



wwPDB EM Validation Summary Report ⓘ

Nov 29, 2022 – 11:28 AM JST

PDB ID : 7WBJ
EMDB ID : EMD-32401
Title : Cryo-EM structure of N-terminal modified human vasoactive intestinal polypeptide receptor 2 (VIP2R) in complex with PACAP27 and Gs
Authors : Xu, Y.N.; Feng, W.B.; Zhou, Q.T.; Liang, A.Y.; Li, J.; Dai, A.T.; Zhao, F.H.; Yan, J.H.; Chen, C.W.; Li, H.; Zhao, L.H.; Xia, T.; Jiang, Y.; Xu, H.E.; Yang, D.H.; Wang, M.W.
Deposited on : 2021-12-16
Resolution : 3.42 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:

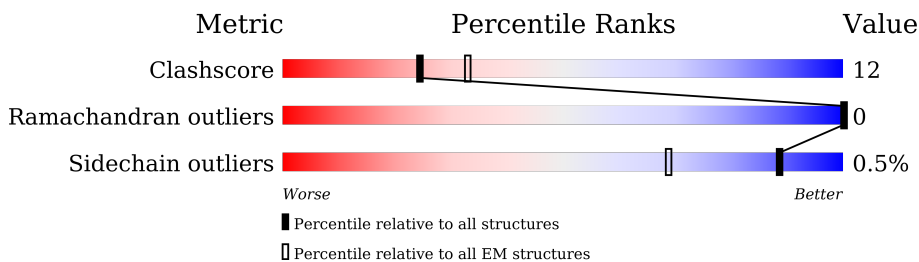
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.42 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	R	432	
2	L	27	
3	A	394	
4	B	400	
5	G	71	
6	N	140	

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 8989 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 Vasoactive intestinal polypeptide receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	R	359	2871	1889	465	496	21	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	7	ASP	-	expression tag	UNP P41587
R	8	TYR	-	expression tag	UNP P41587
R	9	LYS	-	expression tag	UNP P41587
R	10	ASP	-	expression tag	UNP P41587
R	11	ASP	-	expression tag	UNP P41587
R	12	ASP	-	expression tag	UNP P41587
R	13	ASP	-	expression tag	UNP P41587
R	14	VAL	-	expression tag	UNP P41587
R	15	ASP	-	expression tag	UNP P41587
R	16	HIS	-	expression tag	UNP P41587
R	17	HIS	-	expression tag	UNP P41587
R	18	HIS	-	expression tag	UNP P41587
R	19	HIS	-	expression tag	UNP P41587
R	20	HIS	-	expression tag	UNP P41587
R	21	HIS	-	expression tag	UNP P41587
R	22	HIS	-	expression tag	UNP P41587
R	23	HIS	-	expression tag	UNP P41587

- Molecule 2 is a protein called Pituitary adenylate cyclase-activating polypeptide 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	27	221	142	39	39	1	0	0

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	237	1931	1214	348	363	6	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	ASN	SER	engineered mutation	UNP P04896
A	226	ALA	GLY	engineered mutation	UNP P04896
A	268	ALA	GLU	engineered mutation	UNP P04896
A	271	LYS	ASN	engineered mutation	UNP P04896
A	274	ASP	LYS	engineered mutation	UNP P04896
A	280	LYS	ARG	engineered mutation	UNP P04896
A	284	ASP	THR	engineered mutation	UNP P04896
A	285	THR	ILE	engineered mutation	UNP P04896
A	366	SER	ALA	engineered mutation	UNP P04896

- Molecule 4 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		
4	B	340	2590	1599	462	508	21	0	0

There are 61 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-33	MET	-	initiating methionine	UNP P54311
B	-32	HIS	-	expression tag	UNP P54311
B	-31	HIS	-	expression tag	UNP P54311
B	-30	HIS	-	expression tag	UNP P54311
B	-29	HIS	-	expression tag	UNP P54311
B	-28	HIS	-	expression tag	UNP P54311
B	-27	HIS	-	expression tag	UNP P54311
B	-26	SER	-	expression tag	UNP P54311
B	-25	SER	-	expression tag	UNP P54311
B	-24	GLY	-	expression tag	UNP P54311
B	-23	LEU	-	expression tag	UNP P54311
B	-22	VAL	-	expression tag	UNP P54311
B	-21	PRO	-	expression tag	UNP P54311
B	-20	ARG	-	expression tag	UNP P54311
B	-19	GLY	-	expression tag	UNP P54311
B	-18	SER	-	expression tag	UNP P54311
B	-17	HIS	-	expression tag	UNP P54311

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	MET	-	expression tag	UNP P54311
B	-15	ALA	-	expression tag	UNP P54311
B	-14	SER	-	expression tag	UNP P54311
B	-13	HIS	-	expression tag	UNP P54311
B	-12	HIS	-	expression tag	UNP P54311
B	-11	HIS	-	expression tag	UNP P54311
B	-10	HIS	-	expression tag	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
B	341	GLY	-	expression tag	UNP P54311
B	342	SER	-	expression tag	UNP P54311
B	343	SER	-	expression tag	UNP P54311
B	344	GLY	-	expression tag	UNP P54311
B	345	GLY	-	expression tag	UNP P54311
B	346	GLY	-	expression tag	UNP P54311
B	347	GLY	-	expression tag	UNP P54311
B	348	SER	-	expression tag	UNP P54311
B	349	GLY	-	expression tag	UNP P54311
B	350	GLY	-	expression tag	UNP P54311
B	351	GLY	-	expression tag	UNP P54311
B	352	GLY	-	expression tag	UNP P54311
B	353	SER	-	expression tag	UNP P54311
B	354	SER	-	expression tag	UNP P54311
B	355	GLY	-	expression tag	UNP P54311
B	356	VAL	-	expression tag	UNP P54311
B	357	SER	-	expression tag	UNP P54311
B	358	GLY	-	expression tag	UNP P54311
B	359	TRP	-	expression tag	UNP P54311
B	360	ARG	-	expression tag	UNP P54311
B	361	LEU	-	expression tag	UNP P54311
B	362	PHE	-	expression tag	UNP P54311
B	363	LYS	-	expression tag	UNP P54311
B	364	LYS	-	expression tag	UNP P54311

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Chain	Residue	Modelled	Actual	Comment	Reference
B	365	ILE	-	expression tag	UNP P54311
B	366	SER	-	expression tag	UNP P54311

- Molecule 5 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		
5	G	55	418	263	72	80	3	0	0

- Molecule 6 is a protein called Nanobody-35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	N	128	958	597	164	192	5	0	0

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	770771	Depositor
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.549	Depositor
Minimum map value	-3.095	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.064	Depositor
Recommended contour level	0.43	Depositor
Map size (\AA)	308.448, 308.448, 308.448	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.071, 1.071, 1.071	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	R	0.27	0/2949	0.47	0/4015
2	L	0.29	0/225	0.47	0/300
3	A	0.29	0/1966	0.51	0/2649
4	B	0.31	0/2637	0.56	0/3578
5	G	0.24	0/424	0.42	0/573
6	N	0.34	0/978	0.59	1/1328 (0.1%)
All	All	0.29	0/9179	0.52	1/12443 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	106	ASP	CB-CG-OD2	5.17	122.95	118.30

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	R	2871	0	2883	59	0
2	L	221	0	226	4	0
3	A	1931	0	1877	48	0
4	B	2590	0	2481	80	0
5	G	418	0	425	4	0
6	N	958	0	909	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8989	0	8801	209	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 12.

The worst 5 of 209 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)
6:N:35:ASN:HD21	6:N:110:VAL:HG11	1.37	0.89
4:B:54:HIS:HE2	4:B:72:SER:HG	1.12	0.86
6:N:82:GLN:HE22	6:N:84:ASN:HB3	1.45	0.81
4:B:210:LEU:HD22	4:B:255:LEU:HD12	1.66	0.78
4:B:295:ASN:OD1	4:B:304:ARG:NH2	2.19	0.74

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	R	355/432 (82%)	337 (95%)	18 (5%)	0	100	100
2	L	25/27 (93%)	25 (100%)	0	0	100	100
3	A	231/394 (59%)	224 (97%)	7 (3%)	0	100	100
4	B	338/400 (84%)	317 (94%)	21 (6%)	0	100	100
5	G	53/71 (75%)	51 (96%)	2 (4%)	0	100	100
6	N	126/140 (90%)	119 (94%)	7 (6%)	0	100	100
All	All	1128/1464 (77%)	1073 (95%)	55 (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	R	319/389 (82%)	317 (99%)	2 (1%)	86	94
2	L	23/23 (100%)	23 (100%)	0	100	100
3	A	206/351 (59%)	205 (100%)	1 (0%)	88	95
4	B	278/328 (85%)	278 (100%)	0	100	100
5	G	44/58 (76%)	44 (100%)	0	100	100
6	N	103/116 (89%)	101 (98%)	2 (2%)	57	80
All	All	973/1265 (77%)	968 (100%)	5 (0%)	89	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	234	MET
1	R	308	GLN
3	A	42	ARG
6	N	99	CYS
6	N	109	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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.

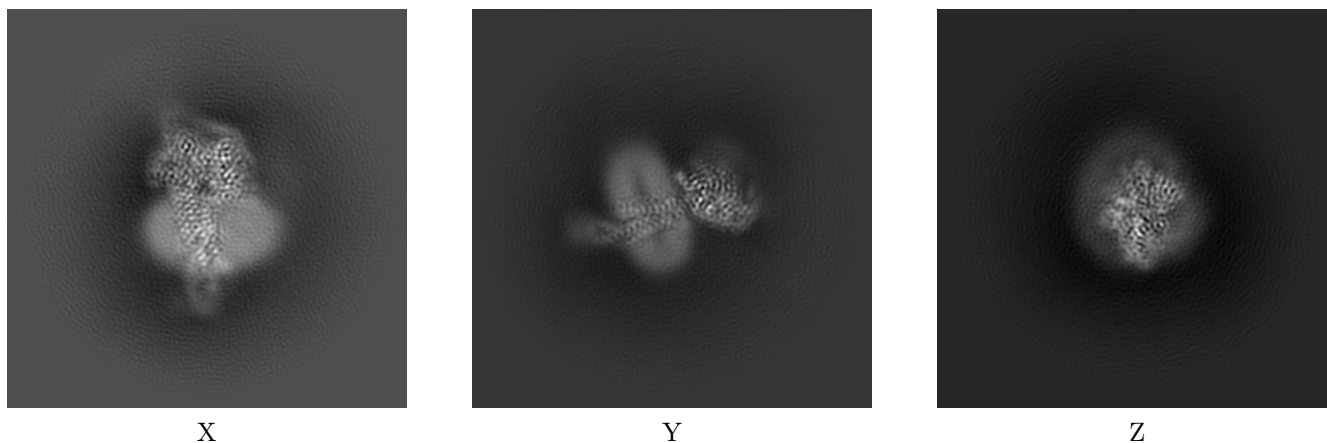
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32401. 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](#)

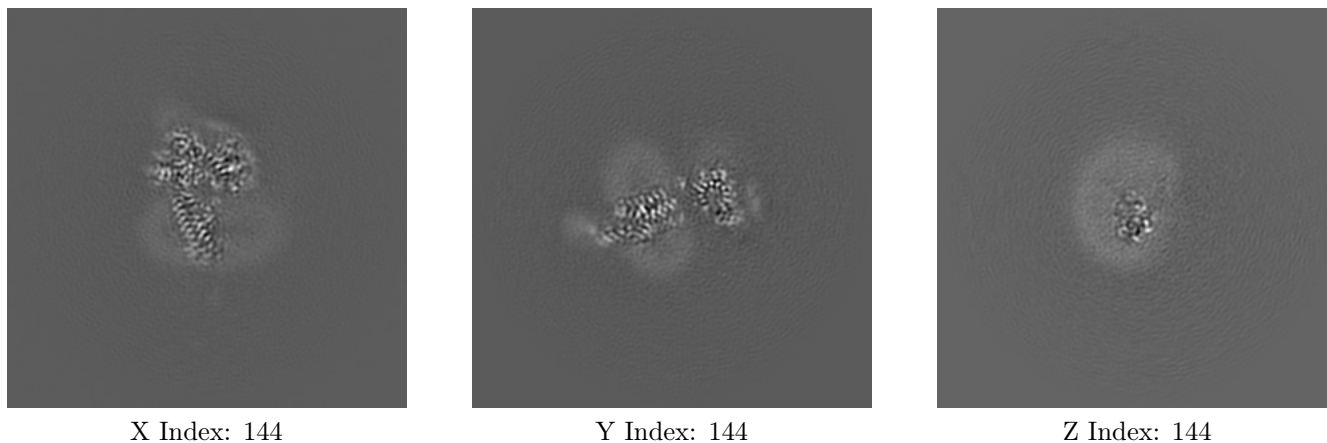
6.1.1 Primary map



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

6.2 Central slices [i](#)

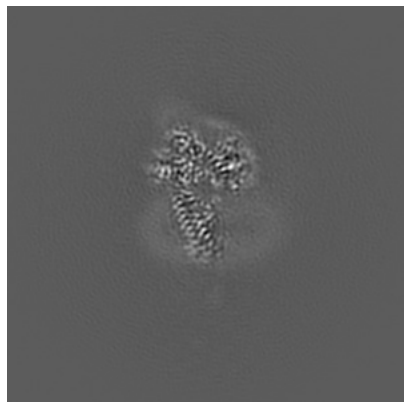
6.2.1 Primary map



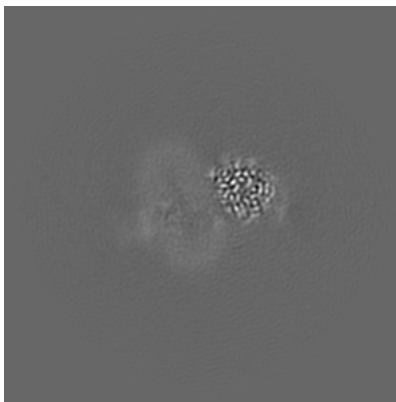
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

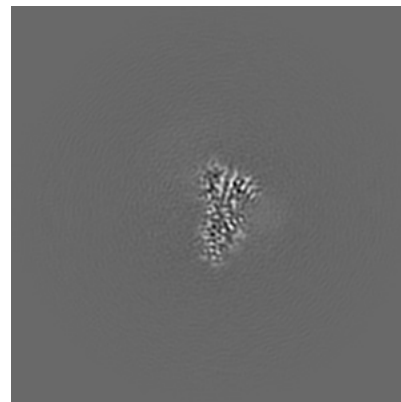
6.3.1 Primary map



X Index: 144



Y Index: 157



Z Index: 168

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

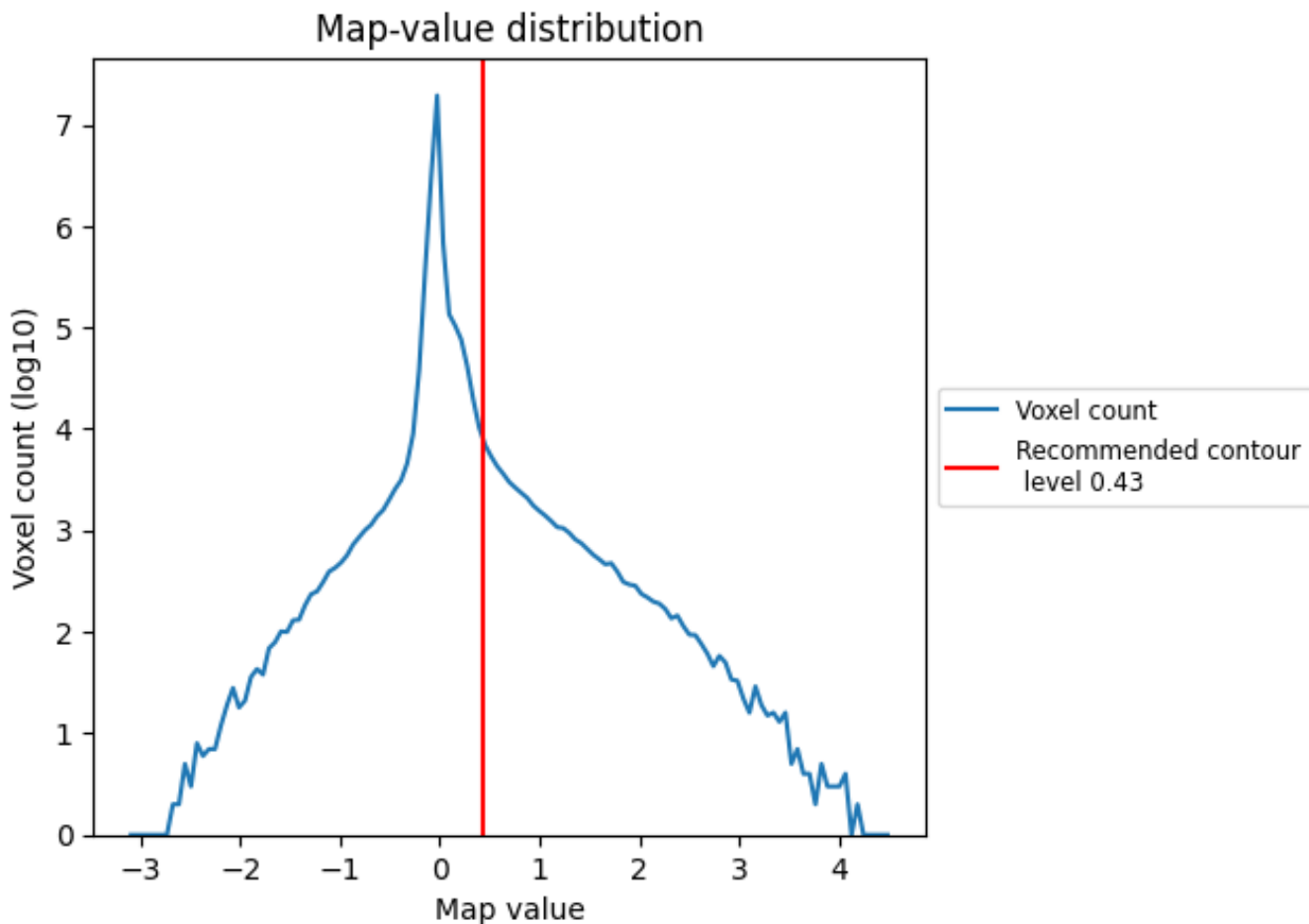
6.5 Mask visualisation

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

7 Map analysis [i](#)

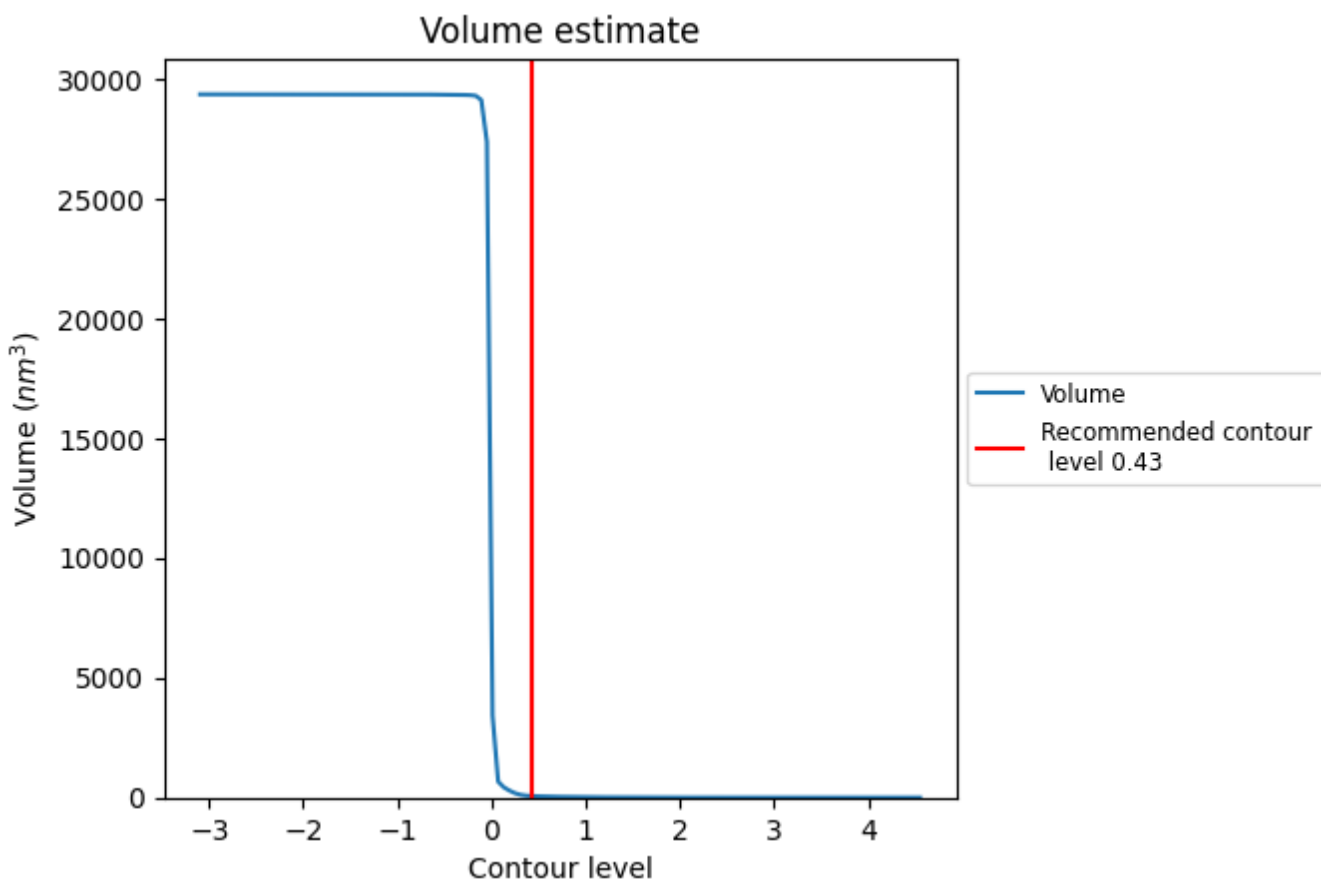
This section contains the results of statistical analysis of the map.

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.

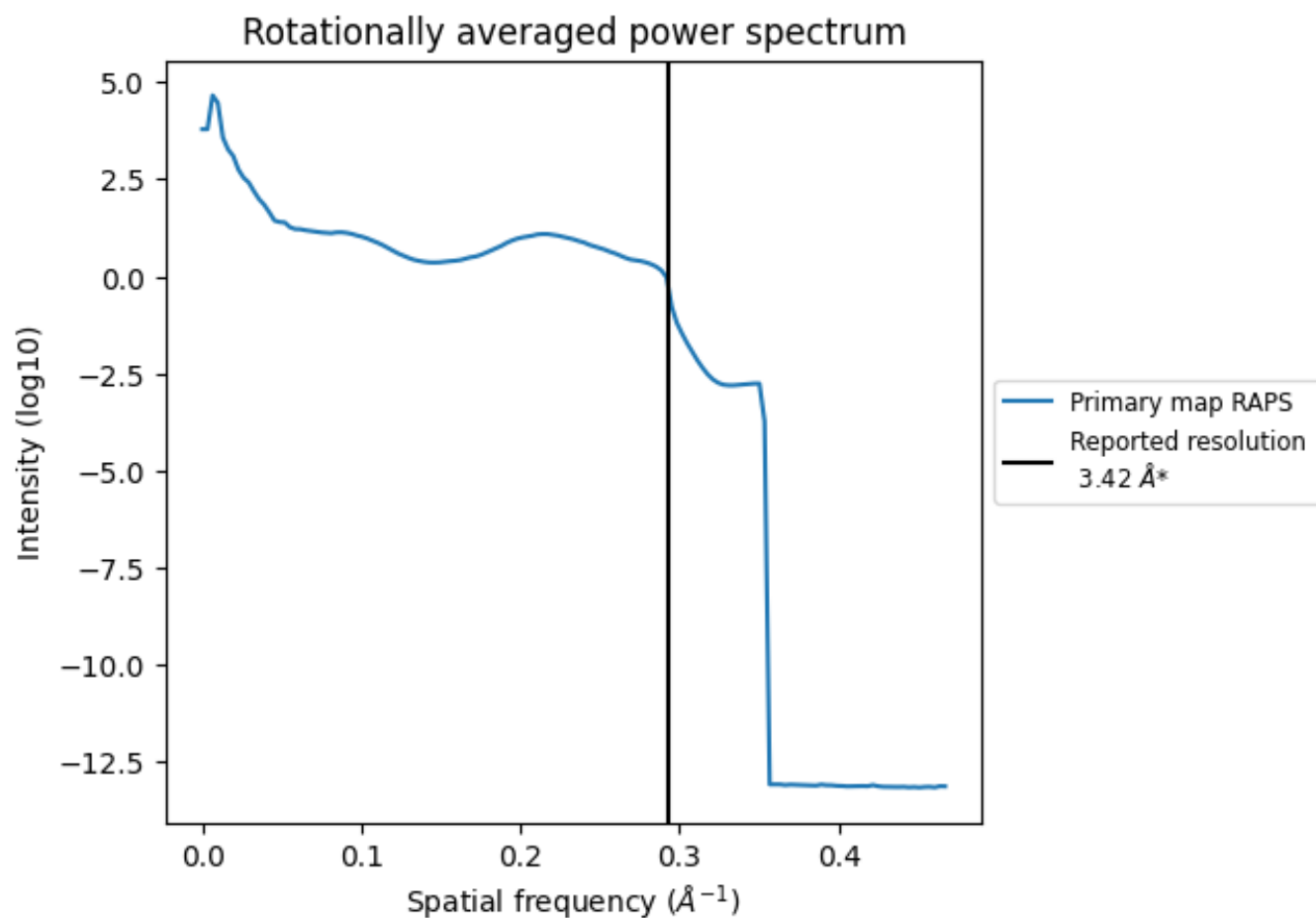
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 62 nm³; this corresponds to an approximate mass of 56 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.292\AA^{-1}

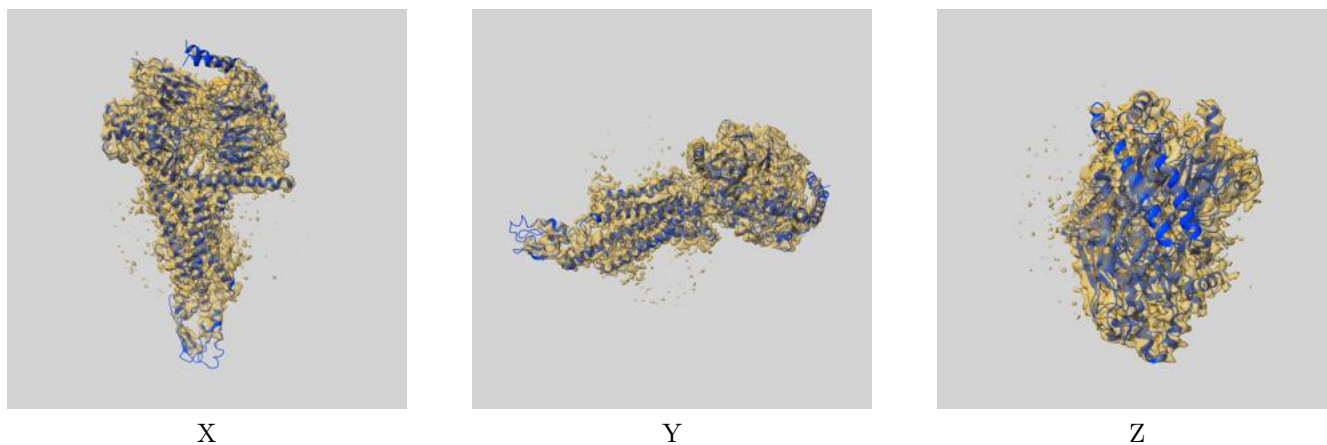
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

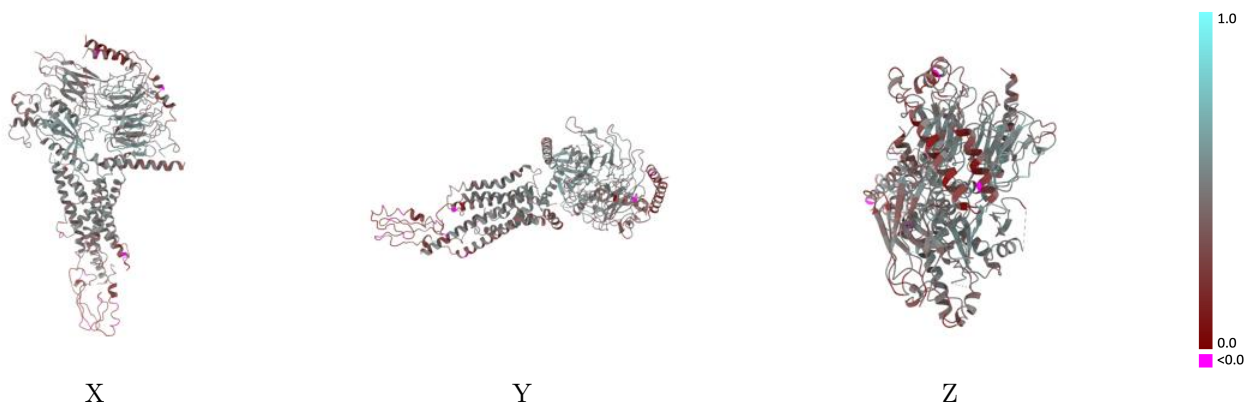
This section contains information regarding the fit between EMDB map EMD-32401 and PDB model 7WBJ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



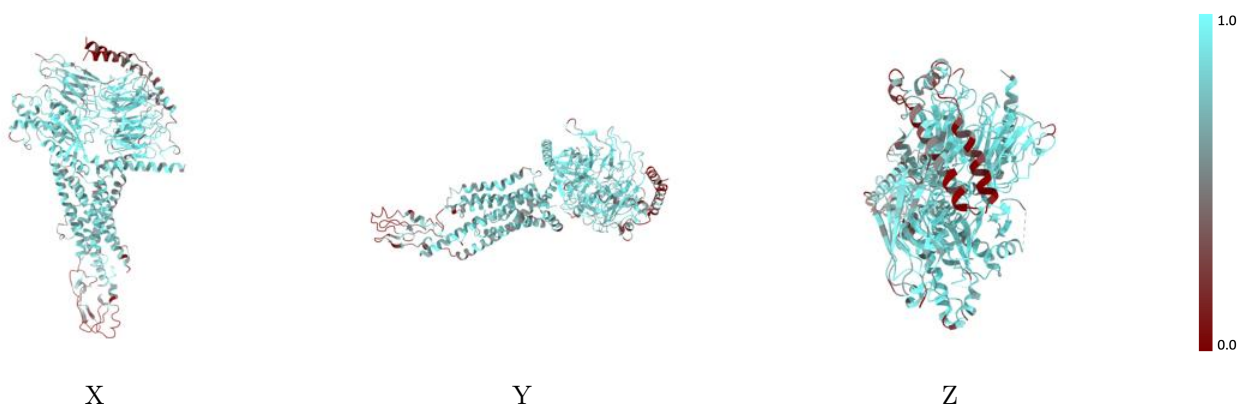
The images above show the 3D surface view of the map at the recommended contour level 0.43 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



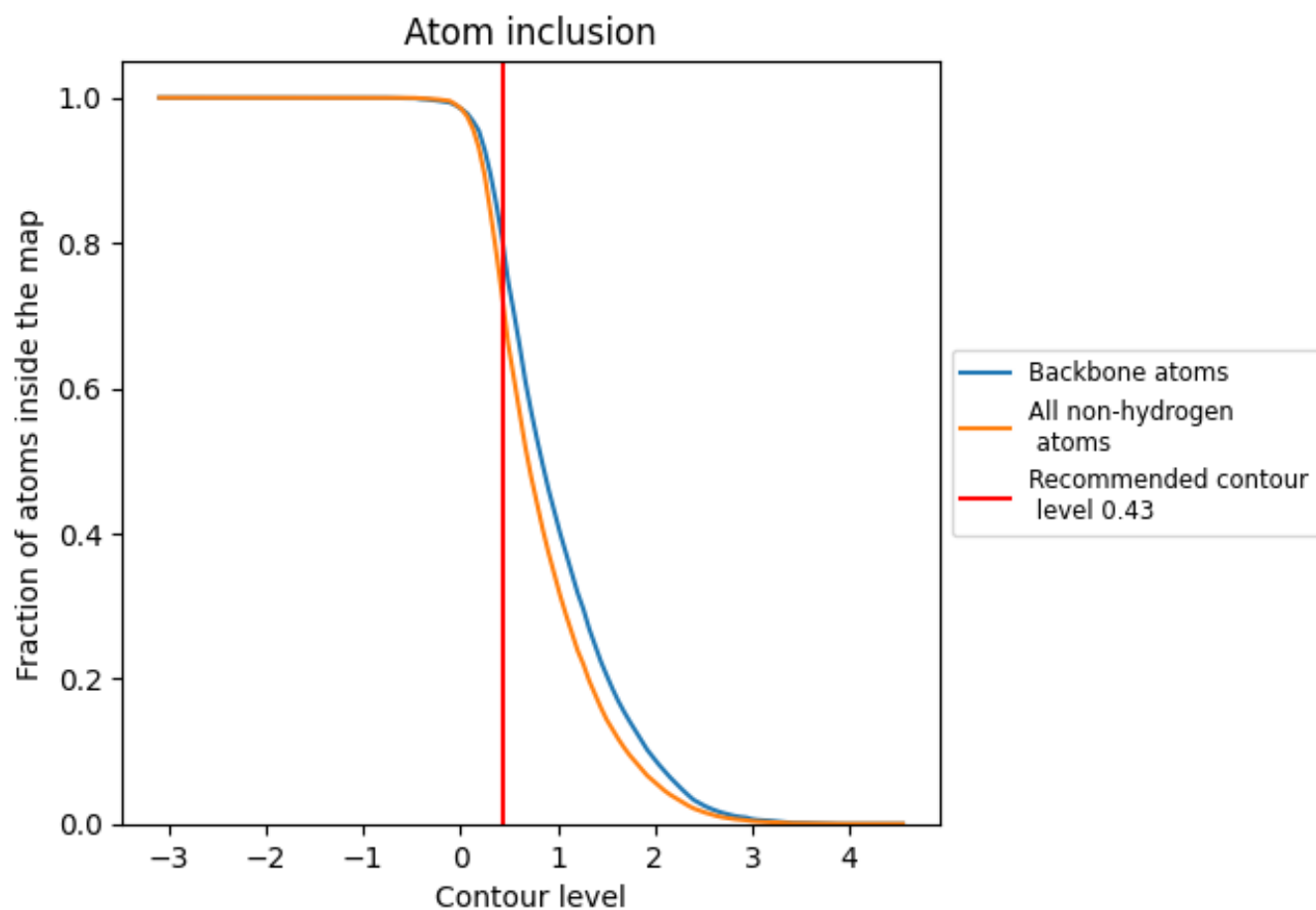
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.43).















9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 73% 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 (0.43) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7262	 0.4250
A	 0.8205	 0.4770
B	 0.7826	 0.4660
G	 0.4407	 0.3120
L	 0.8131	 0.4360
N	 0.7689	 0.4230
R	 0.6337	 0.3700

