Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 07:41 AM EST

PDB ID	:	7N9S
EMDB ID	:	EMD-24261
Title	:	TcdB and frizzled-2 CRD complex
Authors	:	Jiang, M.; Zhang, J.
Deposited on	:	2021-06-18
Resolution	:	5.10 Å(reported)

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

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

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

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

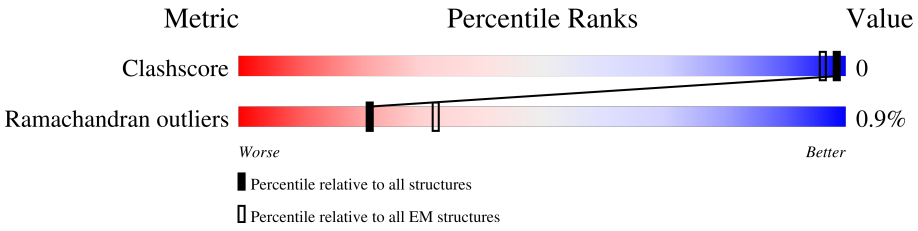
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 5.10 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

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

Mol	Chain	Length	Quality of chain
1	B	121	21% 98%
2	A	2365	18% 98%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7458 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 Frizzled-2.

Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	N		
1	B	121	363	242	121	0	0

- Molecule 2 is a protein called Toxin B.

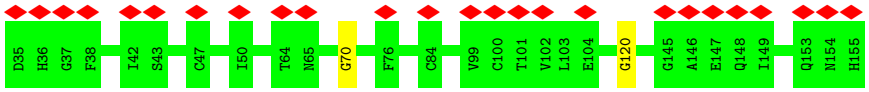
Mol	Chain	Residues	Atoms			AltConf	Trace
			Total	C	N		
2	A	2365	7095	4730	2365	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

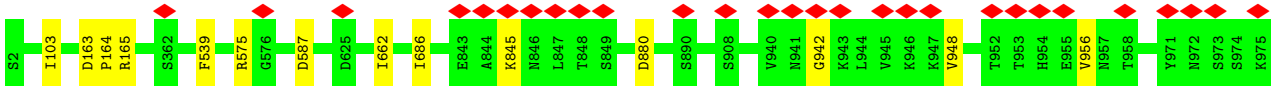
- Molecule 1: Frizzled-2

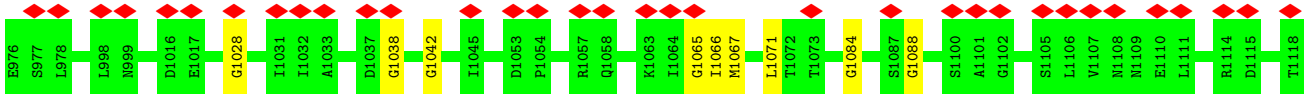
Chain B:

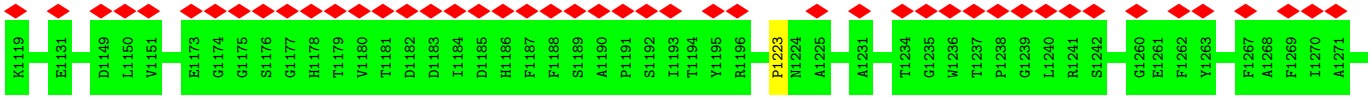


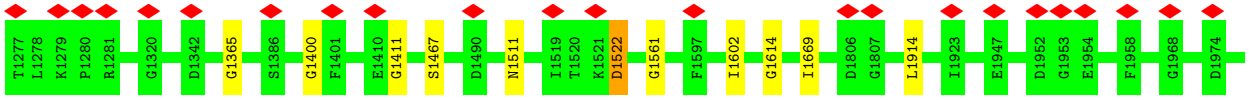
- Molecule 2: Toxin B

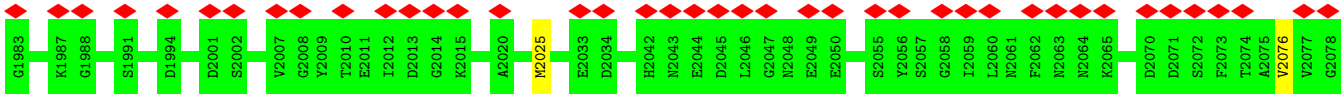
Chain A:

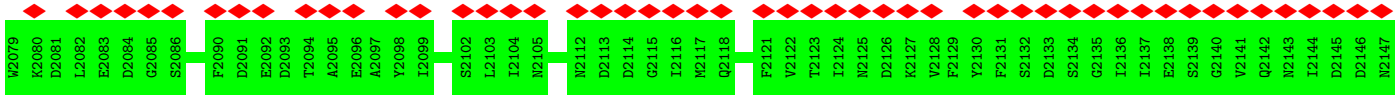


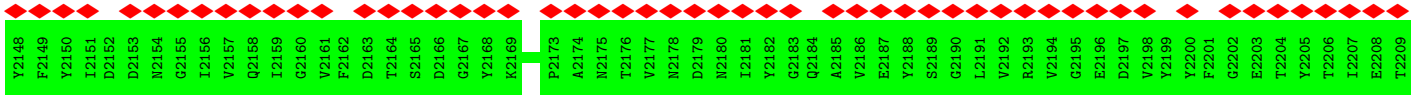


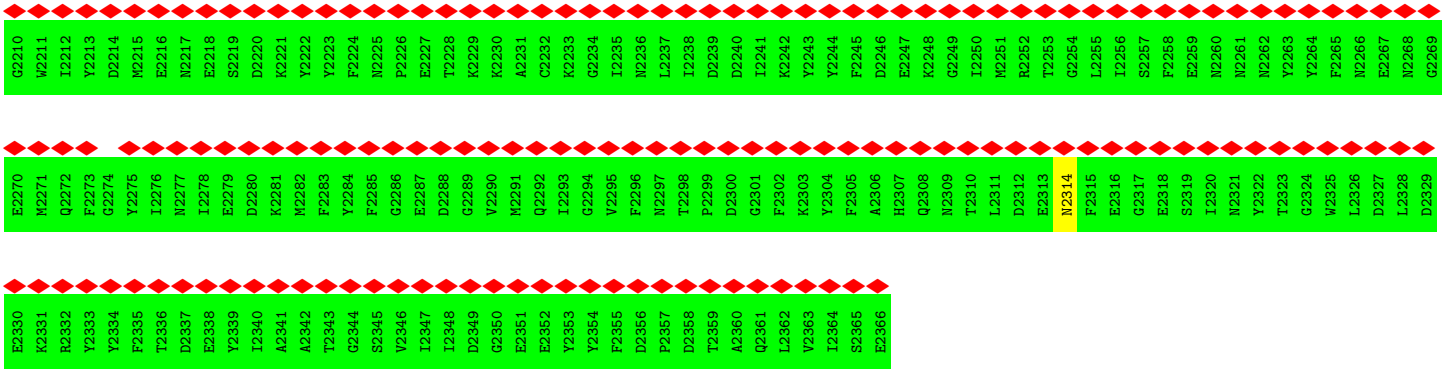











G2210 W2211 I2212 Y2213 D2214 M2215 E2216 N2217 E2218 S2219 D2220 K2221 Y2222 Y2223 F2224 N2225 P2226 E2227 T2228 K2229 K2230 A2231 C2232 K2233 G2234 I2235 N2236 L2237 I2238 D2239 D2240 I2241 K2242 Y2243 Y2244 F2245 D2246 E2247 K2248 G2249 I2250 M2251 R2252 T2253 G2254 L2255 I2256 S2257 F2258 E2259 N2260 N2261 N2262 Y2263 Y2264 F2265 N2266 E2267 N2268 G2269
E2270 M2271 Q2272 F2273 G2274 Y2275 I2276 N2277 I2278 E2279 D2280 K2281 M2282 F2283 Y2284 F2285 G2286 E2287 D2288 G2289 V2290 M2291 Q2292 I2293 G2294 V2295 F2296 N2297 T2298 P2299 D2300 G2301 F2302 K2303 Y2304 F2305 A2306 H2307 Q2308 N2309 T2310 L2311 D2312 E2313 N2314 F2315 E2316 G2317 E2318 S2319 I2320 N2321 Y2322 T2323 G2324 W2325 L2326 D2327 L2328 D2329
E2330 K2331 R2332 Y2333 Y2334 F2335 T2336 D2337 E2338 Y2339 I2340 A2341 A2342 T2343 G2344 S2345 V2346 I2347 I2348 D2349 G2350 E2351 E2352 Y2353 Y2354 F2355 D2356 P2357 D2358 T2359 A2360 Q2361 L2362 V2363 I2364 S2365 E2366

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81240	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	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.097	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	453.9582, 453.9582, 453.9582	wwPDB
Map dimensions	428, 428, 428	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06065, 1.06065, 1.06065	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	B	1.07	2/362 (0.6%)	1.04	0/361
2	A	0.57	11/7094 (0.2%)	0.78	4/7093 (0.1%)
All	All	0.60	13/7456 (0.2%)	0.80	4/7454 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	942	GLY	N-CA	-5.64	1.37	1.46
2	A	1411	GLY	N-CA	-5.59	1.37	1.46
2	A	1400	GLY	N-CA	-5.59	1.37	1.46
2	A	1088	GLY	N-CA	-5.56	1.37	1.46
2	A	1365	GLY	N-CA	-5.52	1.37	1.46
2	A	1038	GLY	N-CA	-5.45	1.37	1.46
2	A	1028	GLY	N-CA	-5.45	1.37	1.46
2	A	1561	GLY	N-CA	-5.44	1.37	1.46
2	A	1084	GLY	N-CA	-5.41	1.38	1.46
2	A	1042	GLY	N-CA	-5.31	1.38	1.46
1	B	120	GLY	N-CA	-5.29	1.38	1.46
2	A	1614	GLY	N-CA	-5.27	1.38	1.46
1	B	70	GLY	N-CA	-5.22	1.38	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1066	ILE	C-N-CA	8.05	141.83	121.70
2	A	1065	GLY	N-CA-C	6.17	128.53	113.10
2	A	1522	ASP	N-CA-C	5.67	126.32	111.00
2	A	1522	ASP	CA-C-N	5.57	129.46	117.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	363	0	124	0	0
2	A	7095	0	2586	1	0
All	All	7458	0	2710	1	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 0.

All (1) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:163:ASP:C	2:A:165:ARG:H	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
2	A	2363/2365 (100%)	2141 (91%)	199 (8%)	23 (1%)	15	54
All	All	2482/2486 (100%)	2257 (91%)	202 (8%)	23 (1%)	21	56

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	103	ILE

Continued on next page...

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Mol	Chain	Res	Type
2	A	164	PRO
2	A	686	ILE
2	A	880	ASP
2	A	1067	MET
2	A	1223	PRO
2	A	1522	ASP
2	A	1669	ILE
2	A	2076	VAL
2	A	539	PHE
2	A	575	ARG
2	A	587	ASP
2	A	662	ILE
2	A	1602	ILE
2	A	956	VAL
2	A	1511	ASN
2	A	1914	LEU
2	A	2025	MET
2	A	948	VAL
2	A	845	LYS
2	A	1071	LEU
2	A	1467	SER
2	A	2314	ASN

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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.

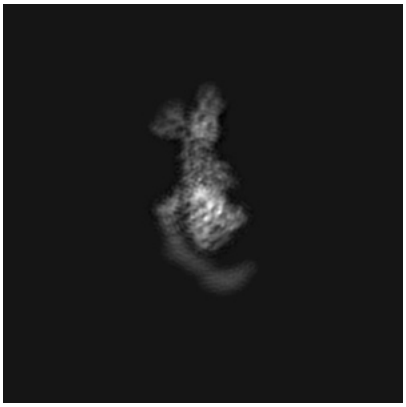
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24261. These allow visual inspection of the internal detail of the map and identification of artifacts.

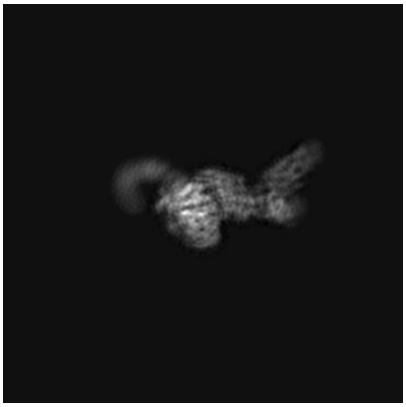
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

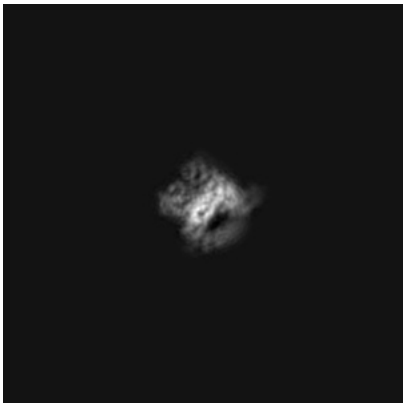
6.1.1 Primary map



X



Y

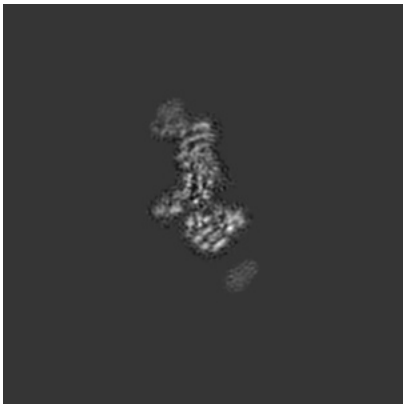


Z

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

6.2 Central slices

6.2.1 Primary map



X Index: 214

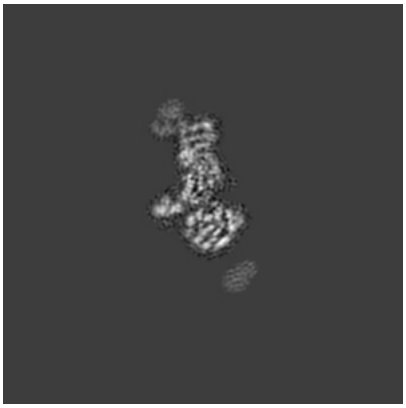
Y Index: 214

Z Index: 214

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

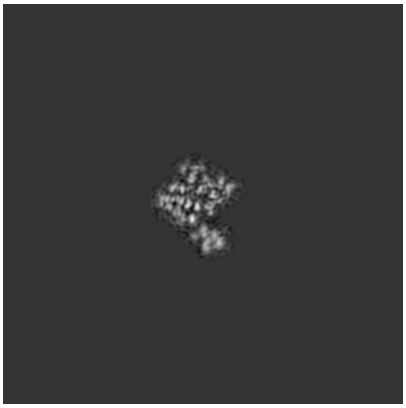
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 216

Y Index: 210



Z Index: 206

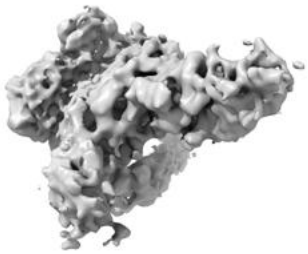
The images above show the largest variance slices of the map in three orthogonal directions.

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

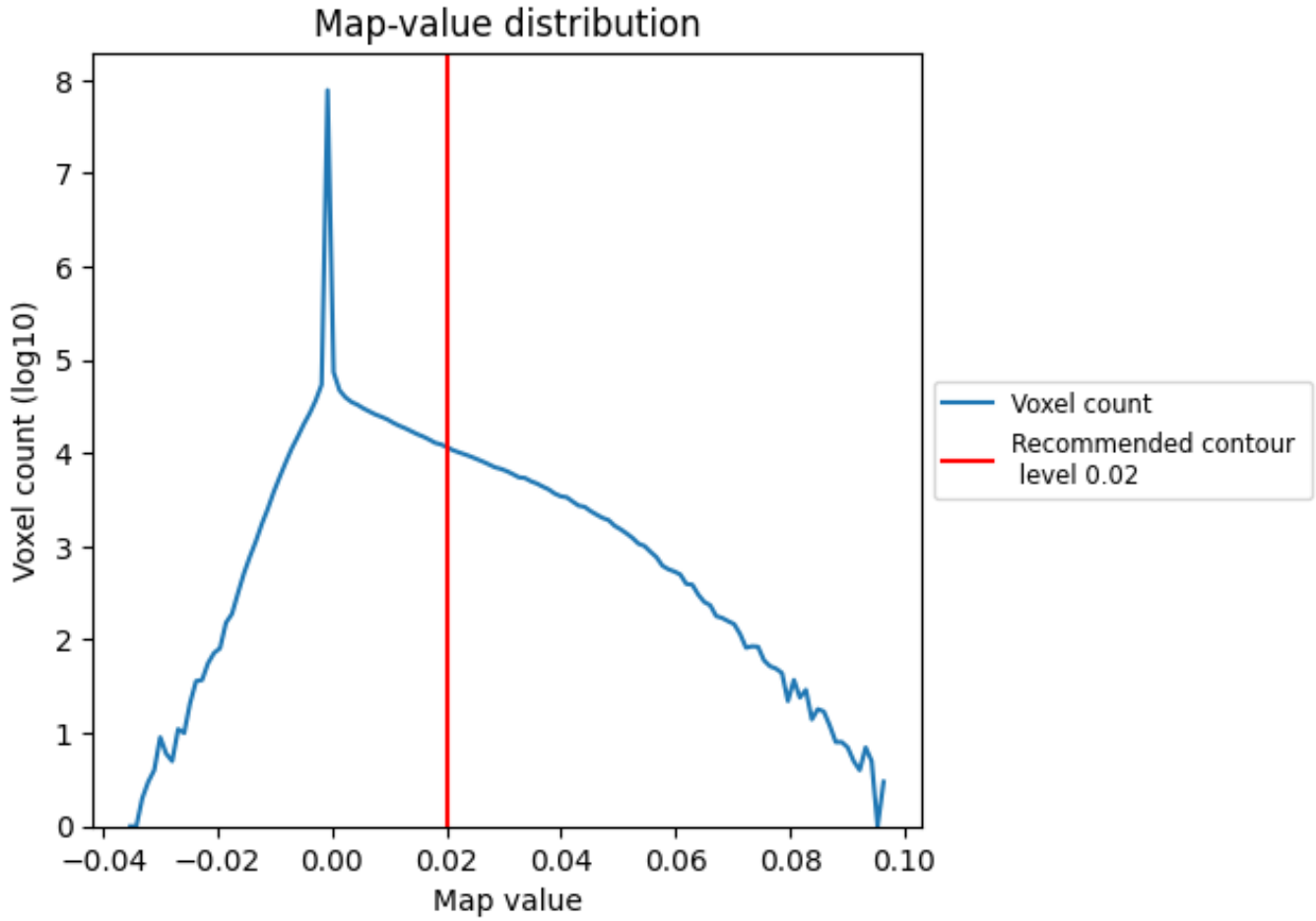
6.5 Mask visualisation (i)

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

7 Map analysis

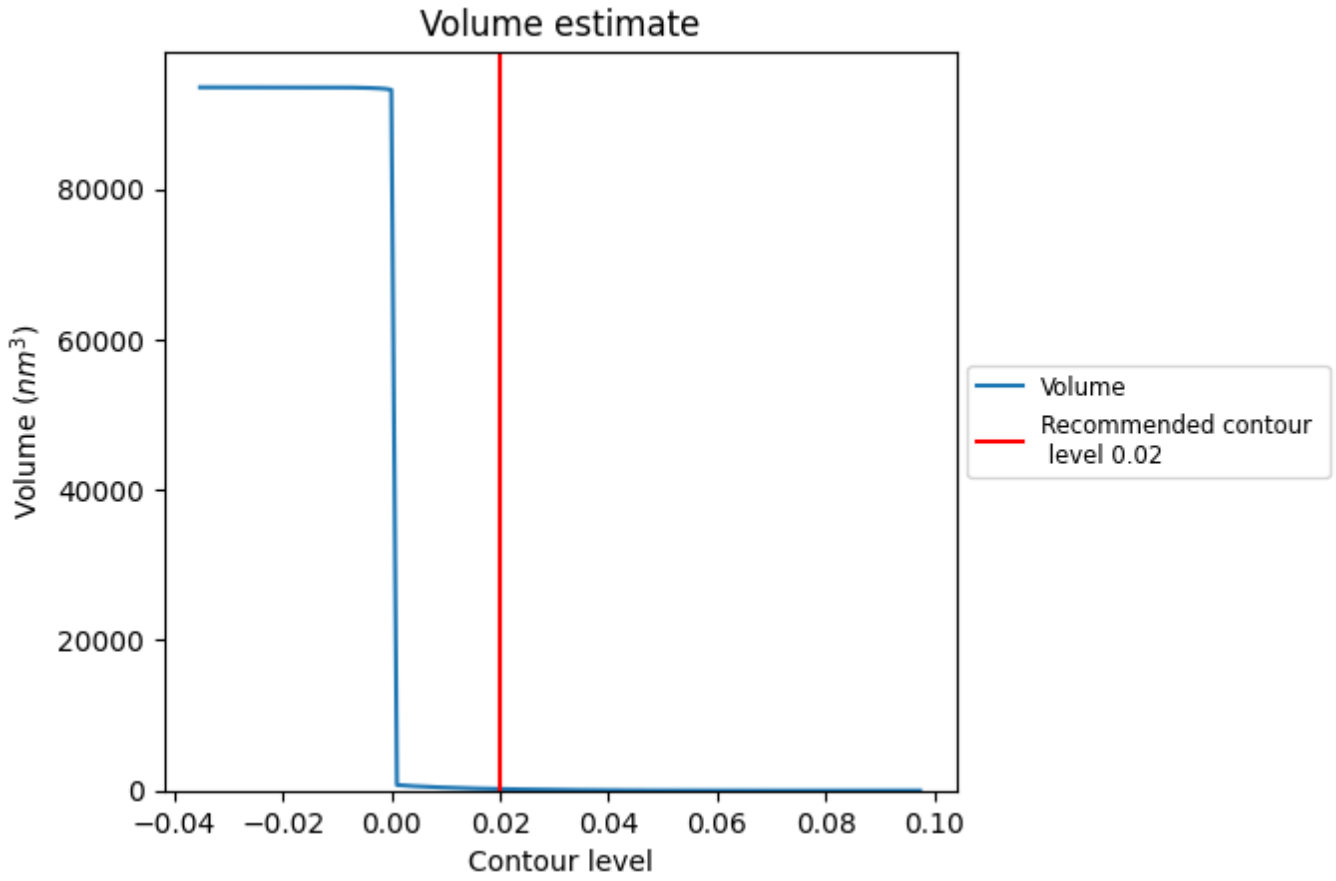
This section contains the results of statistical analysis of the map.

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.

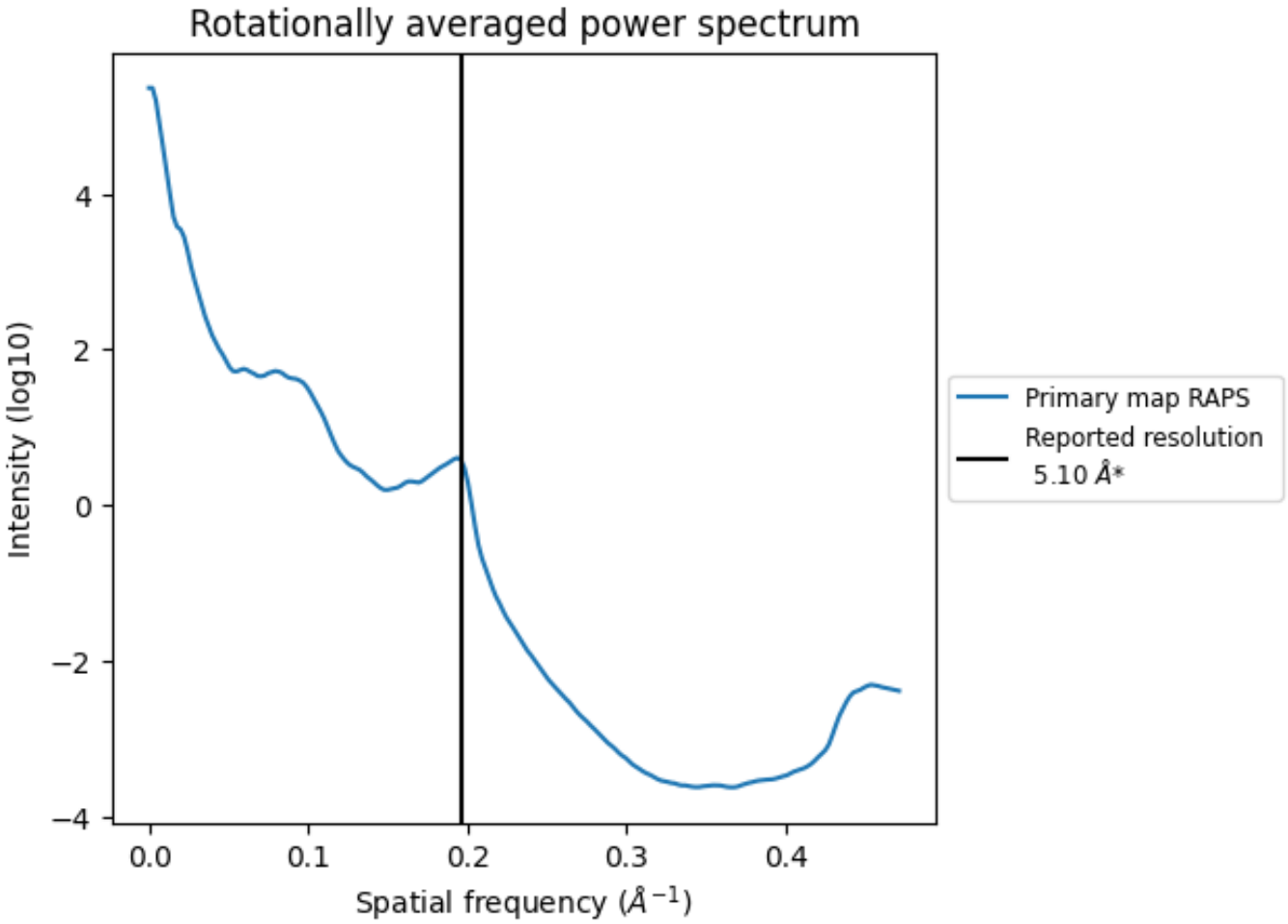
7.2 Volume estimate (i)



The volume at the recommended contour level is 207 nm^3; this corresponds to an approximate mass of 187 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 0.196 $Å^{-1}$

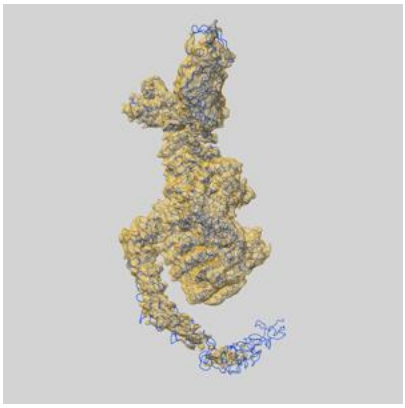
8 Fourier-Shell correlation (i)

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

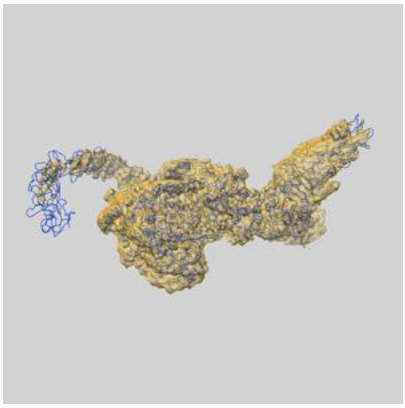
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24261 and PDB model 7N9S. Per-residue inclusion information can be found in section 3 on page 4.

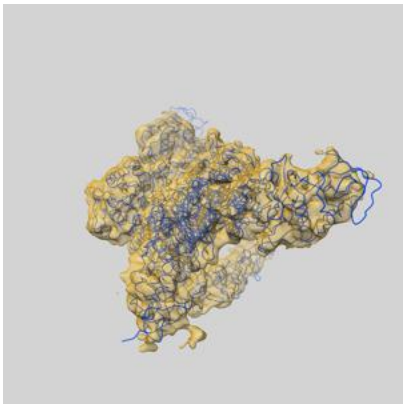
9.1 Map-model overlay



X



Y



Z

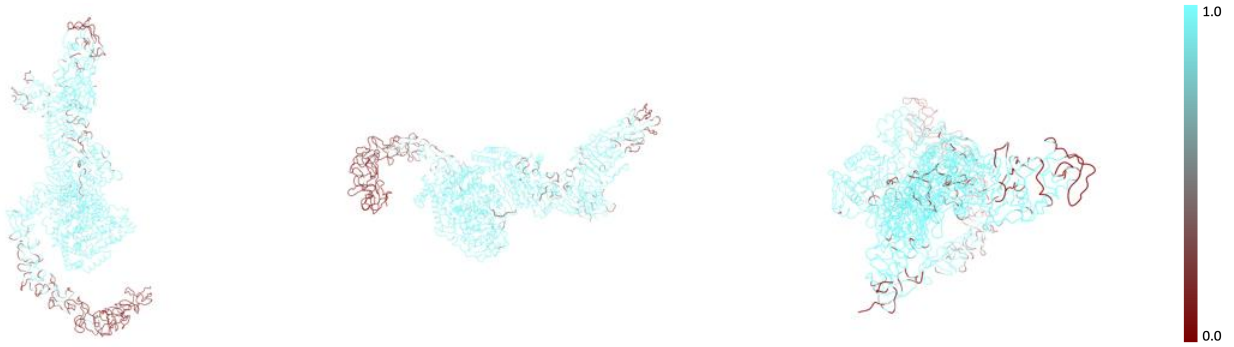
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

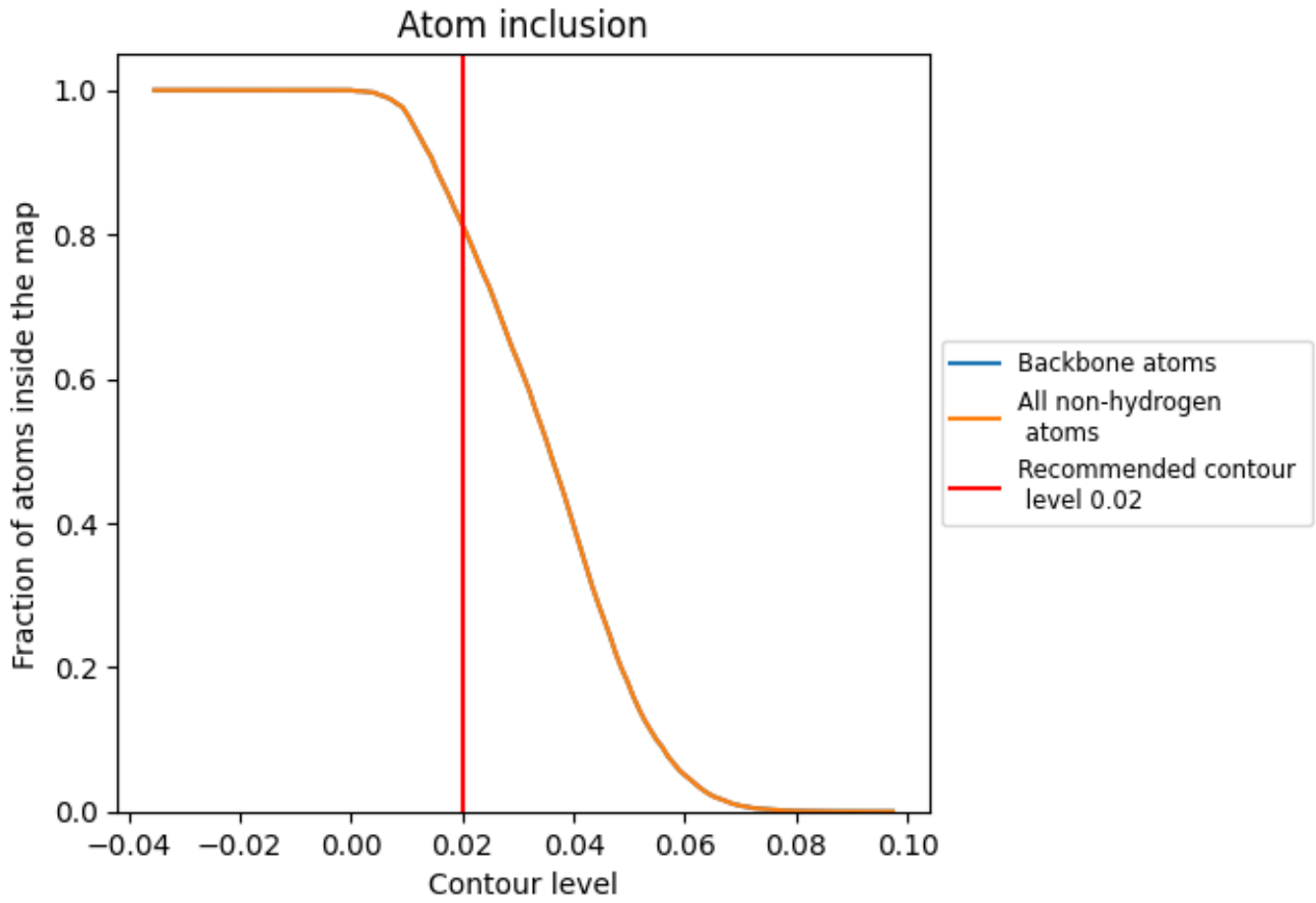
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8142	0.2760
A	0.8155	0.2780
B	0.7879	0.2250