q92466 |
| L | -2 | GLY | - | expression tag | UNP Q92466 |
| L | -1 | GLY | - | expression tag | UNP Q92466 |
| L | 0 | ARG | - | expression tag | UNP Q92466 |

# 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.

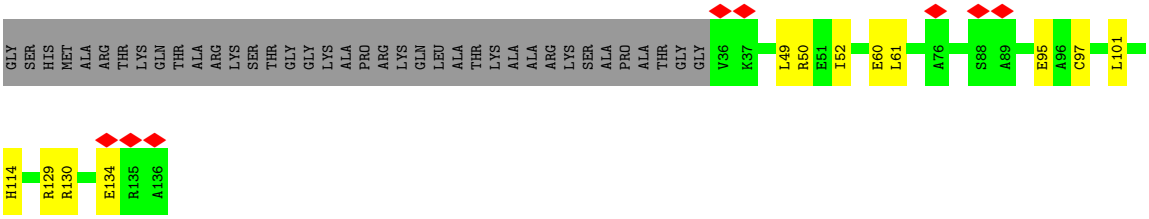
- Molecule 1: Histone H3.1

Chain A:



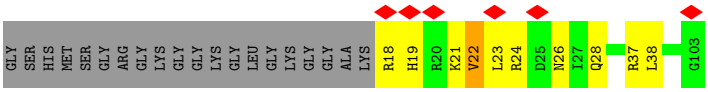

- Molecule 1: Histone H3.1

Chain E:



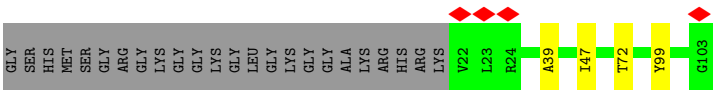

- Molecule 2: Histone H4

Chain B:



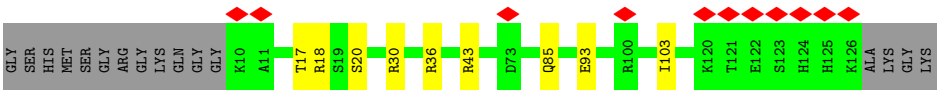

- Molecule 2: Histone H4

Chain F:



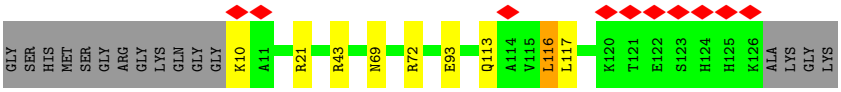

- Molecule 3: Histone H2A type 1-B/E

Chain C:



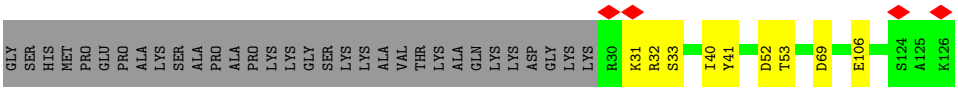

• Molecule 3: Histone H2A type 1-B/E

Chain G:



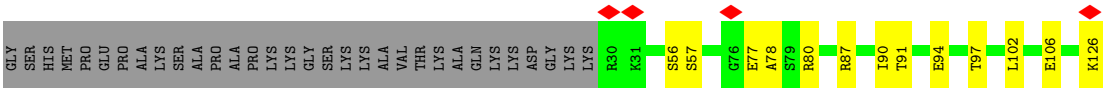

• Molecule 4: Histone H2B type 1-J

Chain D:



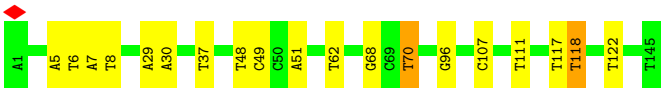

• Molecule 4: Histone H2B type 1-J

Chain H:



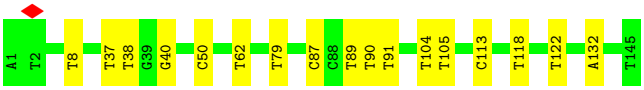

• Molecule 5: Human alpha-satellite DNA (145-MER)

Chain I:



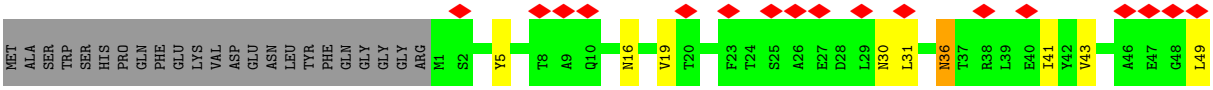

• Molecule 6: Human alpha-satellite DNA (145-MER) with abasic sites at positions 97-98

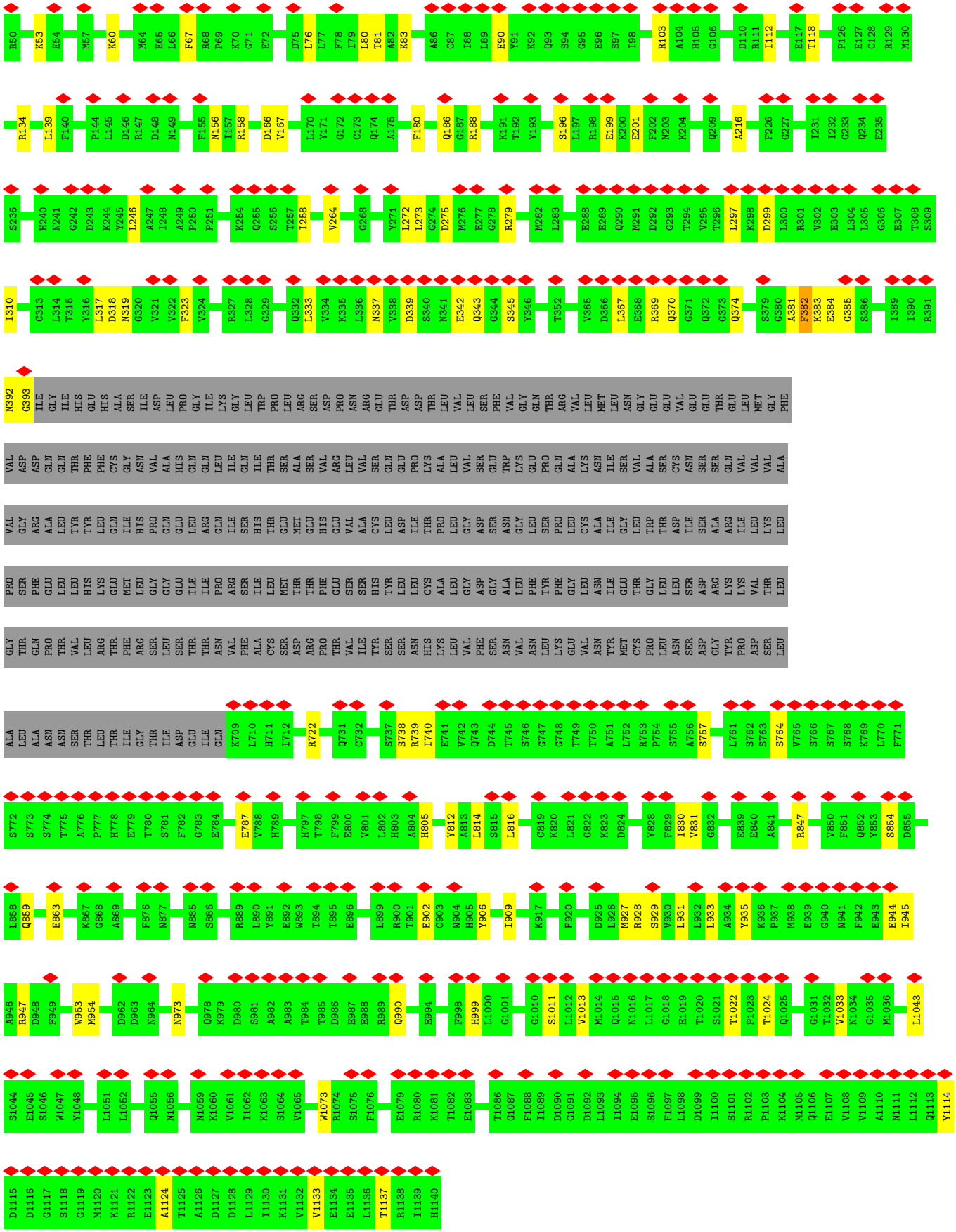
Chain J:




• Molecule 7: DNA damage-binding protein 1

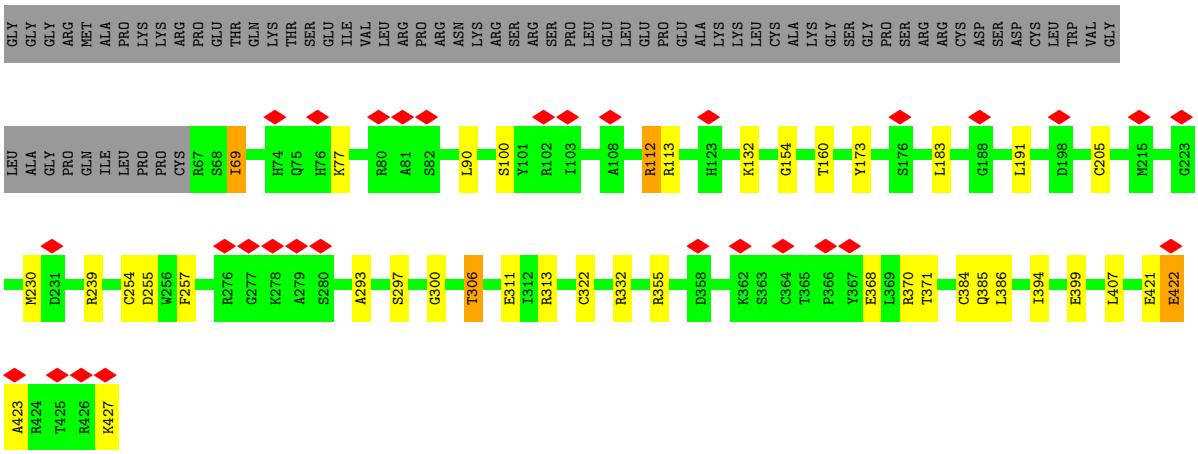
Chain K:




R50 K53 E54 M57 K60 M64 E65 L66 F67 R68 P69 K70 G71 E72 D75 L76 L77 F78 I79 L80 T81 A82 K83 A86 C87 I88 L89 E90 Y91 K92 Q93 S94 G95 E96 S97 I98 R103 A104 H105 G106 D110 R111 I112 E117 T118 P126 E127 C128 R129 M130
R134 L139 F140 P144 L145 D146 R147 D148 N149 F155 N156 I157 R158 D166 V167 L170 Y171 G172 G173 Q174 A175 F180 Q186 G187 R188 K191 T192 Y193 S196 L197 R198 E199 K200 E201 F202 N203 K204 Q209 A216 F226 G227 I231 I232 G233 Q234 E235
S236 H240 N241 G242 D243 K244 Y245 L246 A247 I248 A249 P250 P251 K254 Q255 S256 T257 I258 V264 G268 Y271 L272 L273 G274 D275 M276 E277 G278 R279 M282 L283 E288 E289 Q290 M291 D292 G293 T294 V295 T296 L297 K298 D299 L300 R301 V302 E303 L304 L305 G306 E307 T308 S309
I310 C313 L314 T315 Y316 L317 D318 N319 G320 V321 V322 F323 V324 R327 L328 G329 Q332 L333 V334 K335 L336 N337 V338 D339 S340 N341 E342 Q343 G344 S345 Y346 T352 V365 D366 L367 E368 R369 Q370 G371 Q372 G373 Q374 S379 G380 A381 F382 K383 E384 G385 S386 I389 I390 R391
N392 G393 ILE GLY ILE HIS GLU HIS ALA SER ILE ASP LEU PRO GLY ILE LYS GLY LEU TRP PRO LEU ARG SER ASP PRO ASN ARG GLU THR ASP ASP THR LEU VAL LEU SER PHE VAL GLY GLN THR ARG VAL LEU MET LEU ASN GLY GLU GLU VAL GLU GLU THR GLU LEU VAL PHE
VAL ASP ASP GLN GLN THR PHE PHE CYS GLY ASN VAL ALA HIS GLN GLN LEU ILE GLN ILE THR SER ALA SER VAL ARG LEU VAL SER GLN GLU PRO LYS ALA LEU VAL SER GLU TRP LYS GLU PRO GLN ALA LYS ASN ILE SER VAL ALA SER CYS ASN SER SER GLN VAL VAL VAL ALA
VAL GLY ARG ALA LEU TYR TYR LEU GLN ILE HIS PRO GLN GLU LEU ARG GLN ILE SER HIS THR GLU MET GLU HIS GLU VAL ALA CYS LEU ASP ILE THR PRO LEU GLY ASP SER ASN GLY LEU SER PRO LEU CYS ALA ILE GLY LEU TRP THR ASP ILE SER ALA ARG ILE LEU LYS LEU
PRO SER PHE GLU LEU LEU HIS LYS GLU MET LEU GLY GLY GLU ILE ILE PRO ARG SER ILE LEU MET THR THR PHE GLU SER SER HIS TYR LEU LEU CYS ALA LEU GLY ASP GLY ALA LEU PHE TYR PHE GLY LEU ASN ILE GLU THR GLY LEU LEU SER ASP ARG LYS LYS VAL THR LEU
GLY THR GLN PRO THR VAL LEU ARG THR PHE ARG SER LEU SER THR THR ASN VAL PHE ALA CYS SER ASP ARG PRO THR VAL ILE TYR SER SER ASN HIS LYS LEU VAL PHE SER ASN VAL ASN LEU LYS GLU VAL ASN TYR MET CYS PRO LEU ASN SER ASP GLY TYR PRO ASP SER LEU
ALA LEU ALA ASN ASN SER THR LEU THR ILE GLY THR ILE ASP GLU ILE GLN K709 L710 H711 I712 R722 Q731 C732 S737 S738 R739 I740 E741 V742 Q743 D744 T745 S746 G747 G748 T749 T750 A751 L752 R753 P754 S755 A756 S757 L761 S762 S763 S764 V765 S766 S767 S768 K769 L770 F771
S772 S773 S774 T775 A776 P777 H778 E779 T780 S781 F782 G783 E784 E787 V788 H789 H797 T798 F799 E800 V801 L802 H803 A804 H805 Y812 A813 L814 S815 L816 C819 K820 L821 G822 K823 D824 Y828 F829 I830 V831 G832 E839 E840 A841 R847 V850 F851 Q852 Y853 S854 D855
L858 Q859 E863 K867 G868 A869 F876 N877 N885 S886 R889 L890 Y891 E892 W893 T894 T895 E896 L899 R900 T901 E902 C903 N904 H905 Y906 I909 K917 F920 D925 L926 M927 R928 S929 V930 L931 L932 L933 A934 Y935 K936 P937 M938 E939 G940 N941 F942 E943 E944 I945
A946 R947 D948 F949 W953 N954 D962 D963 N964 N973 Q978 K979 D980 S981 A982 A983 T984 T985 D986 E987 E988 R989 Q990 E994 F998 H999 L1000 G1001 G1010 S1011 L1012 V1013 M1014 Q1015 N1016 L1017 G1018 E1019 T1020 S1021 T1022 P1023 T1024 Q1025 G1031 T1032 V1033 N1034 G1035 M1036 L1043
S1044 E1045 S1046 W1047 Y1048 L1051 L1052 Q1055 N1056 N1059 K1060 V1061 I1062 K1063 S1064 V1065 W1073 R1074 S1075 F1076 E1079 R1080 K1081 T1082 E1083 T1086 G1087 F1088 I1089 D1090 G1091 D1092 L1093 I1094 E1095 S1096 F1097 L1098 D1099 I1100 S1101 R1102 P1103 K1104 M1105 Q1106 E1107 V1108 V1109 A1110 N1111 L1112 Q1113 Y1114
D1115 D1116 G1117 S1118 G1119 M1120 K1121 R1122 E1123 A1124 T1125 A1126 D1127 D1128 L1129 I1130 K1131 V1132 V1133 E1134 E1135 L1136 T1137 R1138 I1139 H1140

• Molecule 8: DNA damage-binding protein 2

Chain L:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 129986 | 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 ($e^-/Å^2$) | 40.0 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | 130000 | Depositor |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 47.031 | Depositor |
| Minimum map value | -16.739 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 1.000 | Depositor |
| Recommended contour level | 4.5 | Depositor |
| Map size (Å) | 308.0, 308.0, 308.0 | wwPDB |
| Map dimensions | 280, 280, 280 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.1, 1.1, 1.1 | 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: 3DR

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 | 0.69 | 0/844 | 0.69 | 0/1130 |
| 1 | E | 0.68 | 0/844 | 0.71 | 0/1130 |
| 2 | B | 0.83 | 0/702 | 0.76 | 0/937 |
| 2 | F | 0.78 | 0/660 | 0.71 | 0/883 |
| 3 | C | 0.64 | 0/921 | 0.68 | 0/1239 |
| 3 | G | 0.65 | 0/921 | 0.74 | 2/1239 (0.2%) |
| 4 | D | 0.76 | 0/777 | 0.67 | 0/1040 |
| 4 | H | 0.74 | 1/777 (0.1%) | 0.64 | 0/1040 |
| 5 | I | 1.13 | 1/3331 (0.0%) | 1.15 | 5/5140 (0.1%) |
| 6 | J | 1.14 | 1/3283 (0.0%) | 1.14 | 15/5062 (0.3%) |
| 7 | K | 0.35 | 0/6595 | 0.59 | 0/8919 |
| 8 | L | 0.55 | 0/2938 | 0.68 | 1/3987 (0.0%) |
| All | All | 0.77 | 3/22593 (0.0%) | 0.84 | 23/31746 (0.1%) |

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 |
|---|---|---|---|
| 2 | B | 0 | 2 |
| 7 | K | 0 | 2 |
| All | All | 0 | 4 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | H | 102 | LEU | C-N | -7.38 | 1.17 | 1.34 |
| 6 | J | 132 | DA | N7-C5 | -5.11 | 1.36 | 1.39 |
| 5 | I | 118 | DT | C5-C7 | -5.06 | 1.47 | 1.50 |

The worst 5 of 23 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | J | 79 | DT | O4'-C1'-N1 | 6.43 | 112.50 | 108.00 |
| 6 | J | 87 | DC | O4'-C4'-C3' | -6.29 | 101.98 | 104.50 |
| 3 | G | 117 | LEU | CA-CB-CG | 5.87 | 128.81 | 115.30 |
| 6 | J | 91 | DT | N3-C4-O4 | 5.47 | 123.18 | 119.90 |
| 6 | J | 90 | DT | N3-C4-O4 | 5.44 | 123.17 | 119.90 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | B | 21 | LYS | Peptide |
| 2 | B | 23 | LEU | Peptide |
| 7 | K | 382 | PHE | Mainchain |
| 7 | K | 928 | ARG | Peptide |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 832 | 876 | 878 | 10 | 0 |
| 1 | E | 832 | 876 | 878 | 9 | 0 |
| 2 | B | 694 | 740 | 742 | 6 | 0 |
| 2 | F | 653 | 695 | 696 | 3 | 0 |
| 3 | C | 909 | 969 | 973 | 7 | 0 |
| 3 | G | 909 | 969 | 973 | 5 | 0 |
| 4 | D | 766 | 793 | 797 | 5 | 0 |
| 4 | H | 766 | 794 | 796 | 10 | 0 |
| 5 | I | 2970 | 1641 | 1641 | 13 | 0 |
| 6 | J | 2949 | 1632 | 1632 | 4 | 0 |
| 7 | K | 6478 | 6422 | 6445 | 64 | 0 |
| 8 | L | 2859 | 2807 | 2822 | 23 | 0 |
| All | All | 21617 | 19214 | 19273 | 137 | 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.

The worst 5 of 137 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) |
|---|---|---|---|
| 4:H:78:ALA:HB1 | 4:H:90:ILE:HD11 | 1.59 | 0.85 |
| 5:I:51:DA:OP1 | 8:L:332:ARG:NH2 | 2.17 | 0.77 |
| 7:K:929:SER:OG | 7:K:954:MET:SD | 2.45 | 0.74 |
| 3:C:43:ARG:NH2 | 5:I:37:DT:O3' | 2.20 | 0.74 |
| 4:D:106:GLU:N | 4:D:106:GLU:OE1 | 2.24 | 0.70 |

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 | 99/139 (71%) | 97 (98%) | 2 (2%) | 0 | 100 | 100 |
| 1 | E | 99/139 (71%) | 98 (99%) | 1 (1%) | 0 | 100 | 100 |
| 2 | B | 84/106 (79%) | 76 (90%) | 7 (8%) | 1 (1%) | 13 | 49 |
| 2 | F | 80/106 (76%) | 78 (98%) | 2 (2%) | 0 | 100 | 100 |
| 3 | C | 115/133 (86%) | 111 (96%) | 4 (4%) | 0 | 100 | 100 |
| 3 | G | 115/133 (86%) | 109 (95%) | 6 (5%) | 0 | 100 | 100 |
| 4 | D | 95/129 (74%) | 90 (95%) | 5 (5%) | 0 | 100 | 100 |
| 4 | H | 95/129 (74%) | 90 (95%) | 5 (5%) | 0 | 100 | 100 |
| 7 | K | 821/1163 (71%) | 802 (98%) | 16 (2%) | 3 (0%) | 34 | 71 |
| 8 | L | 359/431 (83%) | 313 (87%) | 43 (12%) | 3 (1%) | 19 | 57 |
| All | All | 1962/2608 (75%) | 1864 (95%) | 91 (5%) | 7 (0%) | 38 | 71 |

5 of 7 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | K | 382 | PHE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | L | 69 | ILE |
| 8 | L | 112 | ARG |
| 7 | K | 36 | ASN |
| 7 | K | 383 | LYS |

### 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 | 88/113 (78%) | 87 (99%) | 1 (1%) | 73 | 84 |
| 1 | E | 88/113 (78%) | 87 (99%) | 1 (1%) | 73 | 84 |
| 2 | B | 71/81 (88%) | 71 (100%) | 0 | 100 | 100 |
| 2 | F | 67/81 (83%) | 67 (100%) | 0 | 100 | 100 |
| 3 | C | 93/102 (91%) | 93 (100%) | 0 | 100 | 100 |
| 3 | G | 93/102 (91%) | 92 (99%) | 1 (1%) | 73 | 84 |
| 4 | D | 83/107 (78%) | 82 (99%) | 1 (1%) | 71 | 83 |
| 4 | H | 83/107 (78%) | 83 (100%) | 0 | 100 | 100 |
| 7 | K | 720/1018 (71%) | 720 (100%) | 0 | 100 | 100 |
| 8 | L | 313/372 (84%) | 309 (99%) | 4 (1%) | 69 | 82 |
| All | All | 1699/2196 (77%) | 1691 (100%) | 8 (0%) | 89 | 93 |

5 of 8 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | L | 427 | LYS |
| 8 | L | 422 | GLU |
| 8 | L | 306 | THR |
| 3 | G | 10 | LYS |
| 8 | L | 421 | GLU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | K | 1059 | ASN |
| 8 | L | 345 | HIS |
| 7 | K | 93 | GLN |
| 7 | K | 319 | ASN |
| 7 | K | 859 | 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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 6 | 3DR | J | 95 | 6 | 8,11,12 | 0.50 | 0 | 9,14,17 | 0.82 | 0 |
| 6 | 3DR | J | 96 | 6 | 8,11,12 | 0.37 | 0 | 9,14,17 | 0.69 | 0 |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 6 | 3DR | J | 95 | 6 | - | 3/3/15/16 | 0/1/1/1 |
| 6 | 3DR | J | 96 | 6 | - | 1/3/15/16 | 0/1/1/1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 6 | J | 95 | 3DR | O4'-C4'-C5'-O5' |
| 6 | J | 95 | 3DR | C3'-C4'-C5'-O5' |
| 6 | J | 96 | 3DR | C4'-C5'-O5'-P |
| 6 | J | 95 | 3DR | C4'-C5'-O5'-P |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 4 | H | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | H | 102:LEU | C | 103:LEU | N | 1.17 |

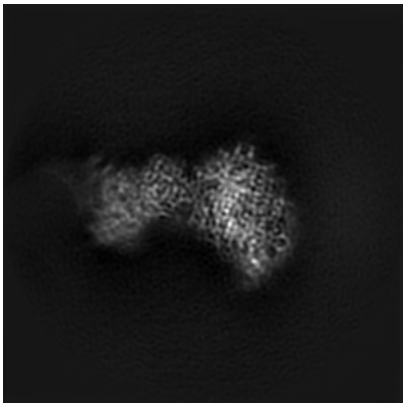
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4763. These allow visual inspection of the internal detail of the map and identification of artifacts.

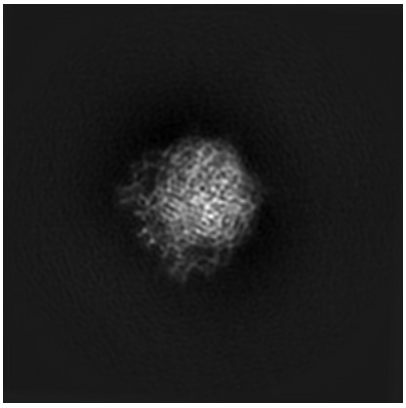
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

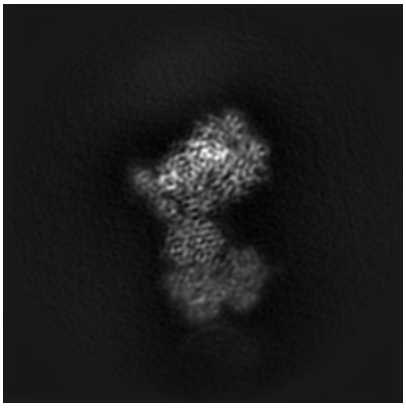
### 6.1.1 Primary map



X



Y

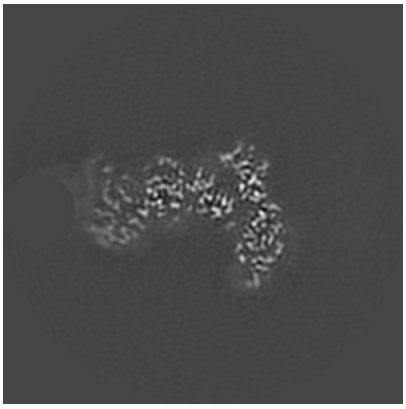


Z

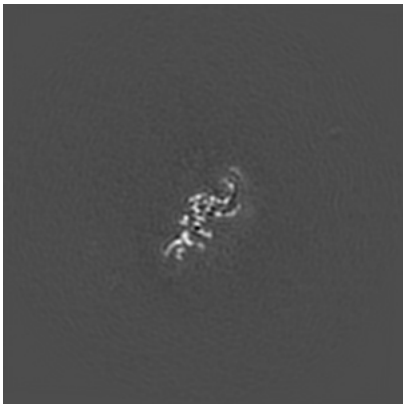
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

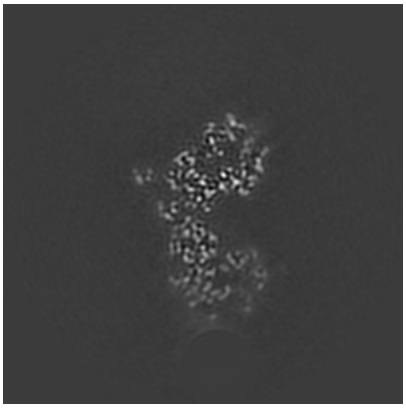
### 6.2.1 Primary map



X Index: 140



Y Index: 140

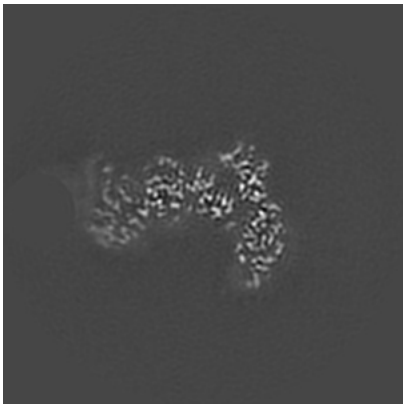


Z Index: 140

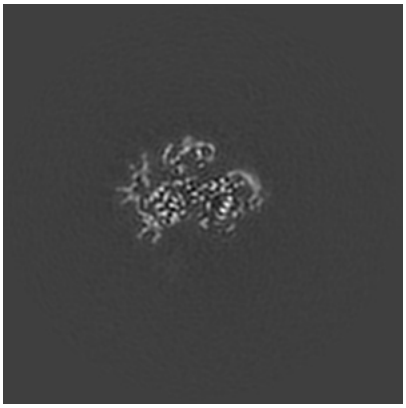
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

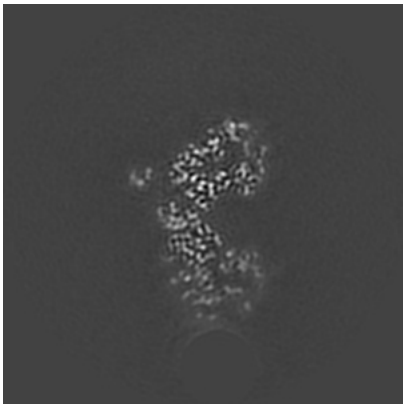
### 6.3.1 Primary map



X Index: 140



Y Index: 174

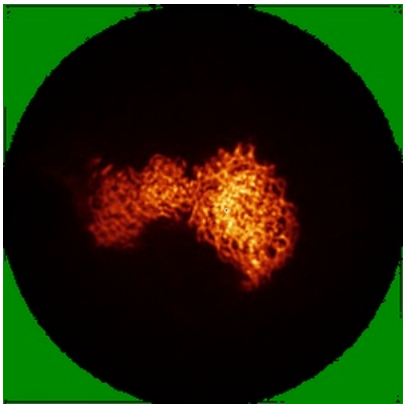


Z Index: 142

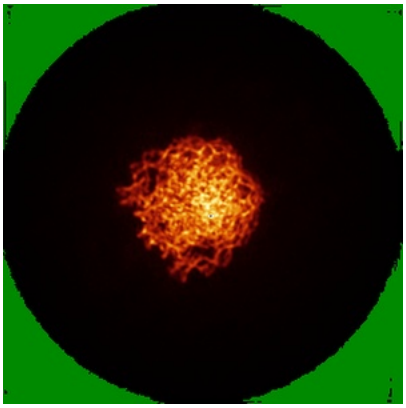
The images above show the largest variance slices of the map in three orthogonal directions.

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

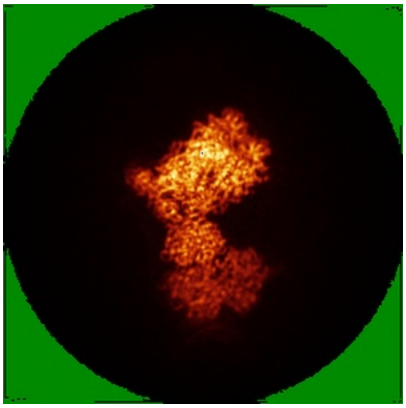
### 6.4.1 Primary map



X



Y

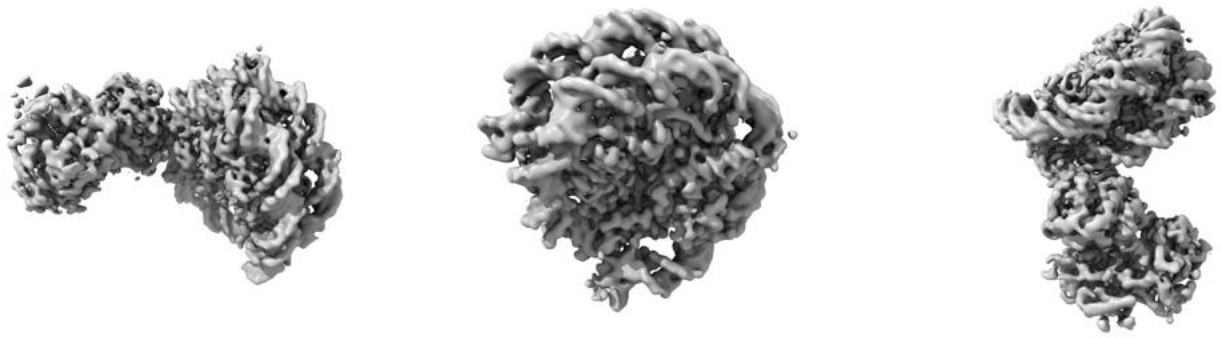


Z

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

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

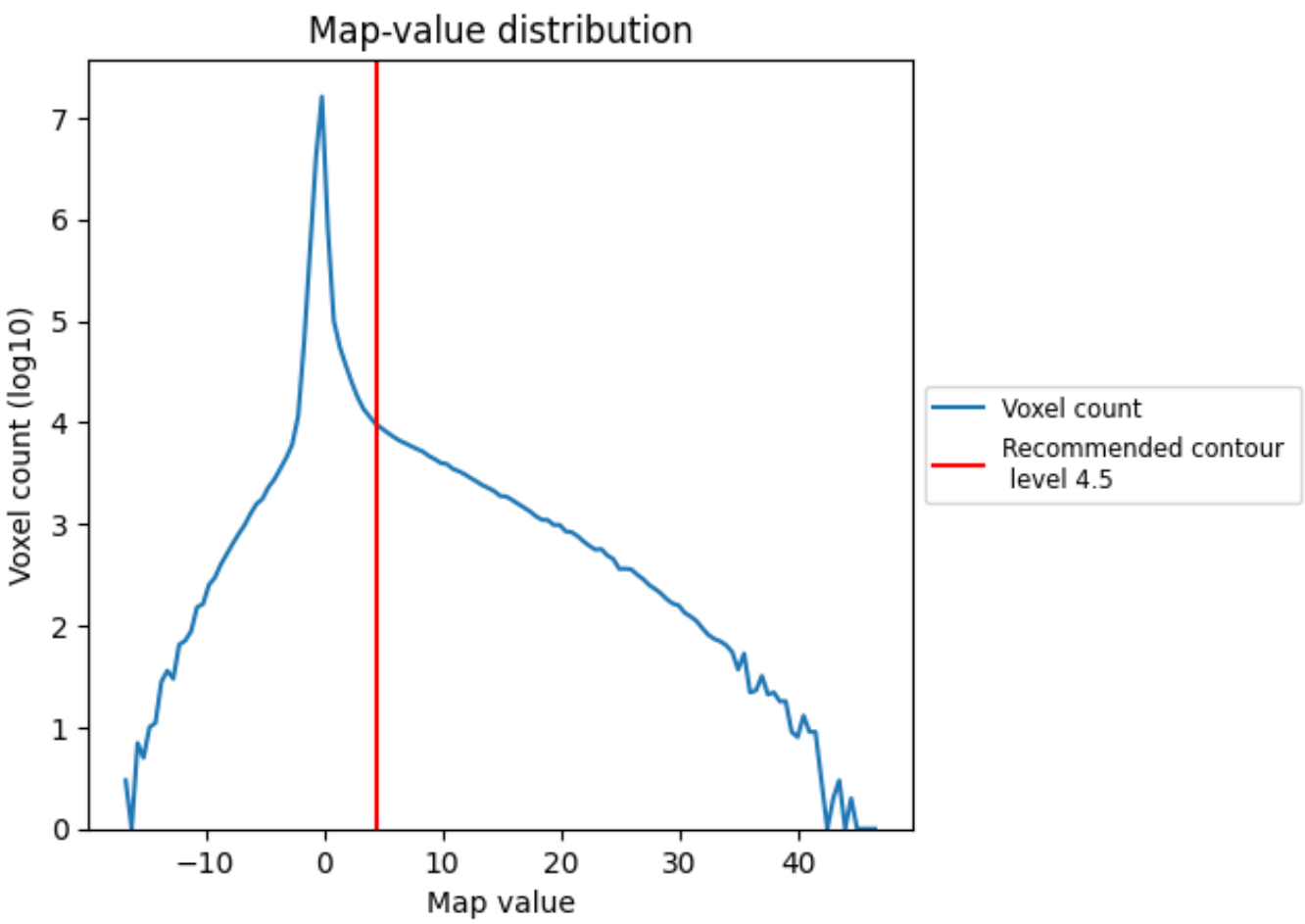
## 6.6 Mask visualisation (i)

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

# 7 Map analysis (i)

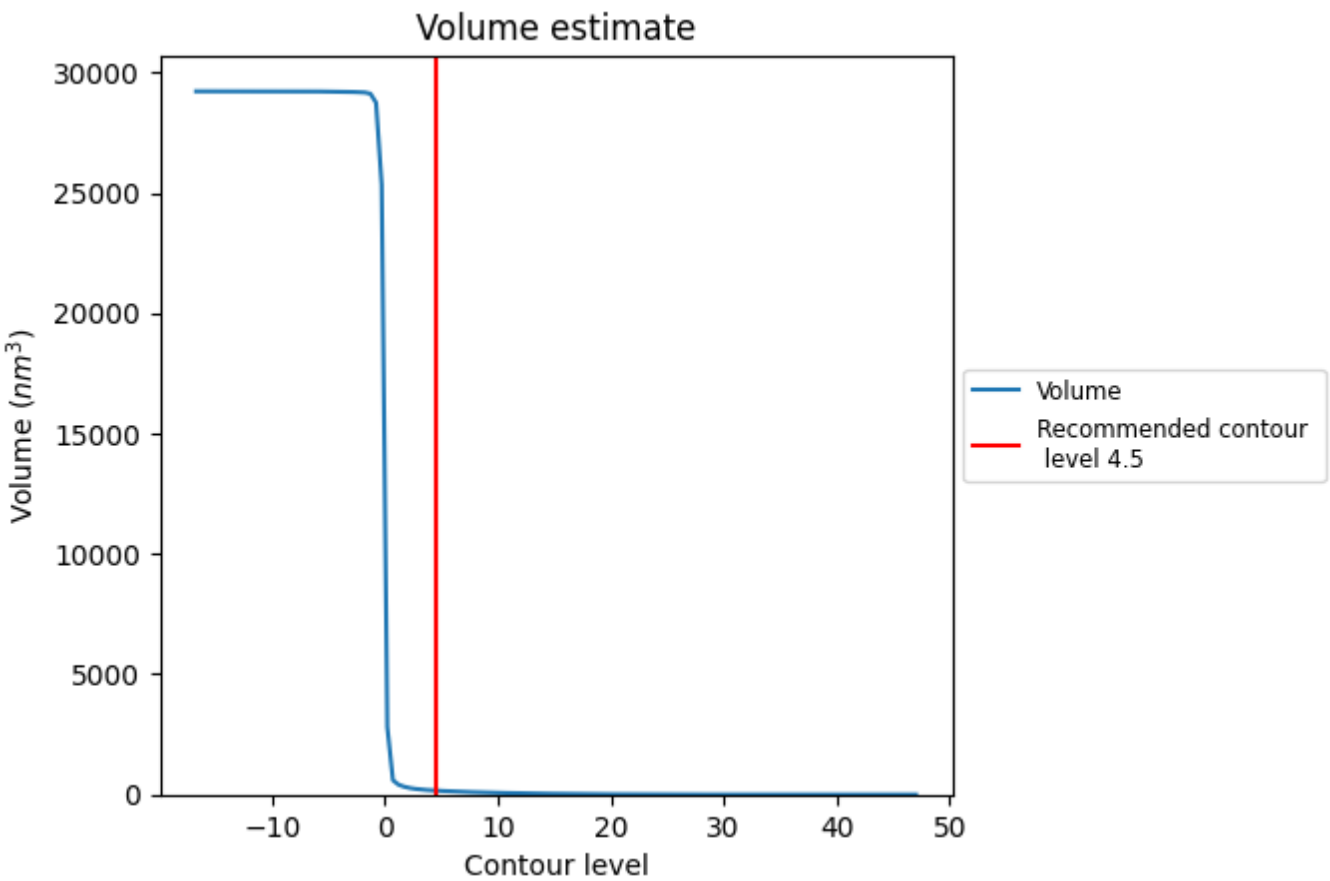
This section contains the results of statistical analysis of the map.

## 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.

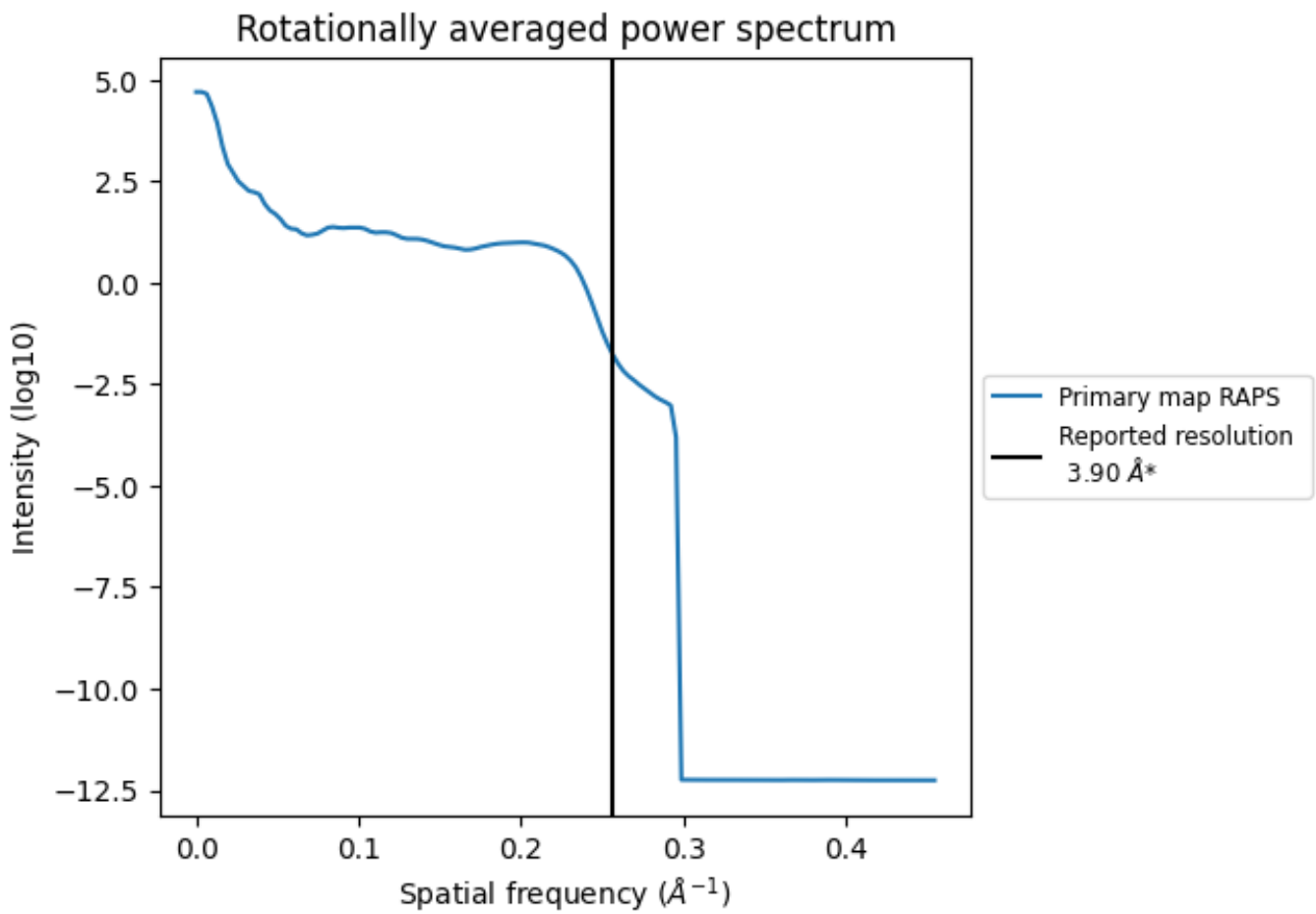
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 165 $nm^3$; this corresponds to an approximate mass of 149 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 0.256 Å$^{-1}$

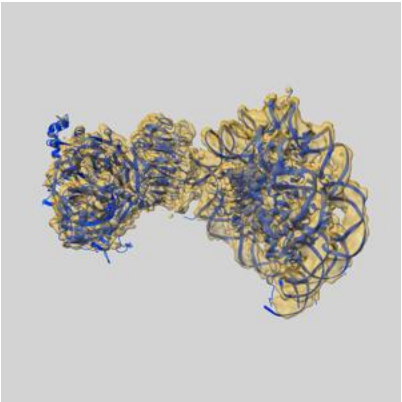
# 8 Fourier-Shell correlation (i)

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

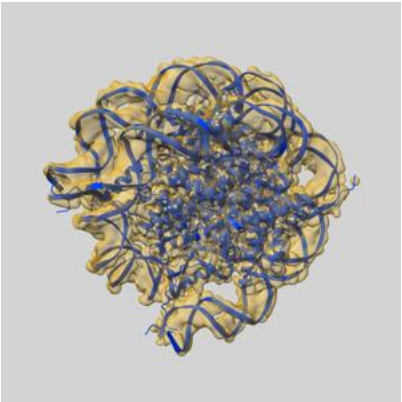
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4763 and PDB model 6R8Z. Per-residue inclusion information can be found in section 3 on page 8.

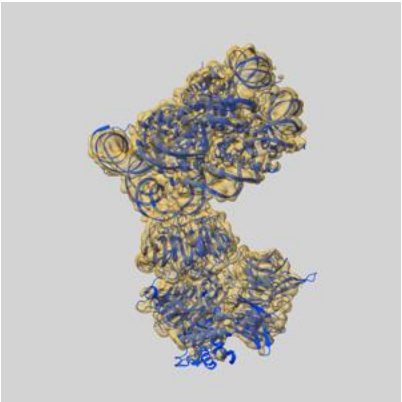
## 9.1 Map-model overlay (i)



X



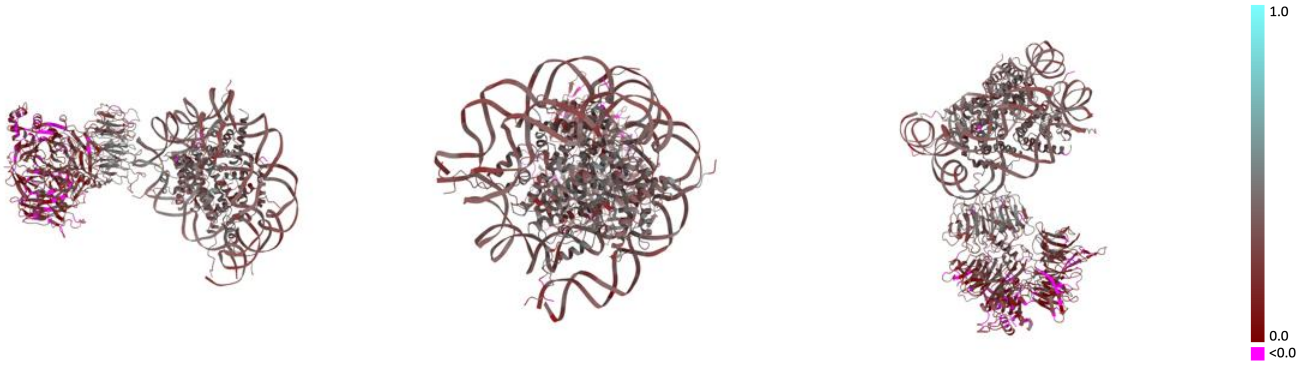
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.5 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.

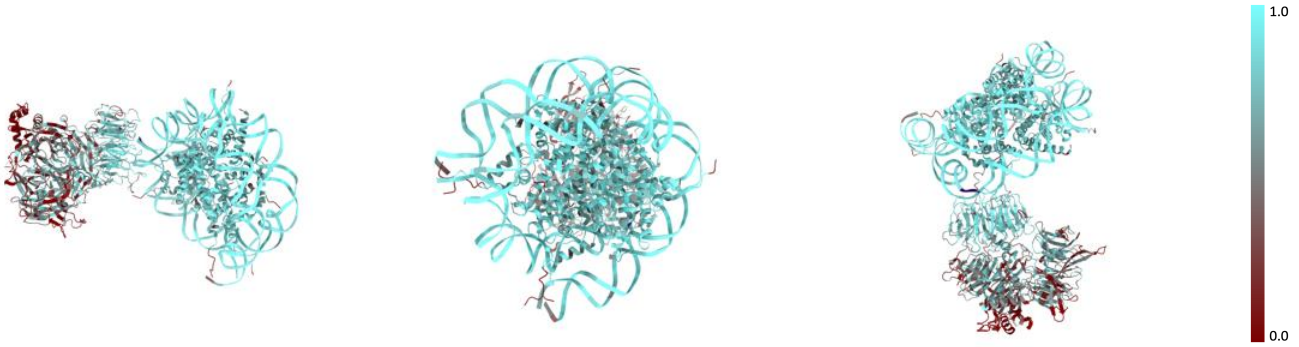
## 9.2 Q-score mapped to coordinate model (i)




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.

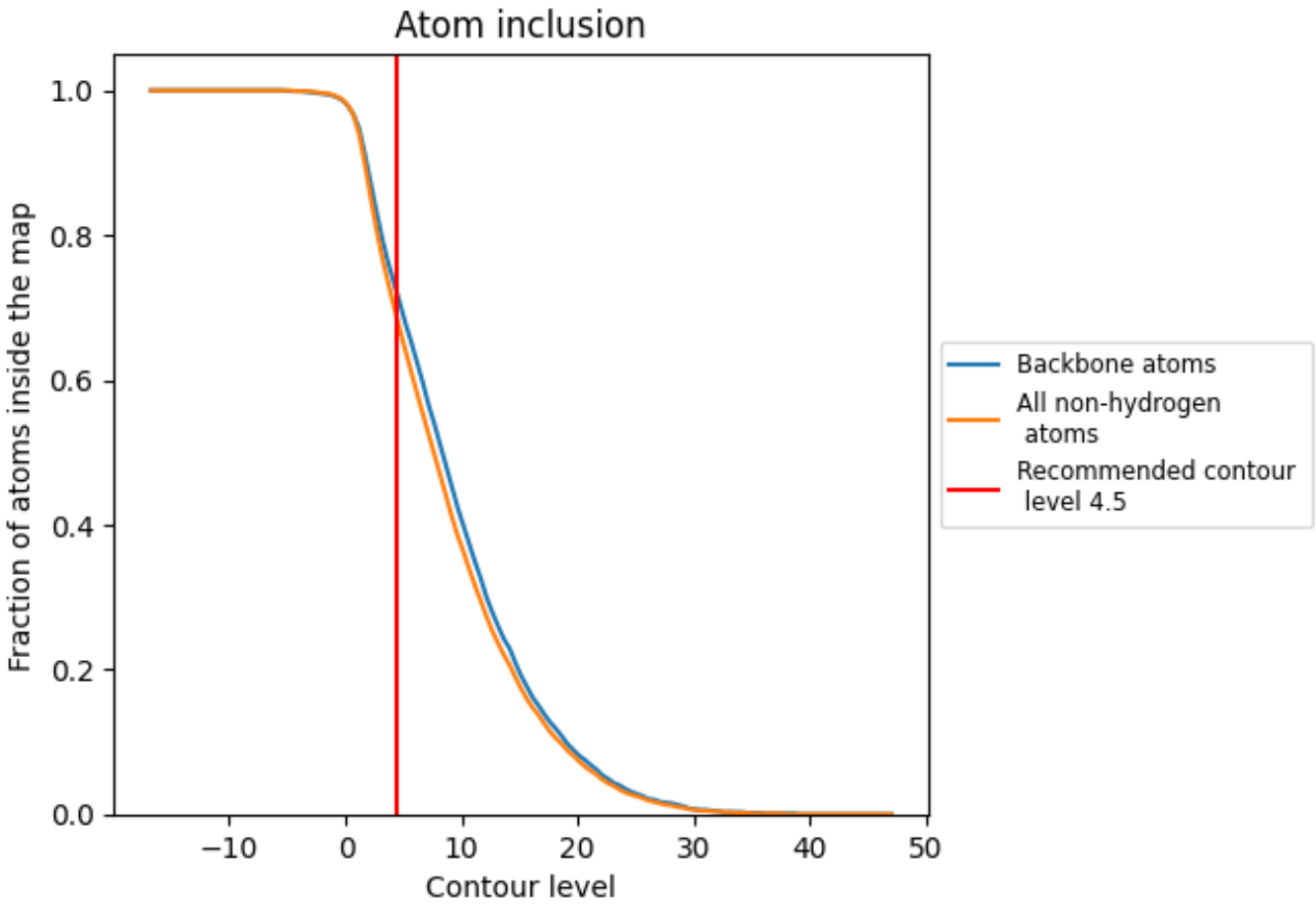
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (4.5).

## 9.4 Atom inclusion (i)




At the recommended contour level, 72% of all backbone atoms, 68% 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 (4.5) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.6820 | 0.3070 |
| A | 0.8110 | 0.3940 |
| B | 0.8090 | 0.3950 |
| C | 0.7630 | 0.3710 |
| D | 0.8090 | 0.3560 |
| E | 0.8050 | 0.3790 |
| F | 0.8280 | 0.3970 |
| G | 0.7820 | 0.3780 |
| H | 0.8050 | 0.3670 |
| I | 0.8820 | 0.3270 |
| J | 0.8870 | 0.3310 |
| K | 0.4280 | 0.1930 |
| L | 0.7470 | 0.3570 |