



## wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 07:40 pm BST

PDB ID : 8A7E  
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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

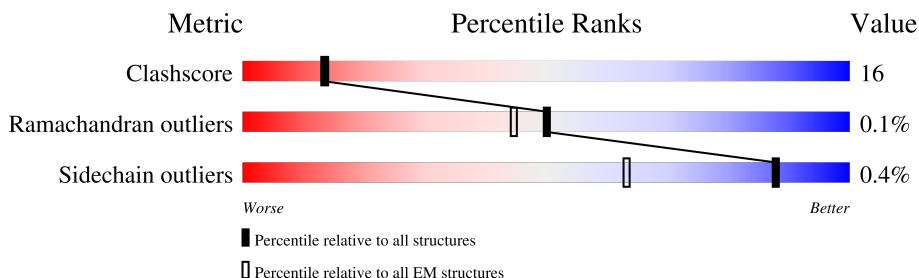
# 1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	70% 30%
1	P	168	57% 43%
2	C	1536	64% 35% .
2	Q	1536	65% 33% .

## 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 (three-letter code: 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	

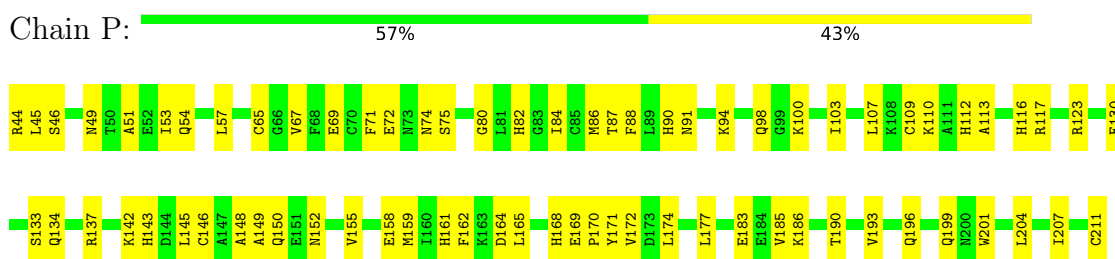
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

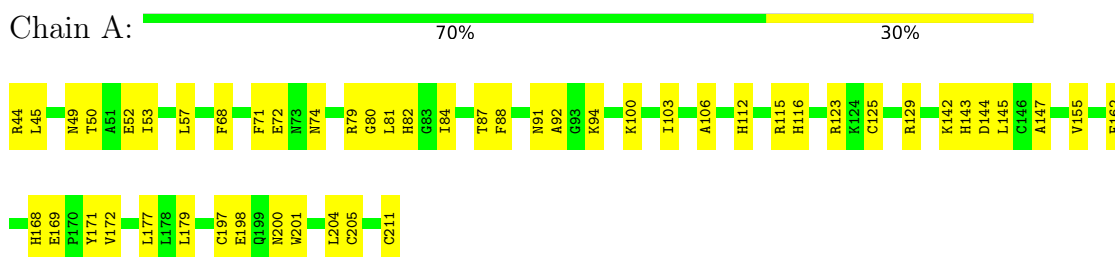
### 3 Residue-property plots

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.

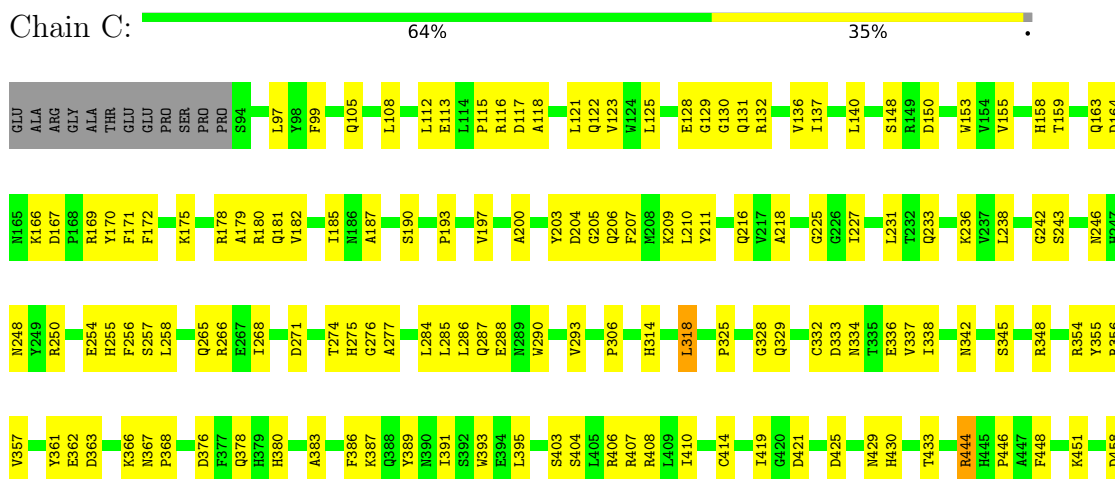
#### • Molecule 1: Stanniocalcin-2

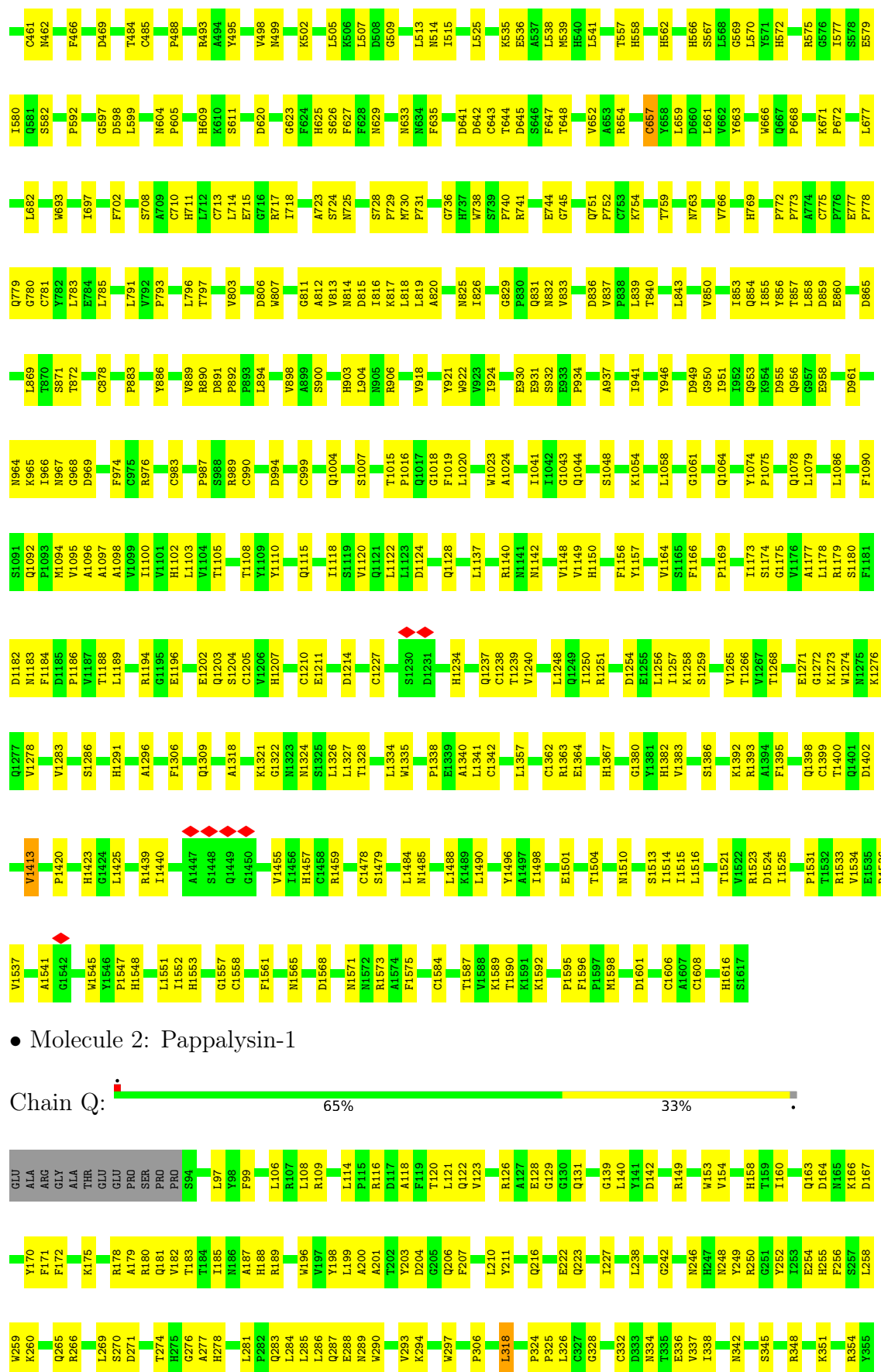


#### • Molecule 1: Stanniocalcin-2



#### • Molecule 2: Pappalysin-1





• Molecule 2: Pappalysin-1

Chain Q: 65% 33%

C1558	R1439	Q1277	F1184	W1085	K965	Y856	A774	P672	C587	C473	R356
E1559	T1440	C1285	D1185	L1086	D969	D859	C775	P679	P592	N480	V357
F1561	D1446	P1288	V1187	Y1089	G970	E860	F776	L682	G597	T464	Y361
M1571	A1447	D1289	T1188	F1090	F974	H861	P778	L682	D598	C485	E362
M1572	S1448	S1190	L1189	Y1096	F981	L869	C780	T690	L599	K366	D363
R1573	Q1449	C1192	S1191	A1096	R982	T870	C781	L691	M604	P488	K367
F1575	G1450	F1298	C983	A1097	C983	T871	L783	W693	P605	P368	N367
	L1451		I984	A1097	I984	T872	L783			R493	D376
	G1452	A1318	D985	I1100	D985	A873	E786	I697	H609	Y495	F377
			E986		E986				K610		Q378
	H1457	T1328	F987	L1103	F987	P876	L791	F702	S611		H379
	V1464	C1329	S988	Y1104	S988	L877	V792	E703		N499	H380
	N1465	Q1203	R989	T1105	R989	L879	C878		P615		F356
		S1204	C999	Y1108	C999		E794	S708	D620		
	H1469	W1335	T1108	Y1109	T1108		S795	A709		G509	Y389
	S1479	S1336	Y1110	Y1110	Y1110		L796	C710		L513	N390
		L1341	Q1115	Q1115	Q1004		T797	H711		N514	I391
	E1483	C1342	Q1118	Q1118	T1006		W800	C713		I515	
	L1484	E1211	L1122	L1122	S1007		T801			F516	D396
	N1485	K1212	L1123	L1123	Y1014		S804	L719		F628	
	S1486	D1214	L1223	L1223	T1015		W807			N629	S403
	N1487	A1223	D1124	D1124	P1016		L894	N725		T630	S404
	L1488	C1227	Q1128	Q1128	Q1017		W808	A726		K535	L405
	K1489		L1132	L1132	G1018		S809	S727		E536	R406
			L1137	L1137	F1019		A899	S728		L538	
	L1507	S1230	L1230	L1230	L1020		S900	P729		M539	I410
	I1514	H1234	L1234	L1234	L1021		H903	W738		H540	
	I1515	Q1237	R1140	R1140	W1023		D815	S739		L541	C414
	L1516	C1238	N1141	N1141	A1024		I816	C643		G542	D415
	T1521	T1239	N1142	N1142	S1025		K817	P740		G543	
	D1524	R1387	D1151	D1151	N1026		L818	E744		H558	K418
	I1525	R1388	L1152	L1152	S1030		L819	G745		T559	I419
			L1157	L1157	P1037		A820	H746		M560	D425
	L1529	R1243	Y1157	Y1157	P1037		N825	P747		I561	
	R1533	R1251	H1158	H1158	V1040		I826	Q751		H562	N429
	V1534	R1252	V1162	V1162	V1040		S827	P752		Q563	H430
	E1535	D1254	F1166	F1166	Q1044		L828	C753		I564	T433
	R1536	E1255	P1169	P1169	S1048		N832	K754		G655	
	V1537	L1256	K1258	K1258	Q1044		W833	S755		H566	R444
		T1257			S1049		D836	W760		S567	H445
	G1542	K1266	T1266	T1266	Q1049		W837	S761		L568	P446
		V1267	V1267	V1267	Y1080		L839	P762		L659	A447
	V1545	T1414	T1268	T1268	C1051		L843	N763		D660	F448
	P1547	D1415	A1177	A1177	K1054		Q953	V766		L661	D458
	H1548	D1415	R1178	R1178	L1058		Z954	N767		R575	
		L1425	S1180	S1180	L1058		D955			G576	C461
	L1551	G1272	F1181	F1181	S1077		Q956	T770		I577	N462
	L1552	K1273	W1182	W1182	Q1078			V771		S578	
	H553	N1274	N1182	N1182	S1077			P772		E579	F466
	C1554	K1276	N1183	N1183	L1079			P773		P586	D469
	G1557										

## 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: ZN, CA

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	0/1337	0.48	0/1799
1	P	0.28	0/1337	0.51	0/1799
2	C	0.25	0/12217	0.49	1/16633 (0.0%)
2	Q	0.25	0/12217	0.48	1/16633 (0.0%)
All	All	0.25	0/27108	0.49	2/36864 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	318	LEU	CA-CB-CG	6.00	129.09	115.30
2	C	318	LEU	CA-CB-CG	5.16	127.17	115.30

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	A	1315	0	1290	34	0
1	P	1315	0	1290	52	0
2	C	11897	0	11211	373	0
2	Q	11897	0	11213	381	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	810	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 810 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%)	50	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 ⓘ

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%)	1334 (100%)	4 (0%)	91	92
2	Q	1338/1347 (99%)	1331 (100%)	7 (0%)	86	89
All	All	2968/2986 (99%)	2957 (100%)	11 (0%)	88	91

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Q	657	CYS
2	Q	882	LYS
2	Q	1536	ARG
2	Q	1439	ARG
2	Q	414	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	Q	656	HIS
2	Q	1049	GLN
2	Q	1183	ASN
2	Q	1022	GLN
2	C	1004	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](#)

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.

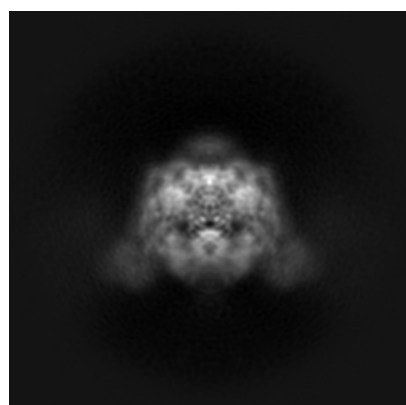
## 6 Map visualisation [i](#)

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.

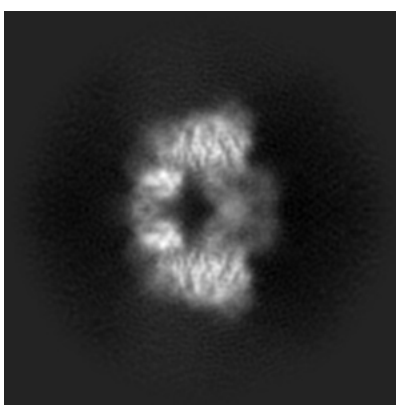
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

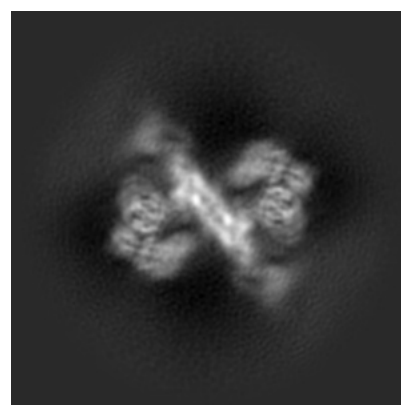
#### 6.1.1 Primary map



X



Y

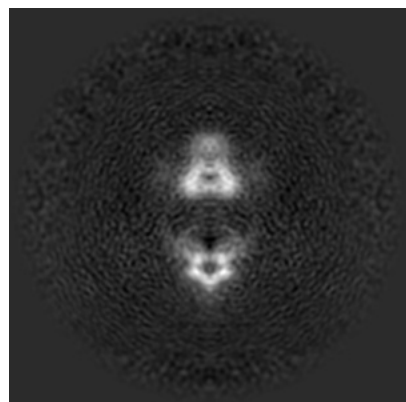


Z

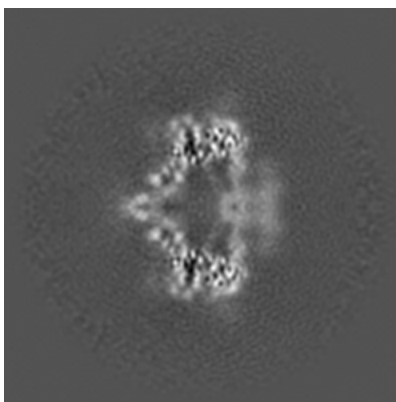
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

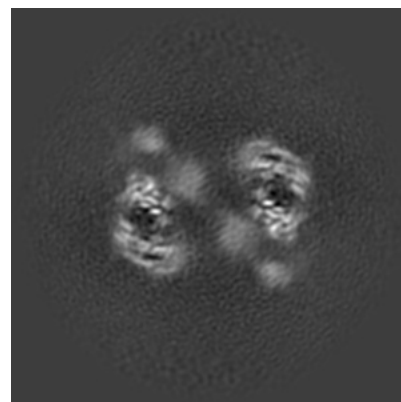
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

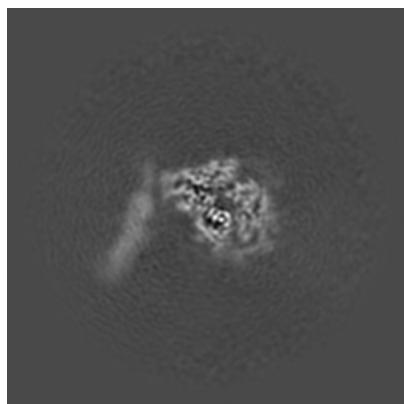


Z Index: 128

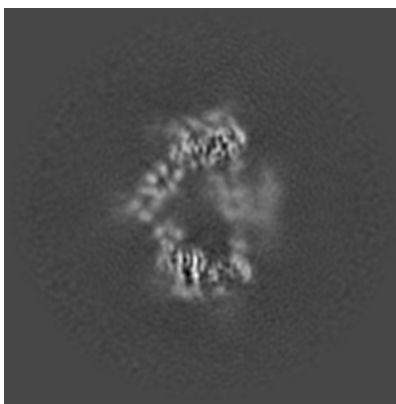
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

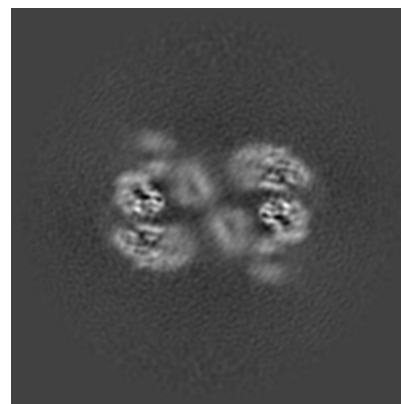
### 6.3.1 Primary map



X Index: 168



Y Index: 124

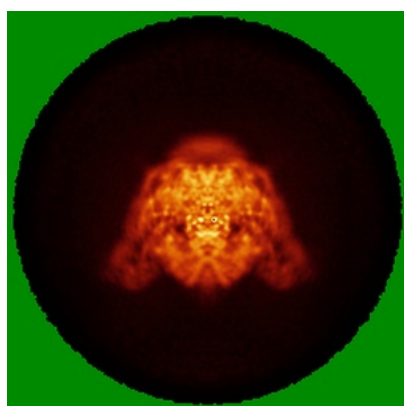


Z Index: 136

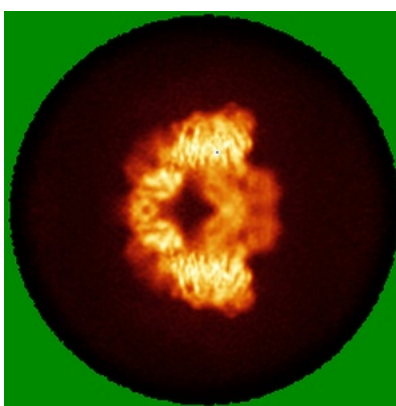
The images above show the largest variance slices of the map in three orthogonal directions.

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

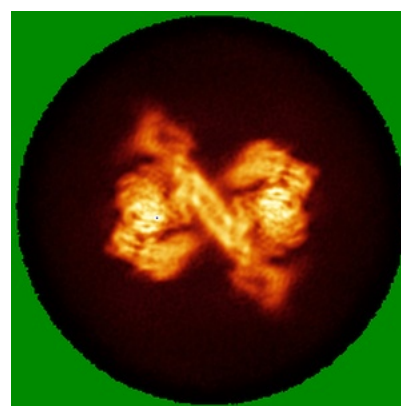
### 6.4.1 Primary map



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.

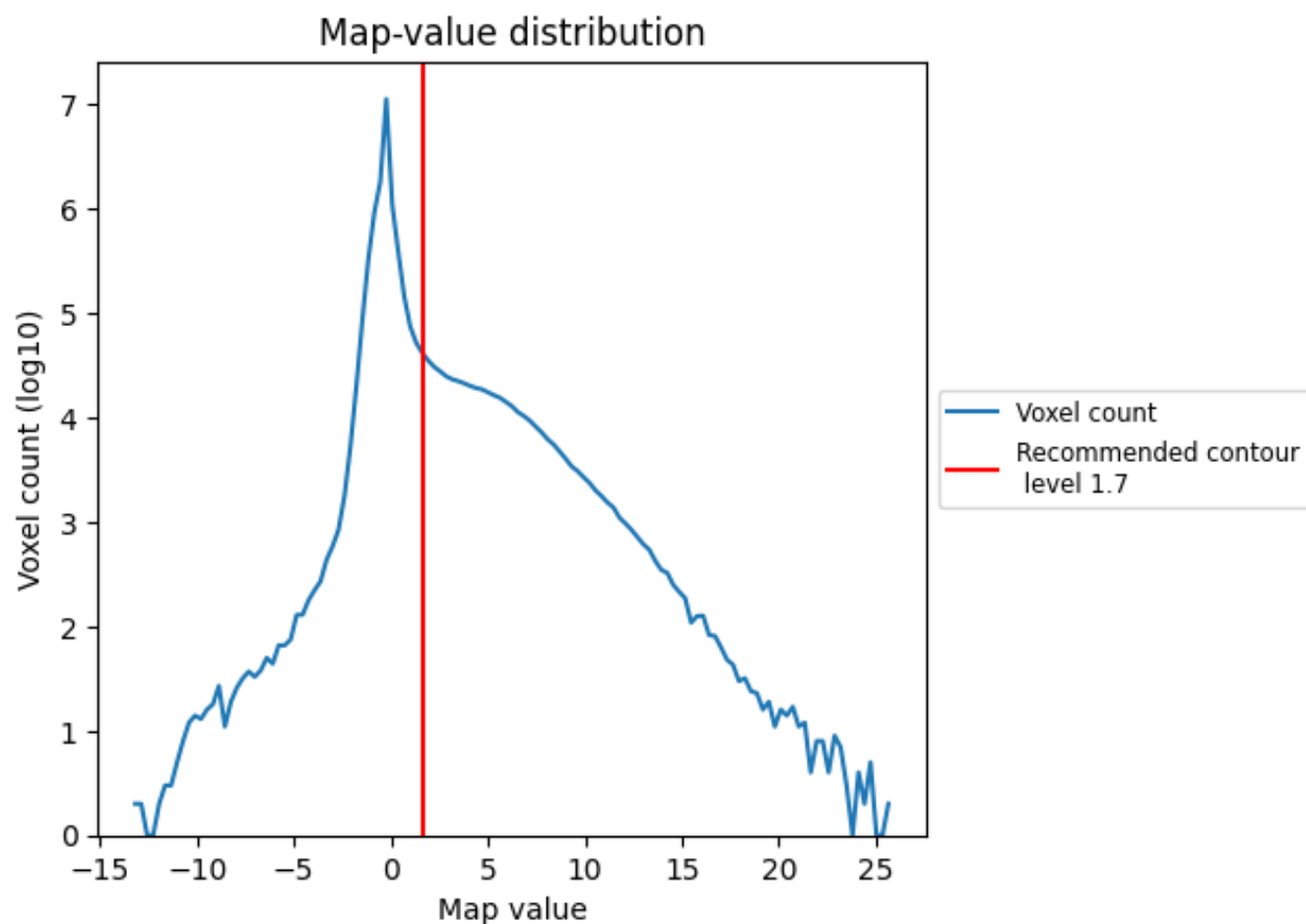
## 6.6 Mask visualisation [i](#)

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.

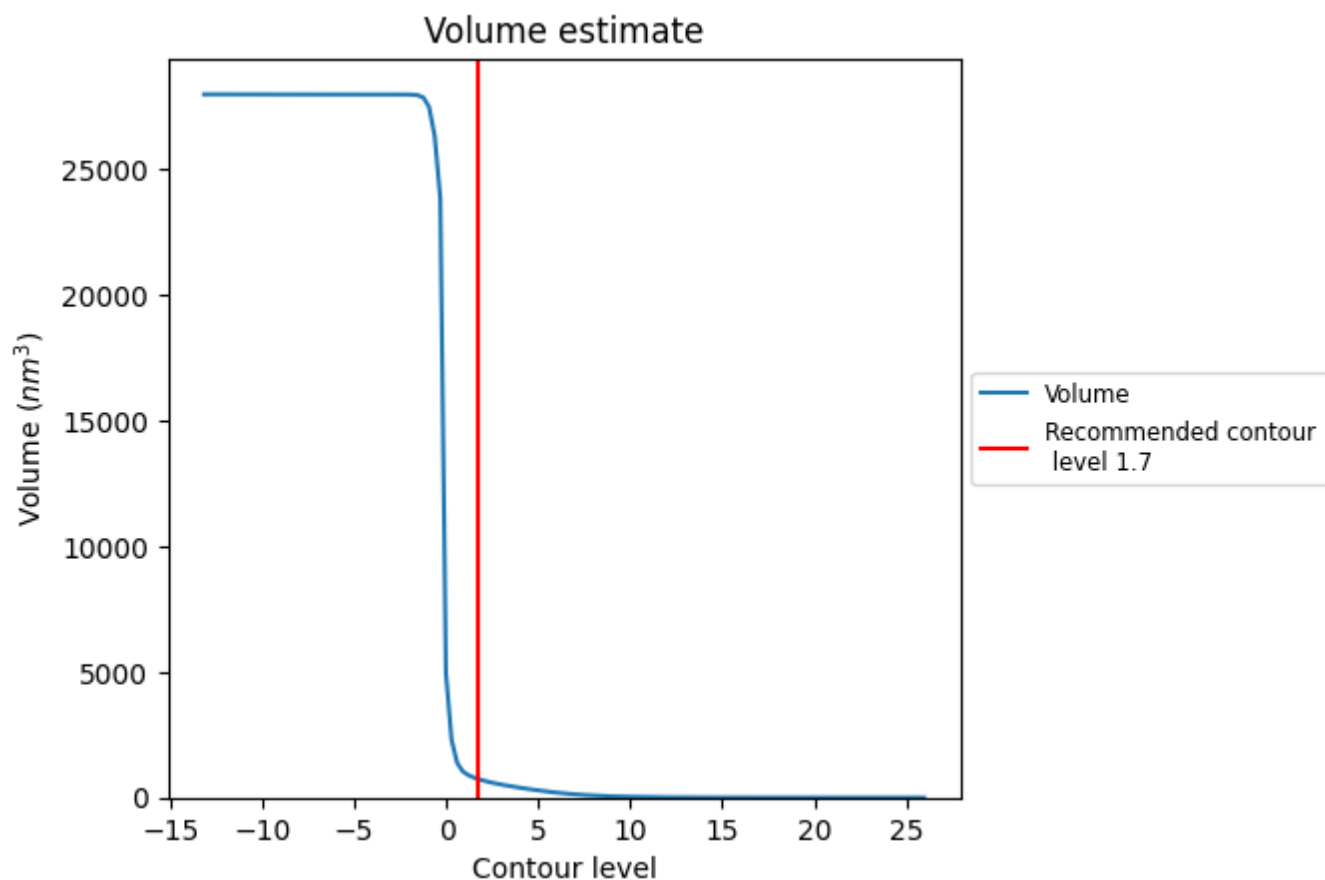
### 7.1 Map-value distribution [i](#)



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.



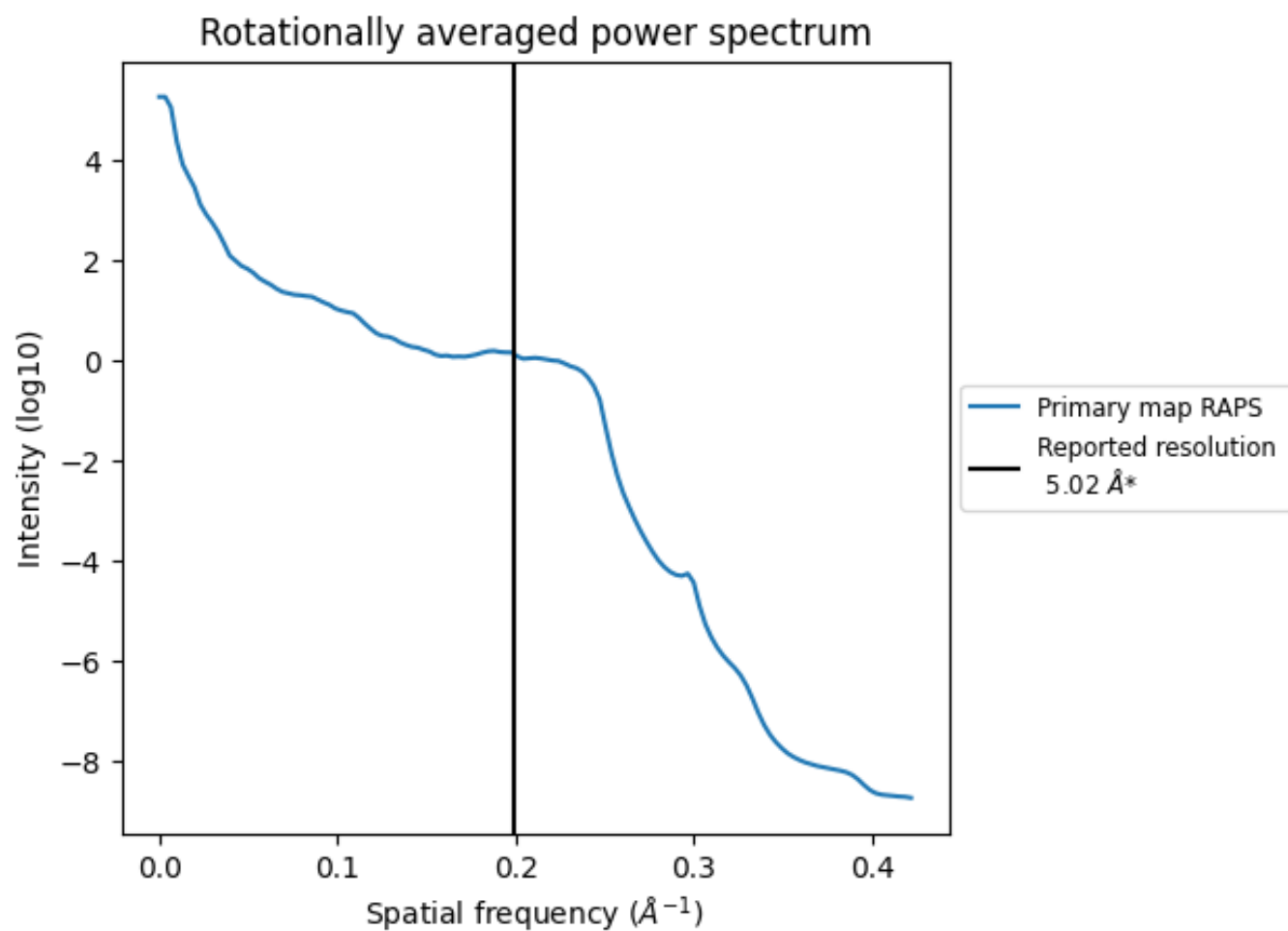
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 743 nm<sup>3</sup>; 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<sup>-1</sup>

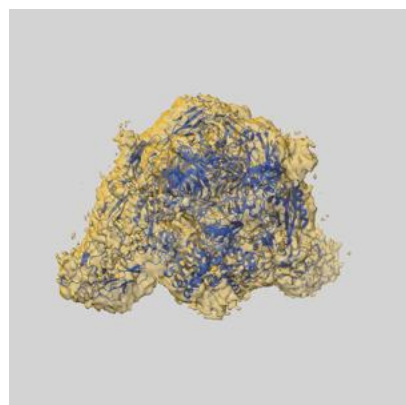
## 8 Fourier-Shell correlation ⓘ

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

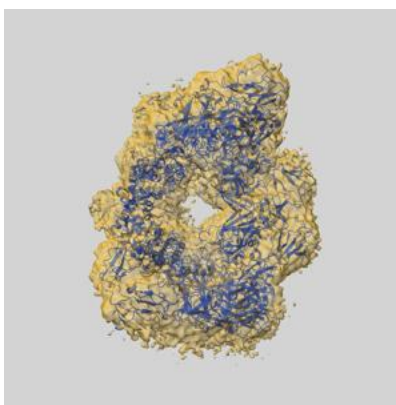
## 9 Map-model fit [i](#)

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

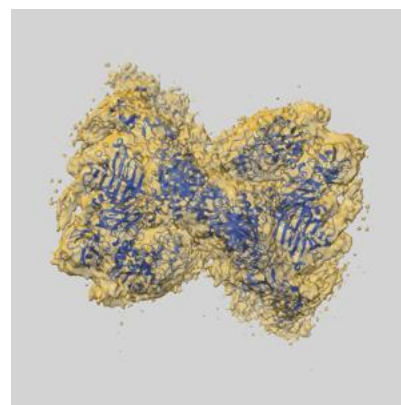
### 9.1 Map-model overlay [i](#)



X



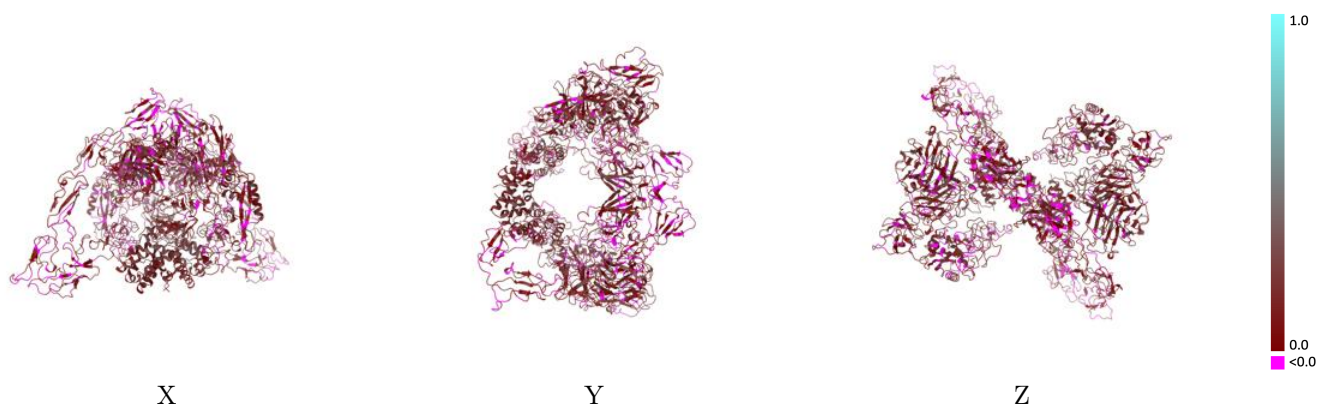
Y



Z

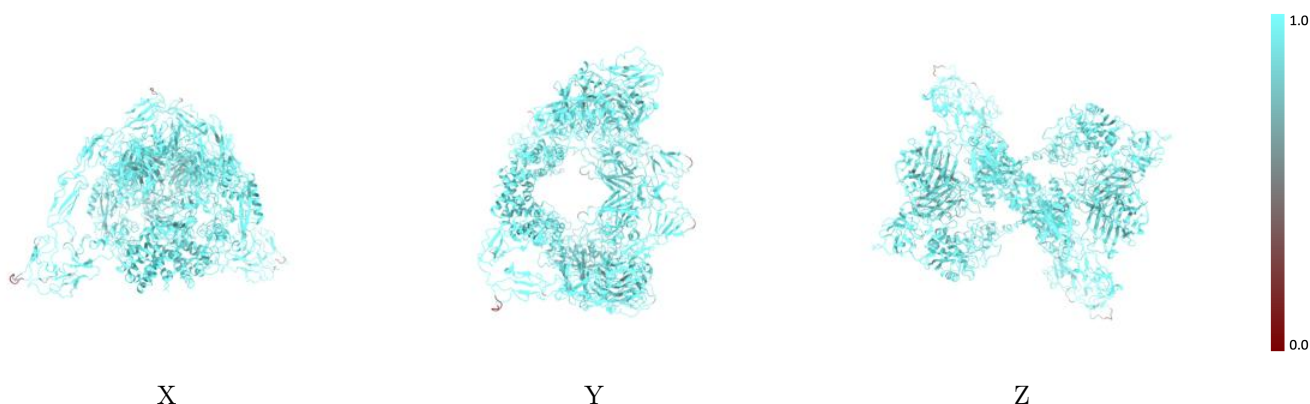
The images above show the 3D surface view of the map at the recommended contour level 1.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



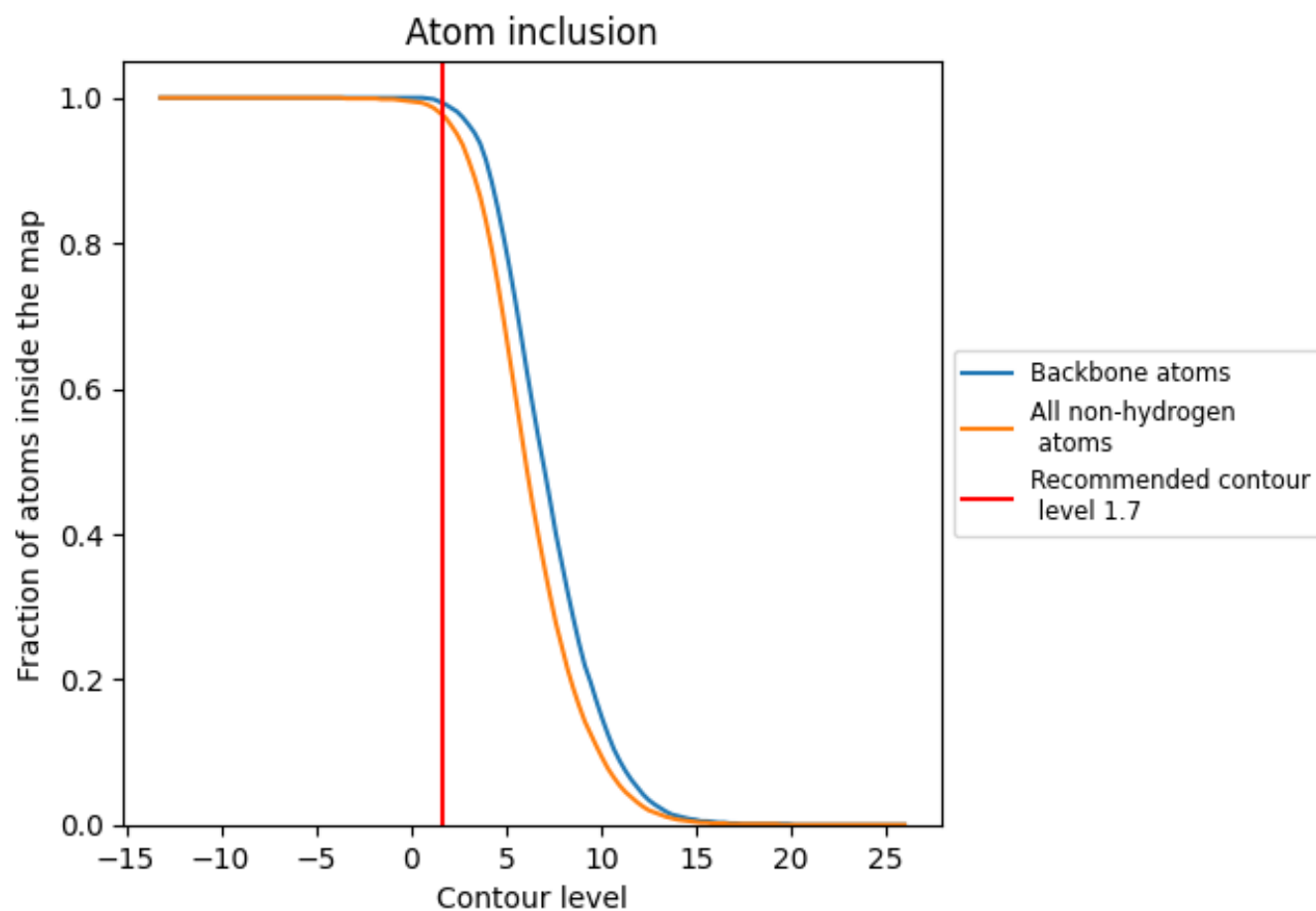
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

