



Full wwPDB EM Validation Report ⓘ

Oct 5, 2024 – 01:56 pm BST

PDB ID : 5O6V
EMDB ID : EMD-3754
Title : The cryo-EM structure of Tick-borne encephalitis virus complexed with Fab fragment of neutralizing antibody 19/1786
Authors : Fuzik, T.; Plevka, P.
Deposited on : 2017-06-07
Resolution : 3.90 Å(reported)

This is a Full wwPDB EM Validation 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
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

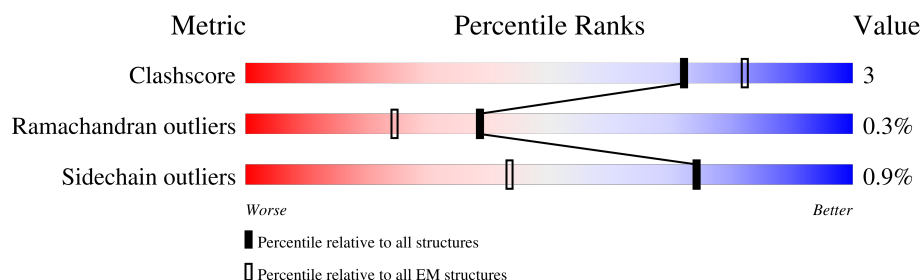
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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 ≥ 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	496	<div> <div>14%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	B	496	<div> <div>17%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
1	C	496	<div> <div>21%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
2	D	75	<div> <div>39%</div> <div>89%</div> <div>5%</div> <div>5%</div> </div>
2	E	75	<div> <div>36%</div> <div>85%</div> <div>9%</div> <div>5%</div> </div>
2	F	75	<div> <div>64%</div> <div>81%</div> <div>13%</div> <div>5%</div> </div>
3	H	212	<div> <div>66%</div> <div>91%</div> <div>9%</div> </div>
3	I	212	<div> <div>81%</div> <div>92%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
4	L	208	<div><div></div><div>74%</div><div></div><div>93%</div><div></div><div>7%</div></div>
4	M	208	<div><div></div><div>88%</div><div></div><div>90%</div><div></div><div>10%</div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19346 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 Envelope protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	492	Total	C	N	O	S	0	0
			3743	2371	654	693	25		
1	B	492	Total	C	N	O	S	0	0
			3743	2371	654	693	25		
1	C	492	Total	C	N	O	S	0	0
			3743	2371	654	693	25		

- Molecule 2 is a protein called Small envelope protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	71	Total	C	N	O	S	0	0
			557	363	100	92	2		
2	E	71	Total	C	N	O	S	0	0
			557	363	100	92	2		
2	F	71	Total	C	N	O	S	0	0
			557	363	100	92	2		

- Molecule 3 is a protein called Fab 19/1786 - Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	212	Total	C	N	O	S	0	0
			1597	1007	259	323	8		
3	I	212	Total	C	N	O	S	0	0
			1597	1007	259	323	8		

- Molecule 4 is a protein called Fab 19/1786 - Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	208	Total	C	N	O	S	0	0
			1605	998	270	330	7		
4	M	208	Total	C	N	O	S	0	0
			1605	998	270	330	7		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

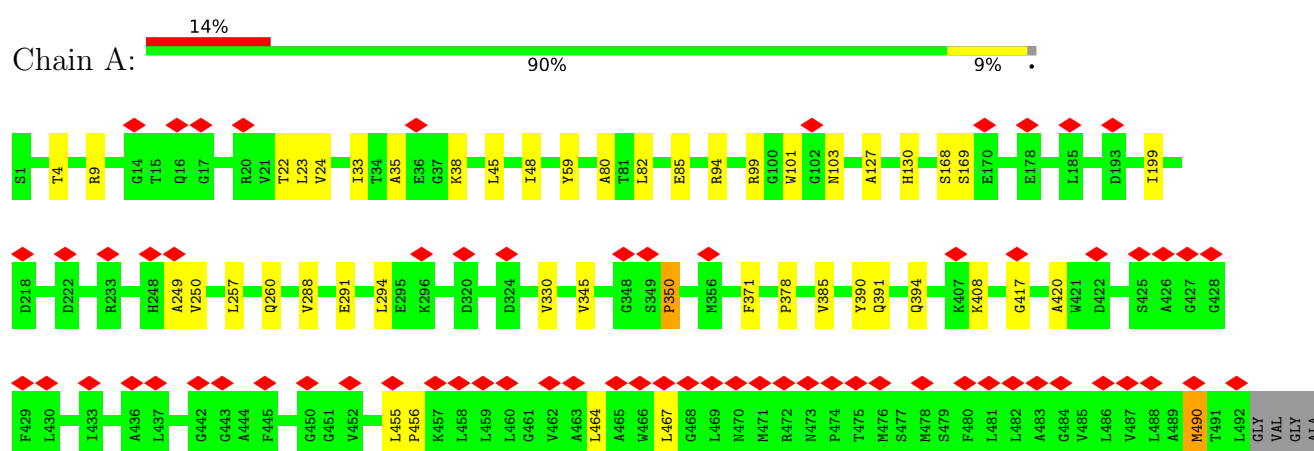


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	

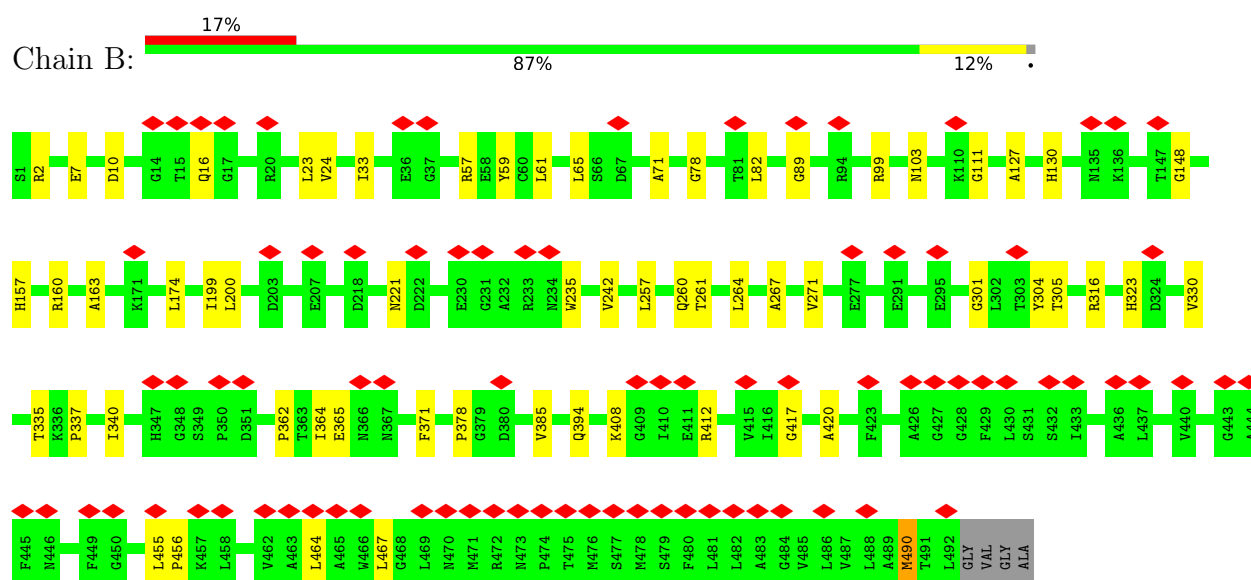
3 Residue-property plots

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.

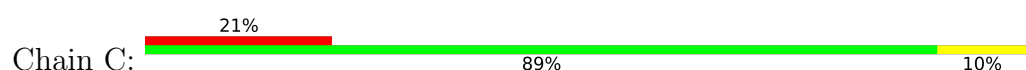
- Molecule 1: Envelope protein

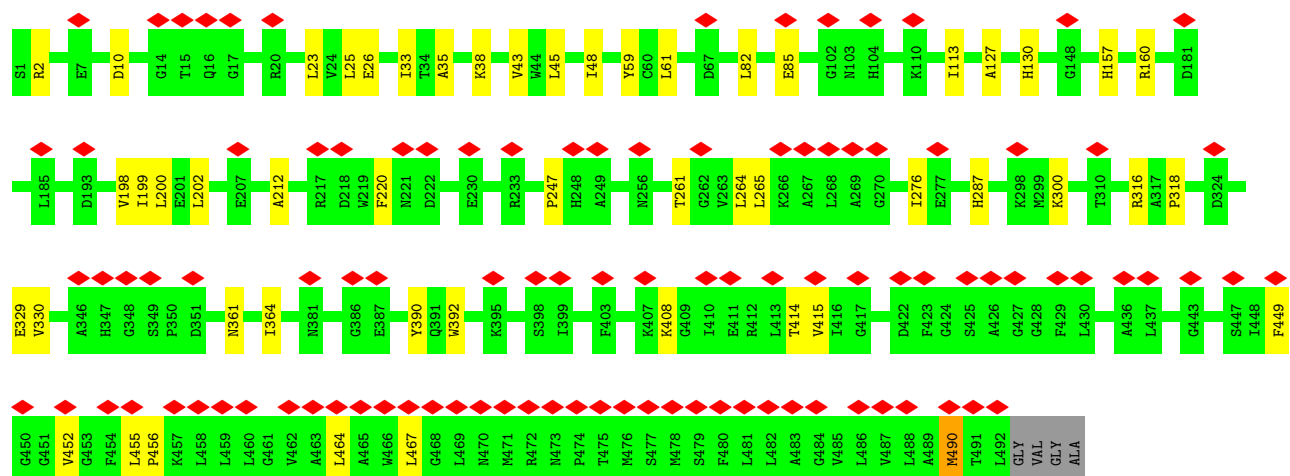


- Molecule 1: Envelope protein

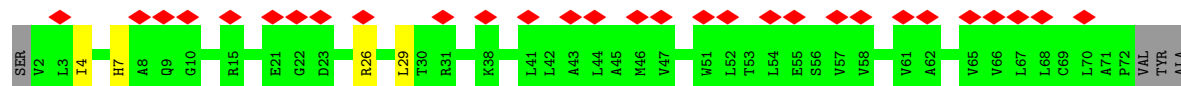
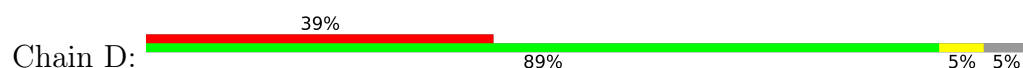


- Molecule 1: Envelope protein

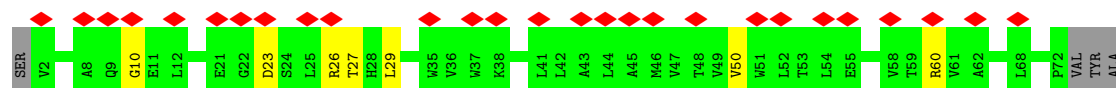
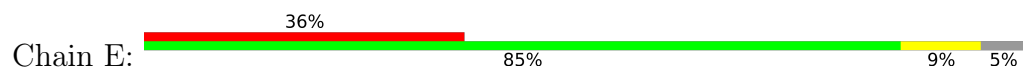




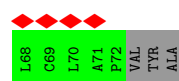
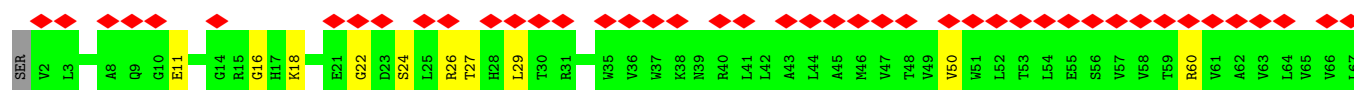
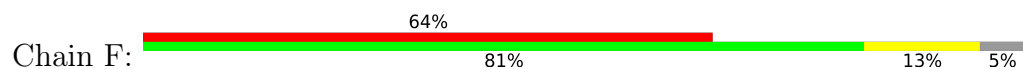
- Molecule 2: Small envelope protein M



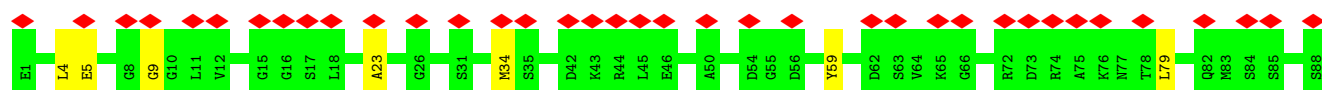
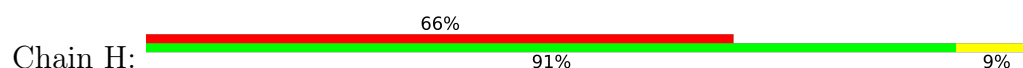
- Molecule 2: Small envelope protein M

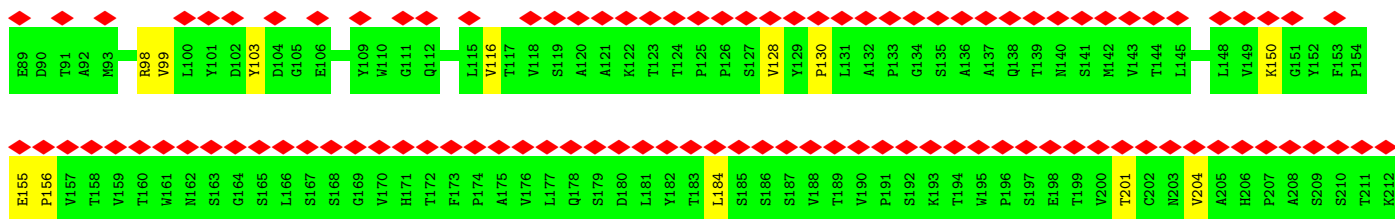


- Molecule 2: Small envelope protein M

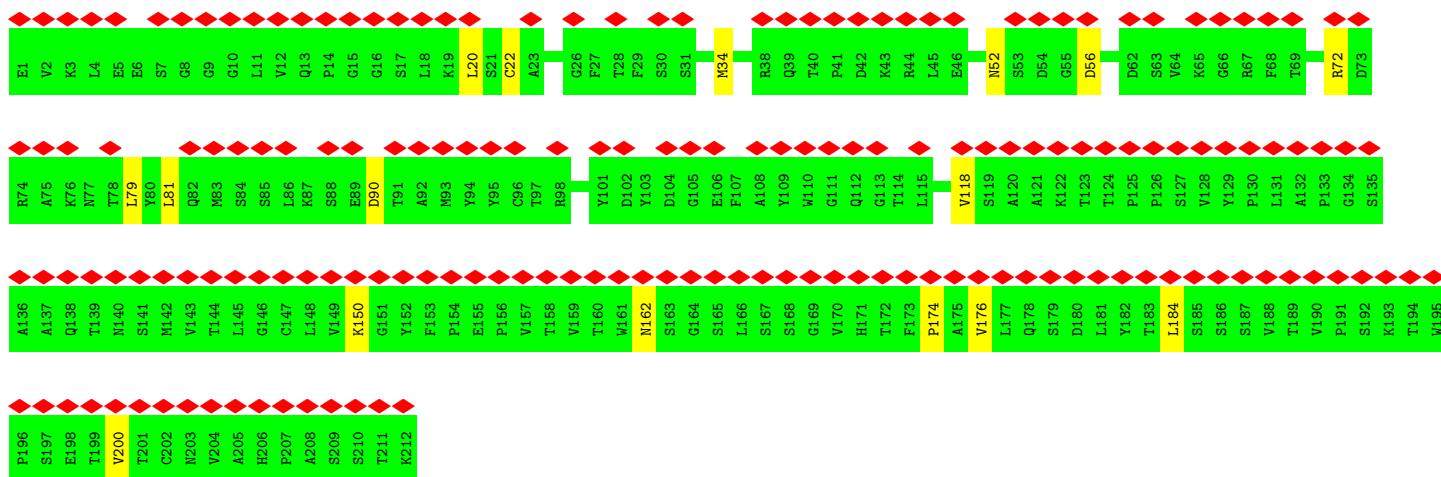
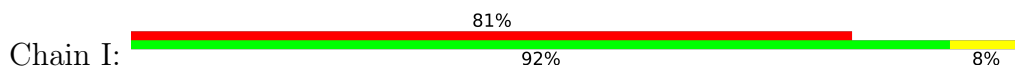


- Molecule 3: Fab 19/1786 - Heavy chain

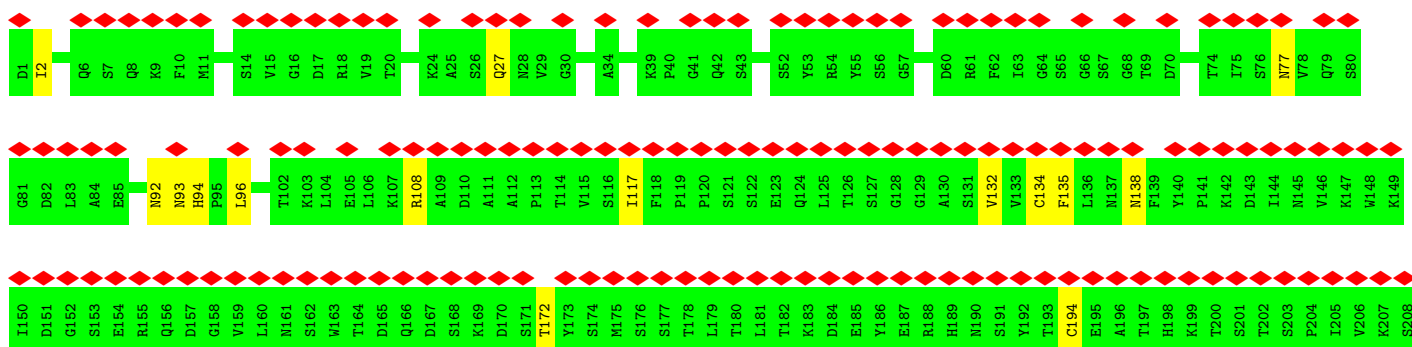
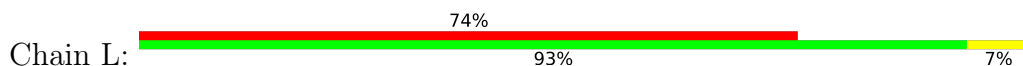




• Molecule 3: Fab 19/1786 - Heavy chain



• Molecule 4: Fab 19/1786 - Light chain



H189	N190	S191	Y192	T193	C194	E195	A196	T197	H198	K199	T200	S201	T202	S203	P204	I205	V206	K207	S208																																								
G68	T69	D70	F71	T72	L73	T74	I75	S76	M77	V78	Q79	S80	G81	D82	L83	A84	E85	Y86	F87	K88	Q89	I90	N91	S92	M93	L96	T97	F98	Q99	A100	G101	T102	K103	L104	E105	I106	K107	R108	A109	D110	A111	A112	P113	T114	V115	S116	I117	F118	P119	T120	S121	E122	E123	Q124	L125	T126	S127	G128	
G129	A130	S131	V132	V133	C134	F135	L136	N137	M138	F139	Y140	P141	K142	D143	I144	N145	V146	K147	M148	K149	I150	D151	G152	S153	E154	R155	Q156	D157	G158	V159	L160	N161	S162	W163	T164	D165	Q166	D167	S168	G169	D170	S171	T172	Y173	S174	M175	S176	S177	T178	L179	T180	L181	T182	K183	D184	E185	Y186	E187	R188

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	9797	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	17.740	Depositor
Minimum map value	-10.508	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.35	Depositor
Map size (Å)	580.0, 580.0, 580.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.45, 1.45, 1.45	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.36	0/3826	0.58	0/5190
1	B	0.35	0/3826	0.59	0/5190
1	C	0.40	0/3826	0.63	3/5190 (0.1%)
2	D	0.40	0/569	0.60	0/779
2	E	0.41	0/569	0.58	0/779
2	F	0.42	0/569	0.58	0/779
3	H	0.38	0/1637	0.56	0/2234
3	I	0.37	0/1637	0.56	0/2234
4	L	0.37	0/1640	0.58	0/2225
4	M	0.38	0/1640	0.56	0/2225
All	All	0.38	0/19739	0.59	3/26825 (0.0%)

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	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	265	LEU	CA-CB-CG	7.62	132.83	115.30
1	C	265	LEU	N-CA-C	5.82	126.71	111.00
1	C	264	LEU	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	SER	Peptide

5.2 Too-close contacts ⓘ

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	3743	0	3732	25	0
1	B	3743	0	3732	34	0
1	C	3743	0	3732	27	0
2	D	557	0	591	3	0
2	E	557	0	591	3	0
2	F	557	0	591	3	0
3	H	1597	0	1548	9	0
3	I	1597	0	1548	8	0
4	L	1605	0	1535	7	0
4	M	1605	0	1535	10	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	14	0	13	0	0
All	All	19346	0	19174	123	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.

All (123) 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:23:LEU:HD11	1:B:33:ILE:HD11	1.70	0.73
1:A:45:LEU:HD21	1:A:48:ILE:HD11	1.77	0.66
1:C:390:TYR:HE2	1:C:392:TRP:CE3	2.16	0.63
1:B:490:MET:N	1:B:490:MET:SD	2.75	0.59
1:C:318:PRO:HG2	1:C:390:TYR:CD2	2.38	0.59
3:H:4:LEU:HD11	3:H:98:ARG:HB2	1.85	0.58
1:C:318:PRO:HB2	1:C:390:TYR:CE2	2.38	0.58
1:C:10:ASP:OD1	1:C:408:LYS:NZ	2.36	0.58
2:F:26:ARG:HG2	2:F:29:LEU:HD12	1.86	0.58
1:B:271:VAL:HG22	2:D:7:HIS:CD2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ALA:HB3	1:A:38:LYS:HB2	1.86	0.57
1:C:59:TYR:HB2	1:C:127:ALA:HB3	1.85	0.57
4:L:2:ILE:HD12	4:L:93:ASN:HB2	1.85	0.57
1:B:163:ALA:HB2	1:B:174:LEU:HD11	1.88	0.56
1:A:345:VAL:HB	1:A:350:PRO:HG2	1.89	0.55
1:C:390:TYR:CE2	1:C:392:TRP:CE3	2.94	0.55
1:A:101:TRP:CH2	1:B:316:ARG:HG3	2.42	0.54
1:B:59:TYR:HB2	1:B:127:ALA:HB3	1.89	0.54
1:C:316:ARG:HB3	1:C:329:GLU:HB3	1.89	0.54
1:A:130:HIS:HB2	1:A:199:ILE:HB	1.90	0.54
4:M:2:ILE:HD11	4:M:27:GLN:HE21	1.73	0.54
1:B:10:ASP:OD1	1:B:408:LYS:NZ	2.40	0.53
2:E:50:VAL:HG13	2:E:60:ARG:HD3	1.89	0.53
1:C:35:ALA:HB3	1:C:38:LYS:HB2	1.91	0.53
1:C:23:LEU:HD11	1:C:33:ILE:HD11	1.89	0.53
1:A:417:GLY:HA2	1:A:420:ALA:HB3	1.91	0.52
1:C:130:HIS:HB2	1:C:199:ILE:HB	1.92	0.52
1:B:257:LEU:O	1:B:260:GLN:NE2	2.43	0.52
1:B:10:ASP:OD2	1:B:412:ARG:NH1	2.43	0.52
1:B:71:ALA:HB2	1:B:82:LEU:HD21	1.91	0.52
2:D:26:ARG:HG2	2:D:29:LEU:HD12	1.92	0.51
1:C:127:ALA:HB1	1:C:200:LEU:HD11	1.92	0.51
1:A:59:TYR:HB2	1:A:127:ALA:HB3	1.92	0.51
1:A:455:LEU:HB2	1:A:456:PRO:HD3	1.93	0.51
1:B:61:LEU:HD13	1:B:261:THR:HA	1.93	0.50
1:B:340:ILE:HD12	1:B:362:PRO:HB2	1.91	0.50
3:I:22:CYS:HB3	3:I:79:LEU:HB3	1.94	0.50
3:H:99:VAL:HG11	3:H:103:TYR:HD1	1.76	0.49
1:A:82:LEU:HB2	1:A:85:GLU:HG3	1.95	0.49
1:C:61:LEU:HD11	1:C:202:LEU:HD22	1.95	0.49
1:B:57:ARG:NH1	1:B:221:ASN:O	2.45	0.49
1:C:45:LEU:HD21	1:C:48:ILE:HD11	1.94	0.49
2:E:23:ASP:O	2:E:27:THR:N	2.46	0.49
1:A:257:LEU:O	1:A:260:GLN:NE2	2.46	0.49
1:A:490:MET:SD	1:A:490:MET:N	2.84	0.48
1:A:103:ASN:ND2	1:A:249:ALA:HB1	2.29	0.48
3:I:162:ASN:HD21	3:I:200:VAL:HA	1.78	0.48
1:A:80:ALA:O	1:A:94:ARG:NH1	2.46	0.48
1:B:417:GLY:HA2	1:B:420:ALA:HB3	1.95	0.48
4:M:117:ILE:HD13	4:M:194:CYS:HB2	1.96	0.48
1:B:455:LEU:HB2	1:B:456:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:LEU:HD23	1:B:467:LEU:HD12	1.97	0.47
1:C:449:PHE:HB3	1:C:452:VAL:HB	1.96	0.47
1:C:212:ALA:HB2	1:C:276:ILE:HG13	1.96	0.47
3:H:5:GLU:HB3	3:H:23:ALA:HB3	1.96	0.47
1:A:330:VAL:HG11	1:A:385:VAL:HG11	1.96	0.47
1:B:130:HIS:HB2	1:B:199:ILE:HB	1.97	0.47
3:I:52:ASN:O	3:I:72:ARG:NH2	2.48	0.47
4:L:138:ASN:HD22	4:L:172:THR:HG21	1.79	0.47
4:M:138:ASN:HD22	4:M:172:THR:HG21	1.80	0.47
3:I:90:ASP:HB2	3:I:118:VAL:HG21	1.97	0.46
3:H:34:MET:HB3	3:H:79:LEU:HD22	1.98	0.46
2:F:50:VAL:HG13	2:F:60:ARG:HD3	1.98	0.46
1:C:113:ILE:HG21	1:C:247:PRO:HG3	1.98	0.46
1:C:490:MET:SD	1:C:490:MET:N	2.85	0.45
3:I:20:LEU:HD12	3:I:81:LEU:HD23	1.98	0.45
1:A:23:LEU:HD11	1:A:33:ILE:HD11	1.98	0.45
1:B:378:PRO:HA	1:B:394:GLN:HB3	1.98	0.45
1:A:99:ARG:HA	1:A:103:ASN:HD21	1.82	0.45
1:B:200:LEU:HD21	1:B:264:LEU:HD21	1.98	0.45
1:C:330:VAL:HG23	1:C:364:ILE:HD11	1.98	0.45
2:E:26:ARG:HG2	2:E:29:LEU:HD12	1.99	0.45
1:A:24:VAL:HG11	1:A:420:ALA:HB2	1.99	0.45
1:B:305:THR:HG21	3:H:59:TYR:HB2	1.98	0.45
3:I:52:ASN:HD21	3:I:56:ASP:HB2	1.82	0.45
1:B:330:VAL:HG11	1:B:385:VAL:HG11	1.99	0.44
1:B:89:GLY:HA2	1:B:235:TRP:HB2	1.98	0.44
1:C:82:LEU:HB2	1:C:85:GLU:HG3	1.99	0.44
1:C:26:GLU:HA	1:C:287:HIS:HA	2.00	0.44
1:C:198:VAL:HG11	1:C:220:PHE:CD1	2.53	0.44
1:B:103:ASN:OD1	1:B:103:ASN:N	2.51	0.43
1:B:337:PRO:HB3	1:B:365:GLU:HA	1.99	0.43
4:L:117:ILE:HD13	4:L:194:CYS:HB2	2.00	0.43
4:L:134:CYS:SG	4:L:135:PHE:N	2.91	0.43
1:A:9:ARG:O	1:A:408:LYS:NZ	2.51	0.43
3:H:155:GLU:HB3	3:H:156:PRO:HA	2.00	0.43
3:H:9:GLY:HA2	3:H:116:VAL:HG22	2.01	0.43
4:L:117:ILE:HD11	4:L:132:VAL:HG12	2.01	0.43
1:B:267:ALA:HB2	2:D:4:ILE:HD13	2.00	0.43
1:A:4:THR:HG21	1:A:371:PHE:HZ	1.84	0.43
1:A:390:TYR:CE2	1:A:391:GLN:O	2.72	0.43
1:A:45:LEU:HD22	1:A:288:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ARG:HG2	1:B:111:GLY:HA3	2.01	0.42
4:M:166:GLN:NE2	4:M:171:SER:OG	2.46	0.42
1:C:464:LEU:HD23	1:C:467:LEU:HD12	2.02	0.42
1:B:148:GLY:O	1:B:371:PHE:N	2.44	0.42
3:H:128:VAL:HG22	3:H:204:VAL:HB	2.02	0.42
3:H:130:PRO:HG3	3:H:201:THR:HG23	2.01	0.42
1:A:378:PRO:HA	1:A:394:GLN:HB3	2.02	0.42
4:M:161:ASN:ND2	4:M:175:MET:SD	2.93	0.42
4:M:90:GLN:HE21	4:M:97:THR:H	1.68	0.41
4:M:138:ASN:ND2	4:M:170:ASP:OD2	2.53	0.41
1:A:464:LEU:HD23	1:A:467:LEU:HD12	2.02	0.41
1:B:24:VAL:HG21	1:B:420:ALA:HB1	2.03	0.41
1:B:65:LEU:HD21	1:B:242:VAL:HG22	2.02	0.41
4:M:149:LYS:HB2	4:M:193:THR:HB	2.03	0.41
1:B:301:GLY:HA2	1:B:304:TYR:CD2	2.56	0.41
1:C:300:LYS:O	1:C:361:ASN:ND2	2.54	0.41
4:M:148:TRP:NE1	4:M:158:GLY:O	2.54	0.41
1:B:157:HIS:HB3	1:B:160:ARG:HB2	2.01	0.41
1:B:340:ILE:HD11	1:B:364:ILE:HD11	2.03	0.41
1:C:455:LEU:HB2	1:C:456:PRO:HD3	2.02	0.41
1:A:33:ILE:HG21	1:A:294:LEU:HD21	2.02	0.41
3:I:34:MET:HB3	3:I:79:LEU:HD22	2.03	0.41
1:A:22:THR:HA	1:A:291:GLU:HA	2.02	0.40
3:I:176:VAL:HG11	4:M:160:LEU:HB3	2.02	0.40
1:B:7:GLU:O	1:B:323:HIS:NE2	2.54	0.40
1:C:414:THR:OG1	1:C:415:VAL:N	2.52	0.40
1:C:25:LEU:HD11	1:C:43:VAL:HG12	2.03	0.40
1:C:157:HIS:HB3	1:C:160:ARG:HB2	2.02	0.40
2:F:24:SER:HA	2:F:27:THR:HG23	2.03	0.40
4:L:2:ILE:HD11	4:L:27:GLN:HE21	1.85	0.40
1:B:335:THR:HB	4:L:94:HIS:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	490/496 (99%)	440 (90%)	48 (10%)	2 (0%)	30	65
1	B	490/496 (99%)	456 (93%)	33 (7%)	1 (0%)	44	75
1	C	490/496 (99%)	443 (90%)	47 (10%)	0	100	100
2	D	69/75 (92%)	56 (81%)	13 (19%)	0	100	100
2	E	69/75 (92%)	57 (83%)	11 (16%)	1 (1%)	9	39
2	F	69/75 (92%)	57 (83%)	9 (13%)	3 (4%)	2	21
3	H	210/212 (99%)	191 (91%)	19 (9%)	0	100	100
3	I	210/212 (99%)	198 (94%)	11 (5%)	1 (0%)	25	60
4	L	206/208 (99%)	186 (90%)	20 (10%)	0	100	100
4	M	206/208 (99%)	183 (89%)	23 (11%)	0	100	100
All	All	2509/2553 (98%)	2267 (90%)	234 (9%)	8 (0%)	38	70

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	22	GLY
2	F	11	GLU
1	A	350	PRO
1	A	169	SER
1	B	78	GLY
2	F	16	GLY
3	I	174	PRO
2	E	10	GLY

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	400/401 (100%)	398 (100%)	2 (0%)	86	90
1	B	400/401 (100%)	397 (99%)	3 (1%)	79	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	400/401 (100%)	397 (99%)	3 (1%)	79	84
2	D	61/64 (95%)	61 (100%)	0	100	100
2	E	61/64 (95%)	61 (100%)	0	100	100
2	F	61/64 (95%)	60 (98%)	1 (2%)	58	73
3	H	180/180 (100%)	178 (99%)	2 (1%)	70	79
3	I	180/180 (100%)	178 (99%)	2 (1%)	70	79
4	L	183/183 (100%)	179 (98%)	4 (2%)	47	65
4	M	183/183 (100%)	180 (98%)	3 (2%)	58	73
All	All	2109/2121 (99%)	2089 (99%)	20 (1%)	74	83

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	250	VAL
1	A	490	MET
1	B	2	ARG
1	B	16	GLN
1	B	490	MET
1	C	2	ARG
1	C	261	THR
1	C	490	MET
2	F	18	LYS
3	H	150	LYS
3	H	184	LEU
3	I	150	LYS
3	I	184	LEU
4	L	77	ASN
4	L	92	ASN
4	L	96	LEU
4	L	108	ARG
4	M	77	ASN
4	M	92	ASN
4	M	108	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN

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Mol	Chain	Res	Type
1	A	208	HIS
1	B	347	HIS
1	C	196	GLN
2	D	7	HIS
2	E	39	ASN
3	H	178	GLN
3	I	162	ASN
4	L	27	GLN
4	L	77	ASN
4	L	92	ASN
4	L	94	HIS
4	L	138	ASN
4	L	161	ASN
4	M	27	GLN
4	M	77	ASN
4	M	137	ASN
4	M	138	ASN
4	M	161	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	B	500	1	14,14,15	0.39	0	17,19,21	0.99	2 (11%)
5	NAG	A	500	1	14,14,15	0.66	0	17,19,21	1.73	1 (5%)
5	NAG	C	500	1	14,14,15	0.35	0	17,19,21	0.95	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	500	1	-	2/6/23/26	0/1/1/1
5	NAG	A	500	1	-	2/6/23/26	0/1/1/1
5	NAG	C	500	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	500	NAG	C1-O5-C5	6.06	120.40	112.19
5	B	500	NAG	O5-C1-C2	-2.16	107.87	111.29
5	C	500	NAG	O5-C1-C2	-2.04	108.06	111.29
5	B	500	NAG	C1-O5-C5	2.00	114.91	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	500	NAG	C4-C5-C6-O6
5	B	500	NAG	C4-C5-C6-O6
5	A	500	NAG	O5-C5-C6-O6
5	B	500	NAG	O5-C5-C6-O6

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.

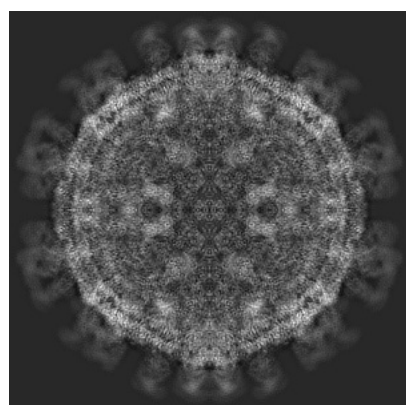
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3754. These allow visual inspection of the internal detail of the map and identification of artifacts.

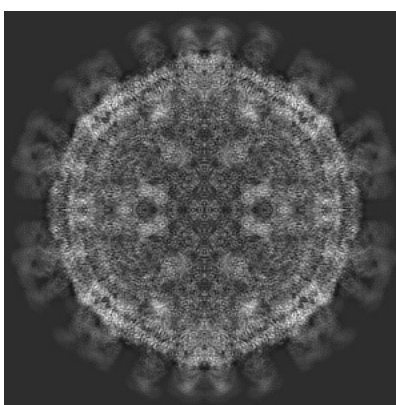
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

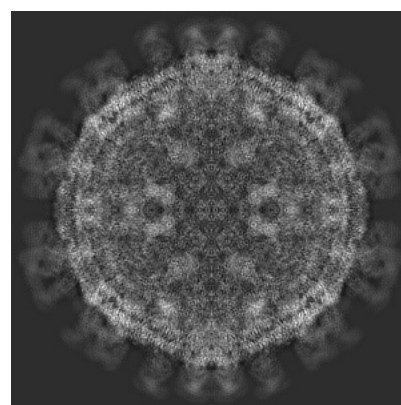
6.1.1 Primary map



X



Y

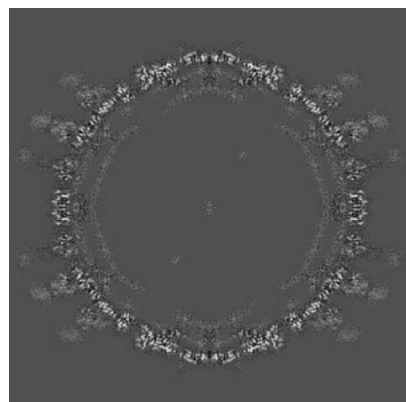


Z

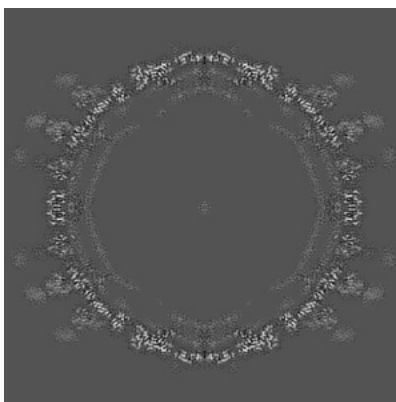
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

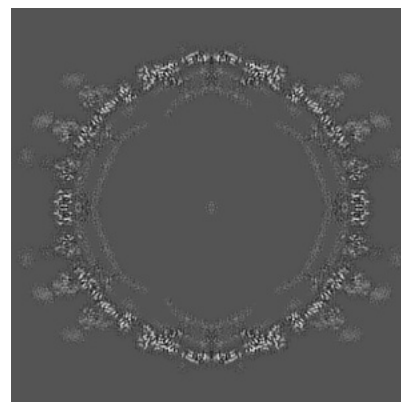
6.2.1 Primary map



X Index: 200



Y Index: 200

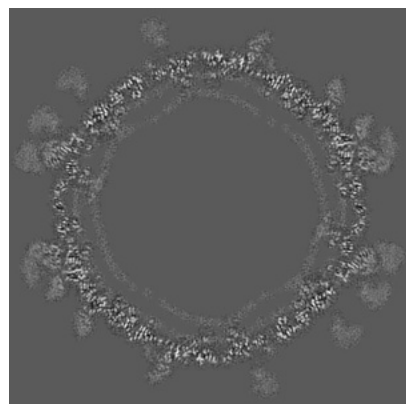


Z Index: 200

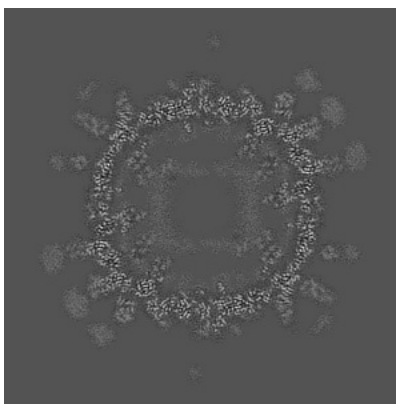
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

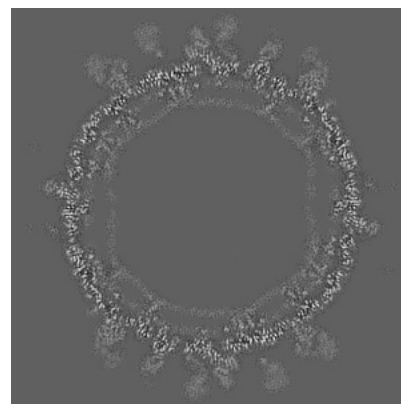
6.3.1 Primary map



X Index: 185



Y Index: 302

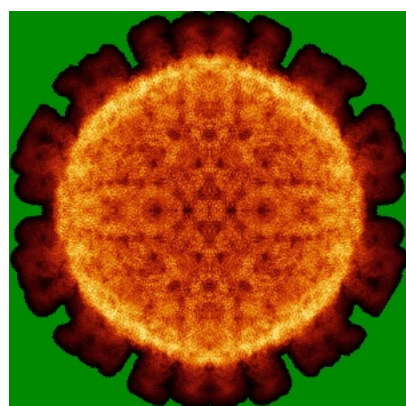


Z Index: 240

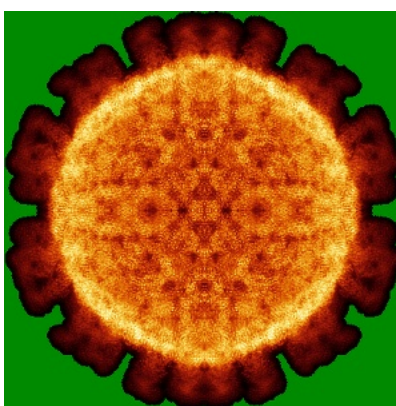
The images above show the largest variance slices of the map in three orthogonal directions.

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

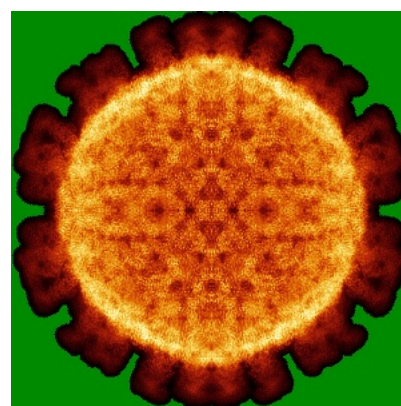
6.4.1 Primary map



X



Y

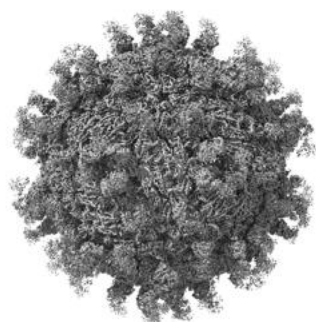


Z

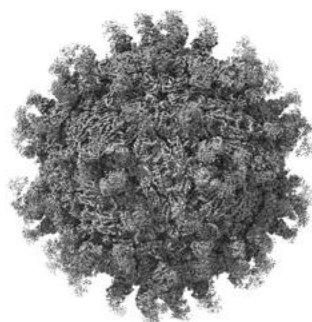
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

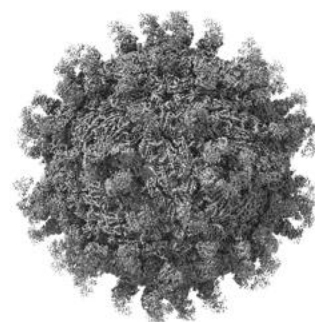
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

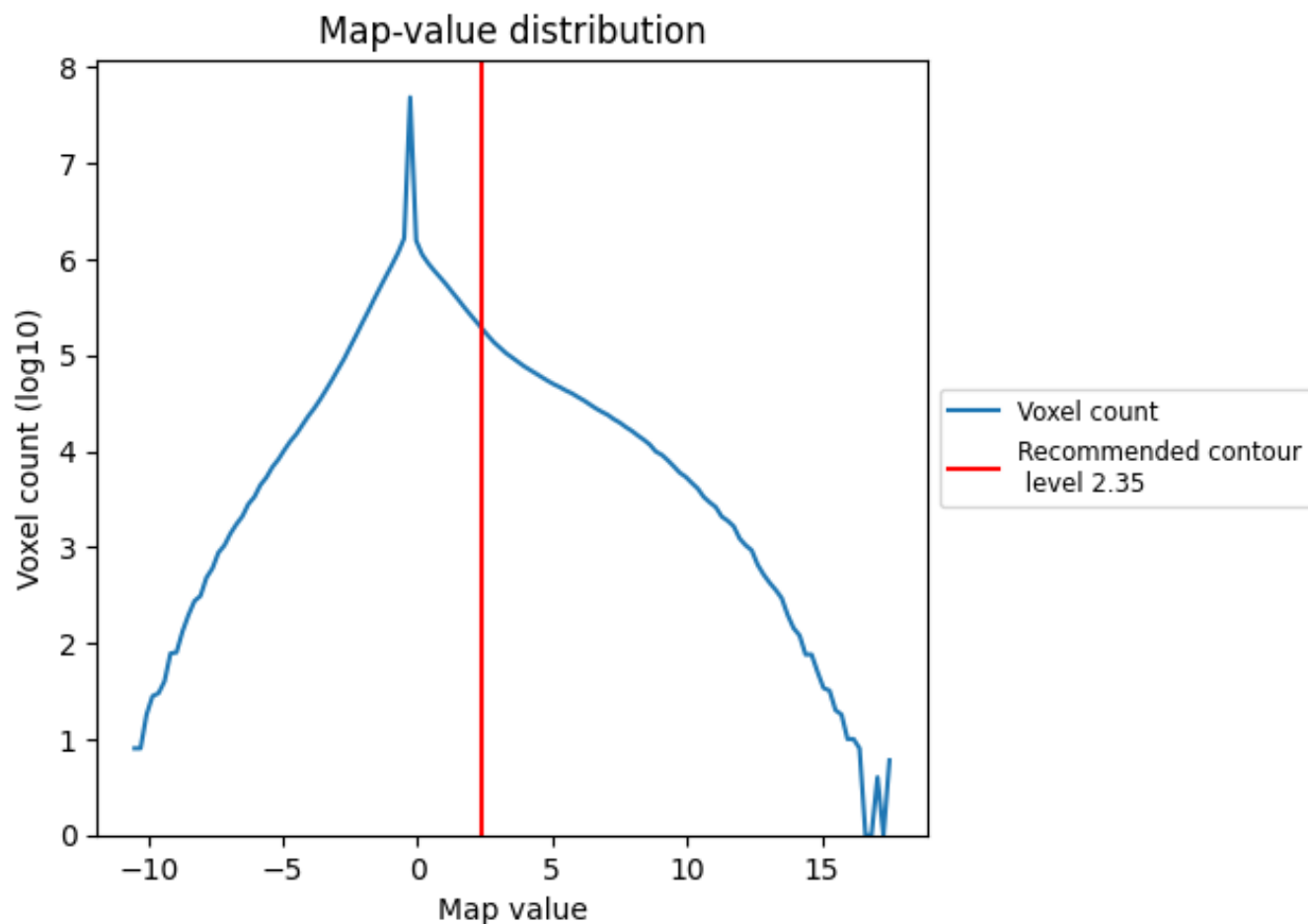
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

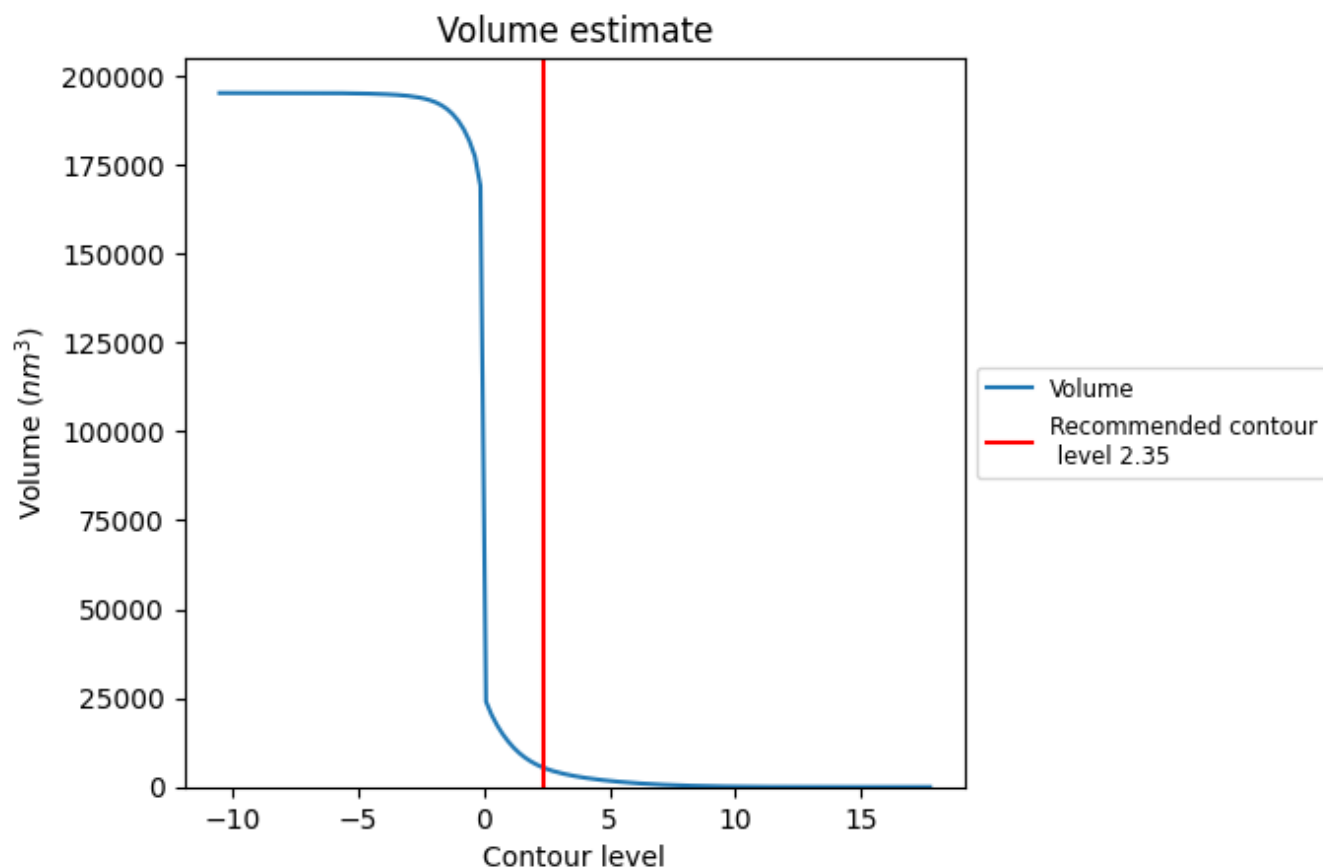
This section contains the results of statistical analysis of the map.

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.

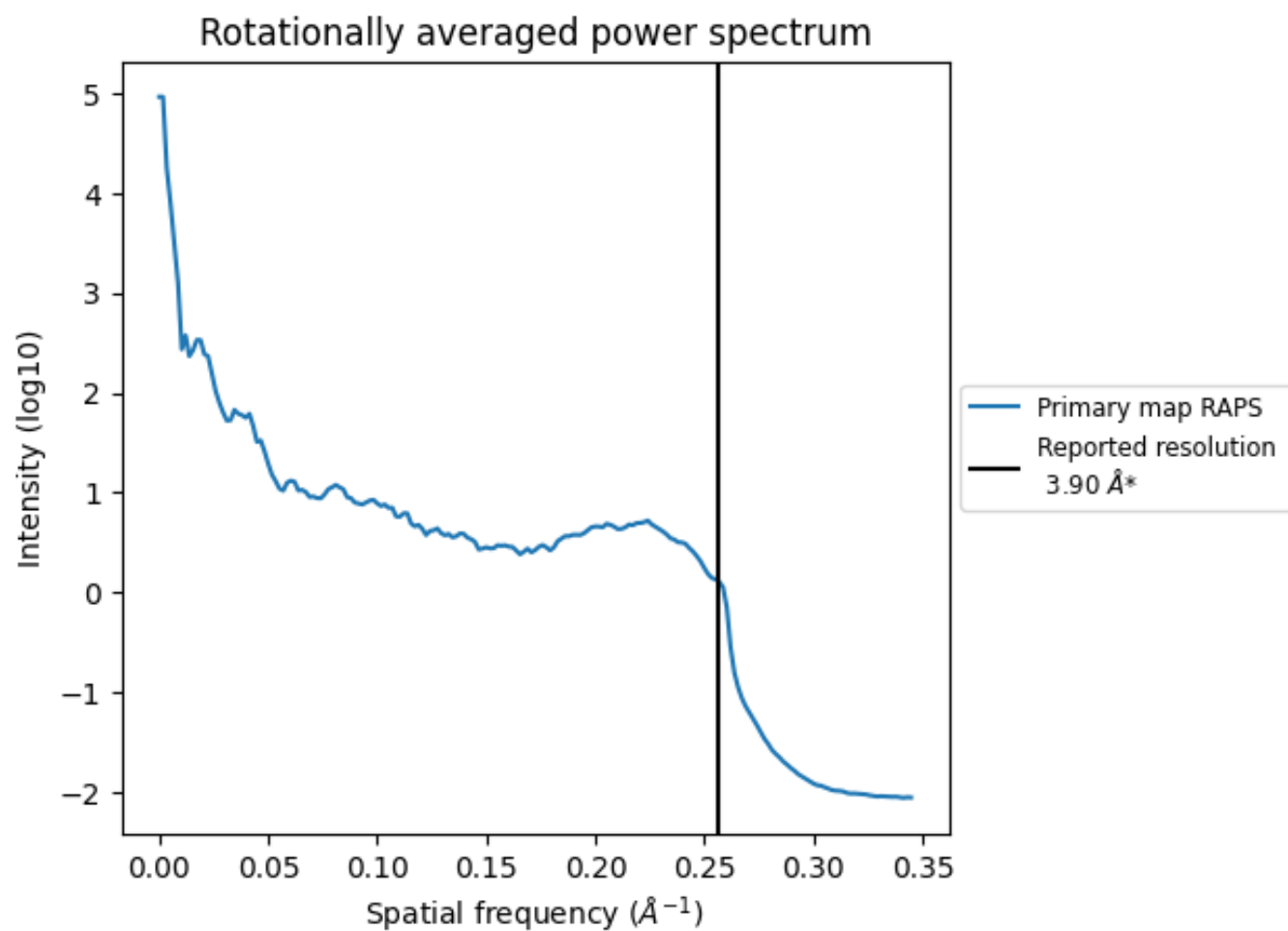
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5490 nm³; this corresponds to an approximate mass of 4959 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 ⓘ

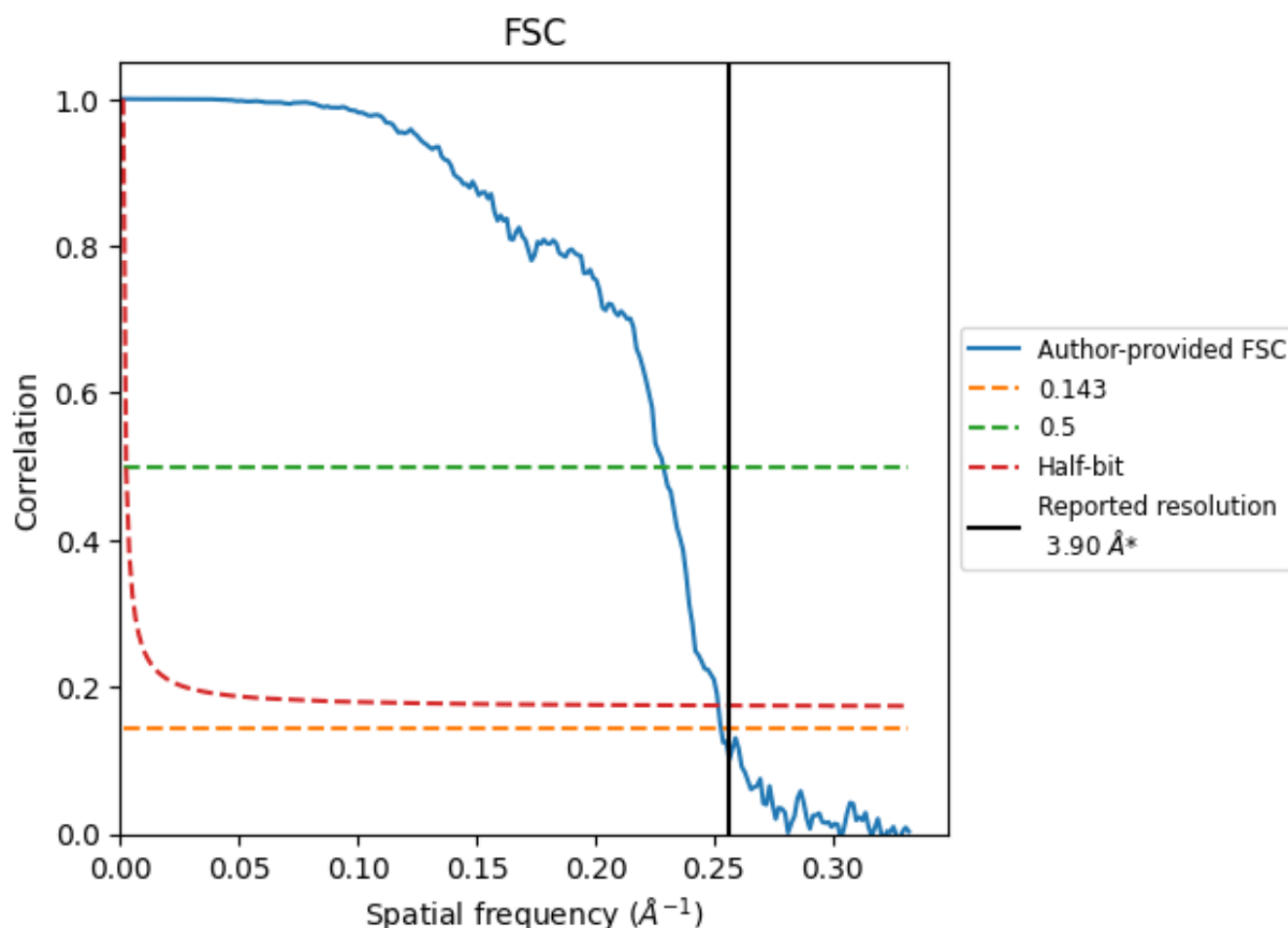


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.95	4.37	3.97
Unmasked-calculated*	-	-	-

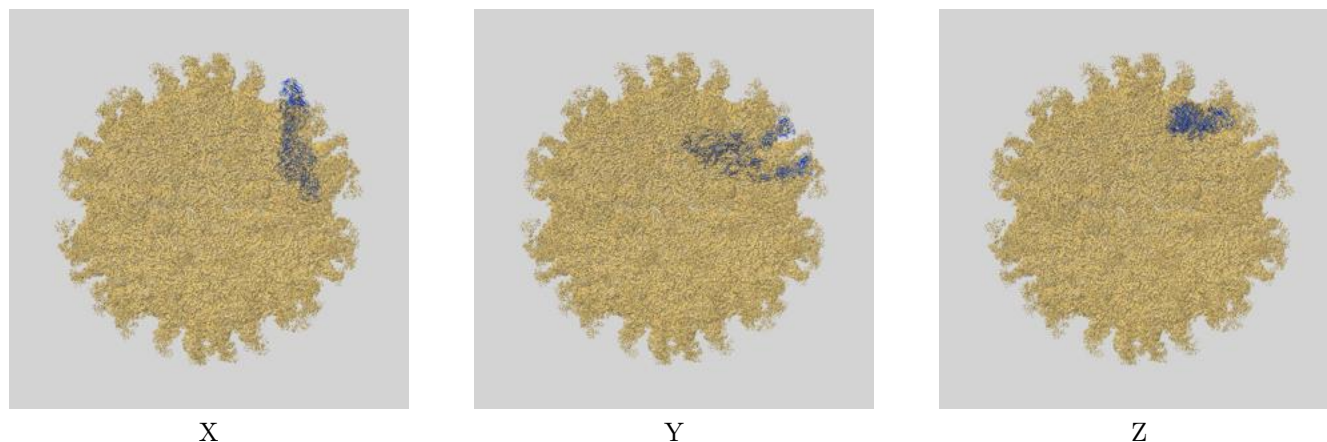
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

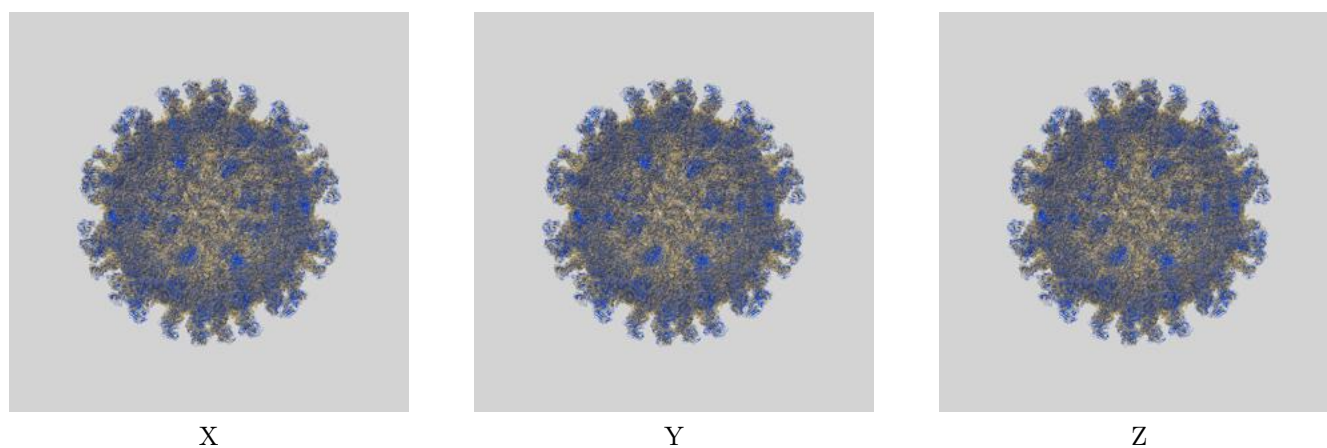
This section contains information regarding the fit between EMDB map EMD-3754 and PDB model 5O6V. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

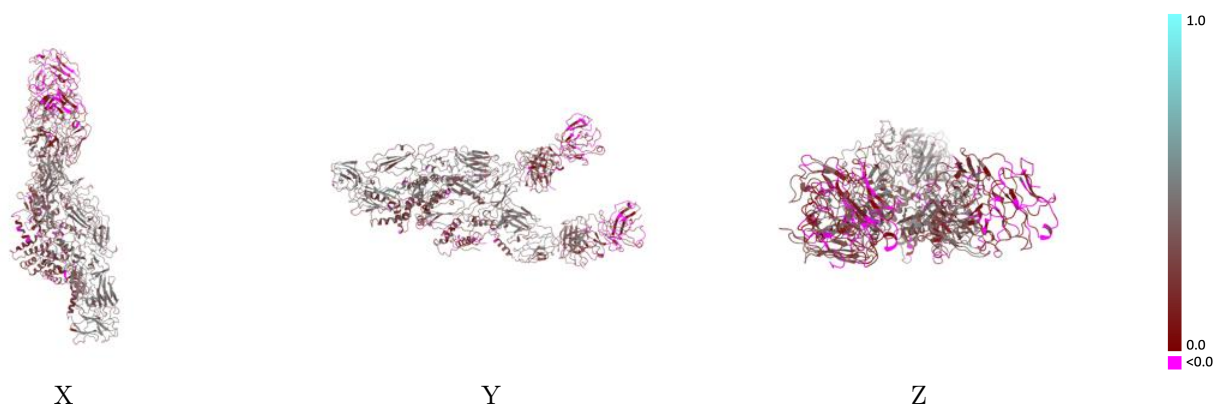


9.1.2 Map-model assembly overlay [i](#)



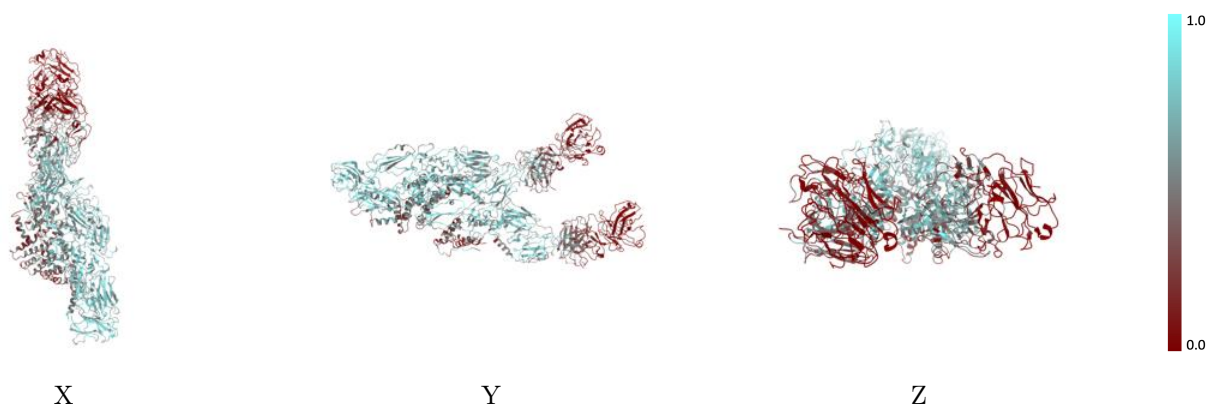
The images above show the 3D surface view of the map at the recommended contour level 2.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



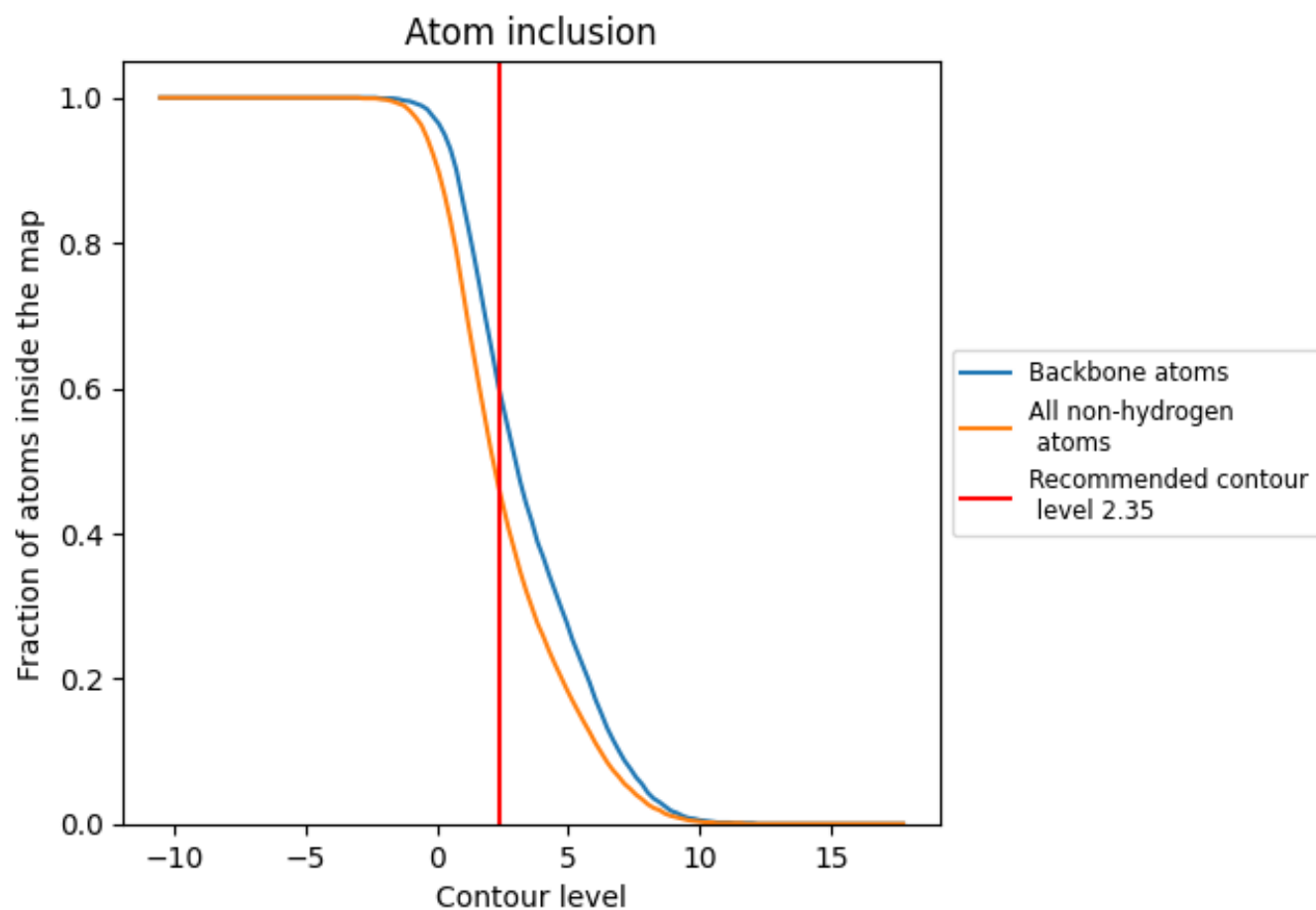
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 46% 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 (2.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4650	<div></div> 0.2770
A	<div></div> 0.6390	<div></div> 0.3800
B	<div></div> 0.6040	<div></div> 0.3450
C	<div></div> 0.5890	<div></div> 0.3240
D	<div></div> 0.4570	<div></div> 0.2170
E	<div></div> 0.4810	<div></div> 0.2810
F	<div></div> 0.3430	<div></div> 0.1930
H	<div></div> 0.2800	<div></div> 0.1710
I	<div></div> 0.2010	<div></div> 0.1840
L	<div></div> 0.2440	<div></div> 0.1420
M	<div></div> 0.1440	<div></div> 0.1500

1.0
0.0
<0.0