wwPDB EM Validation Summary Report ⓘ

Nov 13, 2022 – 07:58 PM EST

|		
PDB ID	:	6WWZ
EMDB ID	:	EMD-21950
Title	:	Cryo-EM structure of the human chemokine receptor CCR6 in complex with CCL20 and a Go protein
Authors	:	Wasilko, D.J.; Johnson, Z.L.; Ammirati, M.; Han, S.; Wu, H.
Deposited on	:	2020-05-09
Resolution	:	3.34 Å(reported)
Based on initial models	:	1M8A, 6DDE, 6G79

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 3.34 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.
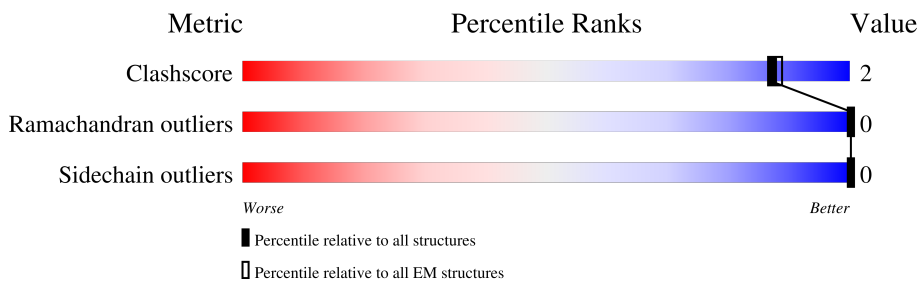
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	B	351	93% · ·
2	C	70	81% 13% 6%
3	Y	68	82% 18%
4	A	250	81% · 16%
5	S	287	79% · 20%
6	R	529	57% · 41%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 9450 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(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	338	2600	1604	467	508	21	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	MET	-	initiating methionine	UNP P54311
B	-9	HIS	-	expression tag	UNP P54311
B	-8	HIS	-	expression tag	UNP P54311
B	-7	HIS	-	expression tag	UNP P54311
B	-6	HIS	-	expression tag	UNP P54311
B	-5	HIS	-	expression tag	UNP P54311
B	-4	HIS	-	expression tag	UNP P54311
B	-3	GLY	-	expression tag	UNP P54311
B	-2	SER	-	expression tag	UNP P54311
B	-1	LEU	-	expression tag	UNP P54311
B	0	LEU	-	expression tag	UNP P54311
B	1	GLN	-	expression tag	UNP P54311

- Molecule 2 is a protein called C-C motif chemokine 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	66	530	343	94	89	4	0	0

- 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
			Total	C	N	O	S		
3	Y	56	433	271	76	83	3	0	0

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(o) subunit alpha,Guanine nucleotide-binding protein G(o) subunit alpha.

| Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	210	Total 1649	C 1046	N 278	O 315	S 10	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP P09471
A	-10	GLY	-	expression tag	UNP P09471
A	-9	HIS	-	expression tag	UNP P09471
A	-8	HIS	-	expression tag	UNP P09471
A	-7	HIS	-	expression tag	UNP P09471
A	-6	HIS	-	expression tag	UNP P09471
A	-5	HIS	-	expression tag	UNP P09471
A	-4	HIS	-	expression tag	UNP P09471
A	-3	GLU	-	expression tag	UNP P09471
A	-2	ASN	-	expression tag	UNP P09471
A	-1	LEU	-	expression tag	UNP P09471
A	0	TYR	-	expression tag	UNP P09471
A	1	PHE	-	expression tag	UNP P09471
A	2	GLN	-	expression tag	UNP P09471
A	3	GLY	-	expression tag	UNP P09471
A	42	ASP	GLY	conflict	UNP P09471
A	43	ASN	GLU	conflict	UNP P09471
A	174	GLY	-	linker	UNP P09471
A	175	GLY	-	linker	UNP P09471
A	176	SER	-	linker	UNP P09471
A	177	GLY	-	linker	UNP P09471
A	178	GLY	-	linker	UNP P09471
A	179	SER	-	linker	UNP P09471
A	180	GLY	-	linker	UNP P09471
A	181	GLY	-	linker	UNP P09471
A	227	ASP	ALA	conflict	UNP P09471
A	230	ASP	GLY	conflict	UNP P09471
A	250	ASP	LEU	conflict	UNP P09471
A	332	ALA	ILE	conflict	UNP P09471
A	335	ILE	VAL	conflict	UNP P09471

- Molecule 5 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	231	Total 1770	C 1125	N 294	O 341	S 10	0	0

- Molecule 6 is a protein called C-C chemokine receptor type 6,C-C chemokine receptor type 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	310	Total 2468	C 1637	N 403	O 406	S 22	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	375	HIS	-	expression tag	UNP P51684
R	376	HIS	-	expression tag	UNP P51684
R	377	HIS	-	expression tag	UNP P51684
R	378	HIS	-	expression tag	UNP P51684
R	379	HIS	-	expression tag	UNP P51684
R	380	HIS	-	expression tag	UNP P51684
R	381	HIS	-	expression tag	UNP P51684
R	382	HIS	-	expression tag	UNP P51684
R	383	HIS	-	expression tag	UNP P51684
R	384	HIS	-	expression tag	UNP P51684

W O R L D W I D E
PDB
PROTEIN DATA BANK

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.

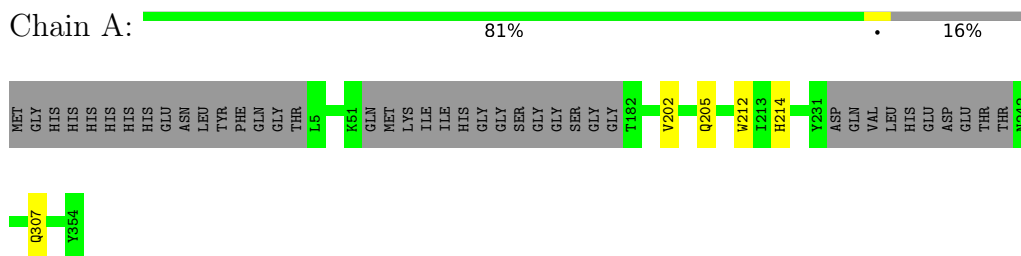• Molecule 1: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:
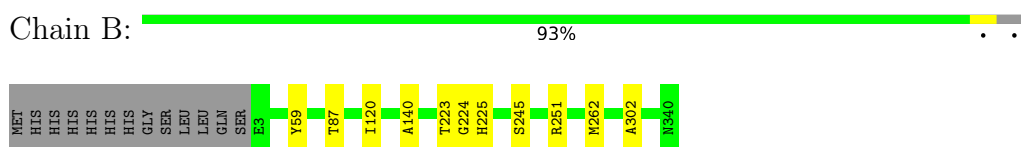
• Molecule 2: C-C motif chemokine 20
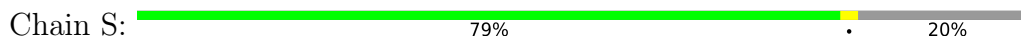
Chain C:
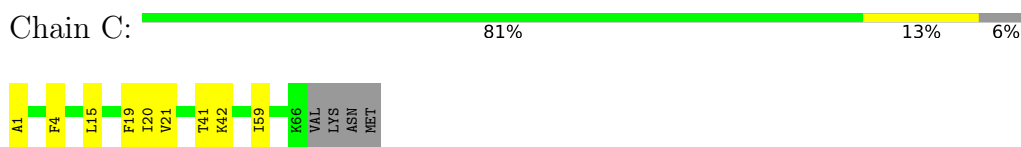
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain Y:
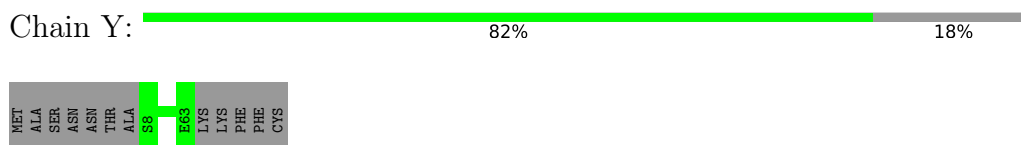
• Molecule 4: Guanine nucleotide-binding protein G(o) subunit alpha,Guanine nucleotide-binding protein G(o) subunit alpha

Chain A:

• Molecule 5: scFv16

Chain S:

MET GLU THR ASP THR LEU LEU TRP VAL LEU LEU TRP VAL PRO GLY SER THR GLY ASP V2 A40 P41 S121 GLY GLY GLY SER GLY GLY GLY SER GLY GLY GLY SER D125 V135 E234 L235 LYS ALA ALA LEU GLU VAL LEU PHE GLN GLY PRO

HIS HIS HIS HIS HIS HIS HIS

• Molecule 6: C-C chemokine receptor type 6,C-C chemokine receptor type 6

Chain R: 57%   •   41%

MET LYS THR ILE ILE ALA LEU SER TYR ILE PHE CYS LEU VAL PHE ALA ASP TYR LYS ASP ASP ASP ALA LYS LEU GLN THR MET GLY THR ALA ASP ASP LEU GLU ASP ASN TRP GLU THR LEU ASN ASP ASN LEU LYS VAL ILE GLU LYS ALA ASP ASN ALA ALA GLN VAL LYS ASP ALA

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

ALA ALA GLU GLN LEU LYS THR THR ARG ASN ALA TYR ILE GLN LYS TYR LEU GLY SER GLU ASN LEU TYR PHE GLN GLY SER GLU GLU MET ASN PHE SER ASP VAL PHE ASP SER GLU GLU ASP TYR PHE VAL SER VAL ASN THR SER TYR Y27 F71 K75 R78 N87

C168 N186 E198 P199 K298 E302 C336 VAL ARG ARG LYS TYR LYS SER SER SER GLY PHE SER CYS ALA GLY ARG TYR SER LYS GLU ASN ILE SER ARG GLN THR SER GLU THR ALA ASP ASN ASP ASN ALA SER SER PHE THR MET HIS HIS HIS HIS HIS HIS HIS HIS

HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	230450	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 $(e^-/\text{Å}^2)$	81.0	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.151	Depositor
Minimum map value	-0.091	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	334.08002, 334.08002, 334.08002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87000006, 0.87000006, 0.87000006	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	B	0.71	0/2647	0.77	0/3589
2	C	0.68	0/541	0.82	0/728
3	Y	0.70	0/439	0.73	0/592
4	A	0.68	0/1676	0.76	0/2255
5	S	0.70	0/1814	0.77	0/2460
6	R	0.71	0/2524	0.74	0/3423
All	All	0.70	0/9641	0.76	0/13047

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	B	2600	0	2505	12	0
2	C	530	0	551	6	0
3	Y	433	0	442	0	0
4	A	1649	0	1627	11	0
5	S	1770	0	1700	5	0
6	R	2468	0	2583	7	0
All	All	9450	0	9408	37	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 2.

The worst 5 of 37 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:B:59:TYR:HE2	4:A:214:HIS:HE1	1.18	0.90
1:B:59:TYR:HE2	4:A:214:HIS:CE1	1.89	0.89
4:A:202:VAL:HG11	4:A:212:TRP:CH2	2.16	0.81
4:A:202:VAL:HG11	4:A:212:TRP:CZ3	2.19	0.78
1:B:59:TYR:CE2	4:A:214:HIS:CE1	2.77	0.72

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	B	336/351 (96%)	325 (97%)	11 (3%)	0	100	100
2	C	64/70 (91%)	59 (92%)	5 (8%)	0	100	100
3	Y	54/68 (79%)	53 (98%)	1 (2%)	0	100	100
4	A	204/250 (82%)	192 (94%)	12 (6%)	0	100	100
5	S	227/287 (79%)	214 (94%)	13 (6%)	0	100	100
6	R	308/529 (58%)	297 (96%)	11 (4%)	0	100	100
All	All	1193/1555 (77%)	1140 (96%)	53 (4%)	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	B	281/293 (96%)	281 (100%)	0	100	100
2	C	59/63 (94%)	59 (100%)	0	100	100
3	Y	46/56 (82%)	46 (100%)	0	100	100
4	A	180/216 (83%)	180 (100%)	0	100	100
5	S	193/234 (82%)	193 (100%)	0	100	100
6	R	274/465 (59%)	274 (100%)	0	100	100
All	All	1033/1327 (78%)	1033 (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. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	3	ASN
4	A	205	GLN
6	R	87	ASN
6	R	192	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-21950. 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 ⓘ

6.1.1 Primary map

| X | Y | Z |
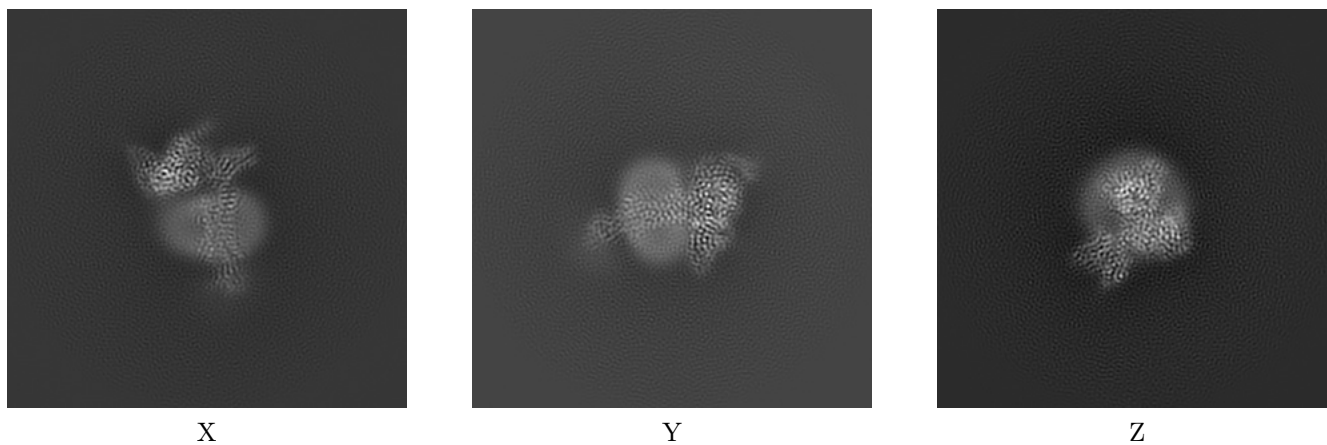
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map

| X Index: 192 | Y Index: 192 | Z Index: 192 |
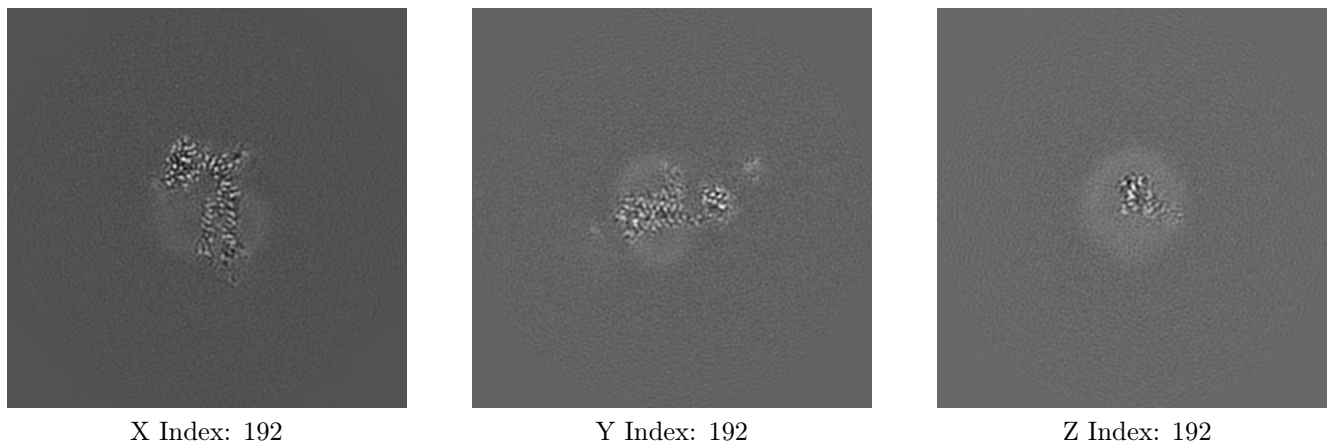
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
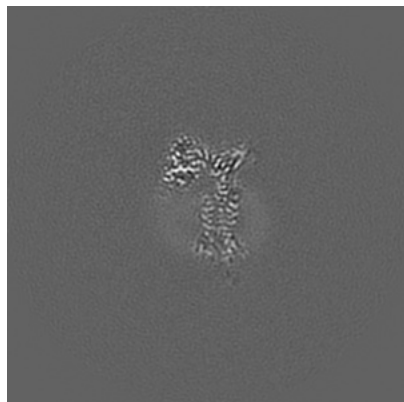
6.3.1 Primary map
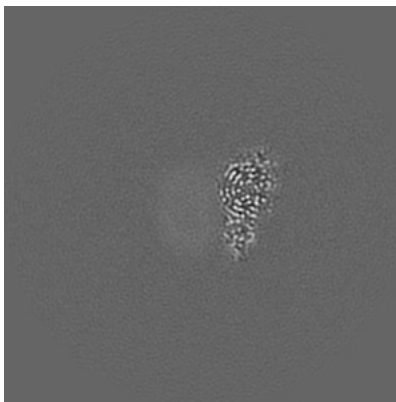
| X Index: 194 | Y Index: 163 | Z Index: 225 |
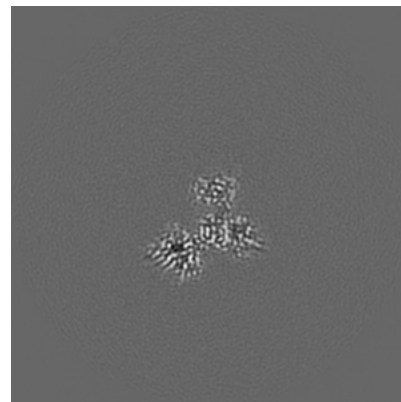
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5   Mask visualisation (i)

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

7   Map analysis ⓘ

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

7.1   Map-value distribution ⓘ
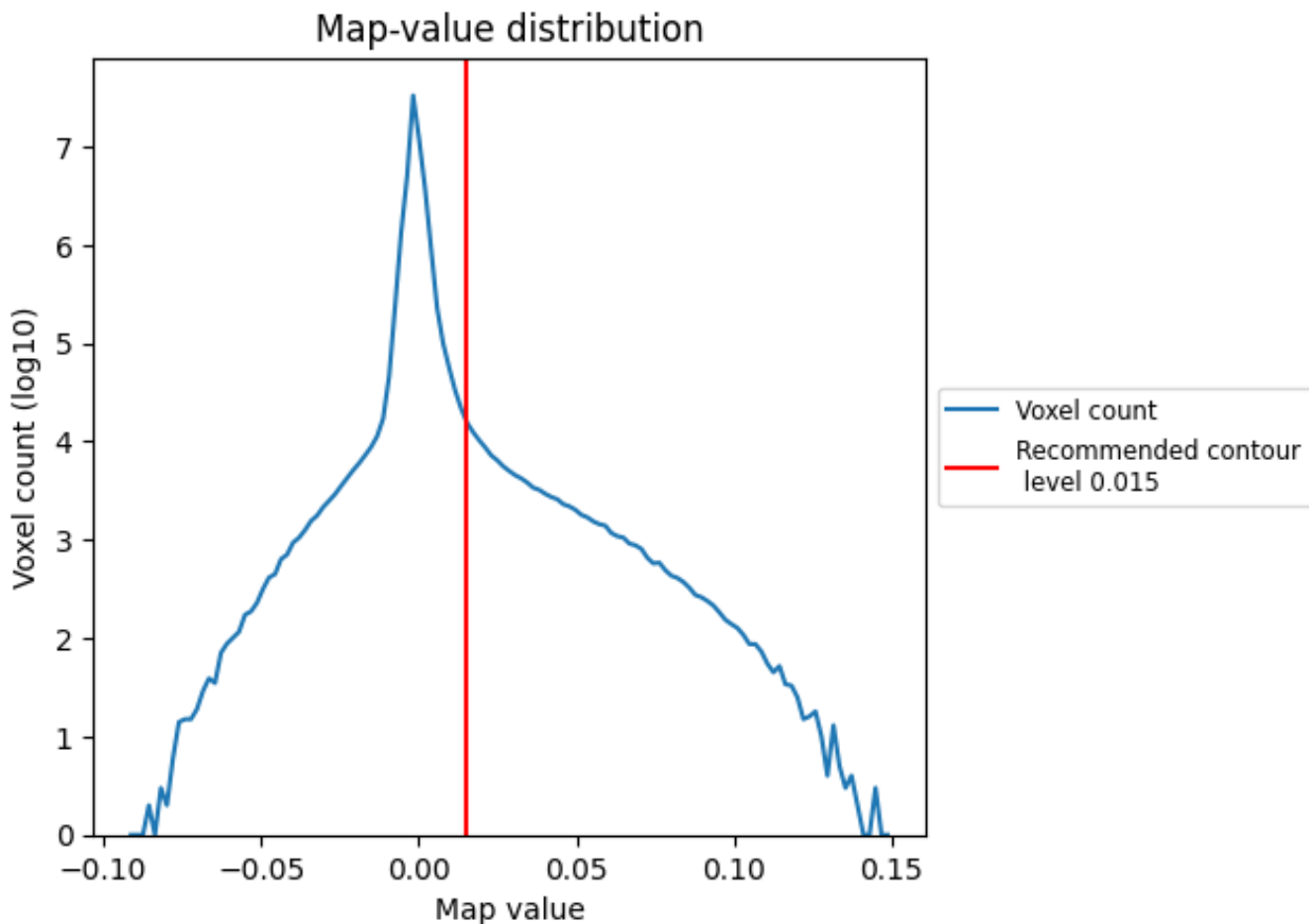
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
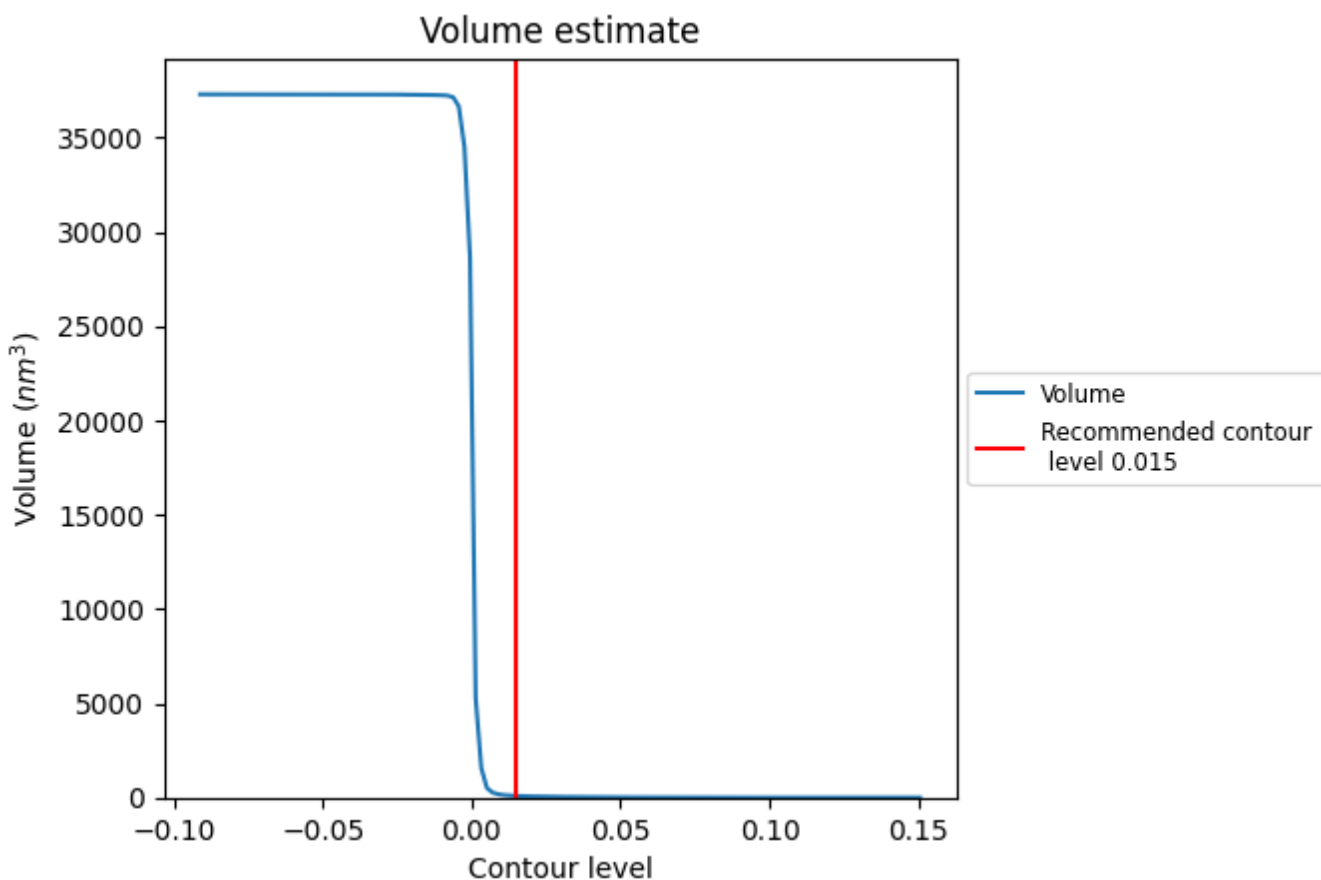
The volume at the recommended contour level is 85 nm^3; this corresponds to an approximate mass of 77 kDa.

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 ⓘ
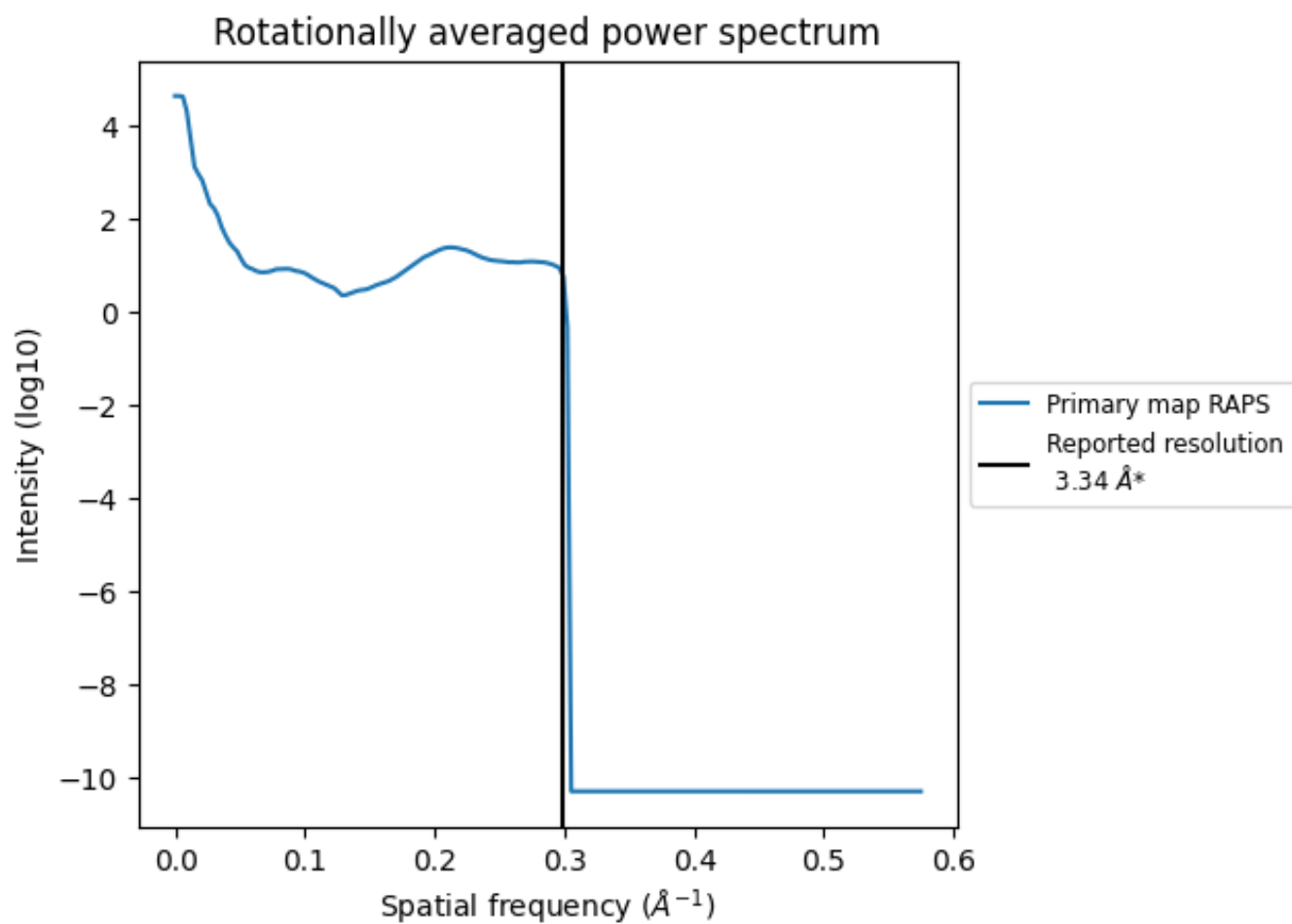
*Reported resolution corresponds to spatial frequency of 0.299 Å^{-1}

8   Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1   FSC ⓘ
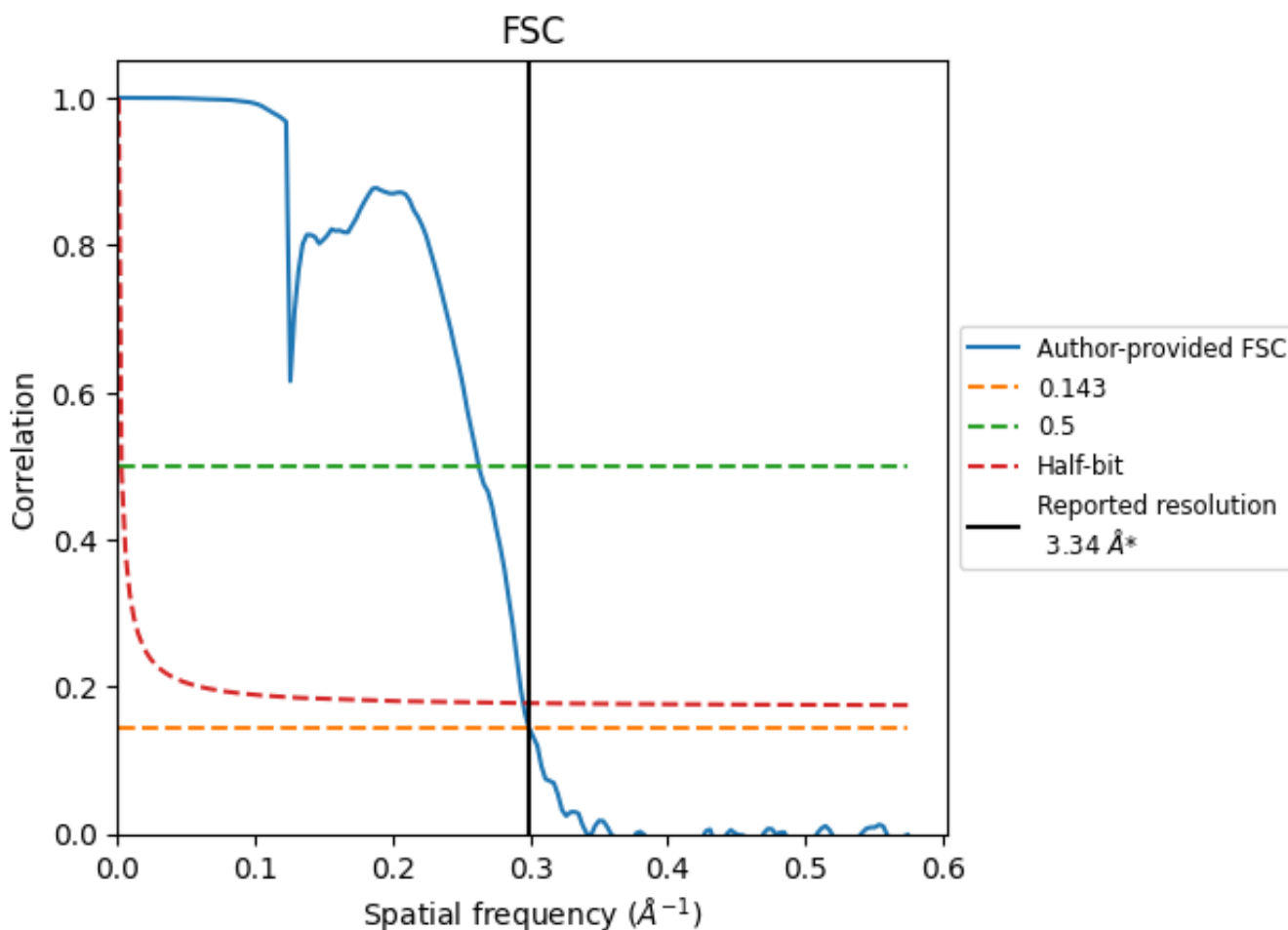
*Reported resolution corresponds to spatial frequency of 0.299 Å^{-1}

8.2   Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.34	-	-
Author-provided FSC curve	3.34	3.81	3.39
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9   Map-model fit   ⓘ

This section contains information regarding the fit between EMDB map EMD-21950 and PDB model 6WWZ. Per-residue inclusion information can be found in section 3 on page 6.

9.1   Map-model overlay   ⓘ

| X | Y | Z |
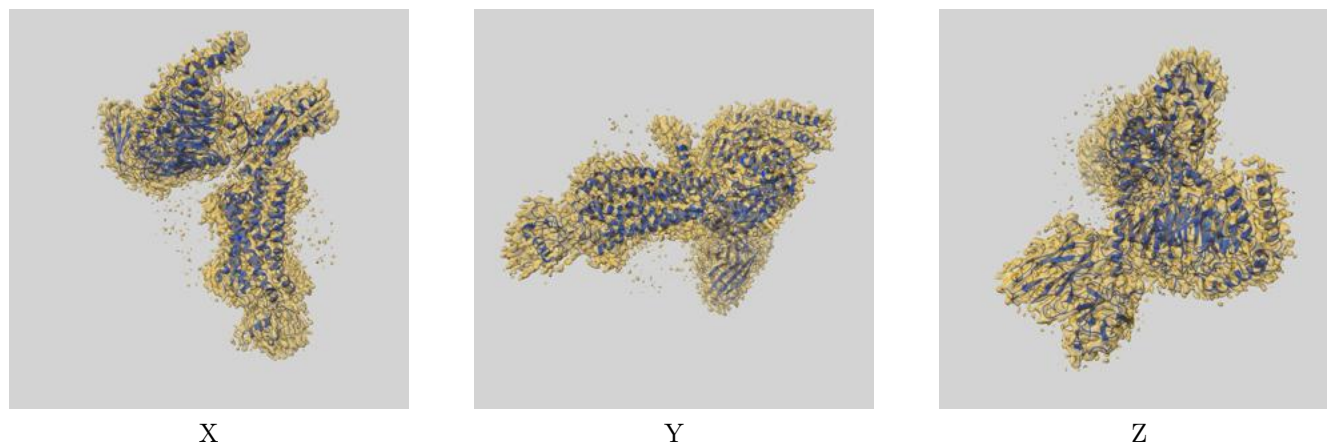
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ
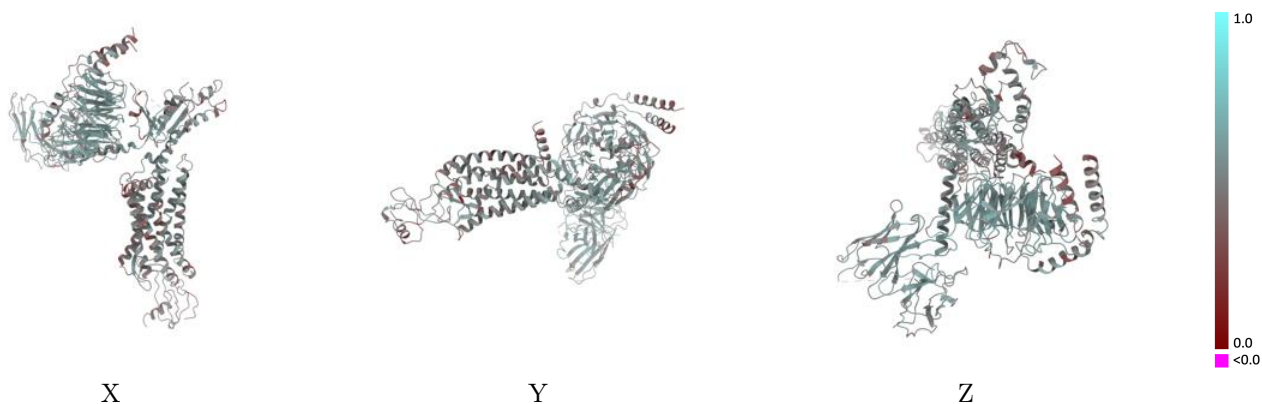
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3   Atom inclusion mapped to coordinate model ⓘ
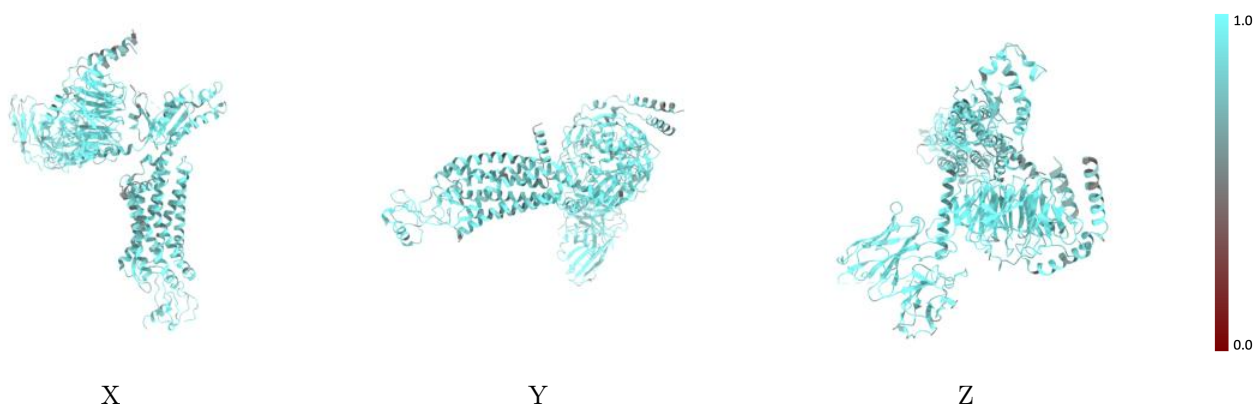
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4   Atom inclusion ⓘ
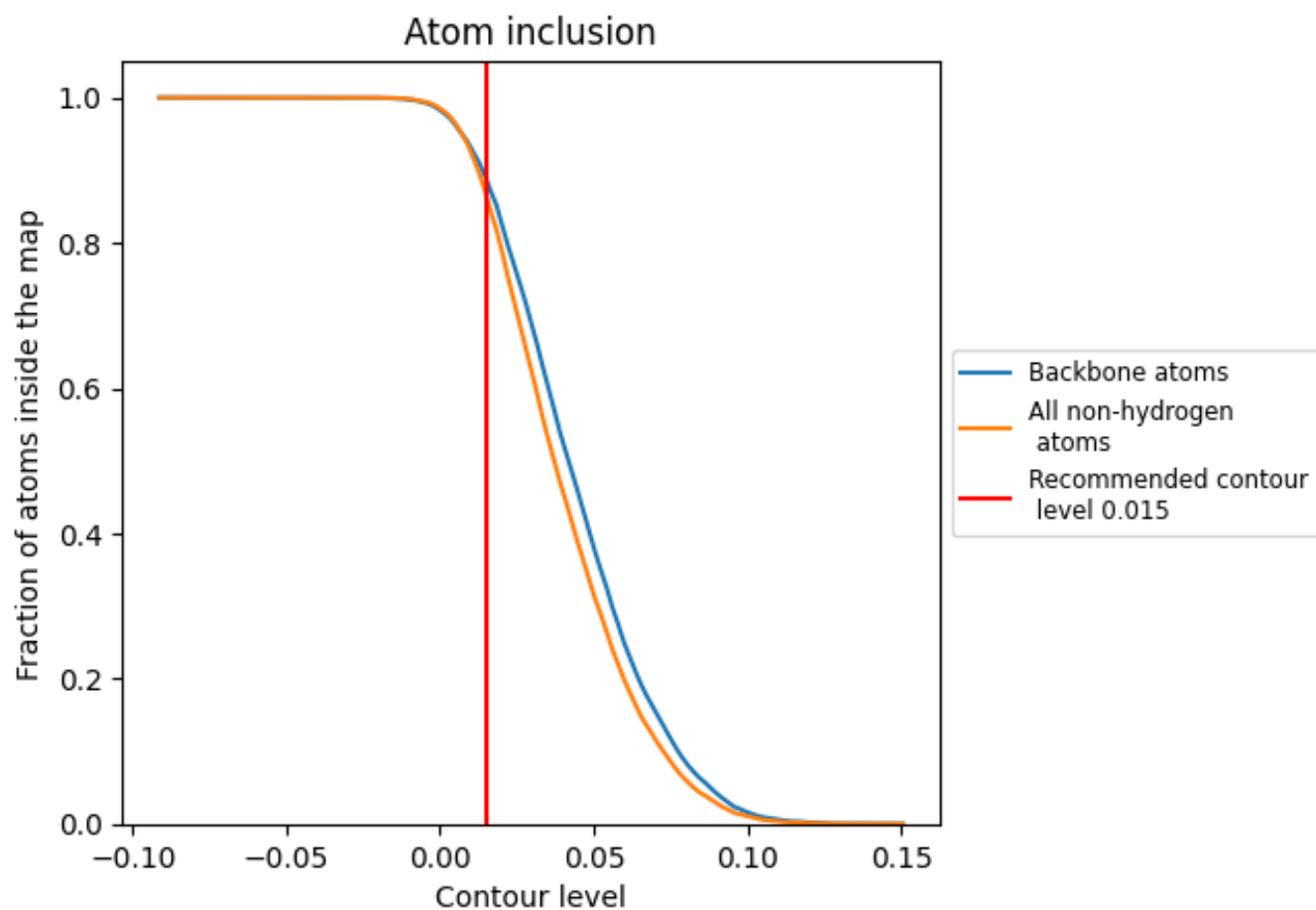
At the recommended contour level, 89% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8670	0.5050
A	0.8514	0.4880
B	0.9142	0.5470
C	0.8369	0.4440
R	0.8272	0.4720
S	0.9000	0.5380
Y	0.7746	0.4500

1.0

0.0
<0.0