



wwPDB EM Validation Summary Report ⓘ

Nov 6, 2022 – 11:11 PM EST

PDB ID : 6CRJ
EMDB ID : EMD-7564
Title : Mouse norovirus model using the crystal structure of MNV P domain and the Norwalkvirus shell domain
Authors : Smith, T.J.
Deposited on : 2018-03-19
Resolution : 8.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

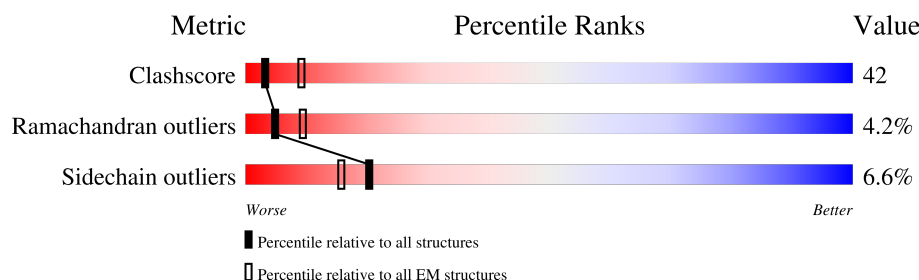
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 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	531	<div> <div>65%</div> <div>58% 30% 6% . .</div> </div>
1	B	531	<div> <div>64%</div> <div>63% 28% 6% . .</div> </div>
1	C	531	<div> <div>60%</div> <div>64% 26% . . .</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11749 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 Norwalk virus, MNV-1 capsid protein chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	527	Total	C	N	O	S	0	0
			3997	2555	672	752	18		
1	A	508	Total	C	N	O	S	0	0
			3876	2484	651	723	18		
1	C	508	Total	C	N	O	S	0	0
			3876	2484	651	723	18		

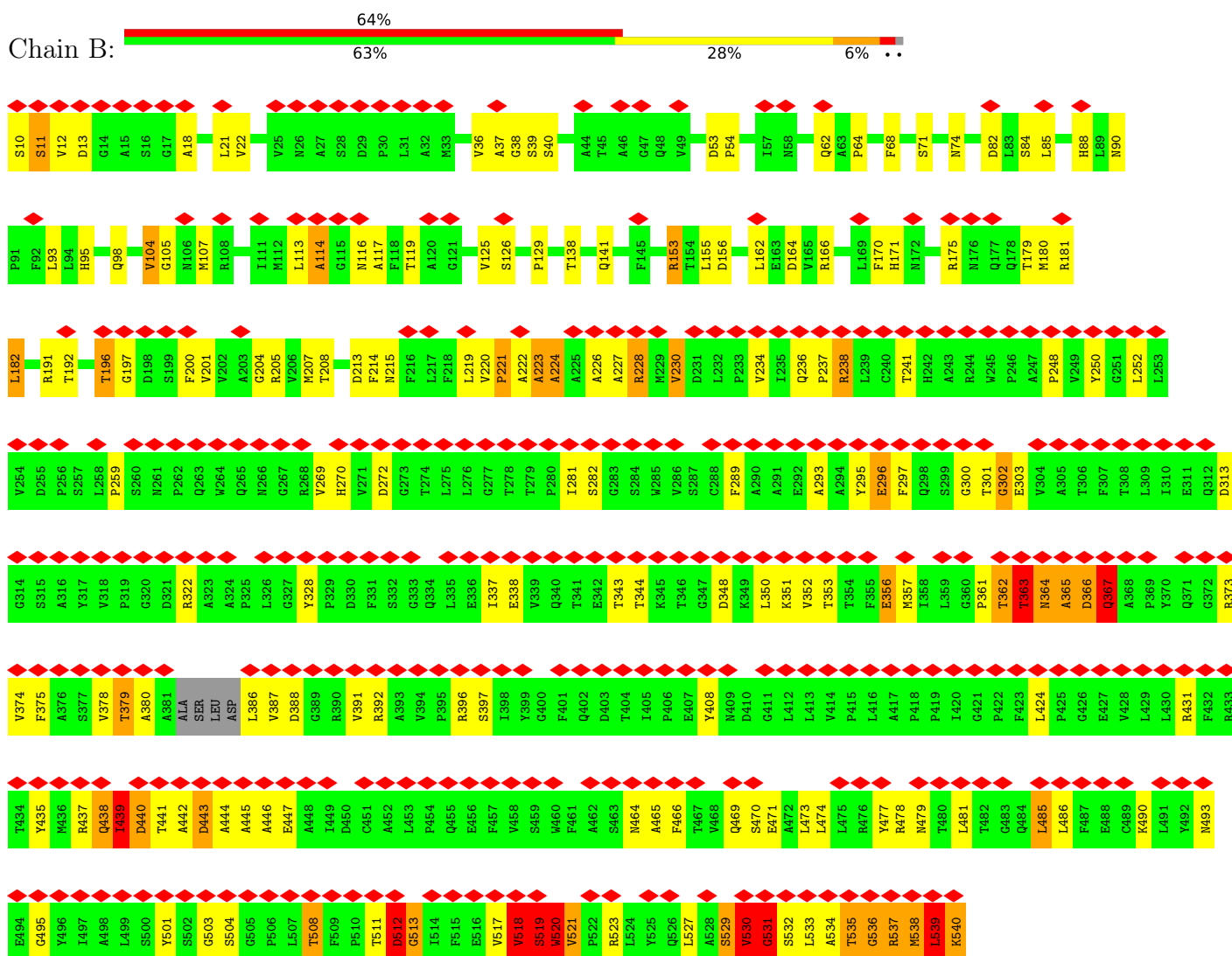
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	222	ALA	-	linker	UNP Q83884
B	223	ALA	-	linker	UNP Q83884
B	224	ALA	-	linker	UNP Q83884
B	225	ALA	-	linker	UNP Q83884
B	226	ALA	-	linker	UNP Q83884
B	227	ALA	-	linker	UNP Q83884
A	222	ALA	-	linker	UNP Q83884
A	223	ALA	-	linker	UNP Q83884
A	224	ALA	-	linker	UNP Q83884
A	225	ALA	-	linker	UNP Q83884
A	226	ALA	-	linker	UNP Q83884
A	227	ALA	-	linker	UNP Q83884
C	222	ALA	-	linker	UNP Q83884
C	223	ALA	-	linker	UNP Q83884
C	224	ALA	-	linker	UNP Q83884
C	225	ALA	-	linker	UNP Q83884
C	226	ALA	-	linker	UNP Q83884
C	227	ALA	-	linker	UNP Q83884

3 Residue-property plots

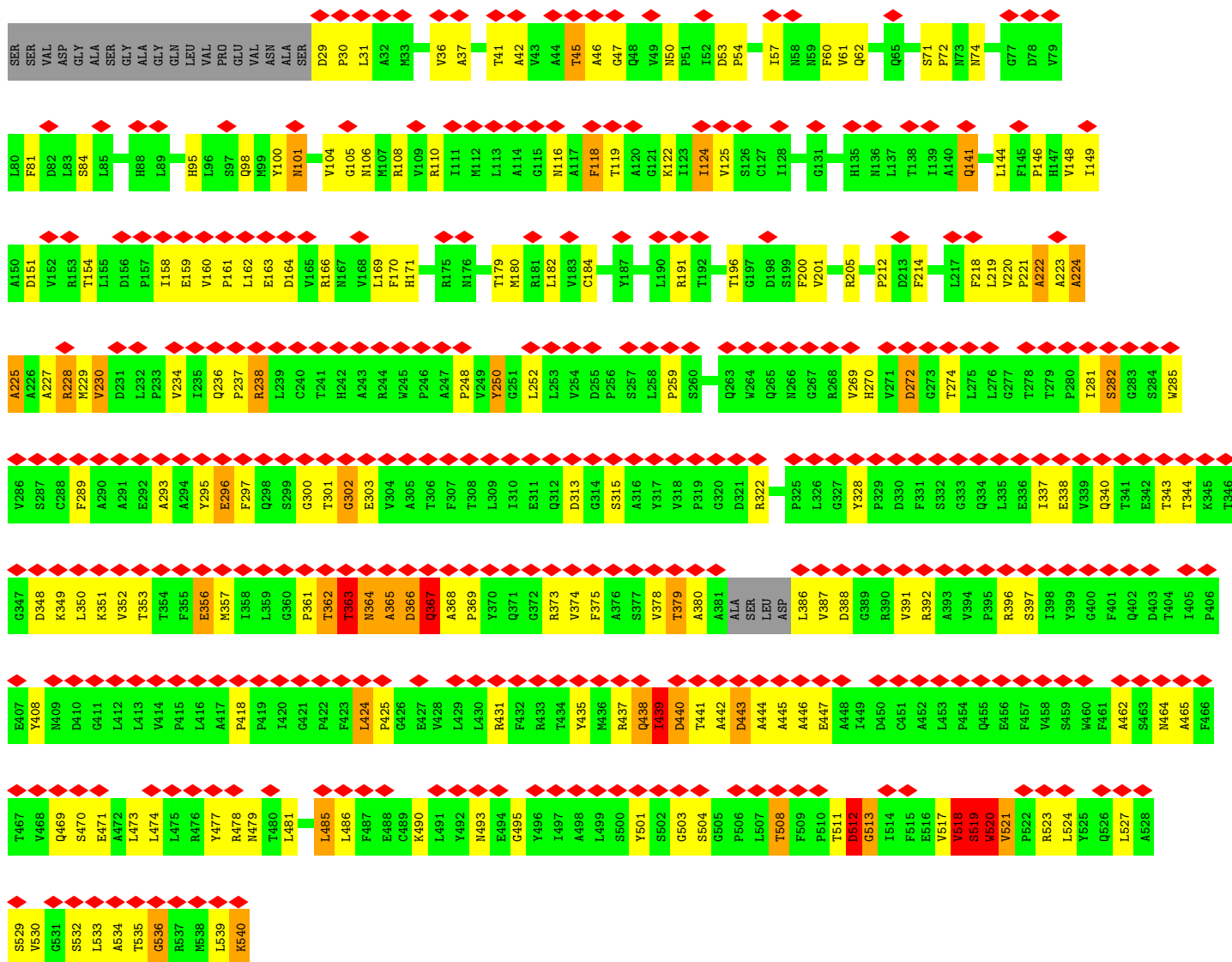
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Norwalk virus, MNV-1 capsid protein chimera

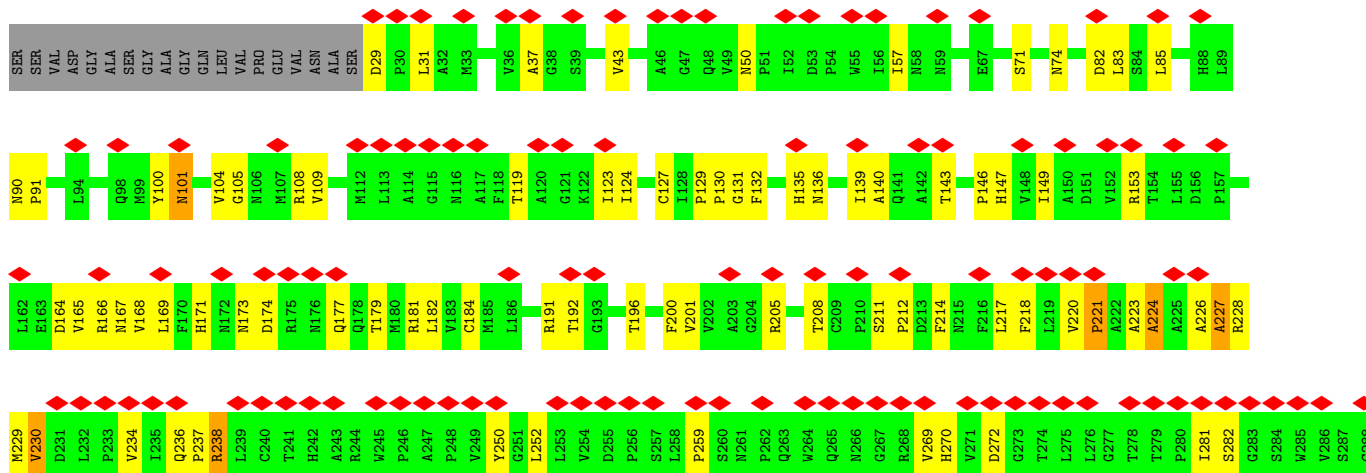


- Molecule 1: Norwalk virus, MNV-1 capsid protein chimera





• Molecule 1: Norwalk virus, MNV-1 capsid protein chimera



F289	K349	D410	Y477	L539
A290	L350	G411	R478	K540
A291	K351	L412	M479	
E292	V352	L413	T480	
A293	T353	V414	L481	
A294	T354	P415	L485	
Y295	F355	L416	L486	
E296	E356	A417	L487	
F297	M357	P418	E488	
Q298	I358	P419	C489	
S299	L359	I420	K490	
G300	G360	G421	L491	
T301	P361	P422	Y492	
G302	T362	F423	M493	
E303	T363	L424	E494	
V304	N364	P425	G495	
A305	A365		Y496	
T306	D366	V428	I497	
F307	Q367	L429	A498	
T308	A368	L430	L499	
L309	P369	R431	S500	
I310		F432	Y501	
E311	G372		S502	
Q312	R373	Y435	G503	
D313	V374	M436	S504	
G314	F375	R437		
S315	A376	Q438	L507	
A316	S377	I439	T508	
Y317	V378	D440	F509	
V318	T379	T441	P510	
P319	A380	A442	T511	
G320	A381	D443	D512	
R321	ALA		G513	
R322	SER	A446	I514	
	LEU	E447	F515	
	ASP	A448	E516	
A323	L386	I449	V517	
A324	V387	D450	V518	
P325	D388	C451	S519	
L326	G389	A452	M520	
G327	R390	L453	V521	
Y328	V391	P454	P522	
P329	R392	Q455	R523	
D330	A393	E456	L524	
F331	V394	F457	Y525	
S332	P395	V458	Q526	
G333	R396	S459	L527	
Q334	S397		A528	
L335	I398	S463	S529	
E336	Y399	M464	V530	
I337	G400	A465	G531	
E338	F401	F466	S532	
V339	Q402	T467	L533	
Q340	D403	V468	A534	
T341	T404	Q469	T535	
E342	I405	S470	G536	
T343	P406	E471	R537	
T344	E407	A472	M538	
K345	Y408	L473		
T346	M409	L474		
G347				
D348				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20425	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	10	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI EAGLE (2k x 2k)	Depositor
Maximum map value	14.876	Depositor
Minimum map value	-11.954	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.934	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	599.0016, 599.0016, 599.0016	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.5598999, 1.5598999, 1.5598999	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	0.97	5/3979 (0.1%)	1.06	14/5449 (0.3%)
1	B	0.97	5/4101 (0.1%)	1.12	26/5616 (0.5%)
1	C	0.97	5/3979 (0.1%)	1.11	20/5449 (0.4%)
All	All	0.97	15/12059 (0.1%)	1.10	60/16514 (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	2	4
1	B	2	4
1	C	2	4
All	All	6	12

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	SER	CB-OG	6.95	1.51	1.42
1	C	282	SER	CB-OG	6.93	1.51	1.42
1	B	282	SER	CB-OG	6.93	1.51	1.42
1	C	513	GLY	N-CA	-6.36	1.36	1.46
1	B	513	GLY	N-CA	-6.34	1.36	1.46

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	532	SER	C-N-CA	-15.40	83.19	121.70
1	B	530	VAL	CB-CA-C	-15.10	82.72	111.40
1	B	539	LEU	C-N-CA	-9.85	97.08	121.70
1	A	272	ASP	CB-CG-OD1	9.77	127.09	118.30
1	B	272	ASP	CB-CG-OD1	9.72	127.05	118.30

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	518	VAL	CA
1	B	521	VAL	CA
1	A	518	VAL	CA
1	A	521	VAL	CA
1	C	518	VAL	CA

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	438	GLN	Peptide
1	B	438	GLN	Peptide
1	B	512	ASP	Peptide
1	B	518	VAL	Peptide
1	B	519	SER	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	3876	0	3810	501	0
1	B	3997	0	3923	427	0
1	C	3876	0	3814	382	0
All	All	11749	0	11547	973	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 42.

The worst 5 of 973 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:B:445:ALA:CA	1:A:350:LEU:HB2	1.24	1.67
1:A:169:LEU:HD12	1:C:168:VAL:CA	1.30	1.62
1:A:425:PRO:HD3	1:C:425:PRO:CG	1.25	1.61
1:B:445:ALA:HA	1:A:350:LEU:CB	1.28	1.57
1:B:446:ALA:CB	1:A:350:LEU:HD21	1.29	1.53

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	504/531 (95%)	446 (88%)	38 (8%)	20 (4%)	3	23
1	B	523/531 (98%)	458 (88%)	41 (8%)	24 (5%)	2	21
1	C	504/531 (95%)	446 (88%)	38 (8%)	20 (4%)	3	23
All	All	1531/1593 (96%)	1350 (88%)	117 (8%)	64 (4%)	5	22

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	114	ALA
1	B	223	ALA
1	B	302	GLY
1	B	362	THR
1	B	363	THR

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	418/434 (96%)	387 (93%)	31 (7%)	13	38
1	B	431/434 (99%)	405 (94%)	26 (6%)	19	44
1	C	418/434 (96%)	392 (94%)	26 (6%)	18	43
All	All	1267/1302 (97%)	1184 (93%)	83 (7%)	20	41

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	31	LEU
1	C	364	ASN
1	C	104	VAL
1	C	237	PRO
1	C	439	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	GLN
1	C	526	GLN
1	A	469	GLN
1	C	364	ASN
1	A	367	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 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 ⓘ

There are no chain breaks in this entry.

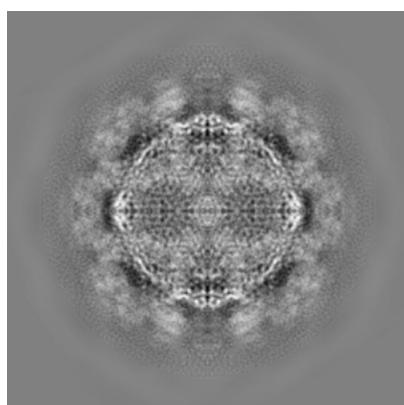
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7564. These allow visual inspection of the internal detail of the map and identification of artifacts.

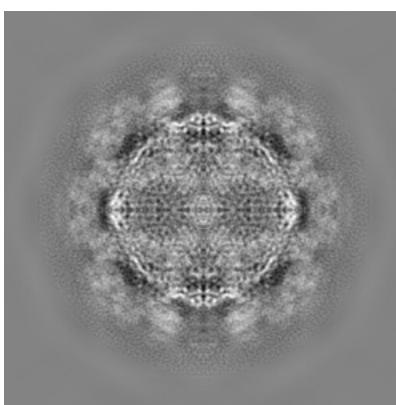
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

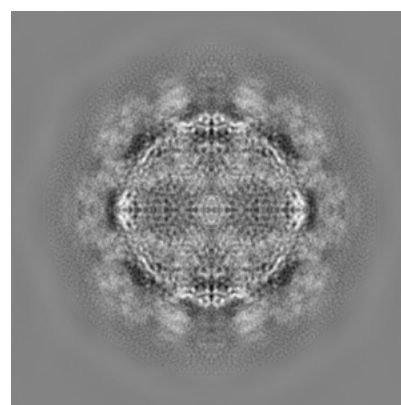
6.1.1 Primary map



X



Y

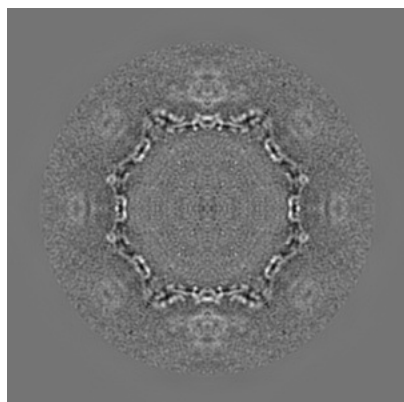


Z

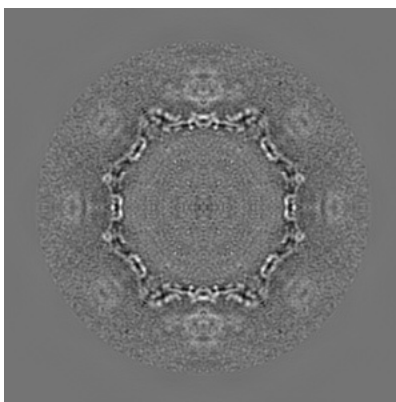
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

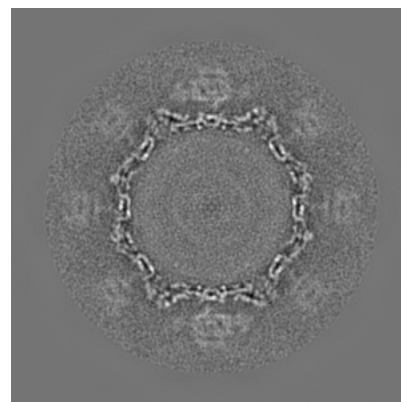
6.2.1 Primary map



X Index: 192



Y Index: 192

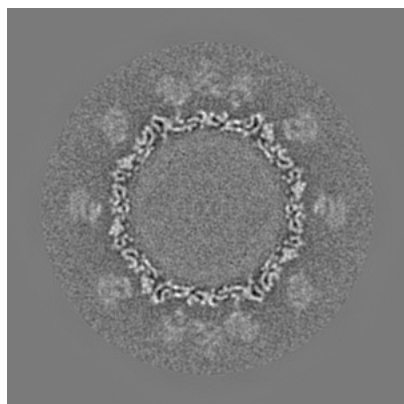


Z Index: 192

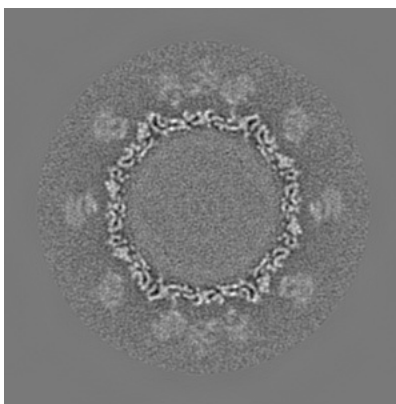
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

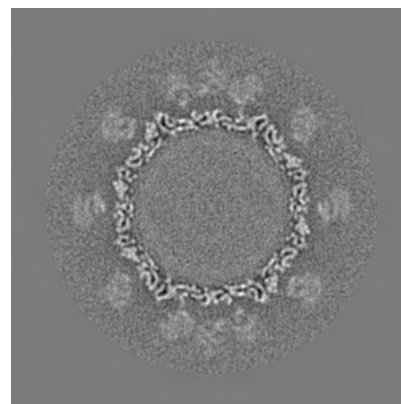
6.3.1 Primary map



X Index: 181



Y Index: 203



Z Index: 202

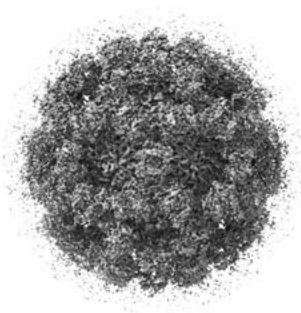
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

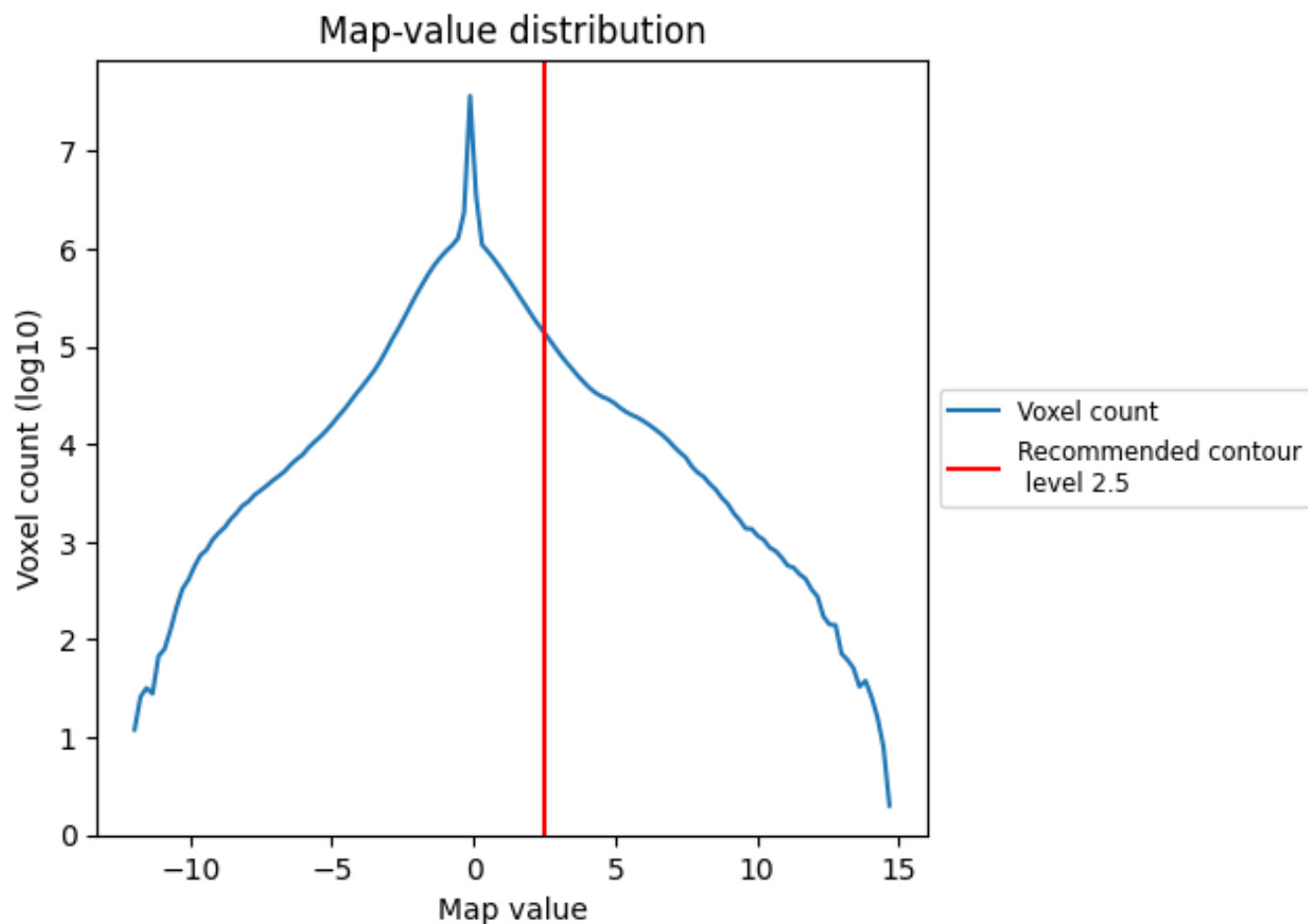
6.5 Mask visualisation

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

7 Map analysis [i](#)

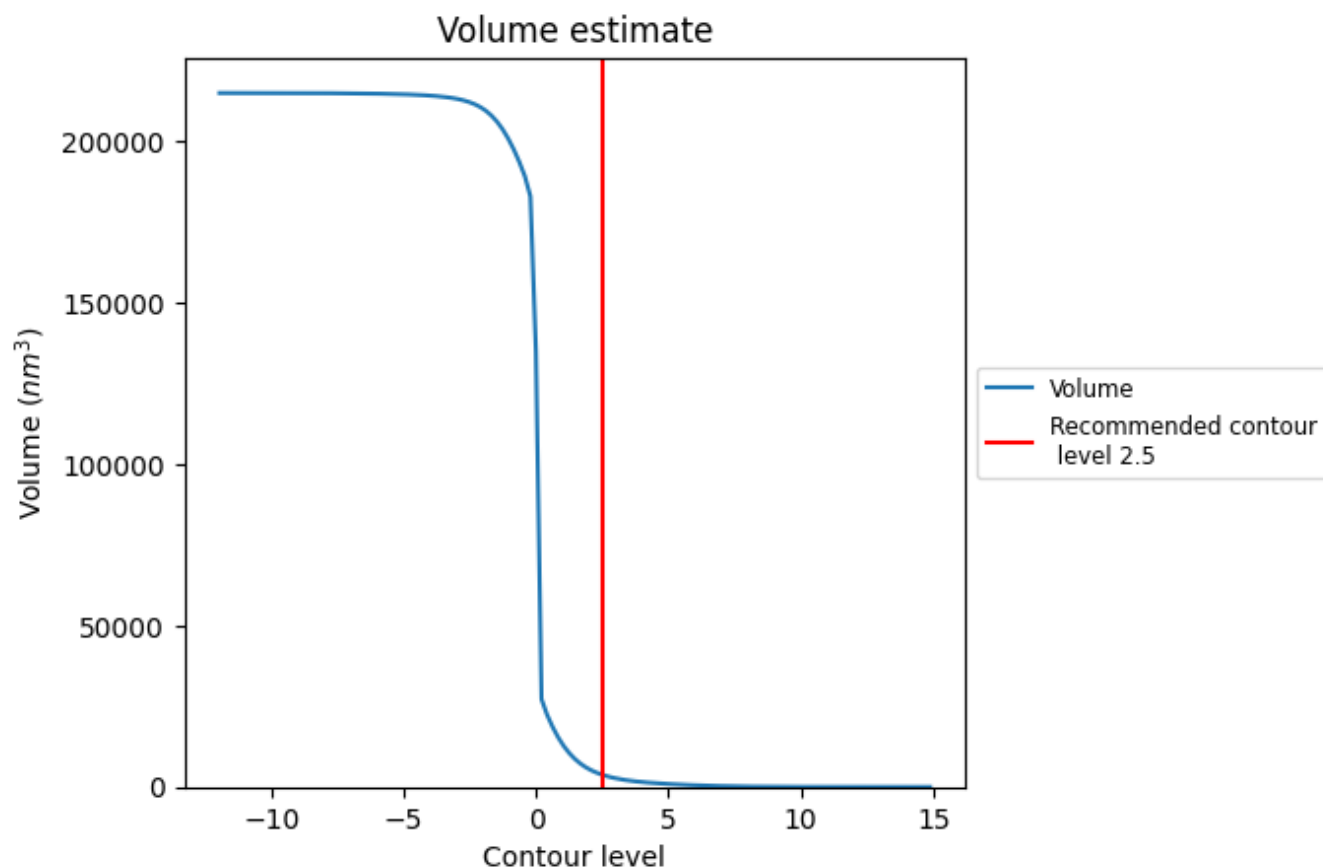
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

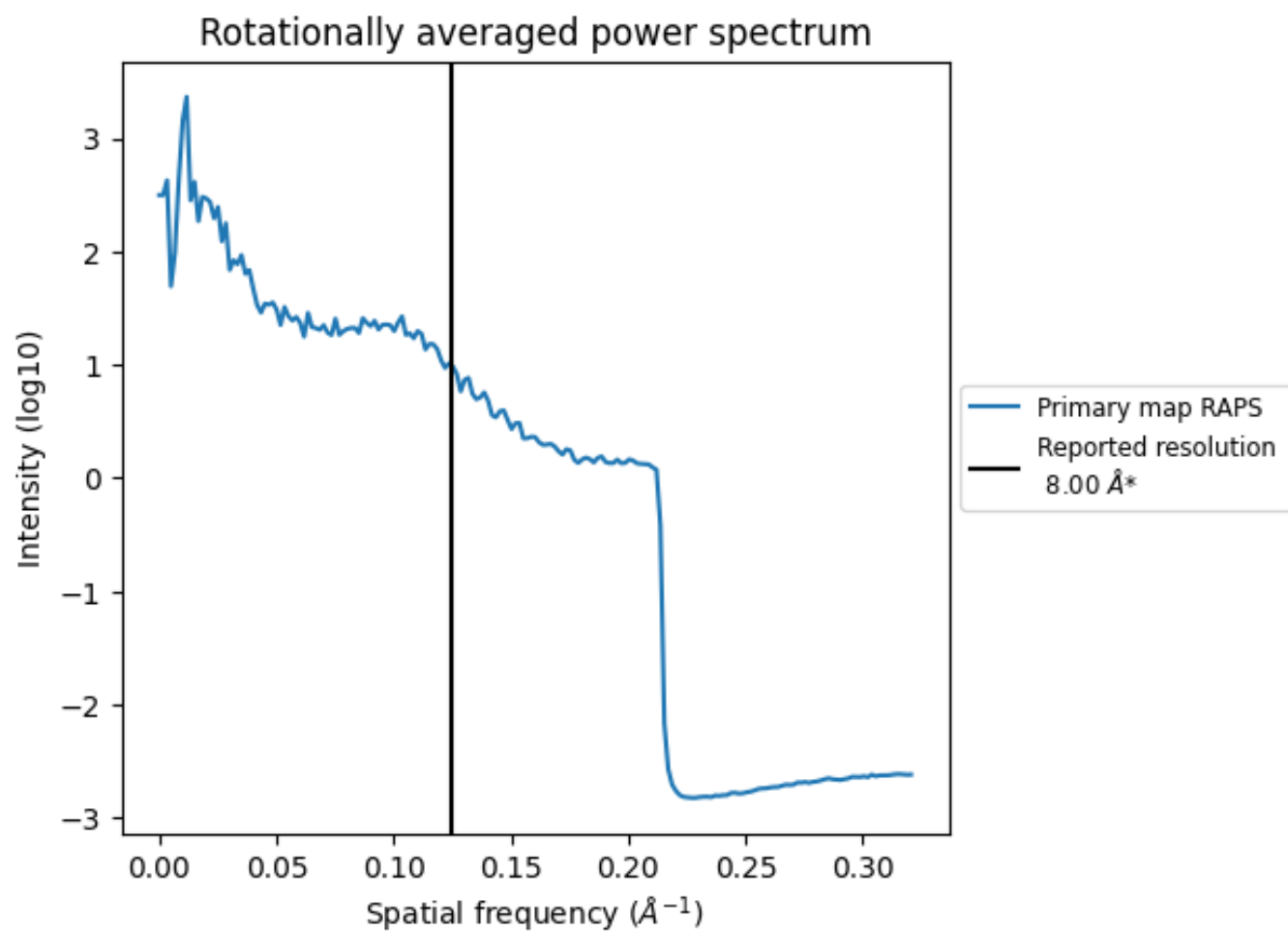
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3779 nm³; this corresponds to an approximate mass of 3414 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 0.125 Å⁻¹

8 Fourier-Shell correlation

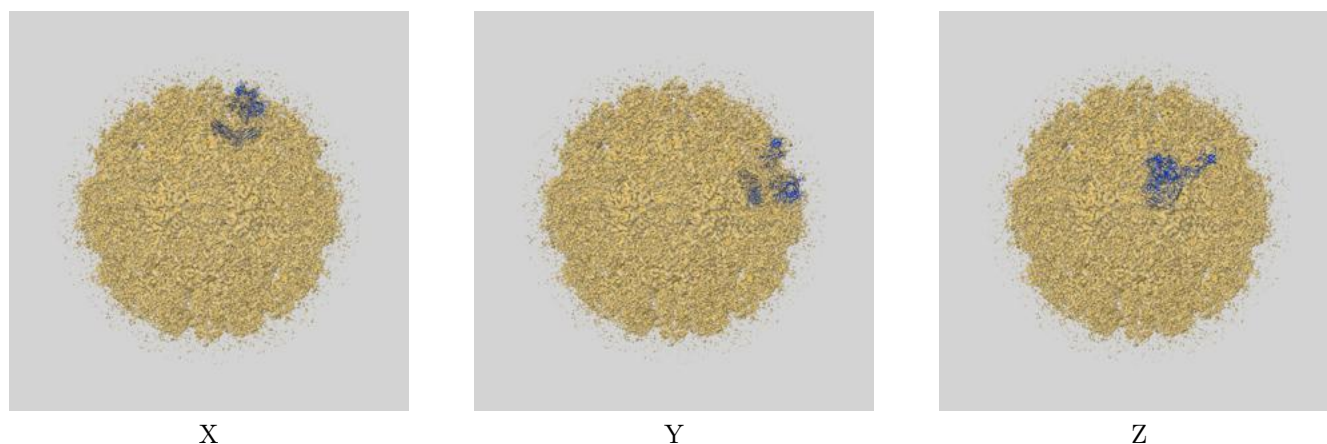
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

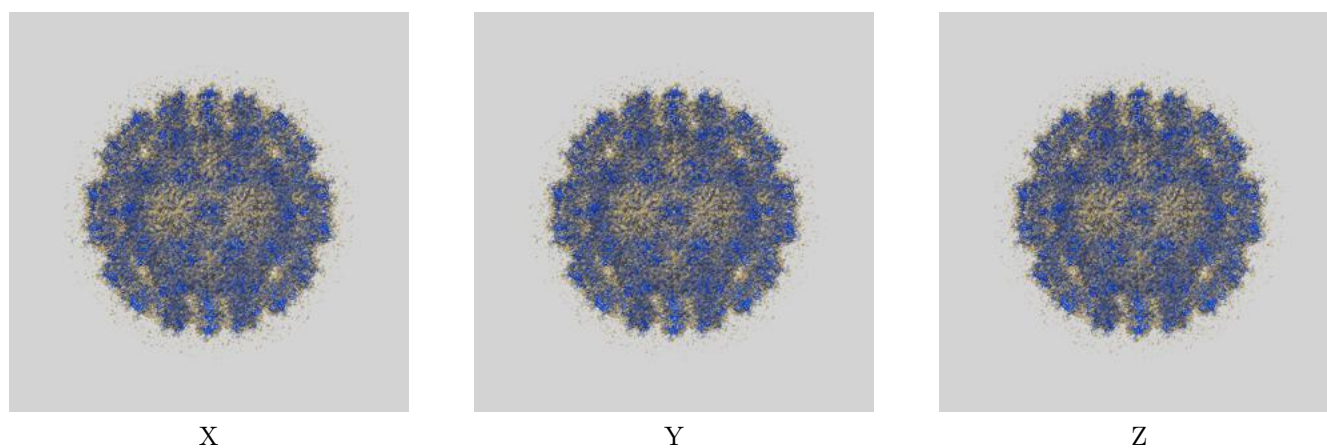
This section contains information regarding the fit between EMDB map EMD-7564 and PDB model 6CRJ. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

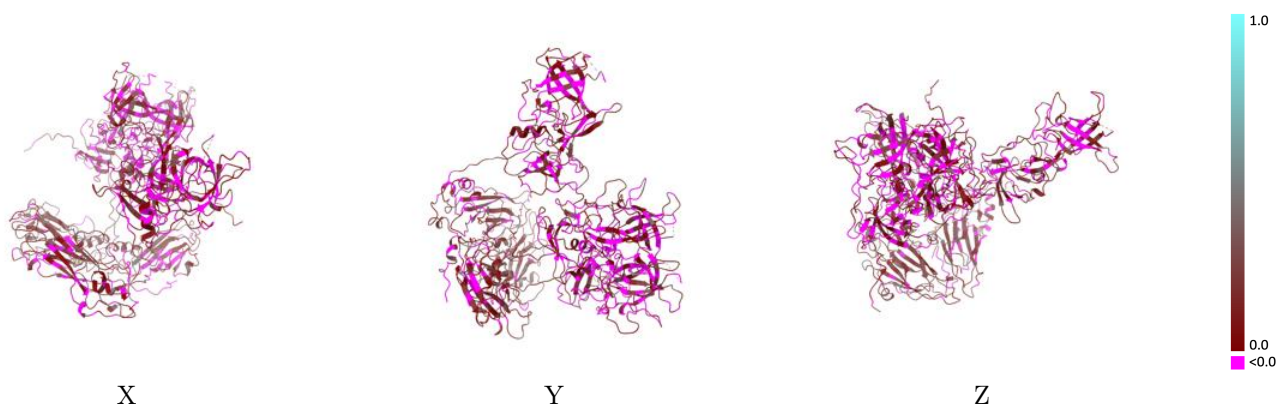


9.1.2 Map-model assembly overlay [i](#)



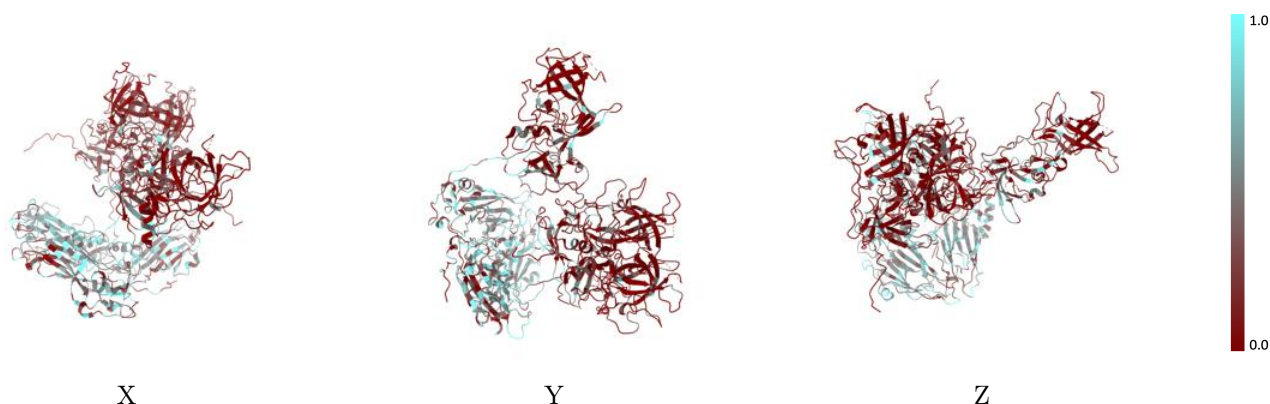
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



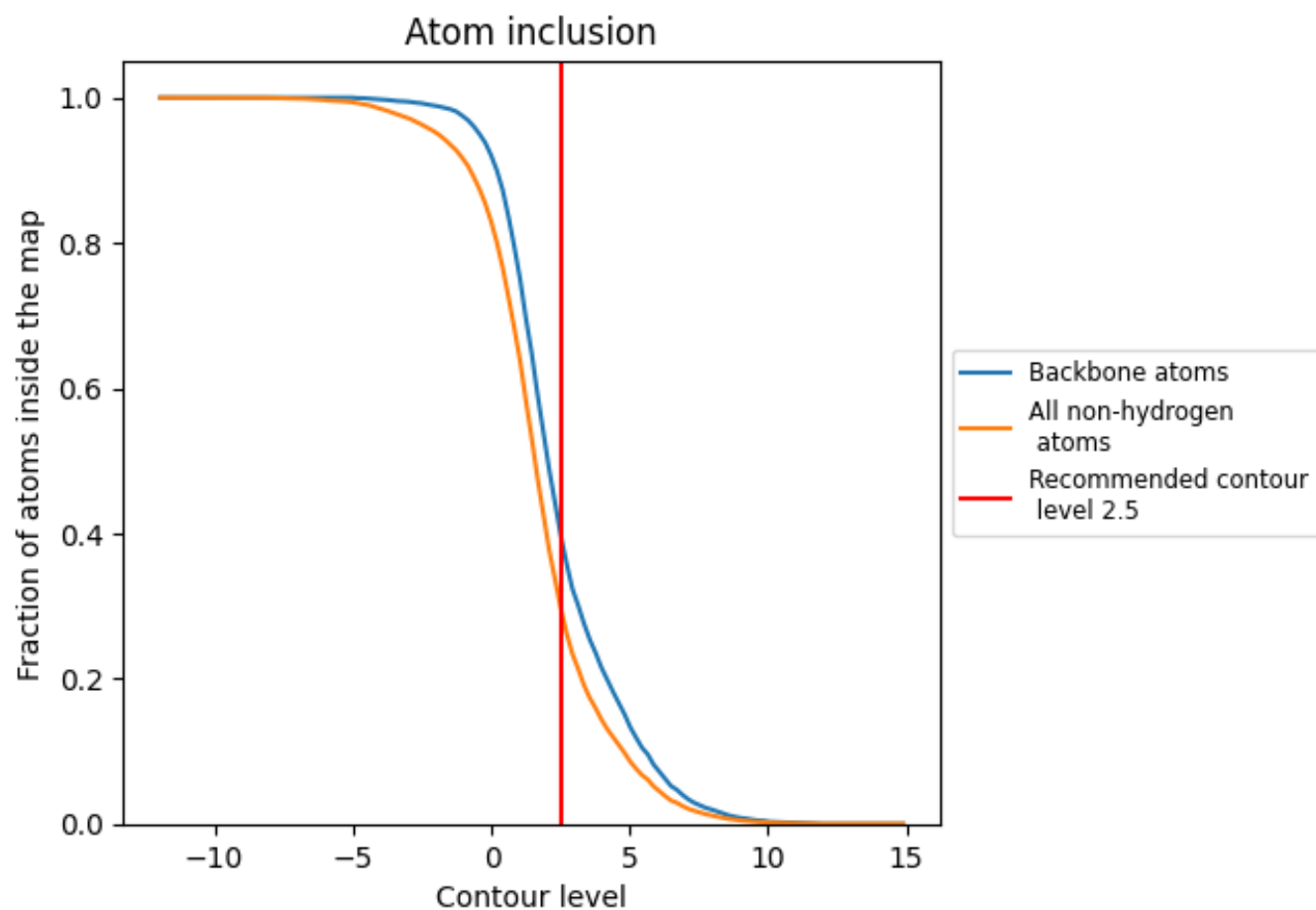
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 40% of all backbone atoms, 30% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.2981	<div></div> 0.0810
A	<div></div> 0.2846	<div></div> 0.0760
B	<div></div> 0.2857	<div></div> 0.0800
C	<div></div> 0.3245	<div></div> 0.0860

