



wwPDB EM Validation Summary Report ⓘ

Mar 14, 2026 – 05:53 AM UTC

PDB ID : 7BLN / pdb_00007bln
EMDB ID : EMD-12220
Title : VPS35/VPS29 arch of metazoan membrane-assembled retromer:SNX3 complex modelled with human proteins
Authors : Leneva, N.; Kovtun, O.; Morado, D.R.; Briggs, J.A.G.; Owen, D.J.
Deposited on : 2021-01-18
Resolution : 8.90 Å (reported)
Based on initial models : 2R17, 5F0L

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:

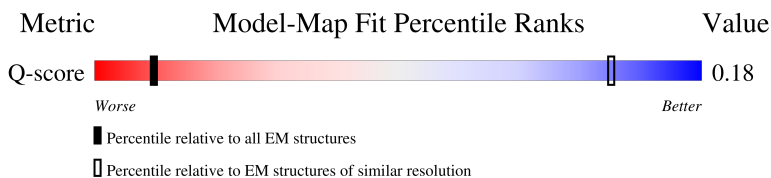
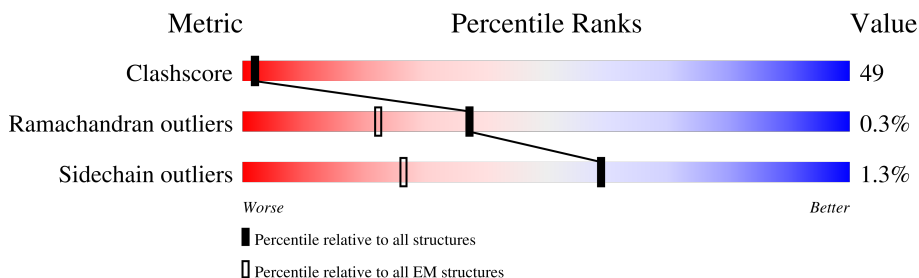
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.90 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	258 (8.40 - 9.40)

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	B	182	60% 53% 38% 8% .
1	D	182	58% 52% 41% 7% .
2	A	796	32% 28% 67% ..
2	C	796	34% 29% 67% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15364 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 Vacuolar protein sorting-associated protein 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	182	Total	C	N	O	S	0	0
			1447	936	242	263	6		
1	D	182	Total	C	N	O	S	0	0
			1447	936	242	263	6		

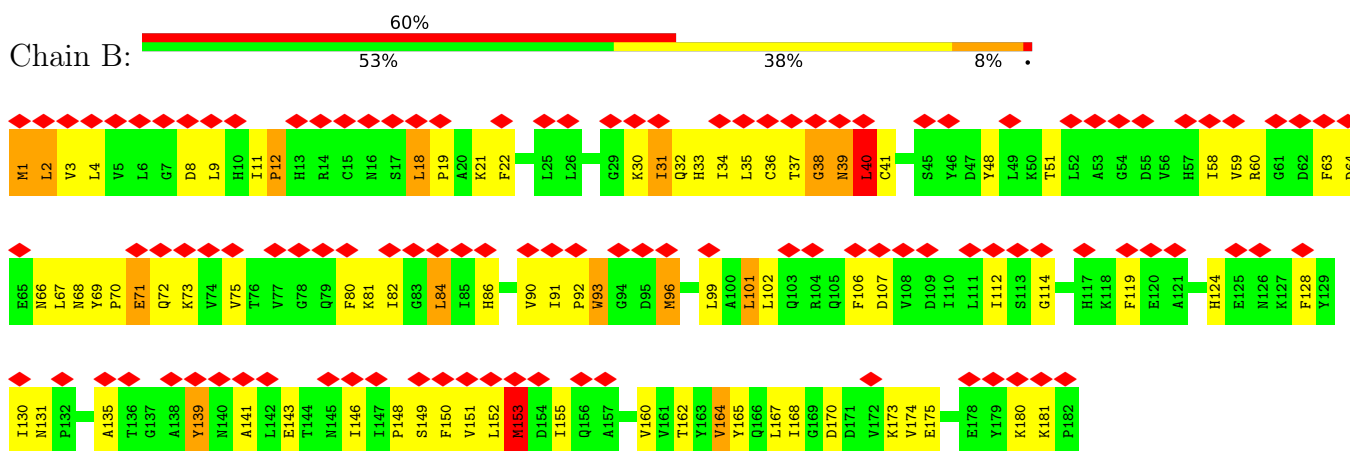
- Molecule 2 is a protein called Vacuolar protein sorting-associated protein 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	769	Total	C	N	O	S	0	0
			6235	3959	1069	1175	32		
2	C	769	Total	C	N	O	S	0	0
			6235	3959	1069	1175	32		

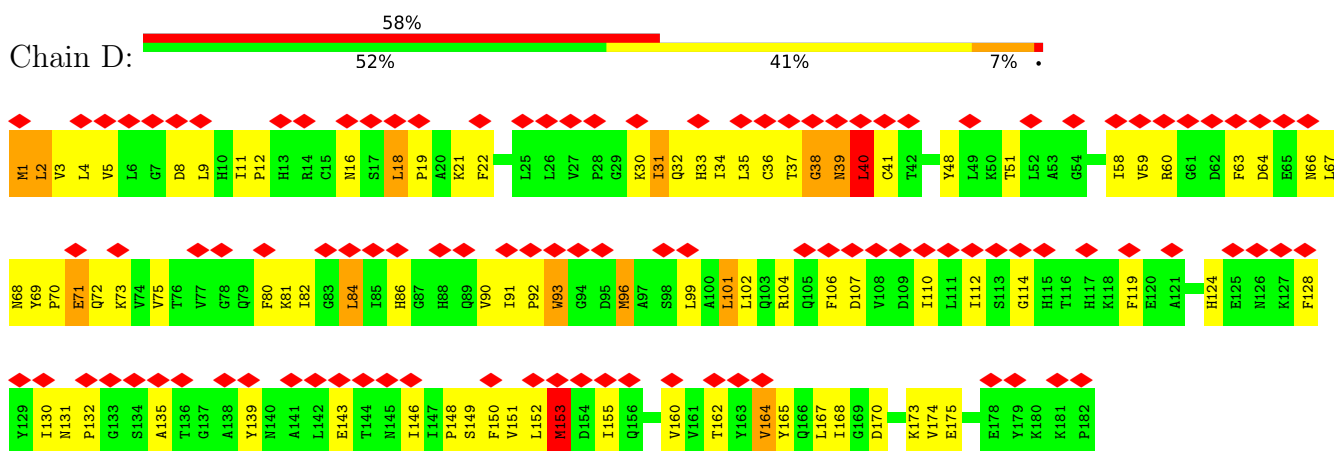
3 Residue-property plots

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.

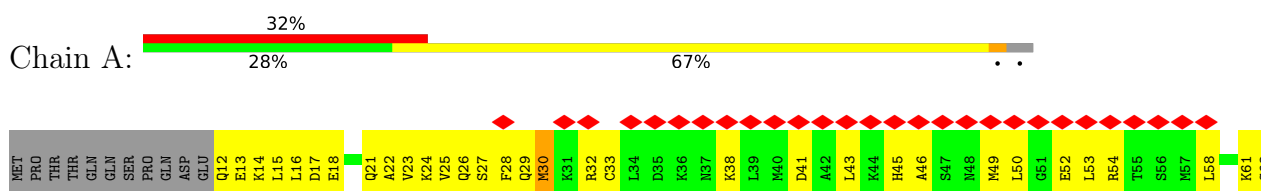
- Molecule 1: Vacuolar protein sorting-associated protein 29

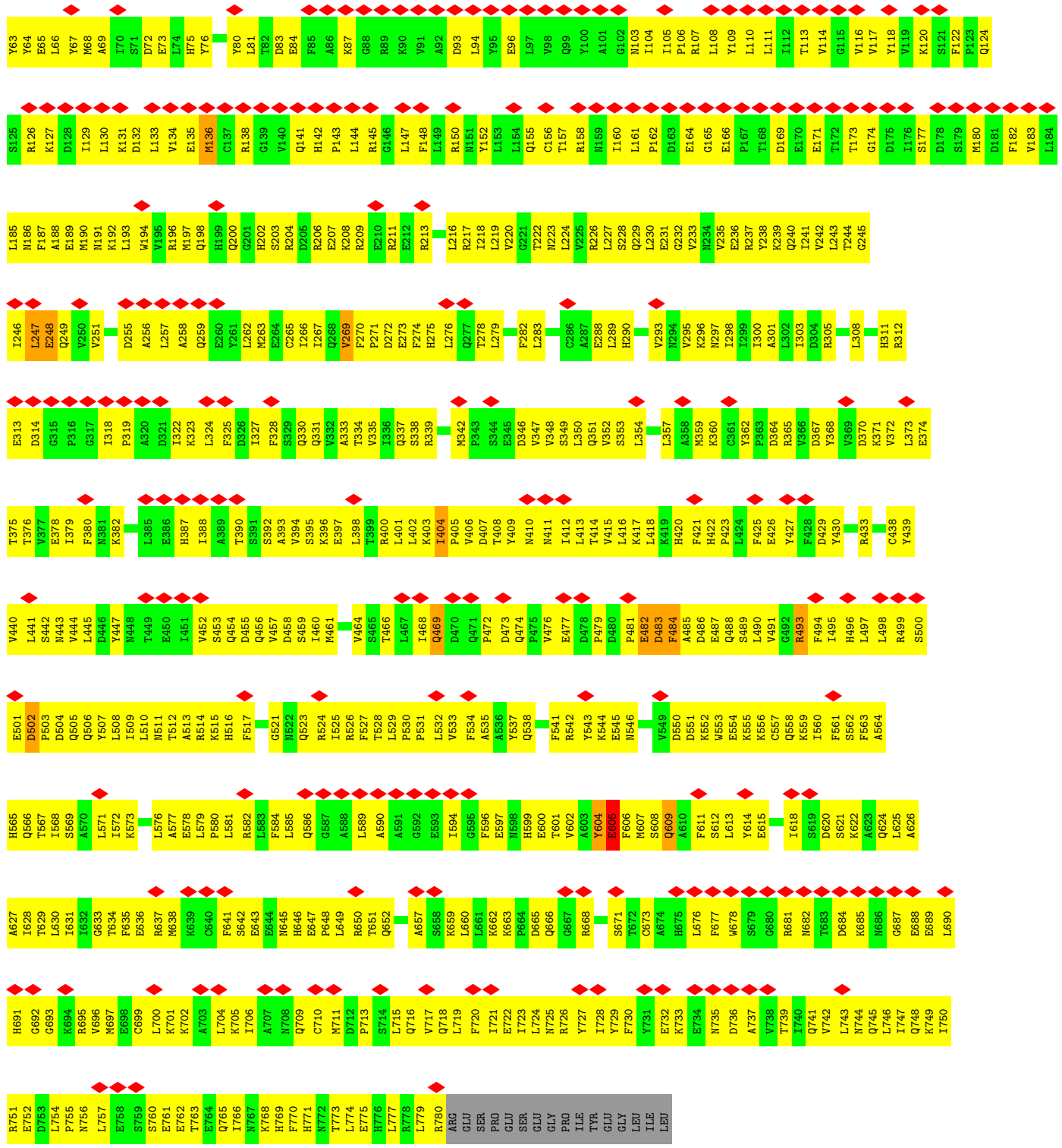


- Molecule 1: Vacuolar protein sorting-associated protein 29



- Molecule 2: Vacuolar protein sorting-associated protein 35





● Molecule 2: Vacuolar protein sorting-associated protein 35



T739	V742	V743	N744	Q745	L746	I747	K748	D684	K685	M686	E687	E688	E689	L690	H691	G692	K693	K694	R695	V696	M697	C698	L700	K701	K702	A703	L704	K705	I706	A707	N708	Q709	C710	C711	M711	D712	P713	Q716	V717	Q718	L719	F720	I721	E722	Q723	L724	N725	R726	Y727	I728	Y729	F730	Y731	E732	K733	E734	N735	D736	A737	V738	D616	E617	I618	S619	D620	S621	K622	A623	Q624	L625	A626	A627	I628	L629	T629	L630	I631	I632	G633	T634	F635	E636	R637	M638	K639	C640	F641	S642	E643	E644	N645	H646	E647	P648	L649	R650	T651	Q652	L655	A656	A657	S658	K659	L660	L661	K662	K663	P664	D665	O666	G667	R668	A669	V670	S671	T672	C673	L676	F677	K556	C557	Q558	K559	L560	F561	S562	F563	A564	H565	T567	I568	S569	A570	L571	I572	K573	A574	E575	L576	A577	E578	L579	P580	L581	R582	L583	F584	L585	Q586	G587	A588	L589	A590	A591	G592	E593	L594	G595	F596	E597	H598	E600	T601	A603	P604	E605	M607	S608	Q609	A610	F611	S612	L613	Y614	E615	K495	H496	L497	L498	R499	S500	E501	D502	F503	D504	O505	O506	Y507	L508	L509	L510	L511	A512	A513	R514	H516	F517	Q523	I525	R526	F527	L528	L529	P530	P531	L532	V533	F534	A535	A536	Y537	O538	L539	A540	F541	R542	Y543	K544	E545	S546	S547	K548	V549	D550	D551	K552	M553	K555	R433	K434	S435	M436	S437	C438	V439	V440	L441	S442	N443	V444	L445	D446	Y447	N448	T449	E450	I451	V452	Q453	D454	Q455	Q456	V457	L460	M461	N462	L463	V464	S465	T466	L467	L468	Q469	D470	Q471	P472	D473	Q474	P475	V476	E477	D478	P479	D480	P481	F482	A485	D486	E487	Q488	S489	S547	L490	G492	V491	G492	Y430	E431	S432	L373	E374	T375	T376	V377	E378	F380	N381	K382	L383	N384	L385	E386	H387	I388	A389	T390	S391	A393	V394	S395	K396	E397	L398	T399	R400	L401	L402	L404	P405	V406	D407	M410	N411	I412	L413	T414	V415	K417	L418	K419	H420	F421	H422	P423	L424	F425	E426	Y427	F428	D429	Y430	E431	S432	A310	H311	R312	E313	D314	G315	P316	G317	L318	P319	A320	D321	K323	L324	F325	O326	L327	F328	S329	Q330	Q331	V332	A333	T334	L335	Q337	S338	R339	Q340	D341	K342	P343	S344	E345	D346	V347	L350	Q351	V352	S353	L354	L355	K356	L357	A358	K359	K360	C361	P363	D364	R366	Y368	V369	K371	L247	E248	Q249	V250	V251	N252	C253	R254	D255	A256	L257	A258	Q259	E260	Y261	L262	M263	E264	C265	L266	L267	Q268	V269	F270	F271	D272	E273	F274	H275	L276	Q277	T278	L279	N280	R284	A285	C286	A287	E288	L289	H290	Q291	N292	V293	N294	V295	R296	N297	L298	I299	L302	I303	D304	R305	L306	A307	L308	F309	L183	L184	L185	N186	F187	A188	E189	M190	N191	K192	L193	V194	L195	R196	L197	Q198	H199	Q200	G201	L202	S203	Q204	R205	R206	E207	L208	R209	E210	R211	E212	R213	Q214	E215	L216	R217	L218	Q219	V220	N223	L224	V225	R226	L227	S228	Q229	L230	E231	G232	E233	N234	R237	Y238	L302	I303	D304	R305	L306	A307	L308	F309	P123	Q124	S125	R126	K127	D128	I129	L130	K131	D132	L133	V134	E135	M136	C137	R138	G139	V140	Q141	H142	P143	L144	R145	G146	L147	F148	E212	R213	Q214	E215	L216	R217	L218	Q219	V220	N223	L224	V225	R226	L227	S228	Q229	L230	E231	G232	E233	N234	R237	Y238	L302	I303	D304	R305	L306	A307	L308	F309	K61	S62	Y64	E65	L66	Y67	A68	M69	I70	S71	D72	E73	L74	H75	Y76	L77	E78	T82	D83	E84	F85	A86	K87	G88	R89	K90	A91	V92	D93	L94	Y95	E96	L97	V98	Q99	Y100	A101	G102	M103	I104	I105	F106	R107	L108	Y109	L110	L111	I112	T113	V114	T115	G115	V116	Y117	Y118	V119	K120	S121	F122	P162	D163	E164	G165	E166	P167	T168	D169	E170	T171	T172	T173	T174	G175	I176	S177	D178	S179	M180	S181	F182
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4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	89313	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 ($e^-/\text{\AA}^2$)	3	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	0.068	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.021	Depositor
Map size (Å)	285.768, 285.768, 285.768	wwPDB
Map dimensions	168, 168, 168	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.701, 1.701, 1.701	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	B	0.56	5/1481 (0.3%)	0.95	6/2008 (0.3%)
1	D	0.56	5/1481 (0.3%)	0.95	6/2008 (0.3%)
2	A	0.54	0/6348	0.97	17/8578 (0.2%)
2	C	0.49	0/6348	0.89	7/8578 (0.1%)
All	All	0.52	10/15658 (0.1%)	0.94	36/21172 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	5
2	C	0	1
All	All	0	6

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	MET	CG-SD	6.26	1.96	1.80
1	D	1	MET	CG-SD	6.25	1.96	1.80
1	D	153	MET	CG-SD	6.16	1.96	1.80
1	B	153	MET	CG-SD	6.14	1.96	1.80
1	D	1	MET	SD-CE	6.01	1.94	1.79

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	269	VAL	CA-C-N	-7.93	105.31	121.48
2	A	269	VAL	C-N-CA	-7.93	105.31	121.48
1	D	40	LEU	N-CA-C	-7.64	103.41	112.89
1	B	40	LEU	N-CA-C	-7.63	103.42	112.89
1	B	93	TRP	N-CA-C	6.96	122.86	111.37

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	469	GLN	Peptide
2	A	482	GLU	Peptide
2	A	483	ASP	Peptide
2	A	502	ASP	Peptide
2	A	605	GLU	Mainchain

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	B	1447	0	1459	96	0
1	D	1447	0	1459	94	0
2	A	6235	0	6251	702	0
2	C	6235	0	6251	645	0
All	All	15364	0	15420	1497	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 49.

The worst 5 of 1497 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:D:92:PRO:HB3	2:C:637:ARG:NH2	1.58	1.15
2:A:647:GLU:HA	2:A:650:ARG:HE	1.17	1.10
1:B:8:ASP:H	1:B:38:GLY:HA3	1.15	1.10
1:D:8:ASP:H	1:D:38:GLY:HA3	1.15	1.09
2:C:471:GLN:HB2	2:C:476:VAL:H	1.28	0.96

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	B	180/182 (99%)	157 (87%)	22 (12%)	1 (1%)	21	59
1	D	180/182 (99%)	157 (87%)	22 (12%)	1 (1%)	21	59
2	A	767/796 (96%)	726 (95%)	40 (5%)	1 (0%)	48	83
2	C	767/796 (96%)	723 (94%)	42 (6%)	2 (0%)	36	72
All	All	1894/1956 (97%)	1763 (93%)	126 (7%)	5 (0%)	37	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	484	PHE
2	C	473	ASP
2	C	693	GLY
1	B	38	GLY
1	D	38	GLY

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	B	160/160 (100%)	149 (93%)	11 (7%)	14	36
1	D	160/160 (100%)	149 (93%)	11 (7%)	14	36
2	A	695/720 (96%)	695 (100%)	0	100	100
2	C	695/720 (96%)	695 (100%)	0	100	100
All	All	1710/1760 (97%)	1688 (99%)	22 (1%)	59	74

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	18	LEU
1	D	84	LEU
1	D	40	LEU
1	D	101	LEU
1	B	84	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	337	GLN
2	C	725	ASN
2	C	443	ASN
2	C	586	GLN
2	A	586	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](#)

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

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12220. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

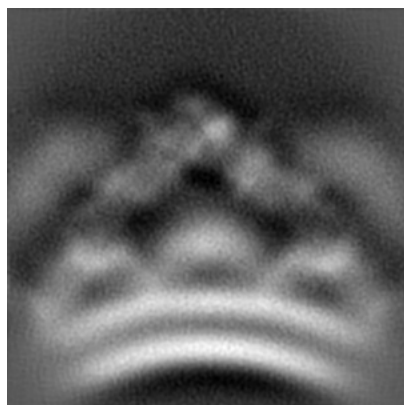


Y

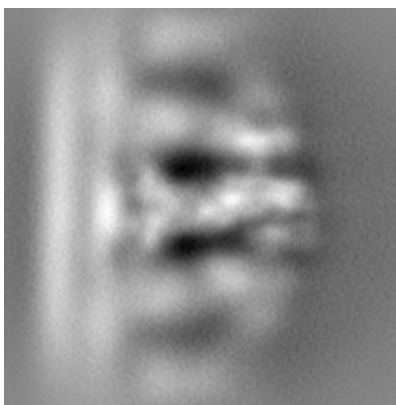


Z

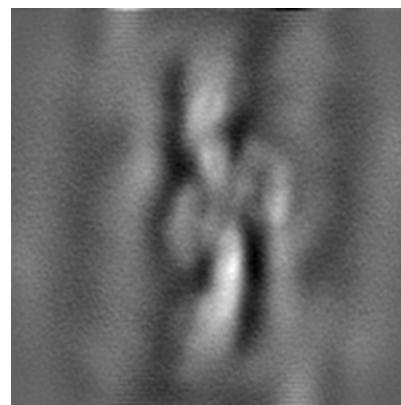
6.1.2 Raw map



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: 84

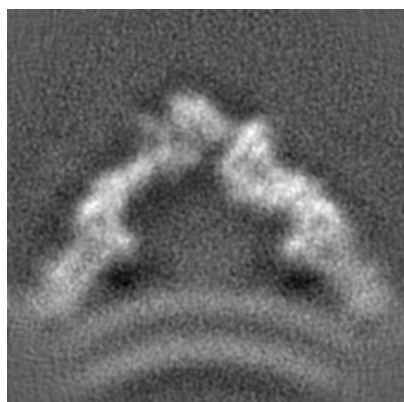


Y Index: 84

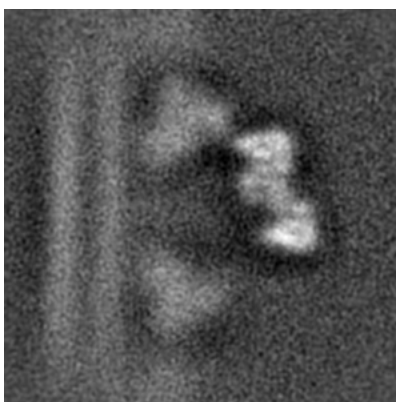


Z Index: 84

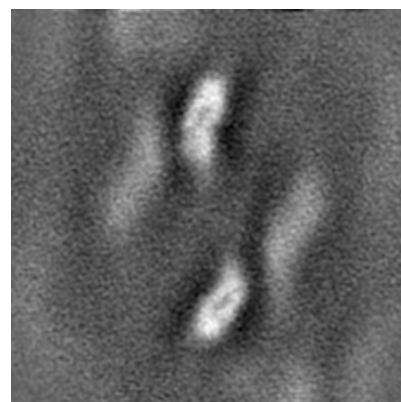
6.2.2 Raw map



X Index: 84



Y Index: 84



Z Index: 84

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: 88

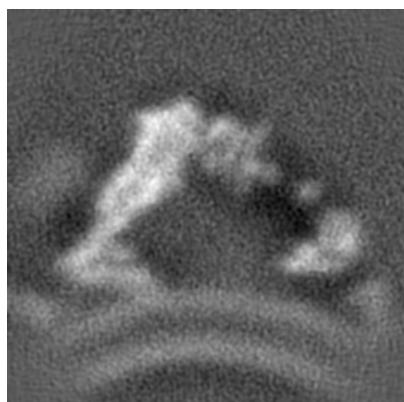


Y Index: 86

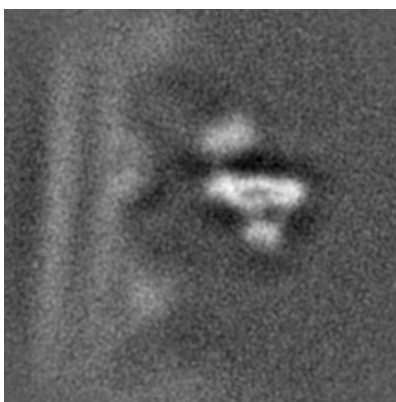


Z Index: 107

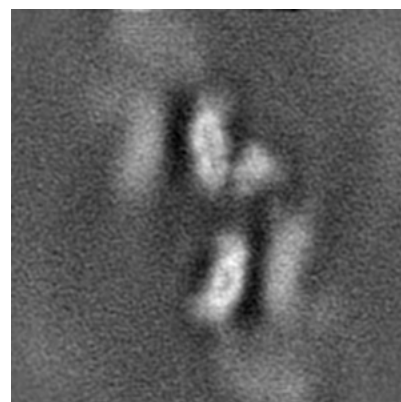
6.3.2 Raw map



X Index: 92



Y Index: 61



Z Index: 95

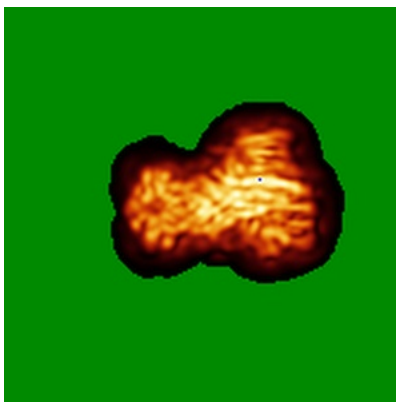
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

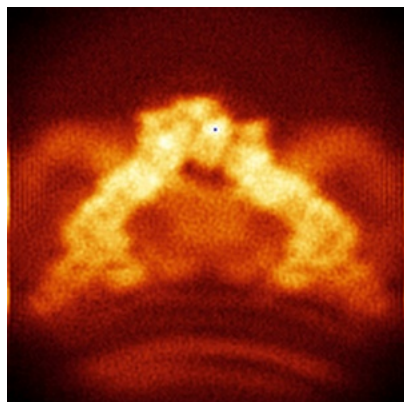


Y

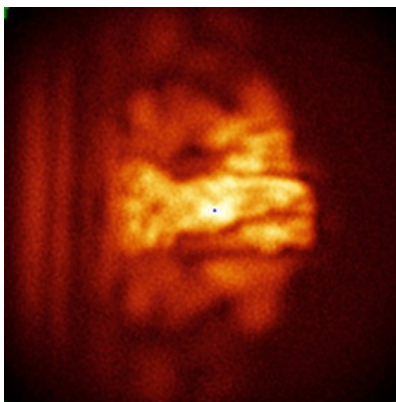


Z

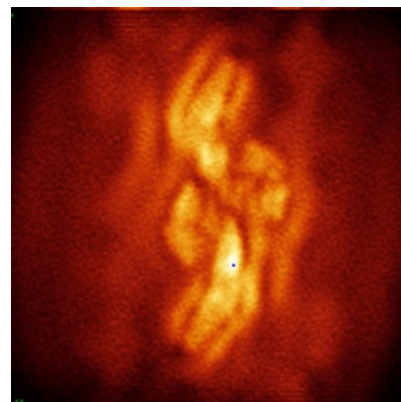
6.4.2 Raw map



X



Y

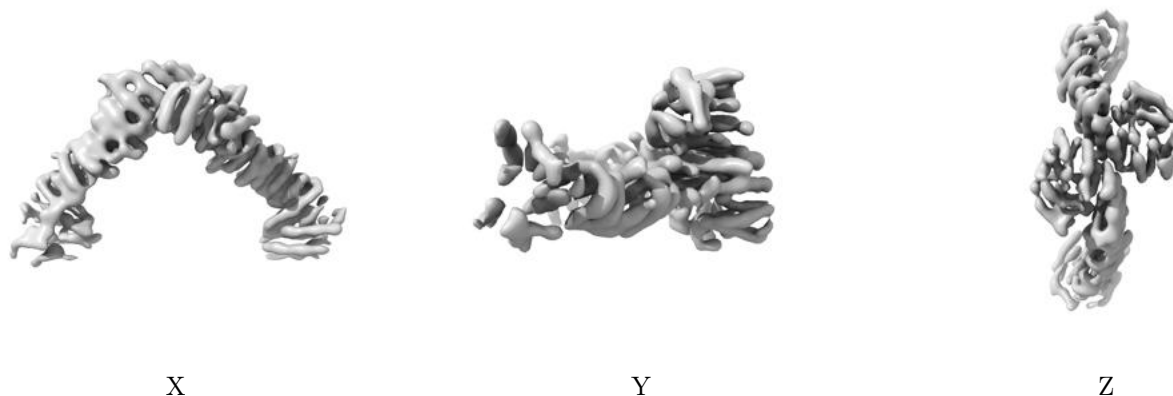


Z

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.

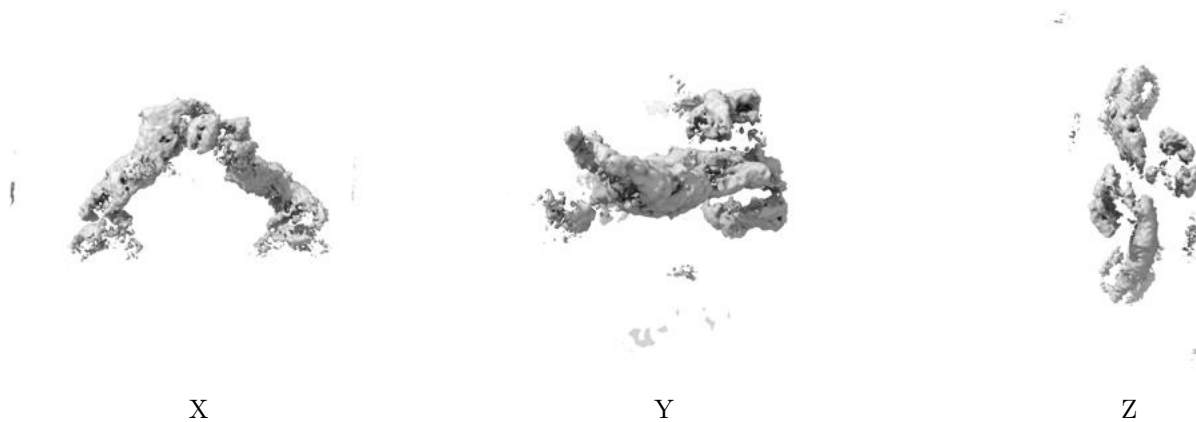
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.021. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

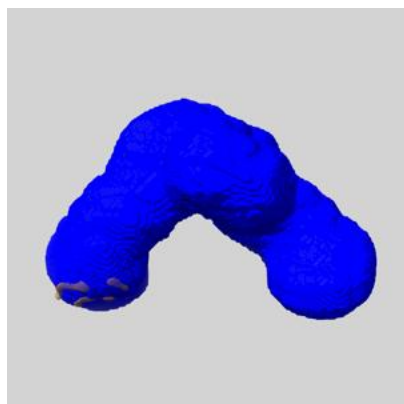
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

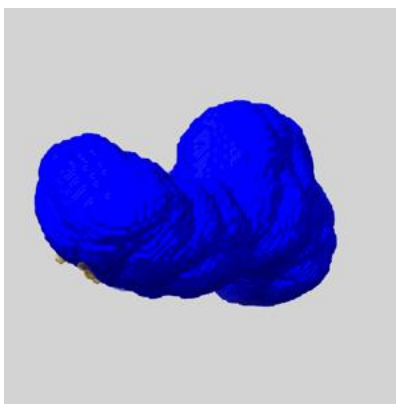
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

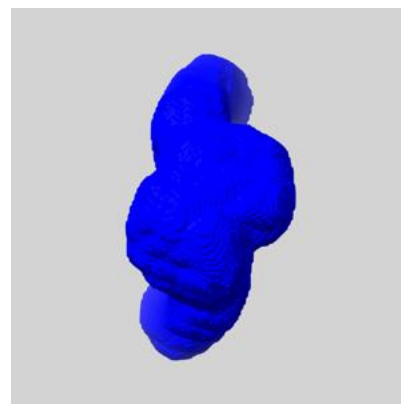
6.6.1 emd_12220_msk_1.map [i](#)



X



Y

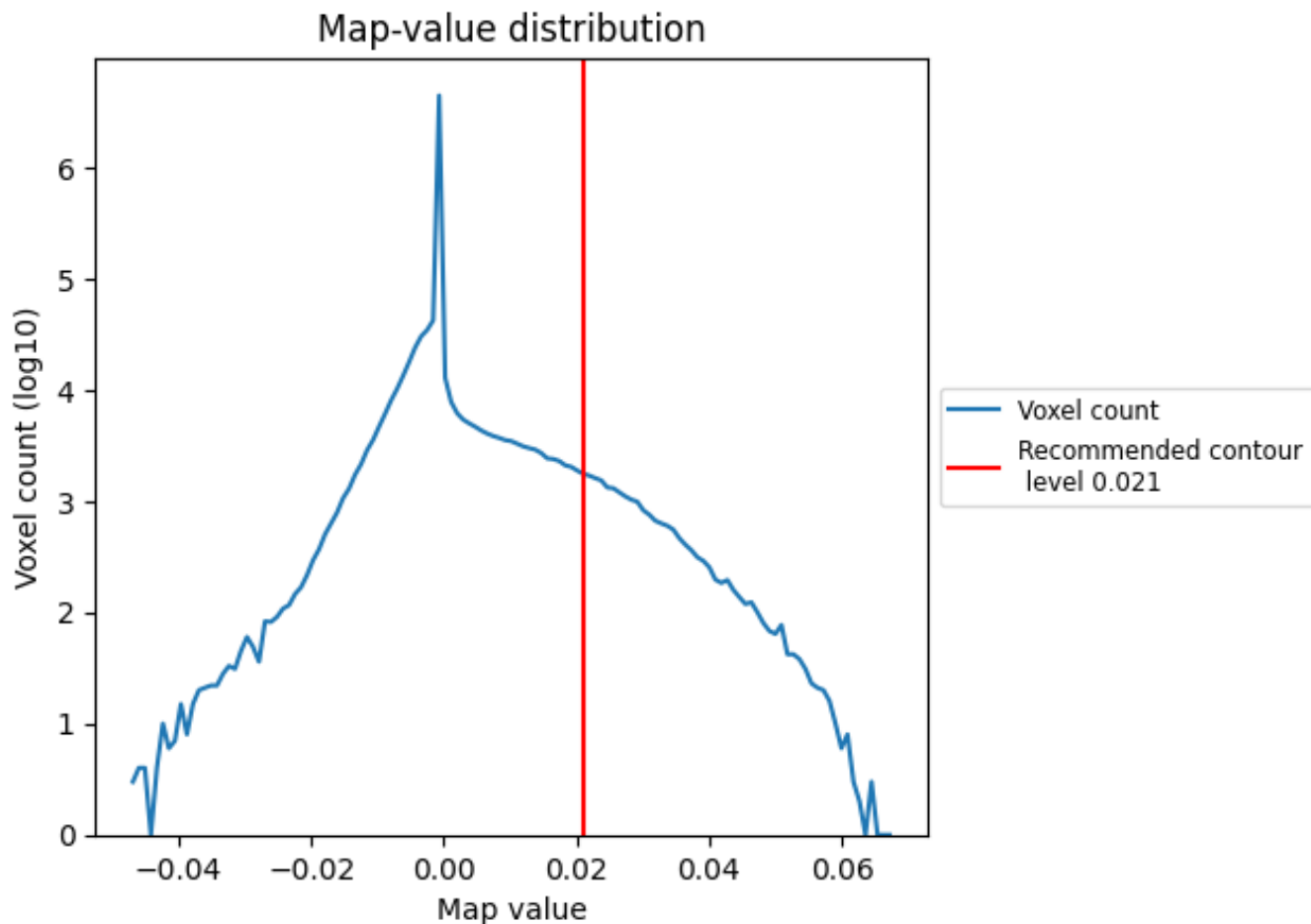


Z

7 Map analysis [i](#)

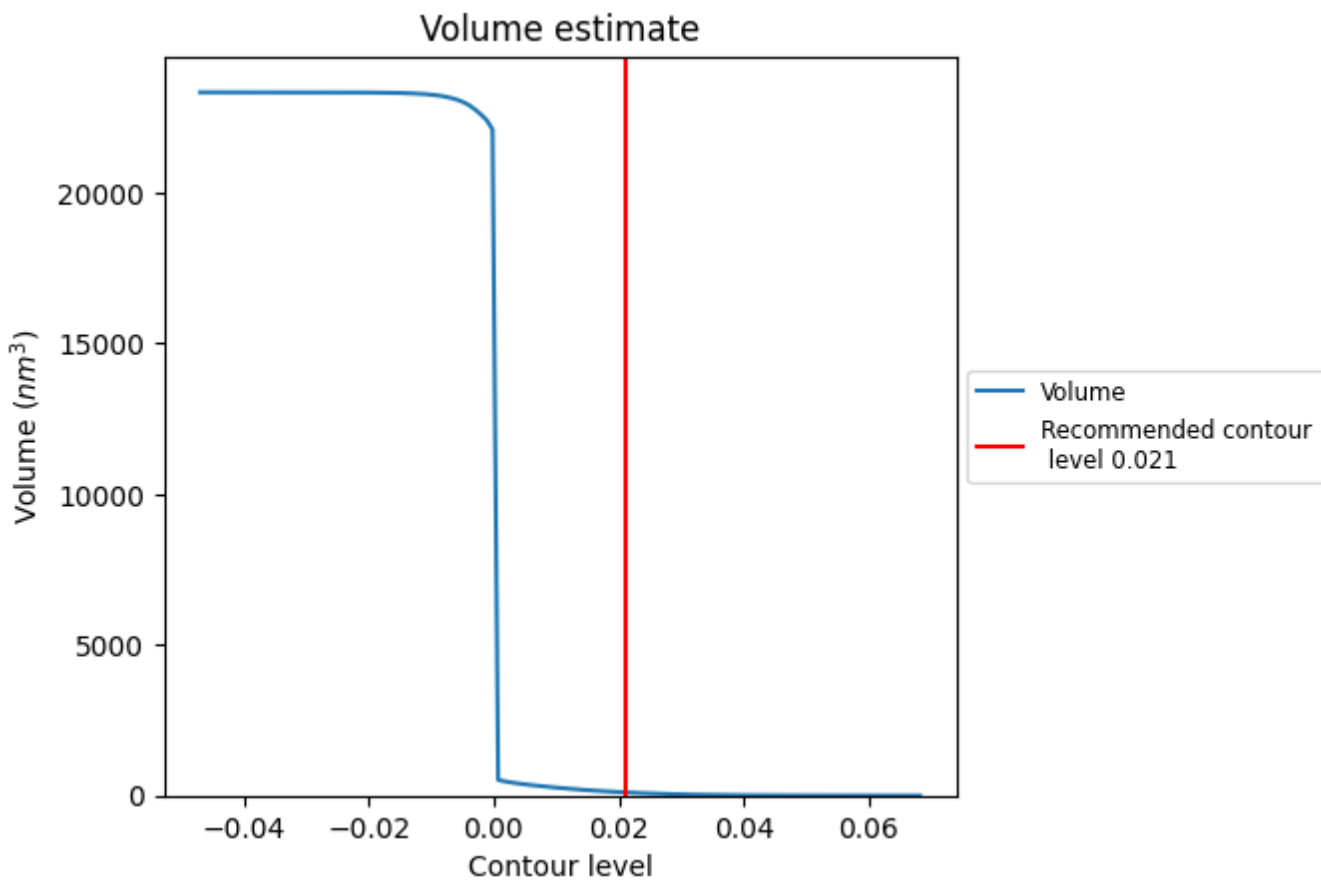
This section contains the results of statistical analysis of the map.

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.

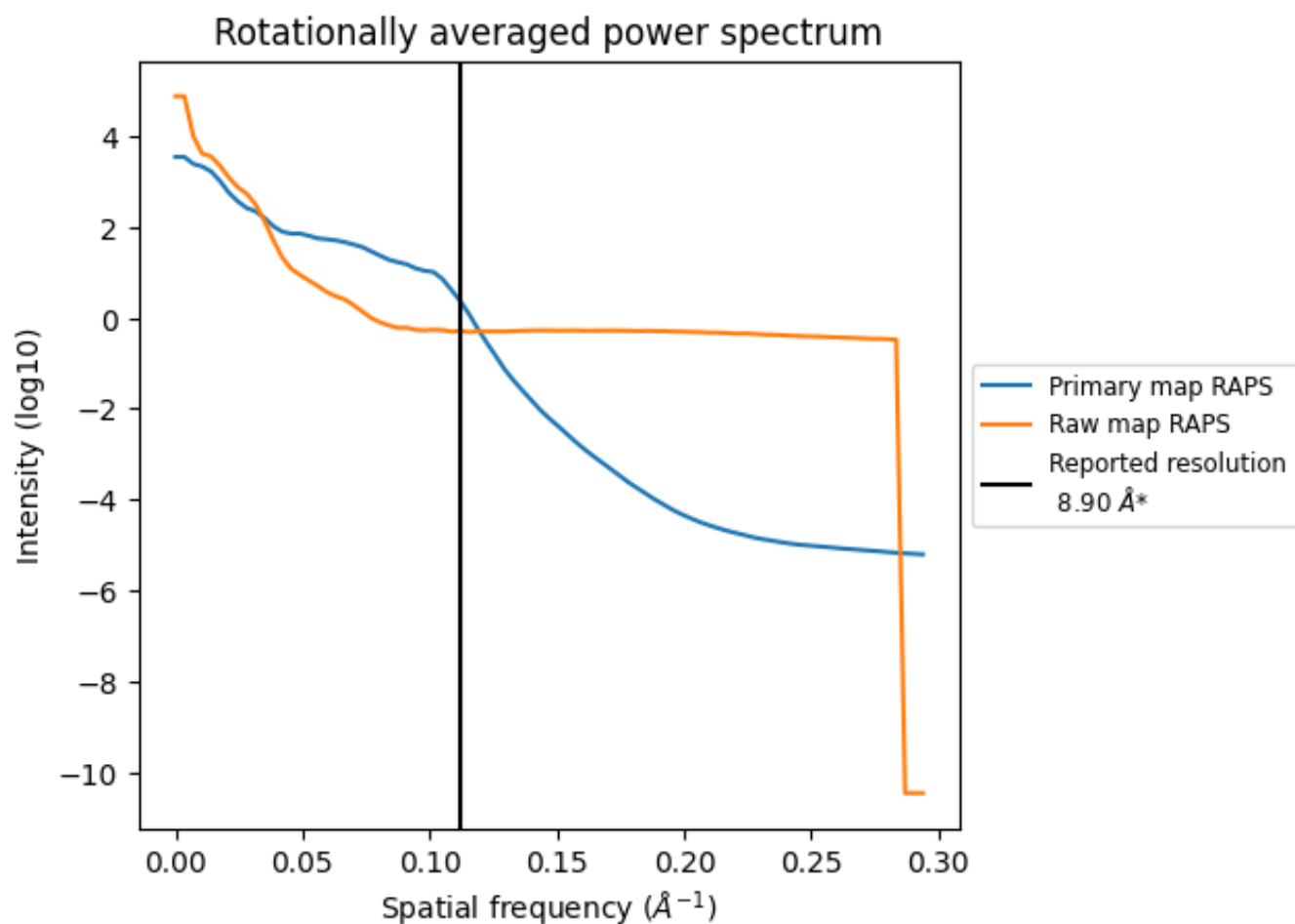
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 106 nm³; this corresponds to an approximate mass of 96 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 [\(i\)](#)

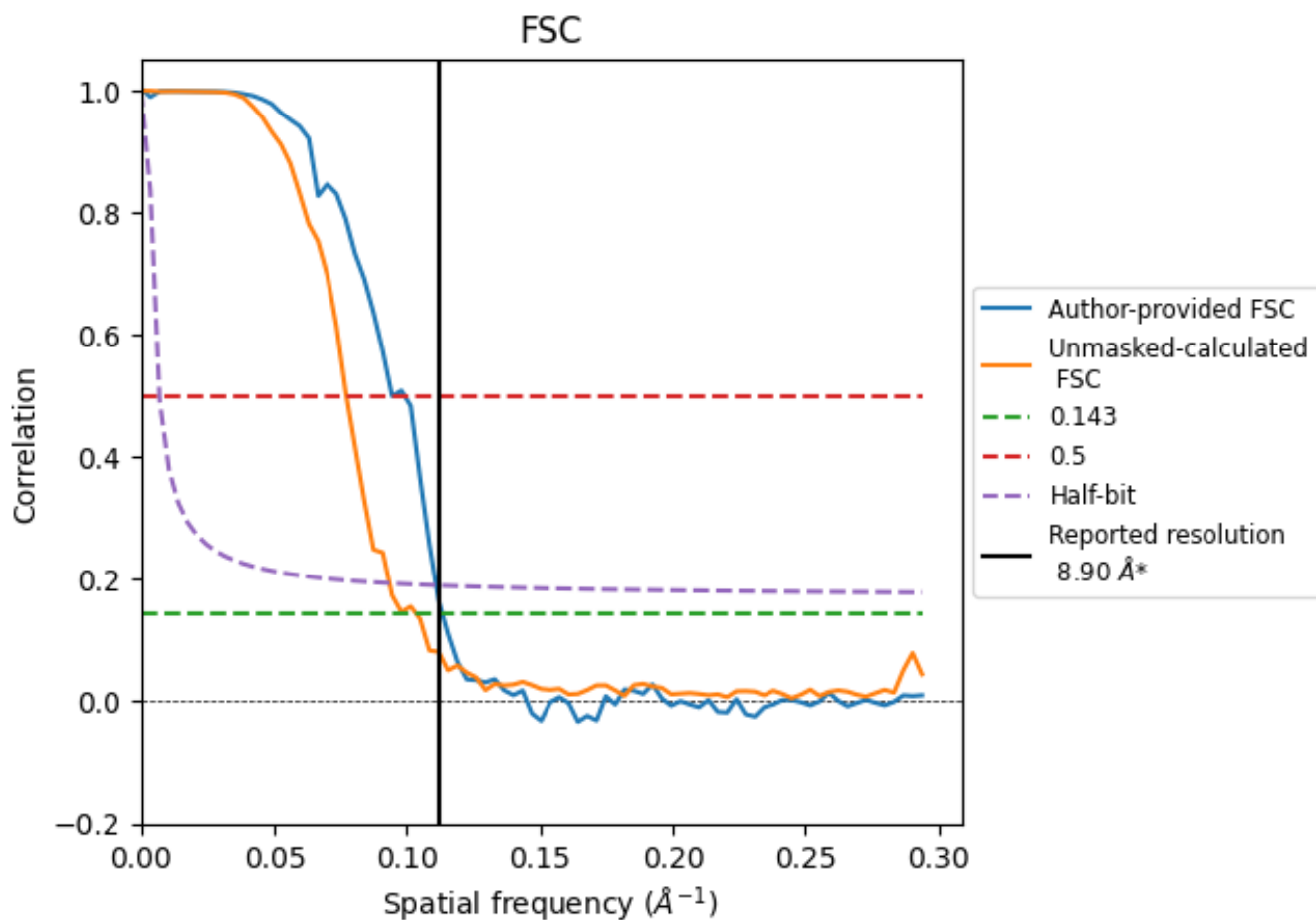


*Reported resolution corresponds to spatial frequency of 0.112 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.112 Å⁻¹

8.2 Resolution estimates [i](#)

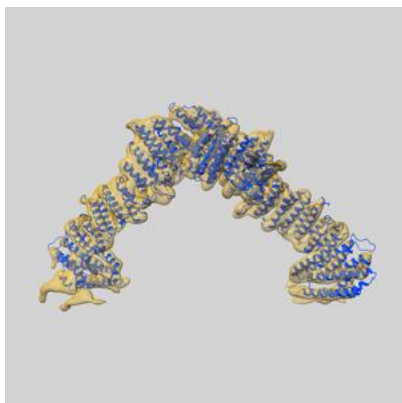
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.90	-	-
Author-provided FSC curve	8.82	10.58	9.01
Unmasked-calculated*	9.65	12.94	10.70

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

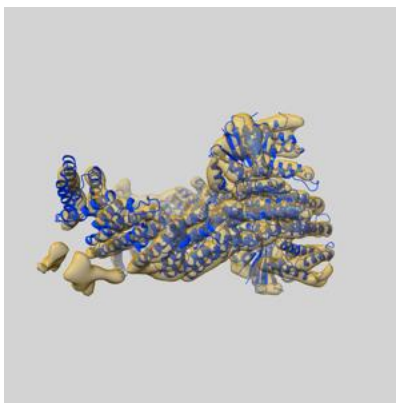
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12220 and PDB model 7BLN. Per-residue inclusion information can be found in section 3 on page 4.

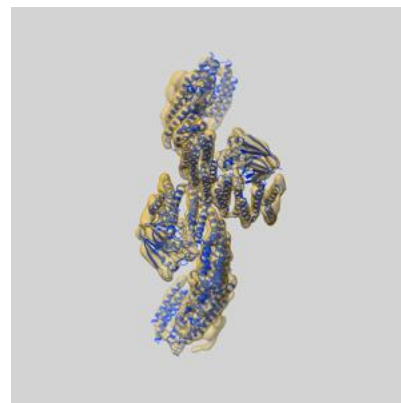
9.1 Map-model overlay [i](#)



X



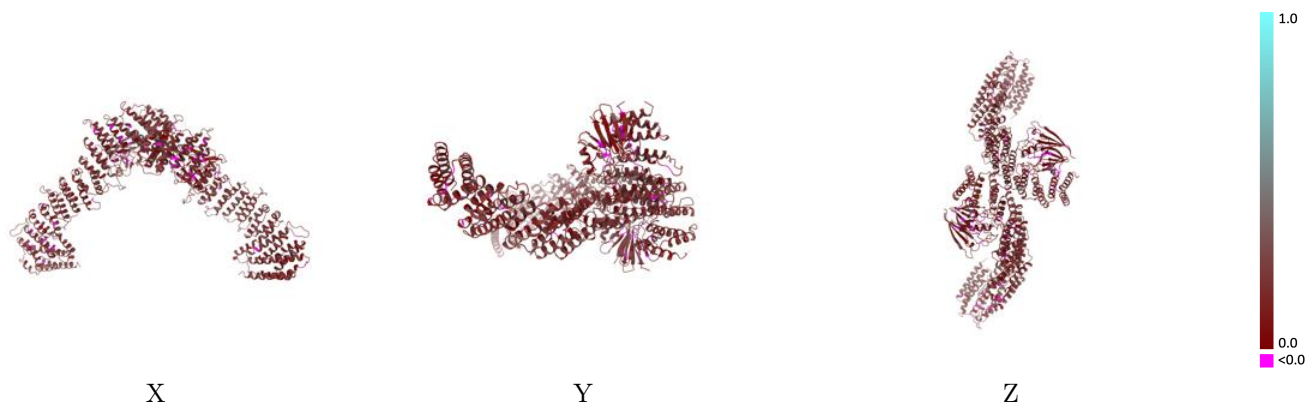
Y



Z

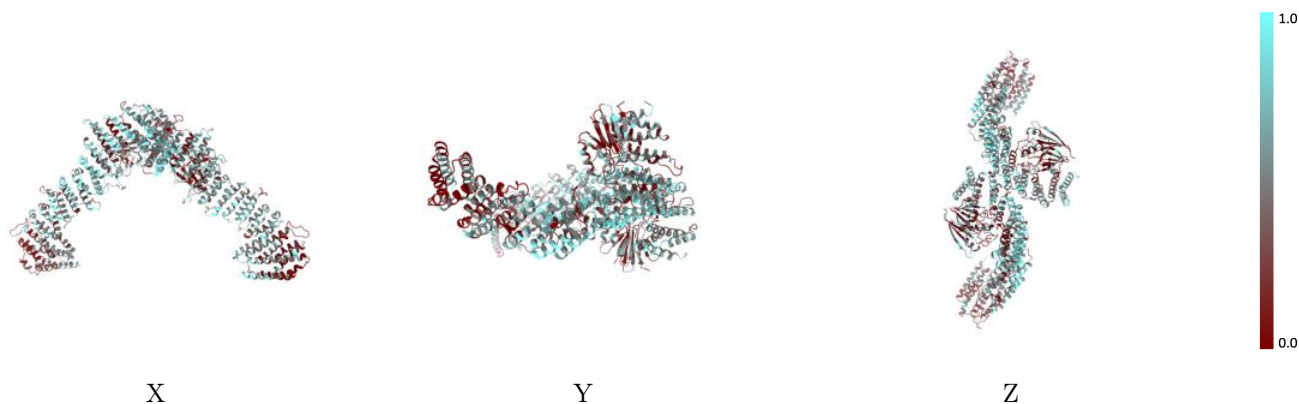
The images above show the 3D surface view of the map at the recommended contour level 0.021 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



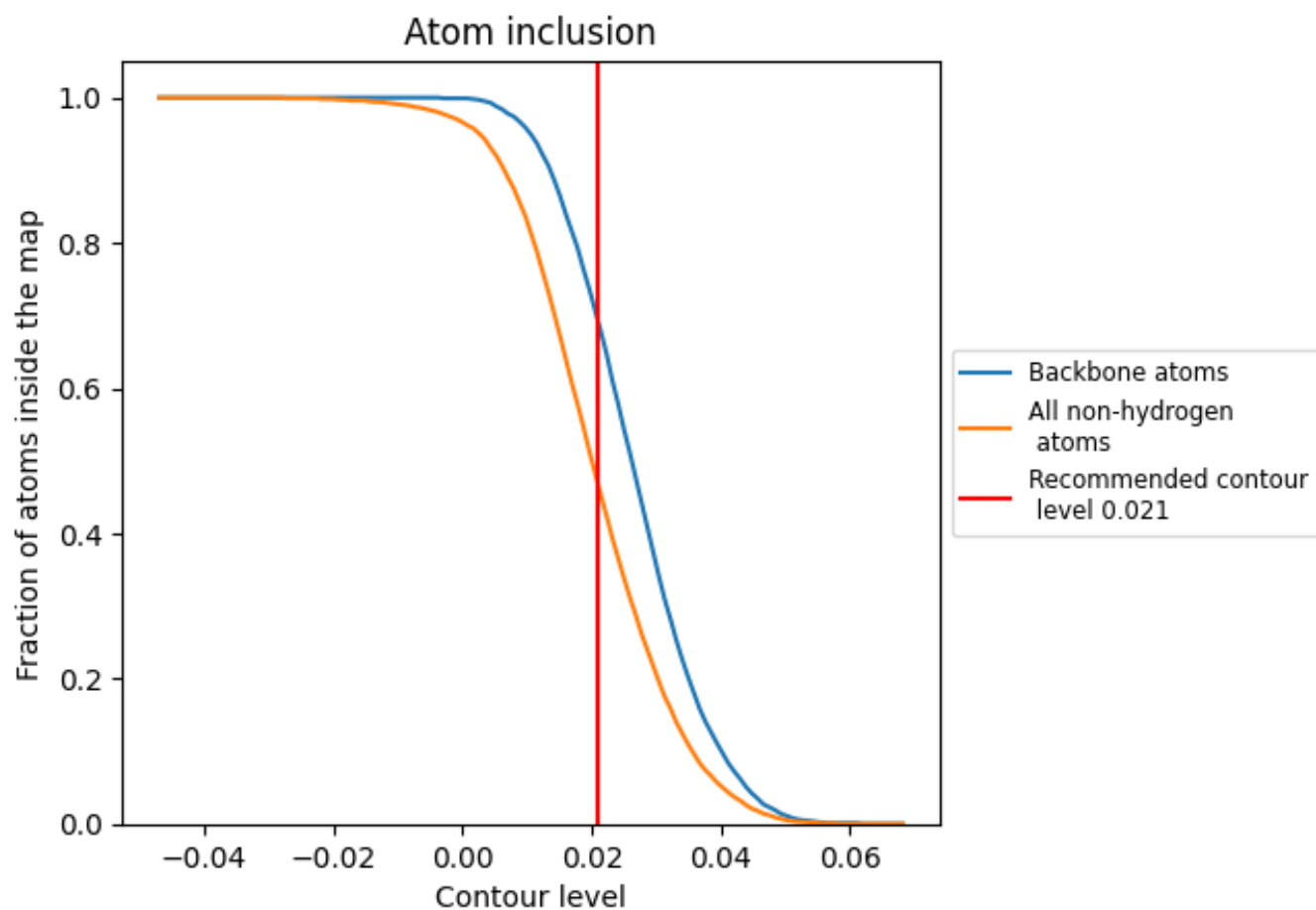
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.021).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 47% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4660	0.1800
A	0.4960	0.1890
B	0.3170	0.1270
C	0.5020	0.1910
D	0.3340	0.1380

