



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 06:21 AM UTC

PDB ID : 7F8W / pdb_00007f8w
EMDB ID : EMD-31494
Title : Cryo-EM structure of the cholecystokinin receptor CCKBR in complex with gastrin-17 and Gq
Authors : Zhang, X.; He, C.; Wang, M.; Zhou, Q.; Yang, D.; Zhu, Y.; Wu, B.; Zhao, Q.
Deposited on : 2021-07-02
Resolution : 3.10 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
Mogul : 2022.3.0, CSD as543be (2022)
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

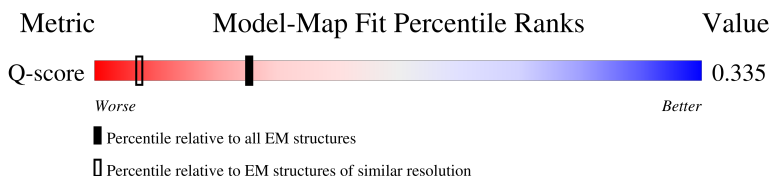
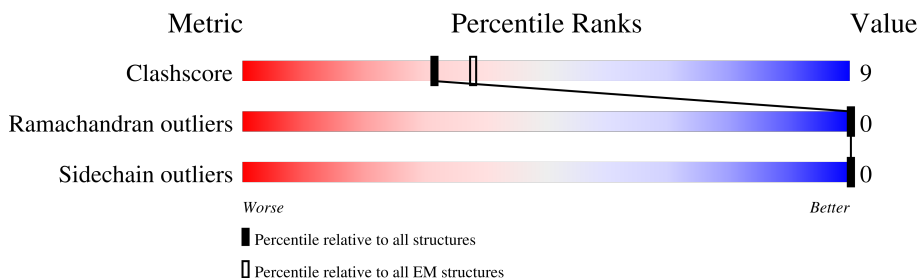
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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 $\leq 5\%$. 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	353	34% 49% 14% 37%
2	B	351	17% 65% 23% 13%
3	C	71	37% 41% 6% 54%
4	D	268	39% 68% 18% 13%

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Mol	Chain	Length	Quality of chain
5	E	17	88% 65% 35%
6	R	465	27% 49% 10% 41%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8486 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 Guanine nucleotide-binding protein G(q) subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	224	Total	C	N	O	S	0	0
			1850	1180	318	343	9		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P50148
A	2	GLY	-	expression tag	UNP P50148
A	3	CYS	-	expression tag	UNP P50148
A	4	THR	-	expression tag	UNP P50148
A	5	LEU	-	expression tag	UNP P50148
A	6	SER	-	expression tag	UNP P50148
A	7	ALA	-	expression tag	UNP P50148
A	8	GLU	-	expression tag	UNP P50148
A	9	ASP	-	expression tag	UNP P50148
A	10	LYS	-	expression tag	UNP P50148
A	11	ALA	-	expression tag	UNP P50148
A	12	ALA	-	expression tag	UNP P50148
A	13	VAL	-	expression tag	UNP P50148
A	14	GLU	-	expression tag	UNP P50148
A	15	ARG	-	expression tag	UNP P50148
A	16	SER	-	expression tag	UNP P50148
A	17	LYS	-	expression tag	UNP P50148
A	18	MET	-	expression tag	UNP P50148
A	19	ILE	-	expression tag	UNP P50148
A	20	ASP	-	expression tag	UNP P50148
A	21	ARG	-	expression tag	UNP P50148
A	22	ASN	-	expression tag	UNP P50148

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	306	Total	C	N	O	S	0	0
			2347	1453	418	456	20		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	MET	-	expression tag	UNP P62873
B	-9	HIS	-	expression tag	UNP P62873
B	-8	HIS	-	expression tag	UNP P62873
B	-7	HIS	-	expression tag	UNP P62873
B	-6	HIS	-	expression tag	UNP P62873
B	-5	HIS	-	expression tag	UNP P62873
B	-4	HIS	-	expression tag	UNP P62873
B	-3	GLY	-	expression tag	UNP P62873
B	-2	SER	-	expression tag	UNP P62873
B	-1	LEU	-	expression tag	UNP P62873
B	0	LEU	-	expression tag	UNP P62873
B	1	GLN	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	33	Total	C	N	O	S	0	0
			245	156	39	48	2		

- Molecule 4 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	232	Total	C	N	O	S	0	0
			1783	1131	295	347	10		

- Molecule 5 is a protein called Gastrin-17.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	17	Total	C	N	O	S	0	0
			133	89	20	23	1		

- Molecule 6 is a protein called Gastrin/cholecystokinin type B receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	275	Total	C	N	O	S	0	0
			2128	1412	359	339	18		

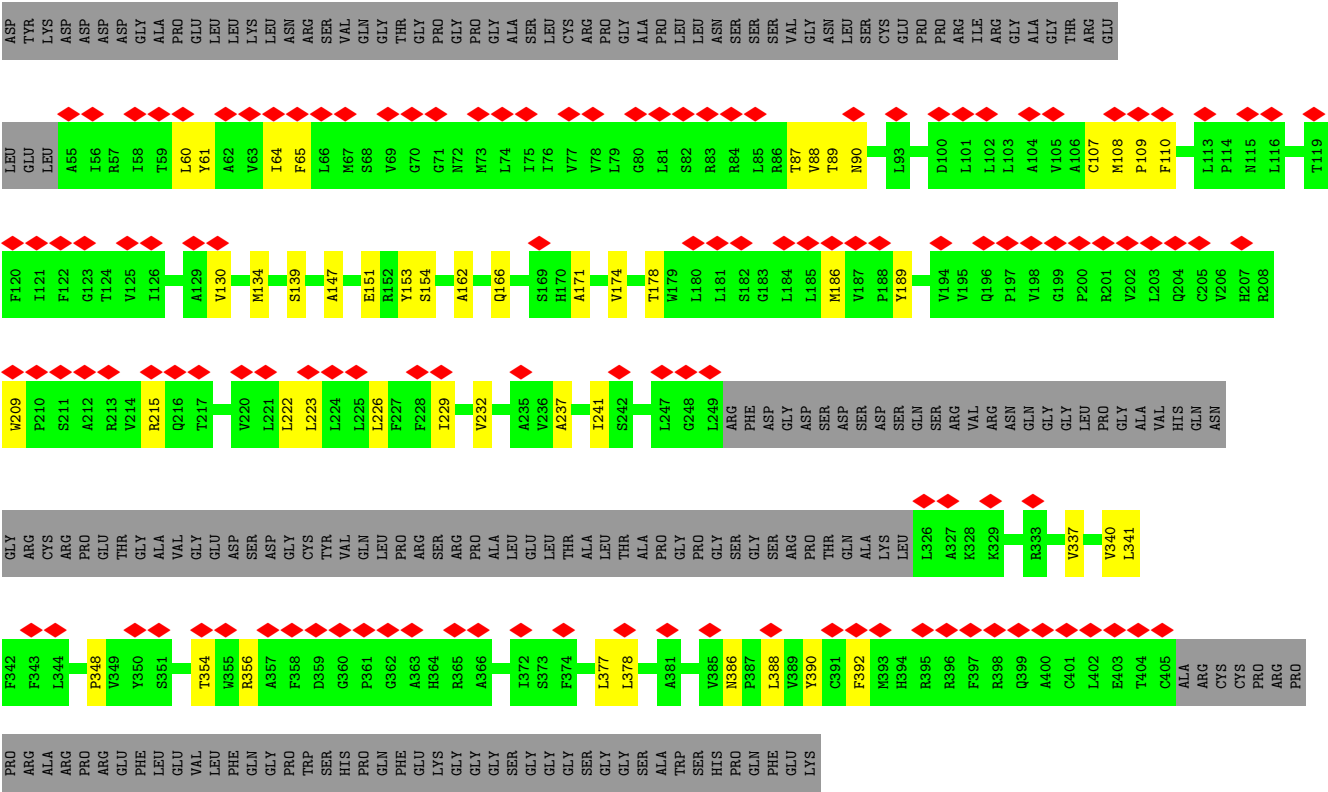
There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-8	ASP	-	expression tag	UNP P32239
R	-7	TYR	-	expression tag	UNP P32239
R	-6	LYS	-	expression tag	UNP P32239
R	-5	ASP	-	expression tag	UNP P32239
R	-4	ASP	-	expression tag	UNP P32239
R	-3	ASP	-	expression tag	UNP P32239
R	-2	ASP	-	expression tag	UNP P32239
R	-1	GLY	-	expression tag	UNP P32239
R	0	ALA	-	expression tag	UNP P32239
R	1	PRO	-	expression tag	UNP P32239
R	419	GLU	-	expression tag	UNP P32239
R	420	PHE	-	expression tag	UNP P32239
R	421	LEU	-	expression tag	UNP P32239
R	422	GLU	-	expression tag	UNP P32239
R	423	VAL	-	expression tag	UNP P32239
R	424	LEU	-	expression tag	UNP P32239
R	425	PHE	-	expression tag	UNP P32239
R	426	GLN	-	expression tag	UNP P32239
R	427	GLY	-	expression tag	UNP P32239
R	428	PRO	-	expression tag	UNP P32239
R	429	TRP	-	expression tag	UNP P32239
R	430	SER	-	expression tag	UNP P32239
R	431	HIS	-	expression tag	UNP P32239
R	432	PRO	-	expression tag	UNP P32239
R	433	GLN	-	expression tag	UNP P32239
R	434	PHE	-	expression tag	UNP P32239
R	435	GLU	-	expression tag	UNP P32239
R	436	LYS	-	expression tag	UNP P32239
R	437	GLY	-	expression tag	UNP P32239
R	438	GLY	-	expression tag	UNP P32239
R	439	GLY	-	expression tag	UNP P32239
R	440	SER	-	expression tag	UNP P32239
R	441	GLY	-	expression tag	UNP P32239
R	442	GLY	-	expression tag	UNP P32239
R	443	GLY	-	expression tag	UNP P32239
R	444	SER	-	expression tag	UNP P32239
R	445	GLY	-	expression tag	UNP P32239

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Chain	Residue	Modelled	Actual	Comment	Reference
R	446	GLY	-	expression tag	UNP P32239
R	447	SER	-	expression tag	UNP P32239
R	448	ALA	-	expression tag	UNP P32239
R	449	TRP	-	expression tag	UNP P32239
R	450	SER	-	expression tag	UNP P32239
R	451	HIS	-	expression tag	UNP P32239
R	452	PRO	-	expression tag	UNP P32239
R	453	GLN	-	expression tag	UNP P32239
R	454	PHE	-	expression tag	UNP P32239
R	455	GLU	-	expression tag	UNP P32239
R	456	LYS	-	expression tag	UNP P32239



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	354647	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.75	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.180	Depositor
Minimum map value	-0.108	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0252	Depositor
Map size ($\text{\AA}$)	267.52, 267.52, 267.52	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.045, 1.045, 1.045	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PCA, NFA

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	0.24	0/1883	0.61	0/2532
2	B	0.21	0/2394	0.55	0/3248
3	C	0.20	0/251	0.49	0/342
4	D	0.25	0/1827	0.61	2/2477 (0.1%)
5	E	0.20	0/119	0.47	0/165
6	R	0.29	0/2179	0.58	0/2977
All	All	0.25	0/8653	0.58	2/11741 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	208	ARG	CA-C-N	5.87	132.75	121.54
4	D	208	ARG	C-N-CA	5.87	132.75	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1850	0	1851	44	0
2	B	2347	0	2249	51	0
3	C	245	0	240	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1783	0	1719	32	0
5	E	133	0	101	4	0
6	R	2128	0	2256	31	0
All	All	8486	0	8416	147	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 147 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:D:171:SER:HA	4:D:233:ILE:O	1.92	0.70
1:A:13:VAL:HG11	2:B:88:ASN:HD22	1.56	0.69
1:A:15:ARG:HH22	4:D:73:GLY:HA3	1.58	0.68
1:A:18:MET:HA	1:A:21:ARG:HB2	1.76	0.68
1:A:34:LEU:HD22	1:A:218:THR:HB	1.75	0.67

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	220/353 (62%)	209 (95%)	11 (5%)	0	100	100
2	B	304/351 (87%)	288 (95%)	16 (5%)	0	100	100
3	C	31/71 (44%)	31 (100%)	0	0	100	100
4	D	228/268 (85%)	211 (92%)	17 (8%)	0	100	100
5	E	15/17 (88%)	15 (100%)	0	0	100	100
6	R	271/465 (58%)	266 (98%)	5 (2%)	0	100	100
All	All	1069/1525 (70%)	1020 (95%)	49 (5%)	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	204/320 (64%)	204 (100%)	0	100	100
2	B	254/293 (87%)	254 (100%)	0	100	100
3	C	26/58 (45%)	26 (100%)	0	100	100
4	D	197/217 (91%)	197 (100%)	0	100	100
5	E	8/12 (67%)	8 (100%)	0	100	100
6	R	232/383 (61%)	232 (100%)	0	100	100
All	All	921/1283 (72%)	921 (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 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	293	ASN
4	D	20	GLN
6	R	115	ASN
4	D	159	GLN
1	A	281	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](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PCA	E	1	5	7,8,9	0.45	0	9,10,12	0.53	0
5	NFA	E	17	5	12,12,12	0.87	0	15,15,15	0.66	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PCA	E	1	5	-	0/0/11/13	0/1/1/1
5	NFA	E	17	5	-	1/8/8/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	17	NFA	NXT-C-CA-N

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1	PCA	1	0
5	E	17	NFA	1	0

5.5 Carbohydrates

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.

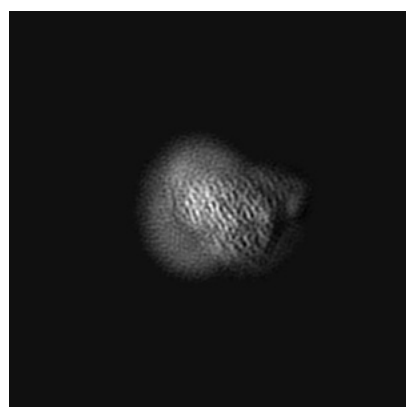
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31494. These allow visual inspection of the internal detail of the map and identification of artifacts.

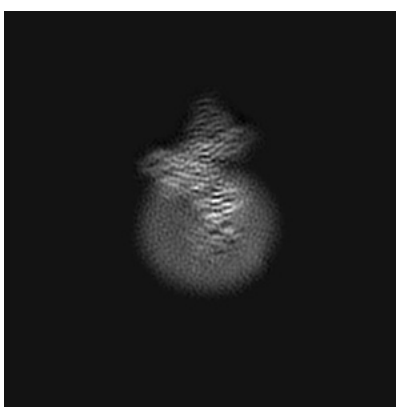
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

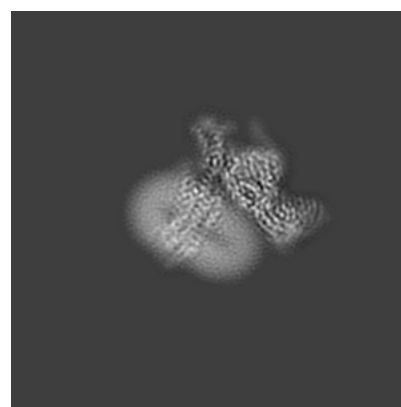
6.1.1 Primary map



X



Y

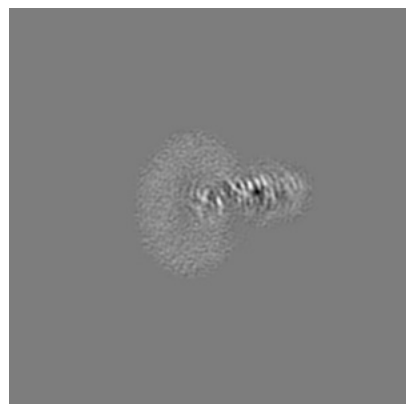


Z

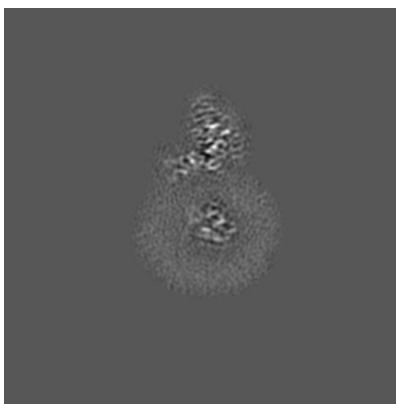
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

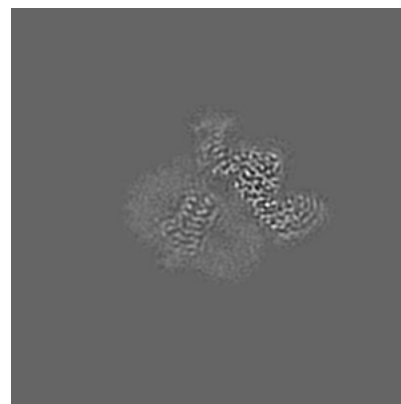
6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

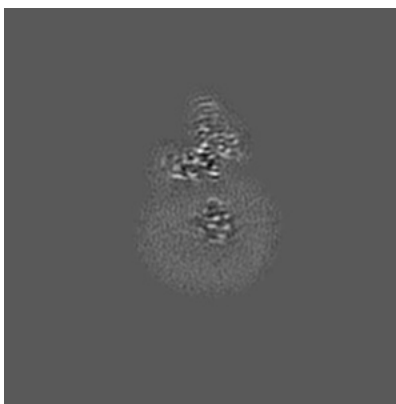
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

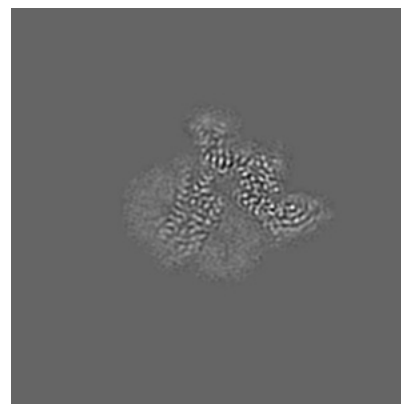
6.3.1 Primary map



X Index: 164



Y Index: 131

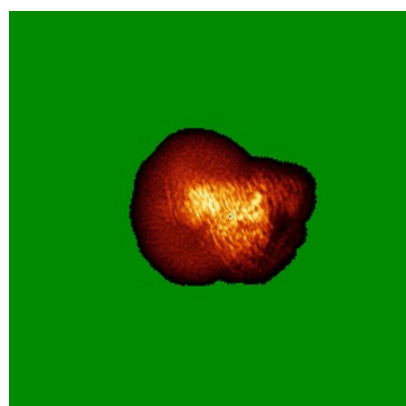


Z Index: 133

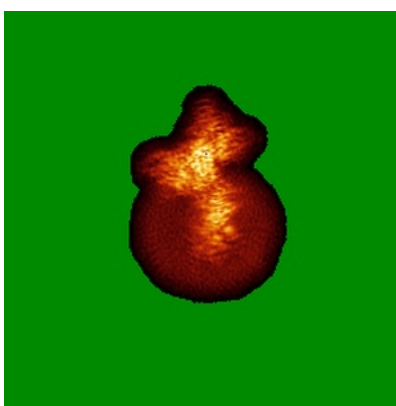
The images above show the largest variance slices of the map in three orthogonal directions.

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

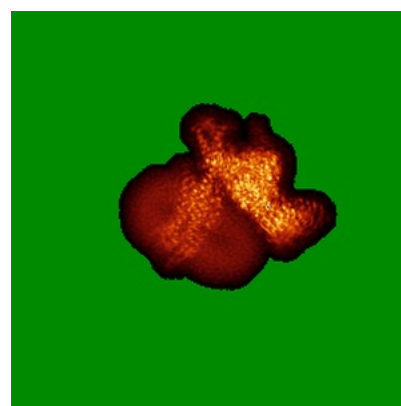
6.4.1 Primary map



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

This section was not generated.

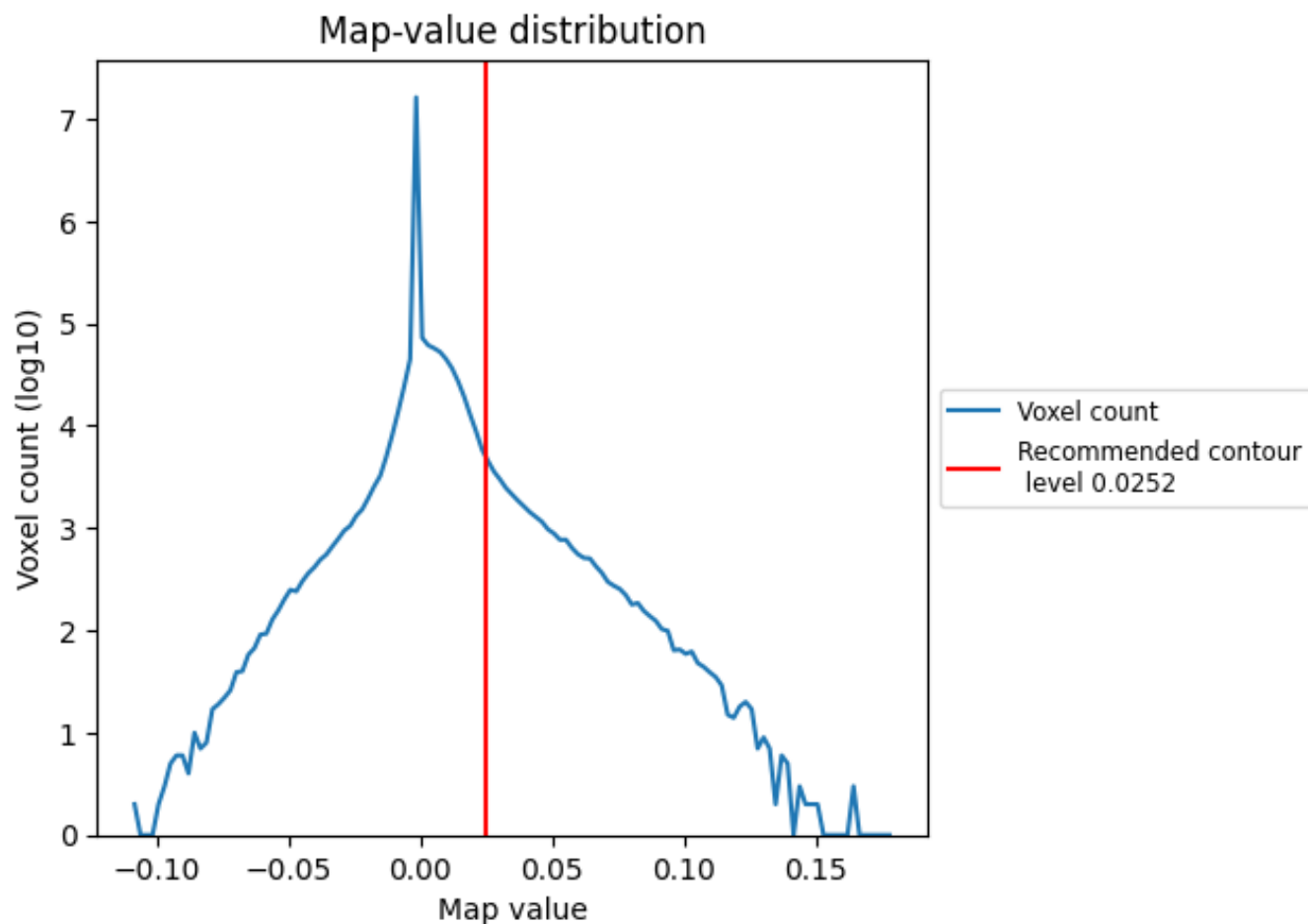
6.6 Mask visualisation

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

7 Map analysis [i](#)

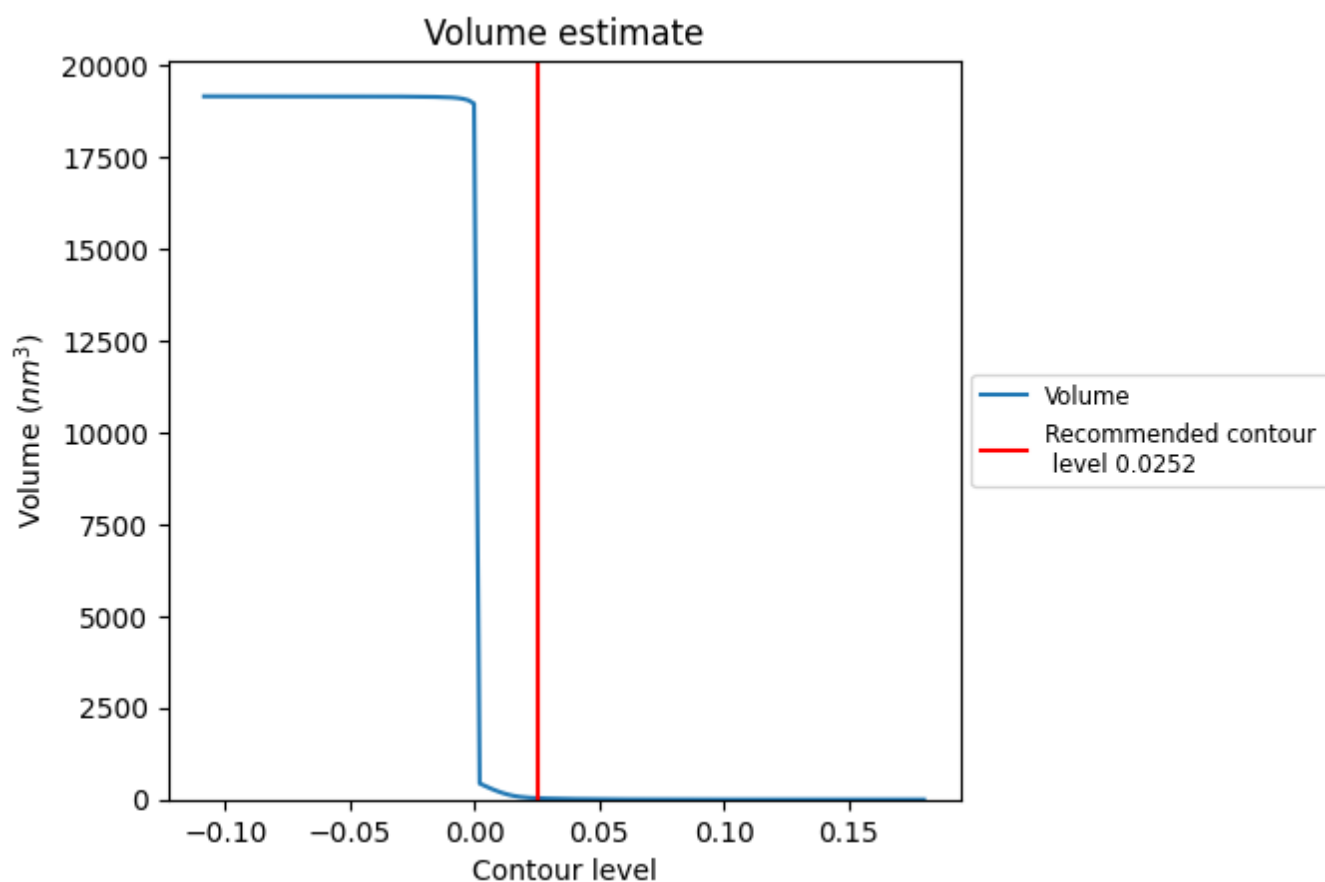
This section contains the results of statistical analysis of the map.

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.

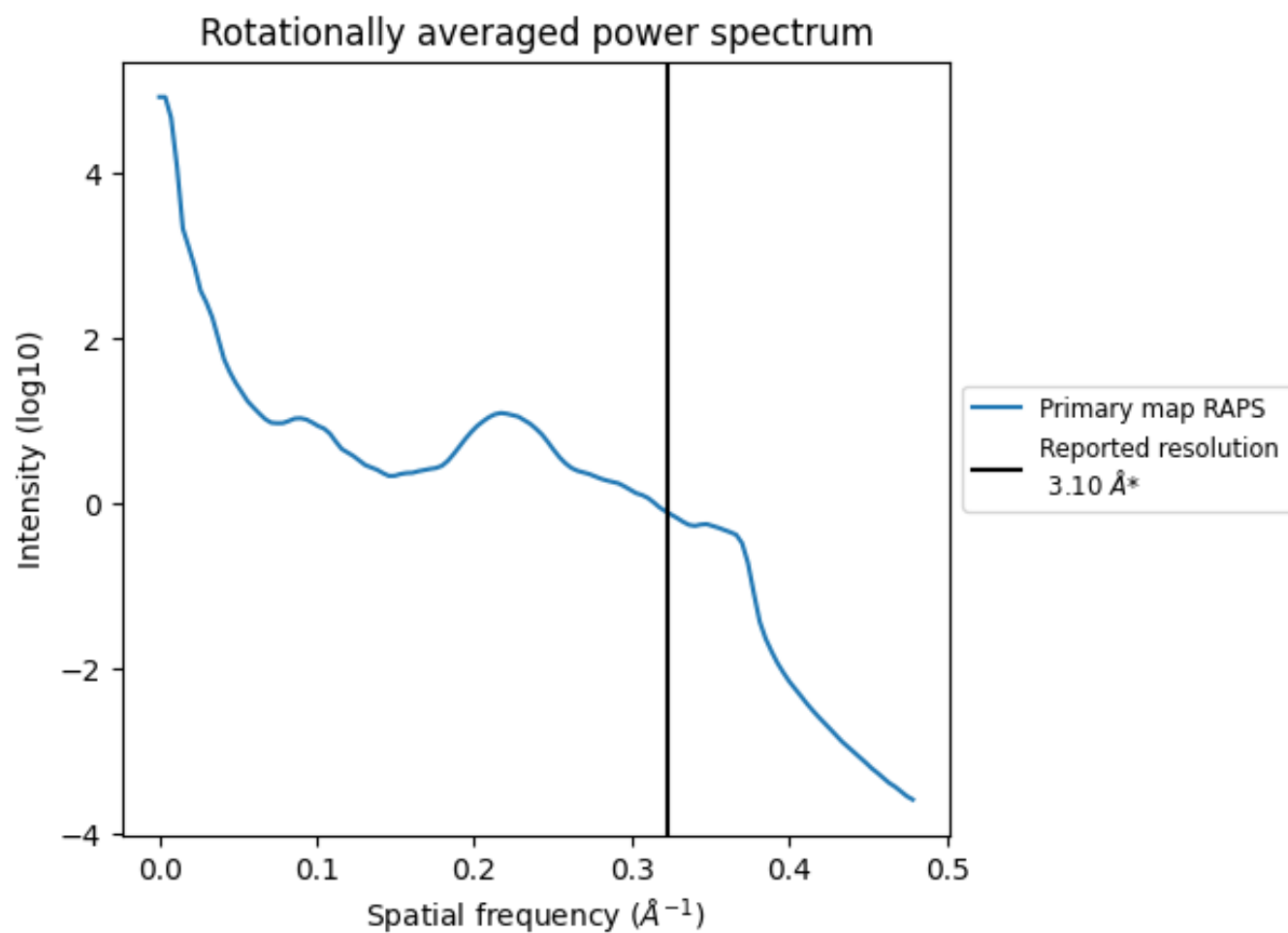
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 38 nm³; this corresponds to an approximate mass of 34 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 0.323 Å⁻¹

8 Fourier-Shell correlation

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

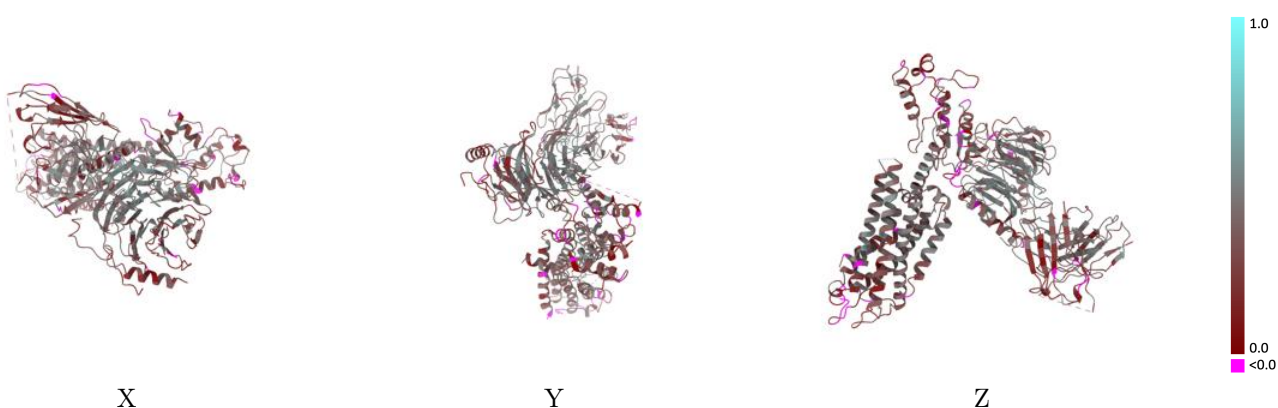
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31494 and PDB model 7F8W. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

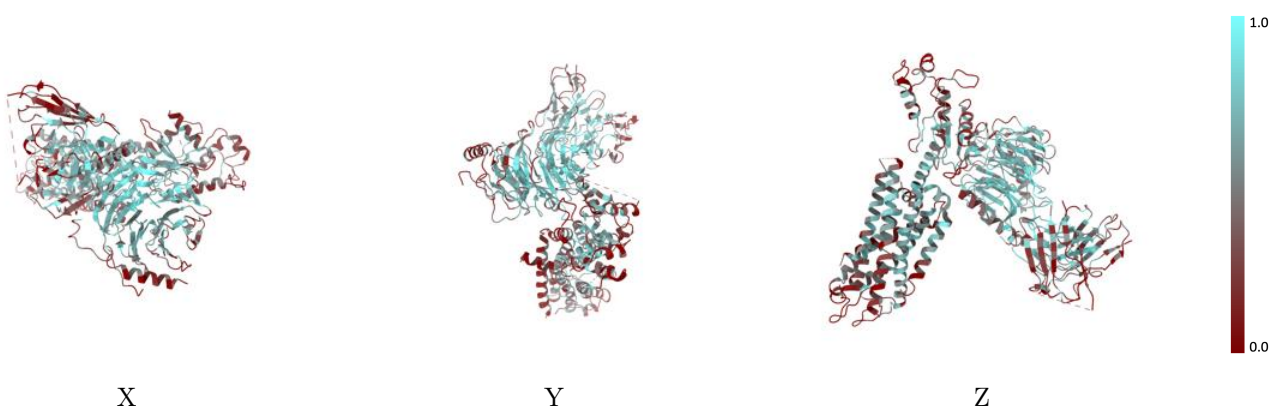
This section was not generated.

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



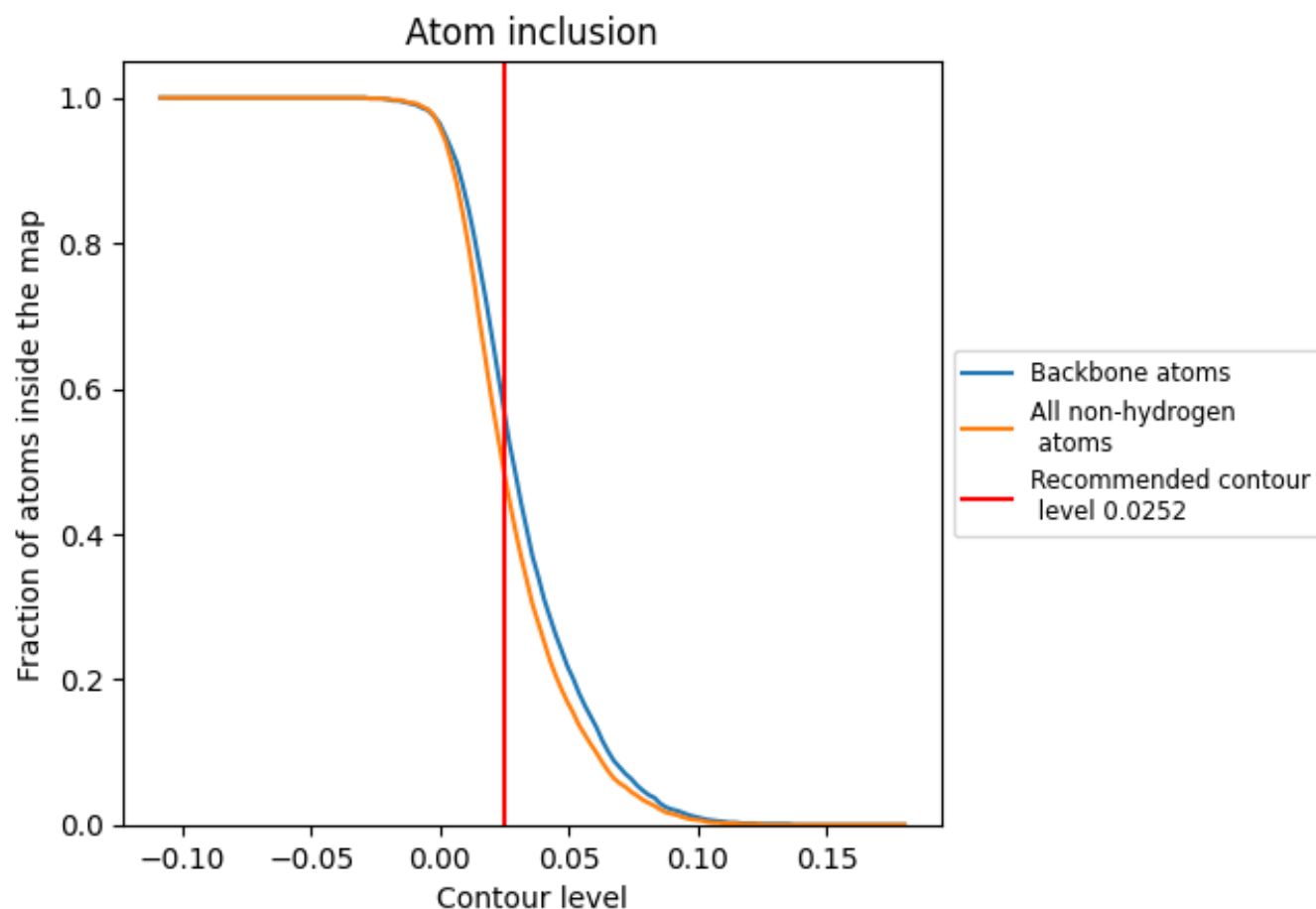
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0252).

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 48% 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 (0.0252) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4790	0.3350
A	0.3980	0.2750
B	0.6290	0.3870
C	0.2710	0.2680
D	0.4840	0.3490
E	0.1620	0.1240
R	0.4250	0.3380

1.0

0.0

<0.0