WORLDWIDE wwPDB
PROTEIN DATA BANK

wwPDB EM Validation Summary Report ⓘ

Mar 14, 2023 – 02:13 PM JST

PDB ID	:	7YON
EMDB ID	:	EMD-33984
Title	:	Complex structure of Neuropeptide Y Y2 receptor in complex with PYY(3-36) and Gi
Authors	:	Kang, H.; Park, C.; Kim, J.; Choi, H.-J.
Deposited on	:	2022-08-01
Resolution	:	2.95 Å(reported)
Based on initial models	:	7VGX, 7DDZ

The following versions of software and data (see references ⓘ) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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)	:	2.32.1

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 2.95 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	Percentile Ranks	Value
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0

Worse   *Better*

▌ Percentile relative to all structures
▯ Percentile relative to all EM structures
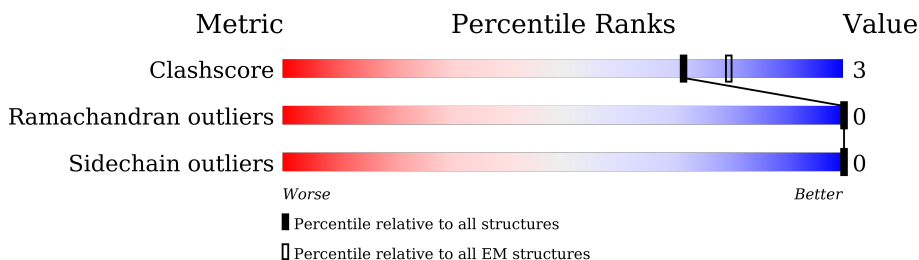
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	354	56%　　6%　　38%
2	B	345	87%　　10%　·
3	G	71	72%　·　24%
4	L	34	12% / 62%　12%　26%
5	R	391	71%　7%　23%
6	S	259	78%　10%　11%

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 9161 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) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	219	Total	C	N	O	S	0	0
			1764	1123	294	334	13		

- 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	336	Total	C	N	O	S	0	0
			2581	1592	465	503	21		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP P62873
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	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	G	54	Total	C	N	O	S	0	0
			418	263	74	78	3		

- Molecule 4 is a protein called Peptide YY(3-36).

Mol	Chain	Residues	Atoms				AltConf	Trace
4	L	25	Total	C	N	O	0	0
			223	143	44	36		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	9	GLY	ARG	variant	UNP P10082

- Molecule 5 is a protein called Neuropeptide Y receptor type 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	302	Total 2402	C 1595	N 385	O 408	S 14	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	0	GLY	-	expression tag	UNP P49146
R	1	PRO	-	expression tag	UNP P49146
R	149	TYR	HIS	engineered mutation	UNP P49146
R	280	CYS	SER	engineered mutation	UNP P49146
R	382	ALA	-	expression tag	UNP P49146
R	383	SER	-	expression tag	UNP P49146
R	384	GLY	-	expression tag	UNP P49146
R	385	LEU	-	expression tag	UNP P49146
R	386	GLU	-	expression tag	UNP P49146
R	387	VAL	-	expression tag	UNP P49146
R	388	LEU	-	expression tag	UNP P49146
R	389	PHE	-	expression tag	UNP P49146
R	390	GLN	-	expression tag	UNP P49146

- Molecule 6 is a protein called single-chain antibody Fv fragment (scFv16).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	230	Total 1771	C 1123	N 293	O 345	S 10	0	0

- Molecule 7 is water.

| Mol	Chain	Residues	Atoms		AltConf
7	L	1	Total 1	O 1	0
7	R	1	Total 1	O 1	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: Guanine nucleotide-binding protein G(i) subunit alpha-1
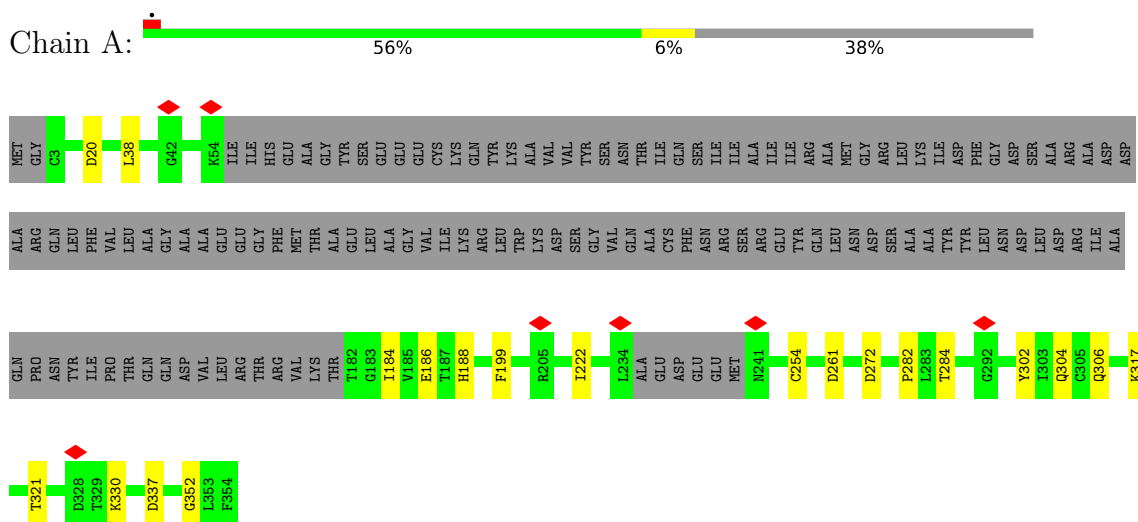
- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1
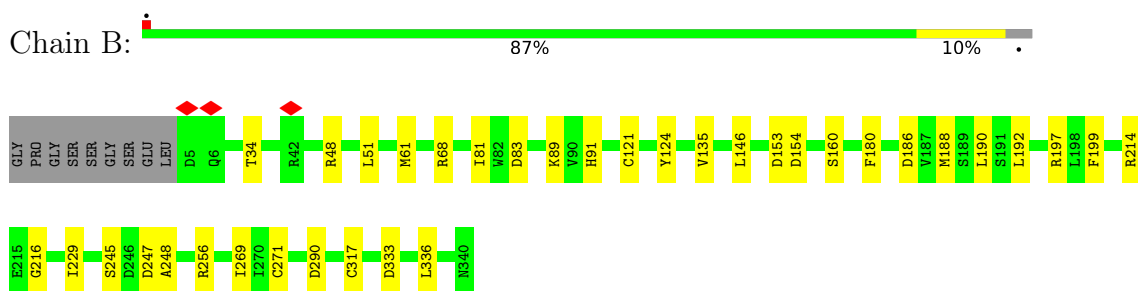
- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2
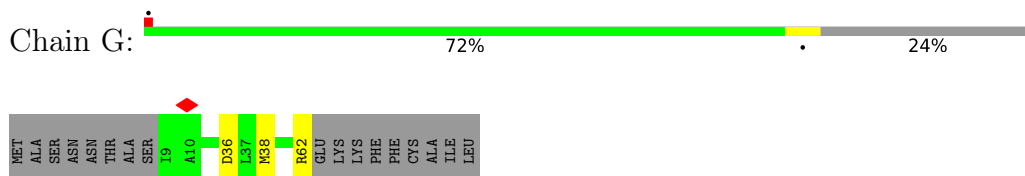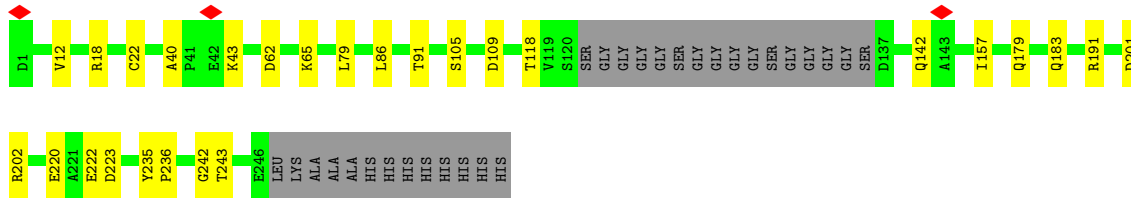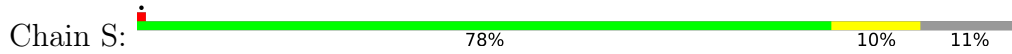

- Molecule 4: Peptide YY(3-36)

Chain L:

12%

62% 12% 26%

I3 K4 P5 E6 A7 PRO GLY GLU ASP ALA SER PRO GLU GLU L17 N18 R19 L24 H25 H26 Y36
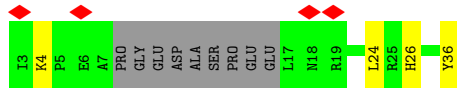
• Molecule 5: Neuropeptide Y receptor type 2

Chain R:

71% 7% 23%

GLY PRO GLY PRO ILE GLY ALA GLU ALA ASP ASN GLN THR VAL GLU GLU MET LYS VAL GLU GLN TYR GLY PRO GLN THR THR PRO ARG GLY GLU LEU VAL PRO ASP PRO GLU PRO GLU L40 I41 D42 K45 L46 I47 E48 N100 L104 M118 L122 Q135 R150

V153 S158 R163 S181 P182 E193 I194 I195 P196 D197 F198 E199 G209 E210 E211 K212 T217 L227 L230 P231 K245 P252 D292 D299 N329 Y332 R341 CYS GLU GLN ARG LEU ASP ALA ILE HIS SER GLU VAL SER VAL THR PHE LYS

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

• Molecule 6: single-chain antibody Fv fragment (scFv16)

Chain S:

78% 10% 11%

D1 V12 R18 C22 A40 P41 E42 K43 D62 K65 L79 L86 T91 S105 D109 T118 V119 S120 SER GLY GLY GLY SER GLY GLY GLY SER GLY GLY GLY SER D137 Q142 A143 I157 Q179 Q183 R191 D201

R202 E220 A221 E222 D223 Y235 P236 G242 T243 E246 LEU LYS ALA ALA HIS HIS HIS HIS HIS HIS

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	359459	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 $(e^-/\text{Å}^2)$	60.5	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.483	Depositor
Minimum map value	-1.148	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	339.59998, 339.59998, 339.59998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8489999, 0.8489999, 0.8489999	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.25	0/1793	0.44	0/2403
2	B	0.25	0/2628	0.53	0/3562
3	G	0.25	0/424	0.43	0/572
4	L	0.23	0/213	0.52	0/285
5	R	0.25	0/2460	0.43	0/3352
6	S	0.28	0/1815	0.52	0/2461
All	All	0.26	0/9333	0.48	0/12635

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	A	1764	0	1760	13	0
2	B	2581	0	2486	21	0
3	G	418	0	431	3	0
4	L	223	0	226	3	0
5	R	2402	0	2515	16	0
6	S	1771	0	1703	16	0
7	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	R	1	0	0	0	0
All	All	9161	0	9121	63	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 3.

The worst 5 of 63 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)
2:B:197:ARG:HH12	2:B:214:ARG:HG2	1.49	0.76
2:B:153:ASP:OD1	2:B:154:ASP:N	2.20	0.75
5:R:217:THR:HG22	5:R:292:ASP:HB3	1.74	0.70
6:S:40:ALA:HB3	6:S:43:LYS:HB2	1.76	0.67
2:B:160:SER:HB3	2:B:190:LEU:HD23	1.77	0.67

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	213/354 (60%)	209 (98%)	4 (2%)	0	100	100
2	B	334/345 (97%)	324 (97%)	10 (3%)	0	100	100
3	G	52/71 (73%)	52 (100%)	0	0	100	100
4	L	21/34 (62%)	20 (95%)	1 (5%)	0	100	100
5	R	300/391 (77%)	293 (98%)	7 (2%)	0	100	100
6	S	226/259 (87%)	217 (96%)	9 (4%)	0	100	100
All	All	1146/1454 (79%)	1115 (97%)	31 (3%)	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	195/305 (64%)	195 (100%)	0	100	100
2	B	278/285 (98%)	278 (100%)	0	100	100
3	G	44/58 (76%)	44 (100%)	0	100	100
4	L	22/29 (76%)	22 (100%)	0	100	100
5	R	269/345 (78%)	269 (100%)	0	100	100
6	S	195/209 (93%)	195 (100%)	0	100	100
All	All	1003/1231 (82%)	1003 (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. There are no such sidechains identified.

5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	TYC	L	36	4	13,13,13	1.63	2 (15%)	17,17,17	0.75	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	TYC	L	36	4	-	2/8/8/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	36	TYC	C-NXT	4.94	1.45	1.32
4	L	36	TYC	O-C	-2.67	1.18	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	36	TYC	O-C-CA-CB
4	L	36	TYC	NXT-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

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-33984. 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 |
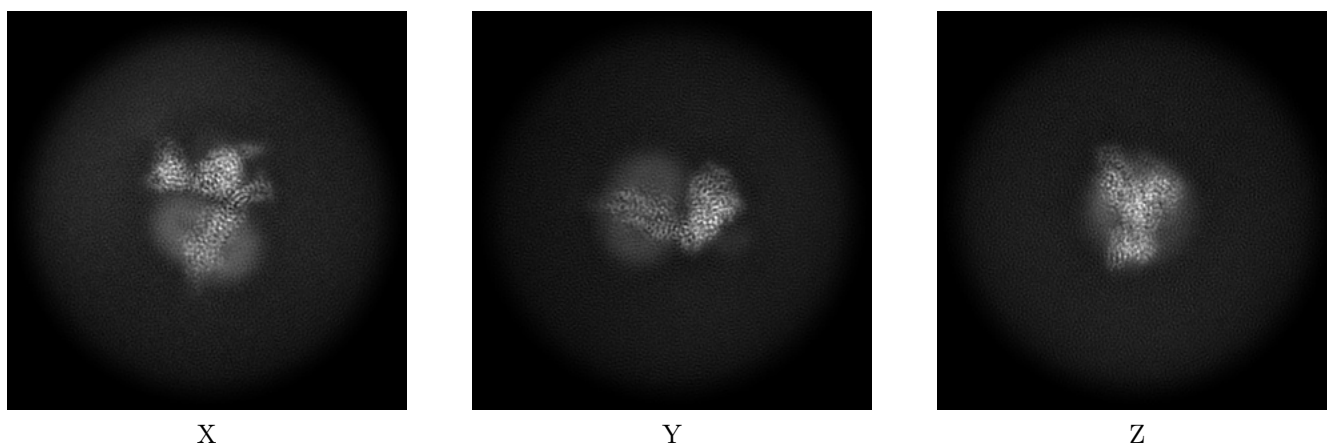
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map

| X Index: 200 | Y Index: 200 | Z Index: 200 |
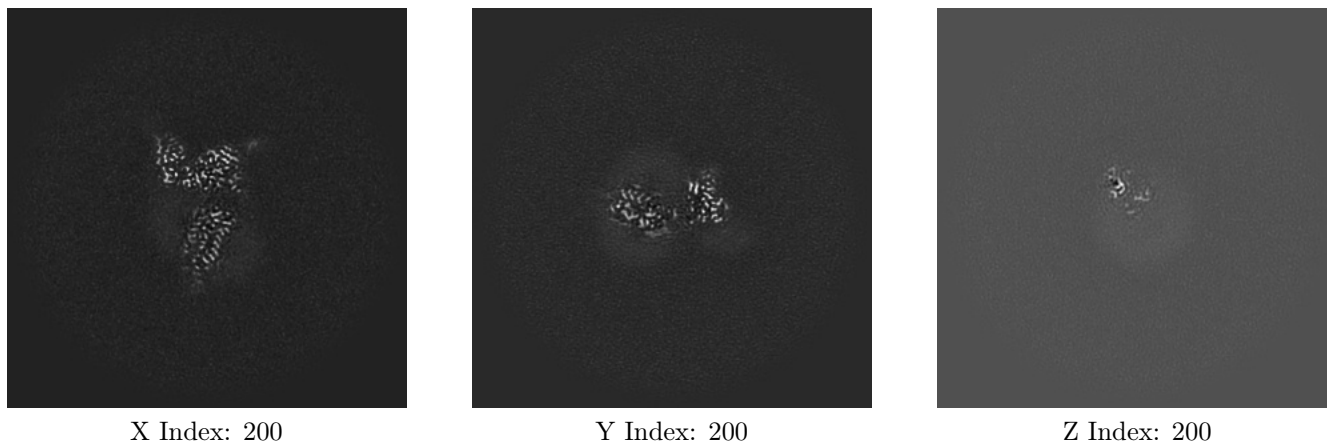
The images above show central slices of the map in three orthogonal directions.

6.3   Largest variance slices   ⓘ
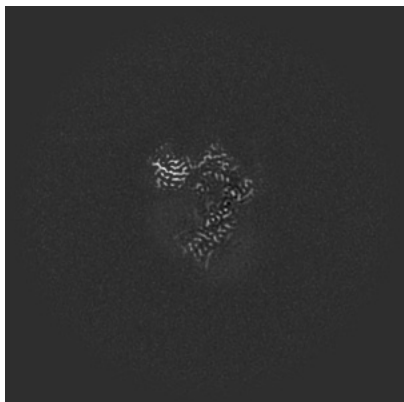
6.3.1   Primary map
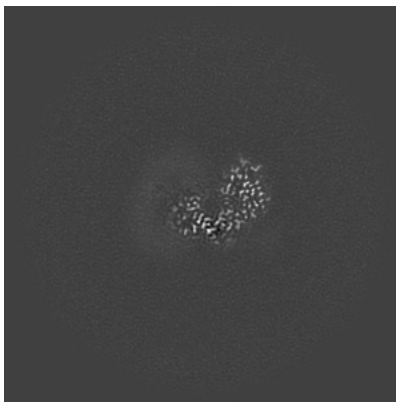
| X Index: 188 | Y Index: 221 | Z Index: 232 |
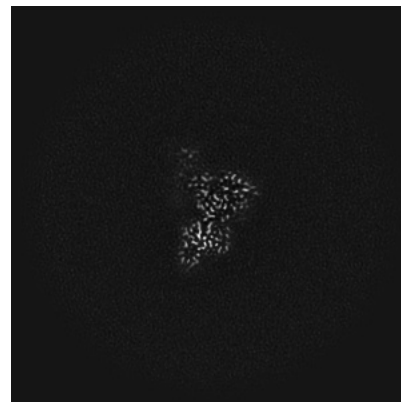
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.2. 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 ⓘ

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

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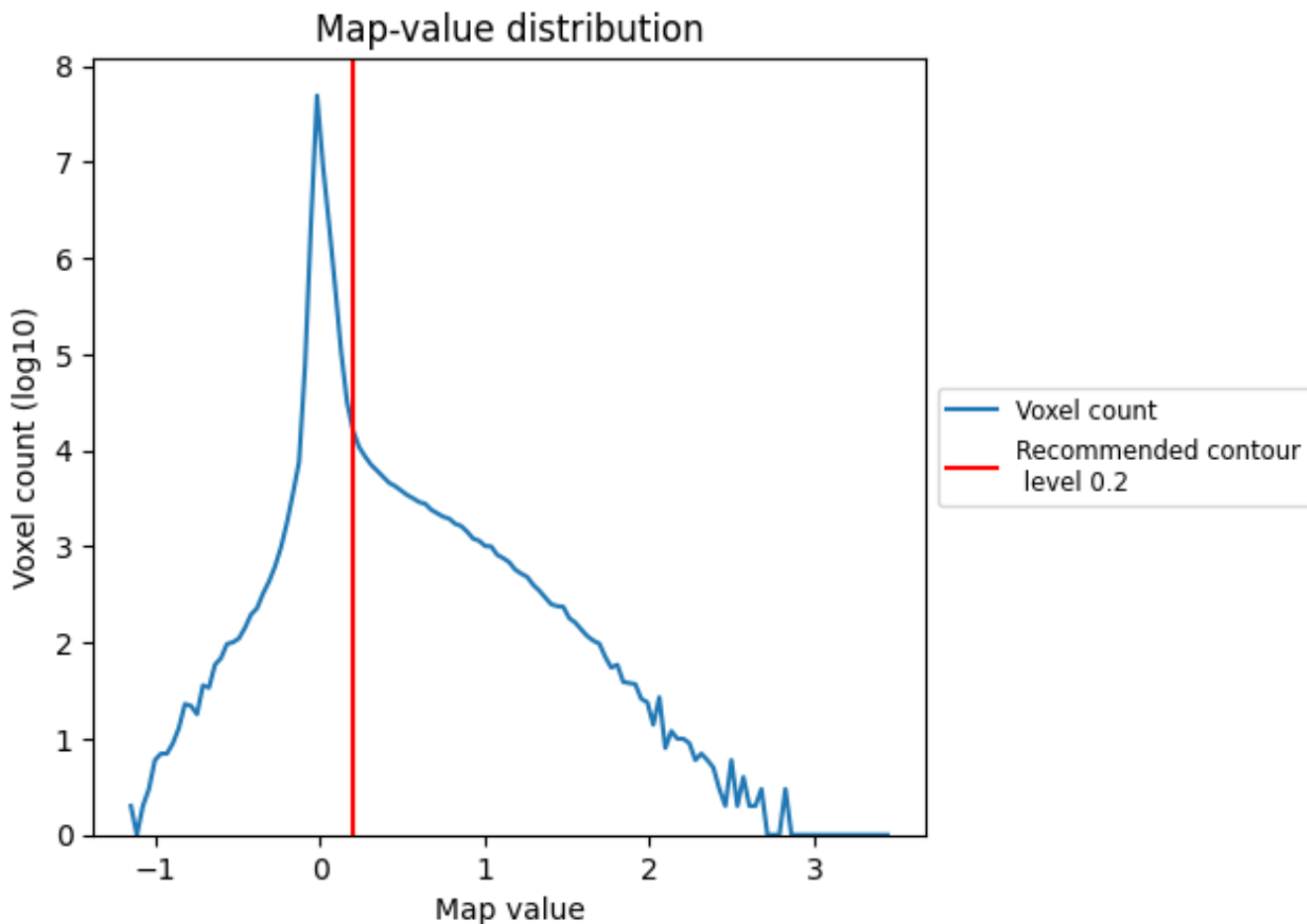
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
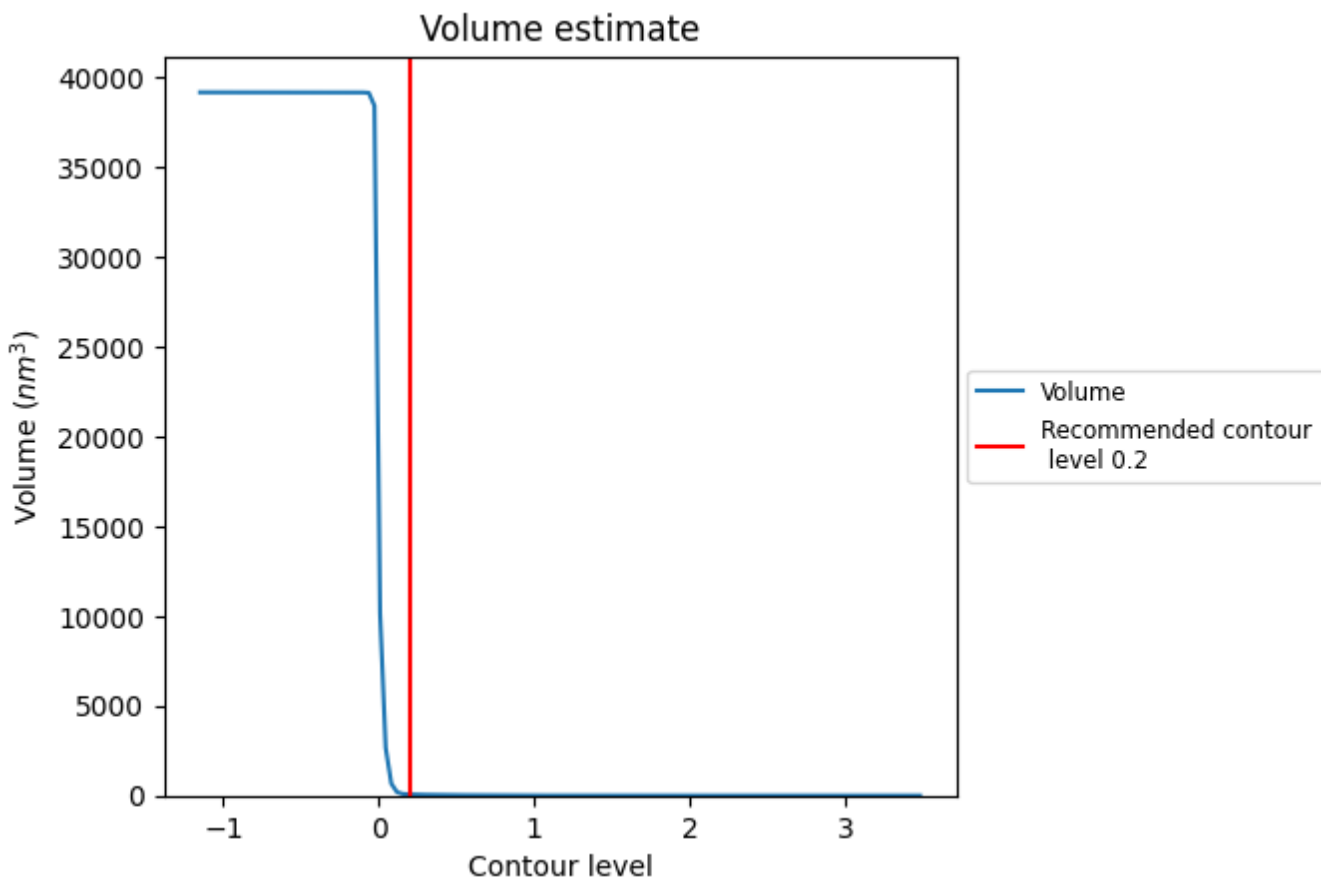
The volume at the recommended contour level is 65 nm^3; this corresponds to an approximate mass of 58 kDa.

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 ⓘ
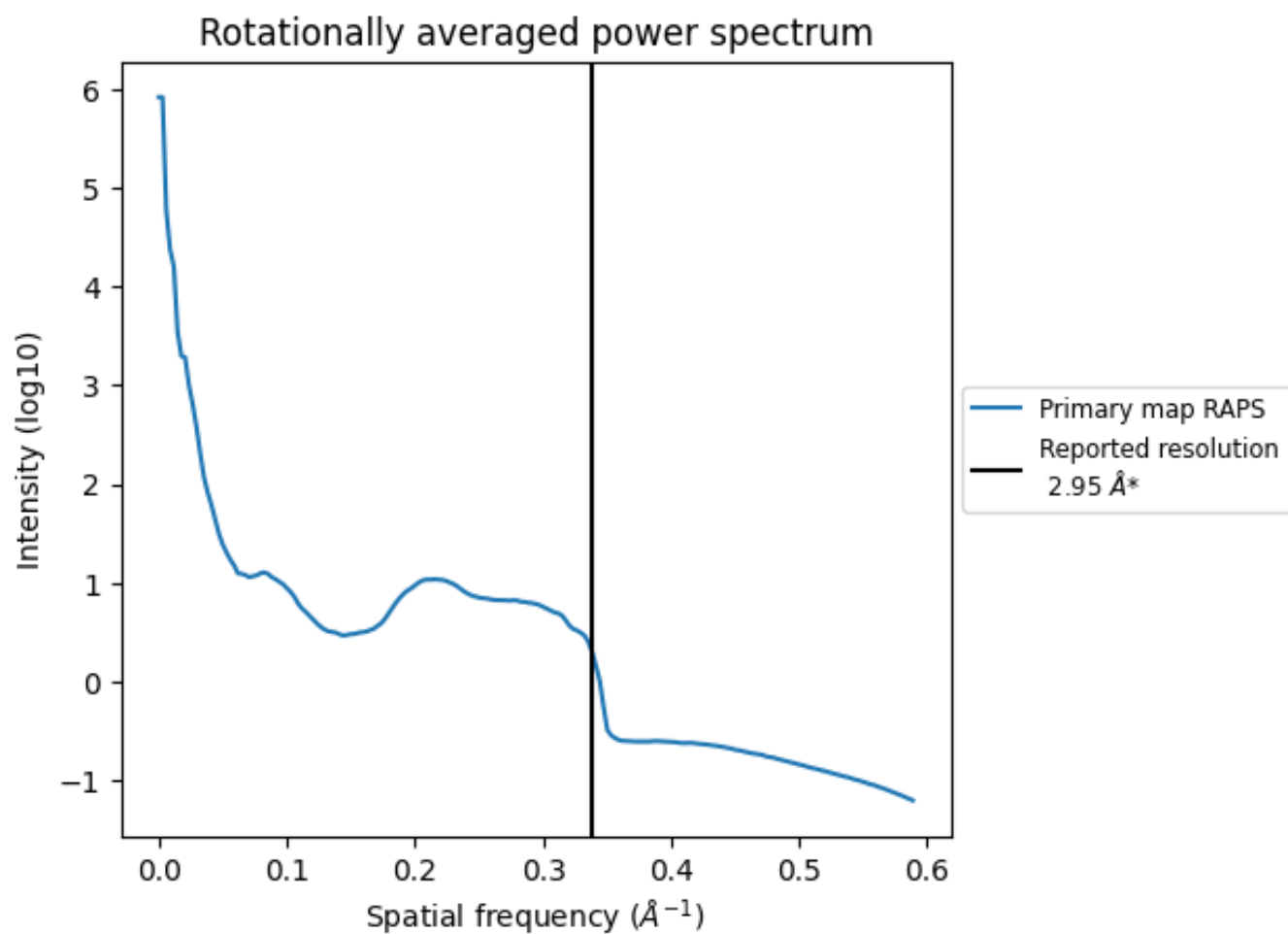
*Reported resolution corresponds to spatial frequency of 0.339 Å^{-1}

8　Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-33984 and PDB model 7YON. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay ⓘ

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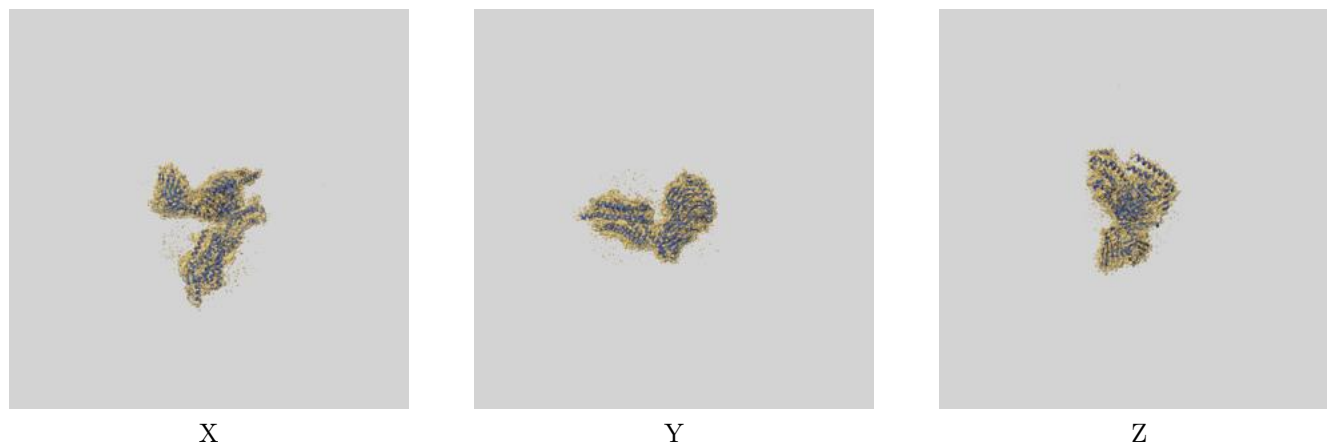
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ
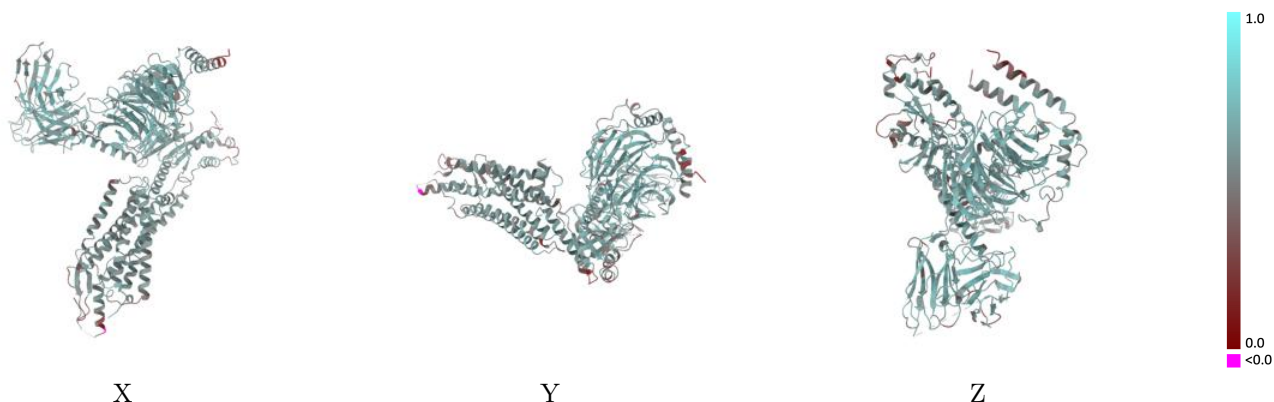
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ
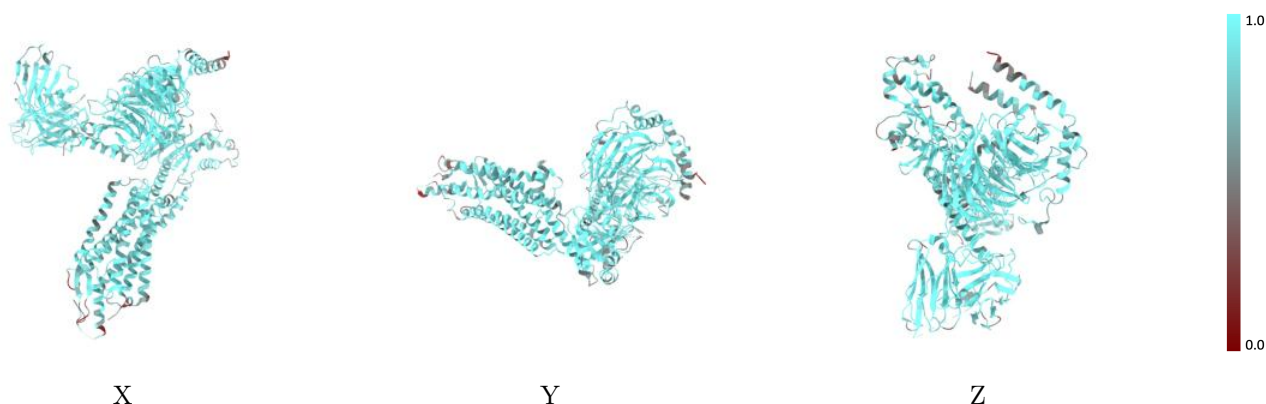
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion ⓘ
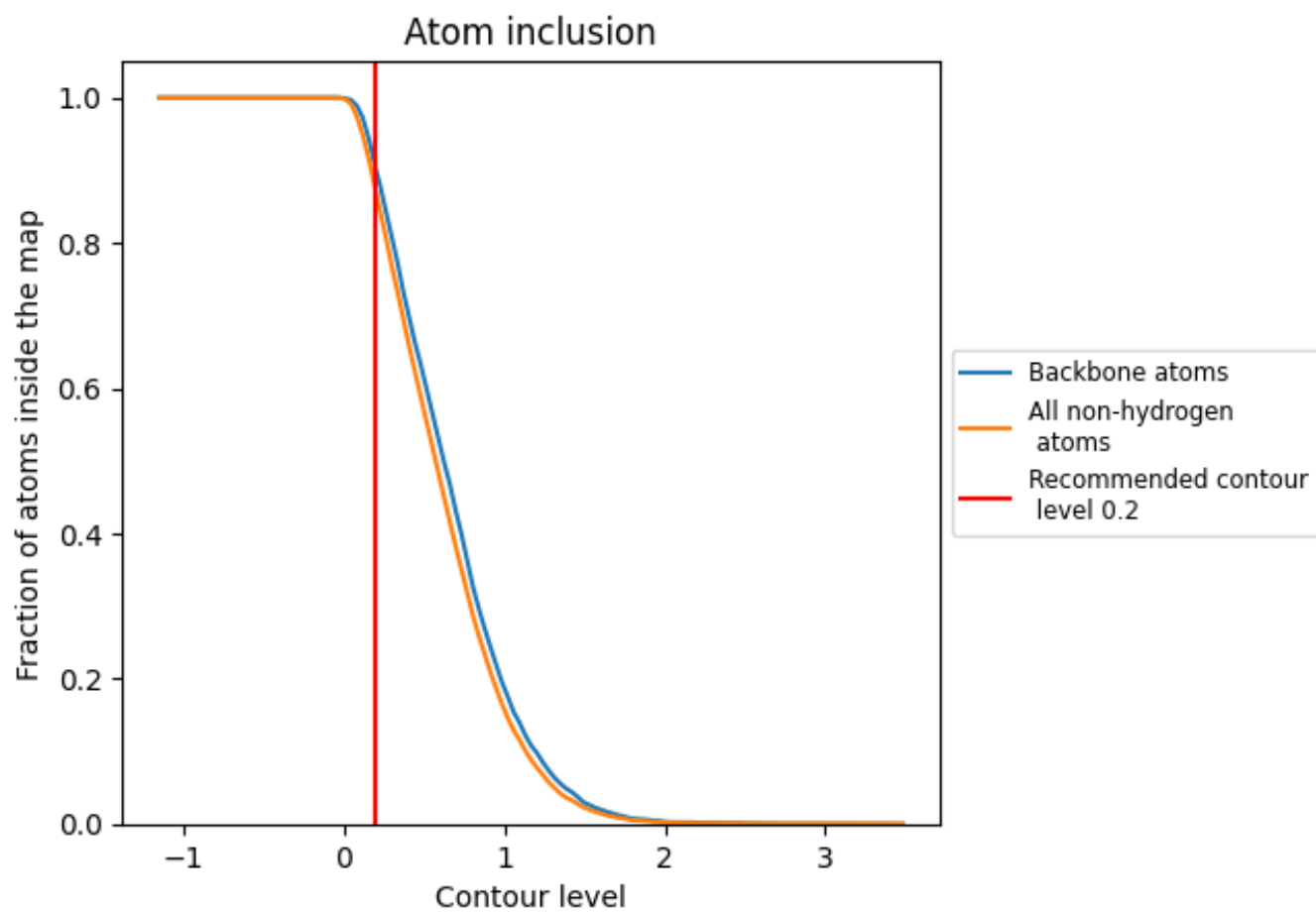
At the recommended contour level, 90% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8698	0.5720
A	0.8500	0.5480
B	0.9183	0.6100
G	0.7810	0.5430
L	0.7488	0.4860
R	0.8336	0.5410
S	0.9093	0.6000

1.0

0.0
<0.0