



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:34 AM UTC

PDB ID : 7WO7 / pdb_00007wo7
EMDB ID : EMD-32641
Title : Locally refined region of SARS-CoV-2 Spike in complex with IgG 553-15
Authors : Zhan, W.Q.; Zhang, X.; Chen, Z.G.; Sun, L.
Deposited on : 2022-01-20
Resolution : 3.80 Å(reported)

This is a Full wwPDB EM Validation 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

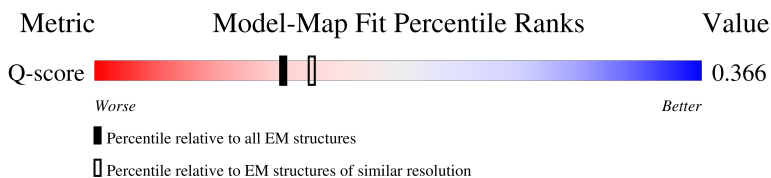
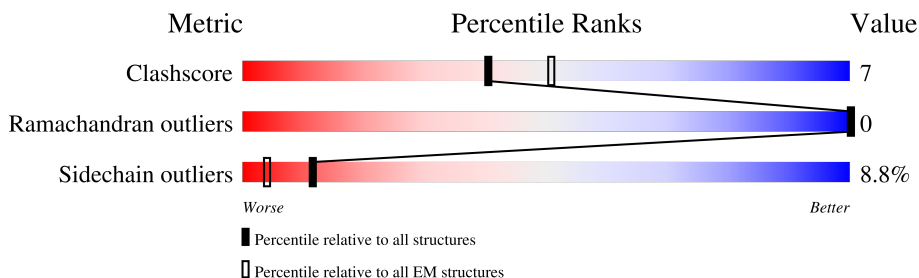
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	225	
2	B	218	
3	C	194	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4870 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 mAb15 VH.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	225	Total	C	N	O	S	0	0
			1704	1077	289	331	7		

- Molecule 2 is a protein called mAb15 VL.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	215	Total	C	N	O	S	0	0
			1616	999	270	342	5		

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	194	Total	C	N	O	S	0	0
			1536	985	256	287	8		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

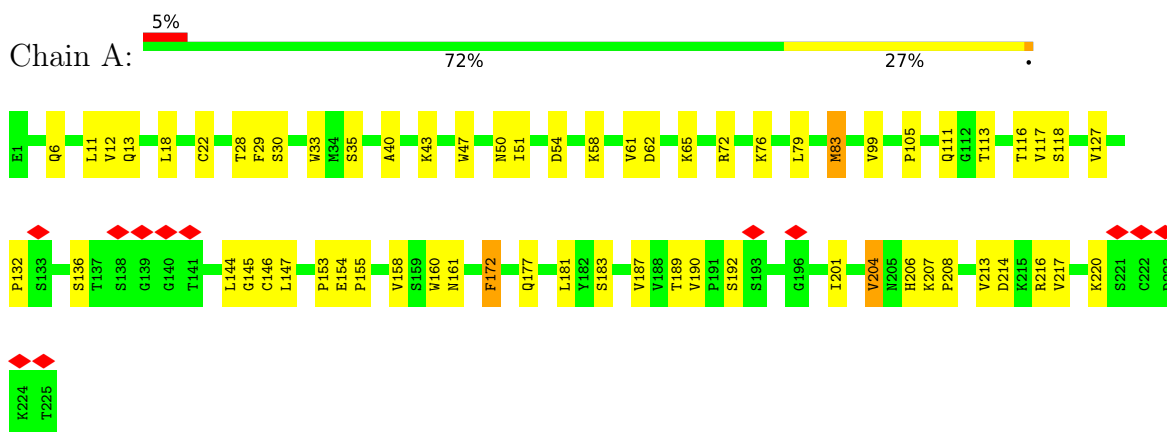


Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	

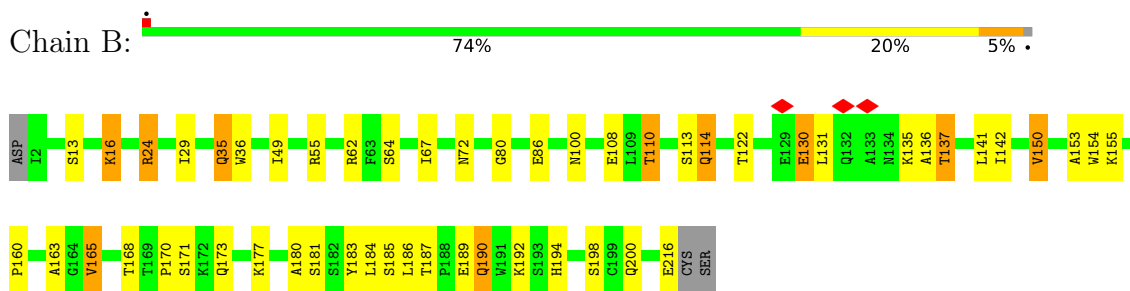
3 Residue-property plots

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.

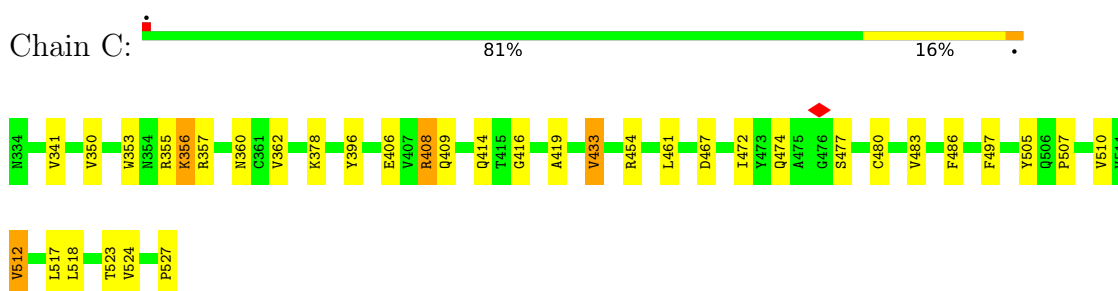
• Molecule 1: mAb15 VH



• Molecule 2: mAb15 VL



• Molecule 3: Spike protein S1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	199441	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 ($e^-/\text{\AA}^2$)	61	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.103	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	513.60004, 513.60004, 513.60004	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: NAG

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	0.18	0/1748	0.45	0/2379
2	B	0.21	0/1654	0.46	2/2260 (0.1%)
3	C	0.17	0/1580	0.45	0/2151
All	All	0.19	0/4982	0.45	2/6790 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	114	GLN	CA-C-N	-5.42	115.18	120.98
2	B	114	GLN	C-N-CA	-5.42	115.18	120.98

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	1704	0	1657	32	0
2	B	1616	0	1538	25	0
3	C	1536	0	1452	14	0
4	C	14	0	13	0	0
All	All	4870	0	4660	67	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 7.

All (67) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLN:HB2	1:A:181:LEU:HB2	1.72	0.72
1:A:201:ILE:HB	1:A:214:ASP:HB3	1.72	0.70
3:C:408:ARG:O	3:C:414:GLN:NE2	2.27	0.67
2:B:187:THR:HB	2:B:190:GLN:HB2	1.77	0.66
1:A:153:PRO:HB2	1:A:155:PRO:HD3	1.77	0.66
2:B:153:ALA:HB3	2:B:200:GLN:HB2	1.78	0.66
2:B:13:SER:O	2:B:16:LYS:NZ	2.31	0.63
1:A:6:GLN:H	1:A:111:GLN:HE21	1.46	0.63
2:B:155:LYS:O	2:B:198:SER:OG	2.16	0.63
1:A:33:TRP:HB2	1:A:99:VAL:HB	1.84	0.60
1:A:29:PHE:O	1:A:72:ARG:NH2	2.35	0.60
1:A:147:LEU:HD11	1:A:183:SER:HB3	1.86	0.57
1:A:28:THR:HG22	1:A:30:SER:H	1.69	0.57
2:B:24:ARG:HB3	2:B:72:ASN:HB3	1.87	0.56
1:A:158:VAL:HA	1:A:204:VAL:HG13	1.88	0.55
1:A:40:ALA:HB3	1:A:43:LYS:HB2	1.88	0.55
3:C:474:GLN:NE2	3:C:477:SER:OG	2.39	0.55
2:B:36:TRP:HB2	2:B:49:ILE:HG22	1.89	0.55
1:A:216:ARG:NH2	1:A:217:VAL:O	2.41	0.54
2:B:122:THR:OG1	2:B:141:LEU:O	2.25	0.54
1:A:145:GLY:HA2	1:A:160:TRP:HZ2	1.73	0.54
2:B:155:LYS:HE2	2:B:160:PRO:HG3	1.90	0.53
1:A:11:LEU:HD13	1:A:116:THR:HG23	1.89	0.53
1:A:47:TRP:NE1	1:A:50:ASN:OD1	2.35	0.53
1:A:105:PRO:HB3	2:B:35:GLN:HG2	1.89	0.53
2:B:170:PRO:HB3	2:B:180:ALA:HB2	1.91	0.52
3:C:406:GLU:OE1	3:C:409:GLN:NE2	2.44	0.51
2:B:86:GLU:HG3	2:B:110:THR:HA	1.93	0.50
3:C:362:VAL:HG13	3:C:527:PRO:HD2	1.95	0.49
1:A:153:PRO:HG2	1:A:208:PRO:HG2	1.95	0.48
1:A:172:PHE:HA	2:B:171:SER:HB2	1.94	0.48
3:C:357:ARG:NH2	3:C:396:TYR:OH	2.46	0.48
3:C:497:PHE:CG	3:C:507:PRO:HG3	2.49	0.48
1:A:220:LYS:NZ	2:B:216:GLU:OE1	2.43	0.48
2:B:142:ILE:HD11	2:B:150:VAL:HG23	1.96	0.47
2:B:163:ALA:O	2:B:185:SER:OG	2.28	0.47
2:B:55:ARG:NH2	2:B:64:SER:OG	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:454:ARG:NH1	3:C:467:ASP:O	2.46	0.47
1:A:190:VAL:HG22	1:A:192:SER:H	1.79	0.47
1:A:22:CYS:HB3	1:A:79:LEU:HB3	1.97	0.46
2:B:62:ARG:HD2	2:B:80:GLY:HA3	1.96	0.46
2:B:141:LEU:HA	2:B:181:SER:HA	1.97	0.46
1:A:154:GLU:N	1:A:155:PRO:HD3	2.31	0.46
1:A:12:VAL:HG21	1:A:18:LEU:HD11	1.96	0.45
3:C:360:ASN:ND2	3:C:523:THR:OG1	2.50	0.45
2:B:173:GLN:HB2	2:B:177:LYS:HB2	1.98	0.45
3:C:353:TRP:HZ3	3:C:355:ARG:HD3	1.82	0.45
2:B:154:TRP:CD2	2:B:184:LEU:HD22	2.52	0.44
1:A:18:LEU:HD13	1:A:83:MET:HE1	1.99	0.44
1:A:62:ASP:HA	1:A:65:LYS:HG3	1.99	0.44
1:A:6:GLN:HE21	1:A:113:THR:HG23	1.83	0.43
3:C:433:VAL:HA	3:C:512:VAL:HG12	2.01	0.43
3:C:416:GLY:H	3:C:419:ALA:HB2	1.84	0.43
2:B:137:THR:HA	2:B:186:LEU:HD11	2.00	0.42
1:A:61:VAL:HG23	2:B:100:ASN:HD21	1.84	0.42
2:B:130:GLU:H	2:B:130:GLU:HG3	1.59	0.42
2:B:165:VAL:HA	2:B:184:LEU:HD12	2.02	0.42
1:A:35:SER:HB3	1:A:50:ASN:ND2	2.36	0.41
1:A:206:HIS:CD2	1:A:208:PRO:HD2	2.55	0.41
1:A:207:LYS:HB2	1:A:208:PRO:HD3	2.02	0.41
1:A:54:ASP:OD1	1:A:54:ASP:N	2.53	0.41
1:A:132:PRO:HG3	1:A:144:LEU:HB3	2.02	0.41
1:A:51:ILE:HG13	1:A:58:LYS:HG2	2.03	0.41
2:B:135:LYS:HE3	2:B:136:ALA:N	2.36	0.41
3:C:353:TRP:CZ3	3:C:355:ARG:HD3	2.56	0.41
3:C:480:CYS:HB3	3:C:486:PHE:H	1.86	0.41
3:C:341:VAL:HG22	3:C:356:LYS:HG3	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	223/225 (99%)	197 (88%)	26 (12%)	0	100	100
2	B	213/218 (98%)	194 (91%)	19 (9%)	0	100	100
3	C	192/194 (99%)	176 (92%)	16 (8%)	0	100	100
All	All	628/637 (99%)	567 (90%)	61 (10%)	0	100	100

There are no Ramachandran outliers to report.

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	189/189 (100%)	175 (93%)	14 (7%)	13	38
2	B	188/191 (98%)	168 (89%)	20 (11%)	6	26
3	C	167/167 (100%)	153 (92%)	14 (8%)	10	34
All	All	544/547 (100%)	496 (91%)	48 (9%)	11	33

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	76	LYS
1	A	83	MET
1	A	117	VAL
1	A	118	SER
1	A	127	VAL
1	A	136	SER
1	A	146	CYS
1	A	161	ASN
1	A	172	PHE
1	A	187	VAL
1	A	189	THR
1	A	204	VAL

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Mol	Chain	Res	Type
1	A	213	VAL
2	B	16	LYS
2	B	24	ARG
2	B	29	ILE
2	B	35	GLN
2	B	67	ILE
2	B	108	GLU
2	B	110	THR
2	B	113	SER
2	B	114	GLN
2	B	130	GLU
2	B	131	LEU
2	B	137	THR
2	B	150	VAL
2	B	165	VAL
2	B	168	THR
2	B	183	TYR
2	B	189	GLU
2	B	190	GLN
2	B	192	LYS
2	B	194	HIS
3	C	350	VAL
3	C	356	LYS
3	C	378	LYS
3	C	408	ARG
3	C	433	VAL
3	C	461	LEU
3	C	472	ILE
3	C	483	VAL
3	C	505	TYR
3	C	510	VAL
3	C	512	VAL
3	C	517	LEU
3	C	518	LEU
3	C	524	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	77	ASN
1	A	111	GLN

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Mol	Chain	Res	Type
1	A	206	HIS
2	B	35	GLN
2	B	39	GLN
2	B	98	ASN
2	B	99	HIS
2	B	100	ASN
2	B	175	ASN
2	B	190	GLN
2	B	200	GLN
3	C	334	ASN
3	C	360	ASN
3	C	409	GLN
3	C	414	GLN
3	C	437	ASN
3	C	439	ASN
3	C	474	GLN
3	C	493	GLN

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](#)

1 ligand is 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
4	NAG	C	601	3	14,14,15	0.25	0	17,19,21	0.43	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
4	NAG	C	601	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	601	NAG	O5-C5-C6-O6
4	C	601	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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-32641. 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

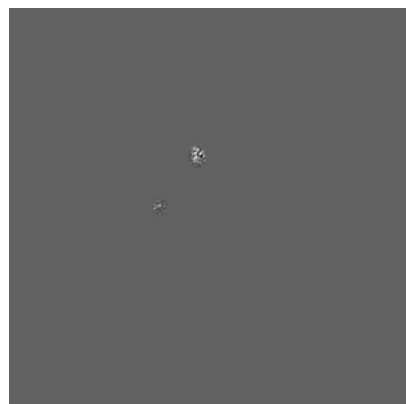


Z

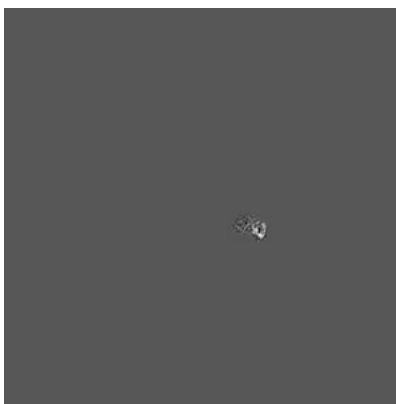
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240



Y Index: 240



Z Index: 240

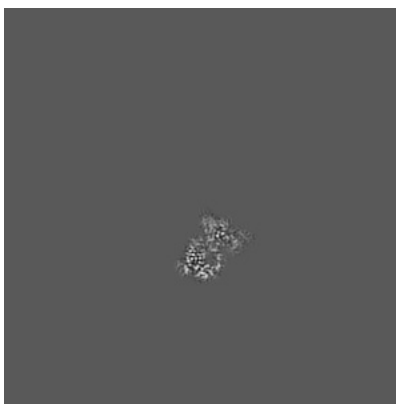
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

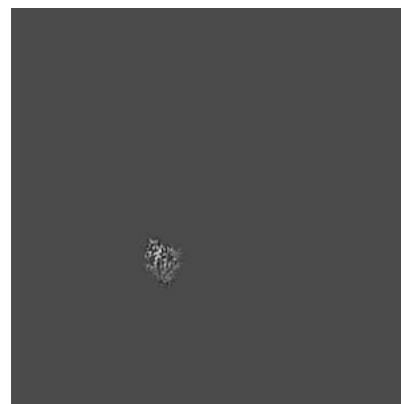
6.3.1 Primary map



X Index: 207



Y Index: 189

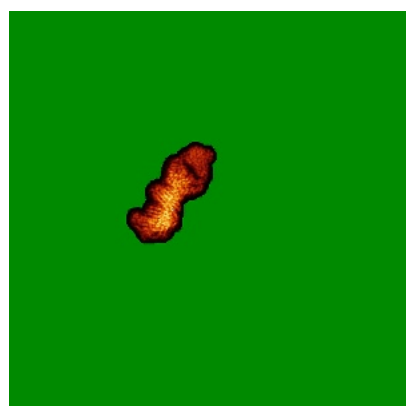


Z Index: 225

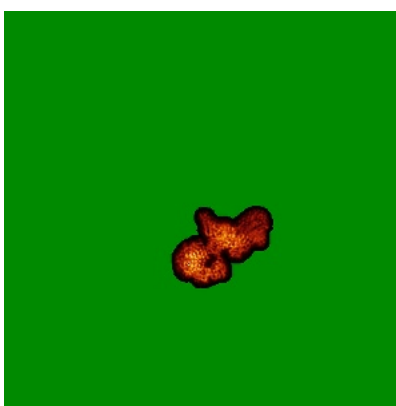
The images above show the largest variance slices of the map in three orthogonal directions.

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

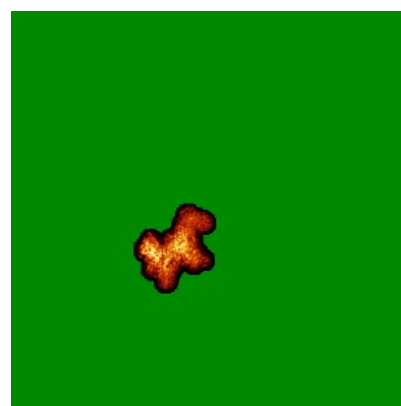
6.4.1 Primary map



X



Y

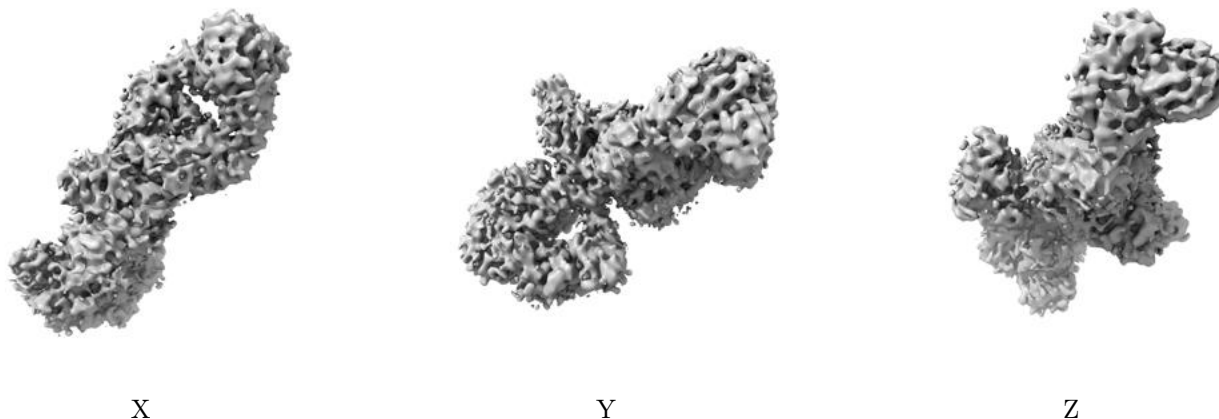


Z

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

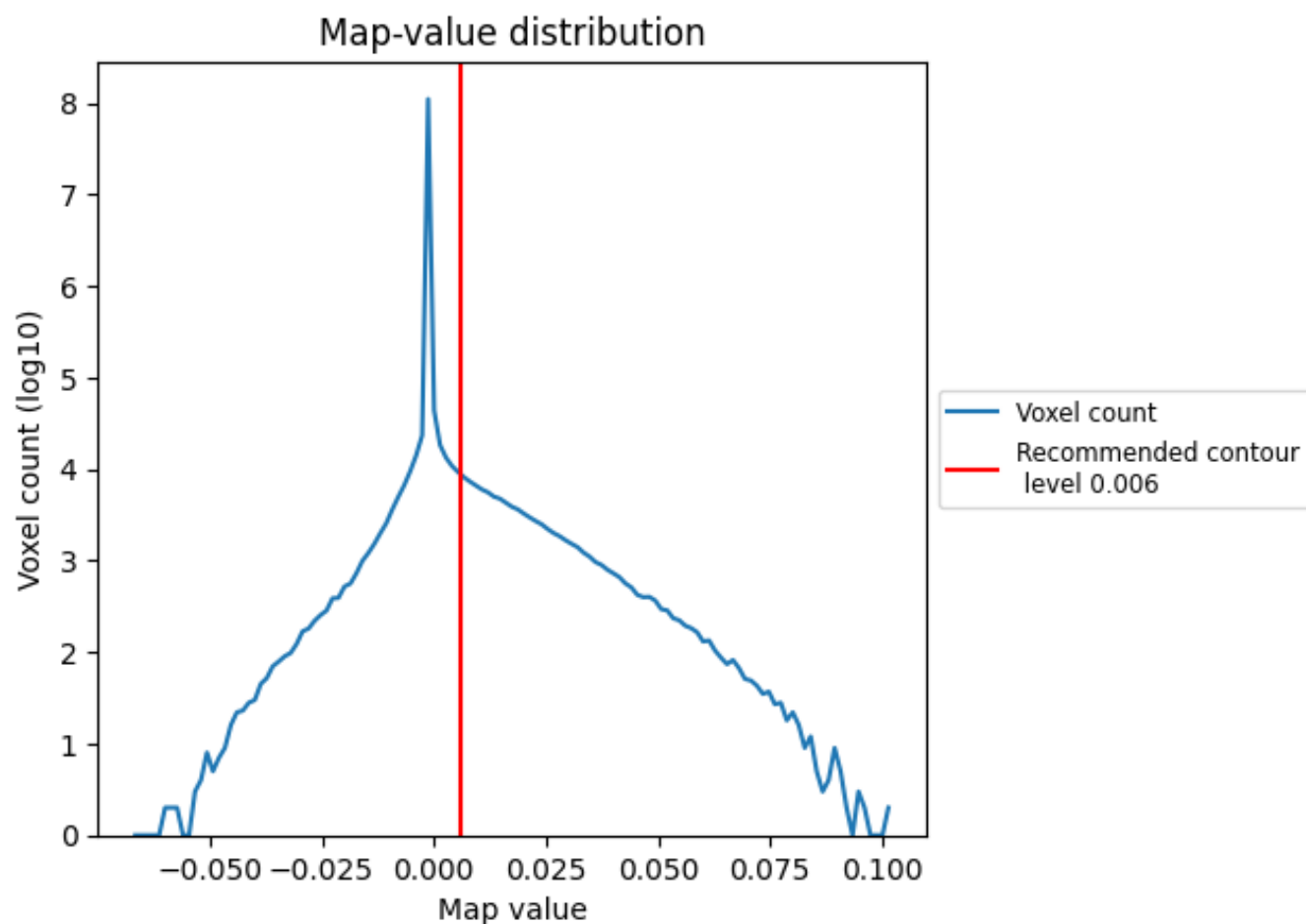
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

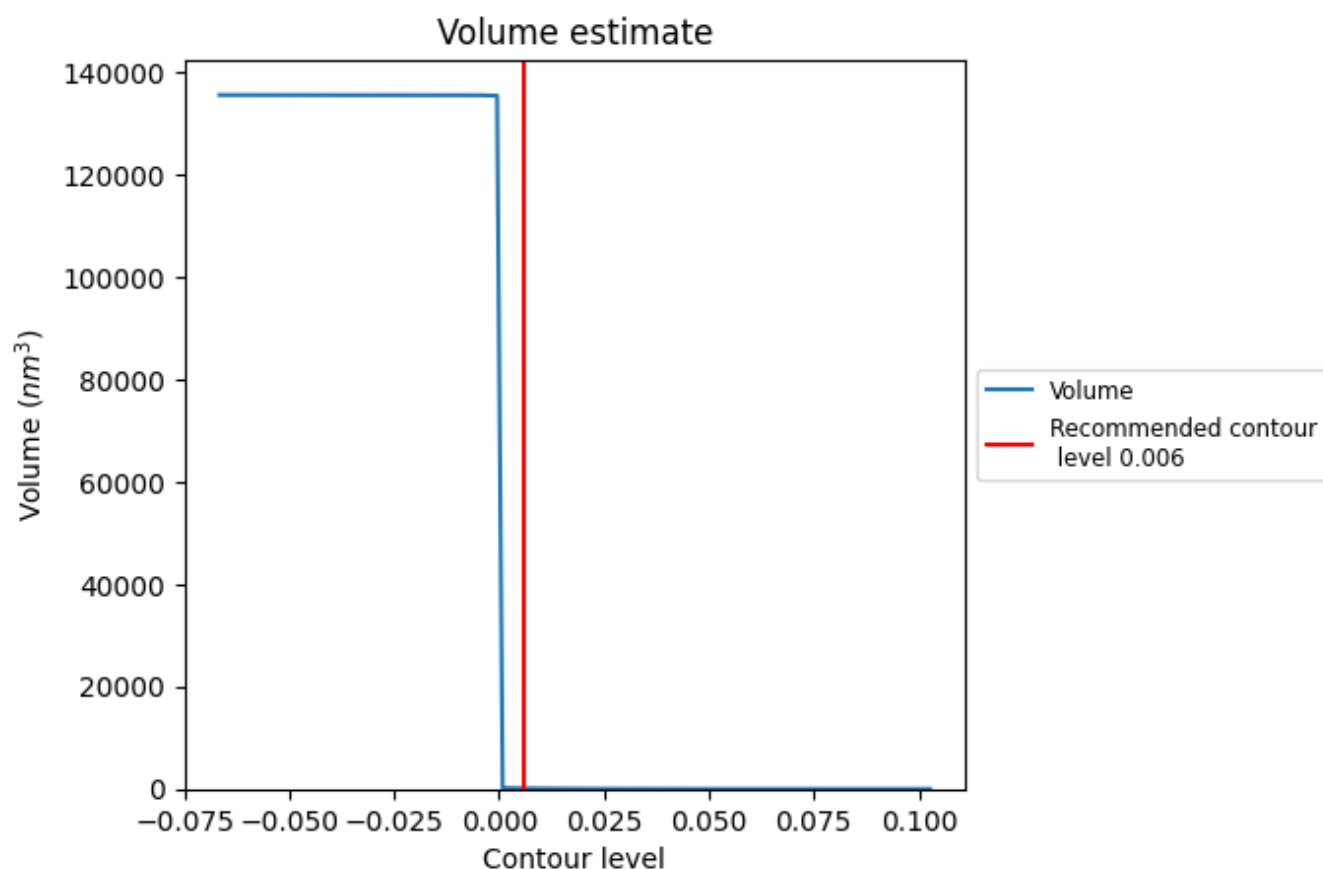
This section contains the results of statistical analysis of the map.

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.

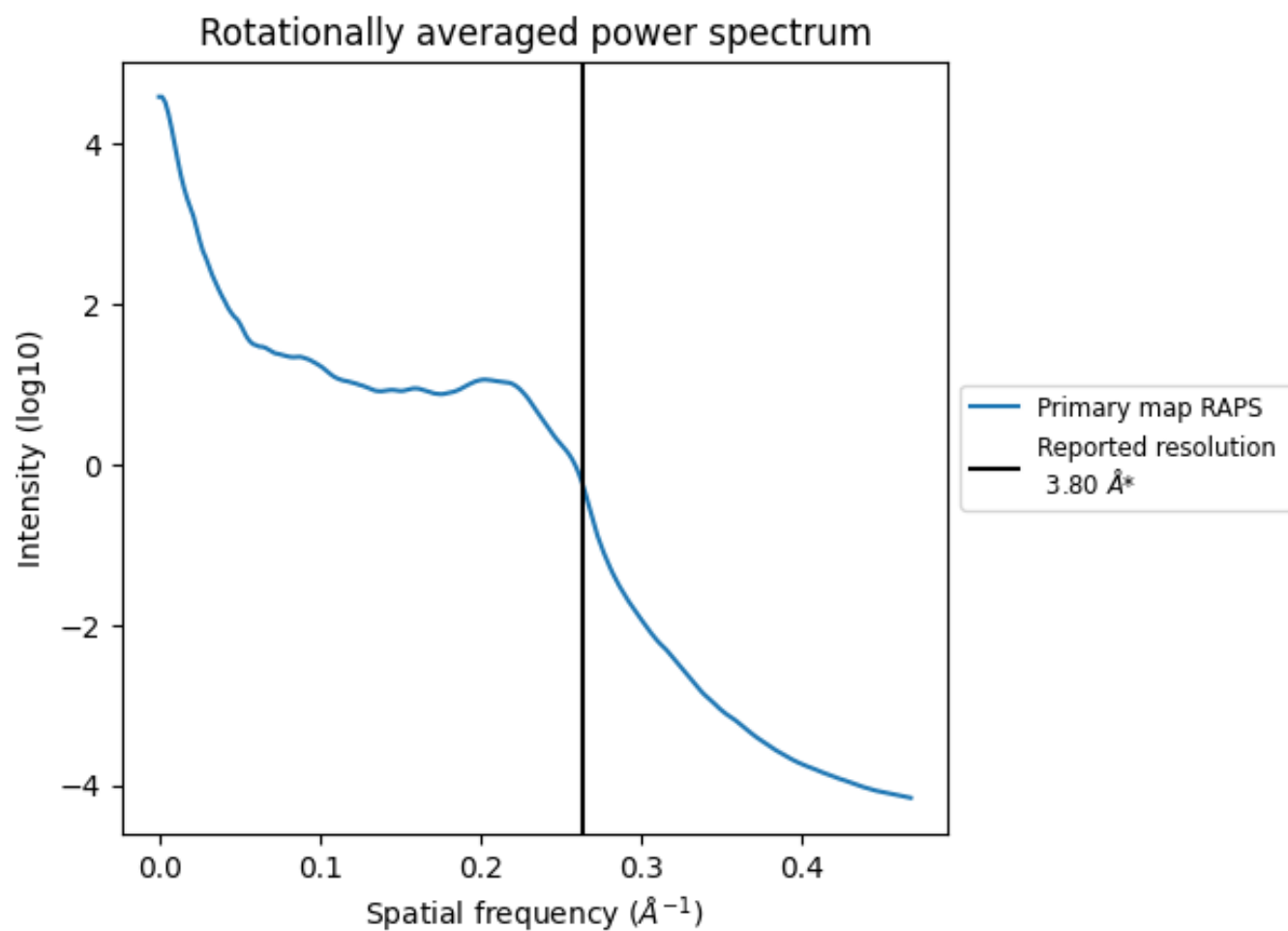
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm^3 ; this corresponds to an approximate mass of 104 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 0.263 Å⁻¹

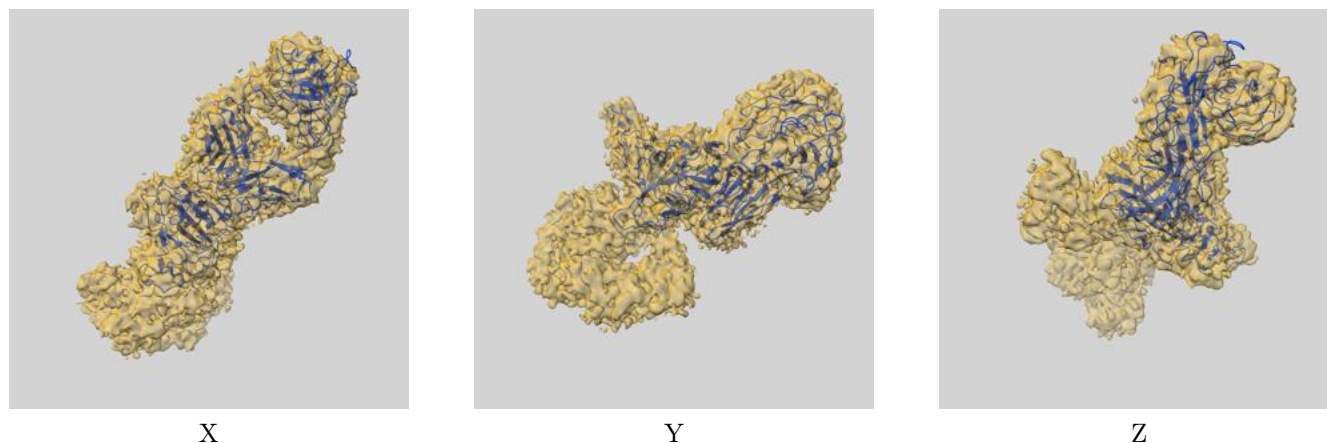
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

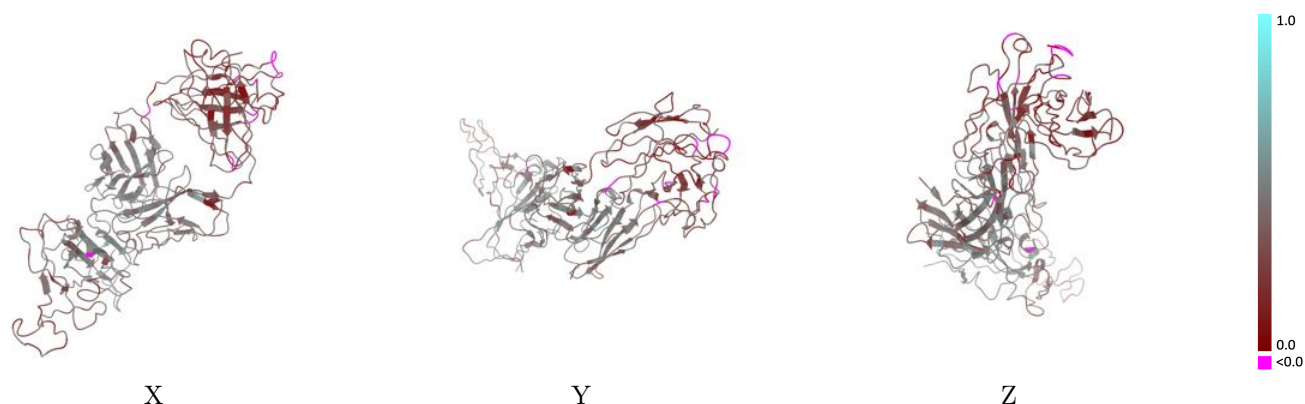
This section contains information regarding the fit between EMDB map EMD-32641 and PDB model 7WO7. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



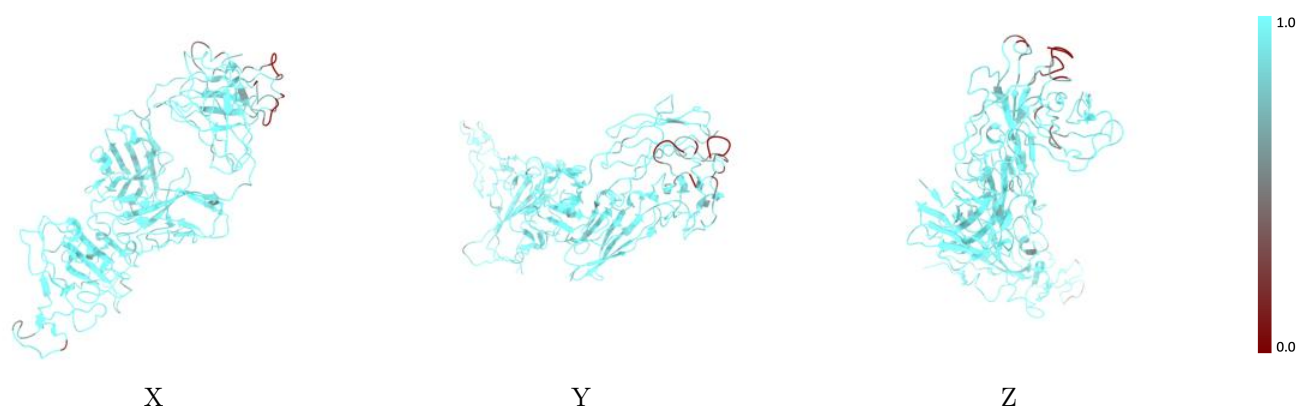
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



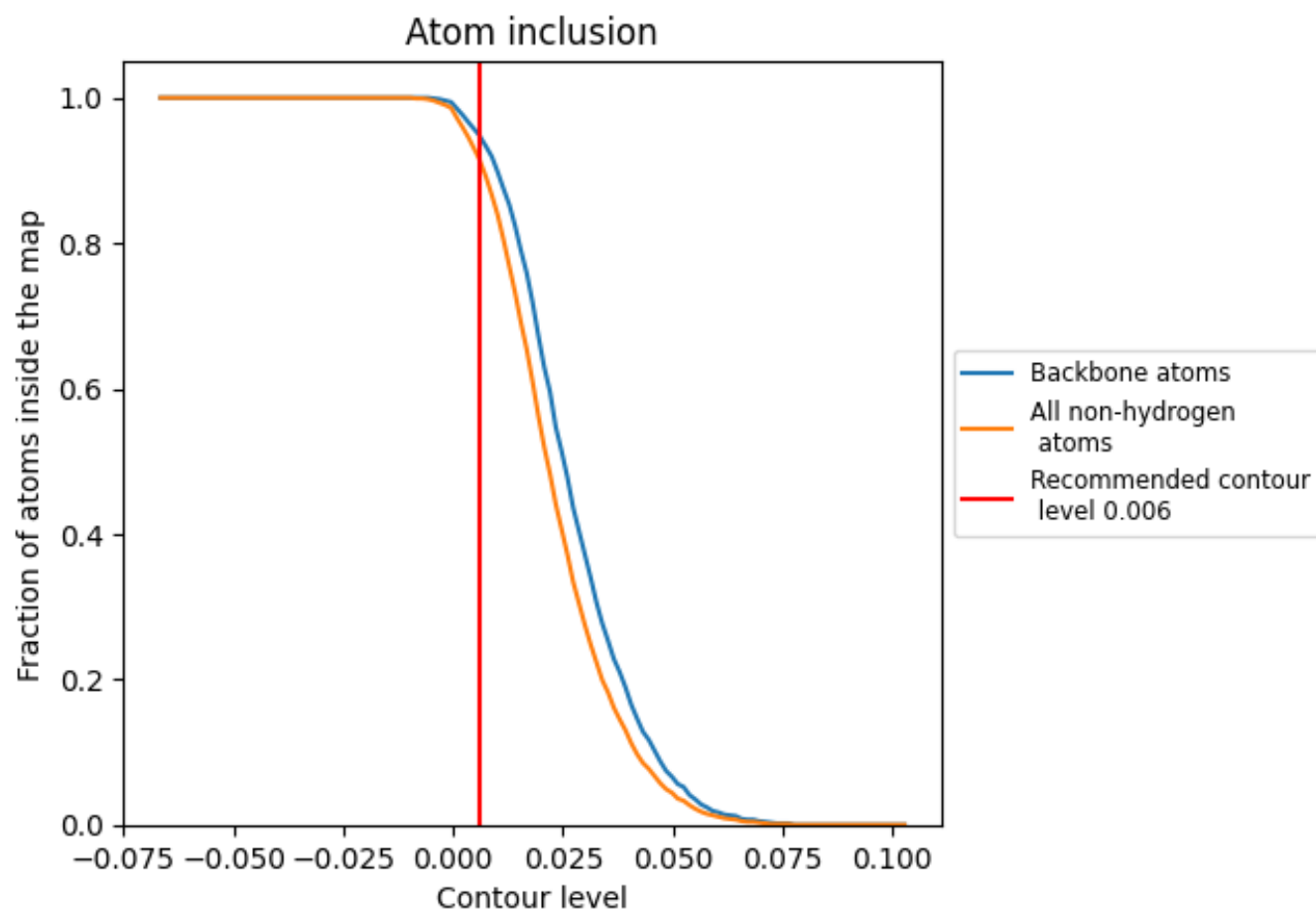
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9150	0.3660
A	0.8770	0.3510
B	0.9210	0.3410
C	0.9500	0.4090

