



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 04:00 am GMT

PDB ID : 6GSH
EMDB ID : EMD-0054
Title : Feline Calicivirus Strain F9
Authors : Conley, M.J.; Bhella, D.
Deposited on : 2018-06-14
Resolution : 3.00 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

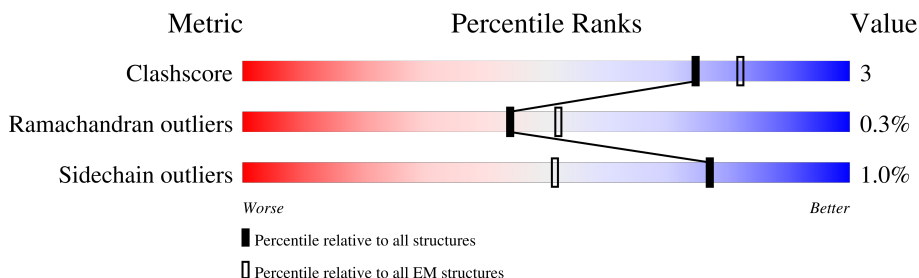
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	669	<p>80% 74% 5% 20%</p>
1	B	669	<p>79% 73% 6% 21%</p>
1	C	669	<p>80% 72% 7% 20%</p>

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 24297 atoms, of which 12040 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 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	533	8100	2606	4014	680	789	11	0	0
1	B	530	8071	2596	4000	680	784	11	0	0
1	C	534	8123	2612	4026	684	790	11	0	0

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ASN	ASP	conflict	UNP A2T4P8
A	21	VAL	ILE	conflict	UNP A2T4P8
A	23	ASP	ASN	conflict	UNP A2T4P8
A	73	ALA	SER	conflict	UNP A2T4P8
A	82	ALA	SER	conflict	UNP A2T4P8
A	90	ALA	GLU	conflict	UNP A2T4P8
A	94	ILE	LEU	conflict	UNP A2T4P8
A	108	GLY	ASN	conflict	UNP A2T4P8
A	127	GLY	-	insertion	UNP A2T4P8
A	133	ALA	THR	conflict	UNP A2T4P8
A	139	PRO	MET	conflict	UNP A2T4P8
A	148	SER	ASN	conflict	UNP A2T4P8
A	149	ALA	THR	conflict	UNP A2T4P8
A	304	SER	THR	conflict	UNP A2T4P8
A	319	ALA	PRO	conflict	UNP A2T4P8
A	345	LYS	ARG	conflict	UNP A2T4P8
A	355	HIS	TYR	conflict	UNP A2T4P8
A	357	THR	SER	conflict	UNP A2T4P8
A	363	VAL	ILE	conflict	UNP A2T4P8
A	392	ILE	MET	conflict	UNP A2T4P8
A	402	ALA	SER	conflict	UNP A2T4P8
A	429	LYS	THR	conflict	UNP A2T4P8
A	440	ASN	ASP	conflict	UNP A2T4P8
A	441	LYS	GLN	conflict	UNP A2T4P8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	442	SER	THR	conflict	UNP A2T4P8
A	447	THR	VAL	conflict	UNP A2T4P8
A	449	ALA	PRO	conflict	UNP A2T4P8
A	450	ALA	SER	conflict	UNP A2T4P8
A	451	GLY	ARG	conflict	UNP A2T4P8
A	452	TYR	PHE	conflict	UNP A2T4P8
A	454	GLY	ALA	conflict	UNP A2T4P8
A	456	ASP	ILE	conflict	UNP A2T4P8
A	457	VAL	THR	conflict	UNP A2T4P8
A	472	SER	ALA	conflict	UNP A2T4P8
A	493	LYS	ARG	conflict	UNP A2T4P8
A	494	VAL	GLU	conflict	UNP A2T4P8
A	495	ASP	ASN	conflict	UNP A2T4P8
A	497	ALA	LYS	conflict	UNP A2T4P8
A	498	ILE	LEU	conflict	UNP A2T4P8
A	499	GLU	ILE	conflict	UNP A2T4P8
A	506	MET	ALA	conflict	UNP A2T4P8
A	515	THR	ALA	conflict	UNP A2T4P8
A	519	LYS	ALA	conflict	UNP A2T4P8
A	529	SER	ALA	conflict	UNP A2T4P8
A	539	GLN	GLU	conflict	UNP A2T4P8
A	543	SER	ALA	conflict	UNP A2T4P8
A	603	PRO	ALA	conflict	UNP A2T4P8
A	615	SER	CYS	conflict	UNP A2T4P8
A	636	SER	ASN	conflict	UNP A2T4P8
A	665	SER	THR	conflict	UNP A2T4P8
B	13	ASN	ASP	conflict	UNP A2T4P8
B	21	VAL	ILE	conflict	UNP A2T4P8
B	23	ASP	ASN	conflict	UNP A2T4P8
B	73	ALA	SER	conflict	UNP A2T4P8
B	82	ALA	SER	conflict	UNP A2T4P8
B	90	ALA	GLU	conflict	UNP A2T4P8
B	94	ILE	LEU	conflict	UNP A2T4P8
B	108	GLY	ASN	conflict	UNP A2T4P8
B	127	GLY	-	insertion	UNP A2T4P8
B	133	ALA	THR	conflict	UNP A2T4P8
B	139	PRO	MET	conflict	UNP A2T4P8
B	148	SER	ASN	conflict	UNP A2T4P8
B	149	ALA	THR	conflict	UNP A2T4P8
B	304	SER	THR	conflict	UNP A2T4P8
B	319	ALA	PRO	conflict	UNP A2T4P8
B	345	LYS	ARG	conflict	UNP A2T4P8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	355	HIS	TYR	conflict	UNP A2T4P8
B	357	THR	SER	conflict	UNP A2T4P8
B	363	VAL	ILE	conflict	UNP A2T4P8
B	392	ILE	MET	conflict	UNP A2T4P8
B	402	ALA	SER	conflict	UNP A2T4P8
B	429	LYS	THR	conflict	UNP A2T4P8
B	440	ASN	ASP	conflict	UNP A2T4P8
B	441	LYS	GLN	conflict	UNP A2T4P8
B	442	SER	THR	conflict	UNP A2T4P8
B	447	THR	VAL	conflict	UNP A2T4P8
B	449	ALA	PRO	conflict	UNP A2T4P8
B	450	ALA	SER	conflict	UNP A2T4P8
B	451	GLY	ARG	conflict	UNP A2T4P8
B	452	TYR	PHE	conflict	UNP A2T4P8
B	454	GLY	ALA	conflict	UNP A2T4P8
B	456	ASP	ILE	conflict	UNP A2T4P8
B	457	VAL	THR	conflict	UNP A2T4P8
B	472	SER	ALA	conflict	UNP A2T4P8
B	493	LYS	ARG	conflict	UNP A2T4P8
B	494	VAL	GLU	conflict	UNP A2T4P8
B	495	ASP	ASN	conflict	UNP A2T4P8
B	497	ALA	LYS	conflict	UNP A2T4P8
B	498	ILE	LEU	conflict	UNP A2T4P8
B	499	GLU	ILE	conflict	UNP A2T4P8
B	506	MET	ALA	conflict	UNP A2T4P8
B	515	THR	ALA	conflict	UNP A2T4P8
B	519	LYS	ALA	conflict	UNP A2T4P8
B	529	SER	ALA	conflict	UNP A2T4P8
B	539	GLN	GLU	conflict	UNP A2T4P8
B	543	SER	ALA	conflict	UNP A2T4P8
B	603	PRO	ALA	conflict	UNP A2T4P8
B	615	SER	CYS	conflict	UNP A2T4P8
B	636	SER	ASN	conflict	UNP A2T4P8
B	665	SER	THR	conflict	UNP A2T4P8
C	13	ASN	ASP	conflict	UNP A2T4P8
C	21	VAL	ILE	conflict	UNP A2T4P8
C	23	ASP	ASN	conflict	UNP A2T4P8
C	73	ALA	SER	conflict	UNP A2T4P8
C	82	ALA	SER	conflict	UNP A2T4P8
C	90	ALA	GLU	conflict	UNP A2T4P8
C	94	ILE	LEU	conflict	UNP A2T4P8
C	108	GLY	ASN	conflict	UNP A2T4P8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	127	GLY	-	insertion	UNP A2T4P8
C	133	ALA	THR	conflict	UNP A2T4P8
C	139	PRO	MET	conflict	UNP A2T4P8
C	148	SER	ASN	conflict	UNP A2T4P8
C	149	ALA	THR	conflict	UNP A2T4P8
C	304	SER	THR	conflict	UNP A2T4P8
C	319	ALA	PRO	conflict	UNP A2T4P8
C	345	LYS	ARG	conflict	UNP A2T4P8
C	355	HIS	TYR	conflict	UNP A2T4P8
C	357	THR	SER	conflict	UNP A2T4P8
C	363	VAL	ILE	conflict	UNP A2T4P8
C	392	ILE	MET	conflict	UNP A2T4P8
C	402	ALA	SER	conflict	UNP A2T4P8
C	429	LYS	THR	conflict	UNP A2T4P8
C	440	ASN	ASP	conflict	UNP A2T4P8
C	441	LYS	GLN	conflict	UNP A2T4P8
C	442	SER	THR	conflict	UNP A2T4P8
C	447	THR	VAL	conflict	UNP A2T4P8
C	449	ALA	PRO	conflict	UNP A2T4P8
C	450	ALA	SER	conflict	UNP A2T4P8
C	451	GLY	ARG	conflict	UNP A2T4P8
C	452	TYR	PHE	conflict	UNP A2T4P8
C	454	GLY	ALA	conflict	UNP A2T4P8
C	456	ASP	ILE	conflict	UNP A2T4P8
C	457	VAL	THR	conflict	UNP A2T4P8
C	472	SER	ALA	conflict	UNP A2T4P8
C	493	LYS	ARG	conflict	UNP A2T4P8
C	494	VAL	GLU	conflict	UNP A2T4P8
C	495	ASP	ASN	conflict	UNP A2T4P8
C	497	ALA	LYS	conflict	UNP A2T4P8
C	498	ILE	LEU	conflict	UNP A2T4P8
C	499	GLU	ILE	conflict	UNP A2T4P8
C	506	MET	ALA	conflict	UNP A2T4P8
C	515	THR	ALA	conflict	UNP A2T4P8
C	519	LYS	ALA	conflict	UNP A2T4P8
C	529	SER	ALA	conflict	UNP A2T4P8
C	539	GLN	GLU	conflict	UNP A2T4P8
C	543	SER	ALA	conflict	UNP A2T4P8
C	603	PRO	ALA	conflict	UNP A2T4P8
C	615	SER	CYS	conflict	UNP A2T4P8
C	636	SER	ASN	conflict	UNP A2T4P8
C	665	SER	THR	conflict	UNP A2T4P8

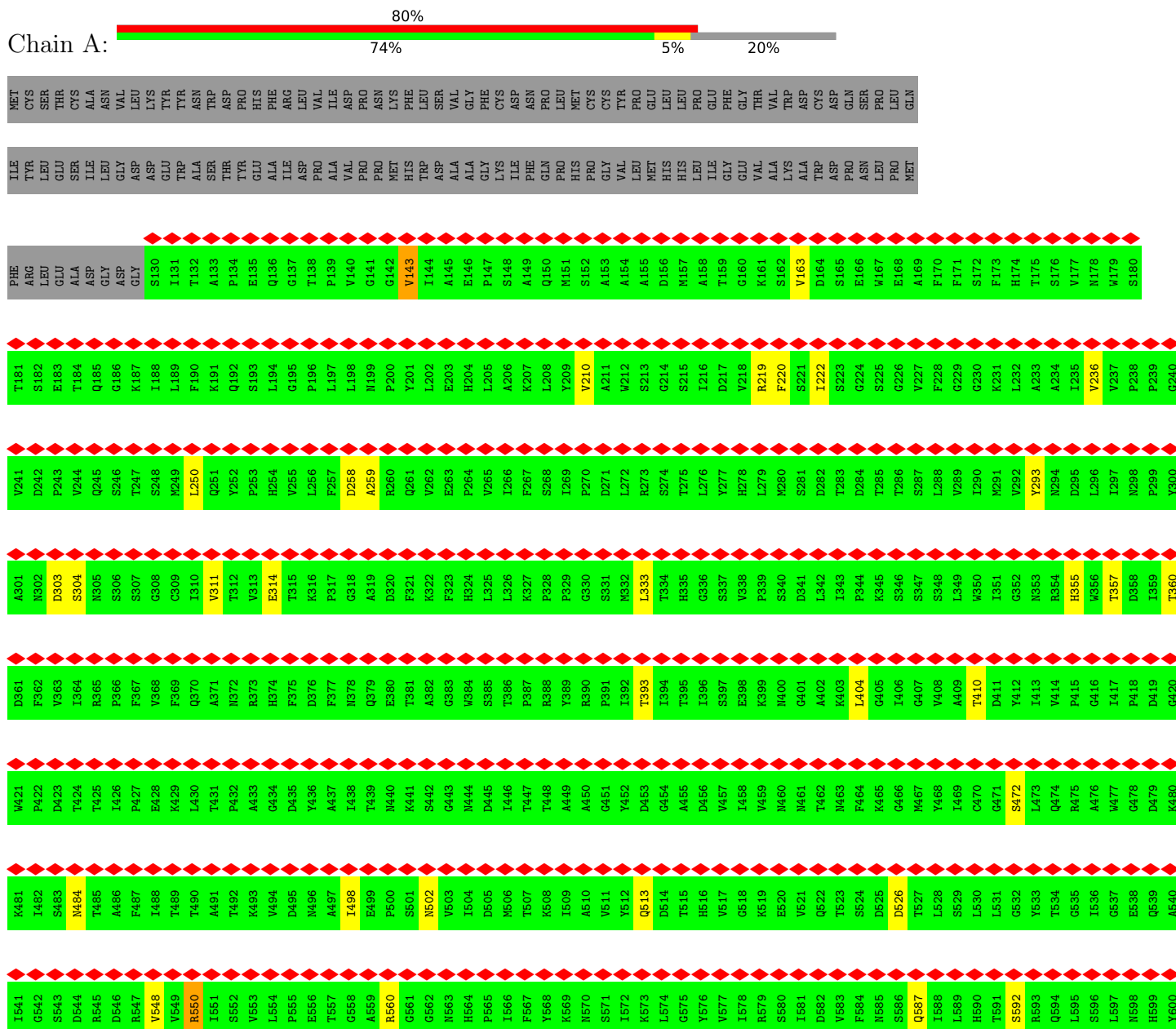
- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total K 1 1	0
2	B	1	Total K 1 1	0
2	C	1	Total K 1 1	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.

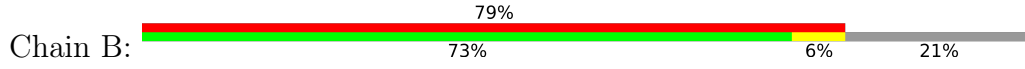
• Molecule 1: VP1



L601	L602	P603	P604	D605	S606	F607	A608	V609	Y610	R611	I612	I613	D614	S615	M616	G617	S618	W619	F620	D621	I622	G623	I624	D625	D626	D627	G628	F629	S630	F631	V632	G633	V634	S635	S636	I637	G638	K639	L640	E641	P642	P643	L644	T645	A646	S647	Y648	M649	G650	I651	Q652	L653	A654	K655	I656	R657	L658	A659	S660
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

M661	I662	ARG	SER	SER	MET	THR	LYS	LEU
------	------	-----	-----	-----	-----	-----	-----	-----

• Molecule 1: VP1



MET	CYS	SER	THR	CYS	ALA	ASN	VAL	LEU	LYS	TYR	TRP	ALA	ASN	SER	TRP	ASP	PRO	HIS	PHE	LEU	SER	ASP	VAL	GLY	PHE	CYS	LYS	ASP	ILE	ASN	PRO	GLN	PRO	LEU	MET	CYS	PRO	GLY	ILE	GLU	PHE	GLY	THR	VAL	TRP	TRP	ASP	CYS	ASP	GLN	SER	LEU	PRO	LEU	GLN					
ILE	TYR	GLU	GLU	SER	ILE	LEU	GLY	ASP	ASP	GLU	TRP	ALA	SER	THR	TYR	THR	TYR	PRO	GLU	ALA	PHE	ILE	ASP	PRO	VAL	GLY	CYS	ILE	PHE	ASN	PRO	GLN	PRO	LEU	HIS	PRO	GLY	ILE	GLU	GLY	VAL	VAL	ALA	TRP	TRP	ASP	TRP	ASP	PRO	ASN	SER	PRO	LEU	PRO	MET					
PHE	ARG	LEU	GLU	ALA	ASP	GLY	ASP	GLY	SER	ILE	THR	THR	ALA	PI34	EI35	QI36	G137	T138	P139	V140	G141	G142	V143	I144	E145	A146	P147	S148	A149	Q150	M151	S152	A153	A154	A155	M157	A158	T159	K161	S162	V163	D164	S165	E166	W167	E168	A169	F170	F171	S172	F173	H174	T175	V176	M178	W179	S180			
T181	S182	E183	T184	Q185	G186	K187	I188	M189	F190	K191	Q192	S193	L194	G195	P196	L197	L198	M199	P200	Y201	L202	E203	H204	L205	A206	K207	L208	Y209	V210	A211	V212	S213	G214	S215	I216	D217	V218	R219	F220	S221	D222	S223	G224	S225	G226	S227	F228	G229	G230	K231	L232	A233	I235	V236	P237	P238	G240			
V241	D242	P243	V244	Q245	S246	T247	S248	M249	L250	Q251	Y252	P253	H254	V255	L256	F257	D258	A259	R260	Q261	V262	E263	P264	V265	F267	S268	I269	P270	D271	L272	R273	S274	T275	L276	Y277	H278	L279	M280	S281	D282	T283	D284	T285	T286	S287	L288	V289	L290	M291	V292	Y293	N294	D295	L296	I297	N298	P299	Y300		
A301	N302	D303	S304	N305	S306	S307	G308	C309	L310	V311	T312	V313	E314	T315	K316	P317	G318	A319	D320	F321	K322	F323	H324	L325	L326	K327	P328	P329	G330	S331	K332	L333	T334	H335	G336	S337	V338	P339	S340	D341	A342	K343	P344	K345	K346	T346	S347	S348	L349	W350	I351	G352	N353	R354	H355	W356	T357	P358	I359	T360
D361	F362	V363	I364	R365	P366	F367	V368	F369	K370	A371	N372	R373	H374	F375	D376	F377	N378	Q379	E380	T381	A382	G383	W384	S385	P387	R388	Y389	R390	P391	I392	T393	I394	T395	I396	S397	E398	K399	N400	G401	A402	K403	L404	G405	L406	G407	V408	A409	T410	D411	Y412	L413	W414	F415	G416	L417	P418	D419	G420		
W421	D422	D423	T424	T425	I426	P427	E428	K429	L430	T431	P432	A433	G434	D435	Y436	A437	I438	T439	M440	K441	S442	G443	M444	D445	T447	T448	I449	A450	A451	G452	D453	G454	A455	D456	V457	I458	V459	N460	M461	T462	M463	F464	K465	G466	D467	Y468	L469	C470	G471	S472	L473	W474	G475	A476	W477	P478	D479	K480		
K481	I482	S483	M484	T485	A486	F487	I488	T489	T490	A491	P492	K493	V494	D495	M496	A497	L498	E499	P500	S501	N502	V503	I504	D505	M506	T507	K508	I509	A510	V511	Y512	Q513	D514	T515	H516	V517	G518	K519	E520	V521	O522	T523	S524	D525	D526	T527	L528	S529	M530	L531	G532	Y533	T534	G535	L536	S537	G538	Q539	A540	
I541	G542	S543	D544	R545	D546	R547	V548	V549	Y550	I551	S552	V553	L554	P555	E556	T557	G558	A559	R560	G561	G562	M563	H564	P565	S566	F567	Y568	S569	N570	S571	I572	K573	L574	G575	Y576	Y577	I578	R579	S580	I581	D582	V583	F584	M585	G586	Q587	I588	L589	H590	T591	S592	R593	O594	L595	S596	L597	N598	H599	Y600	
L601	L602	P603	P604	D605	S606	F607	A608	V609	Y610	R611	I612	I613	D614	S615	M616	G617	S618	W619	F620	D621	I622	G623	I624	D625	D626	D627	G628	F629	S630	F631	V632	G633	V634	S635	S636	I637	G638	K639	L640	E641	P642	P643	L644	T645	A646	S647	Y648	M649	G650	I651	Q652	L653	A654	K655	I656	R657	L658	A659	S660	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	41436	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction was implemented through Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.459	Depositor
Minimum map value	-0.255	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.05	Depositor
Map size (\AA)	545.28, 545.28, 545.28	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.065, 1.065, 1.065	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:
K

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	0.45	0/4188	0.63	1/5711 (0.0%)
1	B	0.44	0/4173	0.62	1/5688 (0.0%)
1	C	0.47	0/4199	0.63	0/5725
All	All	0.45	0/12560	0.63	2/17124 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	642	PHE	N-CA-C	5.97	127.11	111.00
1	A	642	PHE	N-CA-C	5.75	126.54	111.00

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	4086	4014	4017	22	0
1	B	4071	4000	4003	28	0
1	C	4097	4026	4030	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12257	12040	12050	78	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 3.

The worst 5 of 78 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:360:THR:O	1:B:642:PHE:CE1	1.87	1.26
1:C:616:ASN:ND2	1:C:641:GLU:OE2	1.93	1.01
1:B:446:ILE:O	1:B:576:TYR:OH	1.83	0.96
1:B:360:THR:O	1:B:642:PHE:CD1	2.31	0.83
1:C:473:LEU:O	1:C:483:SER:OG	1.97	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	531/669 (79%)	484 (91%)	45 (8%)	2 (0%)	34 72
1	B	528/669 (79%)	478 (90%)	49 (9%)	1 (0%)	47 82
1	C	532/669 (80%)	480 (90%)	50 (9%)	2 (0%)	34 72
All	All	1591/2007 (79%)	1442 (91%)	144 (9%)	5 (0%)	44 76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	VAL
1	B	642	PHE
1	A	642	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	516	HIS
1	C	471	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	A	453/572 (79%)	449 (99%)	4 (1%)	78 92
1	B	451/572 (79%)	447 (99%)	4 (1%)	78 92
1	C	454/572 (79%)	448 (99%)	6 (1%)	69 89
All	All	1358/1716 (79%)	1344 (99%)	14 (1%)	77 91

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	642	PHE
1	C	388	ARG
1	C	642	PHE
1	C	550	ARG
1	C	641	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	400	ASN
1	C	616	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](#)

Of 3 ligands modelled in this entry, 3 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.

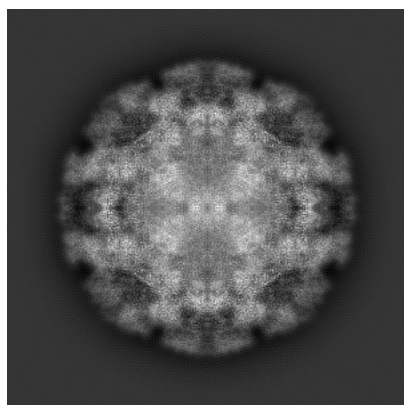
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0054. These allow visual inspection of the internal detail of the map and identification of artifacts.

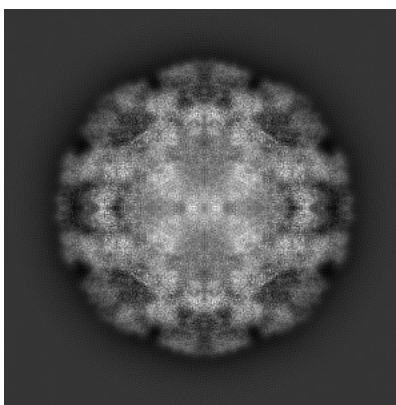
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

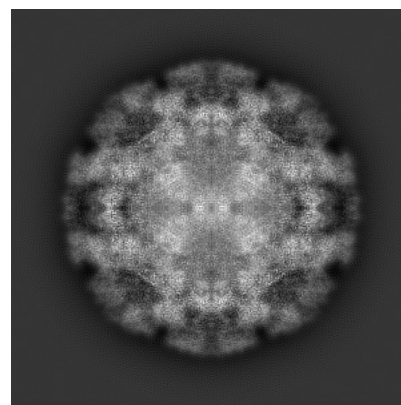
6.1.1 Primary map



X



Y

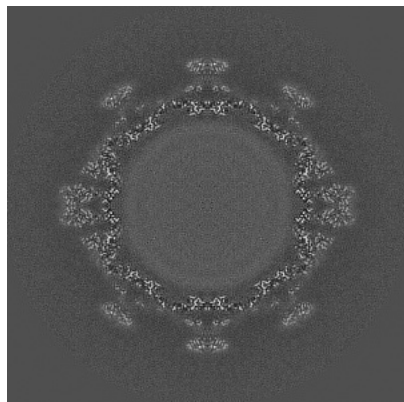


Z

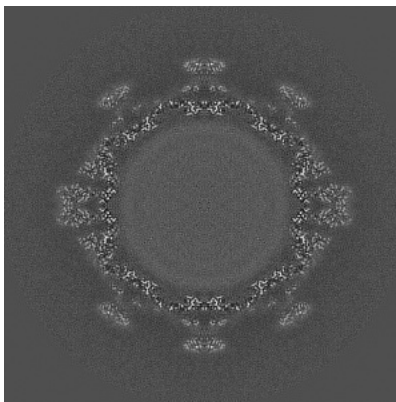
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

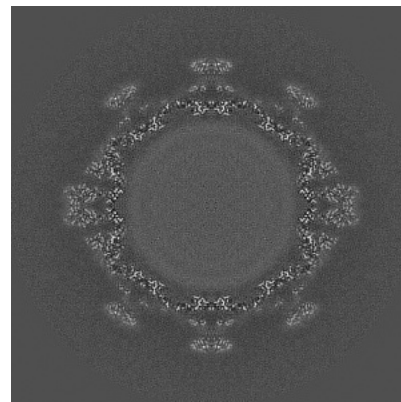
6.2.1 Primary map



X Index: 256



Y Index: 256

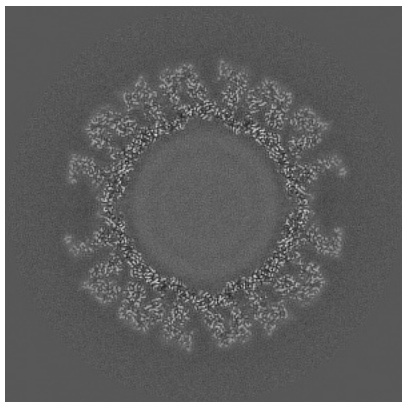


Z Index: 256

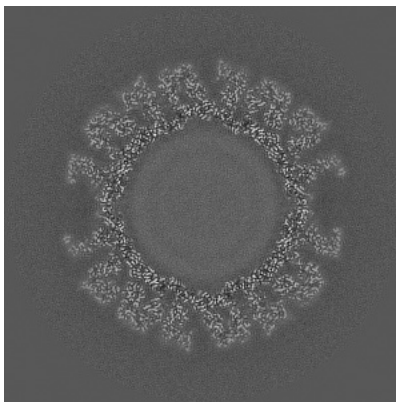
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

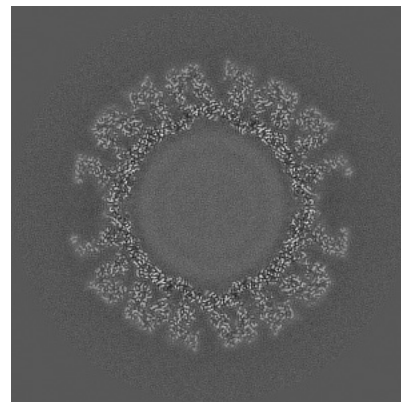
6.3.1 Primary map



X Index: 203



Y Index: 203

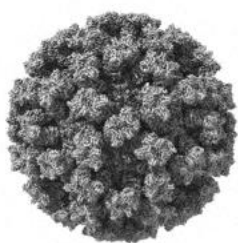


Z Index: 203

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

6.4 Orthogonal surface views [i](#)

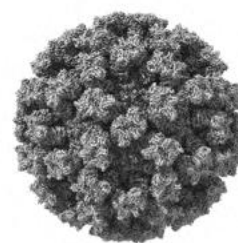
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

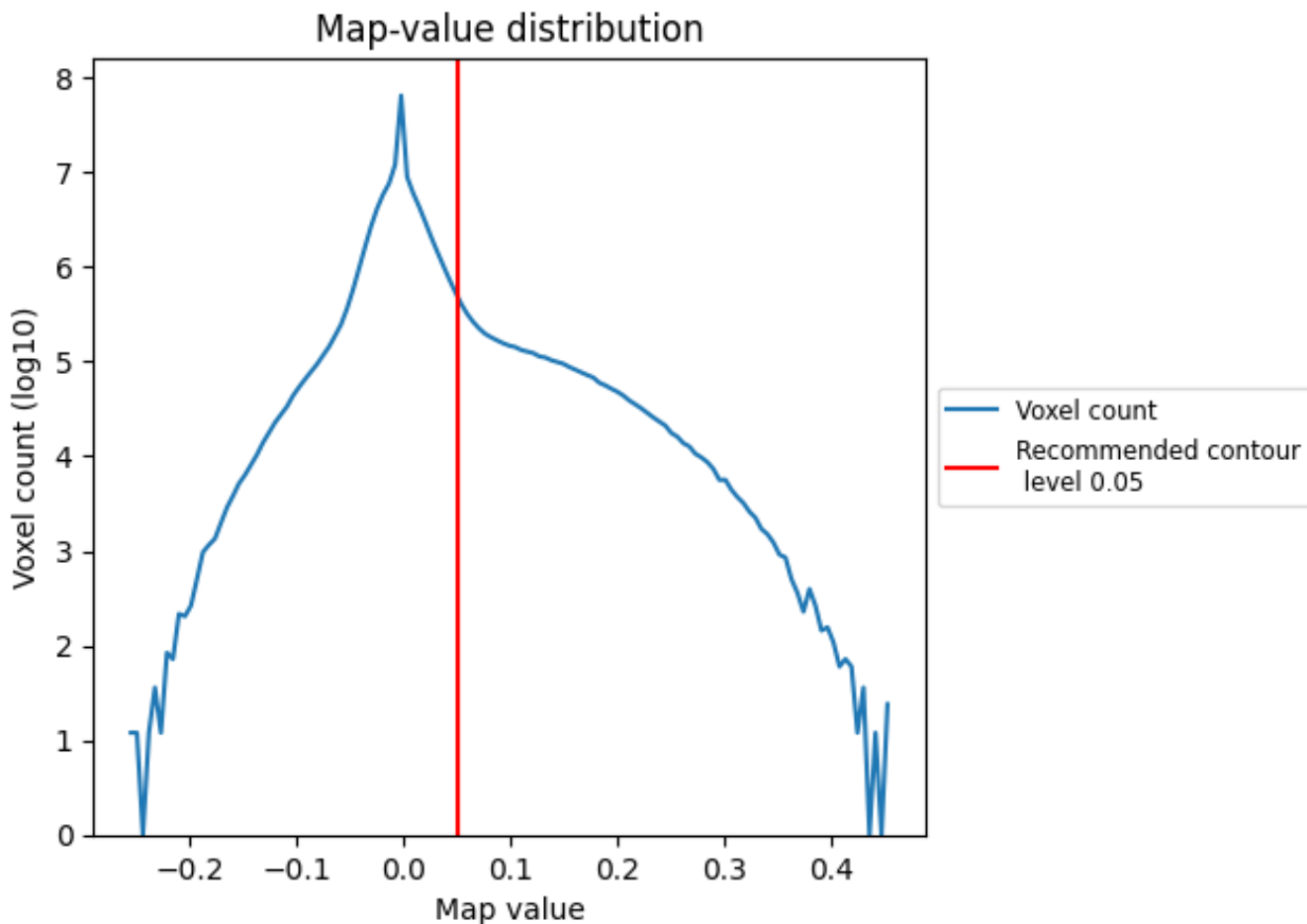
6.5 Mask visualisation

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

7 Map analysis [i](#)

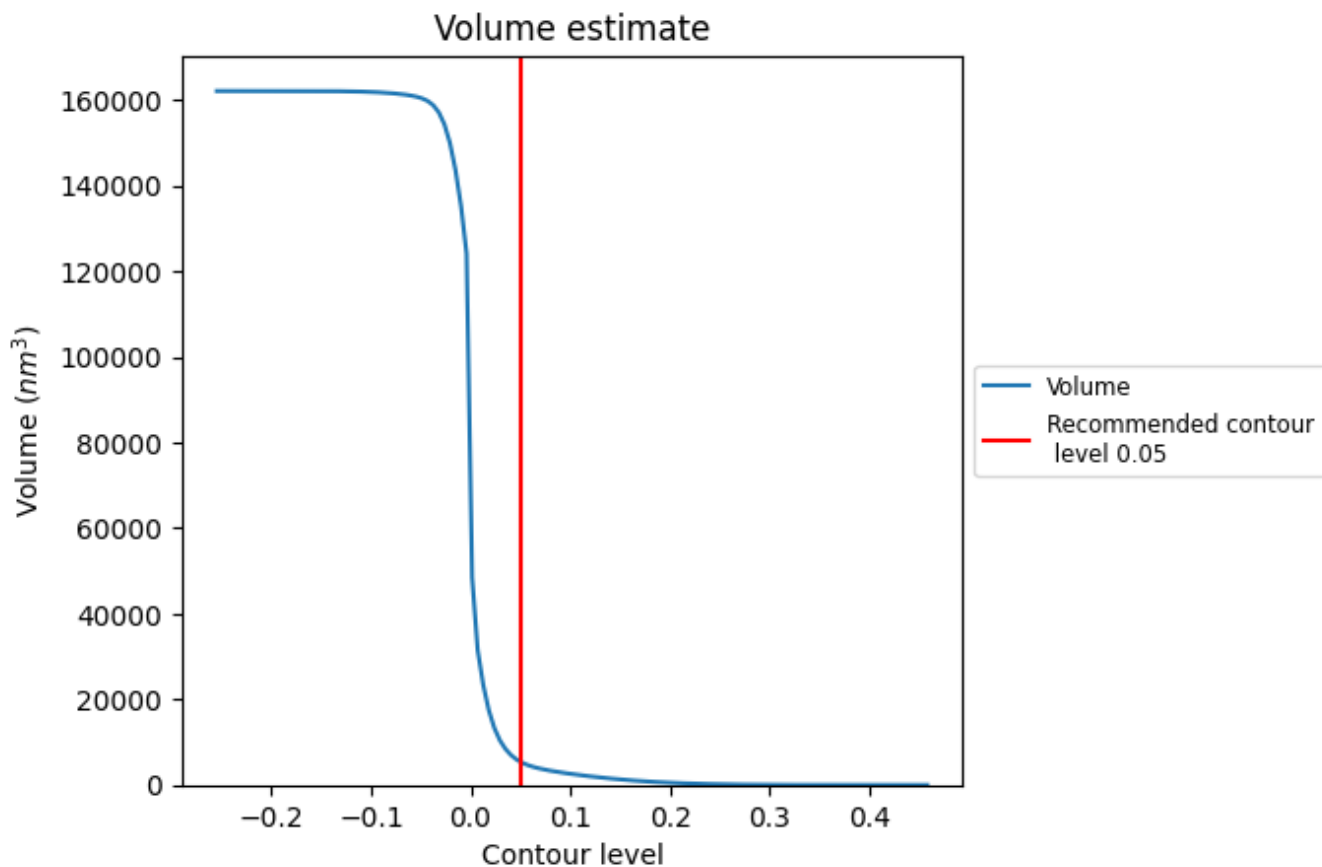
This section contains the results of statistical analysis of the map.

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.

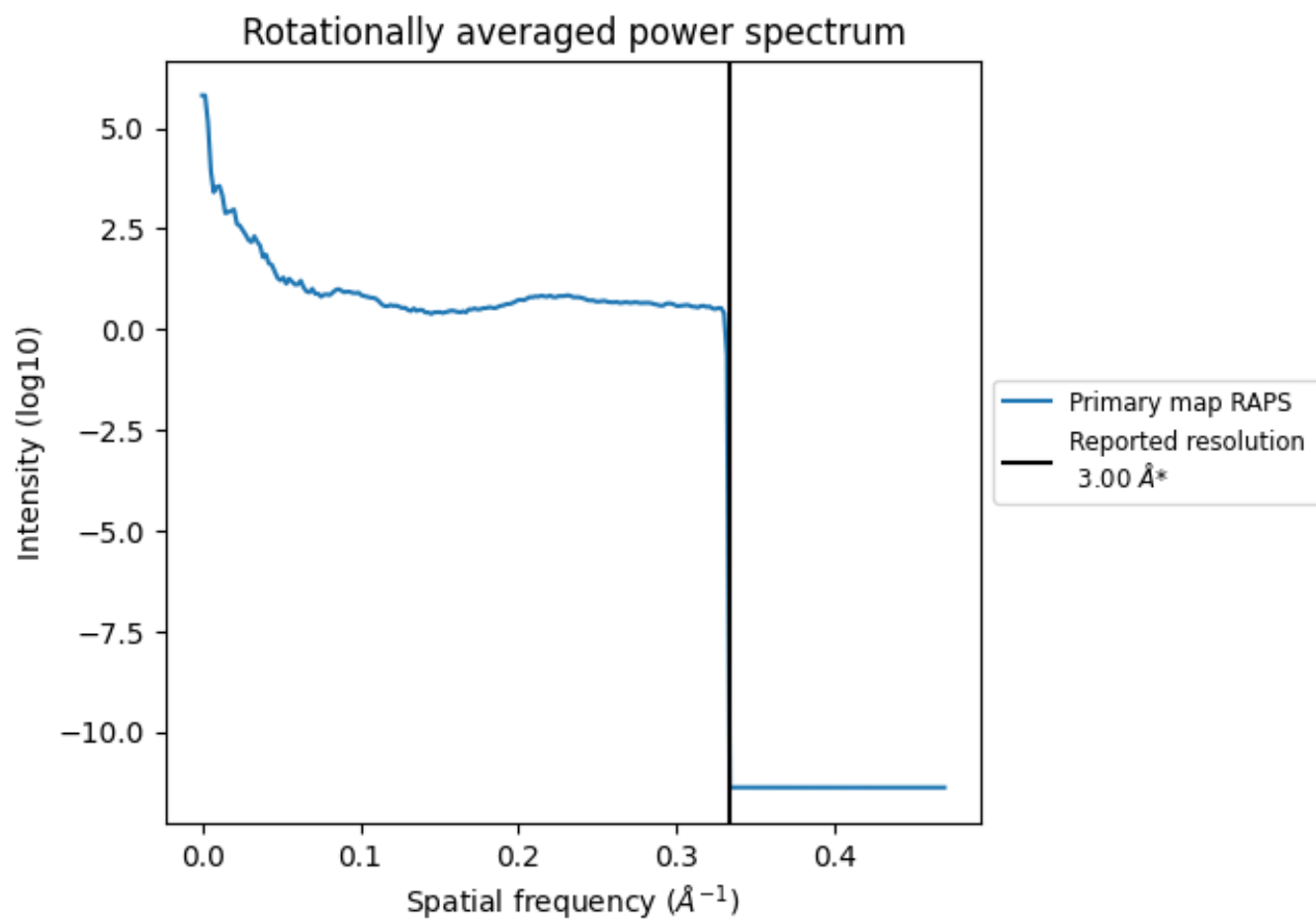
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5428 nm³; this corresponds to an approximate mass of 4903 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](#)

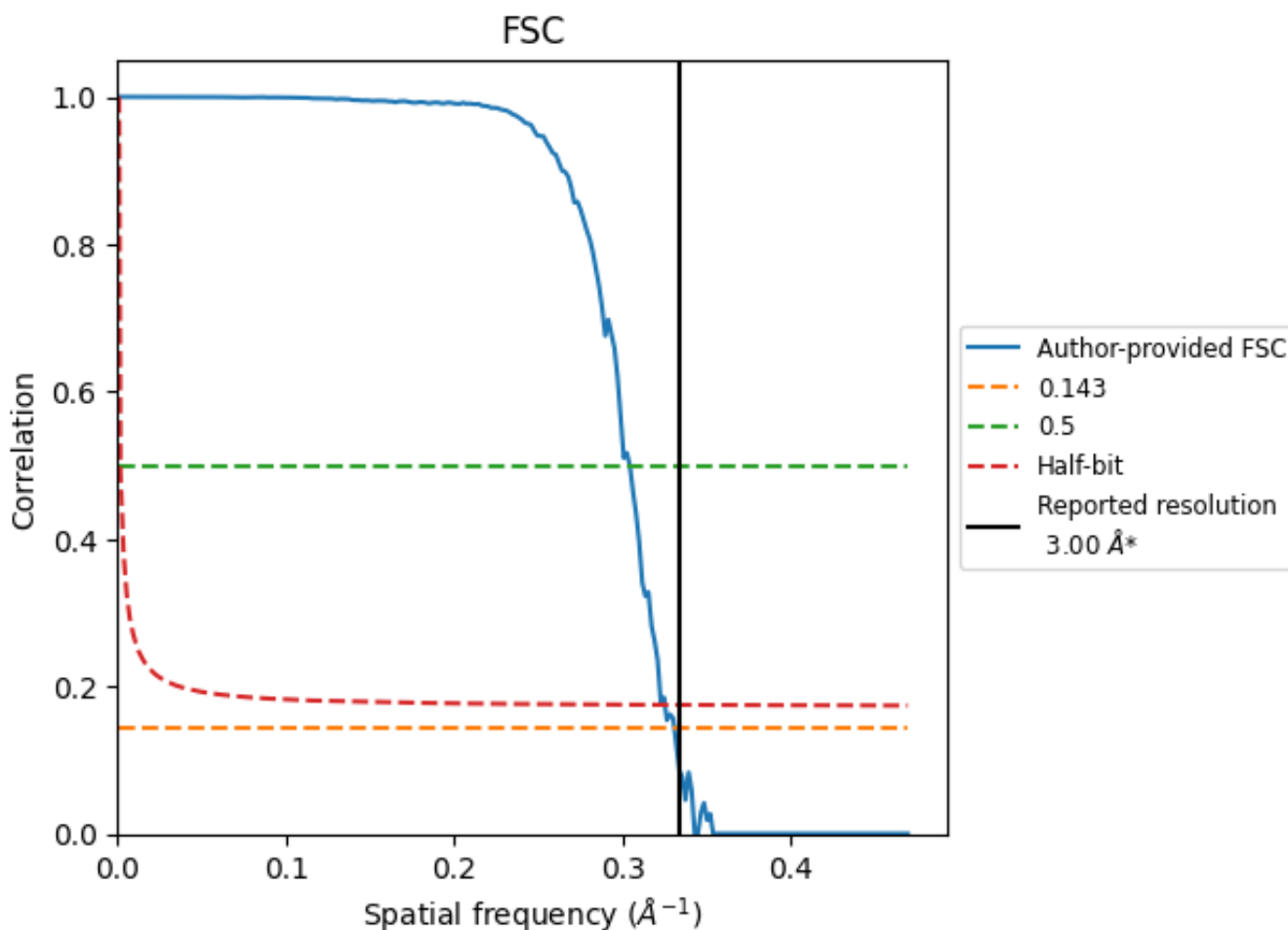


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.02	3.29	3.08
Unmasked-calculated*	-	-	-

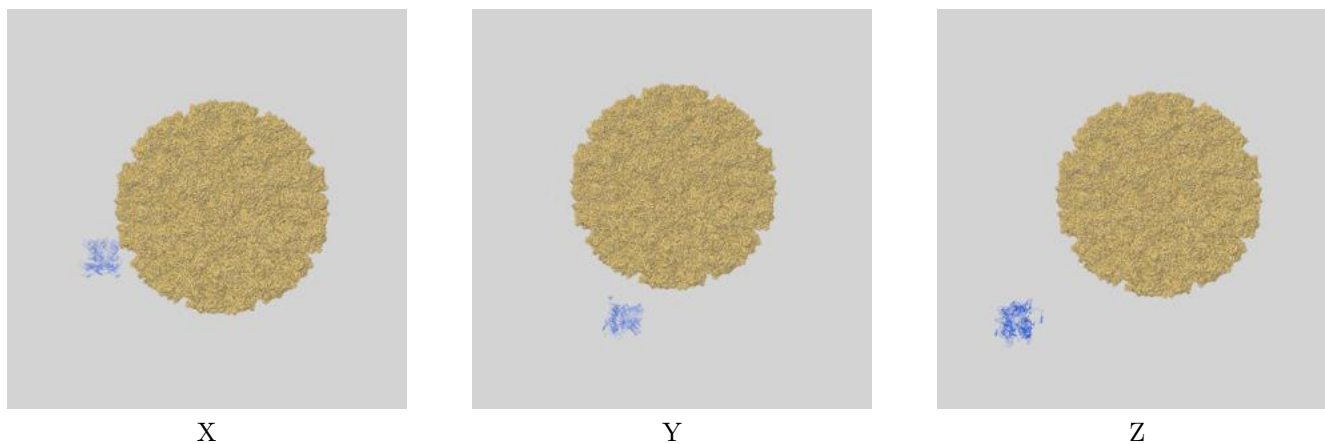
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

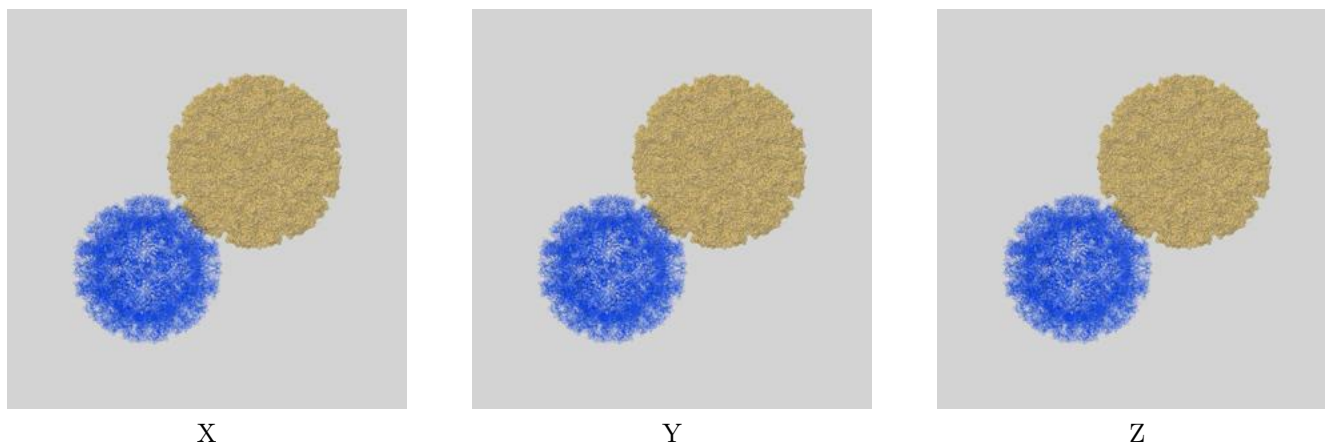
This section contains information regarding the fit between EMDB map EMD-0054 and PDB model 6GSH. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

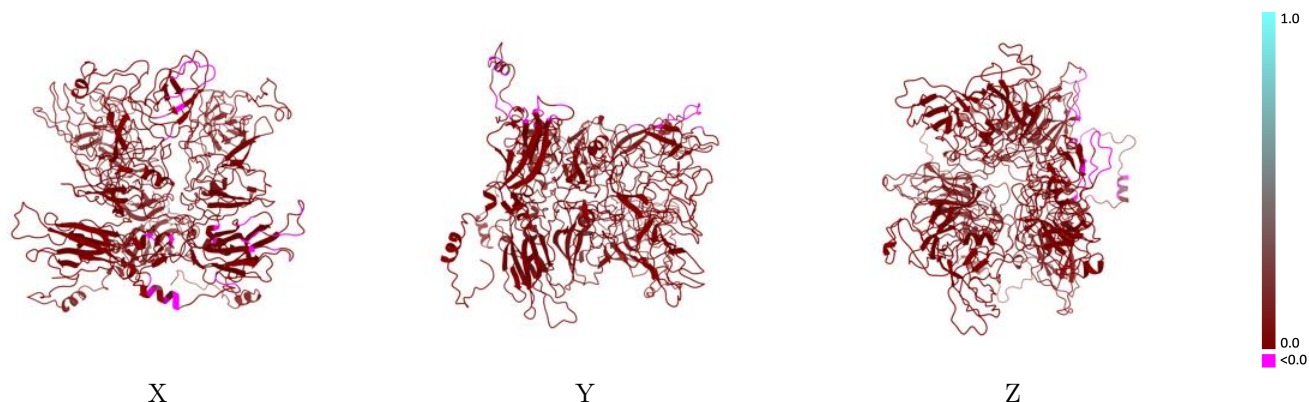


9.1.2 Map-model assembly overlay [i](#)



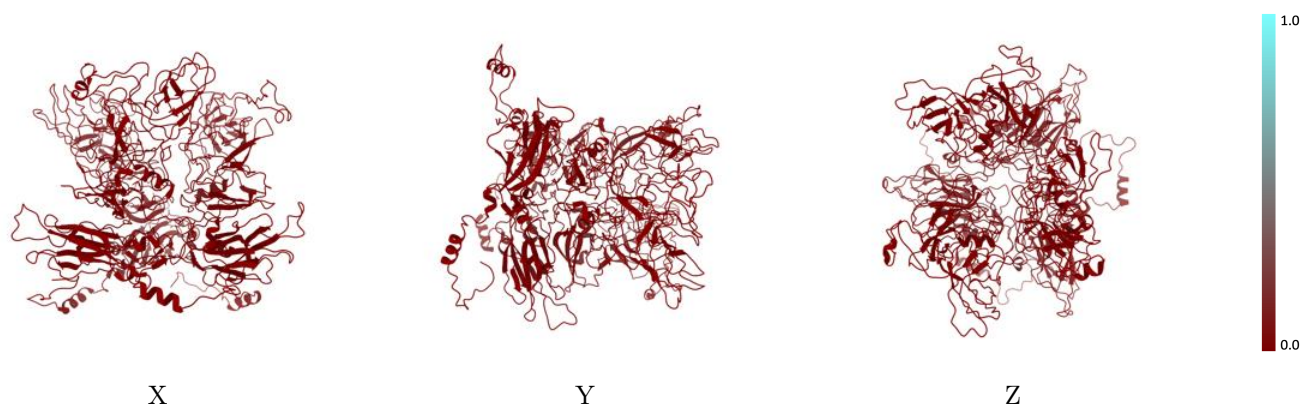
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



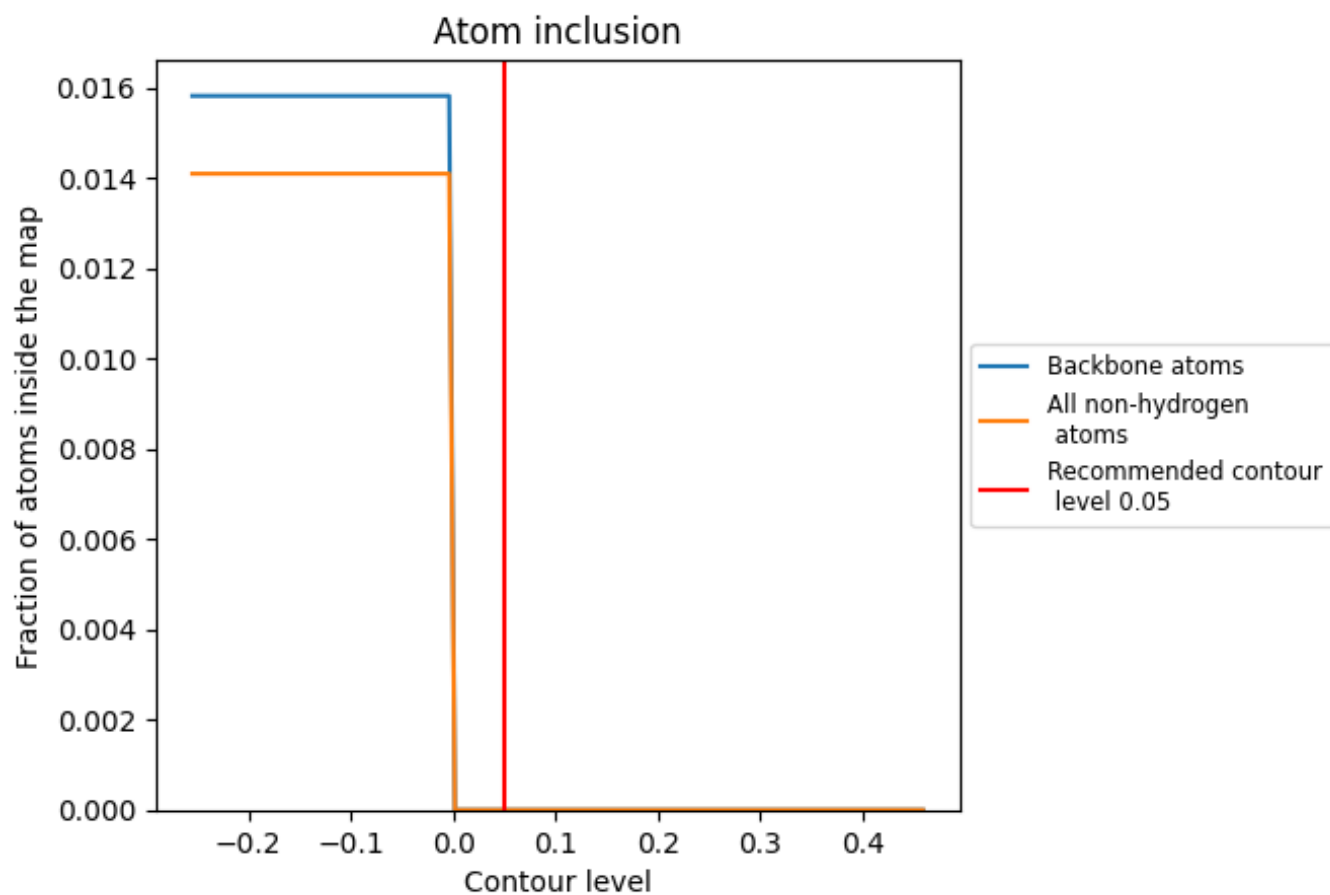
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).









9.4 Atom inclusion [i](#)



At the recommended contour level, 0% of all backbone atoms, 0% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.0000	 -0.0000
A	 0.0000	 0.0000
B	 0.0000	 -0.0000
C	 0.0000	 0.0000

