wwPDB EM Validation Summary Report (i)

Dec 11, 2022 – 05:58 am GMT

PDB ID	:	6RW6
EMDB ID	:	EMD-10033
Title	:	Cryo-EM structure of Photorhabdus luminescens TcdA1
Authors	:	Roderer, D.; Leidreiter, F.; Gatsogiannis, C.; Meusch, D.; Benz, R.; Raunser, S.
Deposited on	:	2019-06-04
Resolution	:	2.75 Å(reported)
Based on initial model	:	1VW1

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:

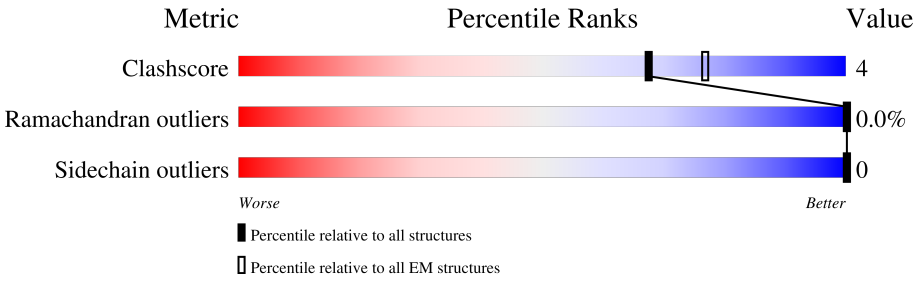
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 2.75 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	2516	88% 11%
1	B	2516	88% 11%
1	C	2516	88% 11%
1	D	2516	88% 11%
1	E	2516	88% 11%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 98645 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 TcdA1.

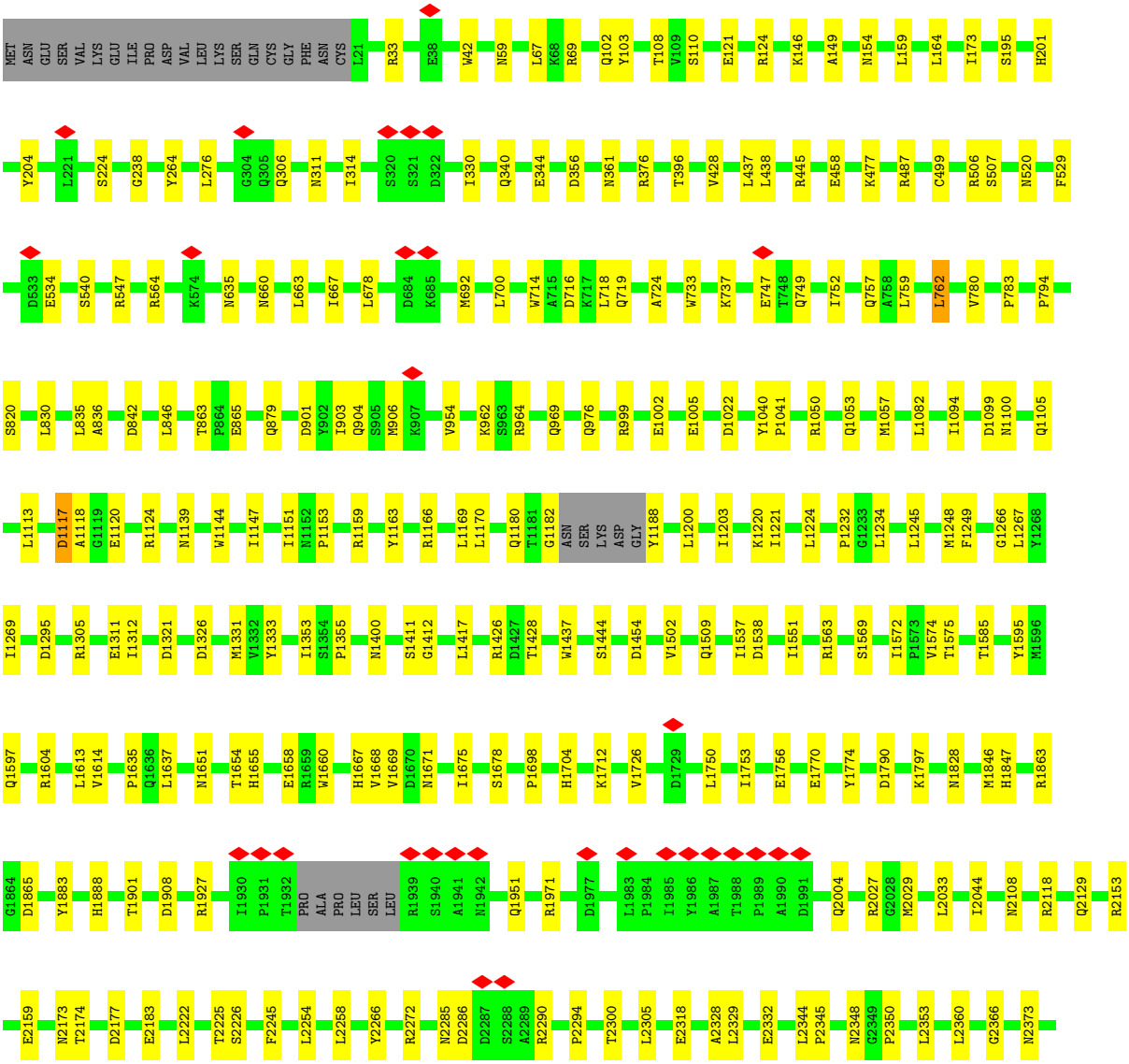
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2485	Total	C	N	O	S	0	0
			19729	12485	3357	3826	61		
1	B	2485	Total	C	N	O	S	0	0
			19729	12485	3357	3826	61		
1	C	2485	Total	C	N	O	S	0	0
			19729	12485	3357	3826	61		
1	D	2485	Total	C	N	O	S	0	0
			19729	12485	3357	3826	61		
1	E	2485	Total	C	N	O	S	0	0
			19729	12485	3357	3826	61		

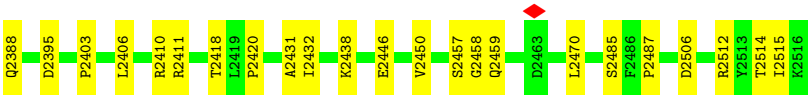
3 Residue-property plots (i)

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: TcdA1

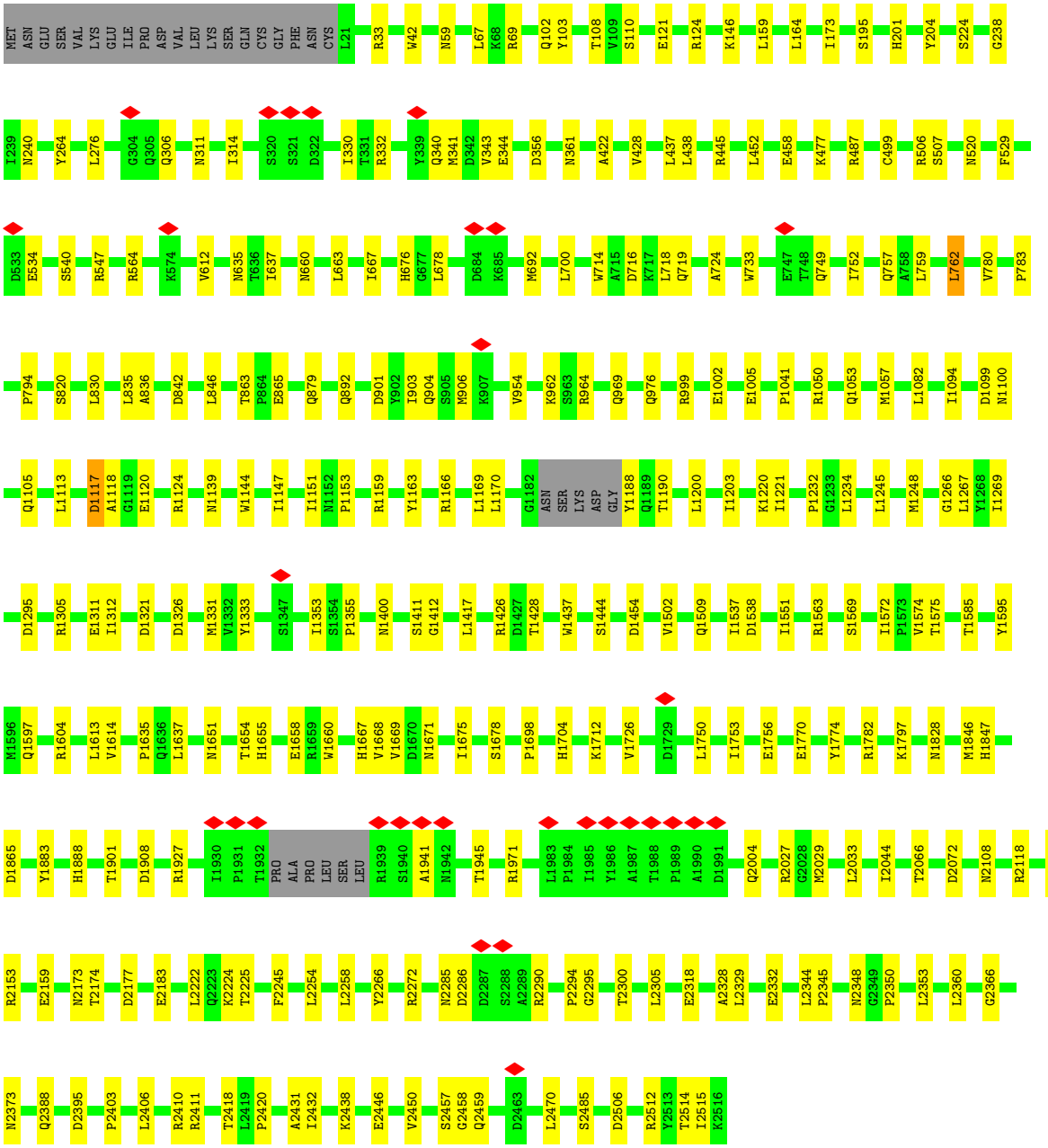
Chain A:





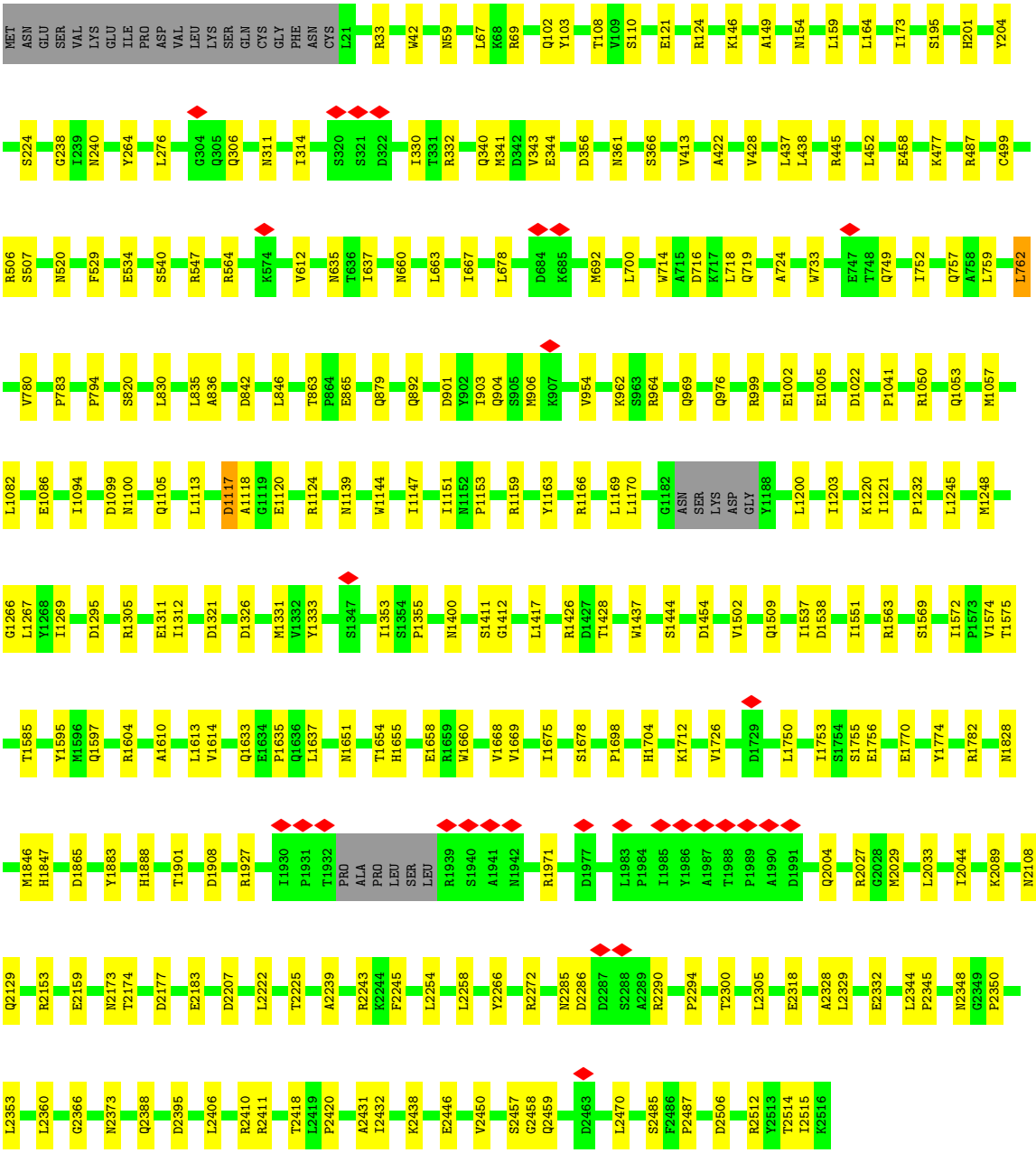
• Molecule 1: TcdA1

Chain B:



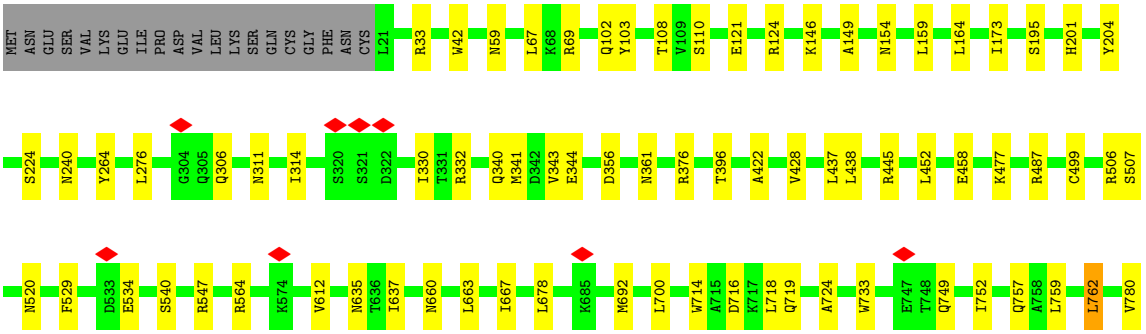
• Molecule 1: TcdA1

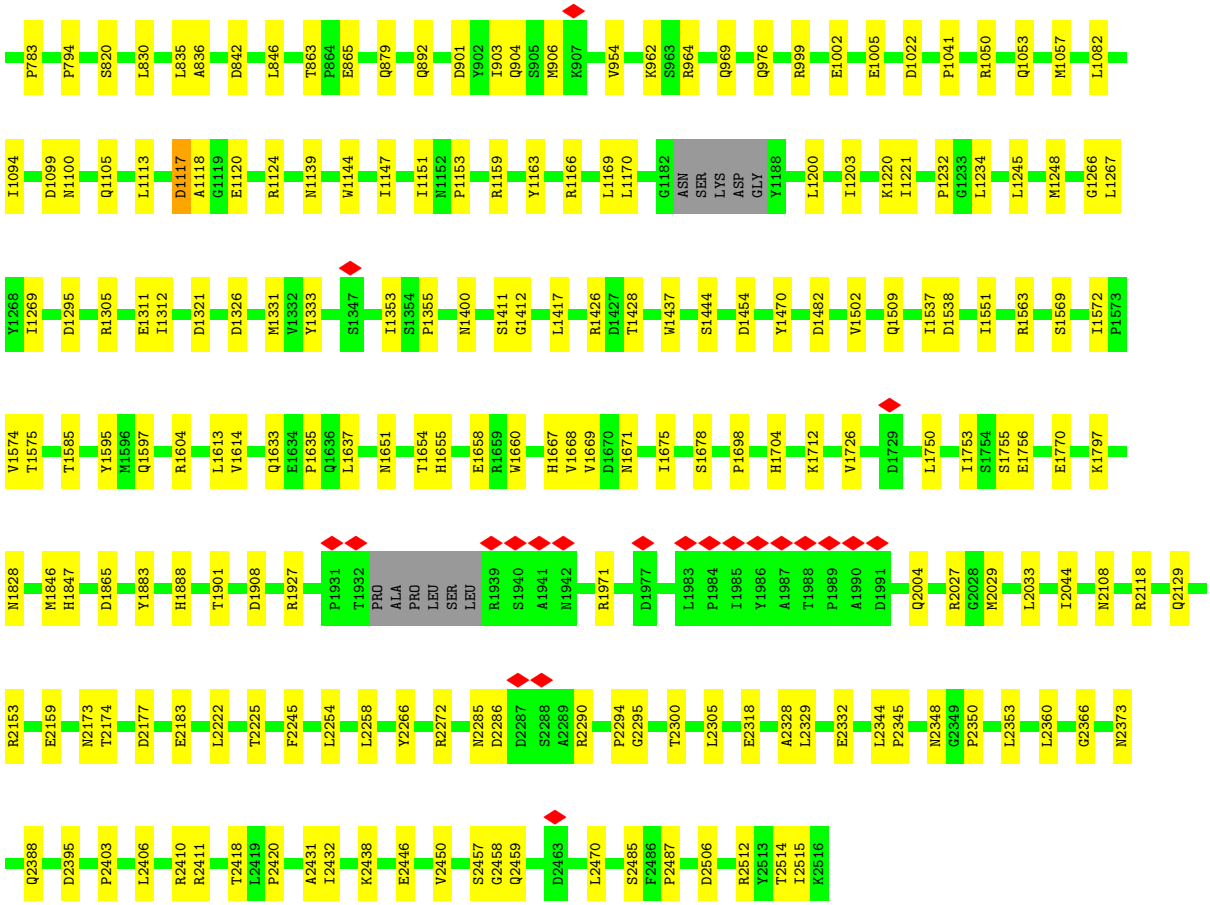
Chain C:



• Molecule 1: TcdA1

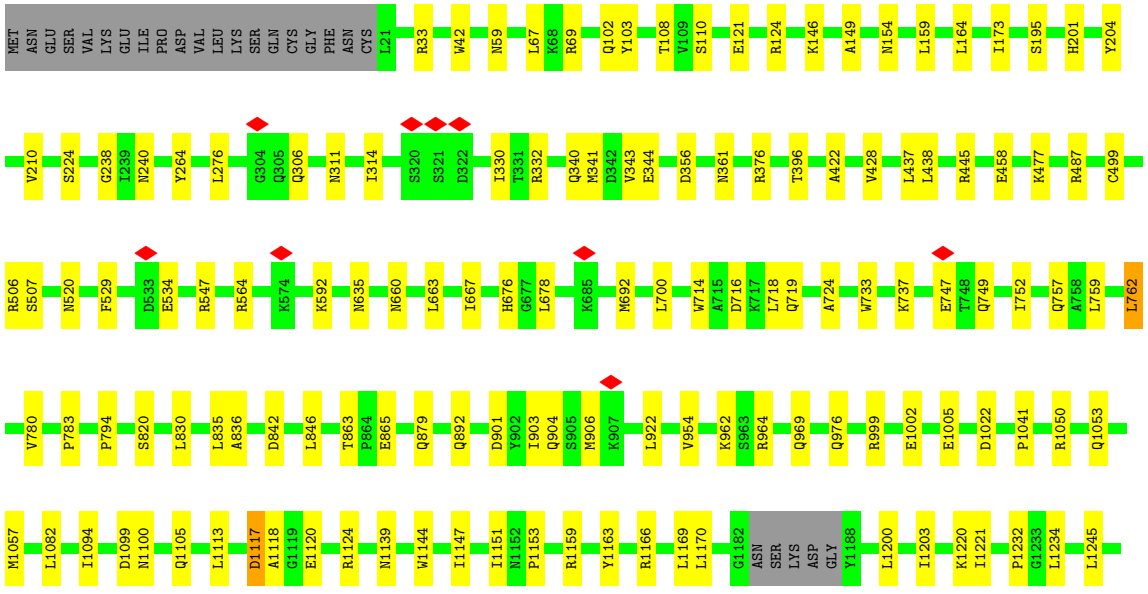
Chain D:

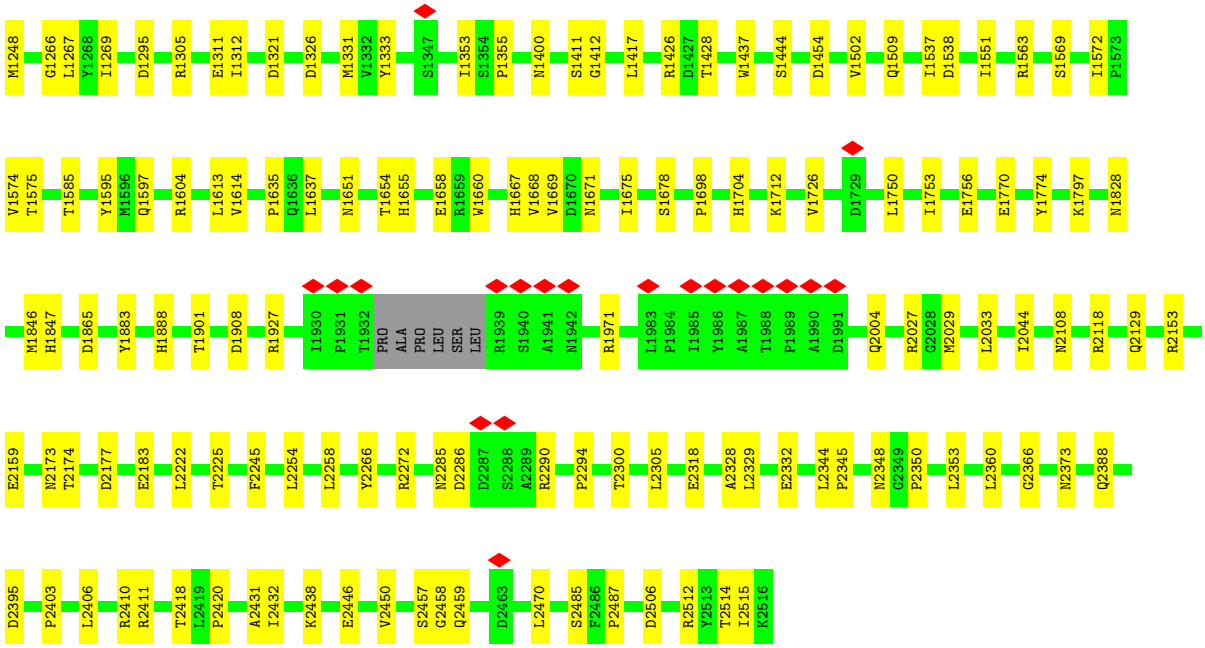




• Molecule 1: TcdA1

Chain E:




M1248 G1266 L1267 Y1268 I1269 D1295 R1305 E1311 I1312 D1321 D1326 M1331 V1332 Y1333 S1347 I1353 S1354 P1355 N1400 S1411 G1412 L1417 R1426 D1427 T1428 W1437 S1444 D1454 V1502 Q1509 I1537 D1538 I1551 R1563 S1569 I1572 P1573
V1574 T1575 T1585 Y1595 M1596 Q1597 R1604 L1613 V1614 P1635 Q1636 L1637 N1651 T1654 H1655 E1658 R1659 W1660 H1667 V1668 V1669 D1670 N1671 I1675 S1678 P1698 H1704 K1712 V1726 D1729 L1750 I1753 E1756 E1770 Y1774 K1797 N1828
M1846 H1847 D1865 Y1883 H1888 T1901 D1908 R1927 T1930 P1931 T1932 PRO ALA PRO LEU SER LEU R1939 S1940 A1941 N1942 R1971 L1983 P1984 I1985 Y1986 A1987 T1988 P1989 A1990 D1991 Q2004 R2027 C2028 M2029 L2033 I2044 N2108 R2118 Q2129 R2153
E2159 N2173 T2174 D2177 E2183 L2222 T2225 F2245 L2254 L2258 Y2266 R2272 N2285 D2286 D2287 S2288 A2289 R2290 P2294 T2300 L2305 E2318 A2328 L2329 E2332 L2344 P2345 N2348 G2349 P2350 L2353 L2360 G2366 N2373 Q2388
D2395 P2403 L2406 R2410 R2411 T2418 L2419 P2420 A2431 I2432 K2438 E2446 V2450 S2457 G2458 Q2459 D2463 L2470 S2485 F2486 P2487 D2506 R2512 Y2513 T2514 I2515 K2516

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	436273	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 ($e^-/Å^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.303	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	437.76, 437.76, 437.76	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.14, 1.14, 1.14	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	0.54	0/20154	0.56	1/27374 (0.0%)
1	B	0.54	0/20154	0.56	1/27374 (0.0%)
1	C	0.54	0/20154	0.56	1/27374 (0.0%)
1	D	0.54	0/20154	0.56	1/27374 (0.0%)
1	E	0.54	0/20154	0.56	1/27374 (0.0%)
All	All	0.54	0/100770	0.56	5/136870 (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	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
All	All	0	15

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	762	LEU	CA-CB-CG	-5.56	102.50	115.30
1	A	762	LEU	CA-CB-CG	-5.56	102.51	115.30
1	C	762	LEU	CA-CB-CG	-5.55	102.54	115.30
1	B	762	LEU	CA-CB-CG	-5.54	102.57	115.30
1	E	762	LEU	CA-CB-CG	-5.53	102.58	115.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1117	ASP	Peptide
1	A	1412	GLY	Peptide
1	A	1668	VAL	Peptide
1	B	1117	ASP	Peptide
1	B	1412	GLY	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	19729	0	19276	168	0
1	B	19729	0	19276	170	0
1	C	19729	0	19276	167	0
1	D	19729	0	19276	166	0
1	E	19729	0	19276	168	0
All	All	98645	0	96380	752	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 4.

The worst 5 of 752 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:340:GLN:HE22	1:A:361:ASN:HD22	1.41	0.69
1:C:340:GLN:HE22	1:C:361:ASN:HD22	1.41	0.69
1:E:340:GLN:HE22	1:E:361:ASN:HD22	1.41	0.69
1:B:340:GLN:HE22	1:B:361:ASN:HD22	1.41	0.69
1:D:340:GLN:HE22	1:D:361:ASN:HD22	1.41	0.69

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	2479/2516 (98%)	2424 (98%)	54 (2%)	1 (0%)	100	100
1	B	2479/2516 (98%)	2423 (98%)	55 (2%)	1 (0%)	100	100
1	C	2479/2516 (98%)	2423 (98%)	55 (2%)	1 (0%)	100	100
1	D	2479/2516 (98%)	2424 (98%)	54 (2%)	1 (0%)	100	100
1	E	2479/2516 (98%)	2423 (98%)	55 (2%)	1 (0%)	100	100
All	All	12395/12580 (98%)	12117 (98%)	273 (2%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1669	VAL
1	B	1669	VAL
1	C	1669	VAL
1	D	1669	VAL
1	E	1669	VAL

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	2129/2157 (99%)	2129 (100%)	0	100	100
1	B	2129/2157 (99%)	2129 (100%)	0	100	100
1	C	2129/2157 (99%)	2129 (100%)	0	100	100
1	D	2129/2157 (99%)	2129 (100%)	0	100	100
1	E	2129/2157 (99%)	2129 (100%)	0	100	100
All	All	10645/10785 (99%)	10645 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 140

such sidechains are listed below:

Mol	Chain	Res	Type
1	E	102	GLN
1	E	584	ASN
1	E	1687	ASN
1	B	1743	HIS
1	B	1704	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

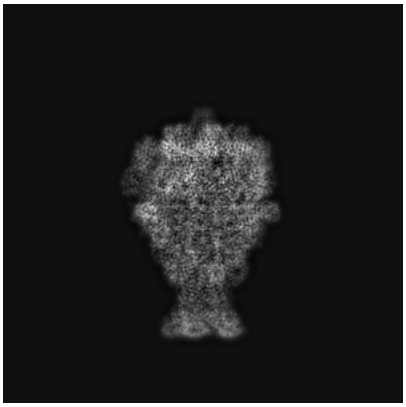
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10033. These allow visual inspection of the internal detail of the map and identification of artifacts.

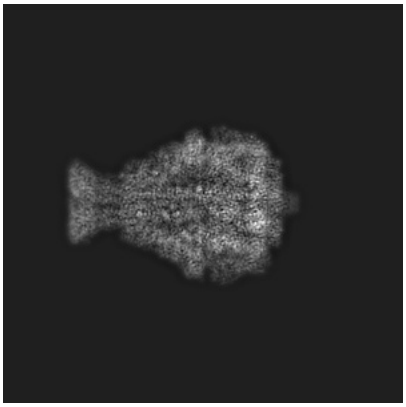
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

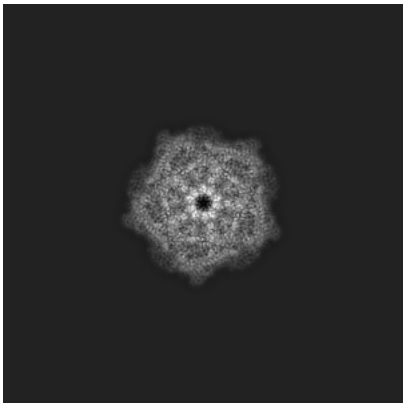
6.1.1 Primary map



X



Y



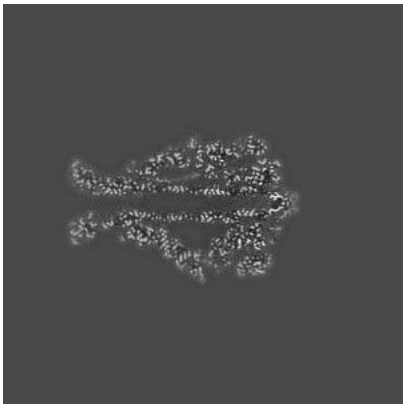
Z

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

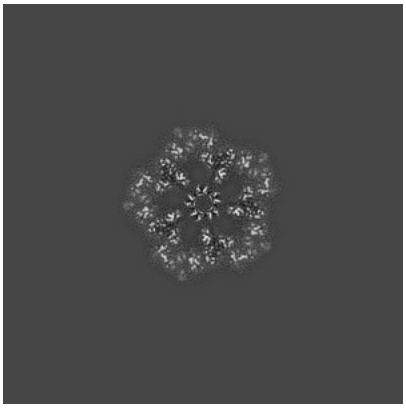
6.2 Central slices

6.2.1 Primary map

X Index: 192



Y Index: 192

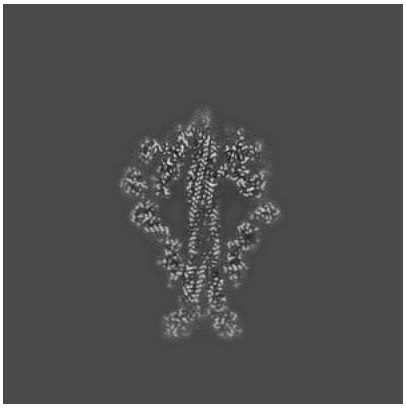


Z Index: 192

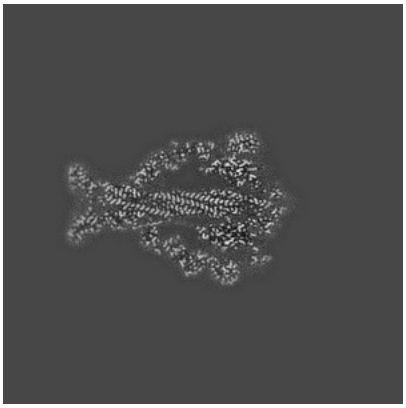
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

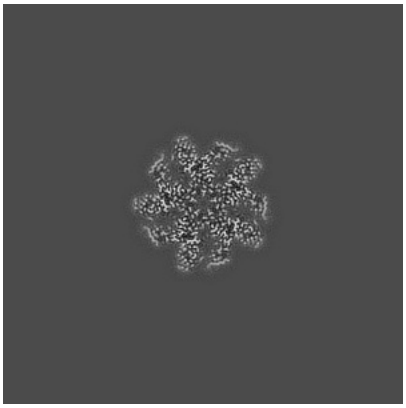
6.3.1 Primary map



X Index: 183



Y Index: 180



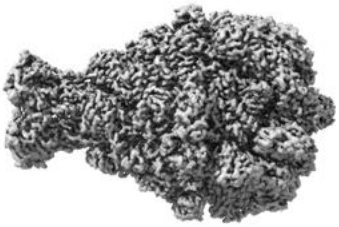
Z Index: 245

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

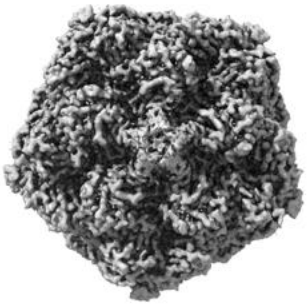
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

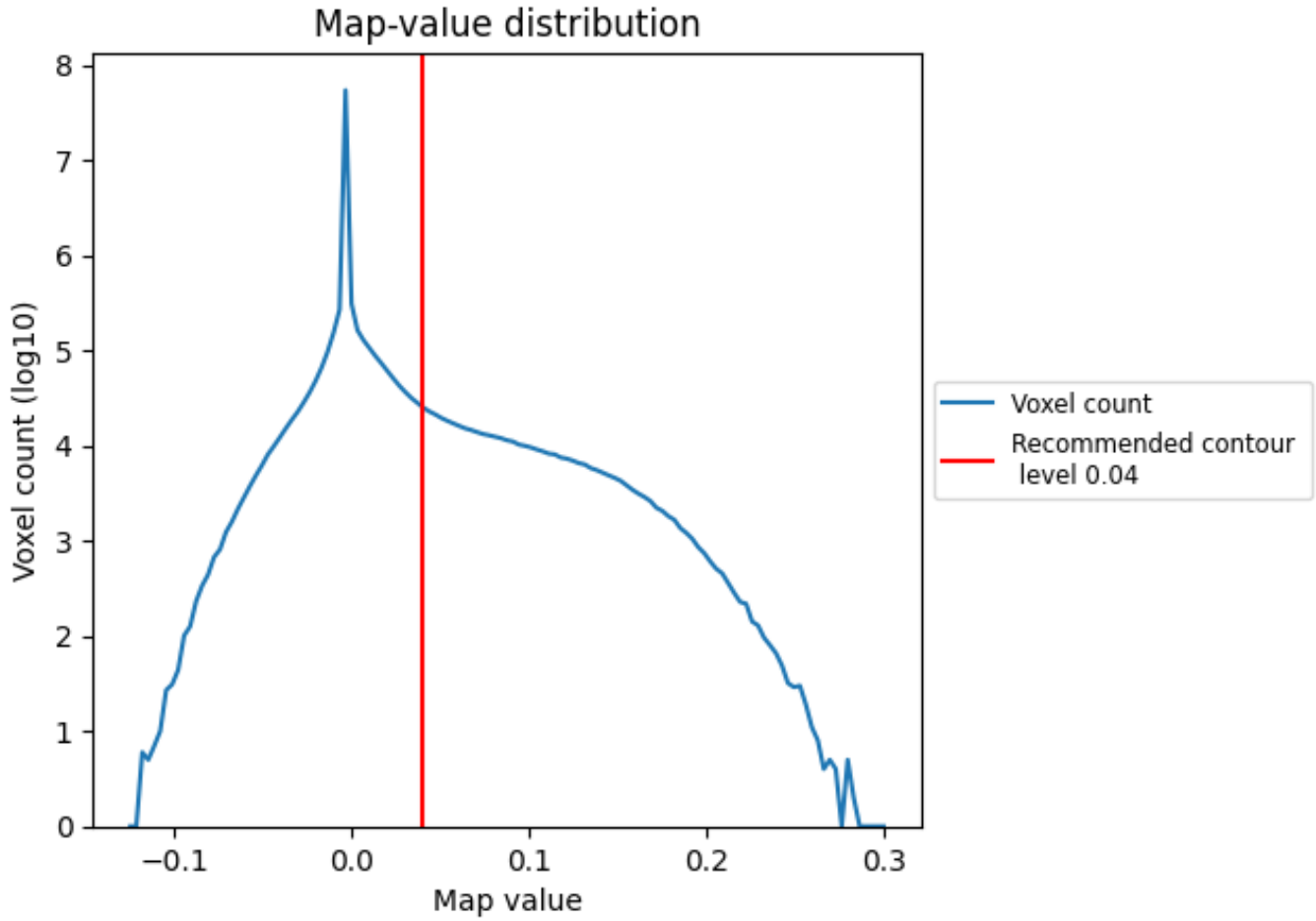
6.5 Mask visualisation (i)

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

7 Map analysis

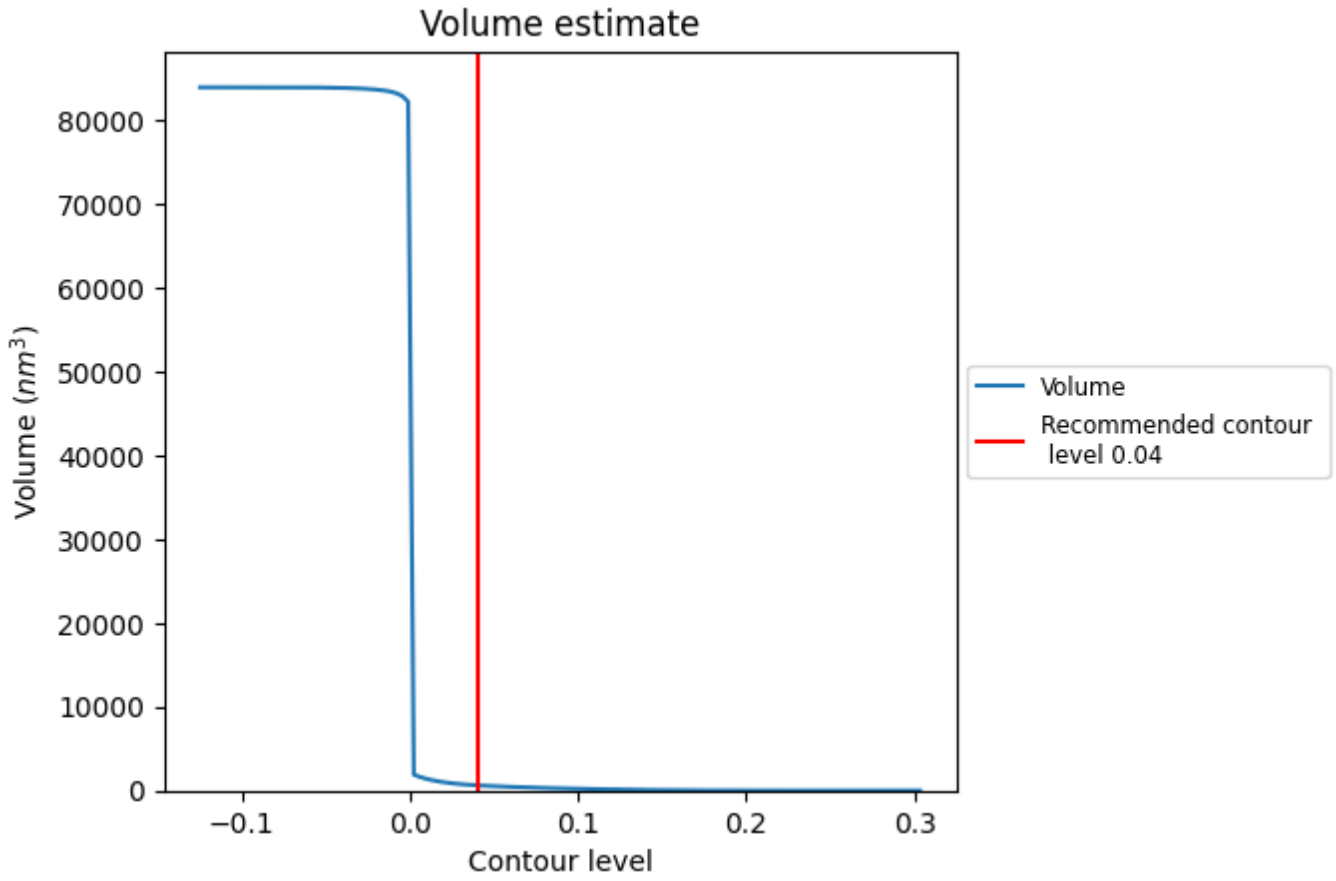
This section contains the results of statistical analysis of the map.

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.

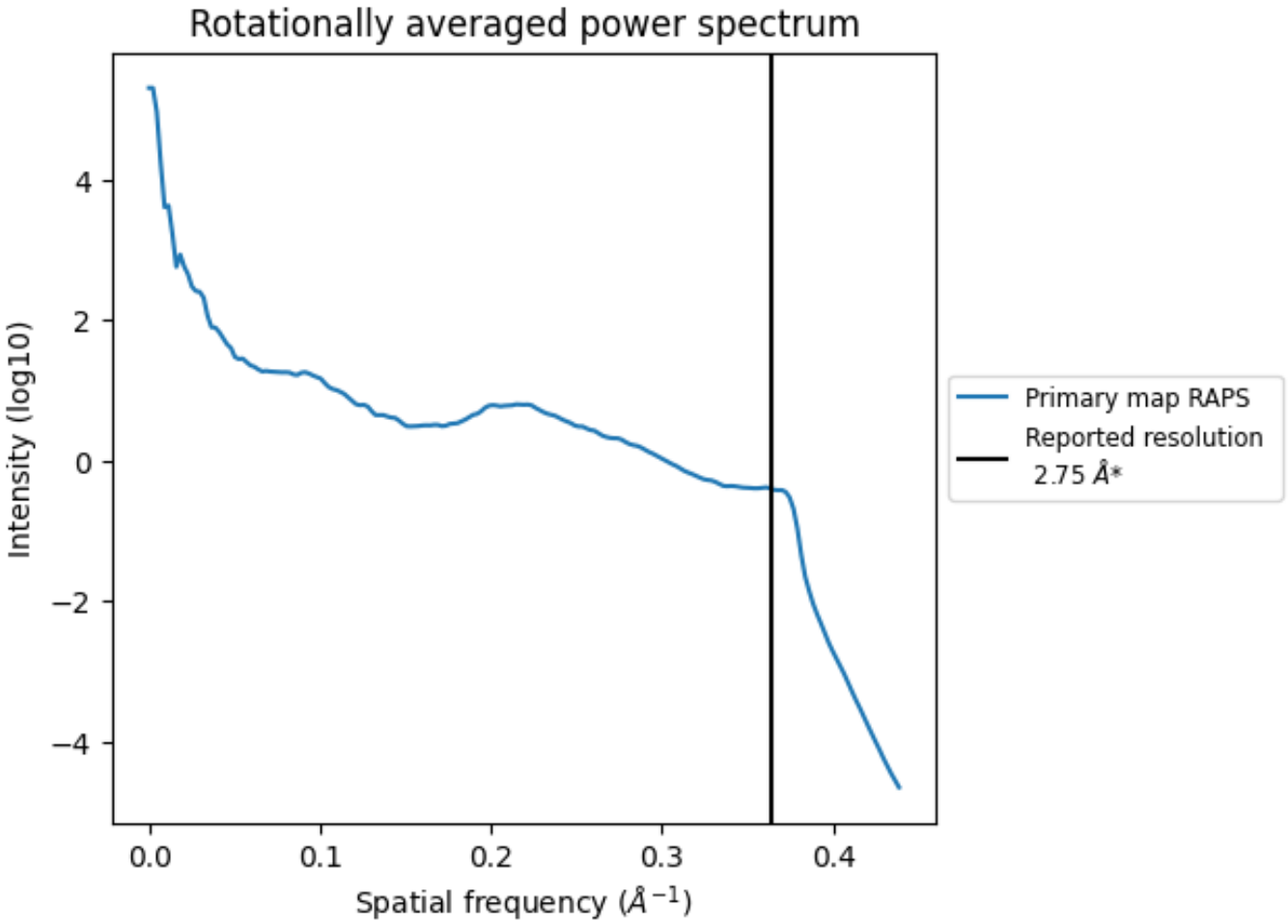
7.2 Volume estimate (i)



The volume at the recommended contour level is 624 nm^3; this corresponds to an approximate mass of 564 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 0.364 Å^{-1}

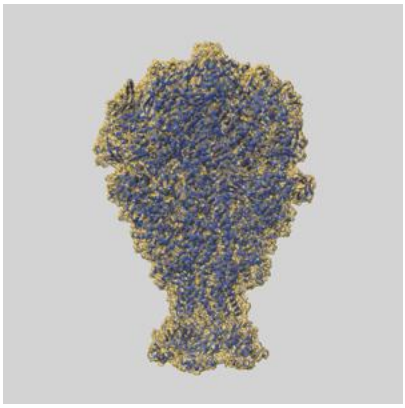
8 Fourier-Shell correlation (i)

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

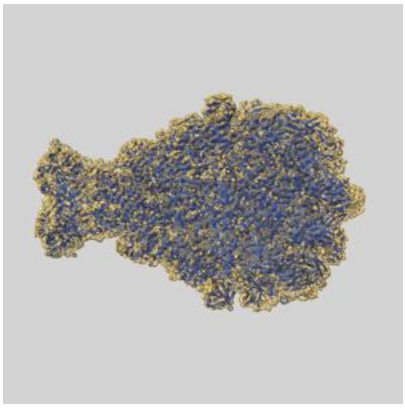
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10033 and PDB model 6RW6. Per-residue inclusion information can be found in section 3 on page 4.

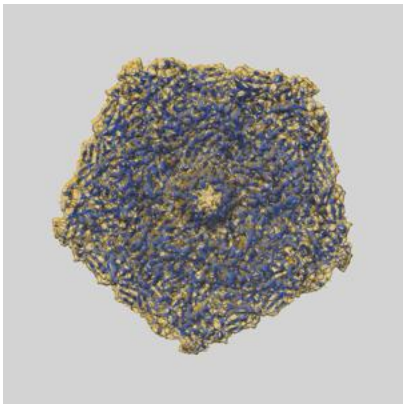
9.1 Map-model overlay



X



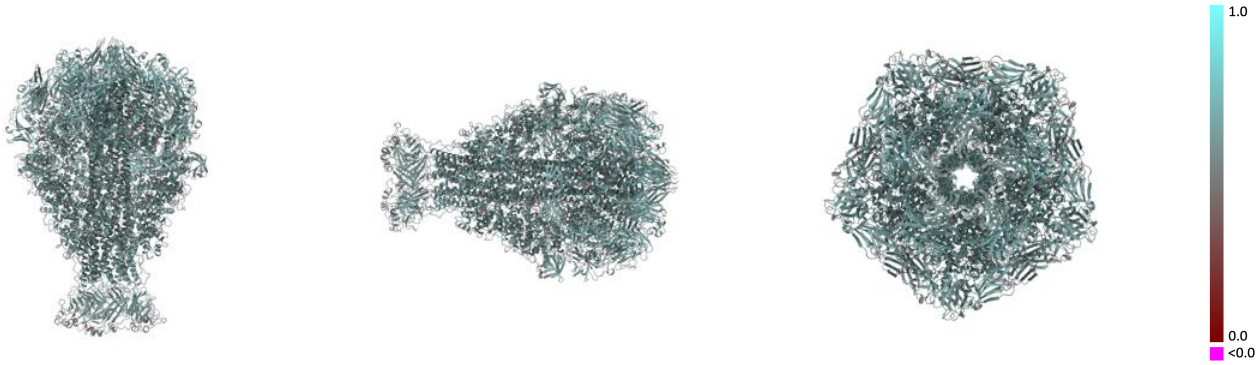
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

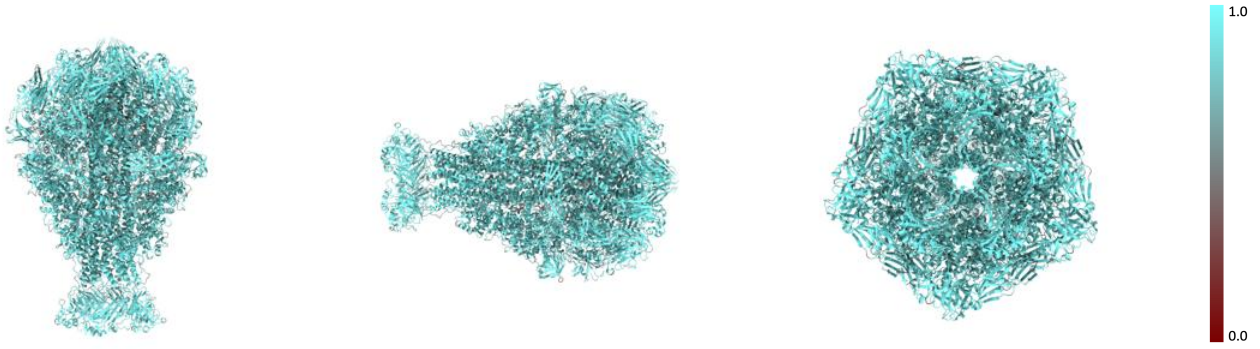
9.2 Q-score mapped to coordinate model (i)



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.

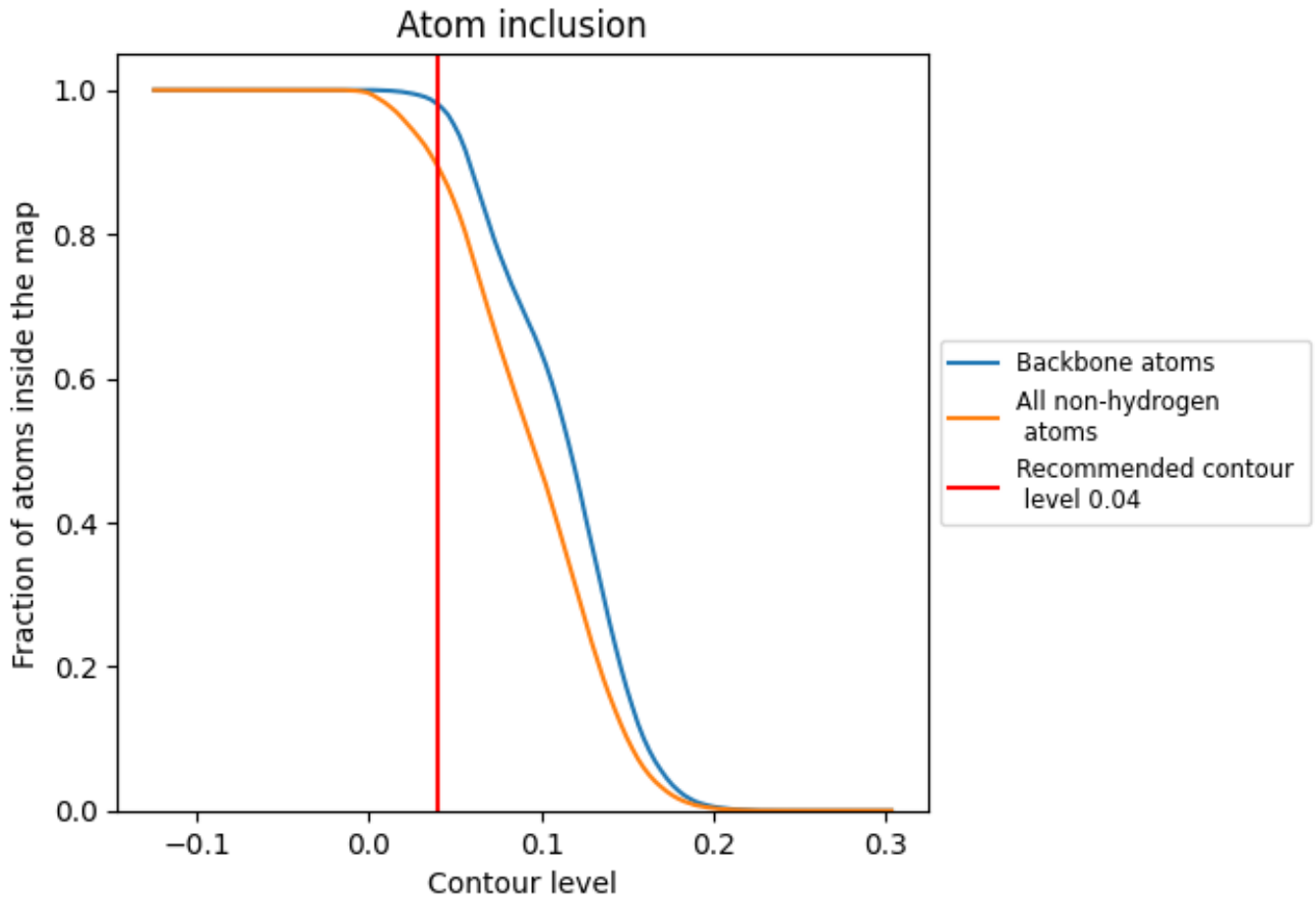
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 89% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8936	0.5850
A	0.8939	0.5850
B	0.8929	0.5840
C	0.8935	0.5850
D	0.8941	0.5850
E	0.8938	0.5850