



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 12:36 AM UTC

PDB ID : 8A7E / pdb_00008a7e
EMDB ID : EMD-15221
Title : PAPP-A dimer in complex with its inhibitor STC2
Authors : Kobbero, S.D.; Gajhede, M.; Mirza, O.A.; Boesen, T.; Oxvig, C.
Deposited on : 2022-06-20
Resolution : 5.02 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.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

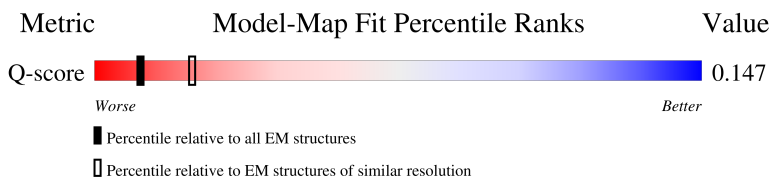
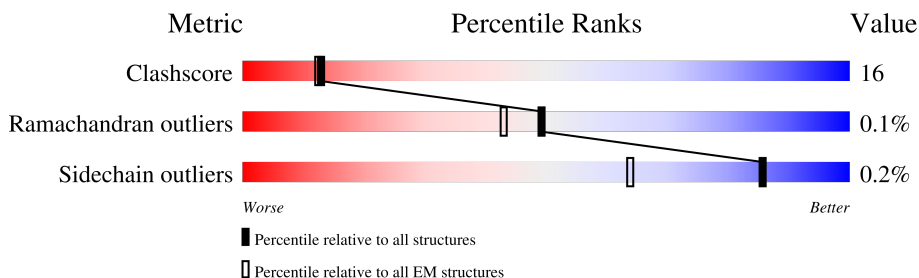
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.02 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	855 (4.52 - 5.51)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	168	67% 33%
1	P	168	58% 42%
2	C	1536	64% 35% .
2	Q	1536	65% 35% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 26442 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 Stanniocalcin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	168	Total	C	N	O	S	0	0
			1315	822	237	239	17		
1	A	168	Total	C	N	O	S	0	0
			1315	822	237	239	17		

- Molecule 2 is a protein called Pappalysin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1524	Total	C	N	O	S	0	0
			11897	7436	2062	2294	105		
2	Q	1524	Total	C	N	O	S	0	0
			11897	7436	2062	2294	105		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	563	GLN	GLU	engineered mutation	UNP Q13219
Q	563	GLN	GLU	engineered mutation	UNP Q13219

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	C	1	Total	Zn	0
			1	1	
3	Q	1	Total	Zn	0
			1	1	

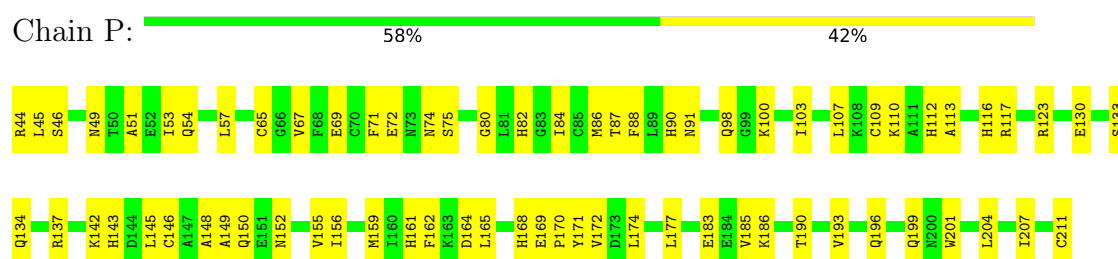
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	C	8	Total 8	Ca 8	0
4	Q	8	Total 8	Ca 8	0

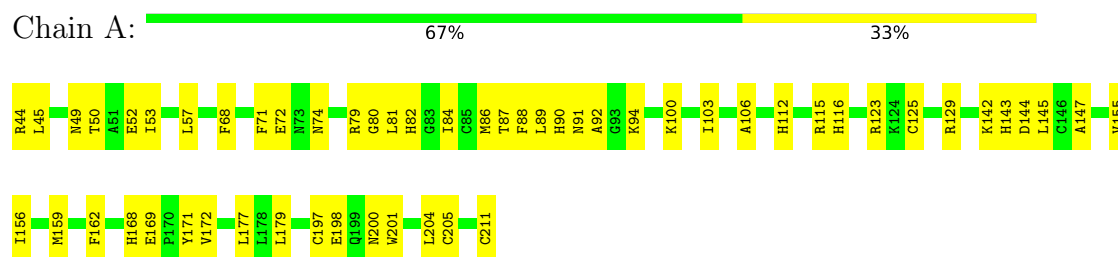
3 Residue-property plots

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.

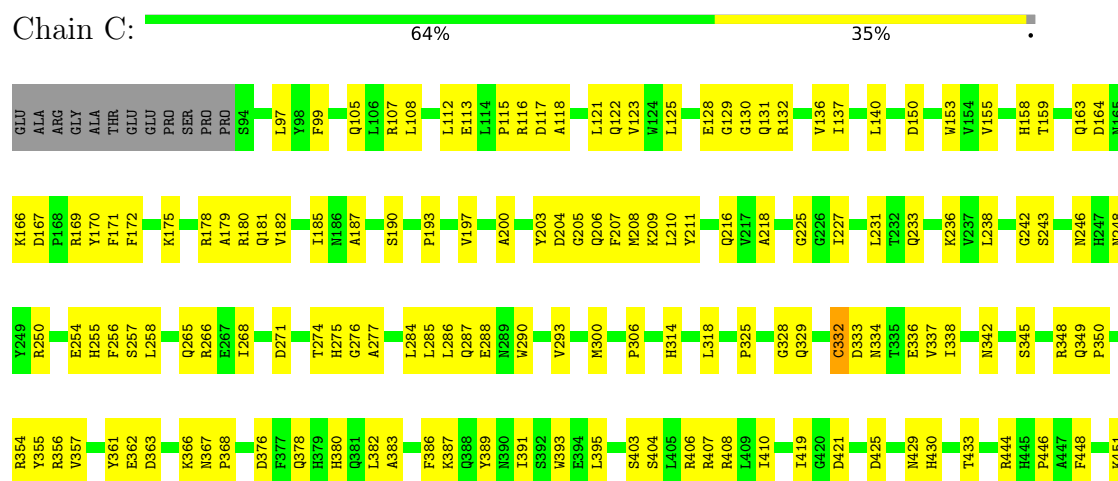
• Molecule 1: Stanniocalcin-2



• Molecule 1: Stanniocalcin-2



• Molecule 2: Pappalysin-1





G1542	D1402	T1266	P1169	Q1049	A937	D836	P762	L661	R575	C461	R354	W259
W1545	Q1406	V1267	I1173	V1050	I941	V837	N763	V662	G576	M462	Y265	K260
P1547	V1413	T1268	I1178	C1051	I941	P838	A765	Y663	R356	I577	R356	Q265
H1546	T1414	E1271	A1177	K1054	C947	L839	N767	W666	V766	F466	V357	R266
L1551	D1416	K1273	R1179	L1058	Q953	L843	T770	P663	S578	D469	Y361	L269
L1552	L1425	W1274	F1181	S1077	Q956	V850	V771	K671	E362	C473	D363	S270
C1554	F1432	K1275	D1182	Q1078	N964	K854	P772	P672	D367	N480	K366	T274
G1557	L1425	W1276	N1183	L1079	K965	V856	P773	P679	E376	T484	N367	H275
C1558	F1432	Q1277	F1184	W1085	D969	T857	C775	L682	S579	C485	P368	A277
C1559	P1186	P1187	D1185	L1086	G970	L888	V776	L682	D598	P488	D377	H278
F1561	T1187	T1188	E1186	E859	G970	D859	E777	T690	L599	N604	F377	L281
F1561	T1188	T1189	F1187	E860	F974	E860	P778	L691	P605	R493	H378	P282
F1561	S1190	L1189	S1190	H861	F974	H861	Q779	E692	N604	A494	H379	Q283
F1561	S1191	L1191	S1191	L862	F981	L862	C781	W693	P605	Y495	Q381	L284
F1561	C1192	G1192	C1192	L869	H882	L869	Y782	H609	H609	N499	L382	L285
F1561	Q1292	Q1292	Q1292	T870	H882	T870	L783	R610	S611	K502	F386	Q287
F1561	F1298	F1298	F1298	S871	I984	S871	L783	S611	S611	P615	Y389	N288
F1561	A1318	A1318	A1318	D985	E986	T872	E786	F702	P615	D620	N350	E288
F1561	G1452	G1452	G1452	E986	E986	A873	L791	E703	D620	G509	I391	N289
F1561	H1457	H1457	H1457	P987	P987	P876	V792	S708	D620	G509	Y389	W290
F1561	H1457	H1457	H1457	S888	S888	L877	P793	A709	G623	L513	D396	V293
F1561	N1464	N1464	N1464	R989	R989	L879	E794	C710	F624	N514	D396	K294
F1561	N1465	N1465	N1465	C999	C999	L879	S795	H711	H625	I515	S403	W297
F1561	H1469	H1469	H1469	E1003	E1003	K882	T797	C713	S626	F516	S403	W297
F1561	S1479	S1479	S1479	Q1004	Q1004	P883	T798	R717	F628	A518	L405	M300
F1561	E1483	E1483	E1483	K1005	K1005	Y886	W799	L718	N629	K519	R406	M300
F1561	L1484	L1484	L1484	T1006	T1006	Y886	T801	L719	T630	K535	R407	P306
F1561	N1485	N1485	N1485	S1007	S1007	R890	S804	N725	P631	E536	L409	L318
F1561	S1486	S1486	S1486	Y1014	Y1014	D891	A726	A726	N633	A537	I410	L318
F1561	N1487	N1487	N1487	T1015	T1015	P892	W807	S727	N634	L538	C414	P324
F1561	L1488	L1488	L1488	P1016	P1016	P893	D808	S728	P635	M539	D415	P325
F1561	K1489	K1489	K1489	Q1017	Q1017	L894	S809	P729	M636	H540	P729	L326
F1561	L1507	L1507	L1507	G1018	G1018	V898	S809	M730	D641	L541	K418	G327
F1561	I1514	I1514	I1514	F1019	F1019	A899	A812	W738	D642	G542	I419	G328
F1561	I1515	I1515	I1515	D1020	D1020	S900	V813	S739	C643	G543	I419	G328
F1561	P1517	P1517	P1517	Q1022	Q1022	H903	N814	P740	C643	H588	D425	C332
F1561	M1518	M1518	M1518	W1023	W1023	P903	D815	S739	T644	T559	N334	D333
F1561	T1521	T1521	T1521	A1024	A1024	K907	I816	E744	D645	T559	N334	D333
F1561	D1524	D1524	D1524	S1025	S1025	N1026	K817	G745	S646	M560	C428	T335
F1561	I1525	I1525	I1525	N1026	N1026	L913	L818	H746	F647	I561	N429	E336
F1561	L1529	L1529	L1529	S1030	S1030	V918	V819	P747	Q651	H562	H430	V337
F1561	R1533	R1533	R1533	S1037	S1037	Y921	N825	Q751	V652	I564	T433	I338
F1561	V1534	V1534	V1534	V1040	V1040	W922	I826	P752	A653	G565	R444	N342
F1561	V1537	V1537	V1537	G1043	G1043	E930	S827	C753	M655	S567	H445	S345
F1561	V1537	V1537	V1537	Q1044	Q1044	S932	L828	K754	H656	L568	P446	P348
F1561	V1537	V1537	V1537	F1166	F1166	S932	N832	S755	C657	G569	A447	Q349
F1561	V1537	V1537	V1537	F1166	F1166	S932	N832	S755	F658	L570	F448	Q349
F1561	V1537	V1537	V1537	F1166	F1166	S932	N832	S755	F658	L570	F448	P350
F1561	V1537	V1537	V1537	F1166	F1166	S932	N832	S755	F658	L570	F448	K351

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	3	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58, 59	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k), GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	25.960	Depositor
Minimum map value	-13.178	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.939	Depositor
Recommended contour level	1.7	Depositor
Map size (Å)	303.59998, 303.59998, 303.59998	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1859374, 1.1859374, 1.1859374	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.13	0/1337	0.32	0/1799
1	P	0.15	0/1337	0.36	0/1799
2	C	0.10	0/12217	0.31	0/16633
2	Q	0.10	0/12217	0.31	0/16633
All	All	0.11	0/27108	0.32	0/36864

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1315	0	1290	39	0
1	P	1315	0	1290	52	0
2	C	11897	0	11211	389	0
2	Q	11897	0	11213	398	0
3	C	1	0	0	0	0
3	Q	1	0	0	0	0
4	C	8	0	0	0	0
4	Q	8	0	0	0	0
All	All	26442	0	25004	847	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 16.

The worst 5 of 847 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:Q:984:ILE:O	2:Q:988:SER:HA	1.69	0.90
1:A:88:PHE:HB3	1:A:103:ILE:HD11	1.54	0.87
2:Q:332:CYS:CB	2:Q:657:CYS:SG	2.64	0.86
2:C:562:HIS:CD2	2:C:566:HIS:NE2	2.45	0.83
2:C:488:PRO:HA	2:C:493:ARG:HD3	1.62	0.81

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	A	166/168 (99%)	162 (98%)	4 (2%)	0	100	100
1	P	166/168 (99%)	163 (98%)	3 (2%)	0	100	100
2	C	1522/1536 (99%)	1422 (93%)	98 (6%)	2 (0%)	48	83
2	Q	1522/1536 (99%)	1427 (94%)	93 (6%)	2 (0%)	48	83
All	All	3376/3408 (99%)	3174 (94%)	198 (6%)	4 (0%)	49	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	1413	VAL
2	Q	1413	VAL
2	C	419	ILE
2	Q	419	ILE

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	A	146/146 (100%)	146 (100%)	0	100	100
1	P	146/146 (100%)	146 (100%)	0	100	100
2	C	1338/1347 (99%)	1336 (100%)	2 (0%)	88	88
2	Q	1338/1347 (99%)	1334 (100%)	4 (0%)	86	84
All	All	2968/2986 (99%)	2962 (100%)	6 (0%)	85	86

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Q	428	CYS
2	Q	587	CYS
2	Q	657	CYS
2	C	657	CYS
2	C	332	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
2	Q	255	HIS
2	Q	1292	GLN
2	Q	650	ASN
2	Q	1064	GLN
2	Q	1354	ASN

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](#)

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

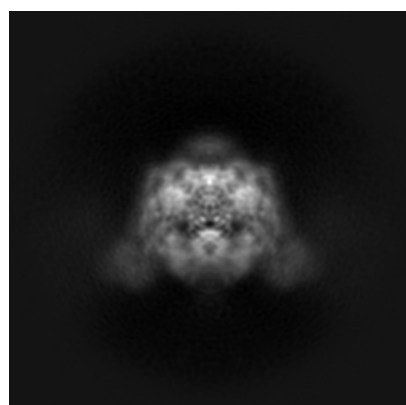
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15221. These allow visual inspection of the internal detail of the map and identification of artifacts.

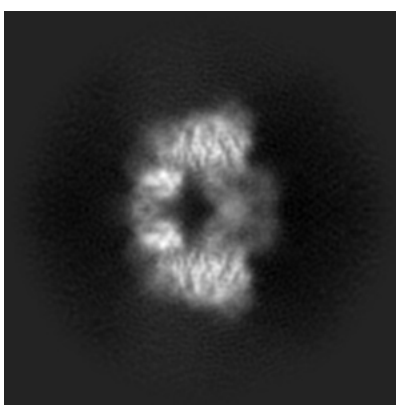
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

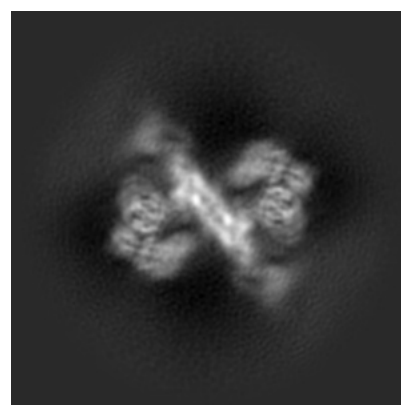
6.1.1 Primary map



X



Y

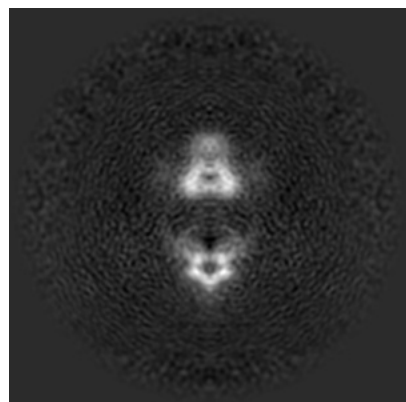


Z

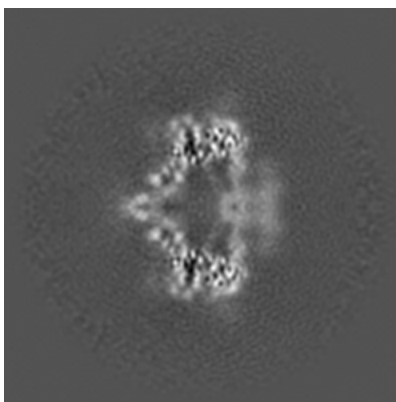
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

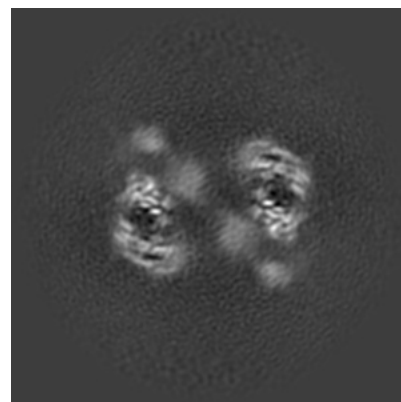
6.2.1 Primary map



X Index: 128



Y Index: 128

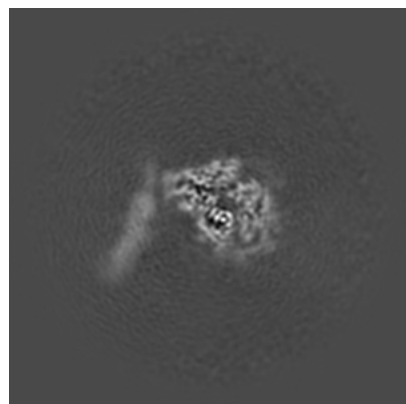


Z Index: 128

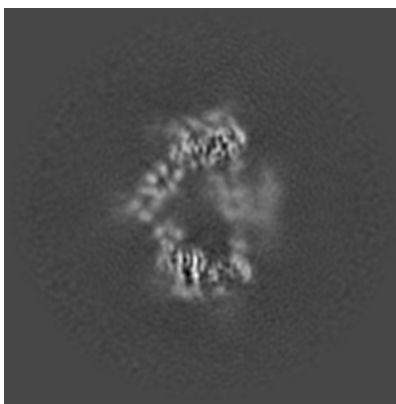
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

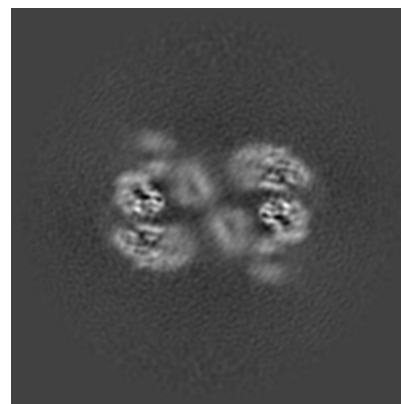
6.3.1 Primary map



X Index: 168



Y Index: 124

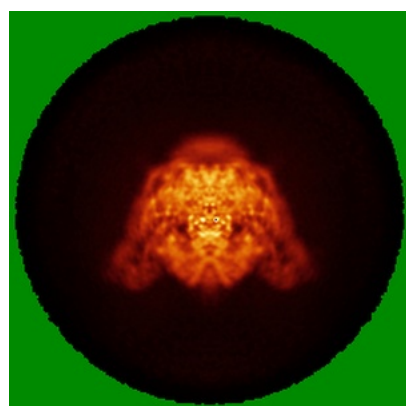


Z Index: 136

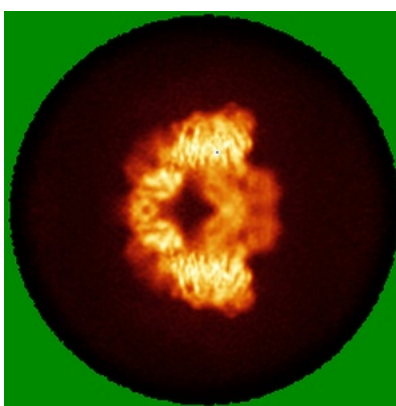
The images above show the largest variance slices of the map in three orthogonal directions.

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

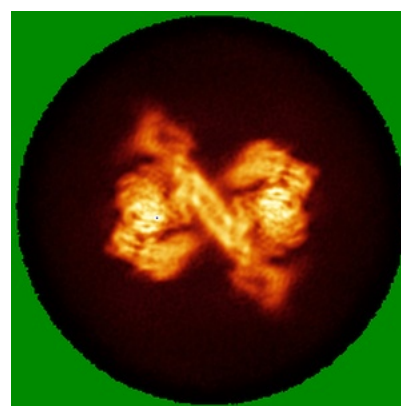
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

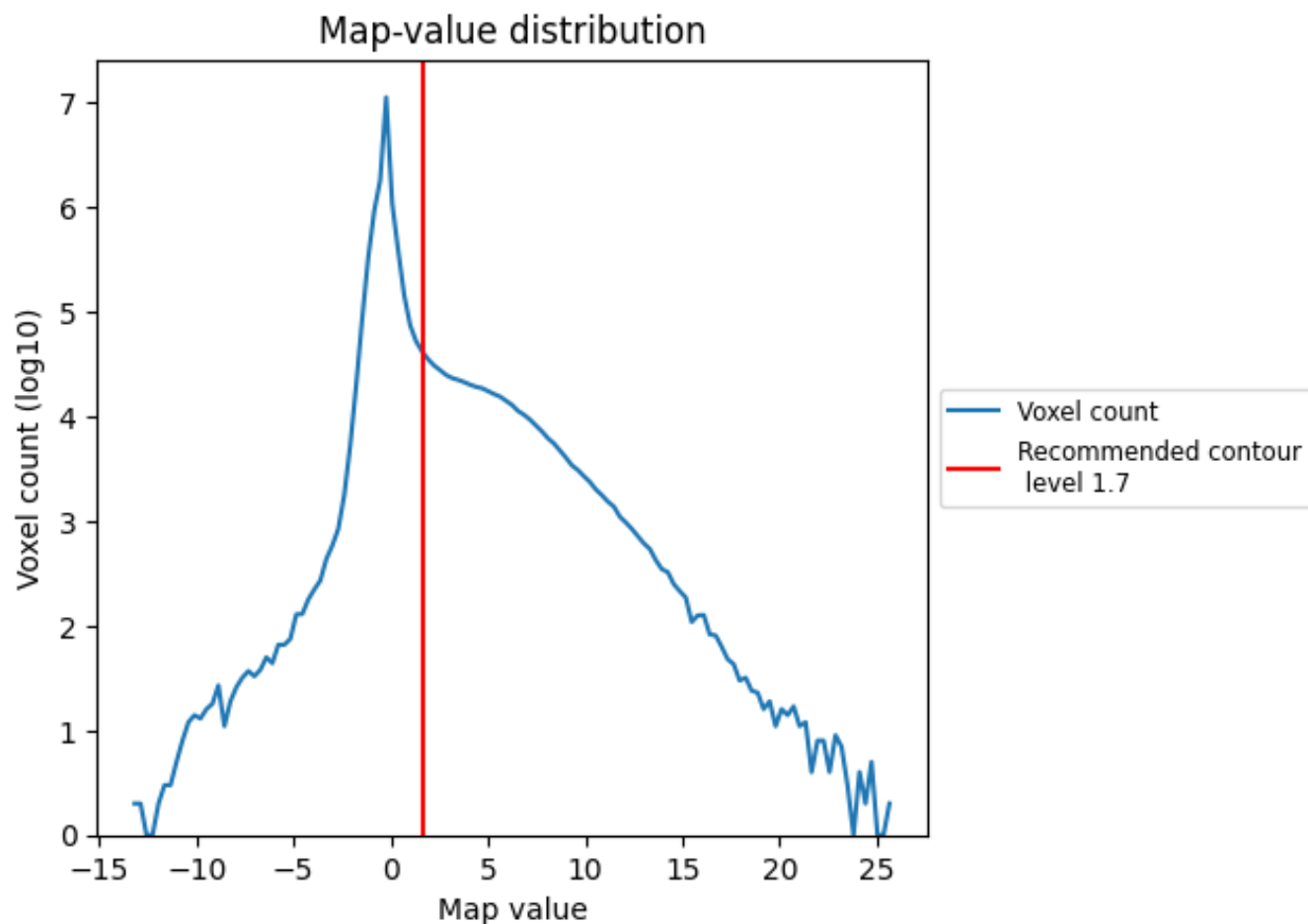
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

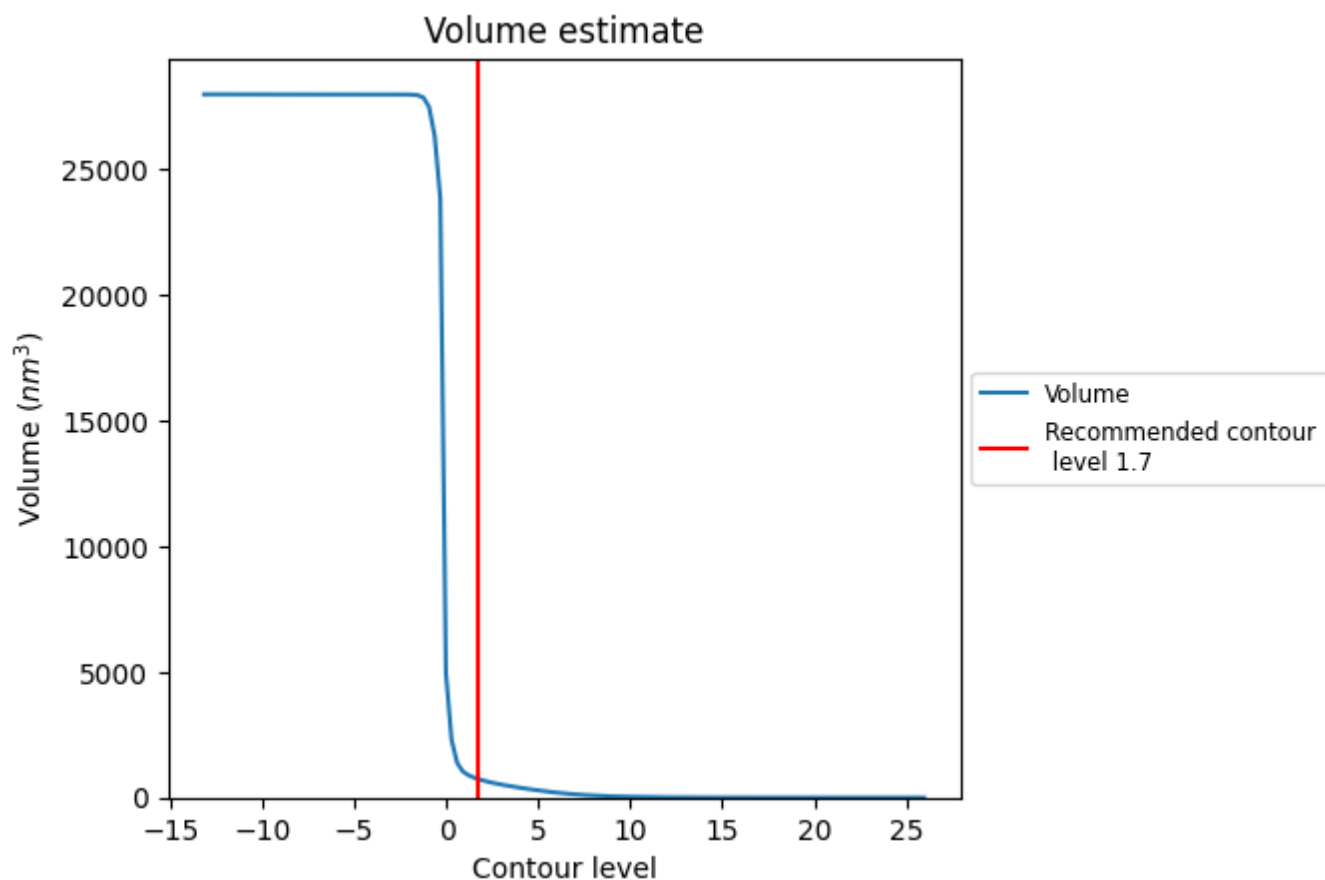
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

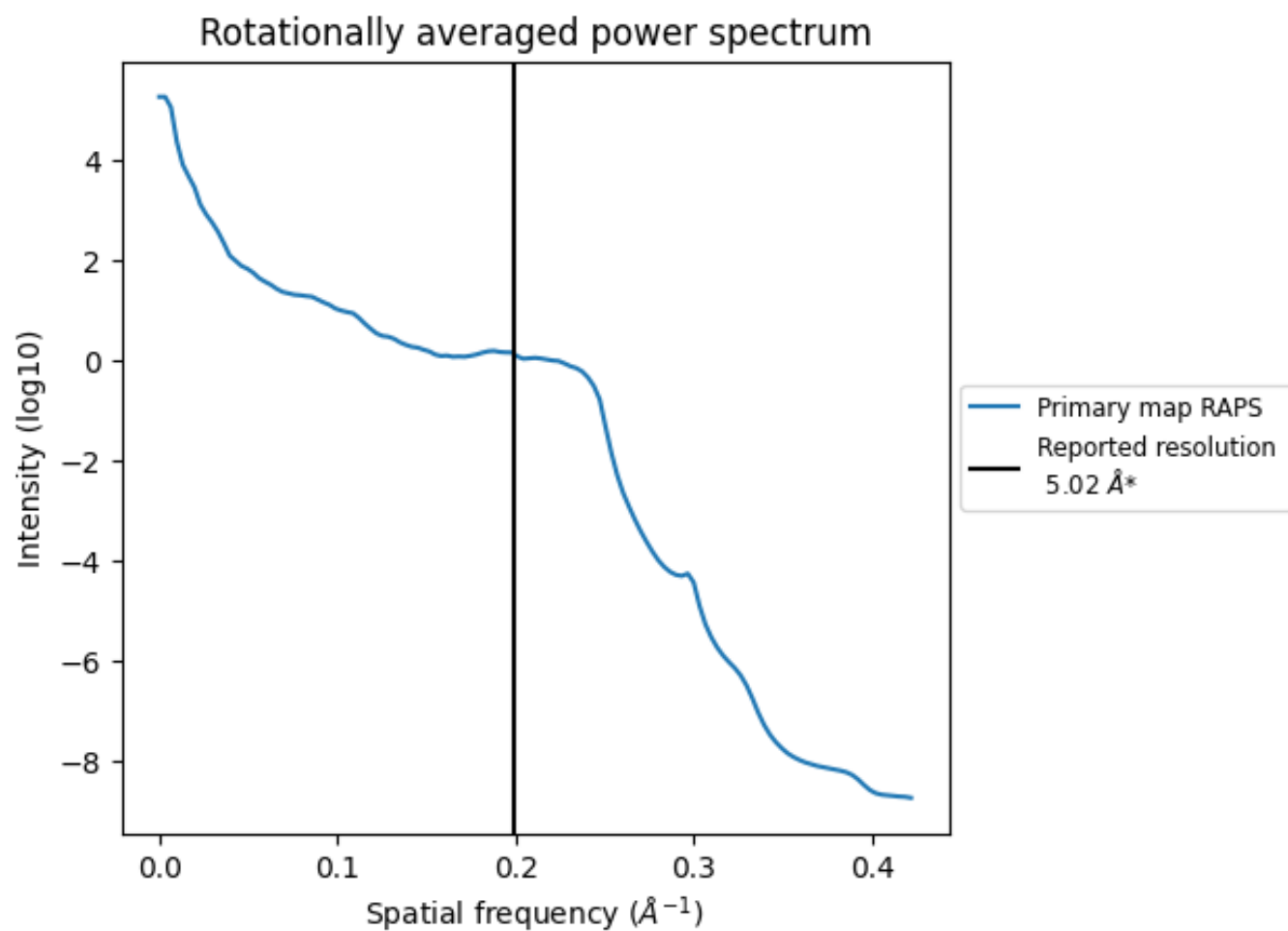
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 743 nm³; this corresponds to an approximate mass of 671 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 0.199 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

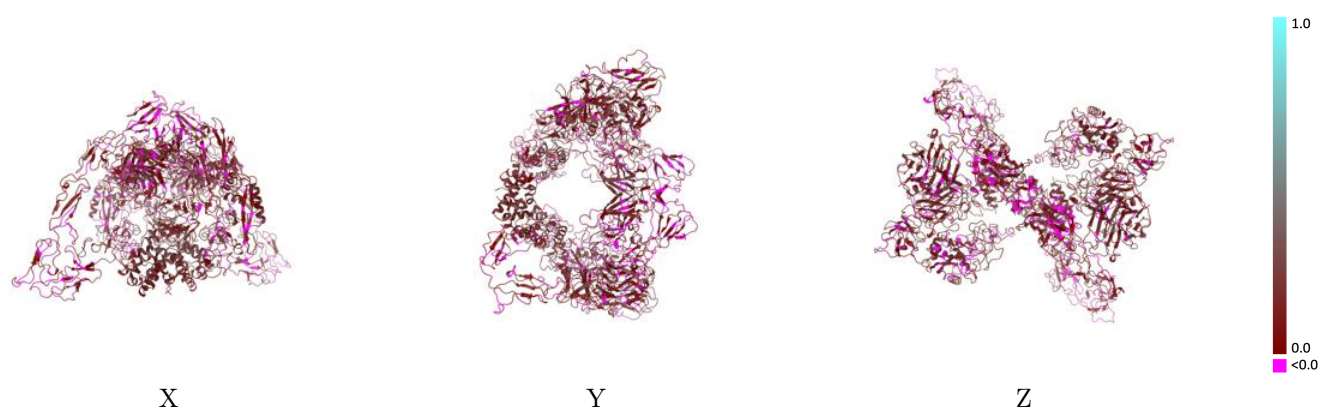
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-15221 and PDB model 8A7E. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

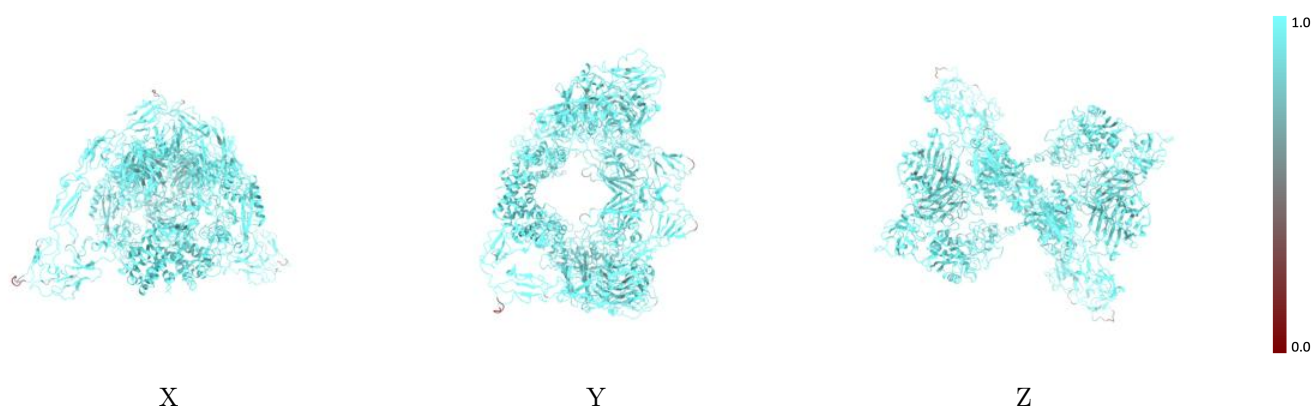
This section was not generated.

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



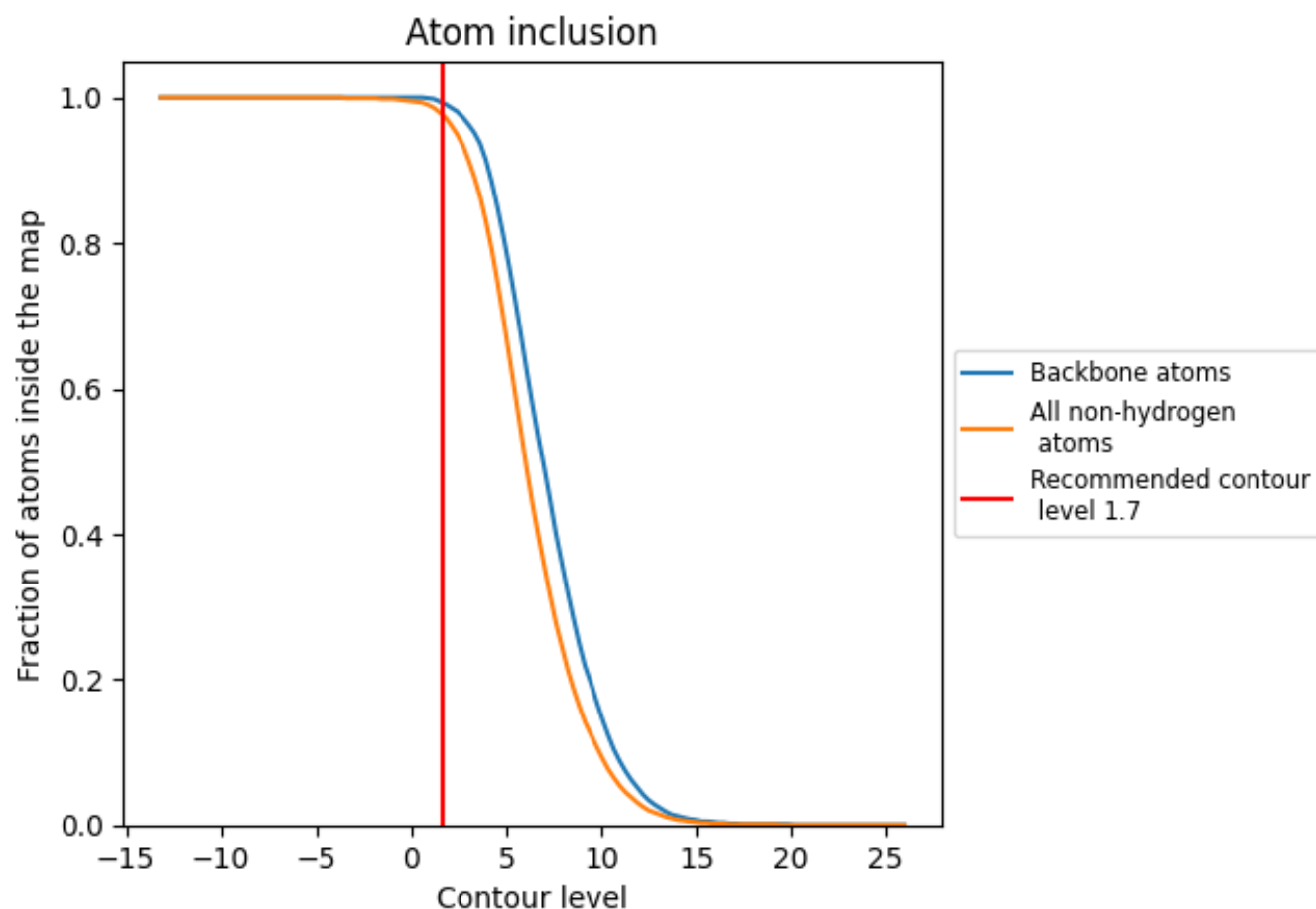
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (1.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9750	<div></div> 0.1470
A	<div></div> 0.9930	<div></div> 0.2210
C	<div></div> 0.9710	<div></div> 0.1300
P	<div></div> 0.9960	<div></div> 0.2160
Q	<div></div> 0.9760	<div></div> 0.1480

