



wwPDB EM Validation Summary Report ⓘ

Jun 4, 2024 – 07:29 pm BST

PDB ID : 5ND1
EMDB ID : EMD-3619
Title : Viral evolution results in multiple, surface-allocated enzymatic activities in a fungal double-stranded RNA virus
Authors : Mata, C.P.; Luque, D.; Gomez Blanco, J.; Rodriguez, J.M.; Suzuki, N.; Ghabrial, S.A.; Carrascosa, J.L.; Trus, B.L.; Caston, J.R.
Deposited on : 2017-03-07
Resolution : 3.70 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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

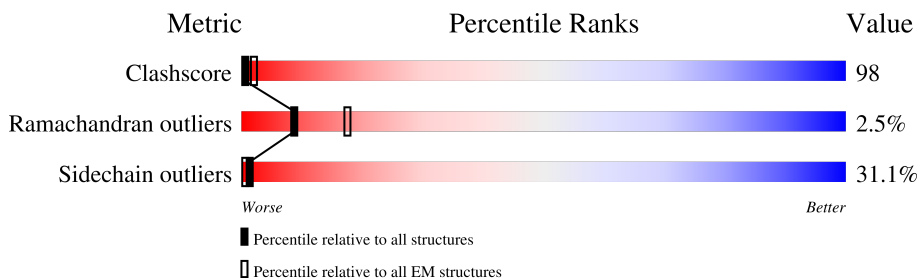
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	A	1357	
2	B	1059	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14963 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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	972	Total	C	N	O	S	0	0
			7371	4561	1355	1400	55		

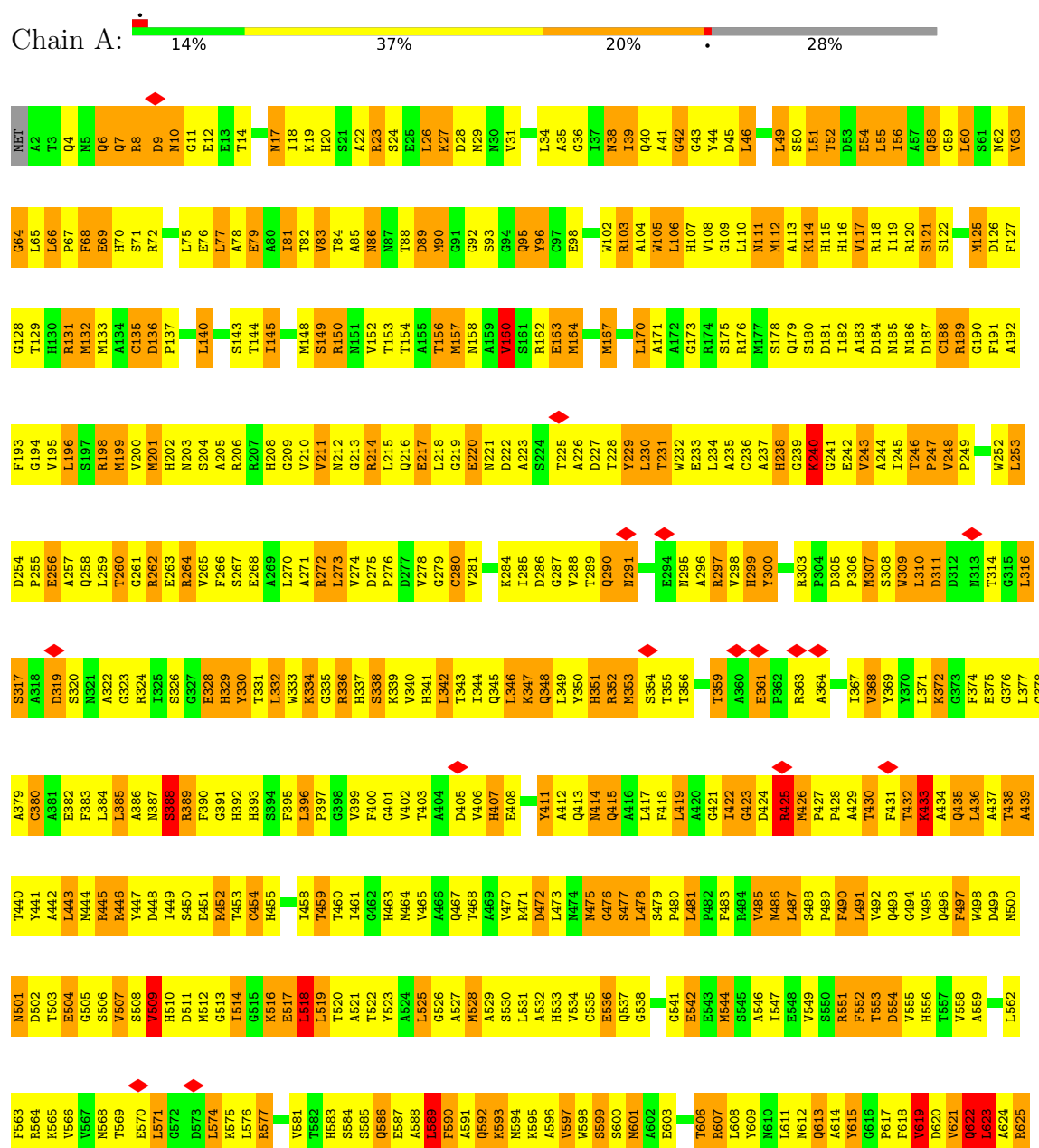
- Molecule 2 is a protein called Capsid protein.

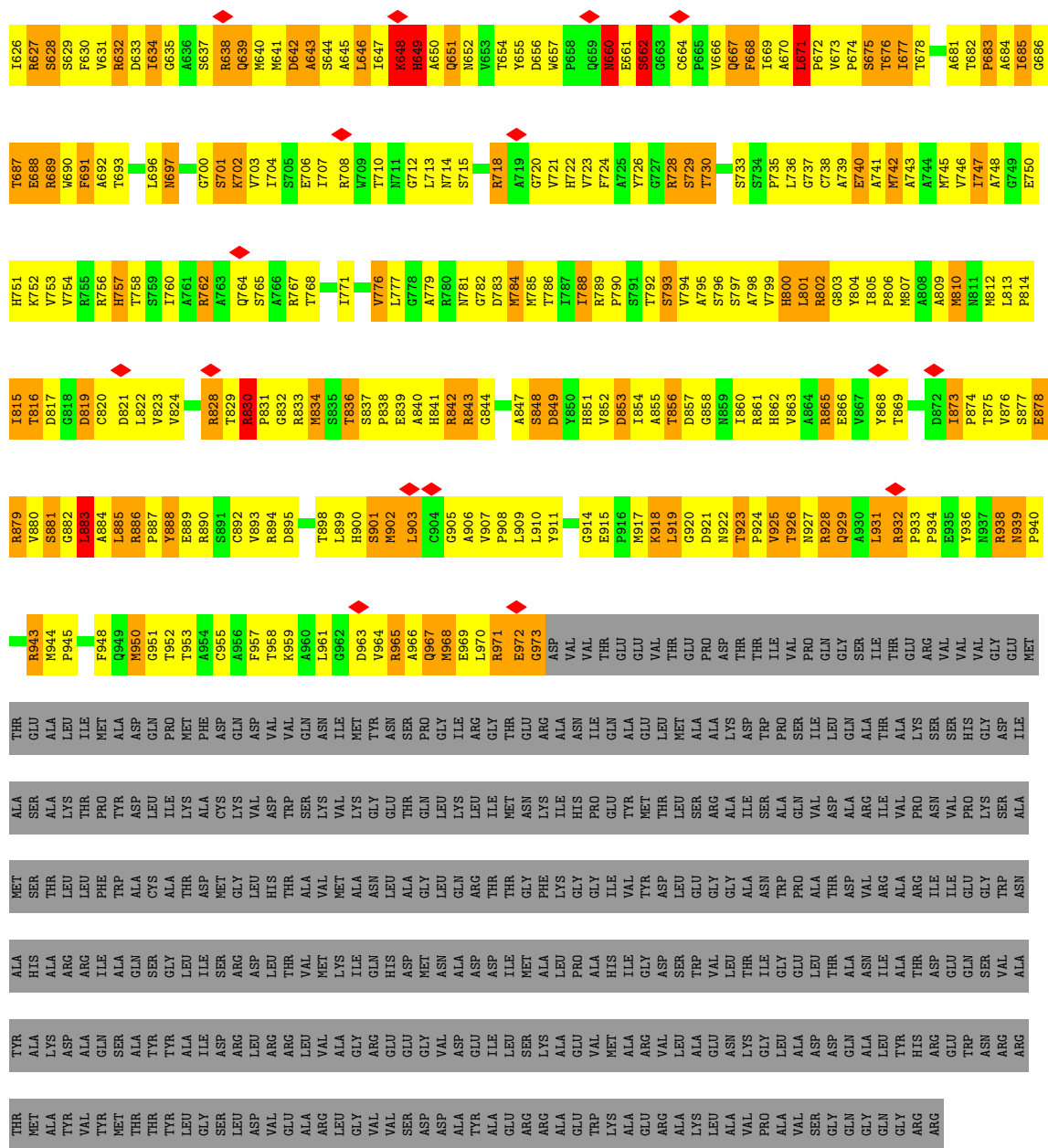
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1005	Total	C	N	O	S	0	0
			7592	4717	1347	1480	48		

3 Residue-property plots

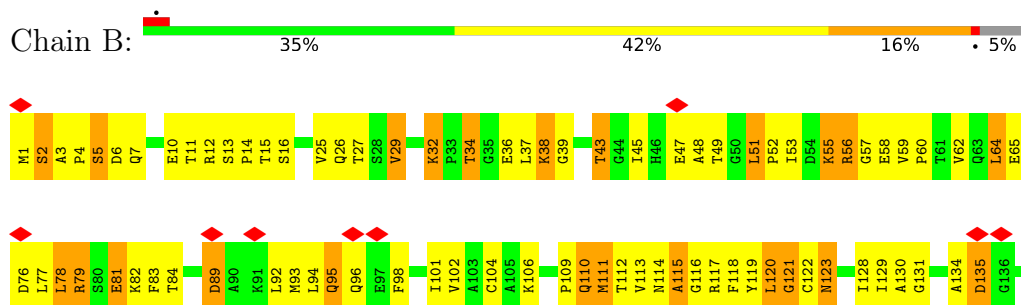
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Capsid protein





• Molecule 2: Capsid protein



SER	L999	V908	H832	R765	D688	A624	H560	G493	K349	M284	R214	Q149
GLU	A1000	N909	G833	D766	I689	T625	G561	M496	P350	E285	D215	C150
	S1001	E910	R835	A767		T627	C563	A497	K351	T286	S216	V152
	T1002	F911	R836	R768	E694		C565	I498		T287	G217	A153
	Y1003	N914	R837	N769	V695	S631	S566	Y499	G354	T288	Q219	L154
	D1004	S915	R838	D770	W701	T632	N666	Q500	A355	D289	H220	E155
	K1005	E916	L839	F772	L702	T633	D667	A501	G356	R290	H221	P156
GLY		E917	F773	W773		T634	S568	G502	H357	A222	A222	
ARG		G918			S706	T635	F569	L503	A358	V291	L224	L161
THR					E707	N636	G571	A504	N359	R292	L224	S162
LYS		H921	R776		E708	N637	G572	A504		A293		G163
GLY		G922	I777		W707	E638	P572	H431	M364	D294	V227	S164
LEU		I923	W778		A709	E639	H573	H432	M365	Y295		T165
THR		E924	K779		H710	A640	C574	W433	S366	A296	T230	S166
LEU		T846	R711		R712	A641	A575	N435	E367	G297	I231	S167
GLU		W781	F713		F713	V643	G576	V436	G368	M299	V234	T168
ASP		M782	R713			D644	D511		V369	V300		Q169
LEU		A853				G645	G512		G370	V301	H237	D170
GLN		R785	A716			G646	D513					N171
LYS		T929	G717			L647	D514		T373	L305	V238	S172
VAL		D855	L718			V648	T515		G374	R306	G239	D173
GLY		L856				T649	R516		V375	K307	D240	S174
GLY		V857				E650	G586		N376		S241	A175
ILE		P858				G651	C587		G377	A242	A242	K176
THR		P859				H652	P588		T378	A243	A243	K177
GLY		M860				V653	G589		R379	K244	K244	L177
GLY		G794				S654	S590		A380	G314	R245	A179
GLY		E795				L655	T591		T381	G314	S246	L180
GLN		D796				T656	G592		P382	T315	R247	
GLY		G797				T657	T593		H383	G316	D248	Q184
MET		G798				T658	G594		A384	D317	G249	V185
THR		R799				T659	G595		D385	T318	W250	V186
GLY		H800				L662	L597		T386	L251	L251	G187
ARG		Q801				N663	S598		V387	E320	D252	G188
GLY		A875				N664	G599		F388	T321	H253	A189
GLY		N876				G665	V599		G389	E322	Q254	S190
GLY		C877				G666	Y600		R390	E322	Q254	T191
GLY		Y806				G667	A601		E391	F257	D256	V192
GLY		F807				L666	V602		E392	G258	F257	G193
GLY		G808				G667	D603		L393	L327	A258	I194
GLY		E809				E669	V604			V259	V259	V195
GLY		A810				N670	N606		L397	L328	K260	A196
GLY		A811				N671	G606		G398	L329	K261	P197
GLY		A812				N672	T607		F399	A330	G261	M198
GLY		L813				G673	D610		A400	L331	M262	L199
GLY		G814				N674	G611		L401	P332	L263	Q200
GLY		H815				L675	Y612		R402	K333	T264	T201
GLY		H816				N676	Y611		H403	C334	P265	V202
GLY		G817				L677	Y612		M404	D335	H266	A203
GLY		H818				N678	Y613		A405	A336	A268	Q204
GLY		G819				G678	A614		D406	G337	S269	E205
GLY		F820				C679	N615		A407	A340	Q206	Q206
GLY		L823				N680	A616		Q408		T207	T207
GLY						T681	G617		E409	L343	F208	F208
ALA						N682	L618		Q410	A344	R209	R209
GLU		Y626				D683	E619		V411	L345	T278	A210
THR		C827				S684	P620			L346	Y279	R211
ILE		A828				G621	G621			V415	S280	V212
GLY		S899				H686	L622			G348	S281	
GLY		T830				E763	L623					
ASP		Y831				L764						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37531	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.7	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.371	Depositor
Minimum map value	-0.852	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.18	Depositor
Map size (\AA)	536.0, 536.0, 536.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

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	0.94	2/7511 (0.0%)	1.12	52/10188 (0.5%)
2	B	0.67	3/7739 (0.0%)	0.88	27/10515 (0.3%)
All	All	0.82	5/15250 (0.0%)	1.00	79/20703 (0.4%)

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
1	A	0	11
2	B	0	6
All	All	0	17

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	ALA	C-N	11.72	1.60	1.34
2	B	600	TYR	CE1-CZ	-5.35	1.31	1.38
2	B	506	PRO	N-CD	5.14	1.55	1.47
2	B	197	PRO	N-CD	5.11	1.55	1.47
1	A	96	TYR	CE2-CZ	-5.04	1.32	1.38

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	GLY	N-CA-C	-8.26	92.46	113.10
1	A	229	TYR	N-CA-C	-7.99	89.43	111.00
1	A	519	LEU	CB-CG-CD2	-7.95	97.49	111.00
1	A	720	GLY	N-CA-C	7.69	132.32	113.10
2	B	706	SER	N-CA-C	-7.52	90.70	111.00

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	GLY	Mainchain
1	A	334	LYS	Peptide
1	A	388	SER	Peptide
1	A	648	LYS	Peptide
1	A	649	HIS	Peptide

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	7371	0	7232	1879	0
2	B	7592	0	7407	1221	0
All	All	14963	0	14639	2903	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 98.

The worst 5 of 2903 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:A:961:LEU:HD11	2:B:284:MET:SD	1.29	1.67
1:A:894:ARG:CA	1:A:902:MET:HE3	1.30	1.59
2:B:327:TYR:CE1	2:B:448:MET:HE1	1.09	1.58
2:B:264:THR:HG22	2:B:265:PRO:CD	1.18	1.58
1:A:105:TRP:CD1	1:A:471:ARG:NH1	1.73	1.57

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	970/1357 (72%)	894 (92%)	60 (6%)	16 (2%)	9	43
2	B	1001/1059 (94%)	874 (87%)	94 (9%)	33 (3%)	4	31
All	All	1971/2416 (82%)	1768 (90%)	154 (8%)	49 (2%)	9	35

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	477	SER
1	A	509	VAL
1	A	554	ASP
1	A	599	SER
1	A	619	VAL

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	774/1083 (72%)	486 (63%)	288 (37%)	0	0
2	B	800/833 (96%)	599 (75%)	201 (25%)	0	4
All	All	1574/1916 (82%)	1085 (69%)	489 (31%)	1	2

5 of 489 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	740	GLU
2	B	735	HIS
1	A	968	MET
2	B	708	GLU
2	B	866	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	485	GLN
2	B	832	HIS
2	B	527	GLN
2	B	705	ASN
2	B	885	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	235:ALA	C	236:CYS	N	1.61

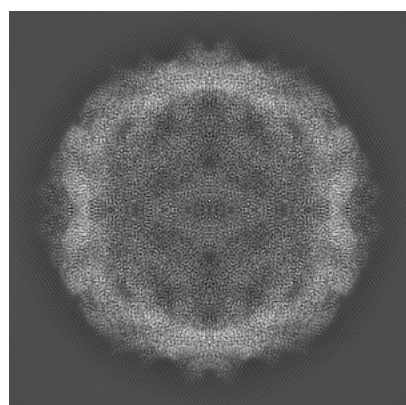
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3619. These allow visual inspection of the internal detail of the map and identification of artifacts.

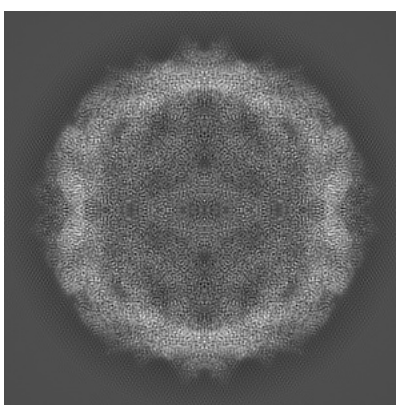
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

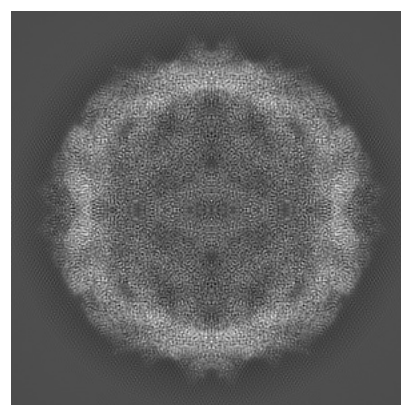
6.1.1 Primary map



X



Y

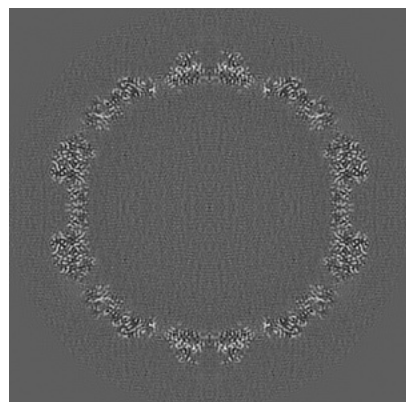


Z

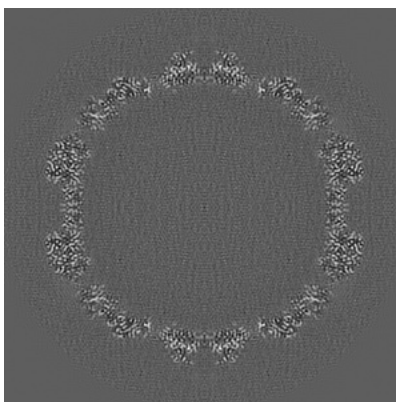
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

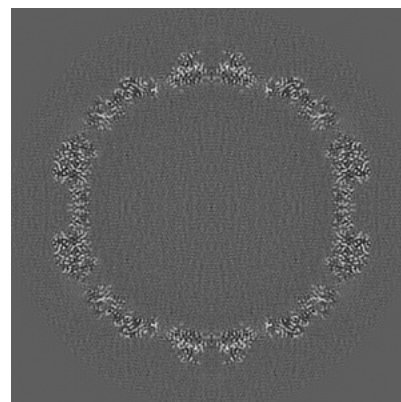
6.2.1 Primary map



X Index: 200



Y Index: 200

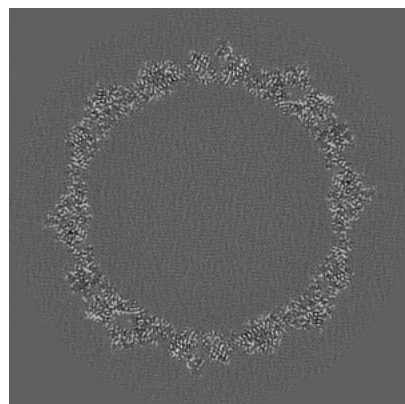


Z Index: 200

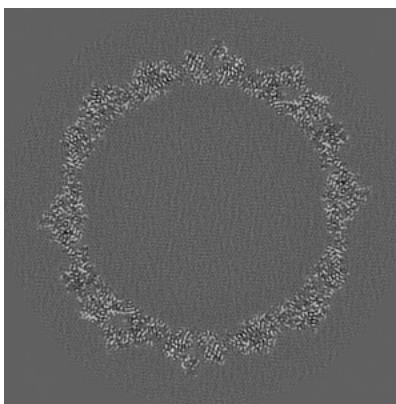
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

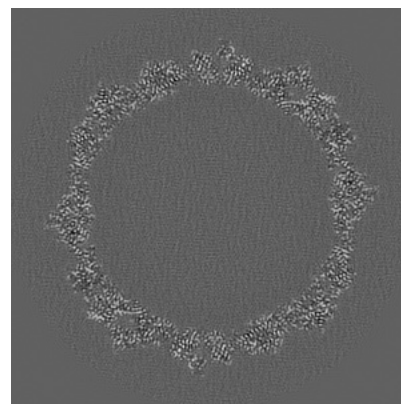
6.3.1 Primary map



X Index: 226



Y Index: 226

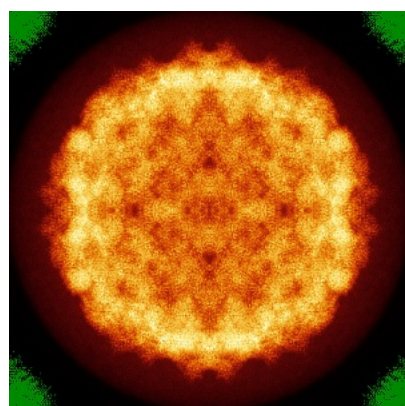


Z Index: 226

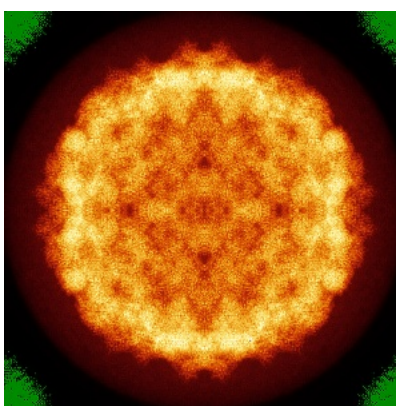
The images above show the largest variance slices of the map in three orthogonal directions.

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

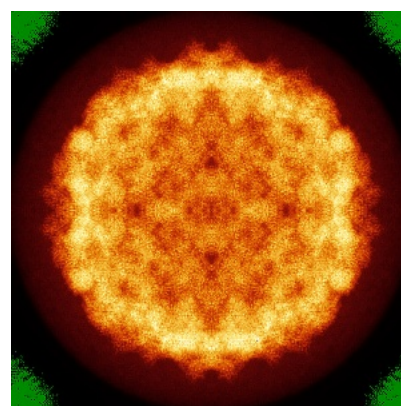
6.4.1 Primary map



X



Y

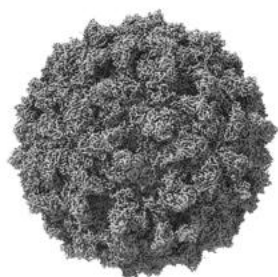


Z

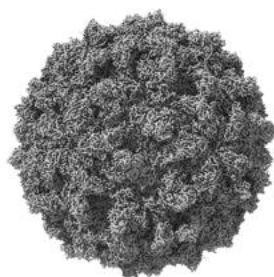
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

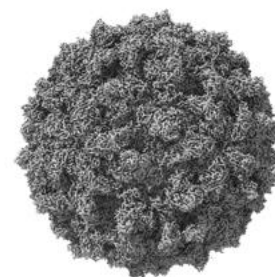
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

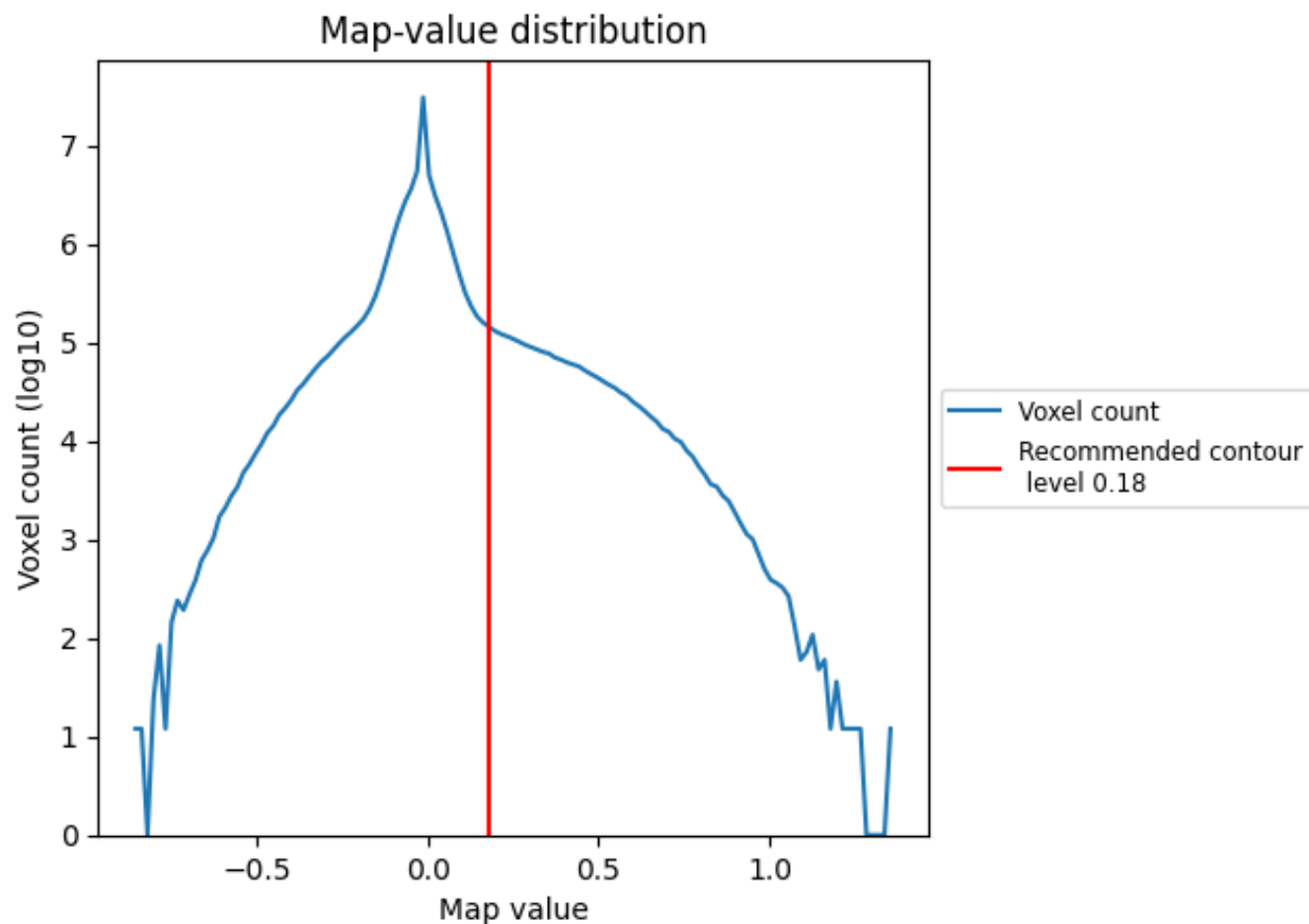
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

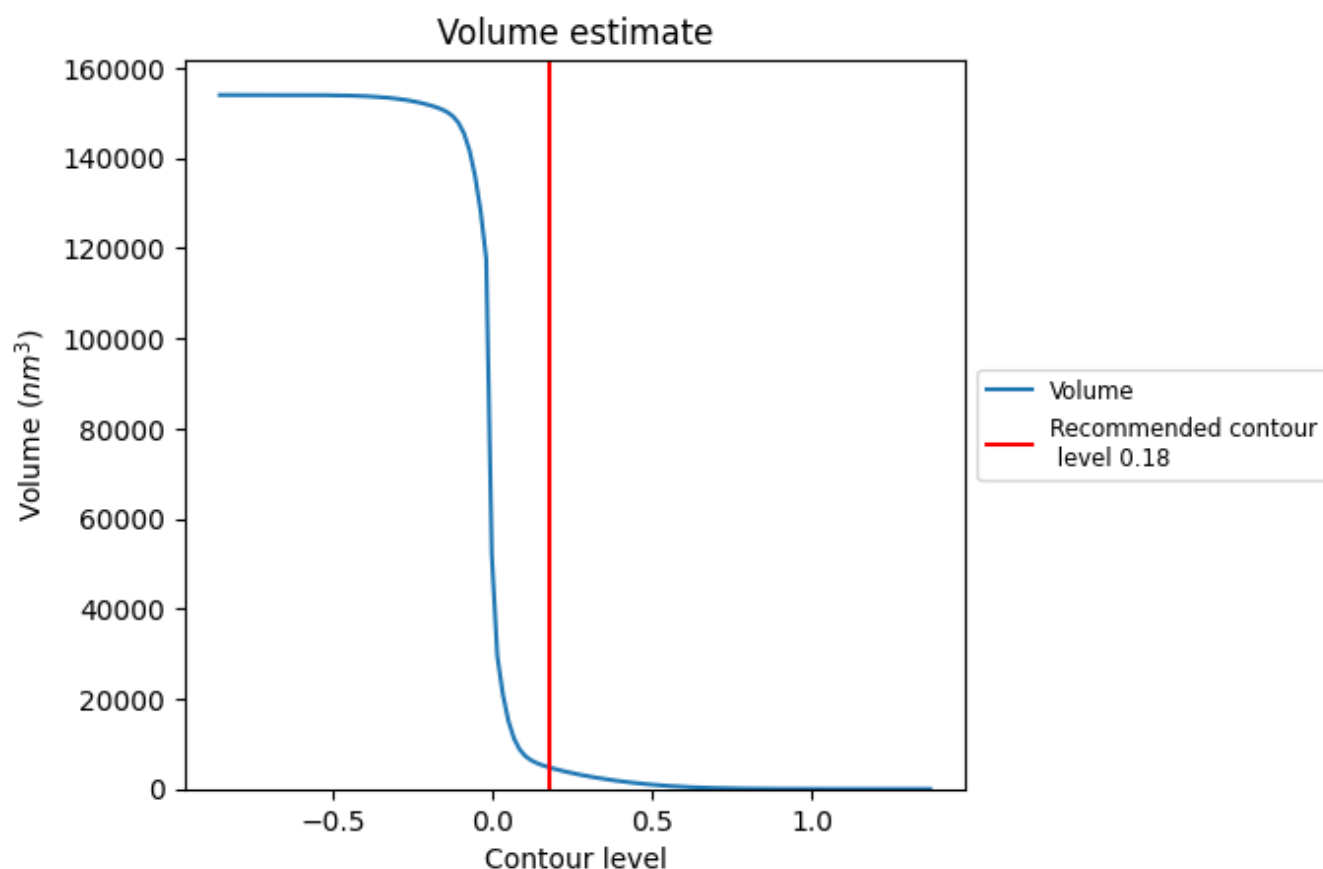
This section contains the results of statistical analysis of the map.

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.

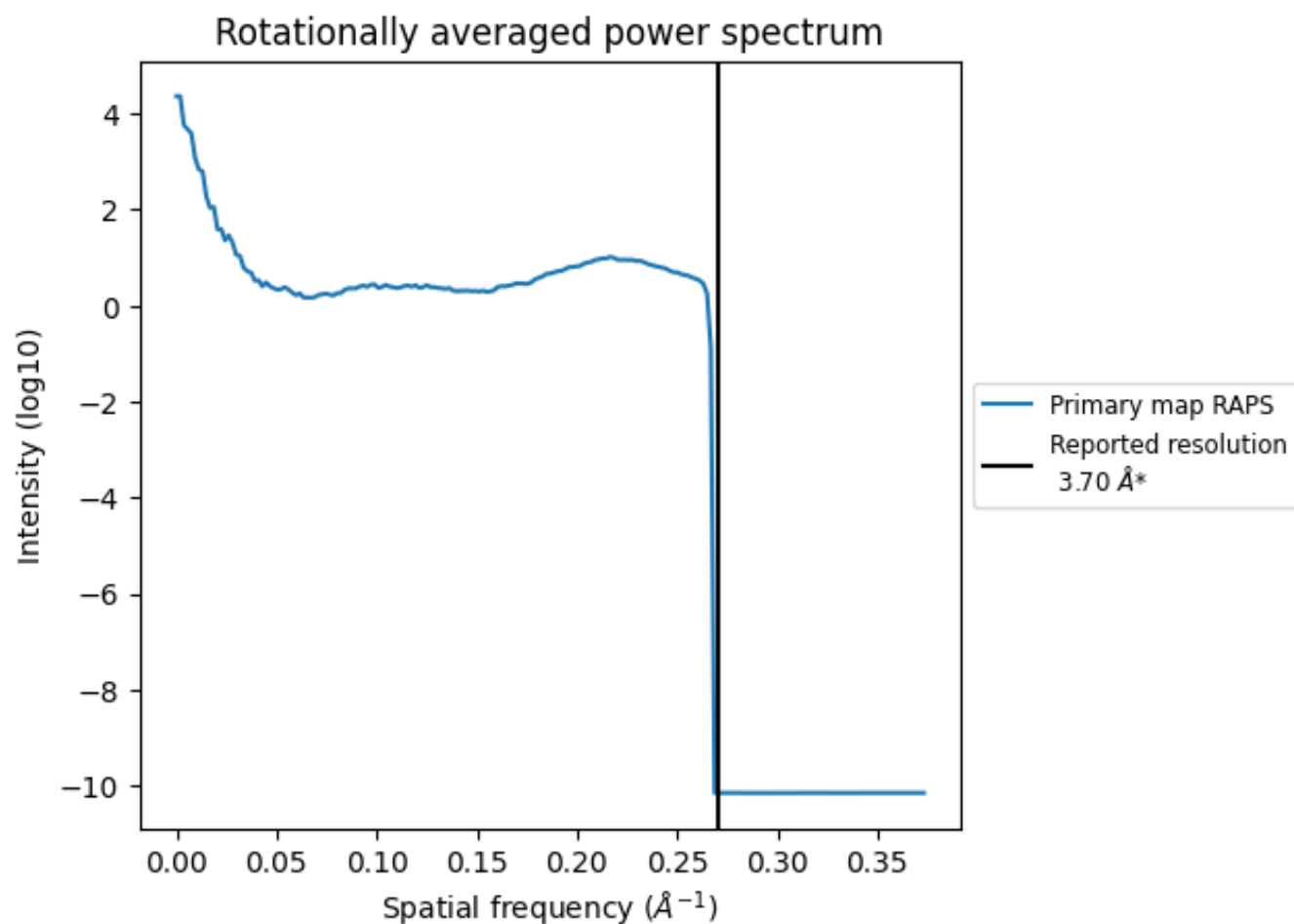
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4755 nm³; this corresponds to an approximate mass of 4296 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 0.270 Å⁻¹

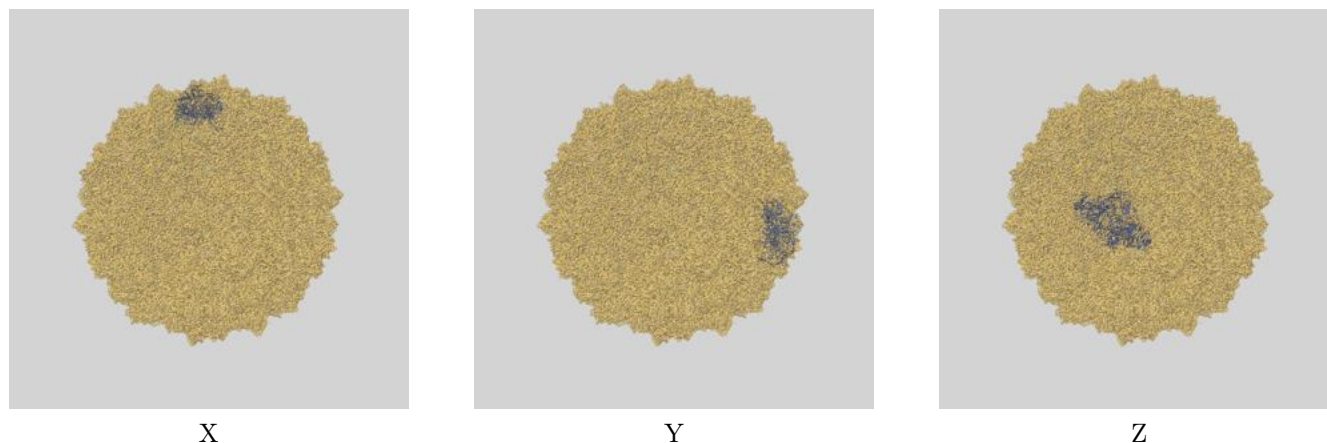
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

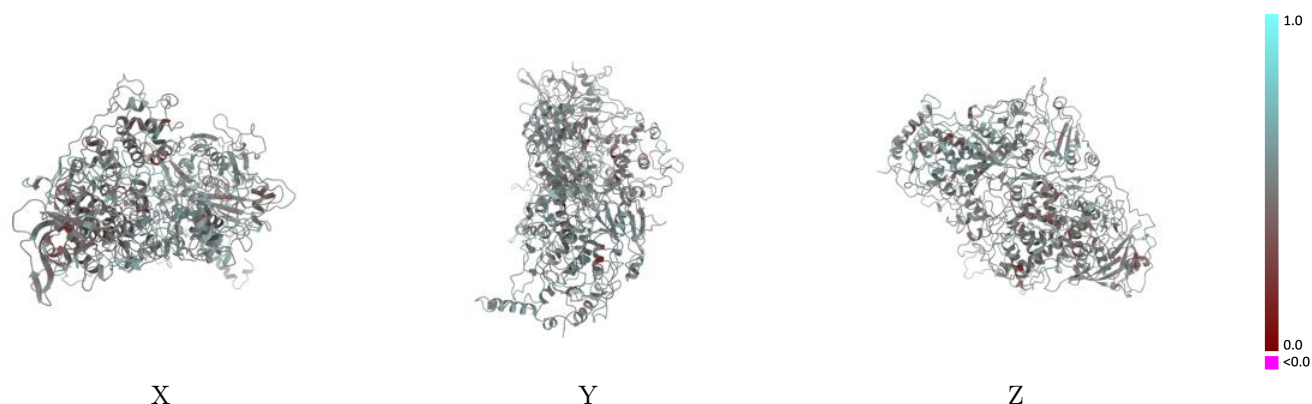
This section contains information regarding the fit between EMDB map EMD-3619 and PDB model 5ND1. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.18 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](#)



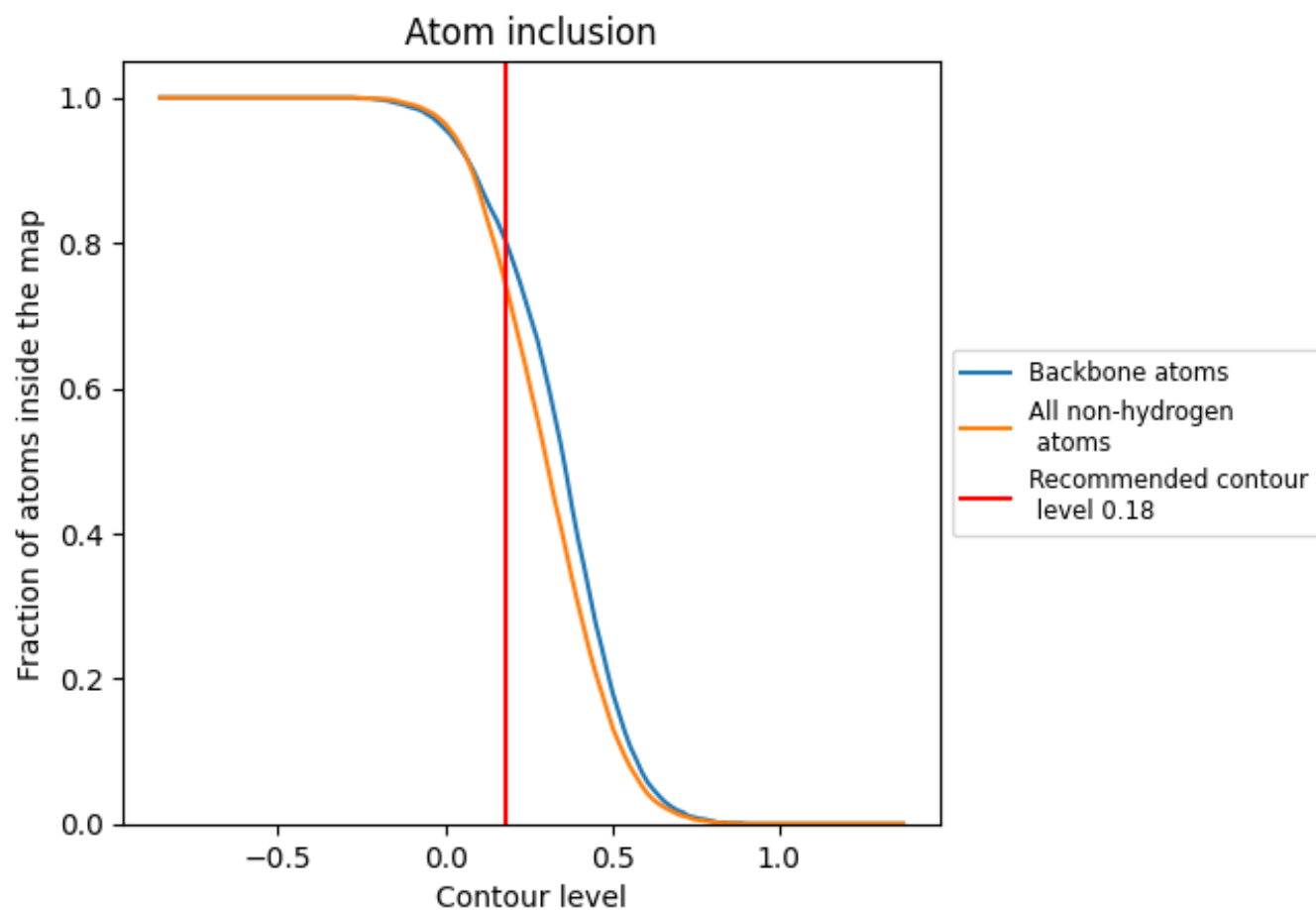
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7450	<div></div> 0.5060
A	<div></div> 0.7630	<div></div> 0.5210
B	<div></div> 0.7270	<div></div> 0.4910

