wwPDB EM Validation Summary Report

May 11, 2024 – 02:31 pm BST

PDB ID	:	6R9T
EMDB ID	:	EMD-4772
Title	:	Cryo-EM structure of autoinhibited human talin-1
Authors	:	Dedden, D.; Schumacher, S.; Zacharias, M.; Biertumpfel, C.; Mizuno, N.
Deposited on	:	2019-04-04
Resolution	:	6.20 Å(reported)
Based on initial models	:	2L7A, 2LQG, 2JSW, 2L10, 2L7N, 1SJ8, 2KVP, 5IC1, 3DYJ, 3IVF

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:

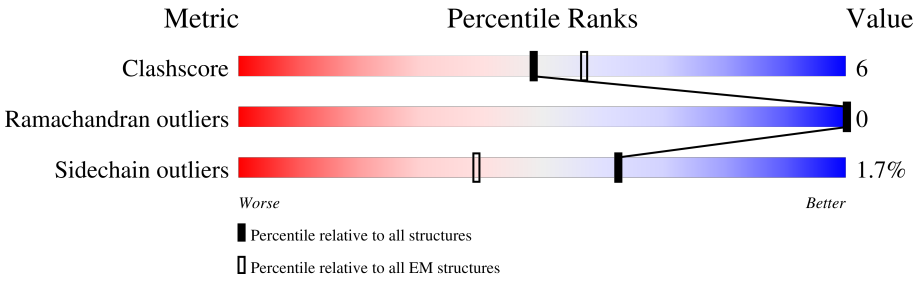
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 6.20 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	2547	16% 71% 14% 14%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 16011 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 Talin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2185	16011	9855	2859	3219	78	0	0

There are 6 discrepancies between the modelled and reference sequences:

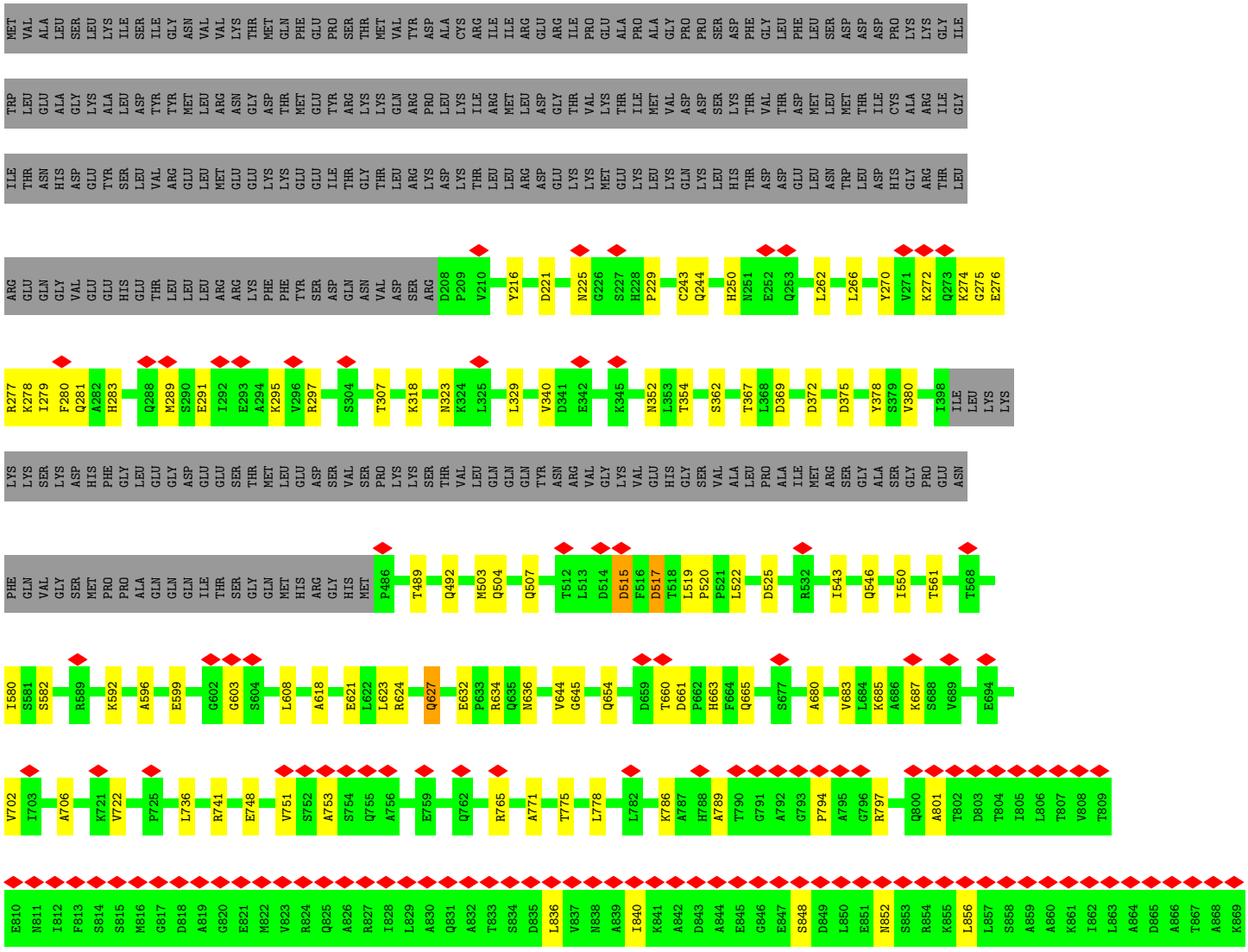
Chain	Residue	Modelled	Actual	Comment	Reference
A	2542	LEU	-	expression tag	UNP Q9Y490
A	2543	VAL	-	expression tag	UNP Q9Y490
A	2544	VAL	-	expression tag	UNP Q9Y490
A	2545	LEU	-	expression tag	UNP Q9Y490
A	2546	PHE	-	expression tag	UNP Q9Y490
A	2547	GLN	-	expression tag	UNP Q9Y490

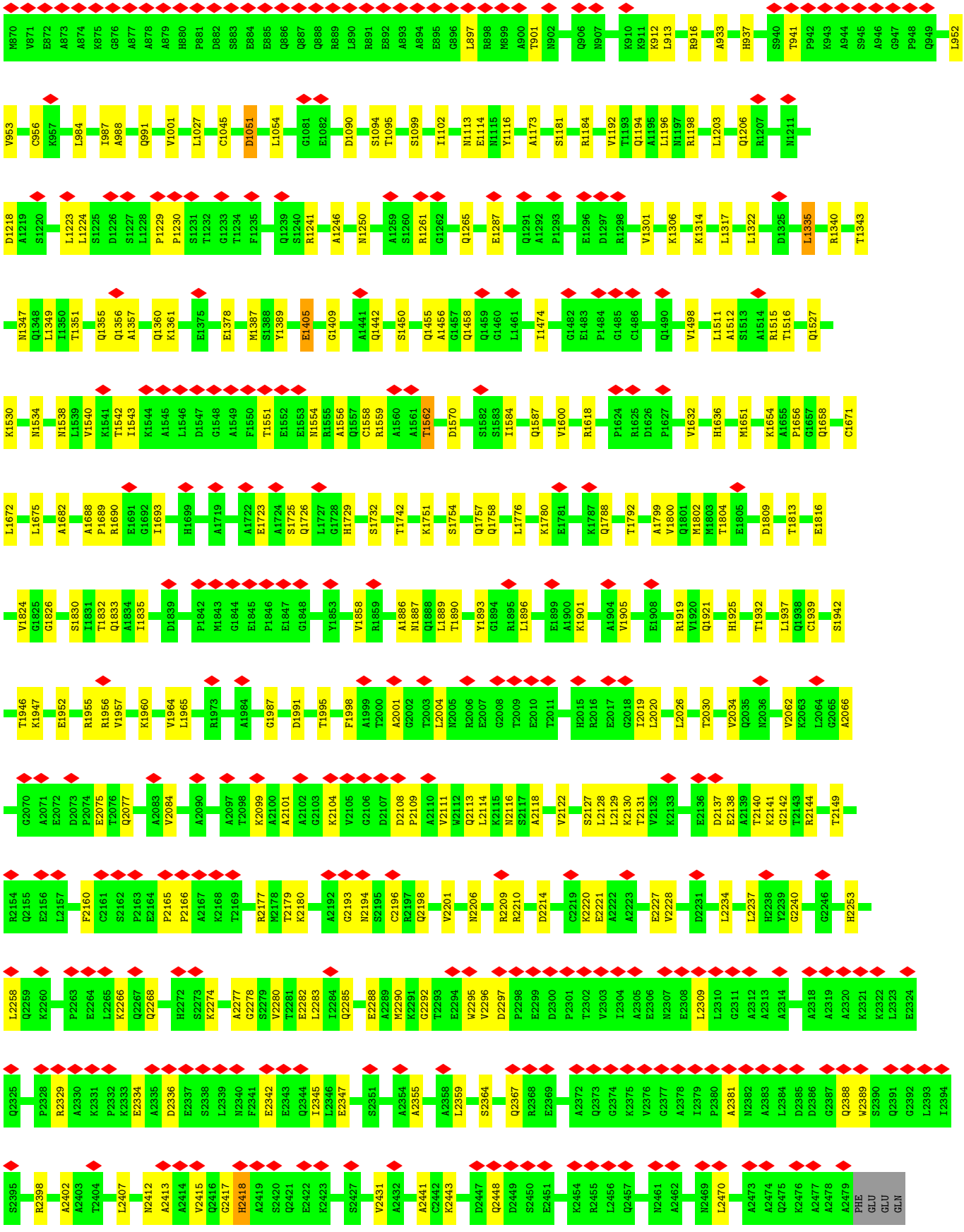
3 Residue-property plots (i)

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: Talin-1

Chain A:




M870 V871 E872 A873 A874 A875 G876 A877 A878 A879 H880 P881 D882 S883 E884 E885 Q886 Q887 Q888 R889 L890 R891 E892 A893 A894 E895 G896 L897 R898 M899 A900 T901 N902 Q906 N907 K910 K911 K912 L913 R916 A933 H937 S940 T941 P942 K943 A944 S945 A946 G947 P948 Q949 L952
V963 C956 K957 L984 I987 A988 Q991 V1001 L1027 C1045 D1051 L1054 G1081 E1082 D1090 S1094 T1095 S1099 I1102 N1113 E1114 N1115 Y1116 A1173 S1181 R1184 V1192 T1193 Q1194 A1195 L1196 N1197 R1198 L1203 Q1206 R1207 N1211
D1218 A1219 S1220 L1223 L1224 S1225 D1226 S1227 L1228 P1229 P1230 S1231 T1232 G1233 T1234 F1235 Q1239 S1240 R1241 A1246 N1250 A1259 S1260 R1261 G1262 Q1265 E1287 Q1291 A1292 P1293 E1296 D1297 R1298 V1301 K1306 K1314 L1317 L1322 D1325 L1335 R1340 T1343
N1347 Q1348 L1349 T1350 T1351 Q1355 Q1356 A1357 Q1360 K1361 E1375 E1378 M1387 S1388 Y1389 E1405 G1409 A1441 Q1442 S1450 Q1455 A1456 G1457 Q1458 Q1459 G1460 L1461 I1474 G1482 E1483 P1484 G1485 C1486 Q1490 V1498 L1511 A1512 S1513 A1514 R1515 T1516 Q1527
K1530 N1534 N1538 L1539 V1540 K1541 T1542 I1543 K1544 A1545 L1546 D1547 G1548 A1549 F1550 T1551 E1552 E1553 N1554 R1555 A1556 Q1557 C1558 R1559 A1560 A1561 T1562 D1570 S1582 S1583 I1584 Q1587 V1600 R1618 P1624 R1625 D1626 P1627 V1632 H1636 M1651 K1654 A1655 P1656 G1657 Q1658 C1671
L1672 L1675 A1682 A1688 P1689 R1690 E1691 G1692 I1693 H1699 A1719 A1722 E1723 A1724 S1725 Q1726 L1727 G1728 H1729 S1732 T1742 K1751 S1754 Q1757 Q1758 L1776 K1780 E1781 K1787 Q1788 T1792 A1799 V1800 Q1801 M1802 M1803 T1804 E1805 D1809 T1813 E1816
V1824 G1825 G1826 S1830 I1831 T1832 Q1833 A1834 I1835 D1839 P1842 M1843 G1844 E1845 P1846 E1847 G1848 Y1853 V1858 R1859 A1886 N1887 Q1888 L1889 T1890 Y1893 G1894 R1895 L1896 E1899 A1900 K1901 A1904 V1905 E1908 R1919 V1920 Q1921 H1925 T1932 L1937 Q1938 C1939 S1942
T1946 K1947 E1952 R1955 R1956 V1957 K1960 V1964 L1965 R1973 A1984 G1987 D1991 T1995 F1998 A1999 T2000 A2001 G2002 T2003 L2004 N2005 R2006 E2007 G2008 T2009 E2010 T2011 H2015 R2016 E2017 G2018 I2019 L2020 L2026 T2030 V2034 Q2035 N2036 V2062 K2063 L2064 G2065 A2066
G2070 A2071 E2072 D2073 P2074 E2075 T2076 Q2077 A2083 V2084 A2090 A2097 T2098 K2099 A2100 A2101 A2102 G2103 K2104 V2105 G2106 D2107 D2108 P2109 A2110 V2111 W2112 Q2113 L2114 K2115 N2116 S2117 A2118 V2122 S2127 L2128 L2129 K2130 T2131 V2132 K2133 E2136 D2137 E2138 A2139 T2140 K2141 G2142 T2143 R2144 T2149
R2154 Q2155 E2156 L2157 F2160 C2161 S2162 P2163 E2164 P2165 P2166 A2167 K2168 T2169 R2177 H2178 T2179 K2180 A2192 G2193 N2194 S2195 C2196 R2197 Q2198 V2201 N2206 R2209 R2210 D2214 C2219 K2220 E2221 A2222 A2223 E2227 V2228 D2231 L2234 L2237 H2238 Y2239 G2240 G2246 H2253
L2258 Q2259 K2260 P2263 E2264 L2265 K2266 Q2267 Q2268 H2272 S2273 K2274 A2277 G2278 S2279 V2280 T2281 E2282 L2283 T2284 Q2285 E2288 A2289 M2290 K2291 G2292 T2293 E2294 W2295 V2296 D2297 P2298 E2299 D2300 P2301 T2302 V2303 G2374 I2304 A2305 E2306 N2307 E2308 L2309 L2310 G2311 A2312 A2313 A2314 A2318 A2319 A2320 K2321 K2322 L2323 E2324
Q2325 P2328 R2329 A2330 K2331 P2332 K2333 E2334 A2335 D2336 E2337 S2338 L2339 N2340 F2341 E2342 E2343 Q2344 I2345 L2346 E2347 S2351 A2354 A2355 A2358 L2359 S2364 Q2367 R2368 E2369 A2372 Q2373 G2374 K2375 V2376 G2377 A2378 I2379 P2380 A2381 N2382 A2383 L2384 D2385 D2386 G2387 Q2388 W2389 S2390 Q2391 G2392 L2393 I2394
S2395 R2398 A2402 A2403 T2404 L2407 N2412 A2413 A2414 V2415 Q2416 G2417 H2418 A2419 S2420 Q2421 E2422 K2423 S2427 V2431 A2432 A2441 C2442 K2443 D2447 Q2448 D2449 S2450 E2451 K2454 R2455 L2456 Q2457 N2461 A2462 N2469 L2470 A2473 A2474 Q2475 K2476 A2477 A2478 A2479 PHE GLU GLU GLN

GLU ASN GLU THR VAL VAL VAL LYS GLU LYS MET VAL GLY GLY ILE ALA GLN ILE ILE ALA ALA GLN GLU GLU MET LEU ARG LYS GLU ARG GLU LEU GLU GLU ALA ARG LYS LYS LEU ALA GLN ILE ARG GLN GLN GLN TYR LYS PHE LEU PRO SER GLU LEU ARG ASP GLU HIS LEU VAL

VAL LEU PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30438	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 ($e^-/Å^2$)	76.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.089	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0232	Depositor
Map size (Å)	237.43999, 237.43999, 237.43999	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.24	0/16192	0.39	0/21946

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	16011	0	16175	200	0
All	All	16011	0	16175	200	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 6.

The worst 5 of 200 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:PHE:O	1:A:283:HIS:HB2	1.97	0.65
1:A:1998:PHE:HB3	1:A:2004:LEU:HB2	1.80	0.63
1:A:1919:ARG:HB3	1:A:1964:VAL:HG12	1.82	0.61
1:A:608:LEU:HG	1:A:654:GLN:HB3	1.84	0.60
1:A:2020:LEU:HD22	1:A:2129:LEU:HD23	1.85	0.58

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	2181/2547 (86%)	2150 (99%)	31 (1%)	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	A	1668/1992 (84%)	1639 (98%)	29 (2%)	60 78

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1265	GLN
1	A	2347	GLU
1	A	1542	THR
1	A	2137	ASP
1	A	1405	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1133	GLN

Continued on next page...

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Mol	Chain	Res	Type
1	A	2285	GLN
1	A	1250	ASN
1	A	2418	HIS
1	A	1764	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

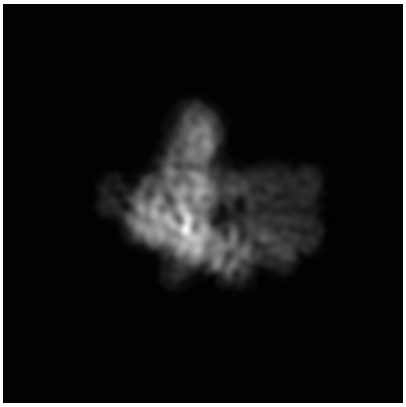
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4772. These allow visual inspection of the internal detail of the map and identification of artifacts.

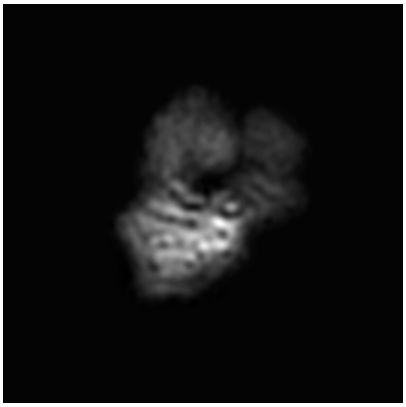
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

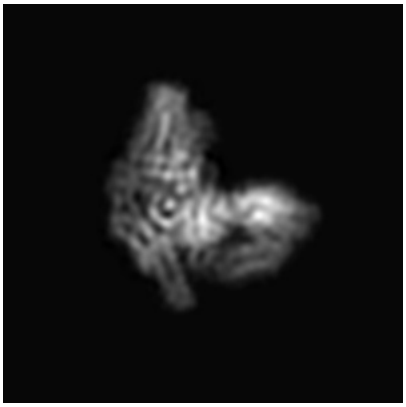
6.1.1 Primary map



X



Y



Z

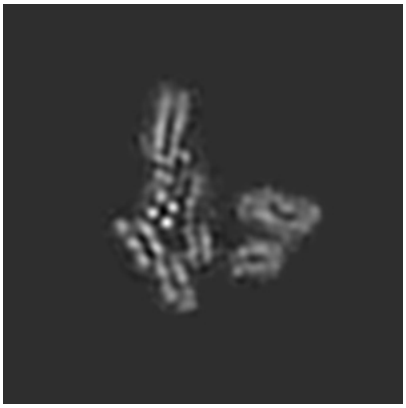
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 112

Y Index: 112

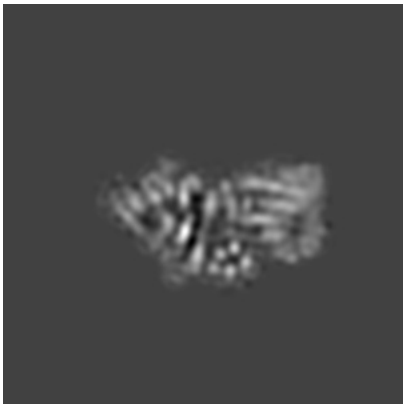


Z Index: 112

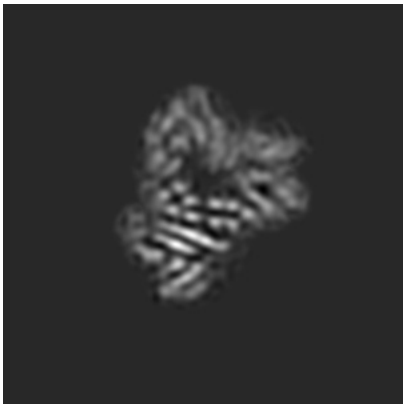
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

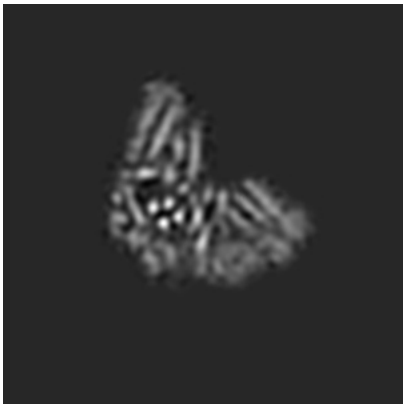
6.3.1 Primary map



X Index: 89



Y Index: 102

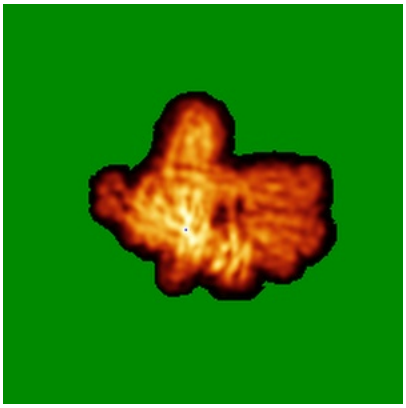


Z Index: 94

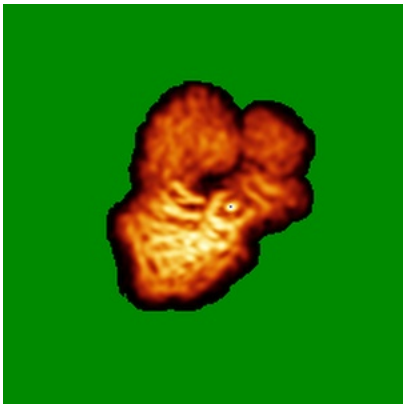
The images above show the largest variance slices of the map in three orthogonal directions.

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

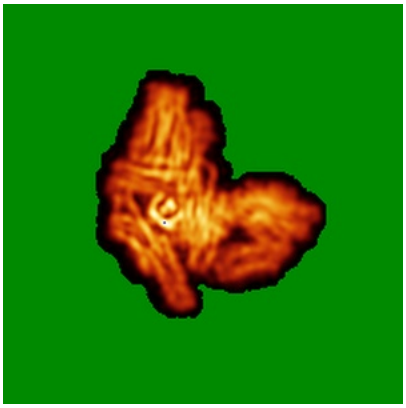
6.4.1 Primary map



X



Y

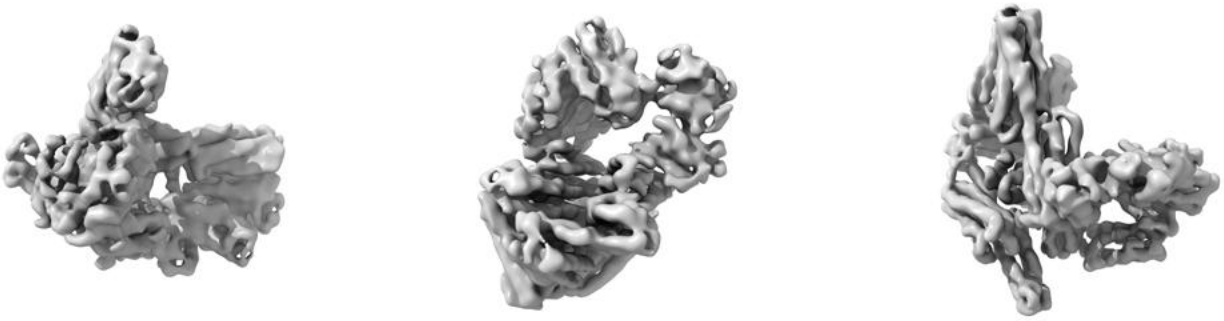


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0232. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

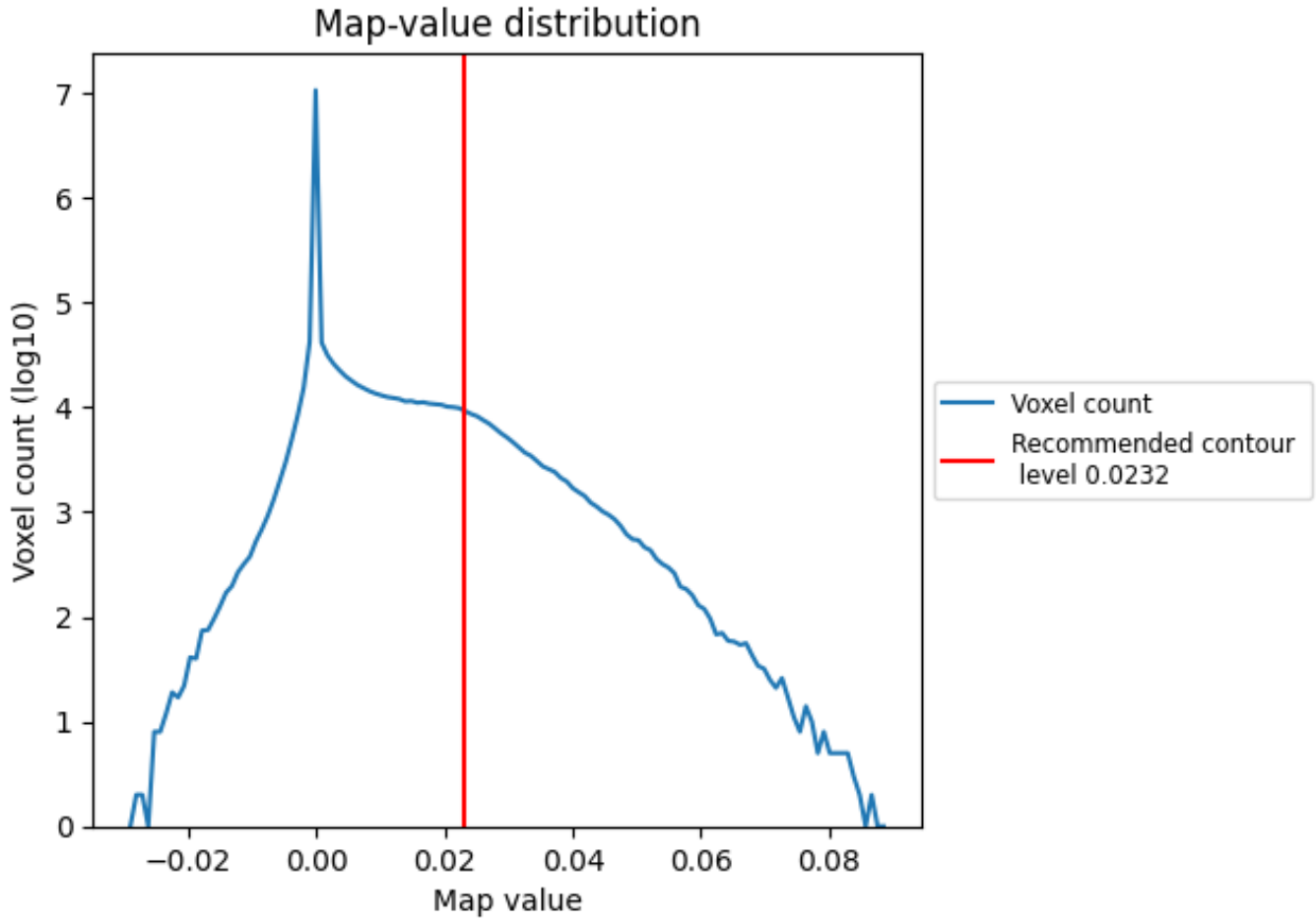
6.6 Mask visualisation (i)

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

7 Map analysis

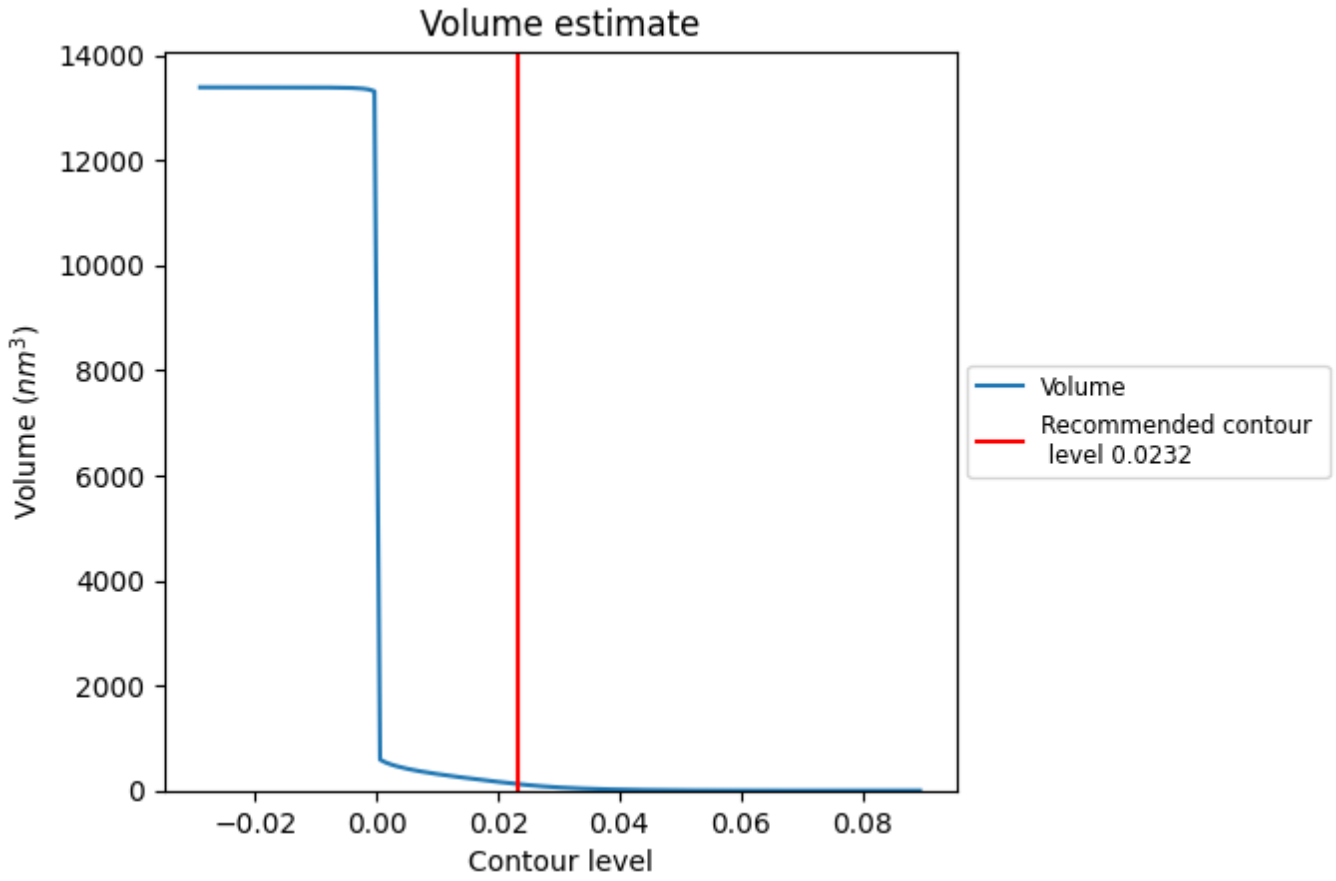
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

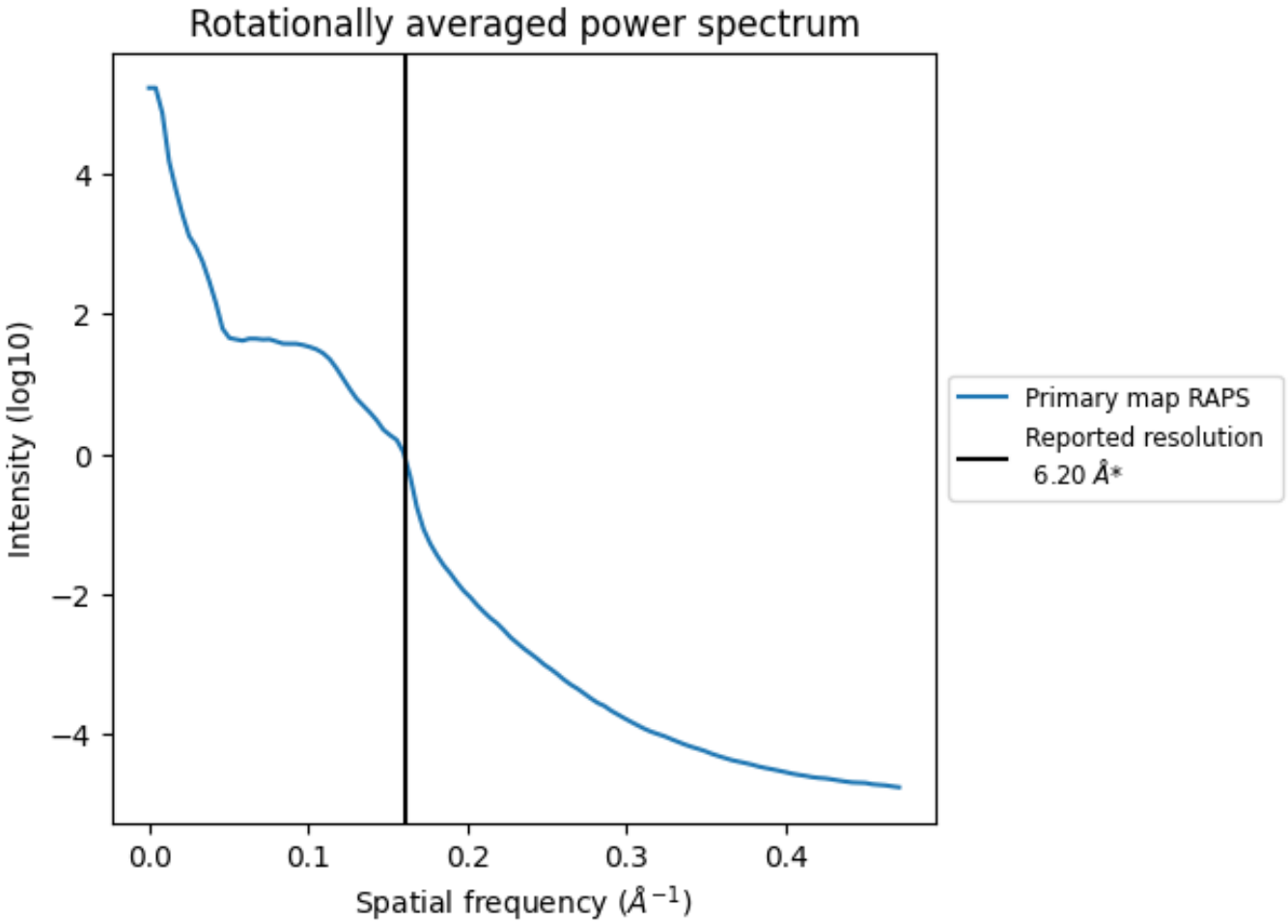
7.2 Volume estimate (i)



The volume at the recommended contour level is 125 nm^3; this corresponds to an approximate mass of 113 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 0.161 Å^{-1}

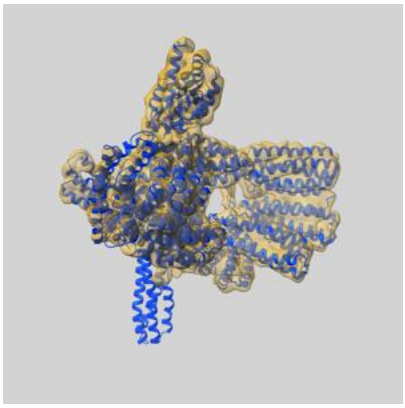
8 Fourier-Shell correlation (i)

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

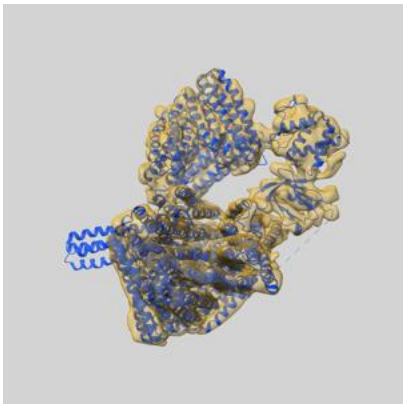
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4772 and PDB model 6R9T. Per-residue inclusion information can be found in section 3 on page 4.

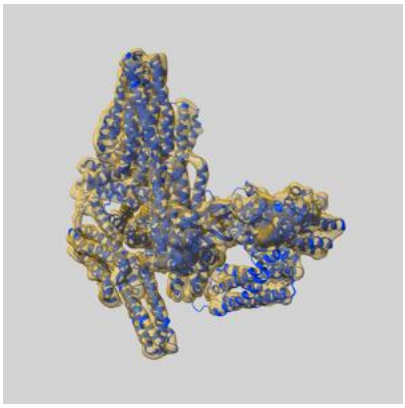
9.1 Map-model overlay



X



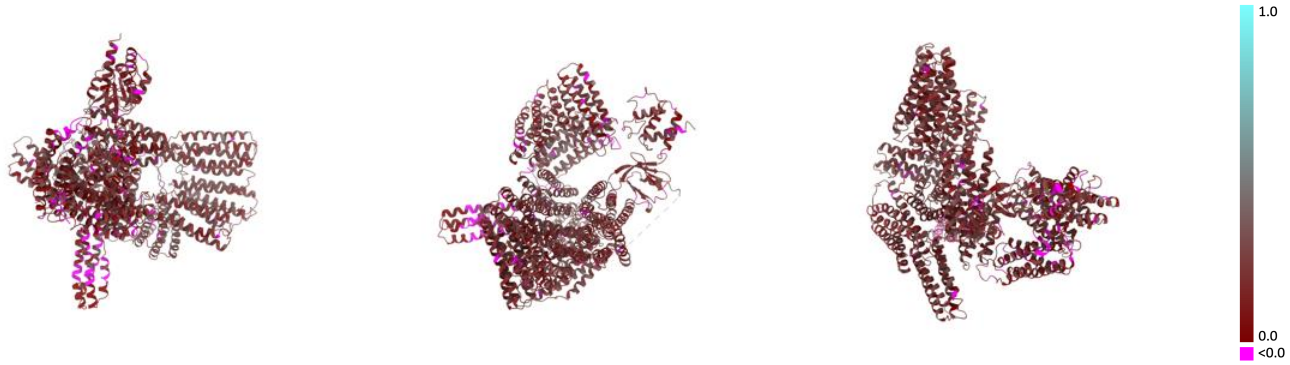
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0232 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

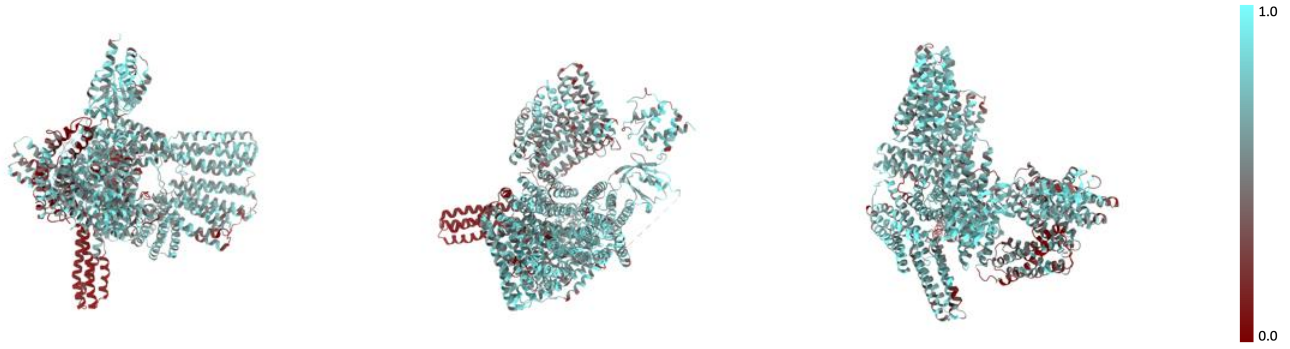
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

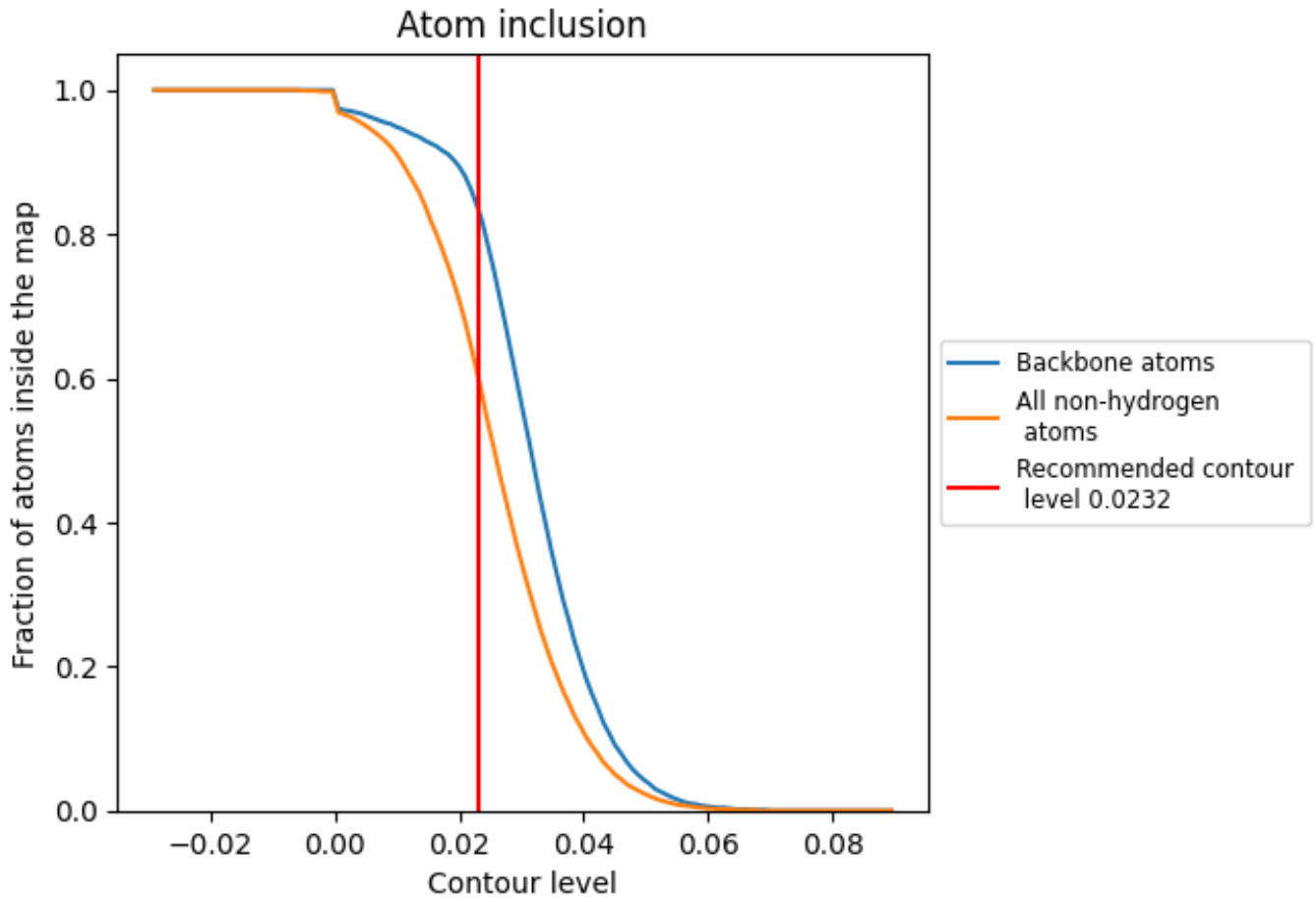
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0232).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 60% 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 (0.0232) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5960	0.1810
A	0.5960	0.1810