



wwPDB EM Validation Summary Report ⓘ

Nov 15, 2022 – 02:02 PM JST

PDB ID : 7BTQ
EMDB ID : EMD-30182
Title : EcoR124I-DNA in the Restriction-Alleviation State
Authors : Gao, Y.; Gao, P.
Deposited on : 2020-04-02
Resolution : 4.54 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.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) : 2.31.2

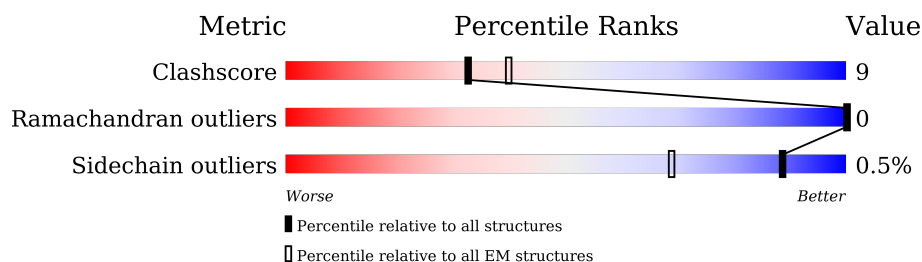
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.54 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 $\leq 5\%$. 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	520	 8% 71% 19% • 9%
1	D	520	 7% 73% 17% • 9%
2	B	64	 6% 34% 34% 31%
3	C	64	 8% 11% 56% • 31%
4	E	404	 6% 74% 20% • 5%
5	F	1038	 8% 77% 18% •

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 20419 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 Type I restriction enzyme EcoR124II M protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	474	Total	C	N	O	S	0	0
			3740	2394	624	716	6		
1	D	474	Total	C	N	O	S	0	0
			3740	2394	624	716	6		

- Molecule 2 is a DNA chain called DNA (64-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	44	Total	C	N	O	P	0	0
			906	432	186	245	43		

- Molecule 3 is a DNA chain called DNA (64-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	44	Total	C	N	O	P	0	0
			892	433	137	279	43		

- Molecule 4 is a protein called Type-1 restriction enzyme EcoR124II specificity protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	384	Total	C	N	O	S	0	0
			3099	2001	505	585	8		

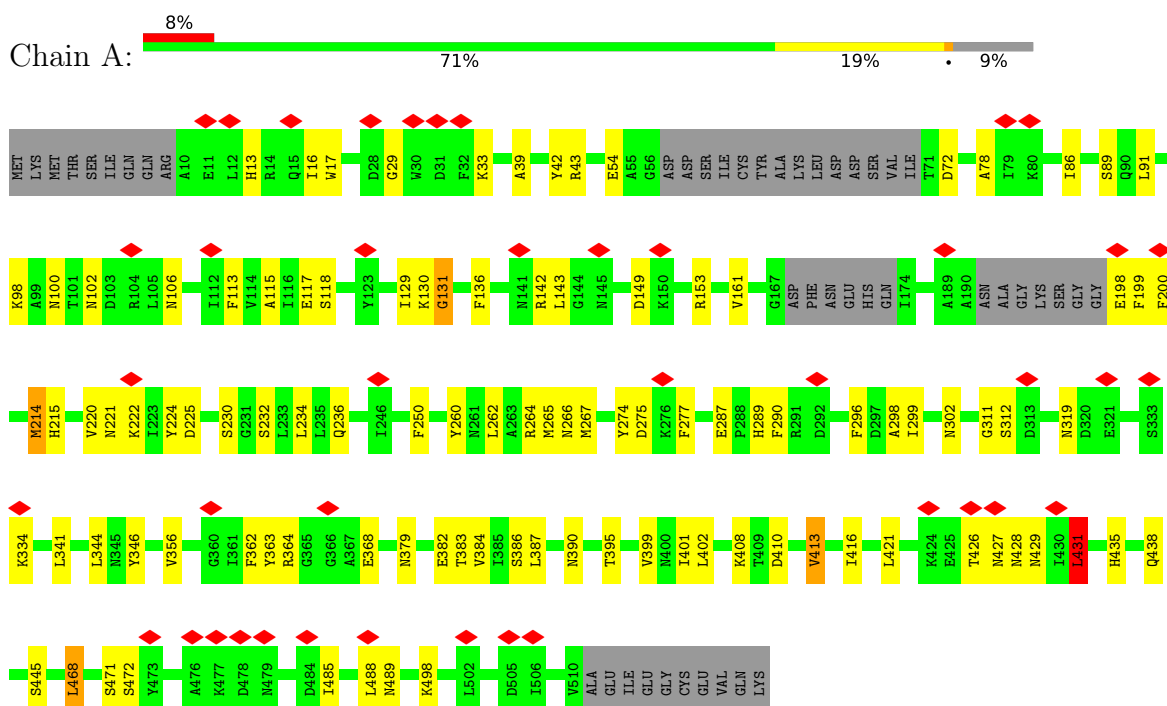
- Molecule 5 is a protein called Type I restriction enzyme R Protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	992	Total	C	N	O	S	0	0
			8042	5108	1363	1554	17		

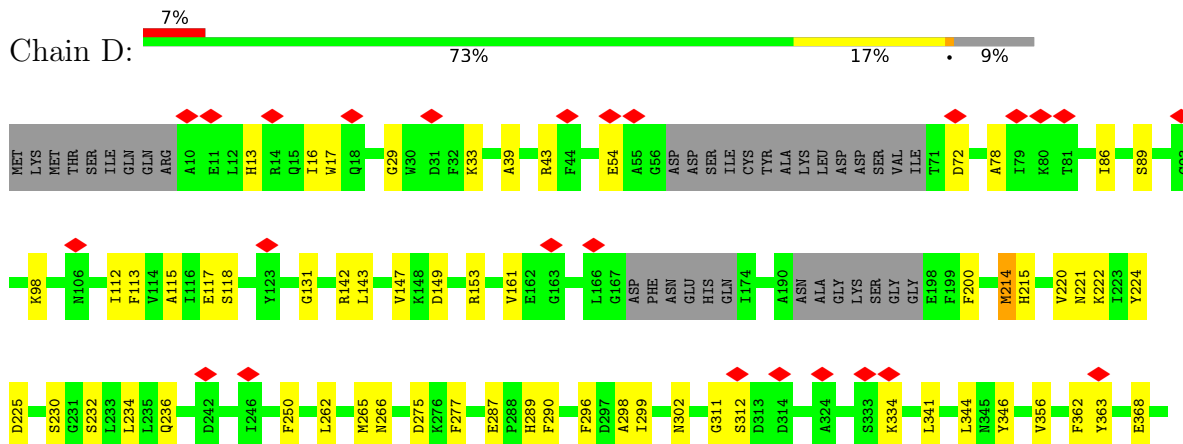
3 Residue-property plots

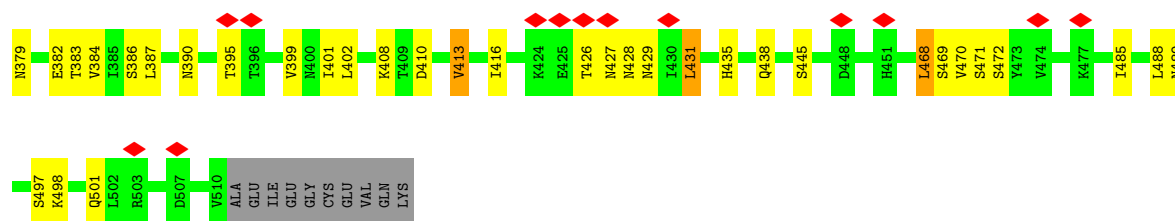
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Type I restriction enzyme EcoR124II M protein

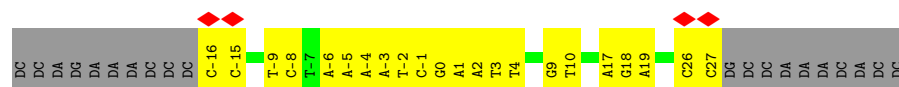


- Molecule 1: Type I restriction enzyme EcoR124II M protein

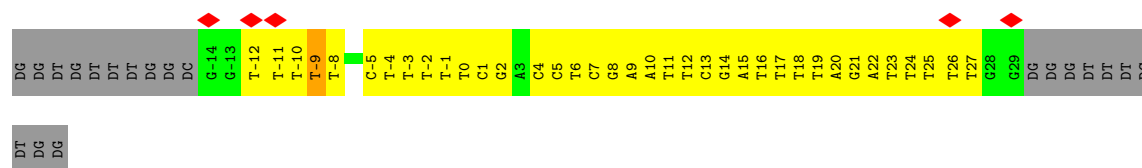
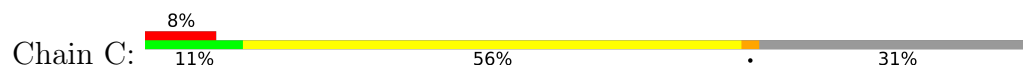




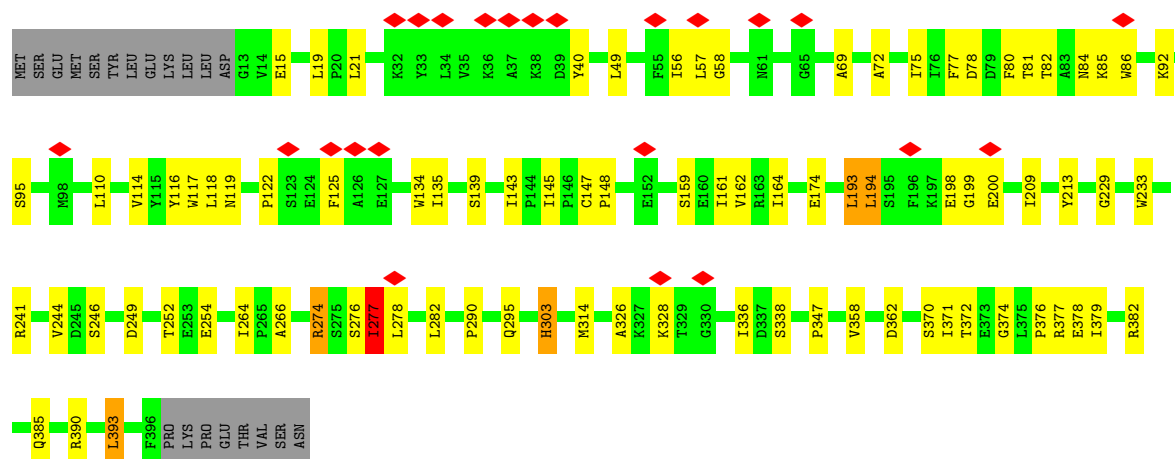
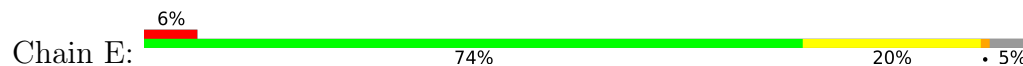
• Molecule 2: DNA (64-MER)



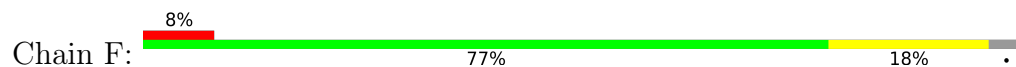
• Molecule 3: DNA (64-MER)



• Molecule 4: Type-1 restriction enzyme EcoR124II specificity protein



• Molecule 5: Type I restriction enzyme R Protein



IIE	S885	Q886	E887	T888	Y892	N901	R902	GLN	ASN	LYS	GLY	LYS	G908	E909	M910	R916	R925	E928	G929	V932	L940	I969	N973	L974	R989	E990	Y991	A992	T993	T997	P1004	K1005	L1006	S1007	P1008	L1009	M1010	P1011	V1025	I1028	G1033	V1034	G1035	GLY	LYS							
	P764	D765	S768	I769	E770	K775	K776	V779	L801	I807	D808	L809	S810	D811	P812	V815	K819	D826	F829	R836	L837	Y846	Y850	R851	D852	R858	R859	E860	K861	GLU	ALA	GLU	LYS	LYS	LYS	LYS	THR	THR	D872	W873	D874	L882	L883	K884								
	Y619	N620	K624	T625	G633	K636	Y637	Y638	R639	D640	R644	V645	Q648	L652	L660	T661	G662	F663	D664	T667	L668	V673	D674	K675	N676	L677	L682	R688	I702	V703	T704	L708	I716	G720	D721	K722	L729	A743	A744	T745	G746	E747										
	F507	L508	R512	Q518	N522	R525	P533	N539	A540	M541	V544	S545	K551	F557	Q561	A569	K572	P573	L574	R575	I576	S581	F582	A583	A584	N585	E586	E587	Q588	N589	A590	I591	G592	E593	I594	S595	D596	E597	T598	F599	D600	S606	S607	K609								
	S361	E362	N363	L367	K368	R369	D372	K373	D374	D375	N376	K377	V380	D395	D408	R412	S413	P438	I439	F440	M443	A444	L445	G446	S447	E448	T449	V453	T464	D465	K476	V477	D478	V482	R483	P484	Q485	F486	K487	S488	L489	E490	D494	A500	Q504							
	R210	Y211	F212	T215	R218	D219	K220	T226	W229	S232	K241	T252	N259	S265	S266	Q267	M272	I277	L284	I287	N295	E300	R322	L323	V337	D338	R339	Q340	D341	Y344	Q345	T346	M347	K348	R352	F353	S354	S357	G360													
	F111	I112	F113	D114	D115	E116	R117	L118	Q135	I136	Q139	F140	E141	GLN	ALA	GLY	SER	HIS	ALA	N148	D151	I154	L155	I164	K167	K168	R169	G170	V171	A172	I173	R174	E175	A176	F177	N178	Q179	I180	HIS	ARG	TYR	SER	LYS	GLU	SER	PHE	ASN	SER	E191	F201	V202	I203

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83797	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.241	Depositor
Minimum map value	-0.108	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.0586	Depositor
Map size (Å)	259.2, 259.2, 259.2	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.33	0/3817	0.69	4/5170 (0.1%)
1	D	0.33	0/3817	0.69	4/5170 (0.1%)
2	B	0.81	4/1023 (0.4%)	1.05	0/1576
3	C	0.73	9/993 (0.9%)	1.02	0/1532
4	E	0.33	0/3173	0.71	5/4301 (0.1%)
5	F	0.32	0/8189	0.56	2/11043 (0.0%)
All	All	0.39	13/21012 (0.1%)	0.69	15/28792 (0.1%)

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	D	0	3
4	E	0	7
5	F	0	4
All	All	0	17

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	27	DC	C1'-N1	5.25	1.56	1.49
3	C	24	DT	C1'-N1	5.21	1.56	1.49
3	C	-10	DT	C1'-N1	5.21	1.56	1.49
2	B	-15	DC	C1'-N1	5.21	1.56	1.49
3	C	23	DT	C1'-N1	5.21	1.56	1.49

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	431	LEU	CA-CB-CG	7.13	131.69	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	LEU	CA-CB-CG	7.12	131.67	115.30
4	E	194	LEU	CA-CB-CG	6.58	130.42	115.30
1	A	468	LEU	CA-CB-CG	6.13	129.41	115.30
1	D	468	LEU	CA-CB-CG	6.12	129.38	115.30

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	GLY	Peptide
1	A	431	LEU	Peptide
1	A	445	SER	Peptide
1	D	131	GLY	Peptide
1	D	431	LEU	Peptide

5.2 Too-close contacts ⓘ

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	3740	0	3653	64	0
1	D	3740	0	3653	56	0
2	B	906	0	492	26	0
3	C	892	0	509	75	0
4	E	3099	0	3118	63	0
5	F	8042	0	7846	107	0
All	All	20419	0	19271	367	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 9.

The worst 5 of 367 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)
3:C:-4:DT:H1'	3:C:-3:DT:C5'	1.76	1.13
3:C:-4:DT:H1'	3:C:-3:DT:H5''	1.43	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:-4:DT:H1'	3:C:-3:DT:H5'	1.46	0.96
2:B:0:DG:H2''	2:B:1:DA:C8	2.01	0.95
3:C:-4:DT:H2''	3:C:-3:DT:C5'	2.00	0.91

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	466/520 (90%)	390 (84%)	76 (16%)	0	100	100
1	D	466/520 (90%)	390 (84%)	76 (16%)	0	100	100
4	E	382/404 (95%)	319 (84%)	63 (16%)	0	100	100
5	F	982/1038 (95%)	885 (90%)	97 (10%)	0	100	100
All	All	2296/2482 (92%)	1984 (86%)	312 (14%)	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	
1	A	399/439 (91%)	395 (99%)	4 (1%)	76	86
1	D	399/439 (91%)	395 (99%)	4 (1%)	76	86

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	344/364 (94%)	341 (99%)	3 (1%)	78	87
5	F	862/927 (93%)	862 (100%)	0	100	100
All	All	2004/2169 (92%)	1993 (100%)	11 (0%)	89	93

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	498	LYS
4	E	277	ILE
4	E	393	LEU
4	E	338	SER
1	D	214	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	91	ASN
5	F	648	GLN
5	F	561	GLN
5	F	676	ASN
1	D	204	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

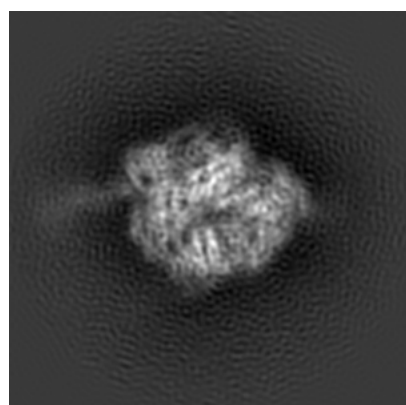
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30182. These allow visual inspection of the internal detail of the map and identification of artifacts.

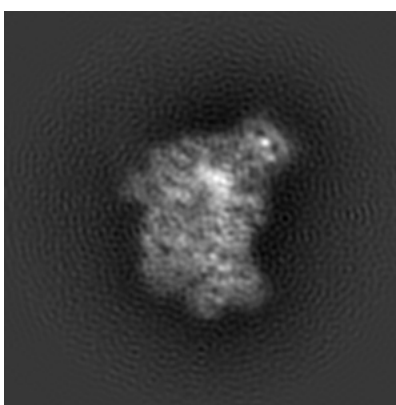
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

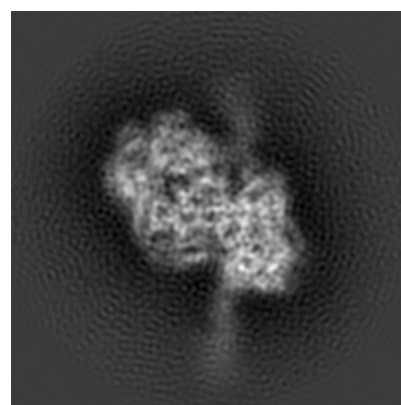
6.1.1 Primary map



X



Y

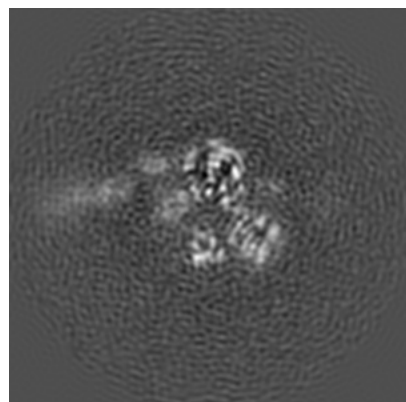


Z

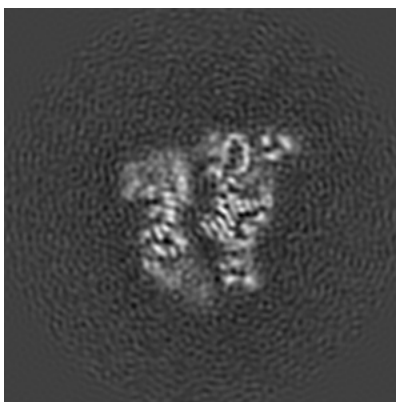
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

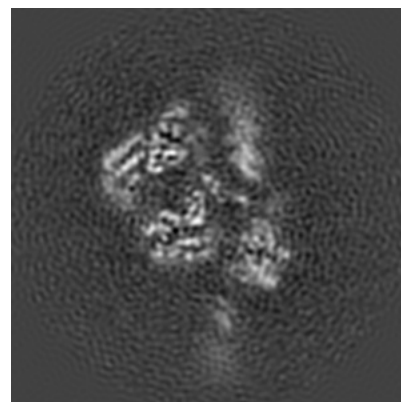
6.2.1 Primary map



X Index: 96



Y Index: 96

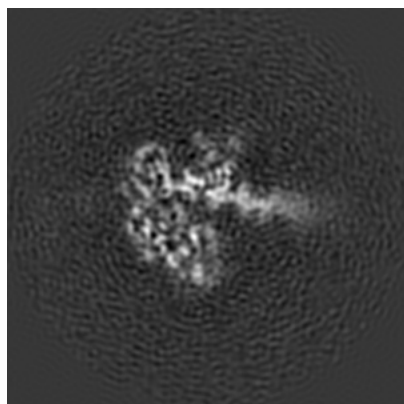


Z Index: 96

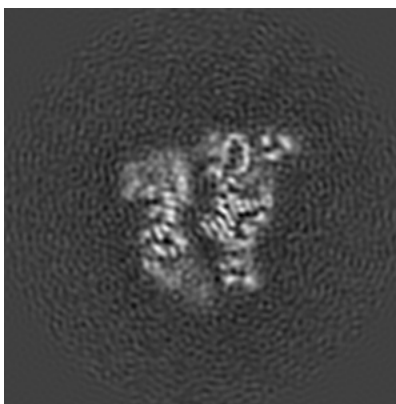
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

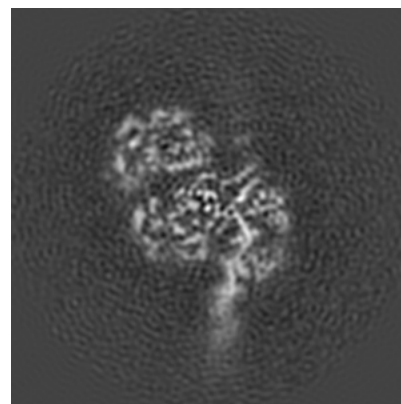
6.3.1 Primary map



X Index: 112



Y Index: 96



Z Index: 105

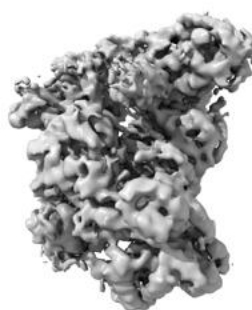
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.0586. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

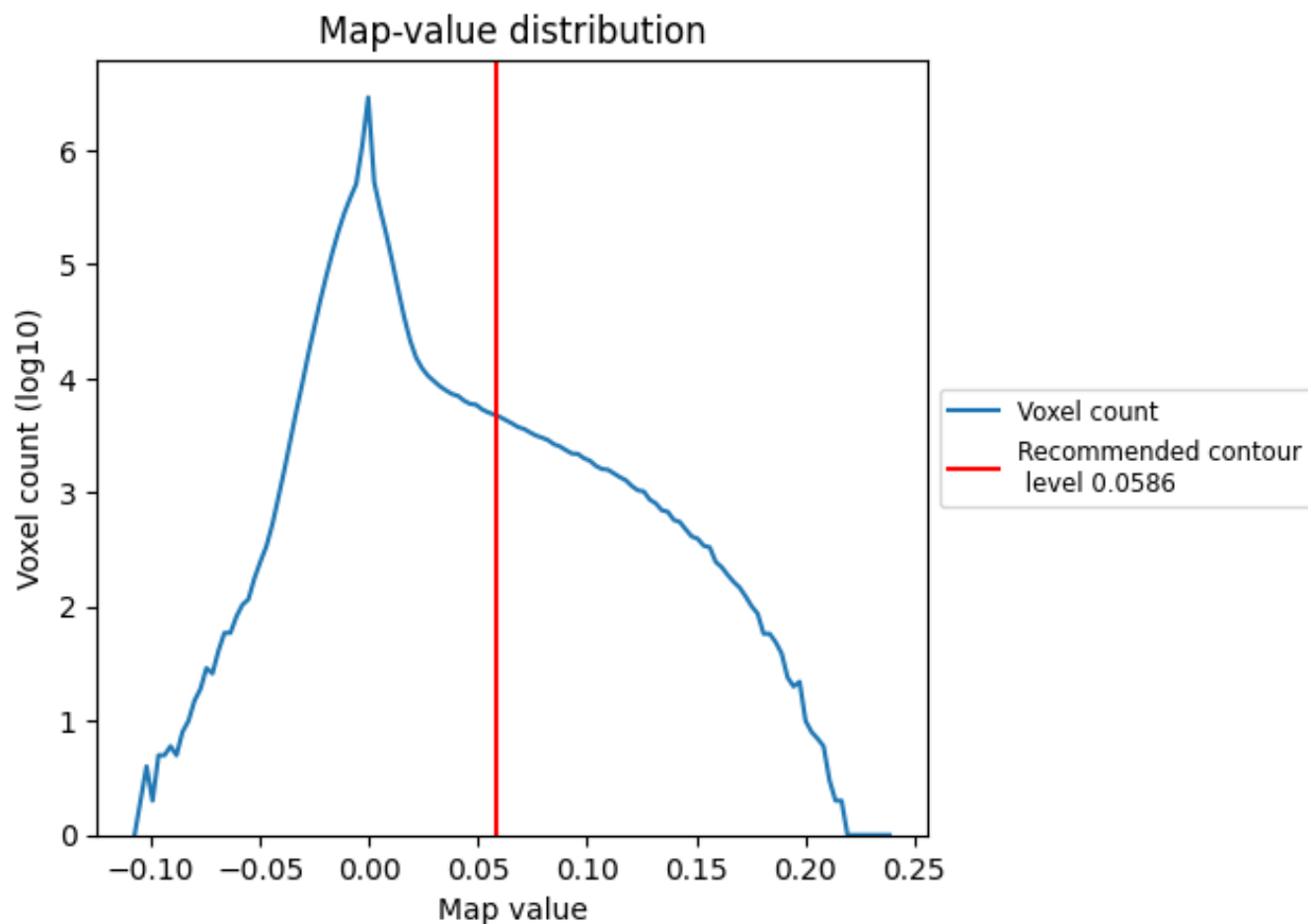
6.5 Mask visualisation

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

7 Map analysis [i](#)

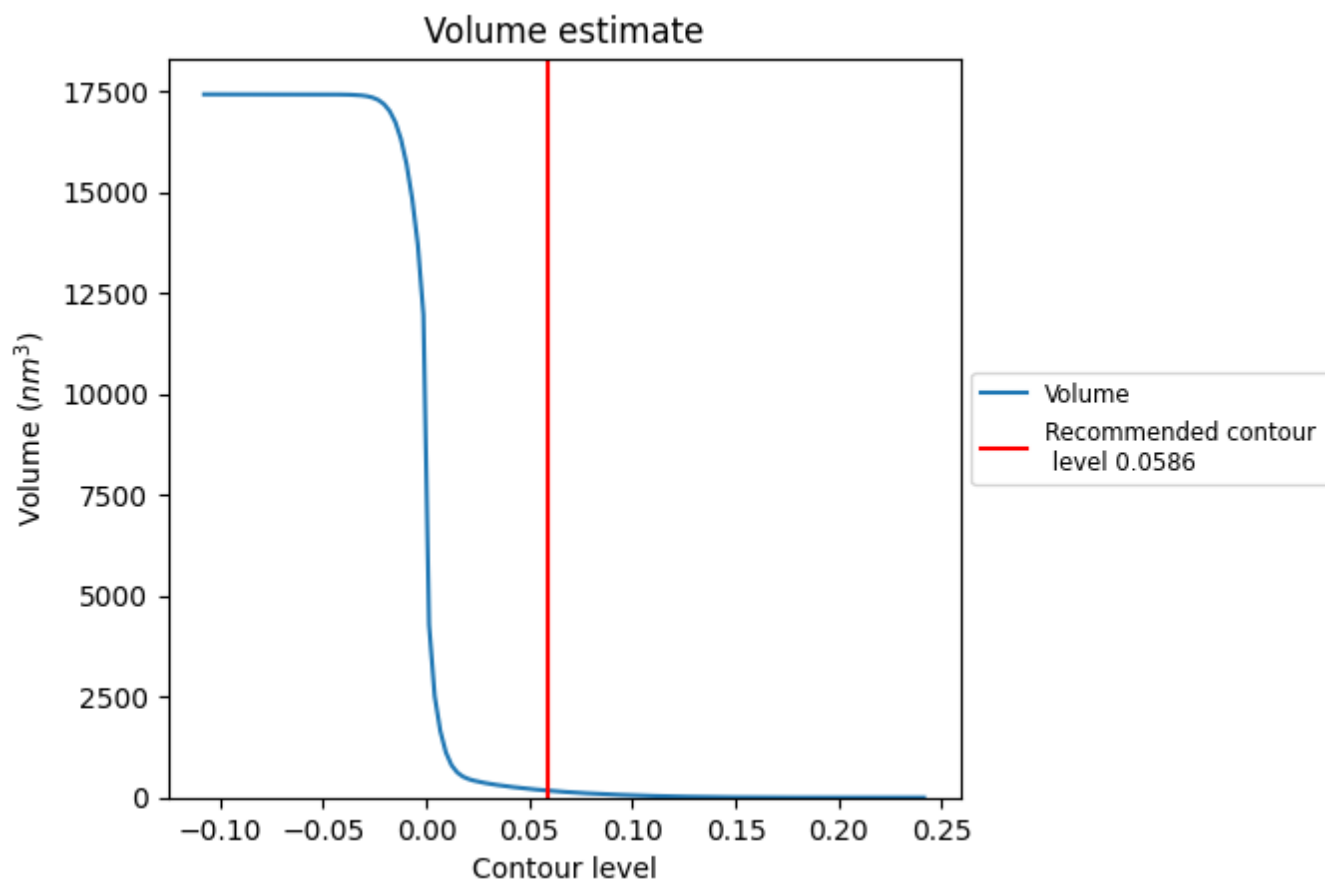
This section contains the results of statistical analysis of the map.

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.

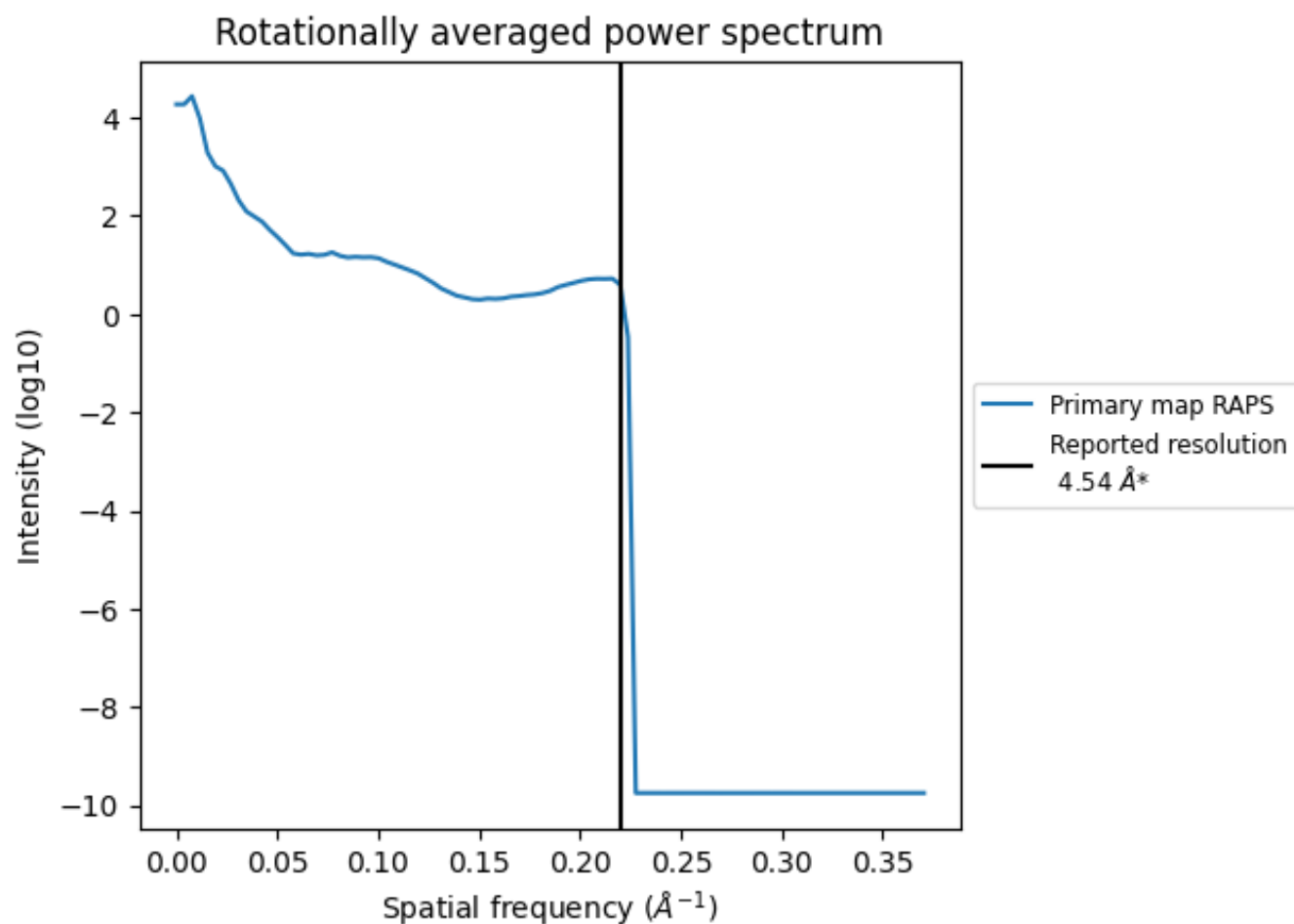
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 174 nm³; this corresponds to an approximate mass of 158 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 0.220 \AA^{-1}

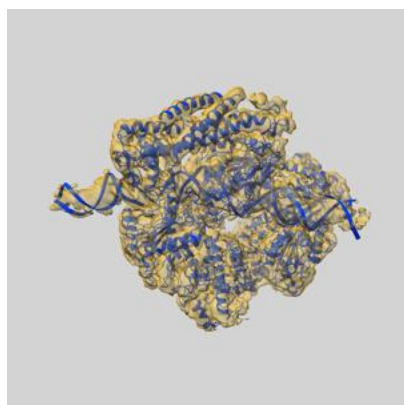
8 Fourier-Shell correlation

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

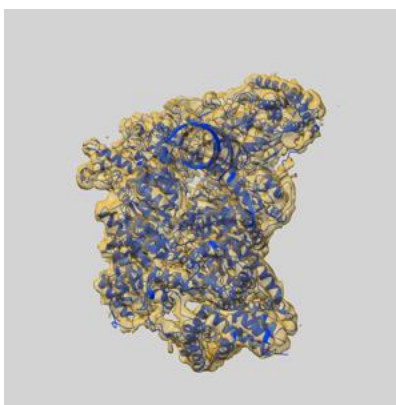
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30182 and PDB model 7BTQ. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

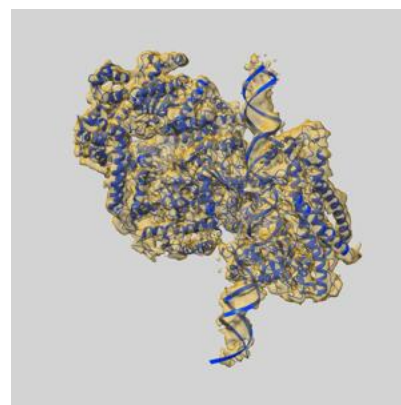
9.1 Map-model overlay [i](#)



X



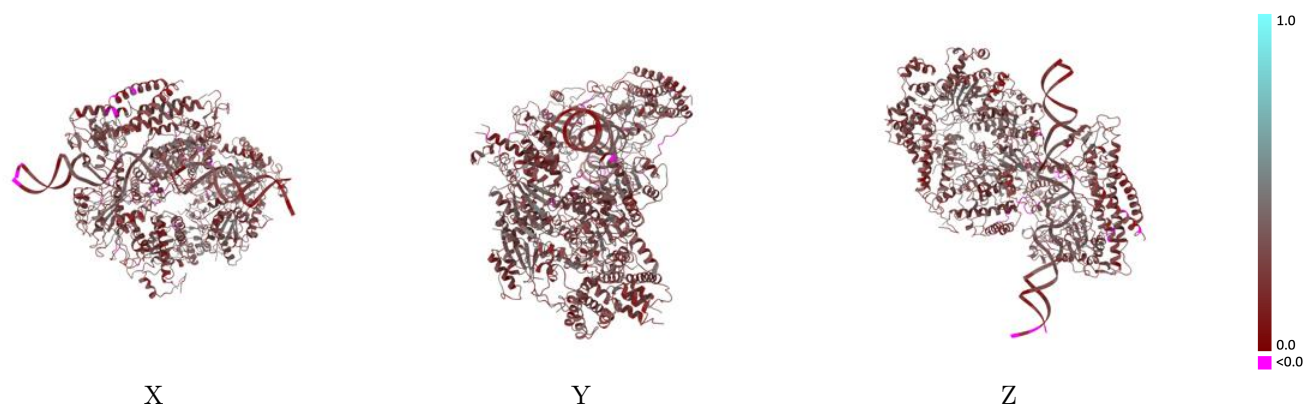
Y



Z

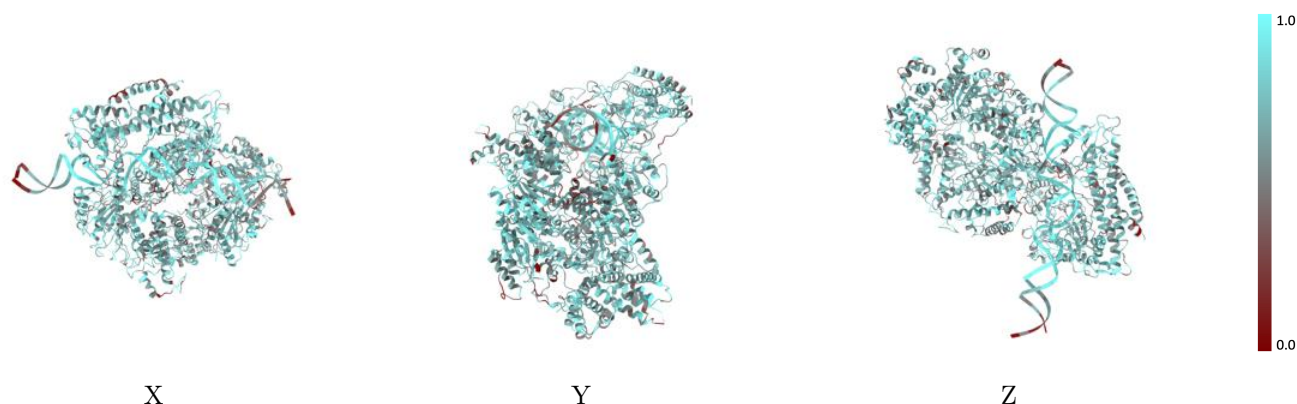
The images above show the 3D surface view of the map at the recommended contour level 0.0586 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



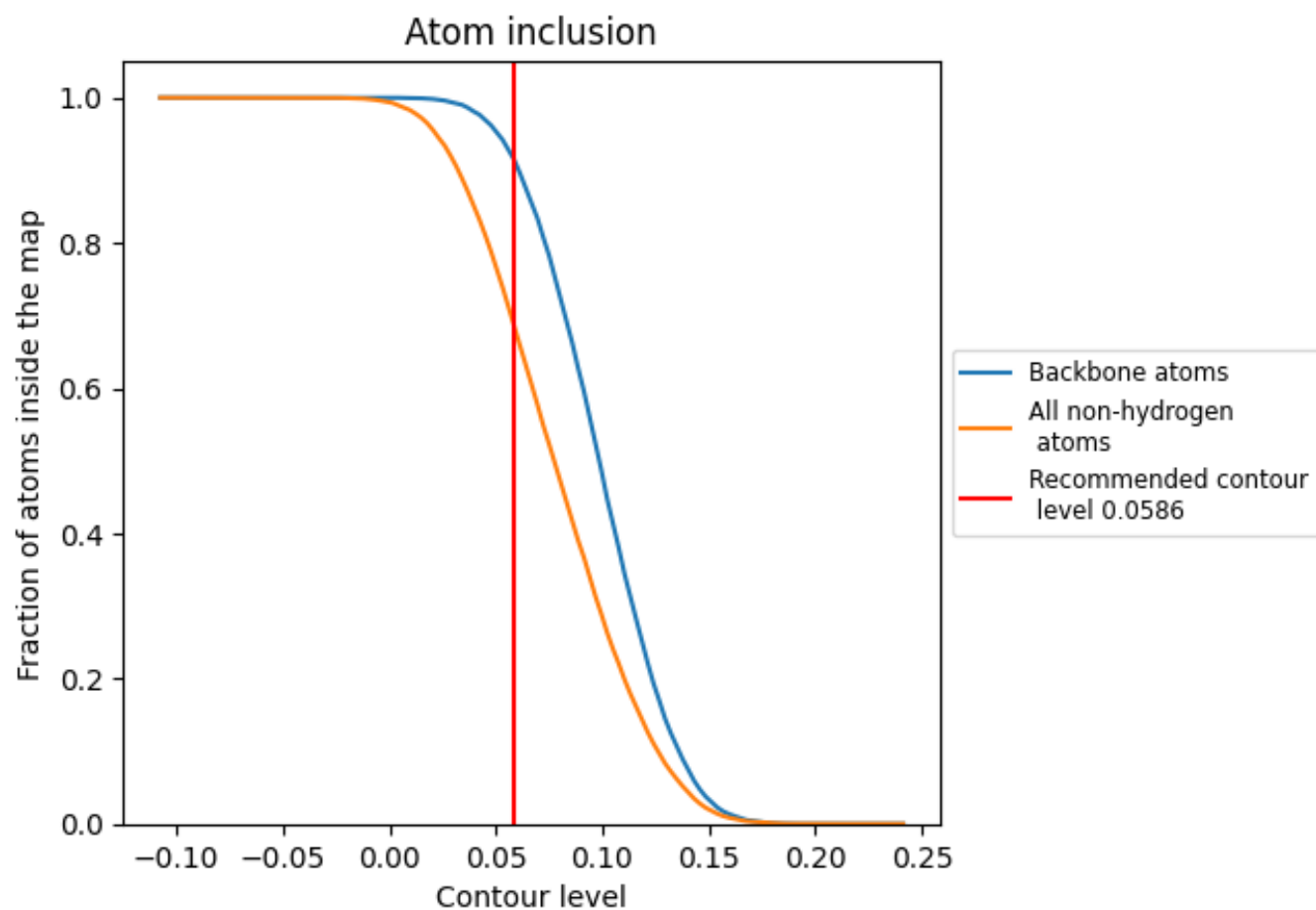
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0586).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 69% 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 (0.0586) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.6861	<div><div></div></div> 0.2770
A	<div><div></div></div> 0.6659	<div><div></div></div> 0.2590
B	<div><div></div></div> 0.7892	<div><div></div></div> 0.2680
C	<div><div></div></div> 0.7433	<div><div></div></div> 0.2460
D	<div><div></div></div> 0.6751	<div><div></div></div> 0.2630
E	<div><div></div></div> 0.6928	<div><div></div></div> 0.2870
F	<div><div></div></div> 0.6798	<div><div></div></div> 0.2920

1.0

0.0

<0.0