wwPDB EM Validation Summary Report

Mar 17, 2026 – 12:05 PM UTC

PDB ID	:	7Z7N / pdb_00007z7n
EMDB ID	:	EMD-14534
Title	:	Mot1E1434Q:TBP:DNA - substrate recognition state
Authors	:	Woike, S.; Eustermann, S.; Jung, J.; Wenzl, S.J.; Hagemann, G.; Bartho, J.D.; Lammens, K.; Butryn, A.; Herzog, F.; Hopfner, K.-P.
Deposited on	:	2022-03-16
Resolution	:	5.10 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 ⓘ 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:

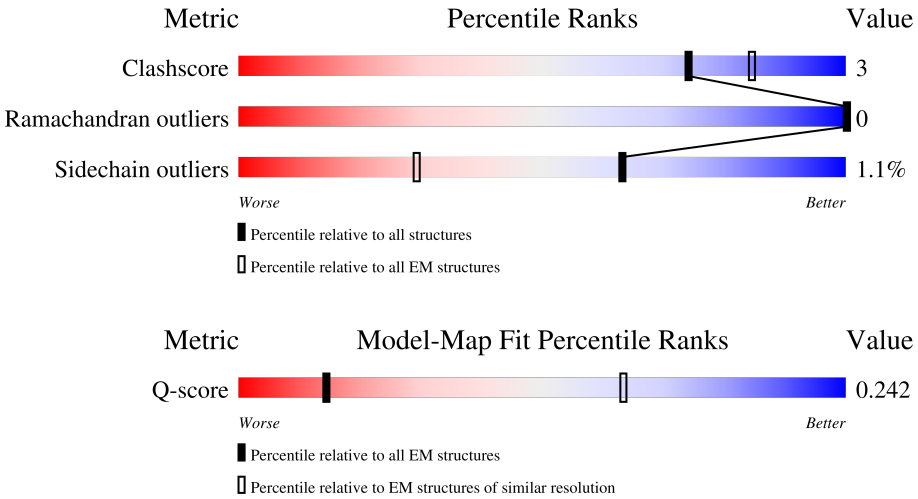
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	844 (4.60 - 5.60)

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	36	6%, 53%, 44%, ·
2	B	36	6%, 61%, 36%, ·
3	D	276	·, 37%, 26%, ·, 36%
4	E	1897	·, 60%, 9%, 31%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 25969 atoms, of which 12825 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 DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	36	1144	348	400	147	213	36	0	0

- Molecule 2 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	B	36	1135	345	403	132	219	36	0	0

- Molecule 3 is a protein called Putative tata-box binding protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	D	178	2907	919	1490	245	247	6	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	initiating methionine	UNP G0SAL6
D	-19	GLY	-	expression tag	UNP G0SAL6
D	-18	SER	-	expression tag	UNP G0SAL6
D	-17	SER	-	expression tag	UNP G0SAL6
D	-16	HIS	-	expression tag	UNP G0SAL6
D	-15	HIS	-	expression tag	UNP G0SAL6
D	-14	HIS	-	expression tag	UNP G0SAL6
D	-13	HIS	-	expression tag	UNP G0SAL6
D	-12	HIS	-	expression tag	UNP G0SAL6
D	-11	HIS	-	expression tag	UNP G0SAL6
D	-10	SER	-	expression tag	UNP G0SAL6
D	-9	SER	-	expression tag	UNP G0SAL6
D	-8	GLY	-	expression tag	UNP G0SAL6
D	-7	GLU	-	expression tag	UNP G0SAL6
D	-6	ASN	-	expression tag	UNP G0SAL6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	LEU	-	expression tag	UNP G0SAL6
D	-4	TYR	-	expression tag	UNP G0SAL6
D	-3	PHE	-	expression tag	UNP G0SAL6
D	-2	GLN	-	expression tag	UNP G0SAL6
D	-1	GLY	-	expression tag	UNP G0SAL6
D	0	HIS	-	expression tag	UNP G0SAL6

- Molecule 4 is a protein called Helicase-like protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	1306	Total	C	H	N	O	S	0	0
			20783	6520	10532	1807	1872	52		

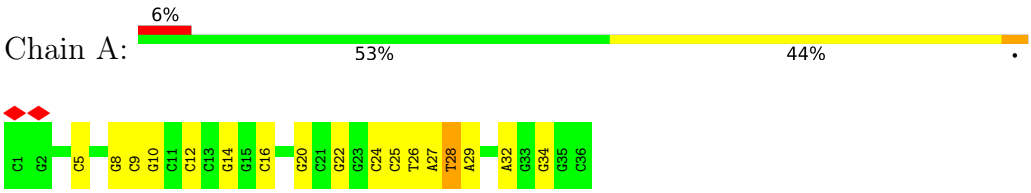
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1434	GLN	GLU	engineered mutation	UNP G0S6C0
E	1887	ALA	-	expression tag	UNP G0S6C0
E	1888	ALA	-	expression tag	UNP G0S6C0
E	1889	ALA	-	expression tag	UNP G0S6C0
E	1890	TRP	-	expression tag	UNP G0S6C0
E	1891	SER	-	expression tag	UNP G0S6C0
E	1892	HIS	-	expression tag	UNP G0S6C0
E	1893	PRO	-	expression tag	UNP G0S6C0
E	1894	GLN	-	expression tag	UNP G0S6C0
E	1895	PHE	-	expression tag	UNP G0S6C0
E	1896	GLU	-	expression tag	UNP G0S6C0
E	1897	LYS	-	expression tag	UNP G0S6C0

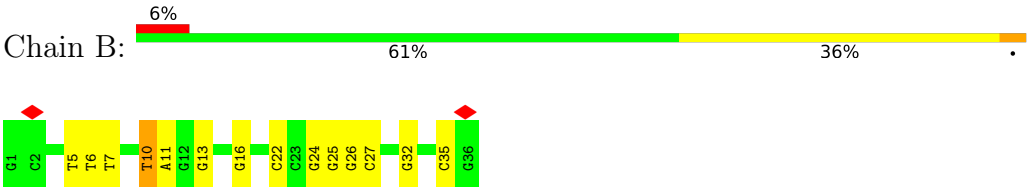
3 Residue-property plots (i)

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.

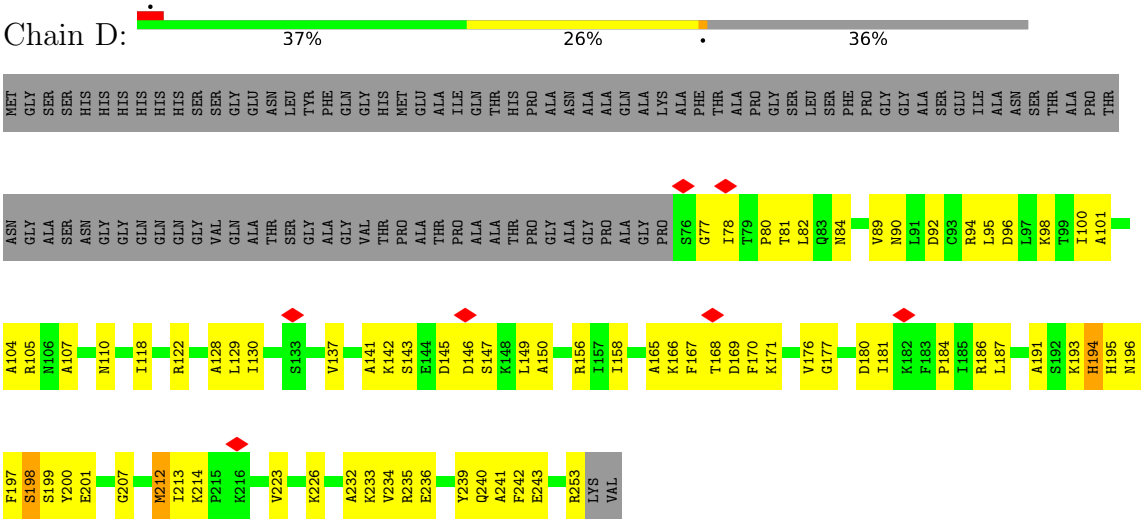
• Molecule 1: DNA (36-MER)



• Molecule 2: DNA (36-MER)

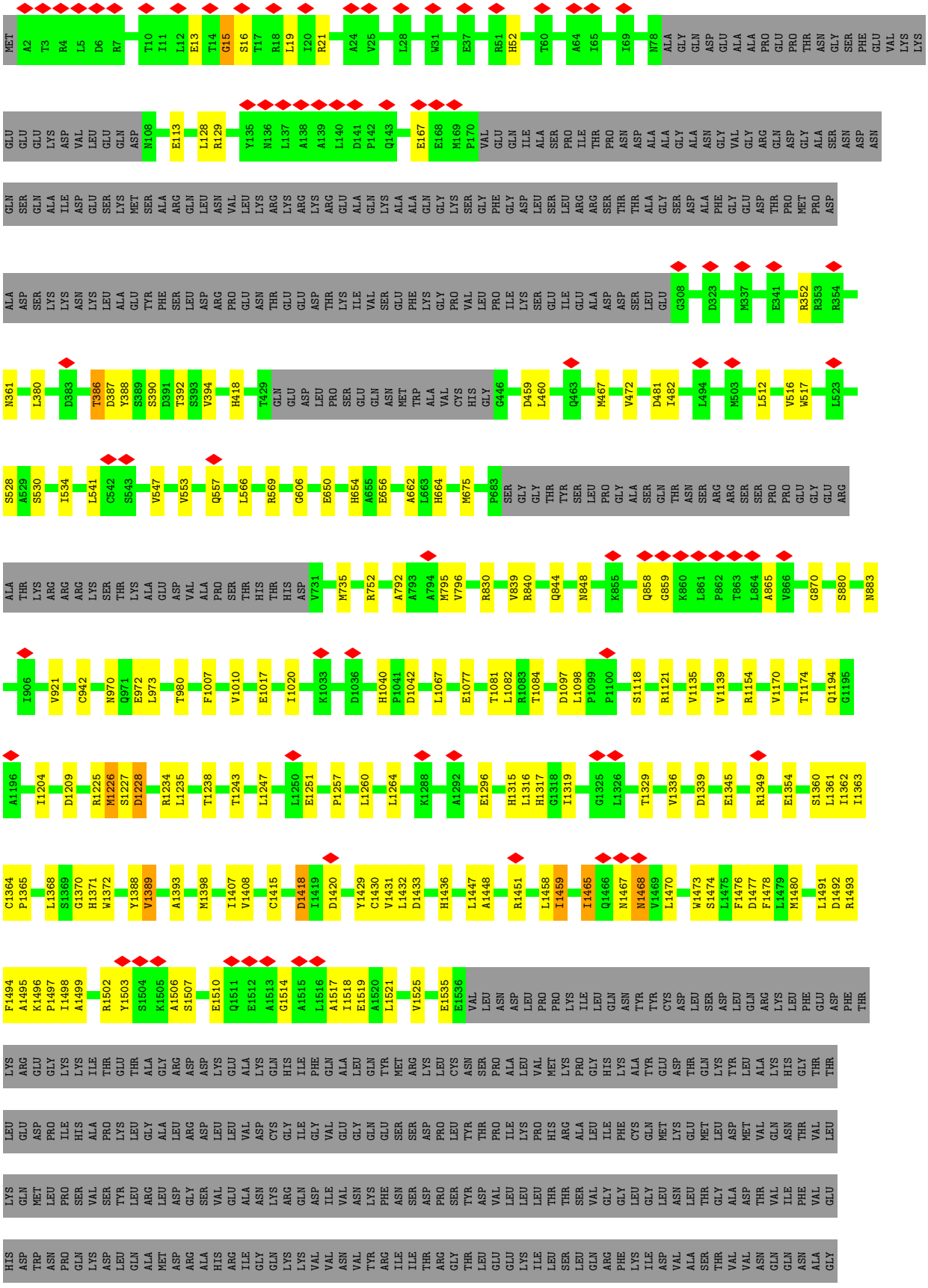


• Molecule 3: Putative tata-box binding protein



• Molecule 4: Helicase-like protein

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GLU GLU GLU LYS ASP VAL LEU GLU GLN ASP N108 E113 L128 R129 Y135 N136 L137 A138 A139 L140 D141 P142 Q143 E167 E168 M169 P170 VAL GLU GLN ILE ALA SER PRO ILE THR PRO ASN ASP ALA ALA GLY ALA ASN GLY VAL GLY ARG GLN ASP GLY ALA SER ASN ASP ASN
GLN SER GLN ALA ILE ASP GLU SER LYS MET SER ALA ARG GLN LEU ASN VAL LEU LYS ARG LYS ARG LYS ARG GLU ALA GLN LYS ALA ALA ALA GLN GLY LYS SER GLY PHE GLY ASP LEU SER LEU ARG ARG SER THR THR ALA GLY SER ASP ALA PHE GLY GLU ASP THR PRO MET PRO ASP
ALA ASP SER LYS LYS ASN LYS LEU ALA GLU TYR PHE SER LEU ASP ARG PRO GLU ASN THR GLU GLU ASP THR LYS ILE VAL SER GLU PHE LYS GLY PRO VAL LEU PRO ILE LYS SER GLU ILE GLU ALA ASP SER LEU G308 D323 M337 E341 R352 R353 R354
N361 L380 D383 T386 D387 Y388 S389 S390 D391 T392 S393 V394 H418 T429 GLN GLU ASP LEU PRO SER GLU GLN ASN MET TRP ALA VAL CYS HIS GLY G446 D459 L460 Q463 M467 V472 D481 I482 L494 M503 L512 V516 W517 L523
S528 A529 S530 I534 L541 C542 S543 V547 V553 Q557 L566 R569 G606 E650 H654 A655 E656 A662 L663 H664 M675 P683 SER GLY GLY THR TYR SER LEU PRO GLY ALA SER GLN THR ASN SER ARG ARG SER SER PRO PRO GLU GLY GLU ARG
ALA THR LYS ARG ARG LYS SER THR LYS ALA GLU ASP VAL ALA PRO SER THR HIS THR HIS ASP V731 M735 R752 A792 A793 A794 M795 V796 R830 V839 R840 Q844 N848 K855 Q858 C859 K860 L861 P862 T863 L864 A865 V866 G870 S880 N883
T906 V921 C942 N970 Q971 E972 L973 T980 F1007 V1010 E1017 I1020 K1033 D1036 H1040 P1041 D1042 L1067 E1077 T1081 L1082 R1083 T1084 D1097 L1098 P1099 P1100 S1118 R1121 V1135 V1139 R1154 V1170 T1174 Q1194 G1196
A1196 I1204 D1209 R1225 M1226 S1227 D1228 R1234 L1235 T1238 T1243 L1247 L1250 E1251 P1257 L1260 L1264 K1288 A1292 E1296 H1315 L1316 H1317 G1318 I1319 G1325 L1326 T1329 V1336 D1339 E1345 R1349 E1354 S1360 L1361 I1362 I1363
C1364 P1365 L1368 S1369 G1370 H1371 W1372 Y1388 V1389 A1393 M1398 I1407 V1408 C1415 D1418 I1419 D1420 Y1429 C1430 V1431 L1432 D1433 H1436 L1447 A1448 R1451 L1458 I1459 I1465 Q1466 N1467 N1468 V1469 L1470 W1473 S1474 L1475 F1476 D1477 F1478 L1479 M1480 L1491 D1492 R1493
F1494 A1495 K1496 P1497 I1498 A1499 R1502 Y1503 S1504 K1505 A1506 S1507 E1510 Q1511 E1512 A1513 G1514 A1515 L1516 A1517 I1518 E1519 A1520 L1521 V1525 E1535 E1536 VAL LEU ASN ASP LEU PRO PRO LYS ILE LEU GLN ASN TYR TYR CYS ASP LEU SER ASP LEU GLN ARG LYS LEU PHE GLU ASP PHE THR
LYS ARG GLU GLY LYS LYS ILE THR GLU THR ALA GLY ARG ASP ASP LYS GLU ALA LYS GLN HIS ILE PHE GLN ALA LEU GLN TYR MET ARG LYS LEU CYS ASN SER PRO ALA LEU VAL MET LYS PRO GLY HIS LYS ALA TYR GLU ASP THR GLN LYS LEU ASP THR GLN LYS LEU ALA LYS HIS GLY THR THR
LEU GLU ASP PRO ILE HIS ALA PRO LYS LEU GLY ALA LEU ARG ASP CYS GLY ILE GLY VAL GLU GLY GLN GLU SER SER ASP PRO LEU TYR THR PRO ILE LYS PRO HIS ARG ALA LEU ILE PHE CYS GLN MET LYS GLU MET LEU LEU ASP MET VAL GLN ASN THR VAL LEU
LYS GLN MET LEU PRO SER VAL SER TYR LEU ARG LEU ASP GLY SER VAL GLU ALA ASN LYS ARG GLN ASP ILE VAL ASN VAL TYR ARG ILE ILE THR ARG GLY THR LEU GLU GLU LYS ILE LEU LEU SER LEU GLN ARG PHE LYS ILE ASP VAL ALA SER THR VAL ASN GLN GLN ASN ALA GLY
HIS ASP TRP ASN PRO GLN LYS ASP LEU GLN ALA MET ASP ARG ALA HIS ARG ILE GLY GLN LYS LYS VAL VAL ASN VAL TYR ARG ILE ILE THR ARG GLY THR LEU GLU GLU LYS ILE LEU LEU SER LEU GLN ARG PHE LYS ILE ASP VAL ALA SER THR VAL ASN GLN GLN ASN ALA GLY


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


LEU TRP ASP ASN ALA GLN TYR GLU GLU SER PHE ASP LEU ASP GLY PHE LEU LYS THR MET GLN ALA ALA ALA TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	44000	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 ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.056	Depositor
Minimum map value	-0.471	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.219	Depositor
Map size (Å)	296.52002, 296.52002, 296.52002	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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	0.72	0/836	1.27	1/1289 (0.1%)
2	B	0.72	0/818	1.33	2/1259 (0.2%)
3	D	2.31	36/1444 (2.5%)	2.41	118/1945 (6.1%)
4	E	0.79	23/10441 (0.2%)	0.87	95/14151 (0.7%)
All	All	1.06	59/13539 (0.4%)	1.19	216/18644 (1.2%)

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	17
2	B	0	13
All	All	0	30

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1371	HIS	CE1-NE2	-8.80	1.23	1.32
4	E	1436	HIS	CE1-NE2	-8.76	1.23	1.32
3	D	195	HIS	ND1-CE1	-8.71	1.23	1.32
3	D	194	HIS	CE1-NE2	-8.66	1.23	1.32
4	E	1371	HIS	ND1-CE1	-8.47	1.24	1.32

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	176	VAL	CA-C-N	9.45	129.71	121.58
3	D	176	VAL	C-N-CA	9.45	129.71	121.58
3	D	137	VAL	CA-C-N	8.20	133.36	123.19
3	D	137	VAL	C-N-CA	8.20	133.36	123.19
3	D	226	LYS	CA-C-N	8.16	133.83	123.14

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	DG	Sidechain
1	A	12	DC	Sidechain
1	A	5	DC	Sidechain
1	A	8	DG	Sidechain
1	A	9	DC	Sidechain

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	744	400	400	0	0
2	B	732	403	403	0	0
3	D	1417	1490	1489	3	0
4	E	10251	10532	10526	80	0
All	All	13144	12825	12818	83	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 83 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:E:1226:MET:O	4:E:1234:ARG:NH2	1.68	1.26
4:E:1227:SER:OG	4:E:1315:HIS:HB3	1.32	1.22
4:E:1227:SER:OG	4:E:1315:HIS:CB	2.22	0.87
4:E:1226:MET:HE2	4:E:1480:MET:SD	2.17	0.85
4:E:606:GLY:N	4:E:650:GLU:OE1	2.24	0.71

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	
3	D	176/276 (64%)	170 (97%)	6 (3%)	0	100	100
4	E	1296/1897 (68%)	1243 (96%)	53 (4%)	0	100	100
All	All	1472/2173 (68%)	1413 (96%)	59 (4%)	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	
3	D	154/219 (70%)	153 (99%)	1 (1%)	78	82
4	E	1114/1620 (69%)	1101 (99%)	13 (1%)	63	74
All	All	1268/1839 (69%)	1254 (99%)	14 (1%)	63	74

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	1067	LEU
4	E	1082	LEU
4	E	1418	ASP
4	E	1363	ILE
4	E	1389	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides 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.

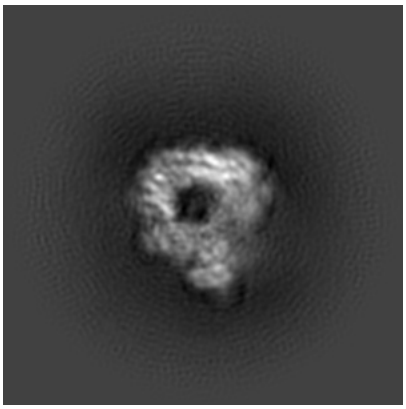
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14534. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

6.1.1 Primary map



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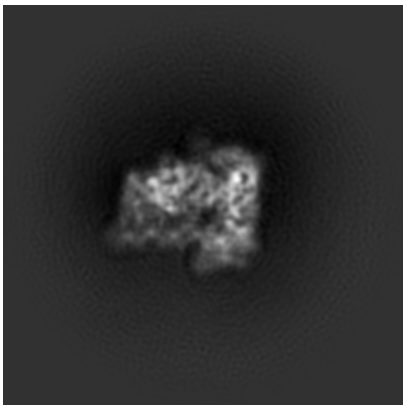

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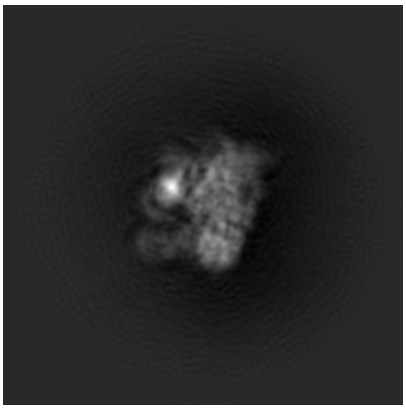
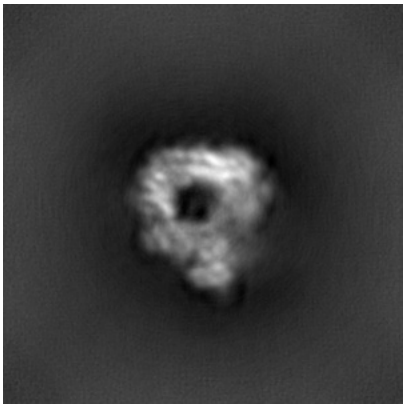


Z

6.1.2 Raw map



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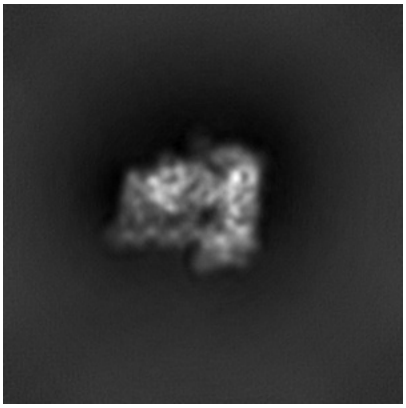

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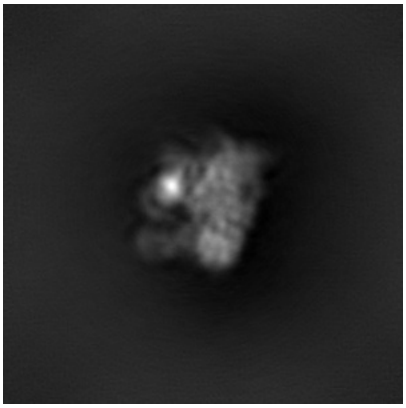
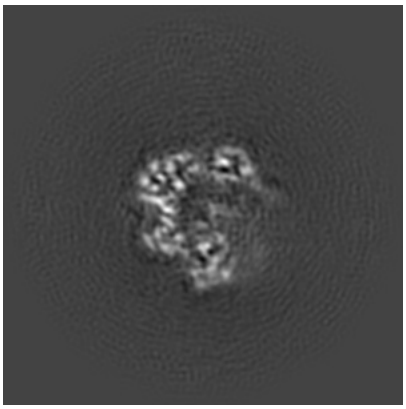


Z

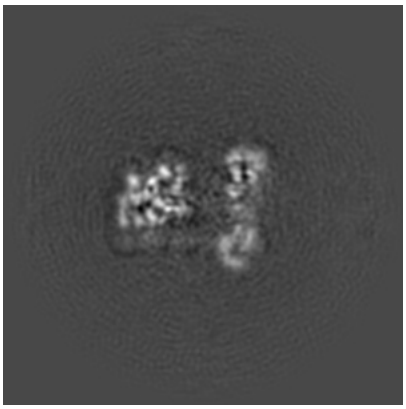
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

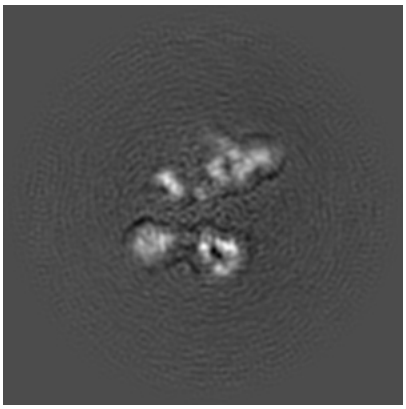
6.2.1 Primary map



X Index: 140

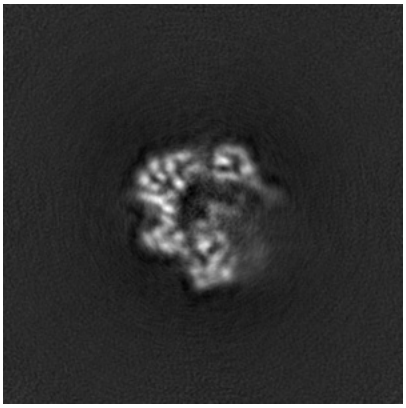


Y Index: 140

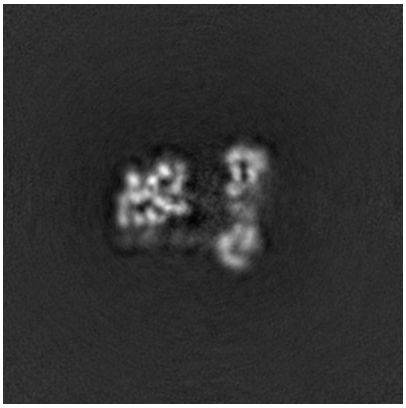


Z Index: 140

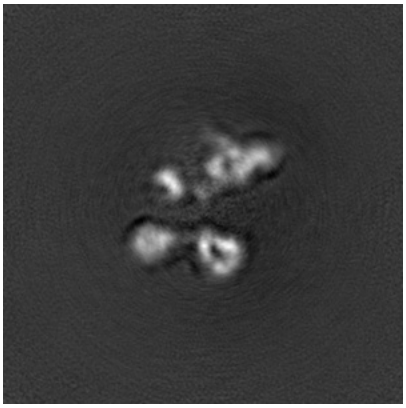
6.2.2 Raw map



X Index: 140



Y Index: 140

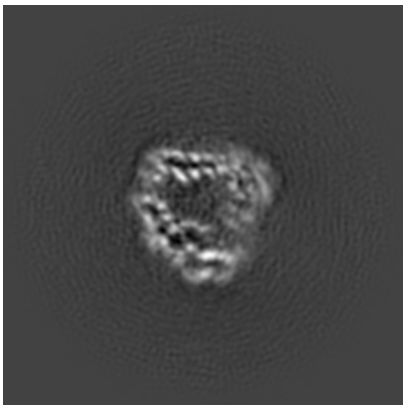


Z Index: 140

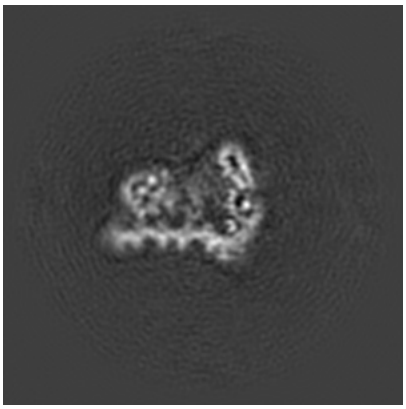
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

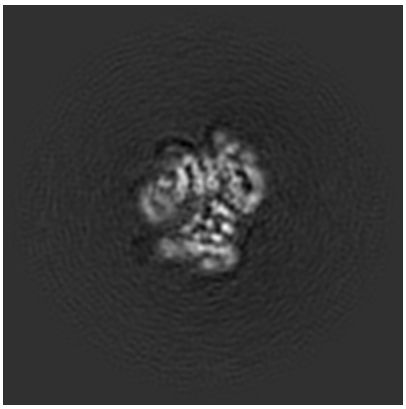
6.3.1 Primary map



X Index: 156

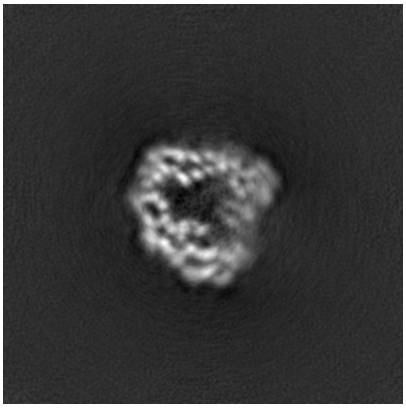


Y Index: 153

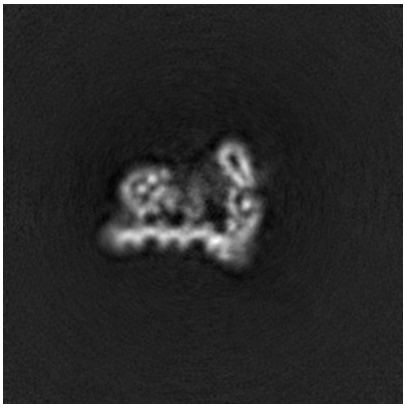


Z Index: 160

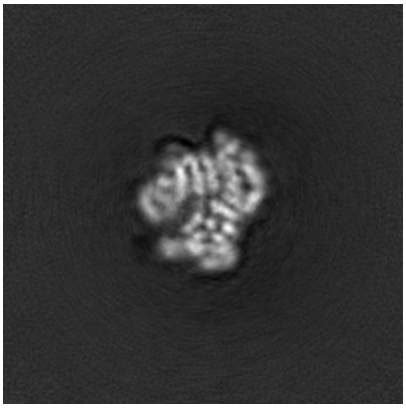
6.3.2 Raw map



X Index: 154



Y Index: 152

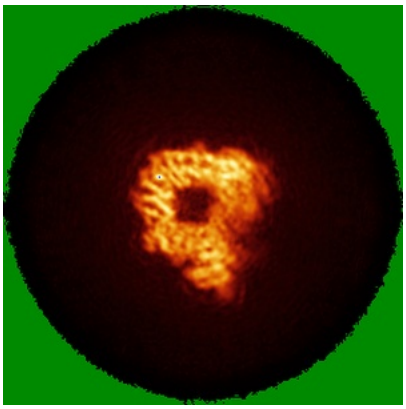


Z Index: 161

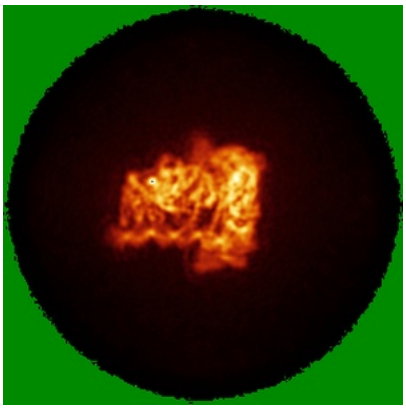
The images above show the largest variance slices of the map in three orthogonal directions.

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

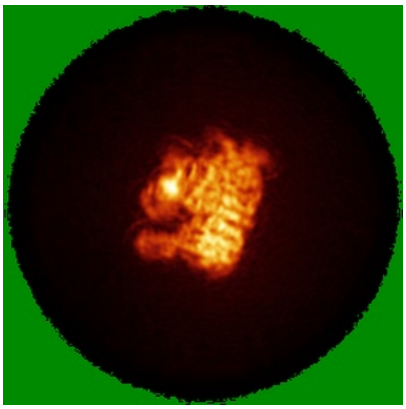
6.4.1 Primary map



X

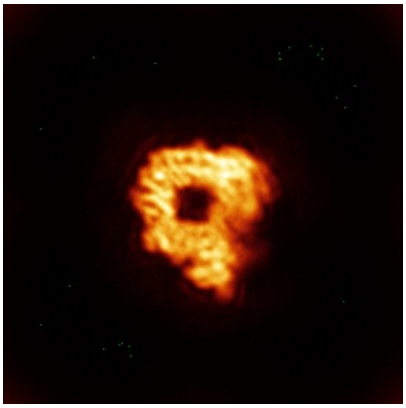


Y

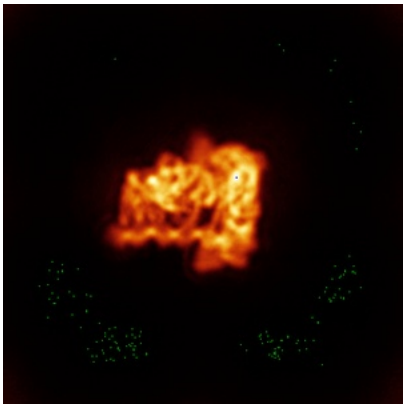


Z

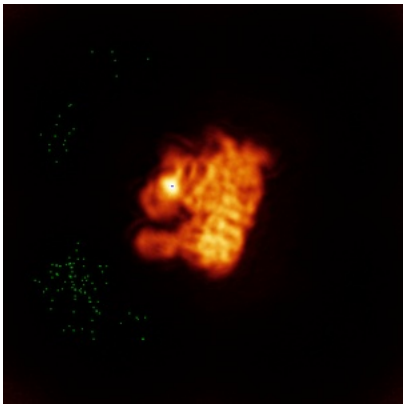
6.4.2 Raw map



X



Y

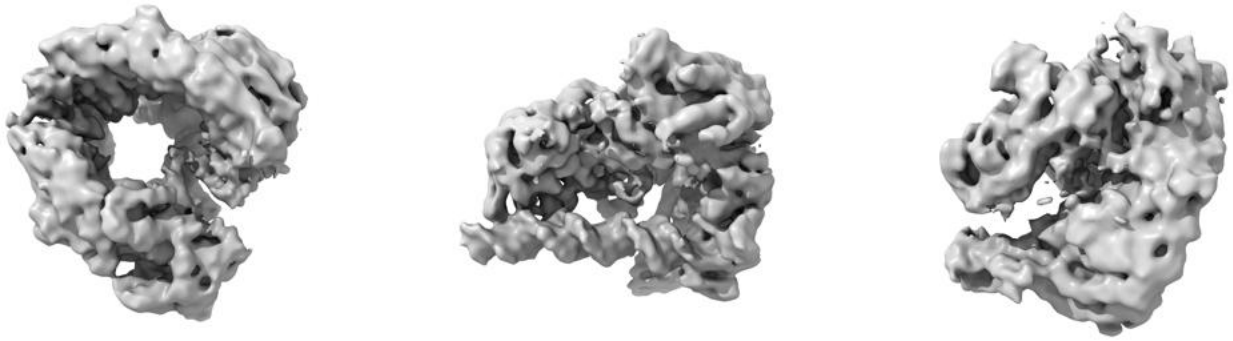


Z

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)

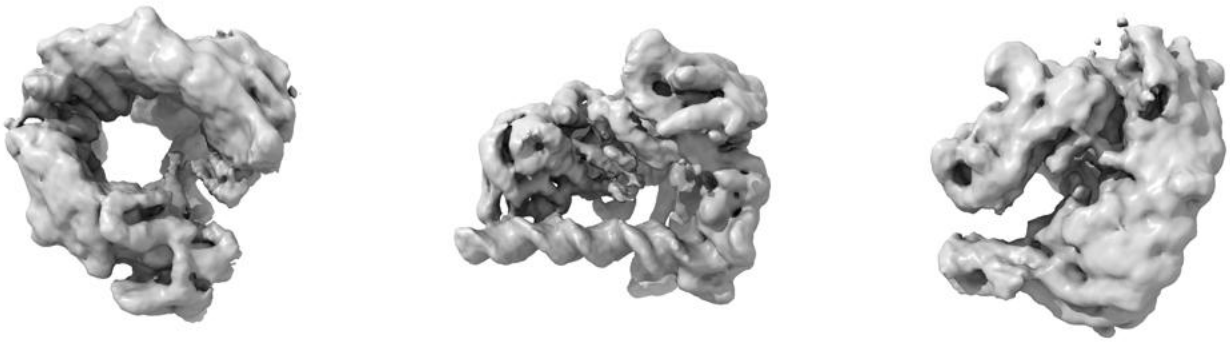
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.219. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

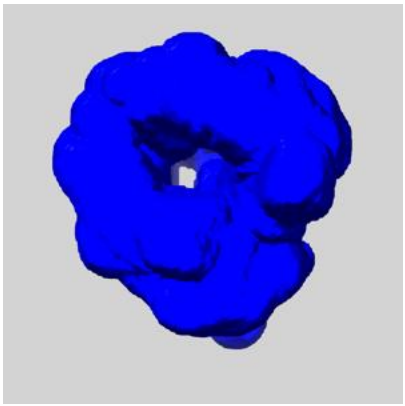
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

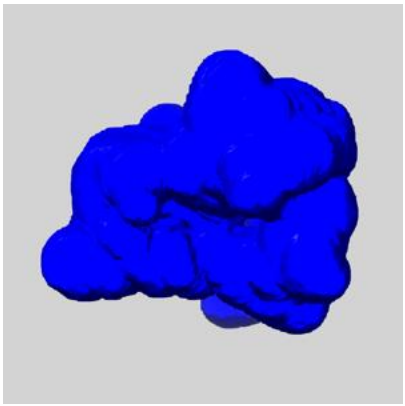
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

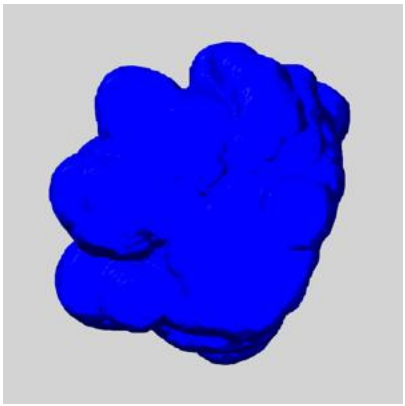
6.6.1 emd_14534_msk_1.map



X



Y

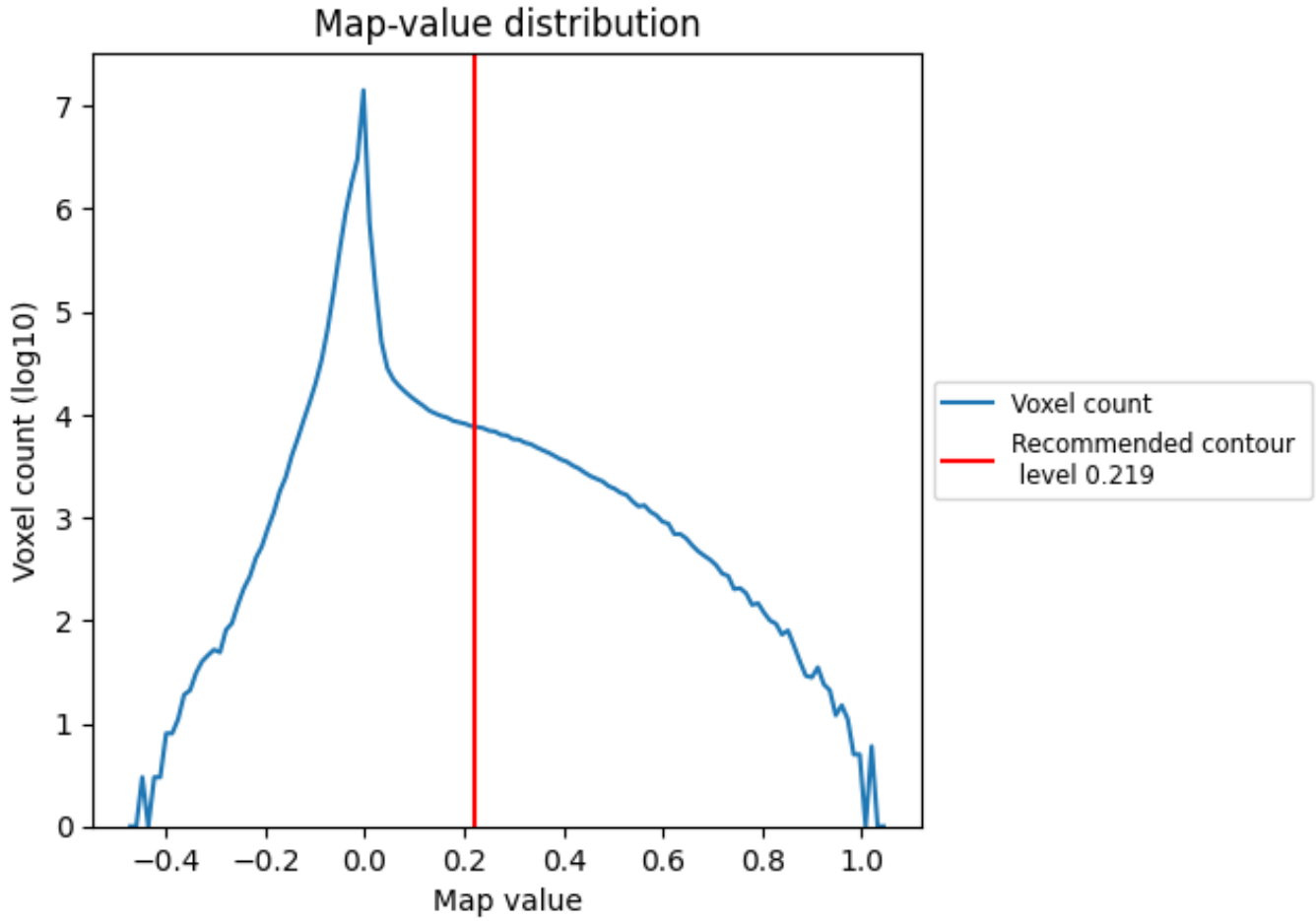


Z

7 Map analysis

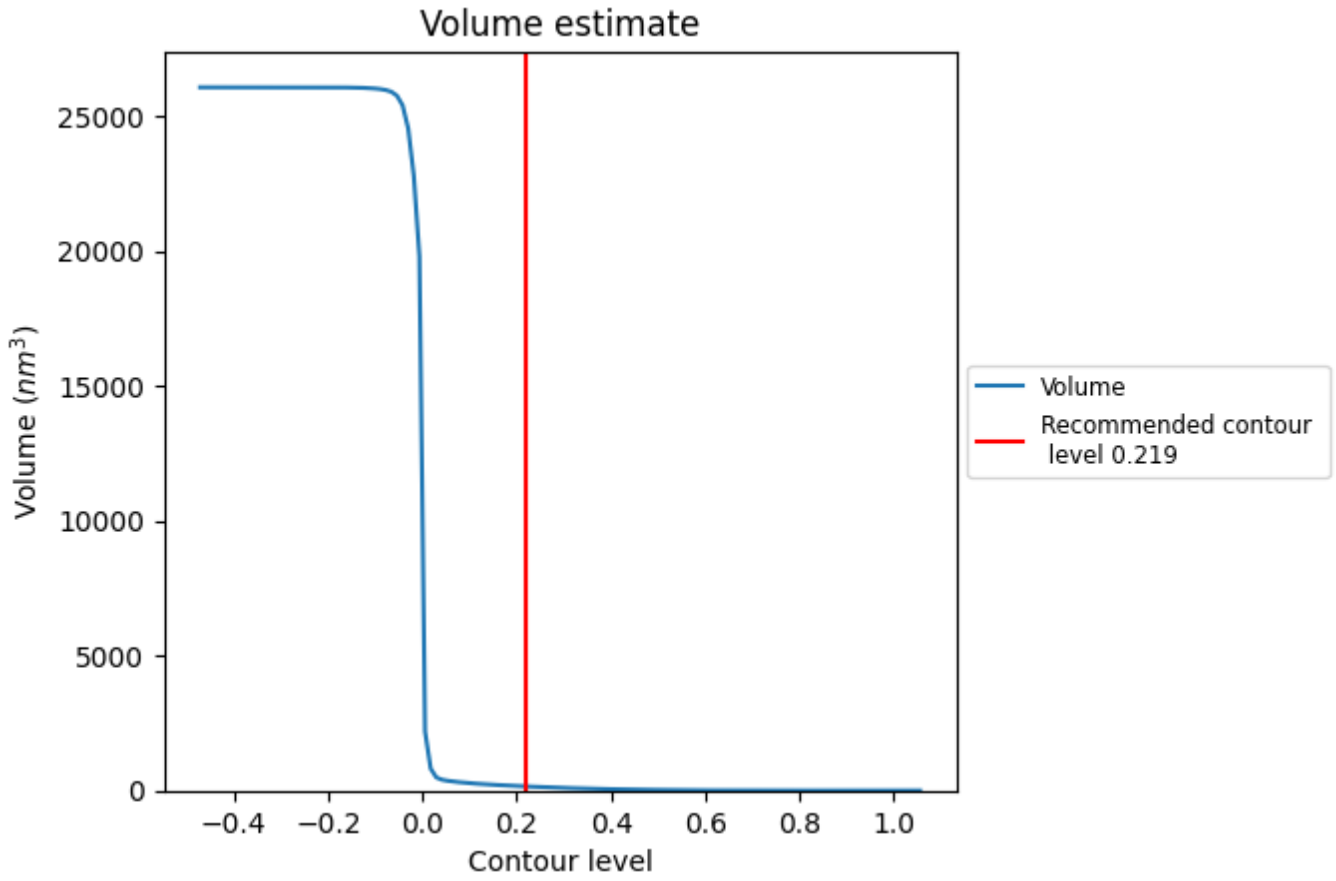
This section contains the results of statistical analysis of the map.

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.

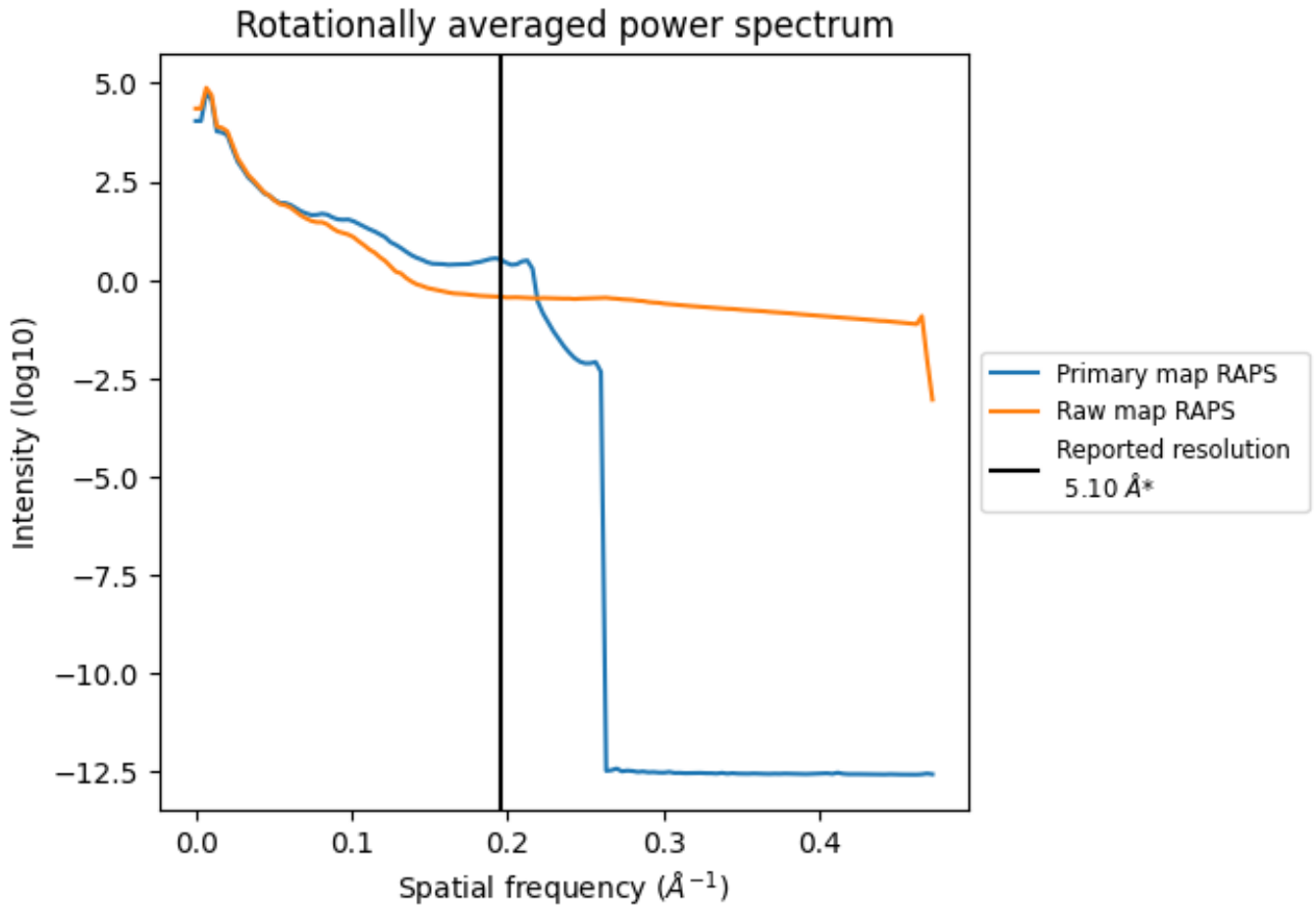
7.2 Volume estimate (i)



The volume at the recommended contour level is 155 nm^3; this corresponds to an approximate mass of 140 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)

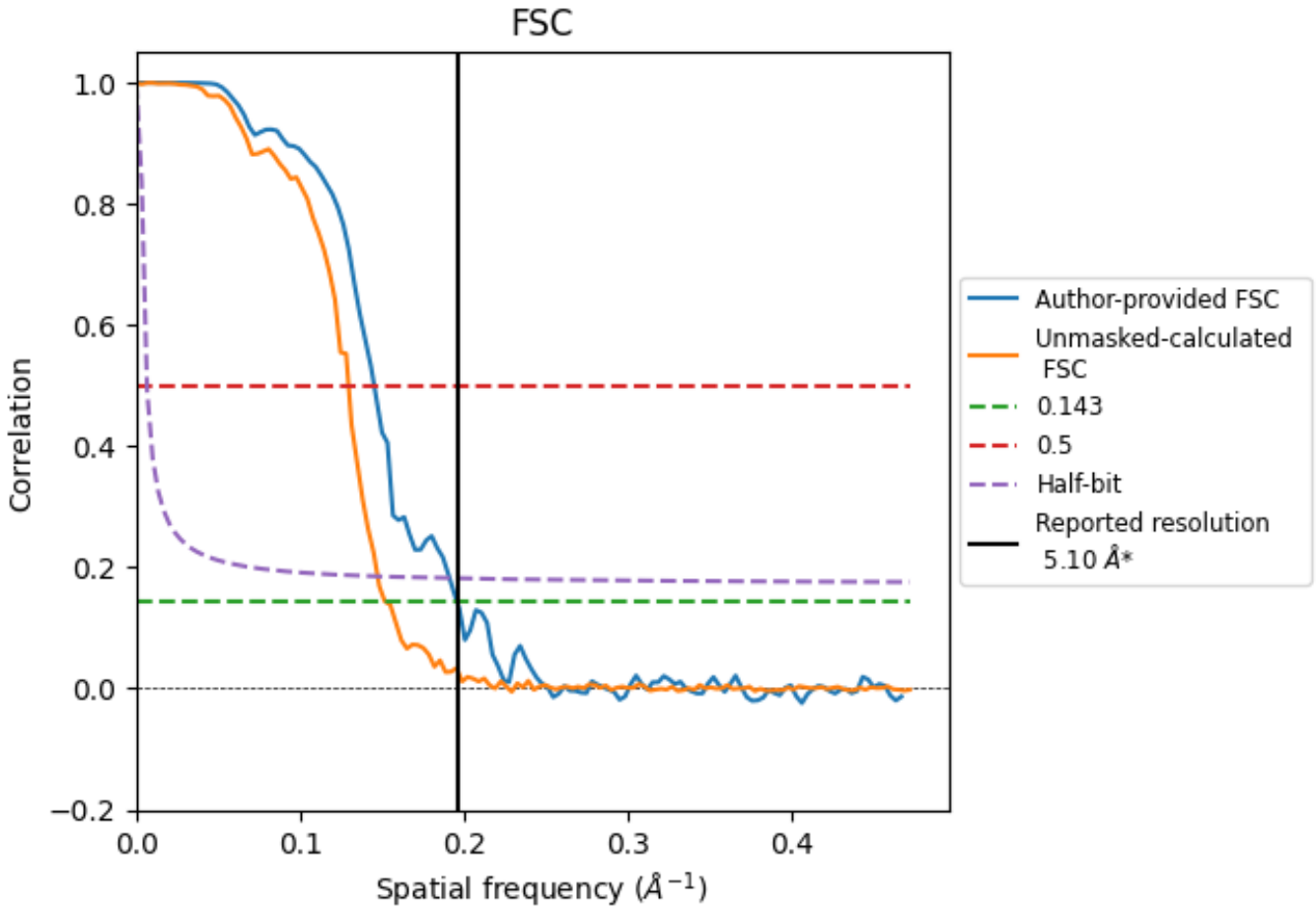


*Reported resolution corresponds to spatial frequency of 0.196 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.196 Å^{-1}

8.2 Resolution estimates (i)

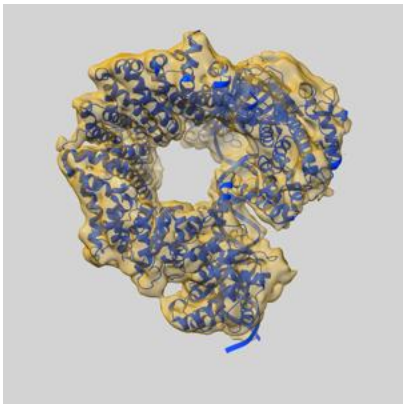
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.10	-	-
Author-provided FSC curve	5.10	6.88	5.22
Unmasked-calculated*	6.57	7.71	6.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.57 differs from the reported value 5.1 by more than 10 %

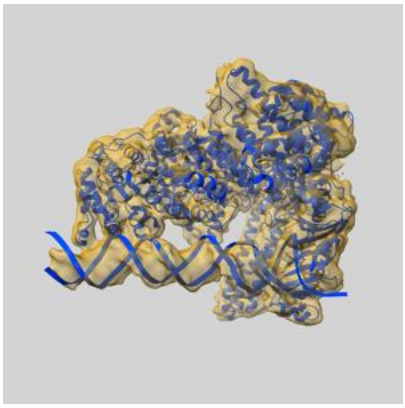
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14534 and PDB model 7Z7N. Per-residue inclusion information can be found in section 3 on page 5.

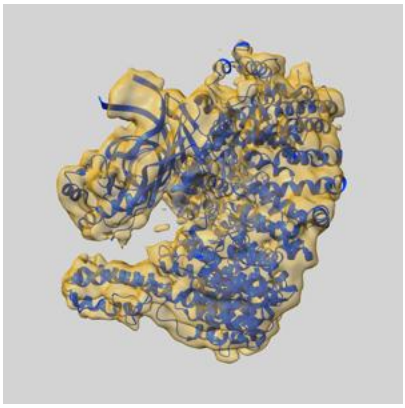
9.1 Map-model overlay



X



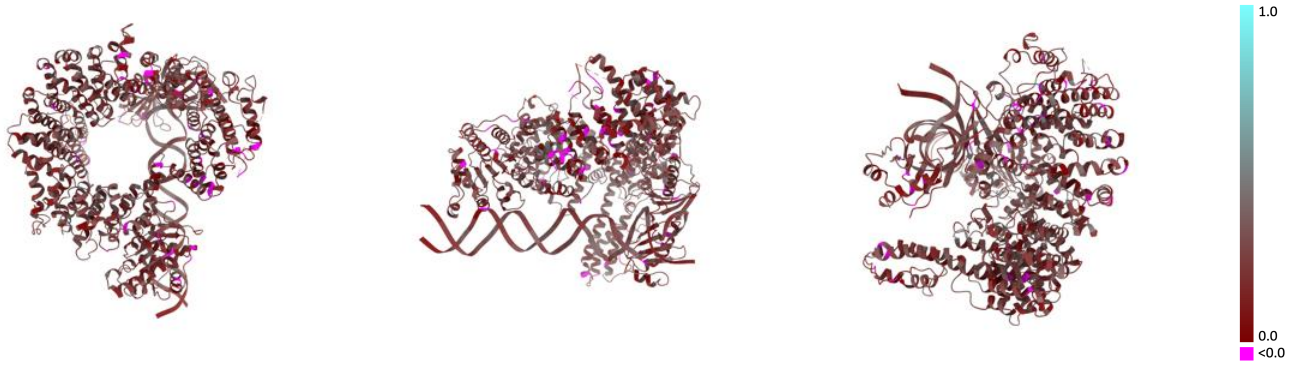
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.219 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.

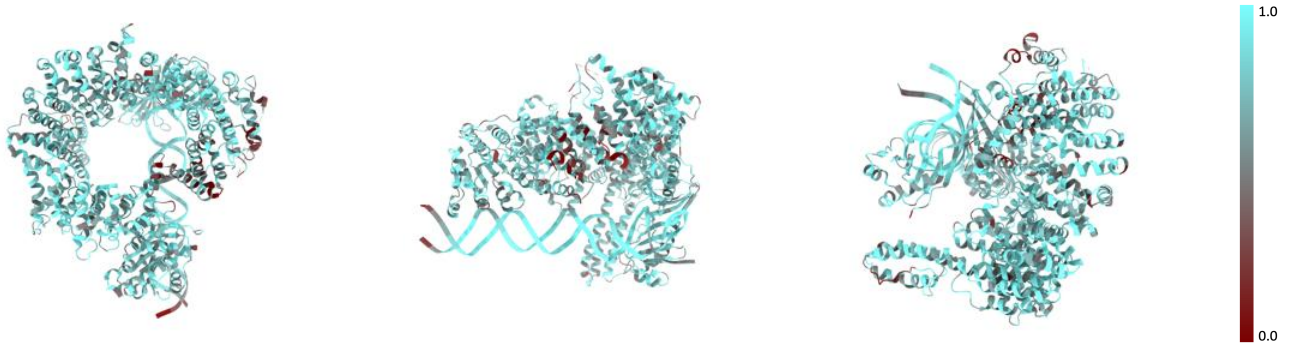
9.2 Q-score mapped to coordinate model (i)



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.

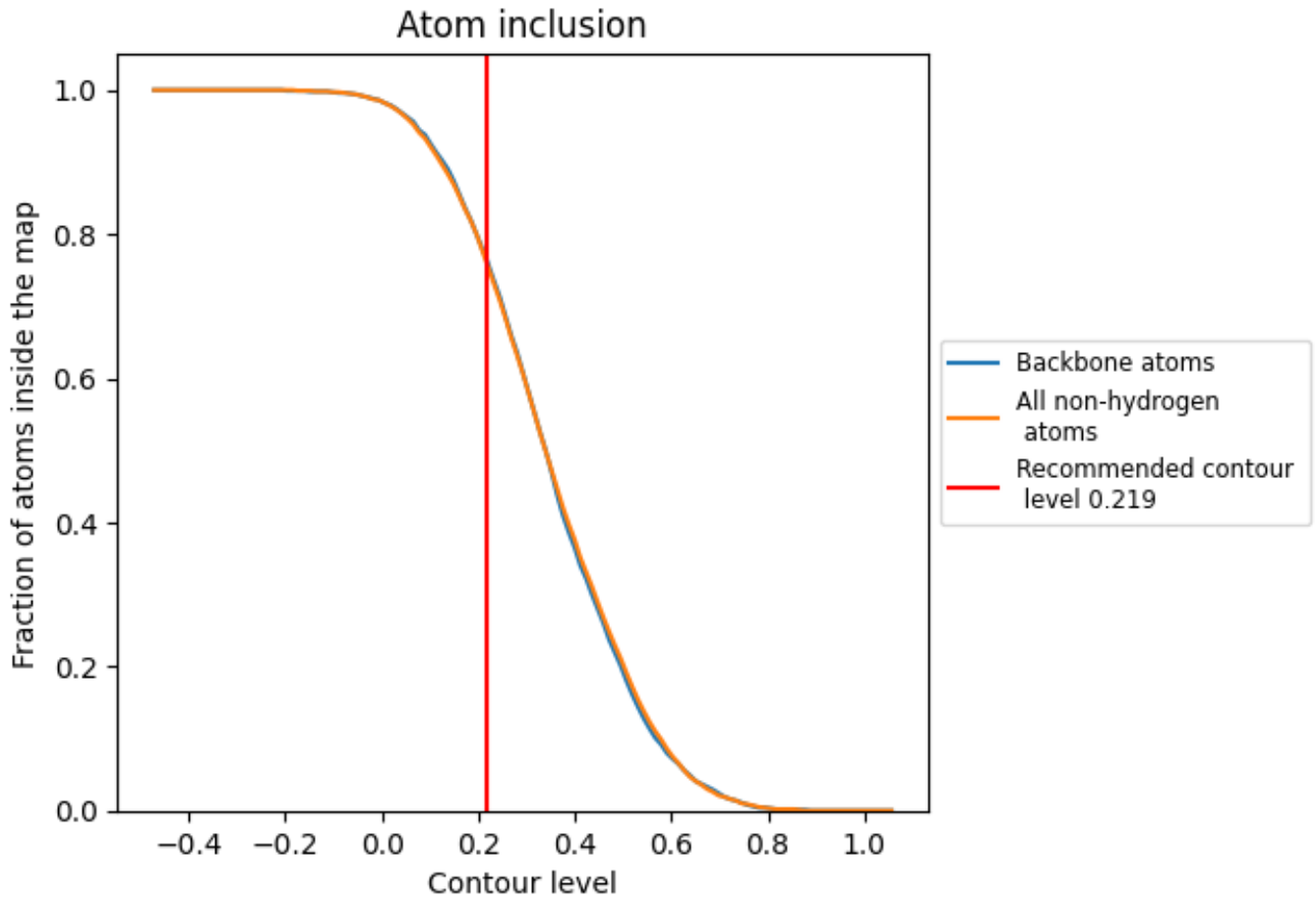
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.219).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (0.219) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.7570	0.2420
A	0.8660	0.2710
B	0.8180	0.2560
D	0.7630	0.2440
E	0.7570	0.2380