



wwPDB EM Validation Summary Report ⓘ

Sep 9, 2026 – 04:27 PM EDT

PDB ID : 9ZP9 / pdb_00009zp9
EMDB ID : EMD-74524
Title : CryoEM structure of DNA-PK bound to N7 nucleosome, state 1
Authors : Lu, W.; He, Y.
Deposited on : 2025-12-16
Resolution : 3.88 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:

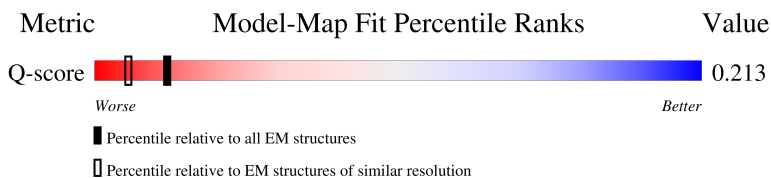
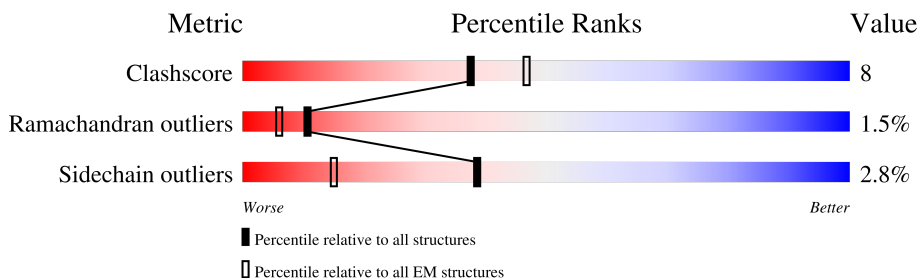
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

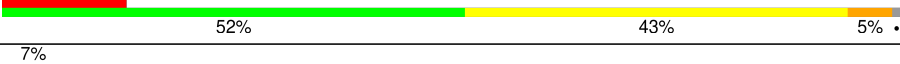
The reported resolution of this entry is 3.88 Å.

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	8773 (3.38 - 4.38)

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 $\leq 5\%$. 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	112	
1	E	112	
2	B	87	
2	F	87	

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Mol	Chain	Length	Quality of chain
3	C	111	
3	G	111	
4	D	96	
4	H	96	
5	I	154	
6	J	154	
7	K	609	
8	L	732	
9	M	4128	
10	N	20	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 98192 atoms, of which 48089 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 Histone H3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	112	Total	C	H	N	O	S	0	0
			1853	566	952	176	156	3		
1	E	90	Total	C	H	N	O	S	0	0
			1522	467	782	140	130	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	86	Total	C	H	N	O	S	0	0
			1453	440	755	141	116	1		
2	F	86	Total	C	H	N	O	S	0	0
			1438	436	744	140	117	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	103	Total	C	H	N	O	0	0
			1609	493	825	152	139		
3	G	111	Total	C	H	N	O	0	0
			1783	539	925	169	150		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	SER	THR	conflict	UNP A0A974HJ06
C	99	ARG	GLY	conflict	UNP A0A974HJ06
G	19	SER	THR	conflict	UNP A0A974HJ06
G	99	ARG	GLY	conflict	UNP A0A974HJ06

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	96	Total	C	H	N	O	S	0	0
			1547	475	789	140	141	2		
4	H	95	Total	C	H	N	O	S	0	0
			1521	469	774	136	140	2		

- Molecule 5 is a DNA chain called DNA (154-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
5	I	154	Total	C	H	N	O	P	0	0
			4904	1503	1730	591	926	154		

- Molecule 6 is a DNA chain called DNA (154-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
6	J	154	Total	C	H	N	O	P	0	0
			4866	1491	1729	573	920	153		

- Molecule 7 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	K	490	Total	C	H	N	O	S	0	0
			7999	2533	4045	671	733	17		

- Molecule 8 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	L	535	Total	C	H	N	O	S	0	0
			8580	2736	4307	713	800	24		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	663	GLN	ARG	conflict	UNP G3R763

- Molecule 9 is a protein called DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	M	3662	Total	C	H	N	O	S	0	0
			58976	18776	29692	4946	5370	192		

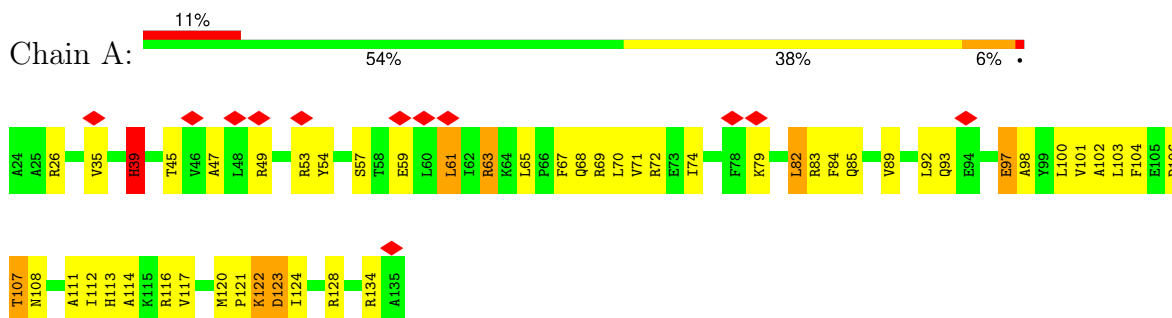
- Molecule 10 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
10	N	20	141	60	40	20	21	0	0

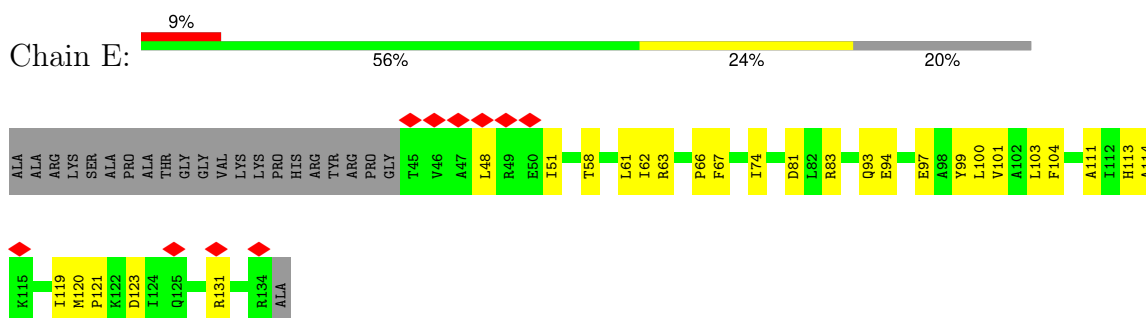
3 Residue-property plots

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.

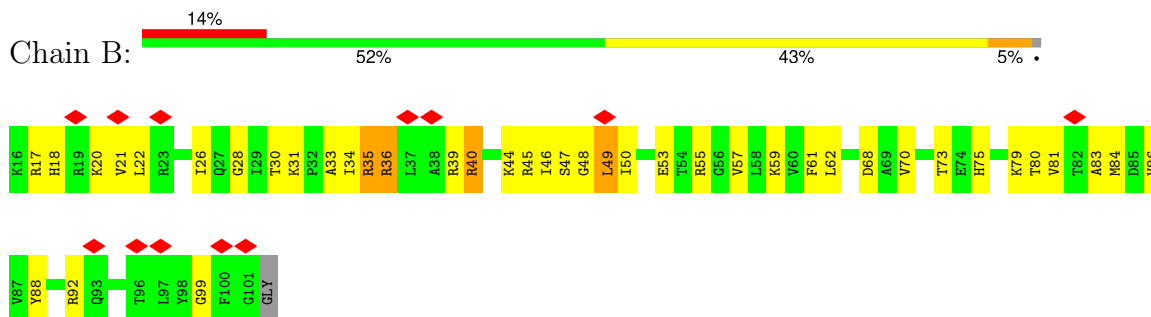
• Molecule 1: Histone H3



• Molecule 1: Histone H3



• Molecule 2: Histone H4

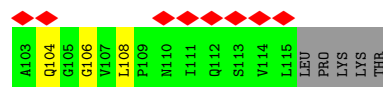
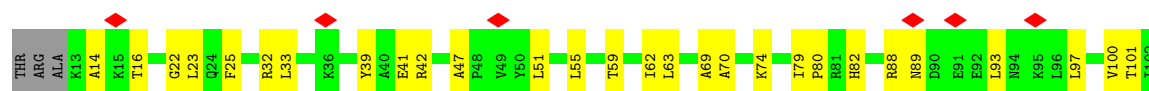


• Molecule 2: Histone H4

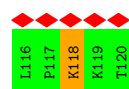
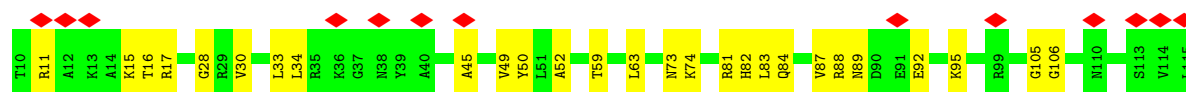
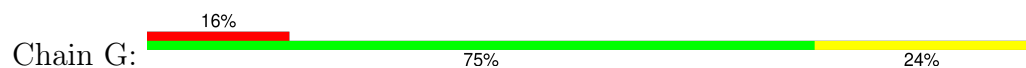




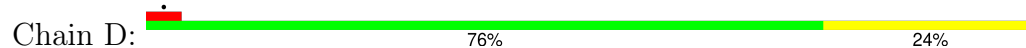
• Molecule 3: Histone H2A



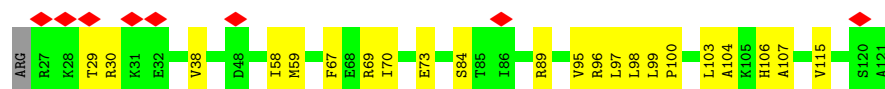
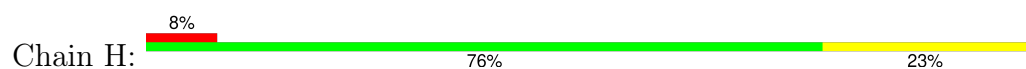
• Molecule 3: Histone H2A



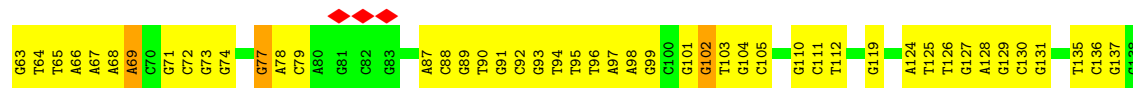
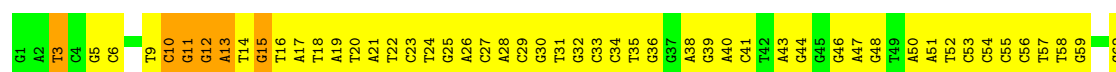
• Molecule 4: Histone H2B



• Molecule 4: Histone H2B

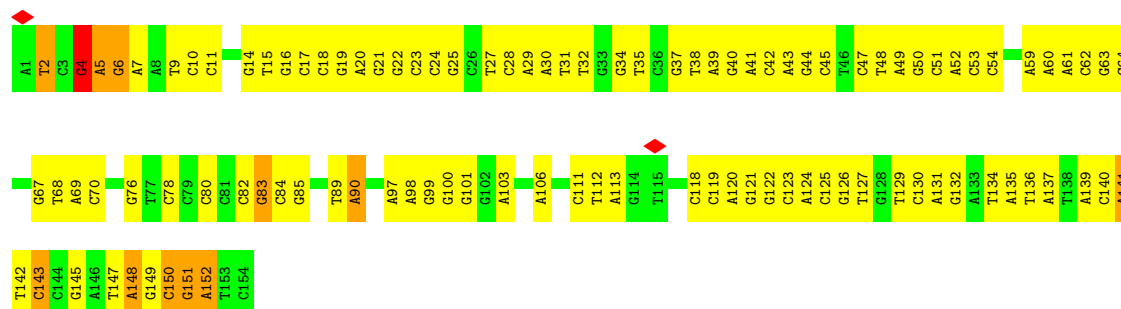


• Molecule 5: DNA (154-MER)

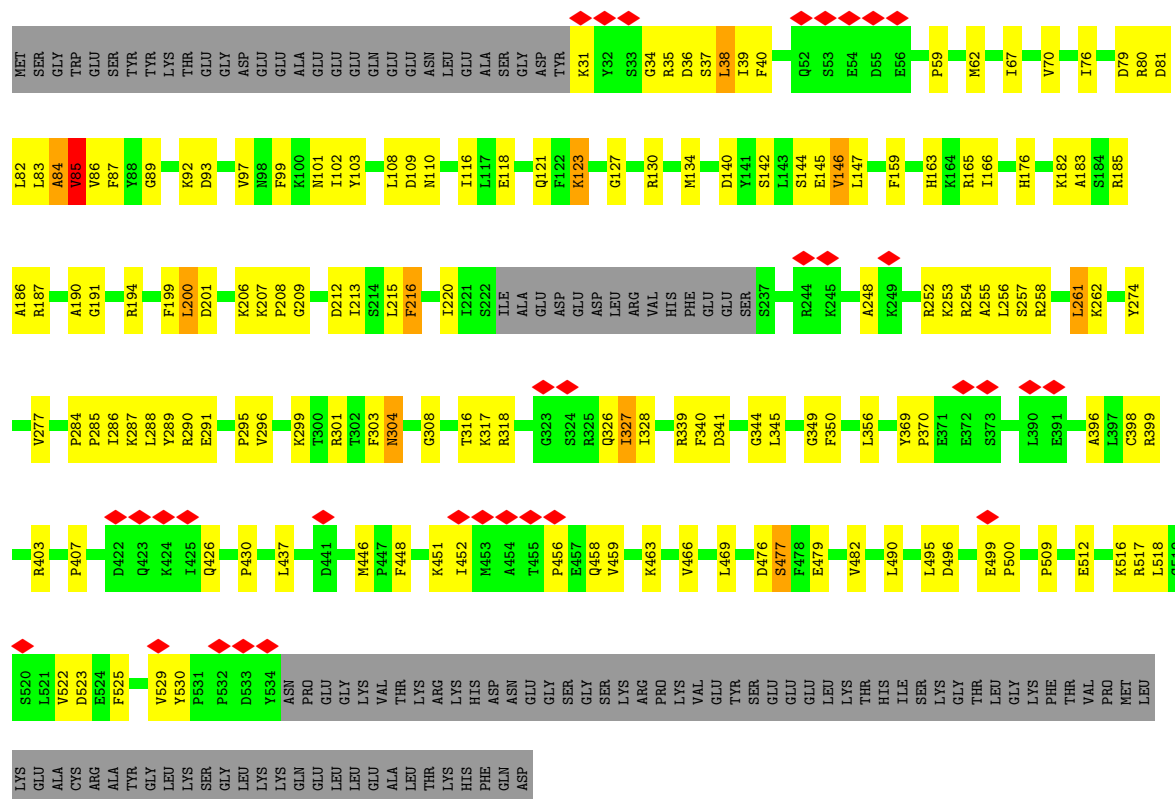




• Molecule 6: DNA (154-MER)

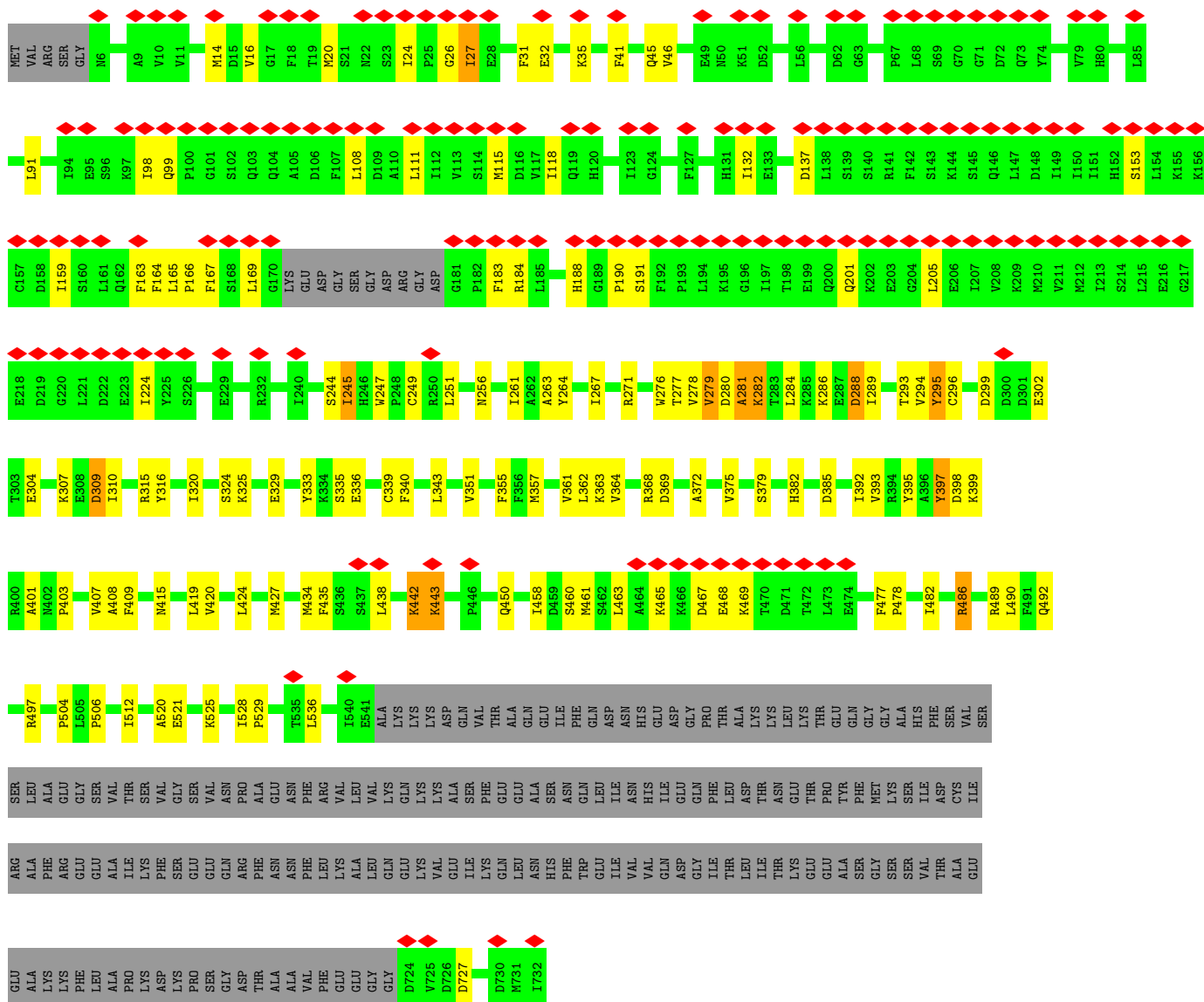


• Molecule 7: X-ray repair cross-complementing protein 6

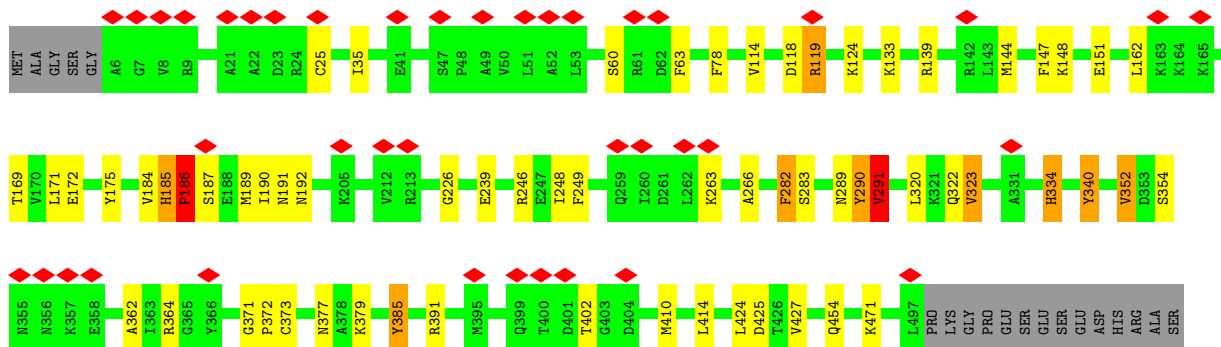


• Molecule 8: X-ray repair cross-complementing protein 5

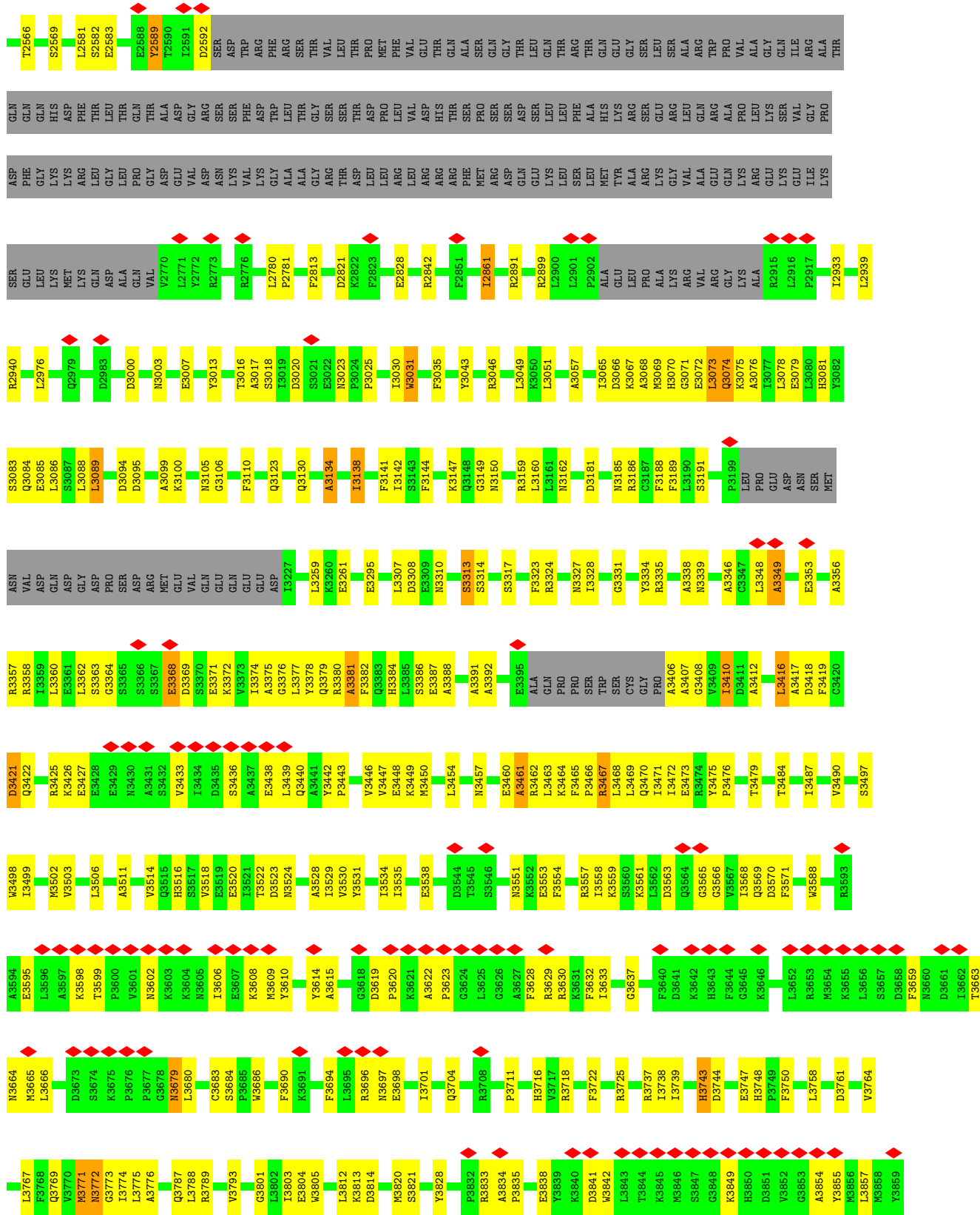


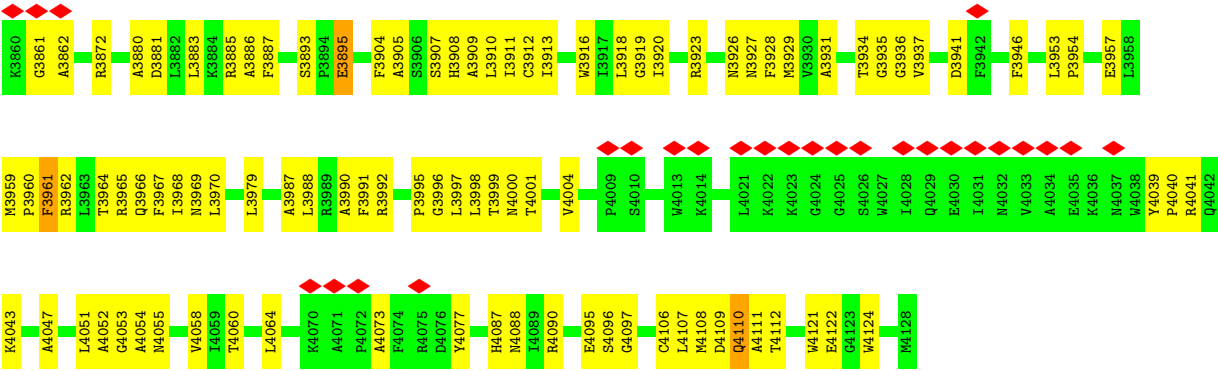


• Molecule 9: DNA-dependent protein kinase catalytic subunit









● Molecule 10: Unknown peptide



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	220128	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.788	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	446.4, 446.4, 446.4	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.86, 1.86, 1.86	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	1.67	8/914 (0.9%)	1.86	36/1225 (2.9%)
1	E	0.18	0/748	0.53	0/1003
2	B	1.42	9/706 (1.3%)	1.45	19/943 (2.0%)
2	F	0.22	0/702	0.60	0/937
3	C	0.19	0/793	0.55	0/1072
3	G	1.41	10/868 (1.2%)	1.32	19/1169 (1.6%)
4	D	0.19	0/769	0.51	0/1032
4	H	0.18	0/758	0.49	0/1018
5	I	0.80	14/3563 (0.4%)	0.98	5/5502 (0.1%)
6	J	0.78	14/3516 (0.4%)	0.94	3/5420 (0.1%)
7	K	1.56	50/4031 (1.2%)	1.53	117/5429 (2.2%)
8	L	0.90	15/4359 (0.3%)	0.97	38/5881 (0.6%)
9	M	1.16	121/29884 (0.4%)	1.49	375/40387 (0.9%)
All	All	1.11	241/51611 (0.5%)	1.34	612/71018 (0.9%)

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	1
5	I	0	7
6	J	0	8
7	K	0	2
8	L	0	1
9	M	0	22
All	All	0	41

The worst 5 of 241 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	3349	ALA	CA-CB	-9.93	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	82	HIS	CE1-NE2	-8.92	1.23	1.32
9	M	3908	HIS	CE1-NE2	-8.88	1.23	1.32
7	K	163	HIS	ND1-CE1	-8.81	1.23	1.32
9	M	3384	HIS	CE1-NE2	-8.78	1.23	1.32

The worst 5 of 612 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	HIS	CA-CB-CG	9.61	123.41	113.80
9	M	186	PRO	CA-N-CD	-8.88	99.56	112.00
5	I	102	DG	OP2-P-O3'	-8.77	81.69	108.00
8	L	288	ASP	CA-CB-CG	8.07	120.67	112.60
9	M	1864	ASP	CA-CB-CG	7.88	120.48	112.60

There are no chirality outliers.

5 of 41 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	82	LEU	Peptide
5	I	3	DT	Sidechain
5	I	5	DG	Sidechain
5	I	6	DC	Sidechain
5	I	74	DG	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	901	952	951	33	0
1	E	740	782	781	32	0
2	B	698	755	752	41	0
2	F	694	744	742	42	0
3	C	784	825	824	31	0
3	G	858	925	922	18	0
4	D	758	789	786	32	0
4	H	747	774	773	25	0
5	I	3174	1730	1683	133	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	3137	1729	1687	102	0
7	K	3954	4045	4042	61	0
8	L	4273	4307	4303	106	0
9	M	29284	29692	29680	219	0
10	N	101	40	23	0	0
All	All	50103	48089	47949	729	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 8.

The worst 5 of 729 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)
8:L:118:ILE:HG21	8:L:159:ILE:HD11	1.54	0.88
8:L:486:ARG:O	8:L:490:LEU:HD23	1.81	0.81
3:G:50:TYR:CD1	4:H:115:VAL:HG21	2.18	0.79
4:D:38:VAL:HG11	4:D:59:MET:HG2	1.65	0.78
1:A:82:LEU:HD22	2:B:81:VAL:HG13	1.65	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	A	110/112 (98%)	102 (93%)	6 (6%)	2 (2%)	6	34
1	E	88/112 (79%)	85 (97%)	3 (3%)	0	100	100
2	B	84/87 (97%)	79 (94%)	5 (6%)	0	100	100
2	F	84/87 (97%)	77 (92%)	7 (8%)	0	100	100
3	C	101/111 (91%)	91 (90%)	10 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	109/111 (98%)	103 (94%)	6 (6%)	0	100	100
4	D	94/96 (98%)	90 (96%)	4 (4%)	0	100	100
4	H	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
7	K	486/609 (80%)	423 (87%)	58 (12%)	5 (1%)	12	45
8	L	529/732 (72%)	455 (86%)	68 (13%)	6 (1%)	11	43
9	M	3632/4128 (88%)	3138 (86%)	427 (12%)	67 (2%)	6	34
All	All	5410/6281 (86%)	4731 (87%)	599 (11%)	80 (2%)	11	37

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	39	HIS
7	K	85	VAL
7	K	216	PHE
8	L	320	ILE

5.3.2 Protein sidechains ⓘ

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	93/93 (100%)	89 (96%)	4 (4%)	26	49
1	E	79/93 (85%)	79 (100%)	0	100	100
2	B	72/72 (100%)	71 (99%)	1 (1%)	59	70
2	F	71/72 (99%)	71 (100%)	0	100	100
3	C	79/88 (90%)	79 (100%)	0	100	100
3	G	88/88 (100%)	88 (100%)	0	100	100
4	D	82/82 (100%)	82 (100%)	0	100	100
4	H	81/82 (99%)	81 (100%)	0	100	100
7	K	444/548 (81%)	442 (100%)	2 (0%)	81	81
8	L	481/649 (74%)	481 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	M	3266/3671 (89%)	3137 (96%)	129 (4%)	28 52
All	All	4836/5538 (87%)	4700 (97%)	136 (3%)	38 59

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	M	2569	SER
9	M	2828	GLU
9	M	3259	LEU
9	M	1184	ARG
9	M	1137	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
9	M	3185	ASN
9	M	3808	ASN
9	M	3327	ASN
9	M	3748	HIS
9	M	3969	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 oligosaccharides 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.

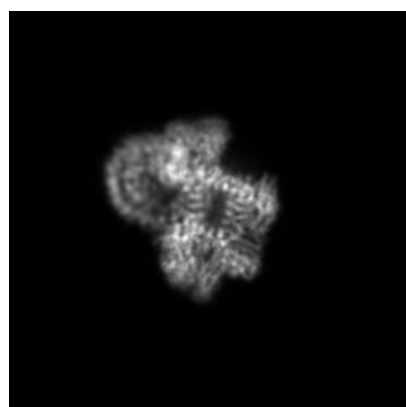
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74524. These allow visual inspection of the internal detail of the map and identification of artifacts.

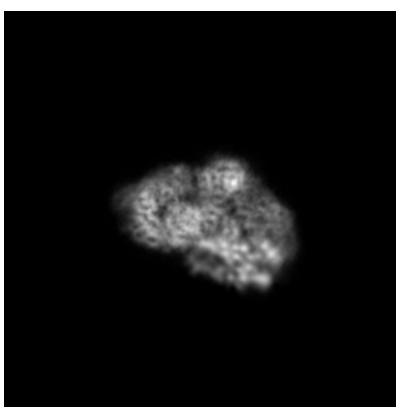
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

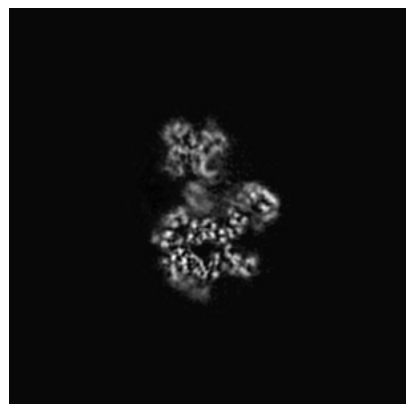


Z

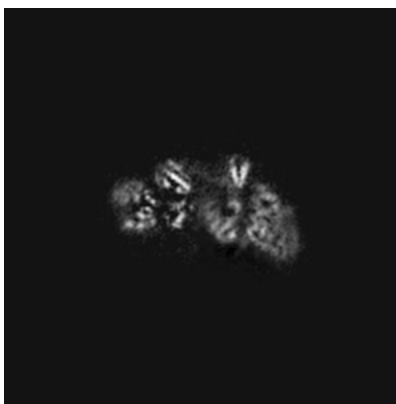
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

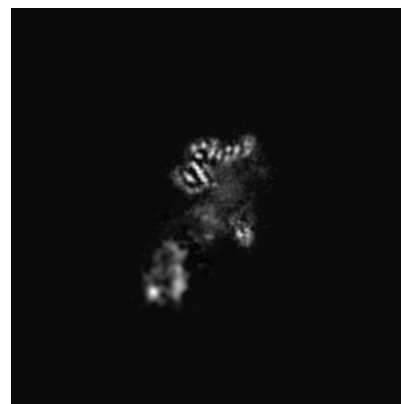
6.2.1 Primary map



X Index: 120



Y Index: 120



Z Index: 120

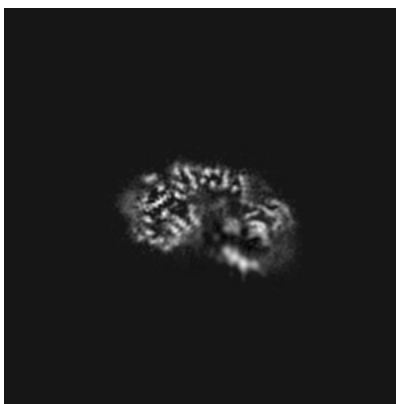
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

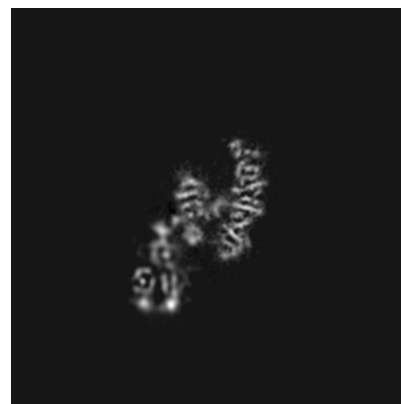
6.3.1 Primary map



X Index: 115



Y Index: 106

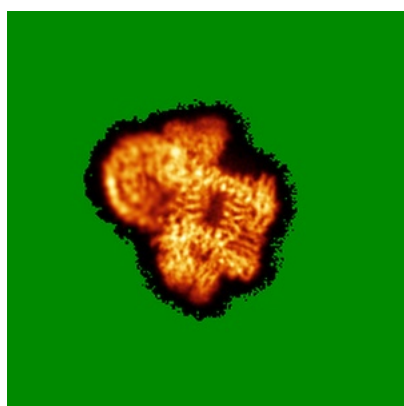


Z Index: 138

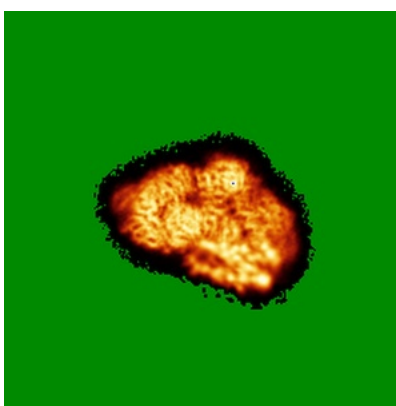
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

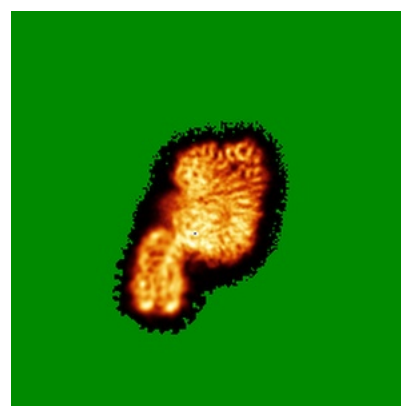
6.4.1 Primary map



X



Y

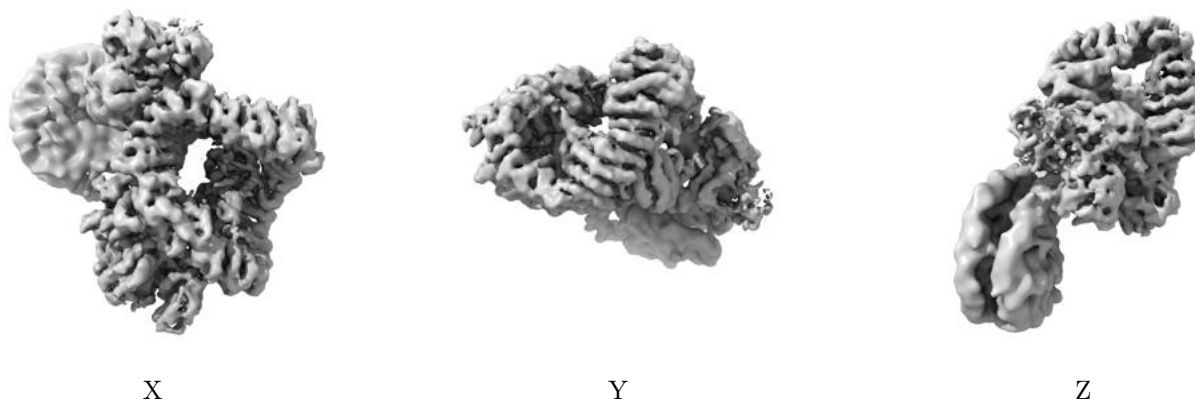


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

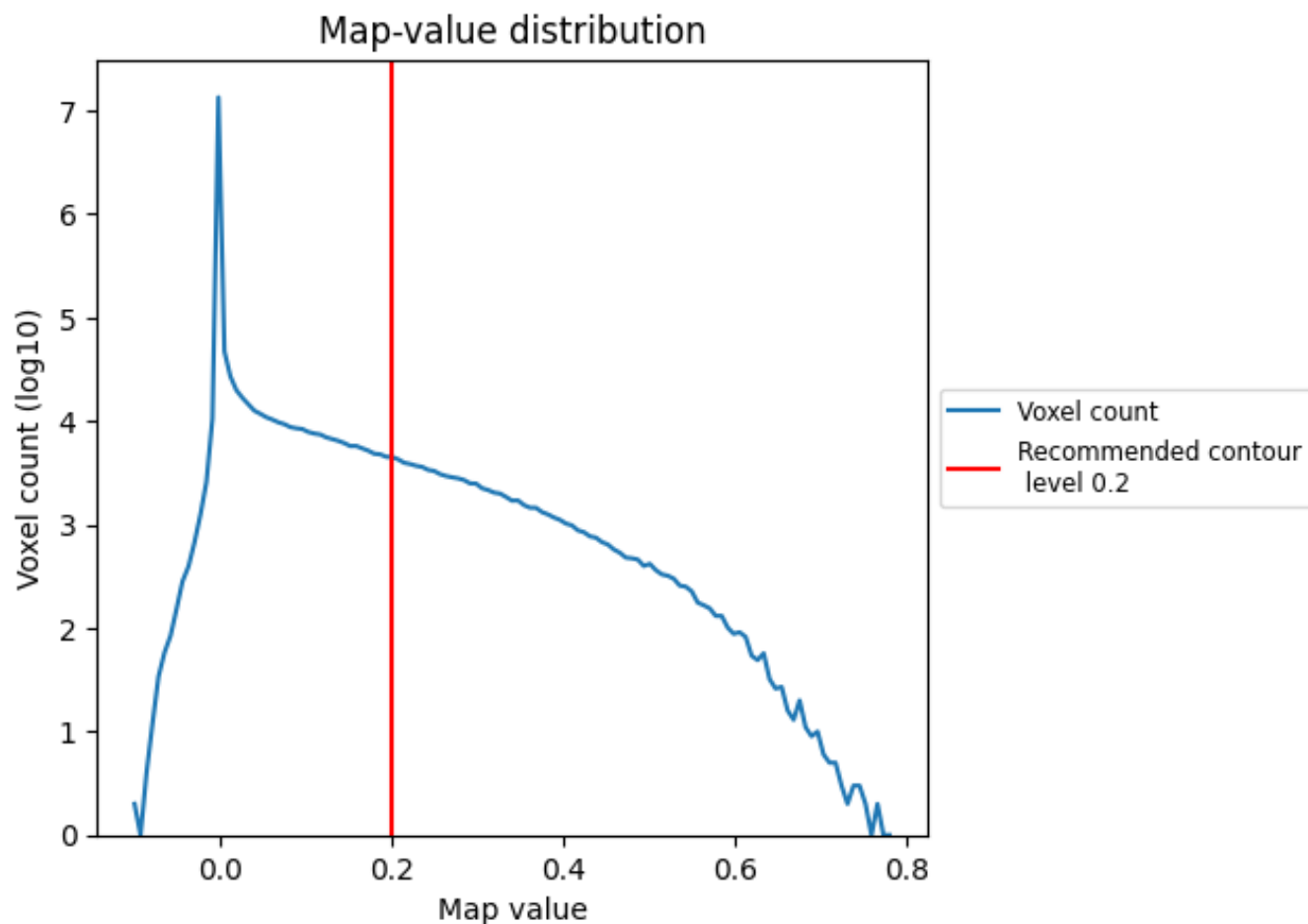
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

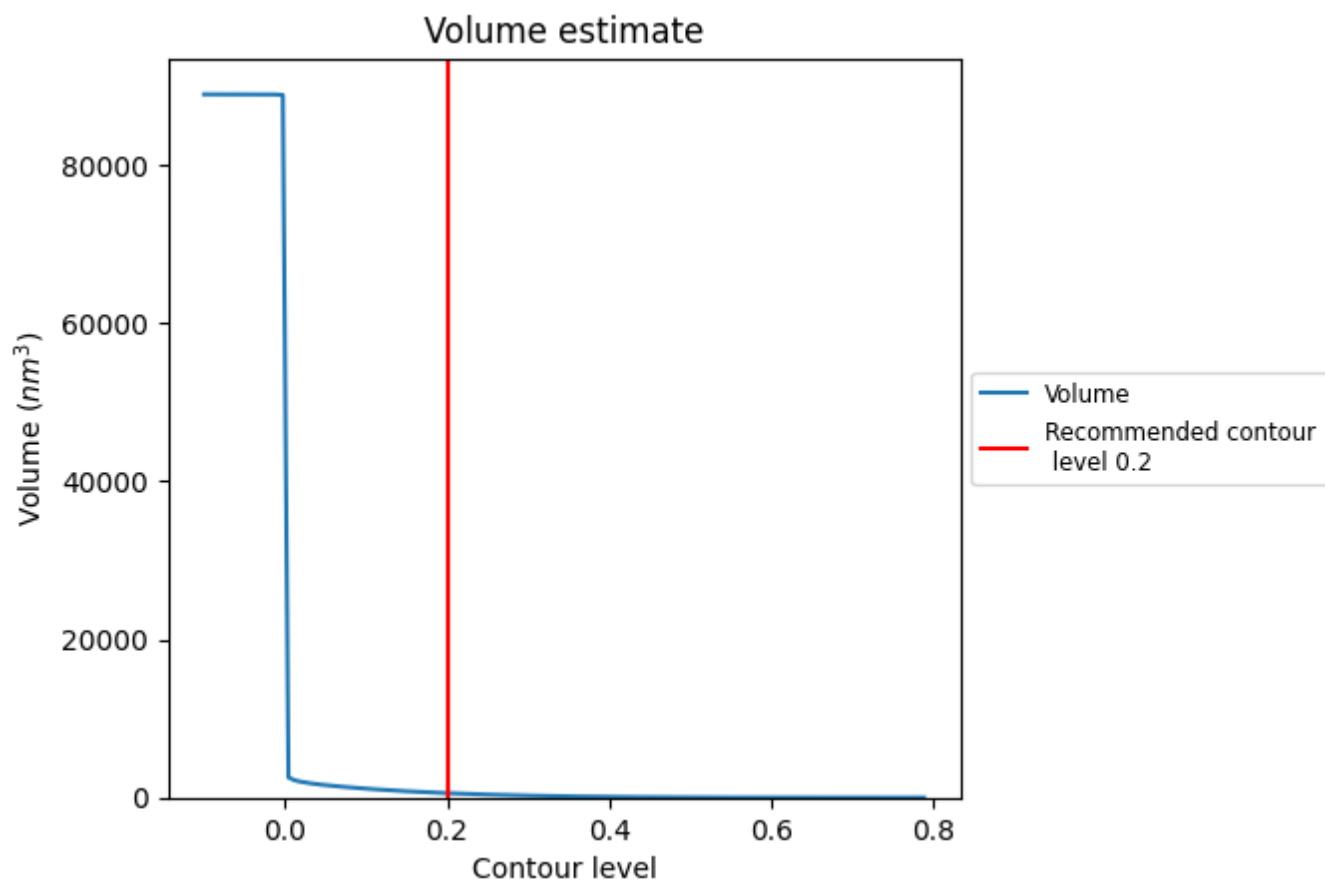
This section contains the results of statistical analysis of the map.

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.

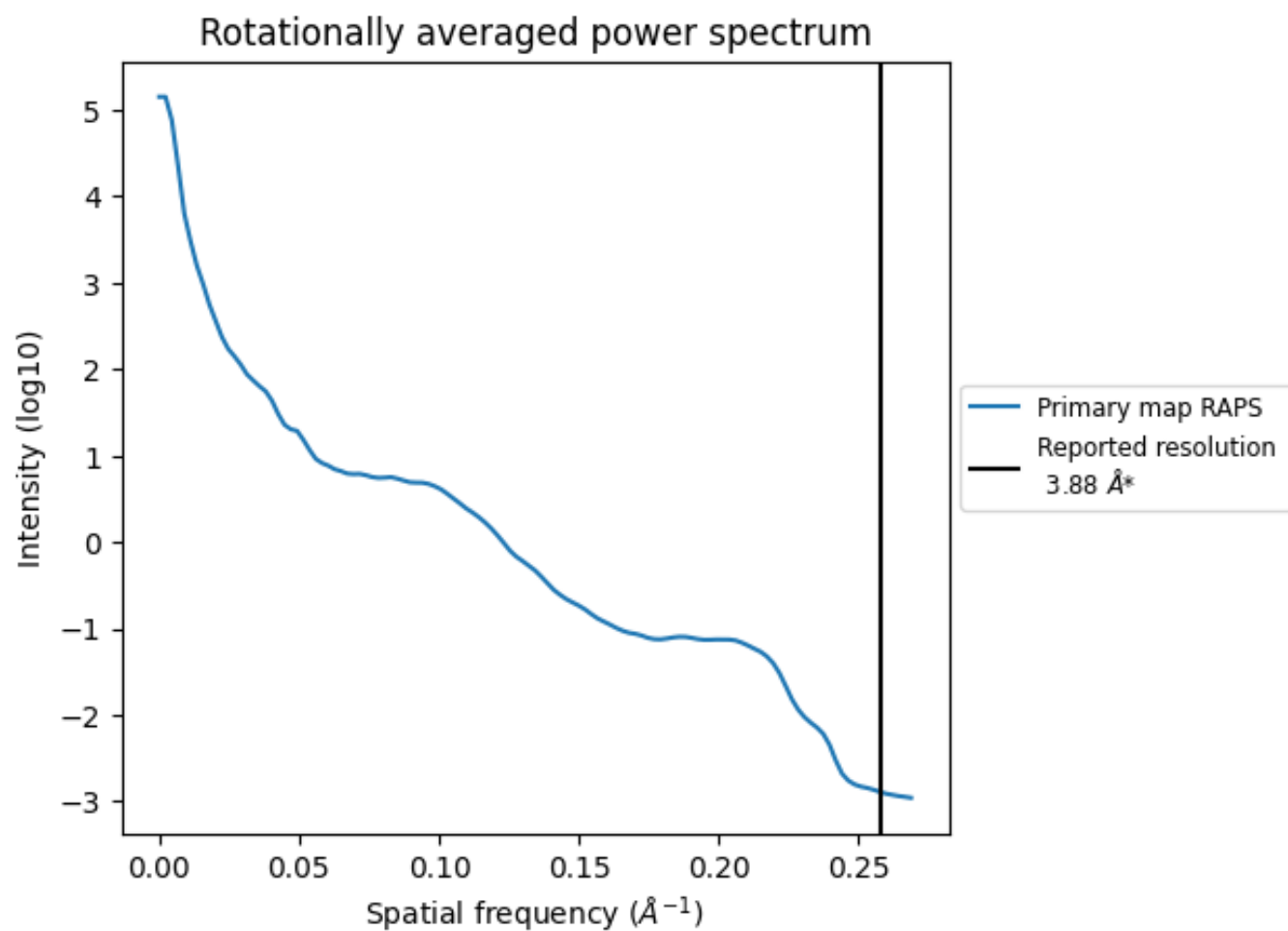
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 559 nm³; this corresponds to an approximate mass of 505 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.258 Å⁻¹

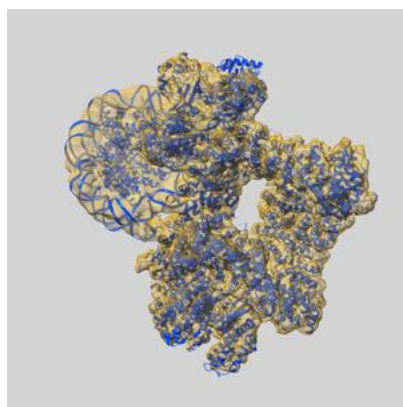
8 Fourier-Shell correlation

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

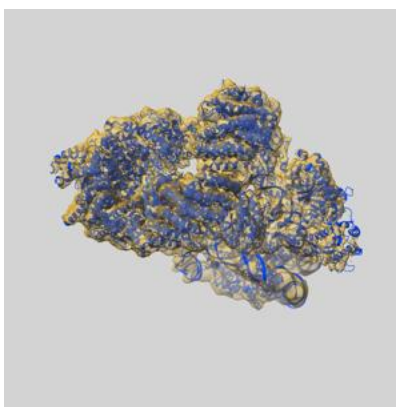
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-74524 and PDB model 9ZP9. Per-residue inclusion information can be found in section [3](#) on page [7](#).

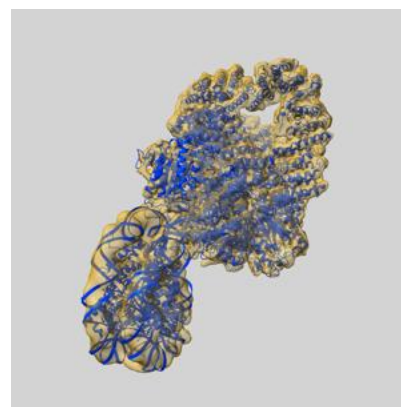
9.1 Map-model overlay [i](#)



X



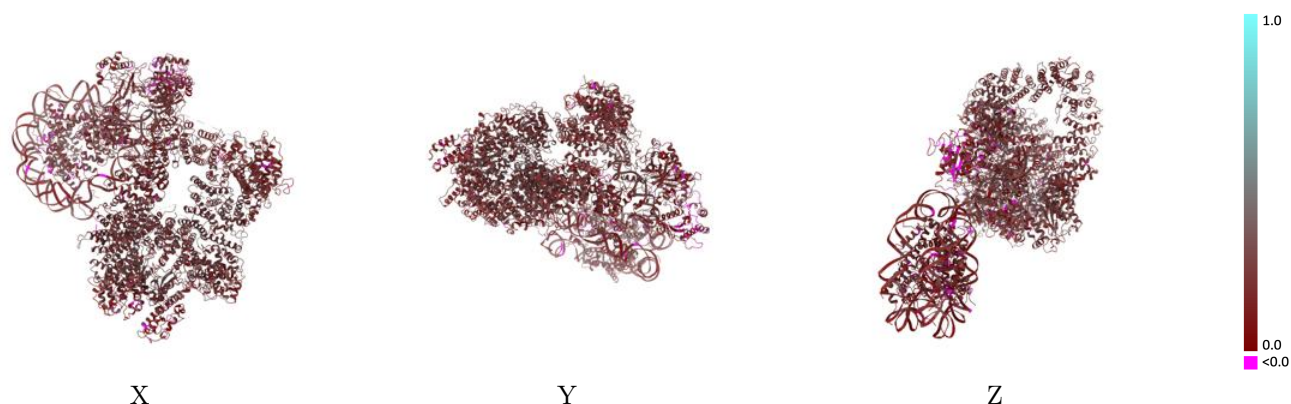
Y



Z

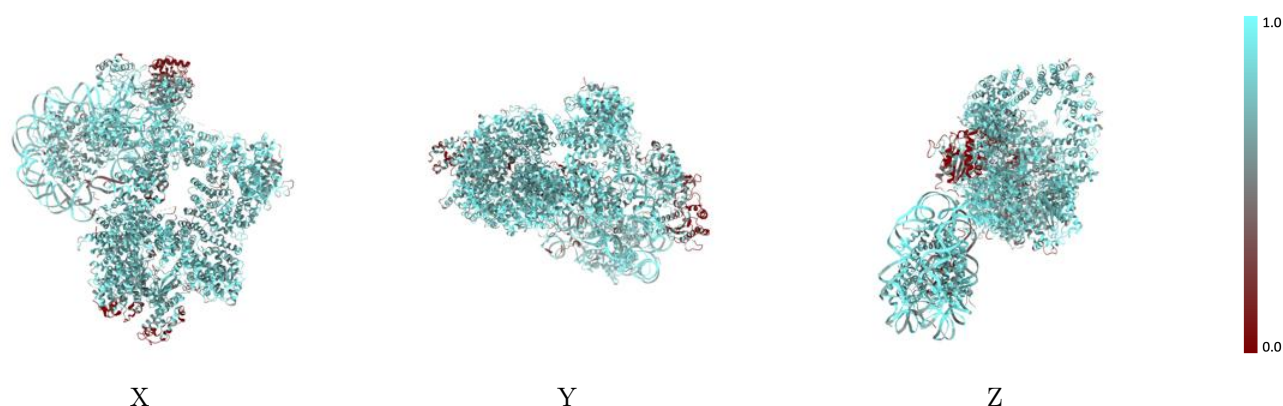
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



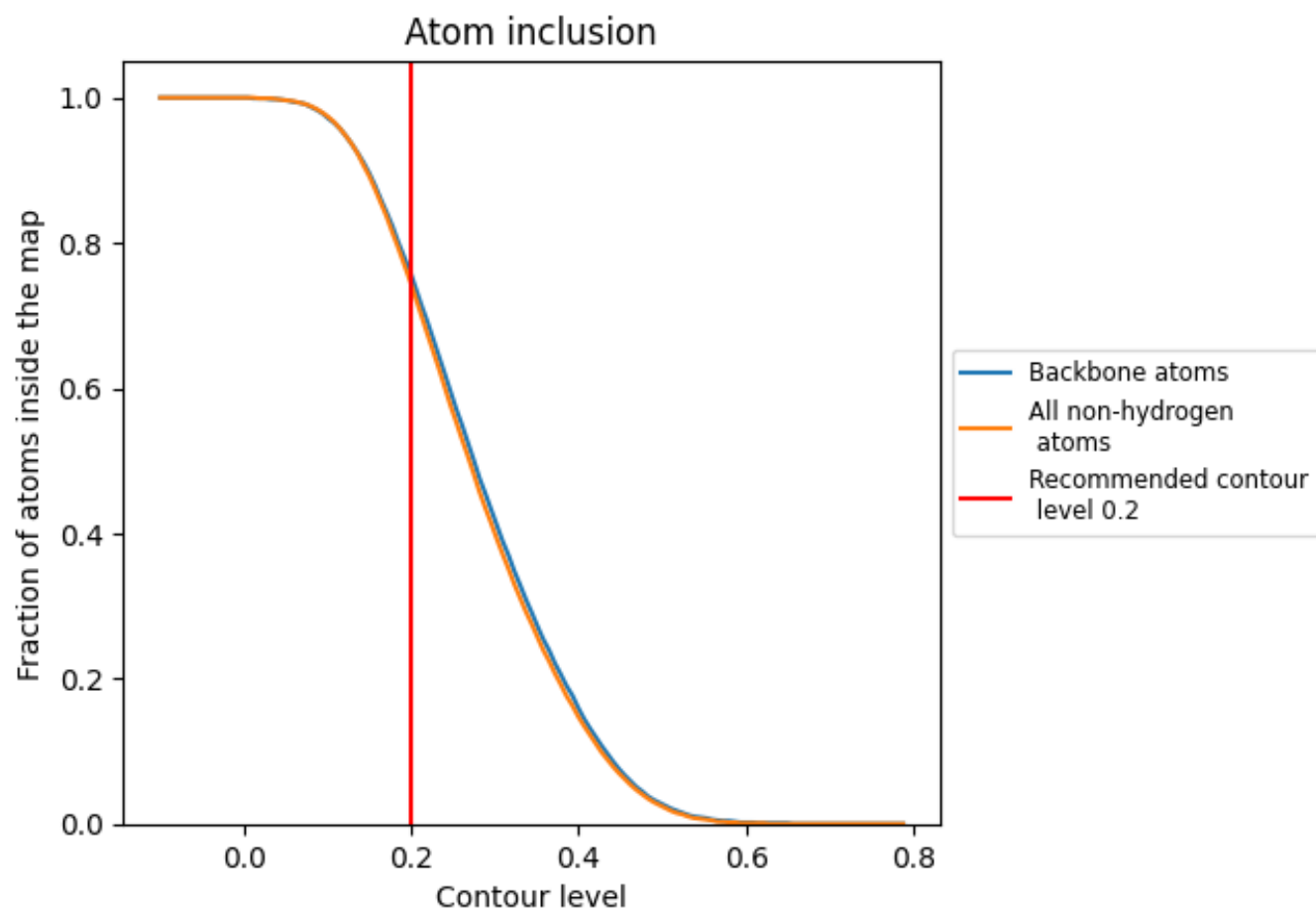
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 74% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7440	 0.2130
A	 0.8010	 0.1600
B	 0.7830	 0.1260
C	 0.7540	 0.1470
D	 0.7900	 0.1680
E	 0.7620	 0.1460
F	 0.8060	 0.1490
G	 0.7000	 0.1550
H	 0.7580	 0.1610
I	 0.8200	 0.1680
J	 0.8330	 0.1760
K	 0.7450	 0.2290
L	 0.5690	 0.1820
M	 0.7560	 0.2360
N	 0.8710	 0.3340

