wwPDB EM Validation Summary Report (i)

Dec 19, 2022 – 10:53 am GMT

PDB ID	:	7NNH
EMDB ID	:	EMD-12477
Title	:	Cryo-EM structure of VAR2CSA FCR3 domain DBL5/6
Authors	:	Wang, K.T.; Dagil, R.; Salanti, A.; Gourdon, P.E.
Deposited on	:	2021-02-24
Resolution	:	4.00 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:

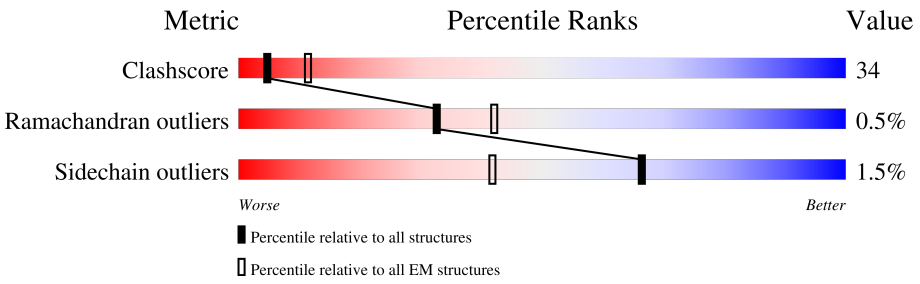
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	X	2649	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5299 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 Erythrocyte membrane protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	X	637	5299	3332	916	1013	38	0	0

There are 4 discrepancies between the modelled and reference sequences:

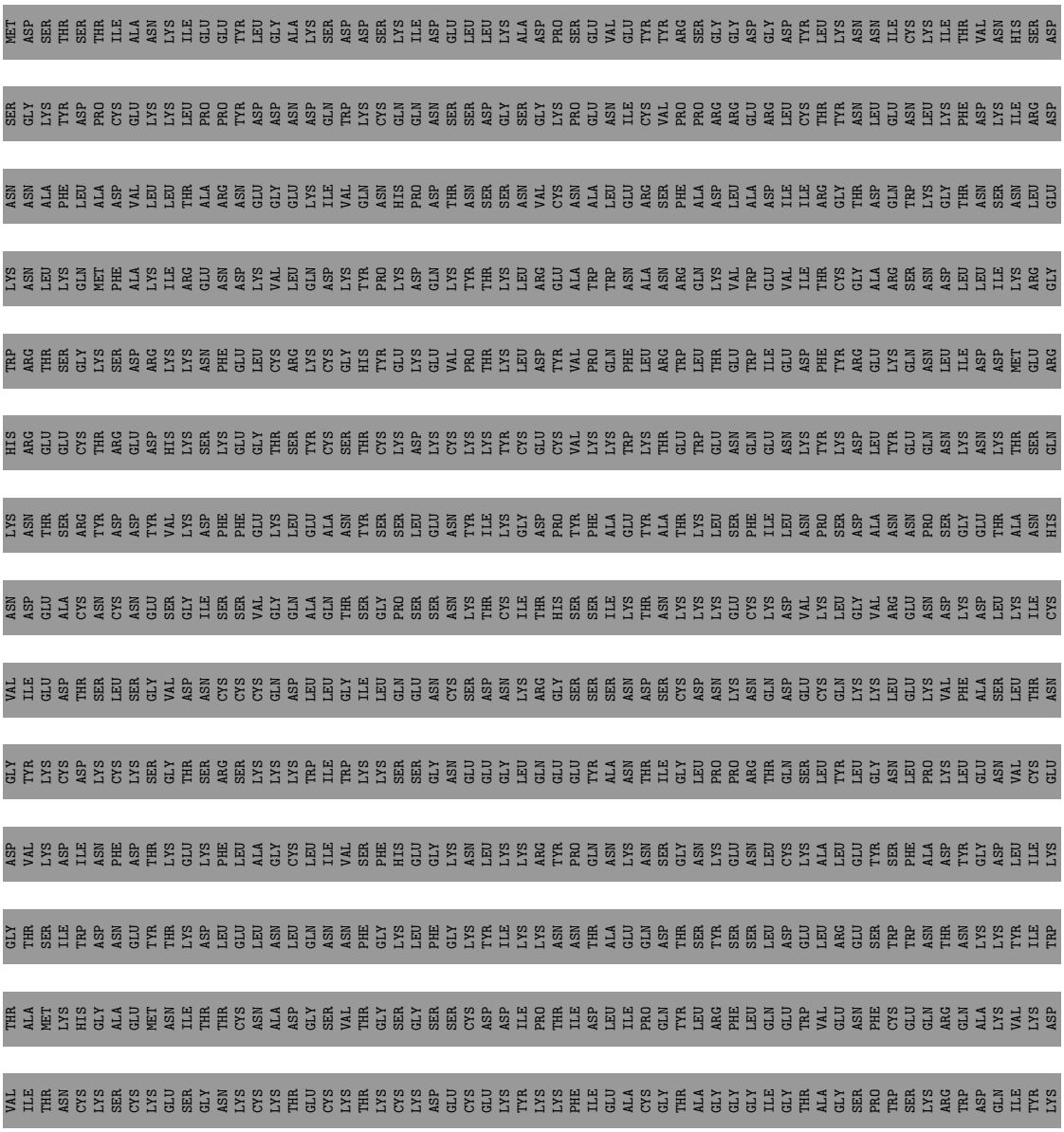
Chain	Residue	Modelled	Actual	Comment	Reference
X	1194	SER	ASN	conflict	UNP Q6UDW7
X	1730	ASN	ASP	conflict	UNP Q6UDW7
X	1878	ASP	GLY	conflict	UNP Q6UDW7
X	2243	GLN	ARG	conflict	UNP Q6UDW7

3 Residue-property plots (i)

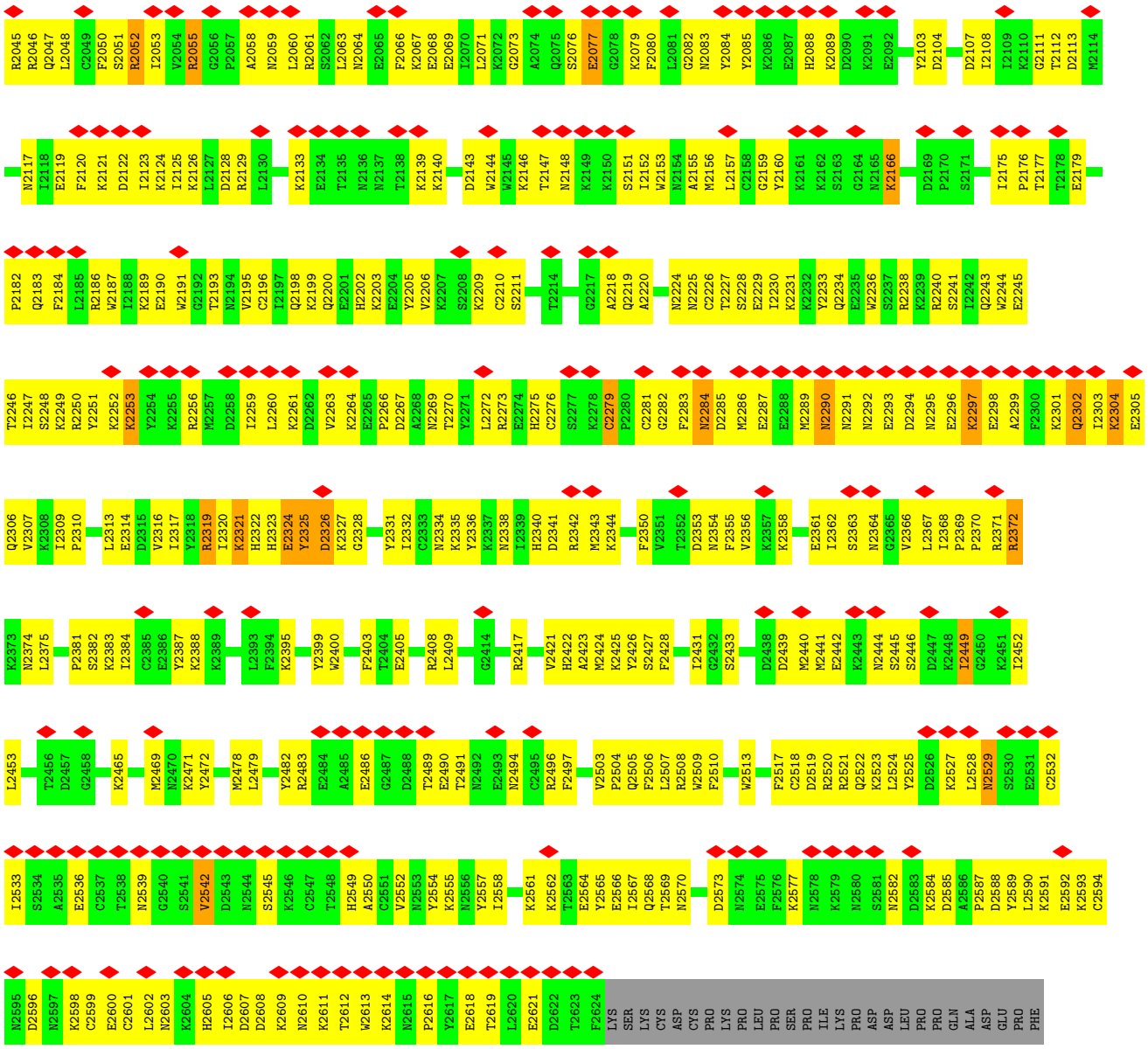
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Erythrocyte membrane protein 1

Chain X:



LYS ASP TYR LYS LEU
Y1988 P1989 L1990 D1991 R1992 C1993 F1994 D1995 D1996 Q1997 T1998 K1999 M2000 K2001 V2002 C2003 D2004 L2005 I2006 A2007 D2008 A2009 I2010
K2013 D2014 K2015 T2016 K2017 L2018 D2019 E2020 L2021 D2022 E2023 W2024
M2027 D2028 L2029 R2030 G2031 T2032 Y2033 N2034 K2035 H2036 K2037 G2038 V2039 L2040 I2041 P2042 P2043 R2044


R2045 R2046 Q2047 L2048 C2049 F2050 S2051 R2052 I2053 V2054 R2055 G2056 P2057 A2058 N2059 L2060 R2061 S2062 L2063 N2064 E2065 F2066 K2067 E2068 E2069 I2070 L2071 K2072 G2073 A2074 Q2075 S2076 E2077 G2078 K2079 F2080 L2081 G2082 N2083 Y2084 Y2085 K2086 E2087 H2088 K2089 D2090 K2091 E2092 Y2103 D2104 D2107 I2108 I2109 K2110 G2111 T2112 D2113 M2114
N2117 I2118 E2119 F2120 K2121 D2122 I2123 K2124 I2125 K2126 L2127 D2128 R2129 L2130 K2133 E2134 T2135 N2136 N2137 T2138 K2139 K2140 D2143 W2144 W2145 K2146 T2147 N2148 K2149 K2150 S2151 I2152 W2153 M2154 A2155 M2156 L2157 C2158 G2159 Y2160 K2161 K2162 S2163 G2164 N2165 K2166 D2169 P2170 S2171 I2175 P2176 T2177 T2178 E2179
P2182 Q2183 F2184 L2185 R2186 W2187 I2188 K2189 E2190 W2191 G2192 T2193 N2194 V2195 C2196 I2197 Q2198 K2199 Q2200 E2201 H2202 K2203 E2204 Y2205 V2206 K2207 S2208 K2209 C2210 S2211 T2214 G2217 A2218 Q2219 A2220 N2224 N2225 C2226 T2227 S2228 E2229 I2230 K2231 K2232 Y2233 Q2234 E2235 W2236 S2237 R2238 K2239 R2240 S2241 I2242 Q2243 W2244 E2245
T2246 I2247 S2248 K2249 R2250 Y2251 K2252 K2253 Y2254 K2255 R2256 M2257 D2258 I2259 L2260 K2261 D2262 V2263 K2264 E2265 P2266 D2267 A2268 N2269 T2270 Y2271 L2272 R2273 E2274 H2275 C2276 S2277 K2278 C2279 P2280 C2281 G2282 F2283 N2284 D2285 M2286 E2287 E2288 M2289 N2290 N2291 N2292 E2293 D2294 N2295 E2296 K2297 E2298 A2299 F2300 K2301 Q2302 I2303 K2304 E2305
Q2306 V2307 K2308 I2309 P2310 L2313 E2314 D2315 V2316 I2317 Y2318 R2319 I2320 K2321 H2322 H2323 E2324 Y2325 D2326 K2327 G2328 Y2331 I2332 C2333 N2334 K2335 Y2336 K2337 N2338 I2339 H2340 D2341 R2342 M2343 K2344 F2350 V2351 T2352 D2353 N2354 F2355 V2356 K2357 K2358 E2361 I2362 S2363 N2364 G2365 V2366 L2367 I2368 P2369 P2370 R2371 R2372
K2373 N2374 L2375 P2381 S2382 K2383 I2384 C2385 E2386 Y2387 K2388 K2389 L2393 F2394 K2395 Y2399 W2400 F2403 T2404 E2405 R2408 L2409 G2414 R2417 V2421 H2422 A2423 M2424 K2425 Y2426 S2427 F2428 I2431 G2432 S2433 D2438 D2439 M2440 M2441 E2442 K2443 N2444 S2445 S2446 D2447 K2448 I2449 G2450 K2451 I2452
L2453 T2456 D2457 G2458 K2465 M2469 N2470 K2471 Y2472 M2478 L2479 Y2482 R2483 E2484 A2485 E2486 G2487 D2488 T2489 E2490 T2491 N2492 E2493 N2494 C2495 R2496 F2497 V2503 P2504 Q2505 F2506 L2507 R2508 W2509 F2510 W2513 F2517 C2518 D2519 R2520 R2521 Q2522 K2523 L2524 Y2525 D2526 K2527 L2528 N2529 S2530 E2531 C2532
I2533 S2534 A2535 E2536 C2537 T2538 N2539 G2540 S2541 V2542 D2543 N2544 S2545 K2546 C2547 T2548 H2549 A2550 C2551 V2552 N2553 Y2554 K2555 N2556 Y2557 I2558 K2561 K2562 T2563 E2564 Y2565 E2566 I2567 Q2568 T2569 N2570 D2573 N2574 E2575 F2576 K2577 N2578 K2579 N2580 S2581 N2582 D2583 K2584 D2585 A2586 P2587 D2588 Y2589 L2590 K2591 E2592 K2593 C2594
N2595 D2596 N2597 K2598 C2599 E2600 C2601 L2602 N2603 K2604 H2605 I2606 D2607 D2608 K2609 N2610 K2611 T2612 W2613 K2614 N2615 P2616 Y2617 E2618 T2619 L2620 E2621 D2622 T2623 F2624
LYS SER LYS CYS ASP CYS PRO LYS PRO LEU PRO SER PRO ILE LYS PRO ASP ASP LEU PRO PRO GLN ALA ASP GLU PRO PHE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	97695	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	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.403	Depositor
Minimum map value	-0.505	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.53	Depositor
Map size (Å)	365.19998, 365.19998, 365.19998	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	X	0.28	0/5414	0.59	2/7269 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	10

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2279	CYS	C-N-CD	-6.08	107.22	120.60
1	X	2326	ASP	N-CA-C	5.17	124.96	111.00

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	2253	LYS	Peptide
1	X	2284	ASN	Peptide
1	X	2290	ASN	Peptide
1	X	2297	LYS	Peptide
1	X	2302	GLN	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	X	5299	0	5167	354	0
All	All	5299	0	5167	354	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 34.

The worst 5 of 354 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:X:2368:ILE:HG21	1:X:2441:MET:HB3	1.56	0.87
1:X:2199:LYS:NZ	1:X:2281:CYS:SG	2.47	0.87
1:X:2338:ASN:HA	1:X:2342:ARG:HH21	1.40	0.84
1:X:2234:GLN:HE21	1:X:2238:ARG:HG3	1.47	0.79
1:X:2290:ASN:OD1	1:X:2292:ASN:ND2	2.16	0.77

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	X	635/2649 (24%)	486 (76%)	146 (23%)	3 (0%)	29 67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	1993	CYS
1	X	1994	PHE
1	X	2077	GLU

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	X	589/2404 (24%)	580 (98%)	9 (2%)	65 80

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	2449	ILE
1	X	2529	ASN
1	X	2166	LYS
1	X	2189	LYS
1	X	2319	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	2083	ASN
1	X	2202	HIS
1	X	2234	GLN
1	X	2291	ASN
1	X	2570	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

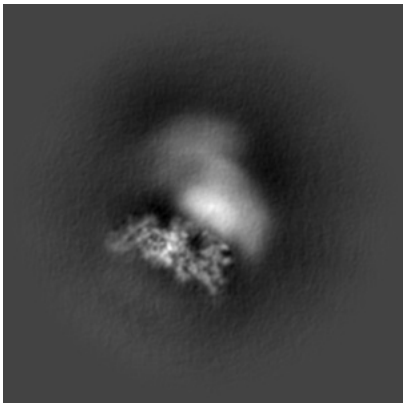
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12477. These allow visual inspection of the internal detail of the map and identification of artifacts.

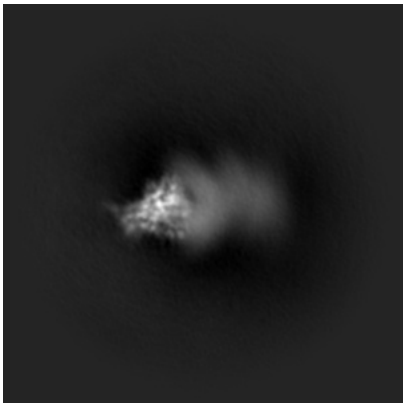
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

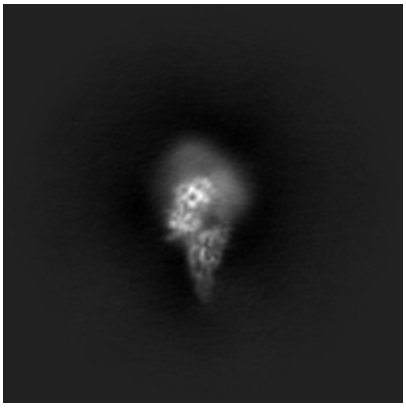
6.1.1 Primary map



X



Y

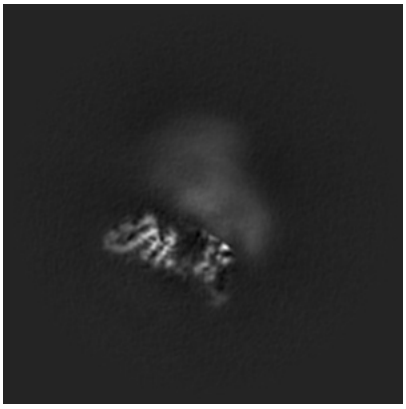


Z

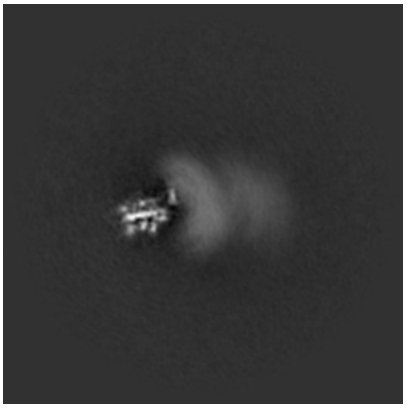
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

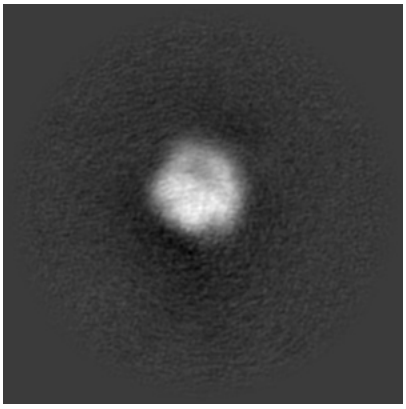
6.2.1 Primary map



X Index: 220



Y Index: 220

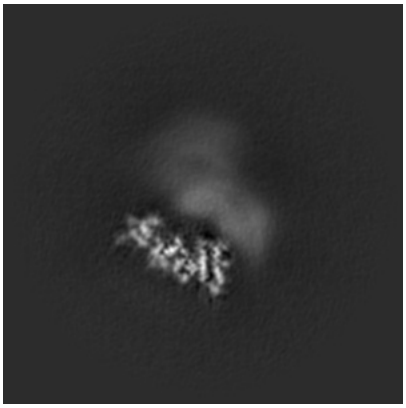


Z Index: 220

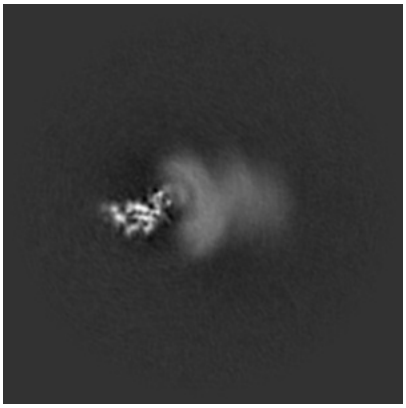
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

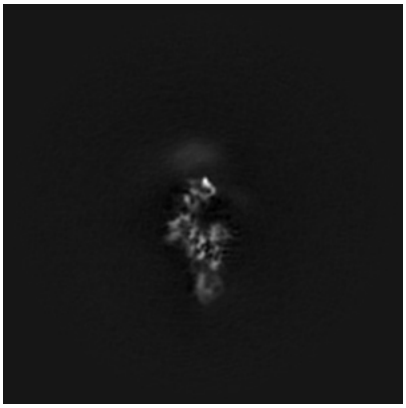
6.3.1 Primary map



X Index: 208



Y Index: 231

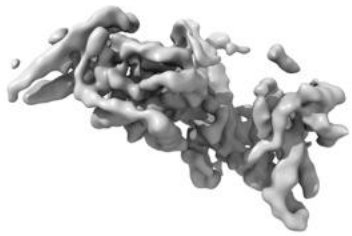


Z Index: 171

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

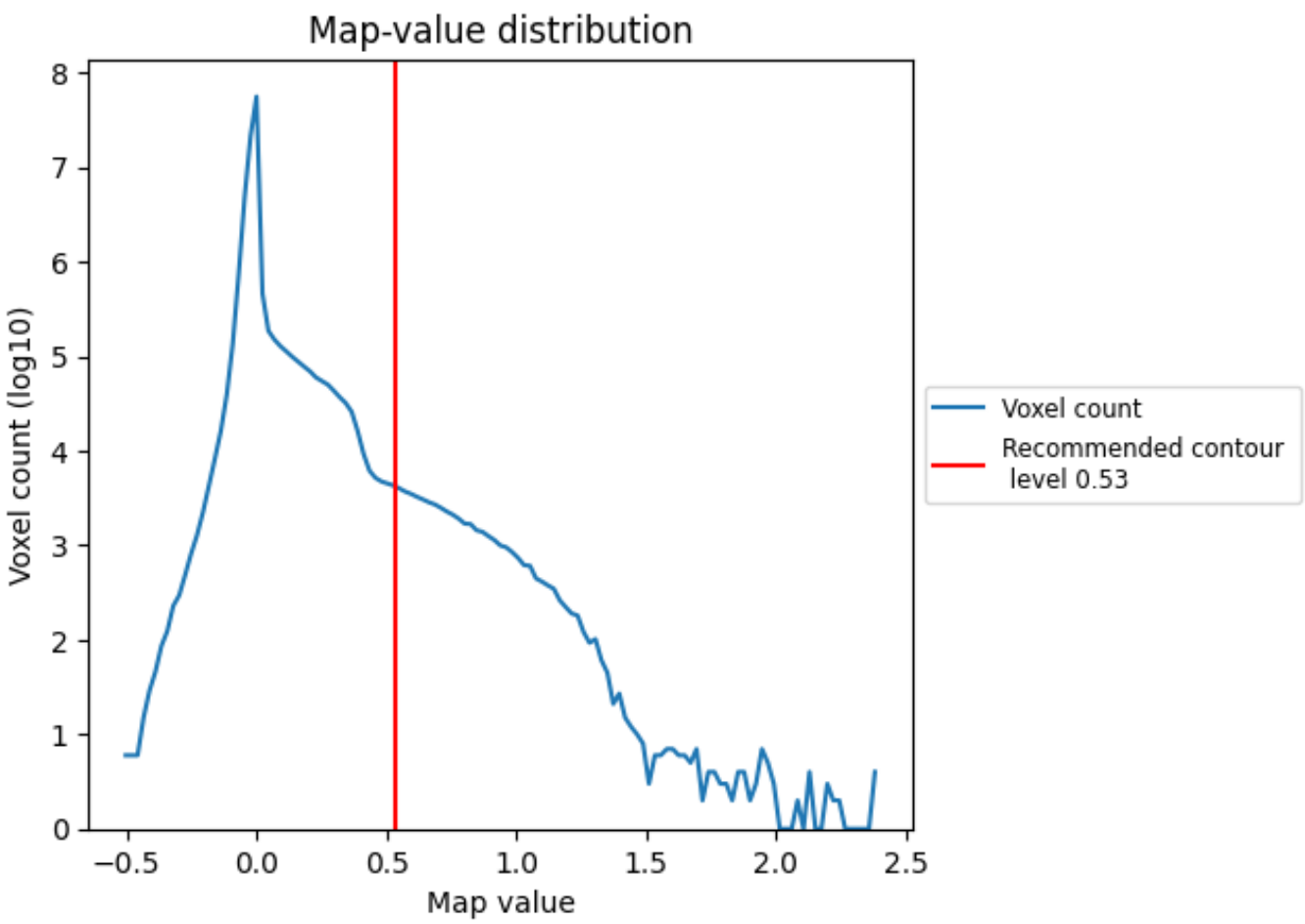
6.5 Mask visualisation (i)

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

7 Map analysis (i)

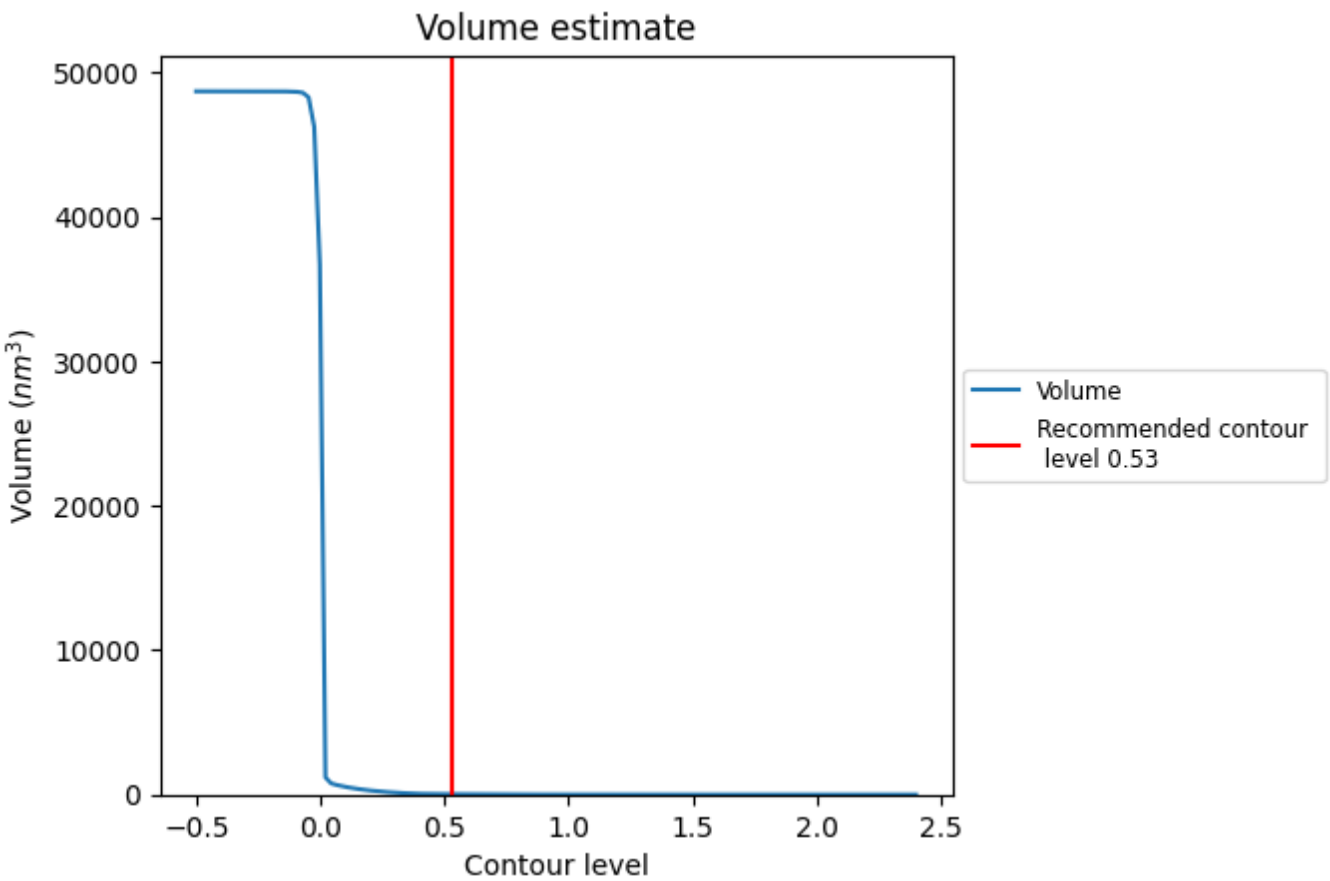
This section contains the results of statistical analysis of the map.

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.

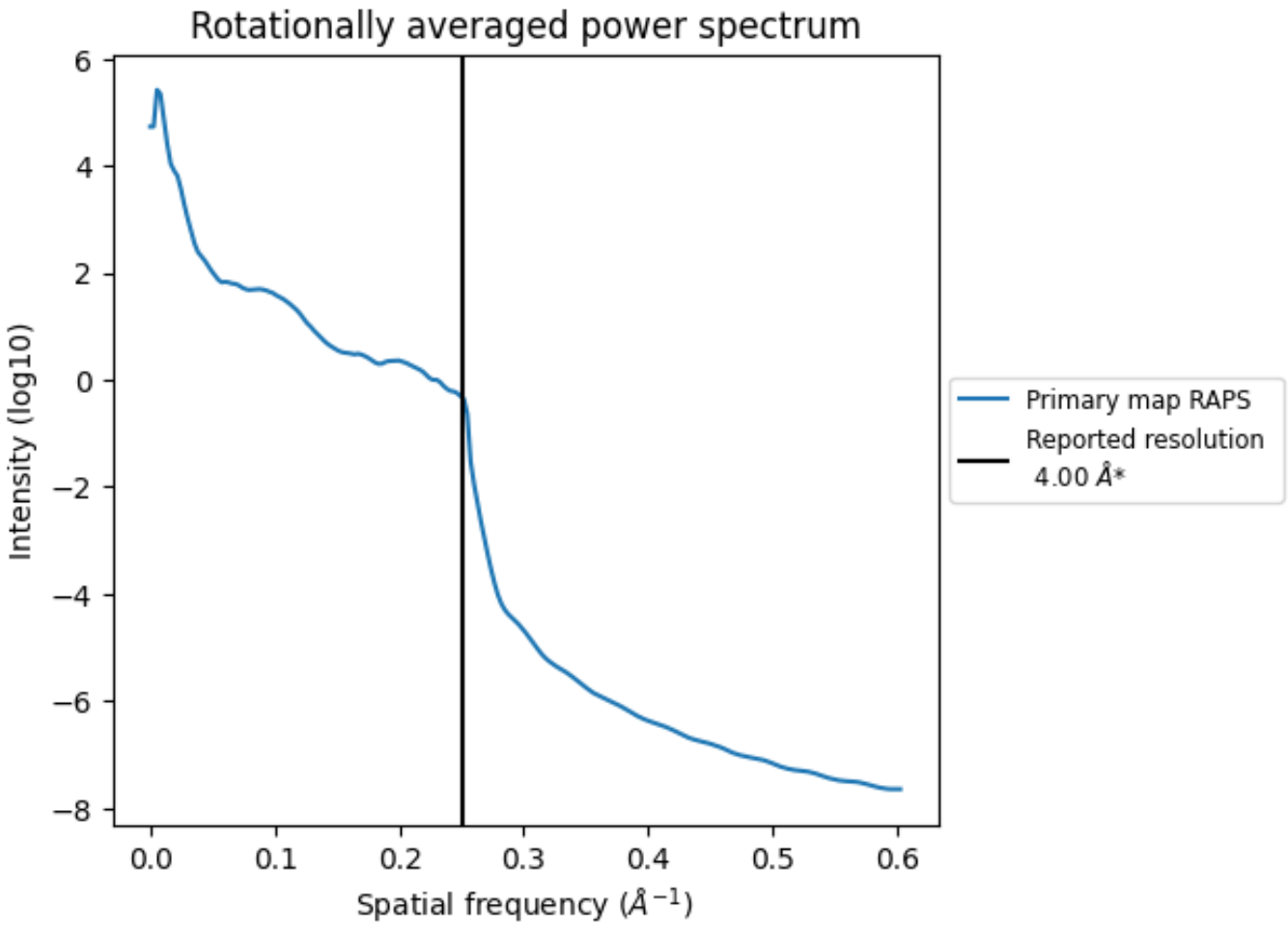
7.2 Volume estimate (i)



The volume at the recommended contour level is 30 nm^3; this corresponds to an approximate mass of 27 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)

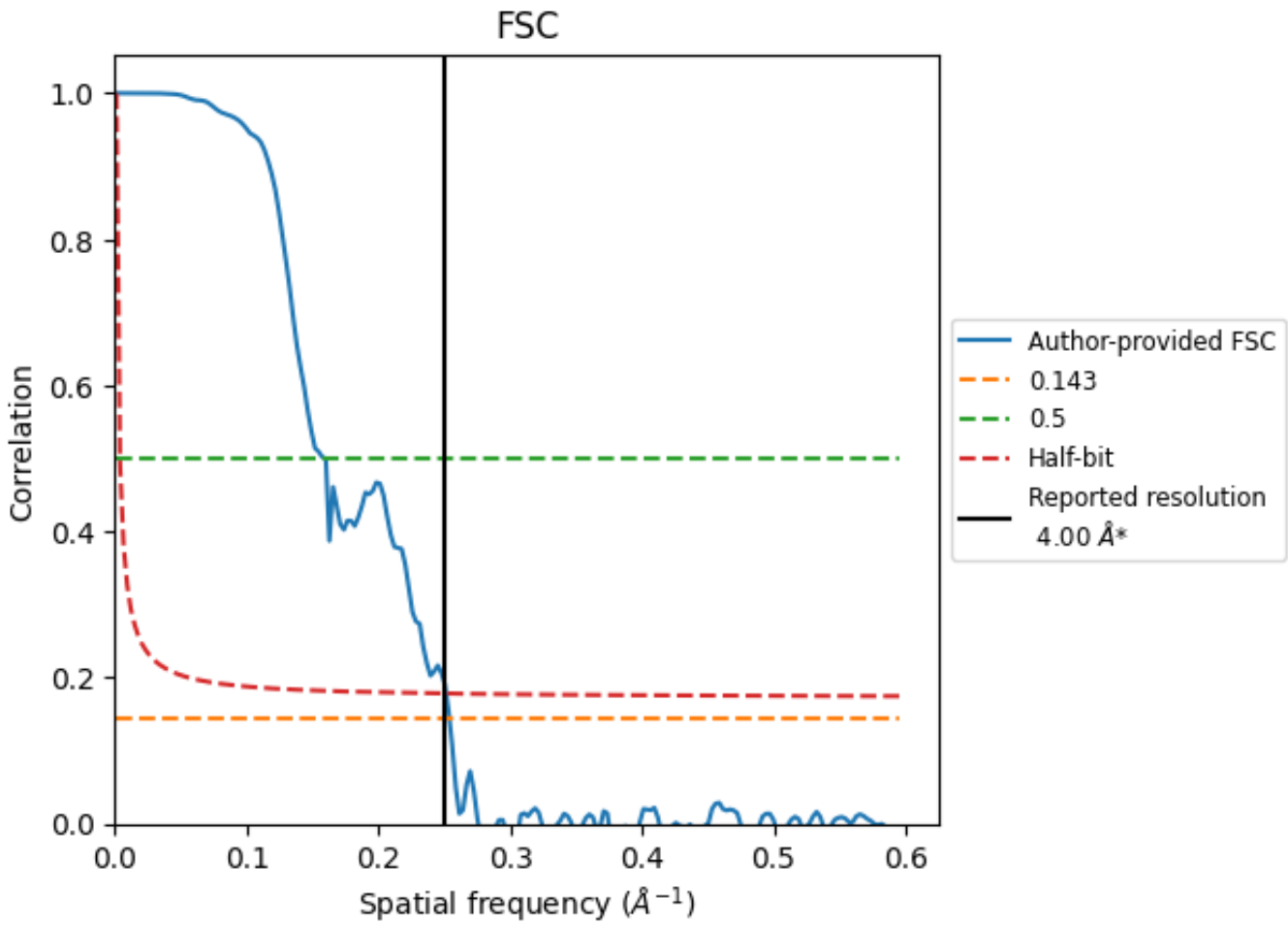


*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8.2 Resolution estimates (i)

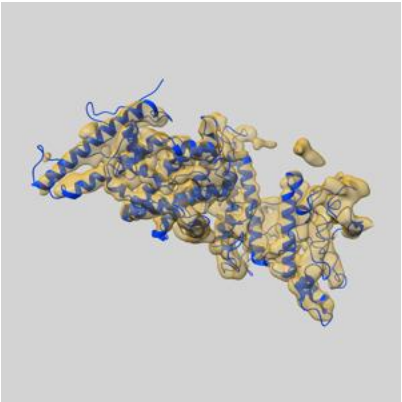
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.94	6.27	3.98
Unmasked-calculated*	-	-	-

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

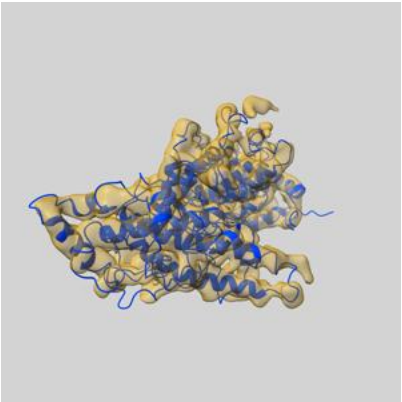
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12477 and PDB model 7NNH. Per-residue inclusion information can be found in section 3 on page 4.

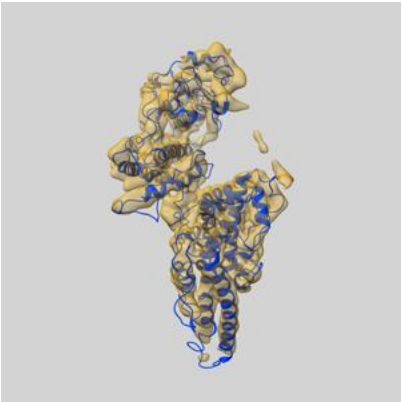
9.1 Map-model overlay (i)



X



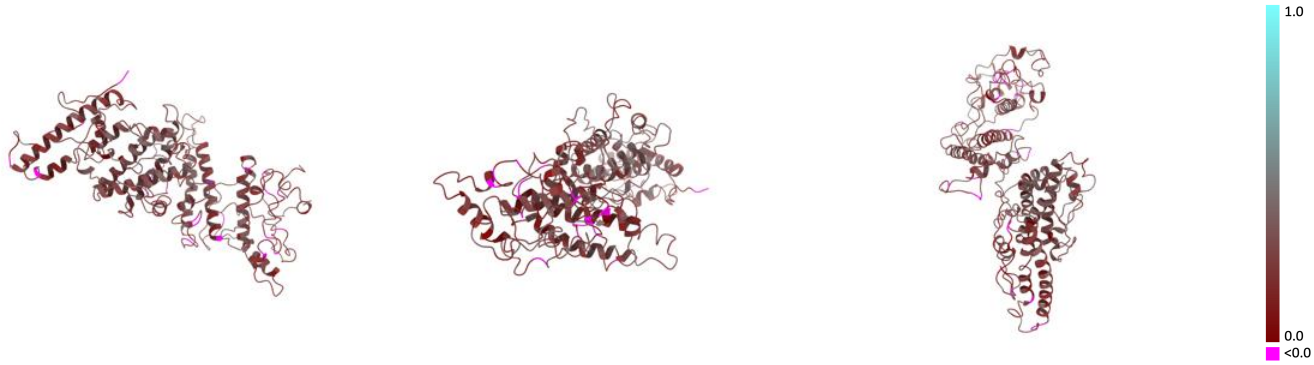
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.53 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.

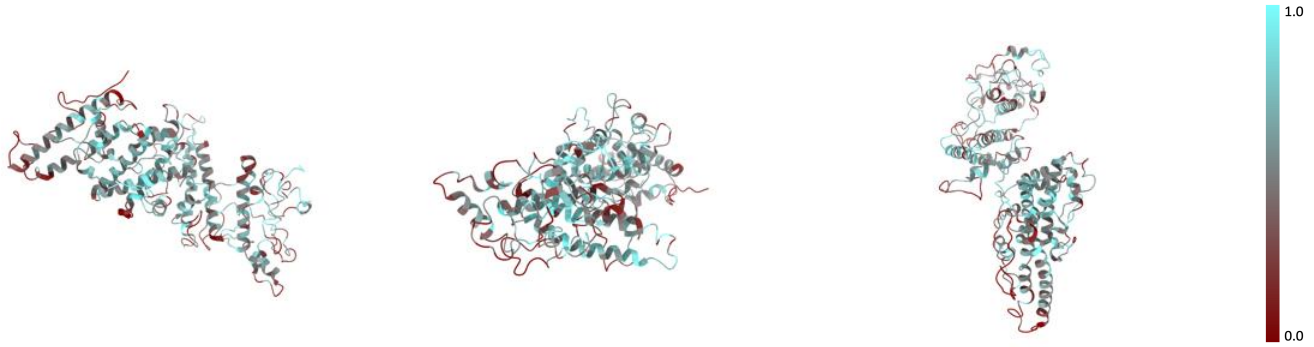
9.2 Q-score mapped to coordinate model (i)



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.

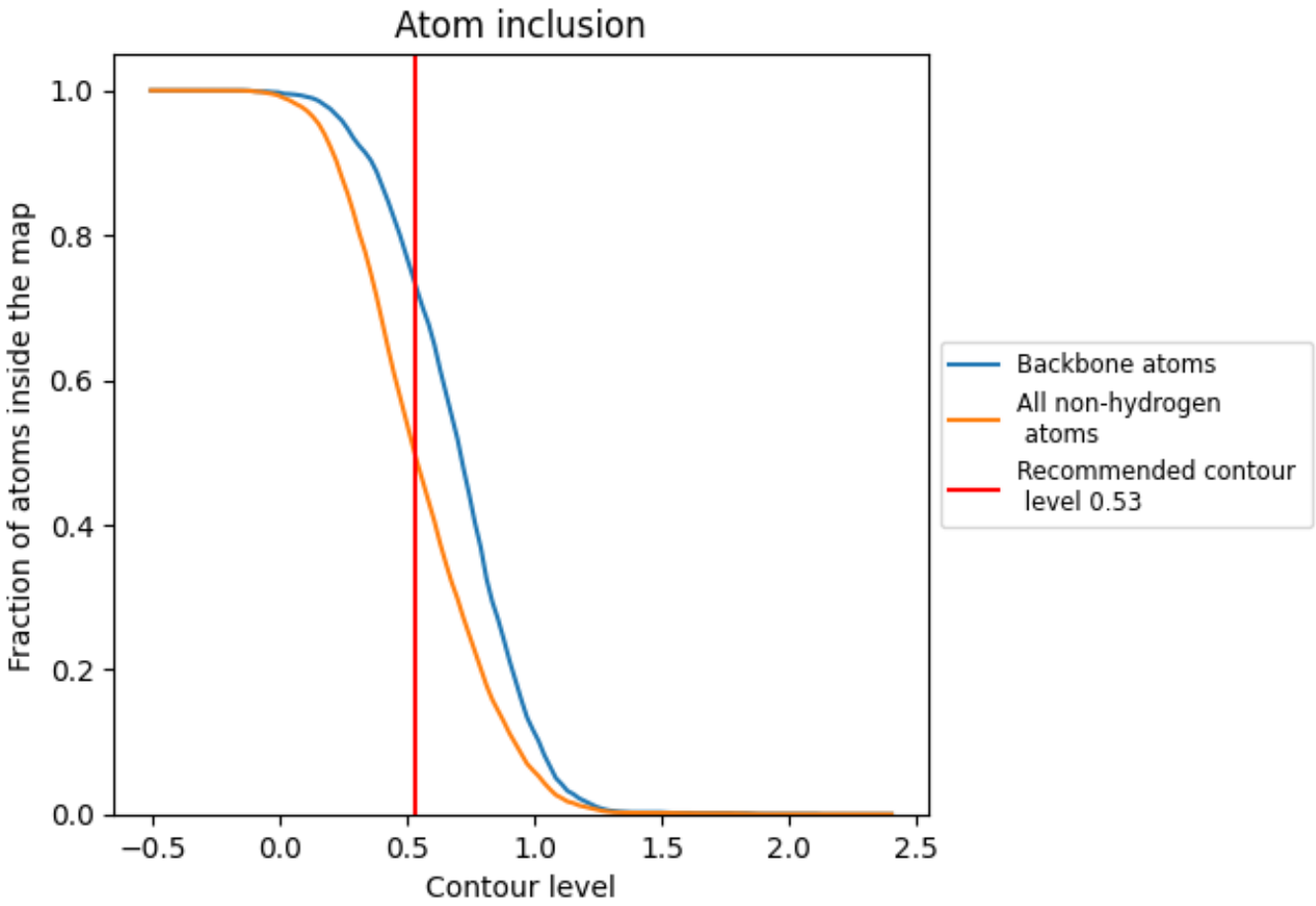
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.53).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.53) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4996	0.2380
X	0.4996	0.2380