Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 06:31 pm GMT

PDB ID	:	5LK8
EMDB ID	:	EMD-4064
Title	:	single particle reconstruction of slow bee paralysis virus empty particle
Authors	:	Kalynych, S.; Fuzik, T.; Plevka, P.
Deposited on	:	2016-07-21
Resolution	:	3.42 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 (i) 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 (i)) were used in the production of this report:

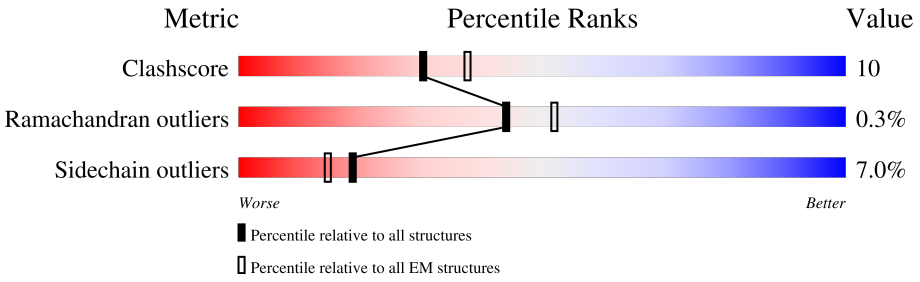
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.42 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 <=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	266	33% 61% 20% • 16%
2	B	261	34% 62% 20% • 18%
3	C	430	23% 44% 13% • 41%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5461 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 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	223	1781	1149	312	313	7	0	0

- Molecule 2 is a protein called VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	215	1725	1128	285	299	13	0	0

- Molecule 3 is a protein called VP3.

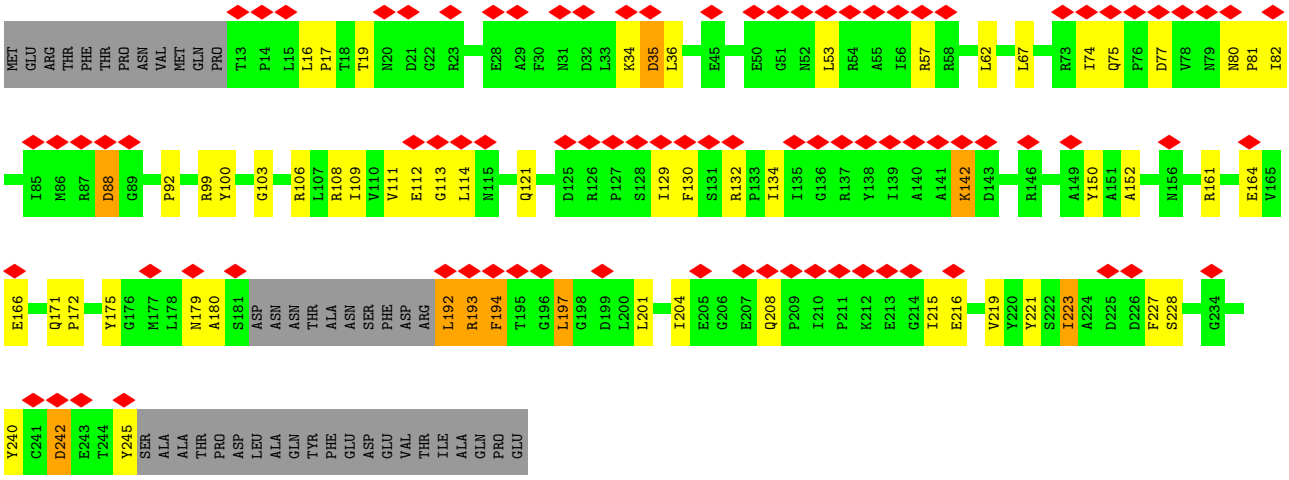
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	255	1955	1265	329	354	7	0	0

3 Residue-property plots (i)

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.

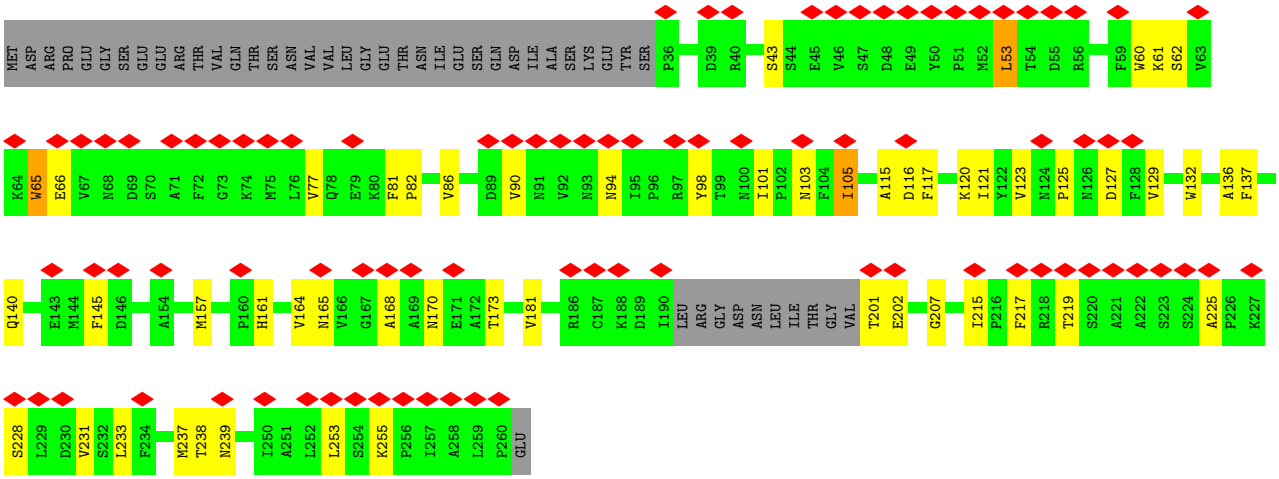
- Molecule 1: VP1

Chain A:



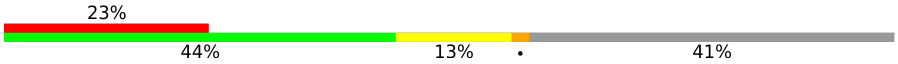
- Molecule 2: VP2

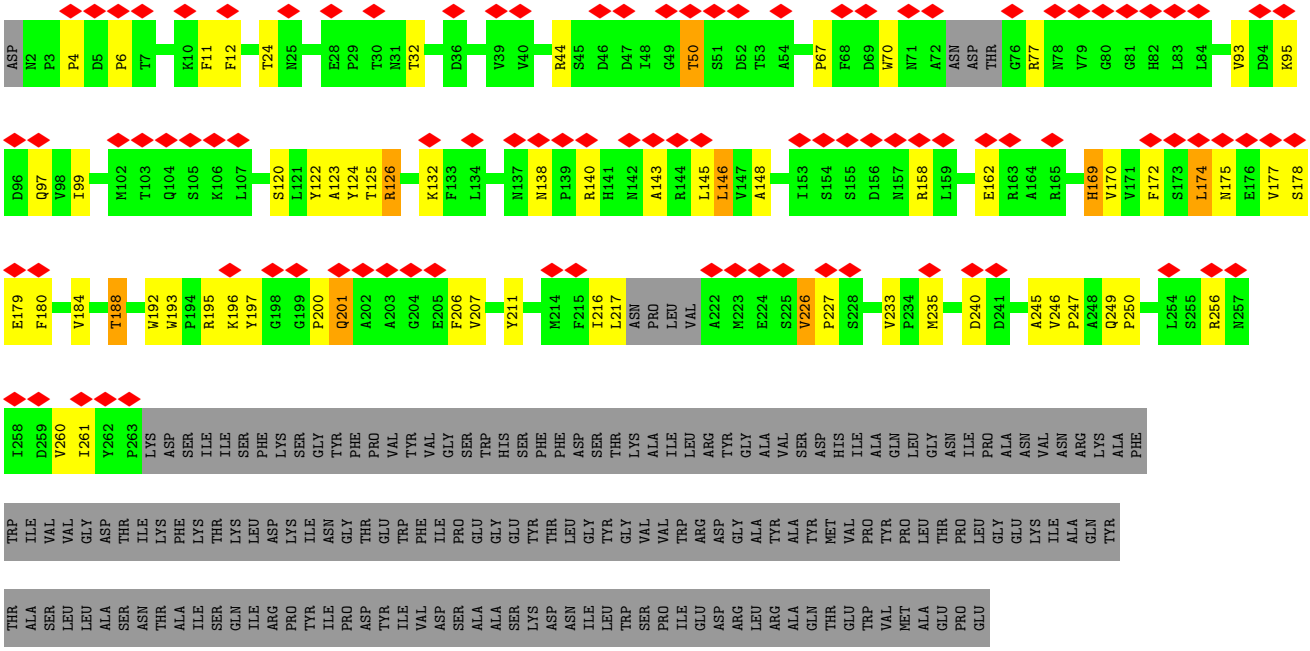
Chain B:



- Molecule 3: VP3

Chain C:


23%
44%
13%
41%


ASP N2 P3 P4 D5 P6 T7 K10 F11 F12 T24 N25 E28 P29 T30 N31 T32 D36 V39 V40 R44 S45 D46 D47 I48 G49 T50 S51 D52 T53 A54 P67 F68 D69 W70 N71 A72 ASN ASP THR G76 R77 N78 V79 G80 G81 H82 L83 L84 V93 D94 K95
D96 Q97 V98 I99 M102 T103 Q104 S105 K106 L107 S120 L121 Y122 A123 Y124 T125 R126 K132 F133 L134 N137 N138 P139 R140 H141 N142 A143 R144 L145 L146 V147 A148 I153 S154 S155 D156 N157 R158 L159 E162 R163 A164 R165 H169 V170 V171 F172 S173 L174 N175 E176 V177 S178
E179 F180 V184 T188 W192 W193 P194 R195 K196 Y197 G198 G199 P200 Q201 A202 A203 G204 E205 F206 V207 Y211 M214 F215 I216 L217 ASN PRO LEU VAL A222 M223 E224 S225 V226 P227 S228 V233 P234 M235 D240 D241 A245 V246 P247 A248 Q249 P250 L254 S255 R256 N257
I258 D259 V260 I261 Y262 P263 LYS ASP SER ILE ILE SER PHE LYS SER GLY TYR PHE PRO VAL TYR VAL GLY SER TRP HIS SER PHE PHE ASP SER THR LYS ALA ILE LEU ARG TYR GLY ALA VAL SER ASP HIS ILE ALA GLN LEU GLY ASN ILE PRO ALA ASN VAL ASN ARG LYS ALA PHE
TRP ILE VAL VAL GLY ASP THR ILE LYS PHE LYS THR LYS LEU ASP LYS ILE ASN GLY THR GLU TRP PHE ILE PRO GLU GLY GLU TYR THR LEU GLY TYR GLY VAL VAL TRP ARG ASP GLY ALA TYR ALA TYR MET VAL PRO TYR PRO LEU THR PRO LEU GLY GLU LYS ILE ALA GLN TYR
THR ALA SER LEU LEU ALA SER ASN THR ALA ILE SER GLN ILE ARG PRO TYR ILE VAL ASP SER ALA ALA SER LYS ASP ASN ILE LEU TRP SER PRO ILE GLU ASP ARG LEU ARG ALA GLN THR GLU TRP VAL MET ALA GLU PRO GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10350	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 ($e^-/Å^2$)	21	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	16.398	Depositor
Minimum map value	-10.148	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.01	Depositor
Map size (Å)	406.6, 406.6, 406.6	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.32	0/1831	0.61	1/2494 (0.0%)
2	B	0.31	0/1775	0.56	0/2414
3	C	0.32	0/2013	0.60	0/2756
All	All	0.32	0/5619	0.59	1/7664 (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
3	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	53	LEU	CA-CB-CG	6.70	130.70	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	201	GLN	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	1781	0	1736	43	0
2	B	1725	0	1715	35	0
3	C	1955	0	1918	45	0
All	All	5461	0	5369	107	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 10.

All (107) 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:192:LEU:HD12	1:A:194:PHE:HB2	1.56	0.86
3:C:143:ALA:HB3	3:C:174:LEU:HD13	1.65	0.78
3:C:124:TYR:HB3	3:C:192:TRP:HB3	1.70	0.72
2:B:123:VAL:HG23	2:B:231:VAL:HG22	1.72	0.71
2:B:101:ILE:HG22	2:B:103:ASN:H	1.59	0.68
1:A:62:LEU:HD21	1:A:215:ILE:HD11	1.74	0.66
2:B:125:PRO:HB3	2:B:170:ASN:HD21	1.60	0.66
3:C:11:PHE:O	3:C:12:PHE:HD1	1.79	0.65
3:C:67:PRO:HD3	3:C:99:ILE:HD11	1.81	0.63
1:A:223:ILE:HG13	1:A:227:PHE:CD1	2.35	0.62
3:C:177:VAL:HG12	3:C:179:GLU:H	1.64	0.62
1:A:240:TYR:CD2	3:C:95:LYS:HE2	2.36	0.61
2:B:165:ASN:HB2	2:B:168:ALA:O	2.00	0.61
1:A:121:GLN:HG2	1:A:152:ALA:HB2	1.83	0.60
1:A:103:GLY:HA3	1:A:227:PHE:HA	1.83	0.59
2:B:60:TRP:CD1	2:B:61:LYS:HG3	2.37	0.59
1:A:88:ASP:OD1	1:A:88:ASP:N	2.35	0.59
1:A:166:GLU:HB3	3:C:32:THR:HG22	1.85	0.57
3:C:67:PRO:HB3	3:C:233:VAL:HG22	1.87	0.56
2:B:116:ASP:HB2	2:B:238:THR:HB	1.87	0.56
1:A:17:PRO:O	3:C:126:ARG:NH2	2.39	0.56
1:A:114:LEU:HD21	1:A:204:ILE:HG22	1.88	0.56
1:A:223:ILE:HG23	1:A:227:PHE:HB3	1.87	0.56
1:A:242:ASP:OD1	1:A:242:ASP:N	2.39	0.55
1:A:34:LYS:NZ	3:C:50:THR:HG21	2.20	0.55
2:B:145:PHE:CE1	3:C:256:ARG:HG3	2.42	0.55
1:A:100:TYR:HB3	1:A:175:TYR:HB3	1.89	0.54
3:C:138:ASN:O	3:C:140:ARG:N	2.42	0.53
1:A:36:LEU:HD13	3:C:247:PRO:HB3	1.90	0.52
2:B:127:ASP:HB3	3:C:140:ARG:HH22	1.75	0.52
3:C:188:THR:HG21	3:C:193:TRP:CZ3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:TYR:CZ	2:B:253:LEU:HD21	2.46	0.51
1:A:228:SER:HB2	3:C:50:THR:HG23	1.92	0.51
2:B:157:MET:O	2:B:157:MET:HG3	2.11	0.51
2:B:53:LEU:O	2:B:103:ASN:HA	2.10	0.51
3:C:132:LYS:HB3	3:C:235:MET:HB2	1.93	0.51
3:C:226:VAL:HG12	3:C:227:PRO:HD2	1.93	0.51
3:C:196:LYS:HG3	3:C:206:PHE:CG	2.47	0.50
3:C:216:ILE:O	3:C:217:LEU:HB2	2.11	0.50
1:A:109:ILE:HG13	1:A:219:VAL:HG13	1.94	0.50
3:C:177:VAL:HG12	3:C:178:SER:N	2.27	0.49
2:B:120:LYS:HB2	2:B:173:THR:HG22	1.95	0.49
1:A:62:LEU:HD21	1:A:215:ILE:CD1	2.43	0.49
2:B:77:VAL:HG21	2:B:233:LEU:HD11	1.95	0.49
2:B:137:PHE:CZ	2:B:207:GLY:HA3	2.47	0.49
3:C:95:LYS:HE3	3:C:197:TYR:CE1	2.47	0.49
2:B:82:PRO:HG3	2:B:117:PHE:CZ	2.47	0.48
2:B:140:GLN:OE1	2:B:181:VAL:HG13	2.13	0.48
1:A:180:ALA:O	2:B:145:PHE:HD2	1.97	0.48
3:C:170:VAL:HG11	3:C:180:PHE:HZ	1.79	0.48
2:B:66:GLU:OE1	2:B:228:SER:HB3	2.14	0.48
3:C:148:ALA:HB2	3:C:169:HIS:HB3	1.96	0.48
2:B:81:PHE:CD1	2:B:82:PRO:HA	2.48	0.47
3:C:177:VAL:HG12	3:C:179:GLU:N	2.29	0.47
2:B:121:ILE:HG23	2:B:164:VAL:HG21	1.97	0.47
1:A:35:ASP:OD2	3:C:24:THR:HB	2.15	0.47
3:C:93:VAL:HG12	3:C:97:GLN:HB2	1.96	0.47
2:B:86:VAL:HG12	2:B:98:TYR:CE1	2.51	0.46
3:C:120:SER:O	3:C:250:PRO:HA	2.15	0.46
1:A:130:PHE:CD2	1:A:134:ILE:HD11	2.51	0.46
3:C:260:VAL:O	3:C:261:ILE:HD13	2.16	0.45
2:B:115:ALA:HA	2:B:239:ASN:O	2.15	0.45
1:A:179:ASN:HA	2:B:145:PHE:CE2	2.51	0.45
2:B:132:TRP:CD1	2:B:215:ILE:HD12	2.52	0.45
1:A:75:GLN:HE21	1:A:77:ASP:HB3	1.81	0.45
2:B:125:PRO:CB	2:B:170:ASN:HD21	2.27	0.45
1:A:112:GLU:HG3	1:A:113:GLY:N	2.32	0.44
1:A:121:GLN:NE2	1:A:150:TYR:HB2	2.32	0.44
1:A:142:LYS:CE	1:A:142:LYS:HA	2.47	0.44
1:A:99:ARG:HA	1:A:99:ARG:HD2	1.73	0.44
1:A:132:ARG:HA	1:A:132:ARG:HD2	1.66	0.44
2:B:65:TRP:CZ3	2:B:217:PHE:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:TRP:HZ3	3:C:174:LEU:HD11	1.82	0.44
3:C:124:TYR:HB2	3:C:245:ALA:HB3	1.98	0.44
2:B:136:ALA:HB2	2:B:161:HIS:HB3	1.98	0.44
2:B:105:ILE:HD12	2:B:105:ILE:HA	1.86	0.44
1:A:106:ARG:O	1:A:221:TYR:HA	2.17	0.44
1:A:130:PHE:CE2	1:A:134:ILE:HD11	2.52	0.43
3:C:70:TRP:CZ3	3:C:174:LEU:HD11	2.54	0.43
1:A:19:THR:HG23	3:C:126:ARG:NH2	2.34	0.43
1:A:74:ILE:O	1:A:74:ILE:HG13	2.18	0.43
1:A:16:LEU:HD12	1:A:17:PRO:HD2	2.00	0.43
3:C:70:TRP:CZ3	3:C:145:LEU:HD21	2.54	0.43
2:B:219:THR:OG1	2:B:225:ALA:HB1	2.18	0.43
2:B:127:ASP:C	3:C:140:ARG:HH12	2.21	0.42
1:A:108:ARG:HE	1:A:164:GLU:HG2	1.83	0.42
3:C:123:ALA:N	3:C:246:VAL:O	2.52	0.42
3:C:193:TRP:HZ2	3:C:207:VAL:O	2.03	0.42
1:A:62:LEU:HD13	1:A:204:ILE:HG23	2.01	0.42
1:A:88:ASP:HB2	1:A:92:PRO:HG2	2.02	0.42
1:A:228:SER:HB3	3:C:44:ARG:NH2	2.34	0.42
2:B:94:ASN:HB3	2:B:255:LYS:HG3	2.02	0.42
1:A:80:ASN:HA	1:A:81:PRO:HD3	1.83	0.42
3:C:122:TYR:O	3:C:195:ARG:HD3	2.20	0.42
3:C:123:ALA:HB3	3:C:246:VAL:HB	2.02	0.41
2:B:86:VAL:HG12	2:B:98:TYR:HE1	1.85	0.41
1:A:179:ASN:HA	2:B:145:PHE:HE2	1.84	0.41
2:B:129:VAL:HG12	2:B:219:THR:HA	2.03	0.41
3:C:146:LEU:HD11	3:C:169:HIS:ND1	2.35	0.41
1:A:67:LEU:HB2	1:A:197:LEU:O	2.21	0.41
2:B:117:PHE:CE1	2:B:237:MET:HG2	2.56	0.41
1:A:34:LYS:HZ1	3:C:50:THR:HG21	1.84	0.40
3:C:172:PHE:CE2	3:C:174:LEU:HA	2.56	0.40
3:C:249:GLN:NE2	3:C:250:PRO:O	2.51	0.40
1:A:171:GLN:HA	1:A:172:PRO:HD3	1.93	0.40
1:A:192:LEU:HG	1:A:193:ARG:H	1.85	0.40
3:C:4:PRO:O	3:C:6:PRO:HD3	2.22	0.40

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	219/266 (82%)	200 (91%)	19 (9%)	0	100	100
2	B	211/261 (81%)	202 (96%)	8 (4%)	1 (0%)	29	65
3	C	249/430 (58%)	229 (92%)	19 (8%)	1 (0%)	34	69
All	All	679/957 (71%)	631 (93%)	46 (7%)	2 (0%)	44	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	202	GLU
3	C	200	PRO

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	187/230 (81%)	169 (90%)	18 (10%)	8	33
2	B	188/234 (80%)	181 (96%)	7 (4%)	34	65
3	C	211/366 (58%)	195 (92%)	16 (8%)	13	43
All	All	586/830 (71%)	545 (93%)	41 (7%)	19	47

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP

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Mol	Chain	Res	Type
1	A	57	ARG
1	A	82	ILE
1	A	88	ASP
1	A	111	VAL
1	A	129	ILE
1	A	142	LYS
1	A	161	ARG
1	A	192	LEU
1	A	193	ARG
1	A	194	PHE
1	A	197	LEU
1	A	201	LEU
1	A	208	GLN
1	A	216	GLU
1	A	223	ILE
1	A	242	ASP
1	A	245	TYR
2	B	43	SER
2	B	53	LEU
2	B	62	SER
2	B	65	TRP
2	B	90	VAL
2	B	105	ILE
2	B	201	THR
3	C	50	THR
3	C	77	ARG
3	C	125	THR
3	C	126	ARG
3	C	146	LEU
3	C	158	ARG
3	C	162	GLU
3	C	169	HIS
3	C	174	LEU
3	C	175	ASN
3	C	184	VAL
3	C	188	THR
3	C	201	GLN
3	C	211	TYR
3	C	226	VAL
3	C	240	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	170	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)

There are no chain breaks in this entry.

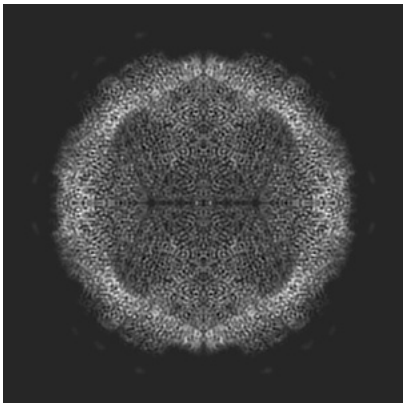
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4064. These allow visual inspection of the internal detail of the map and identification of artifacts.

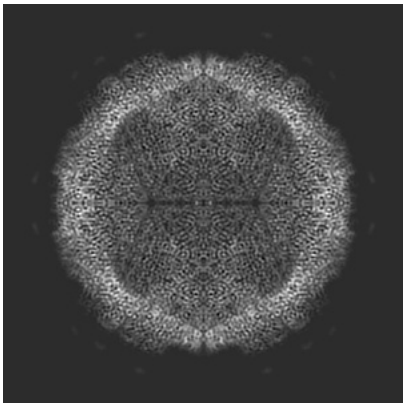
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

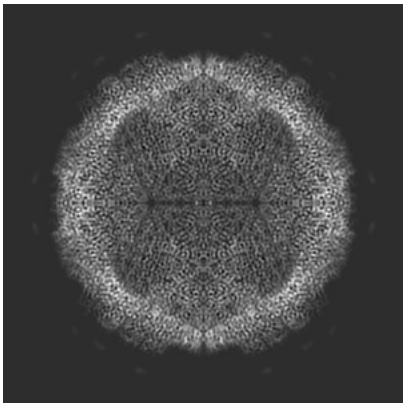
6.1.1 Primary map



X



Y

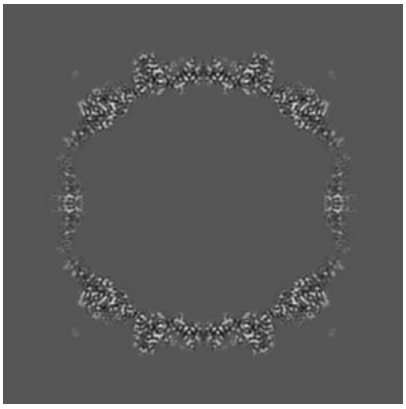


Z

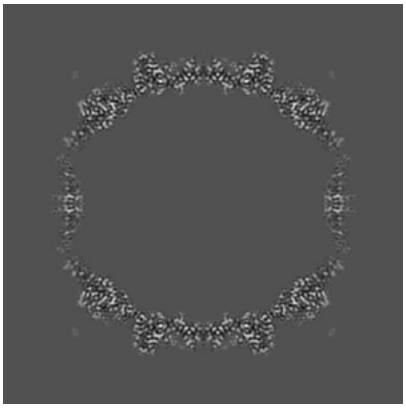
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

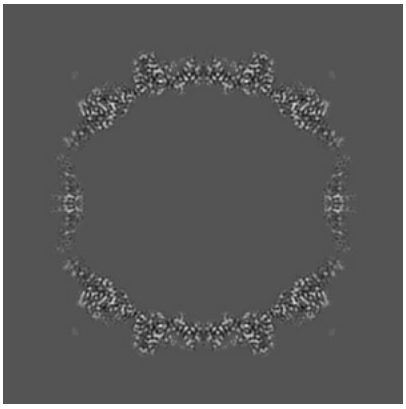
6.2.1 Primary map



X Index: 190



Y Index: 190

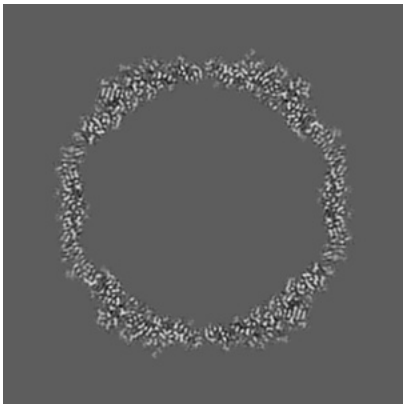


Z Index: 190

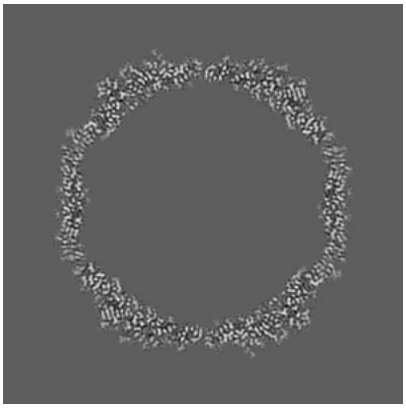
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

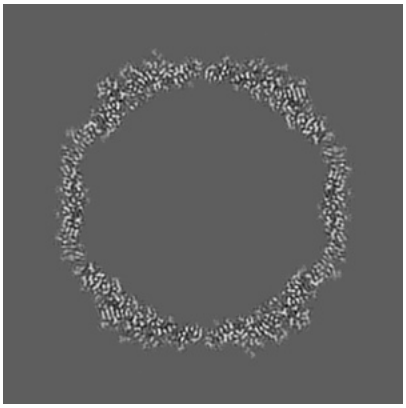
6.3.1 Primary map



X Index: 206



Y Index: 174

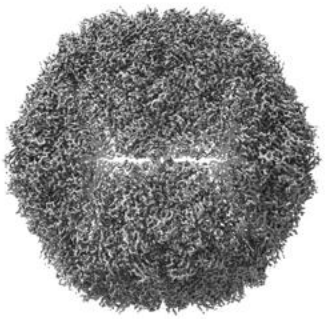


Z Index: 174

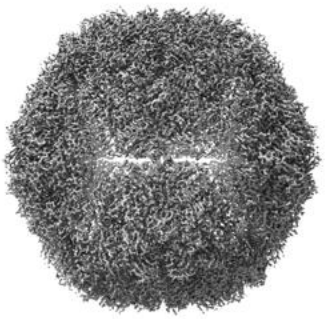
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

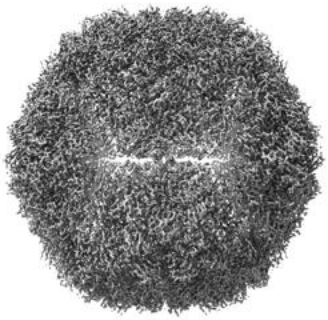
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

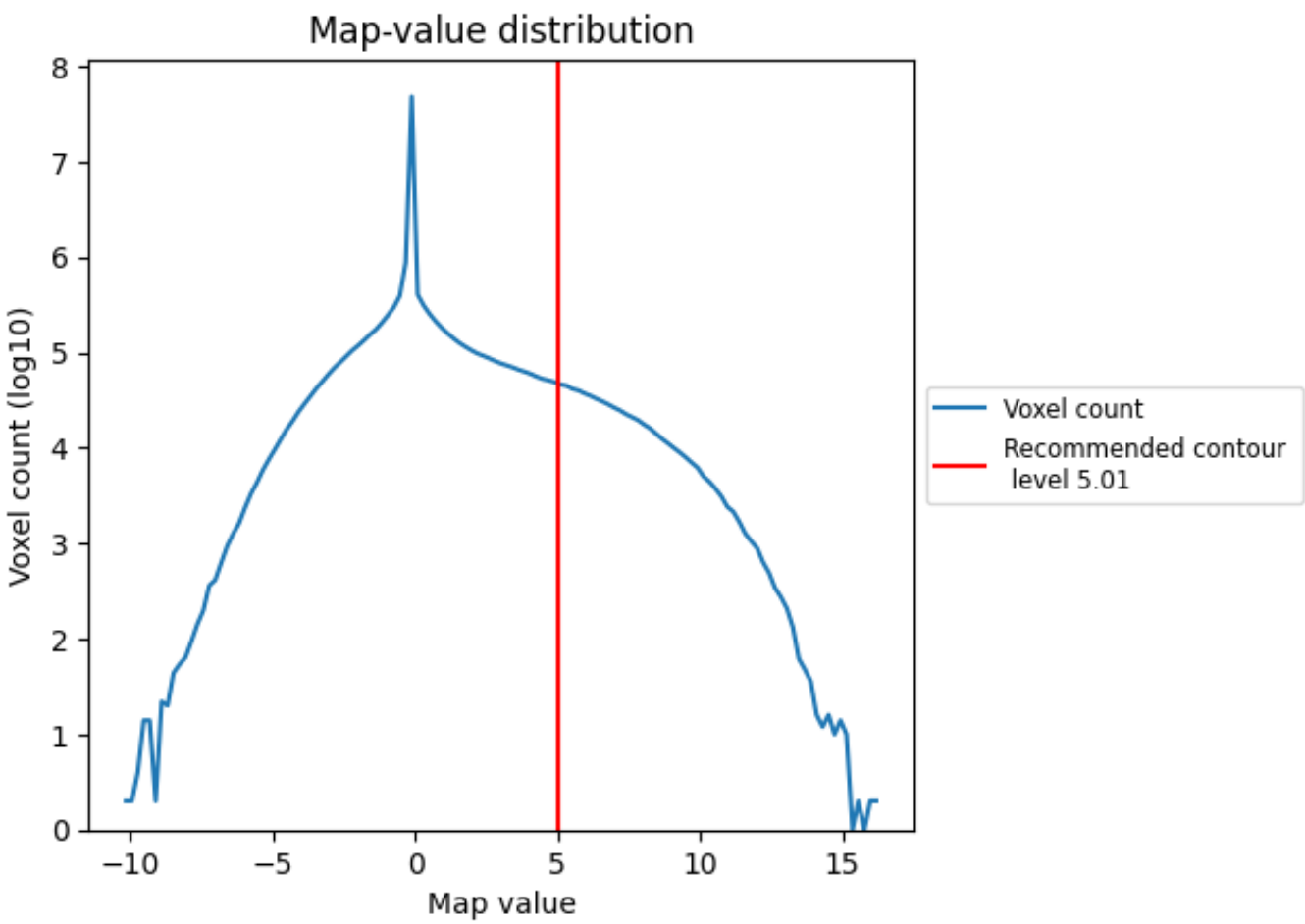
6.5 Mask visualisation (i)

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

7 Map analysis (i)

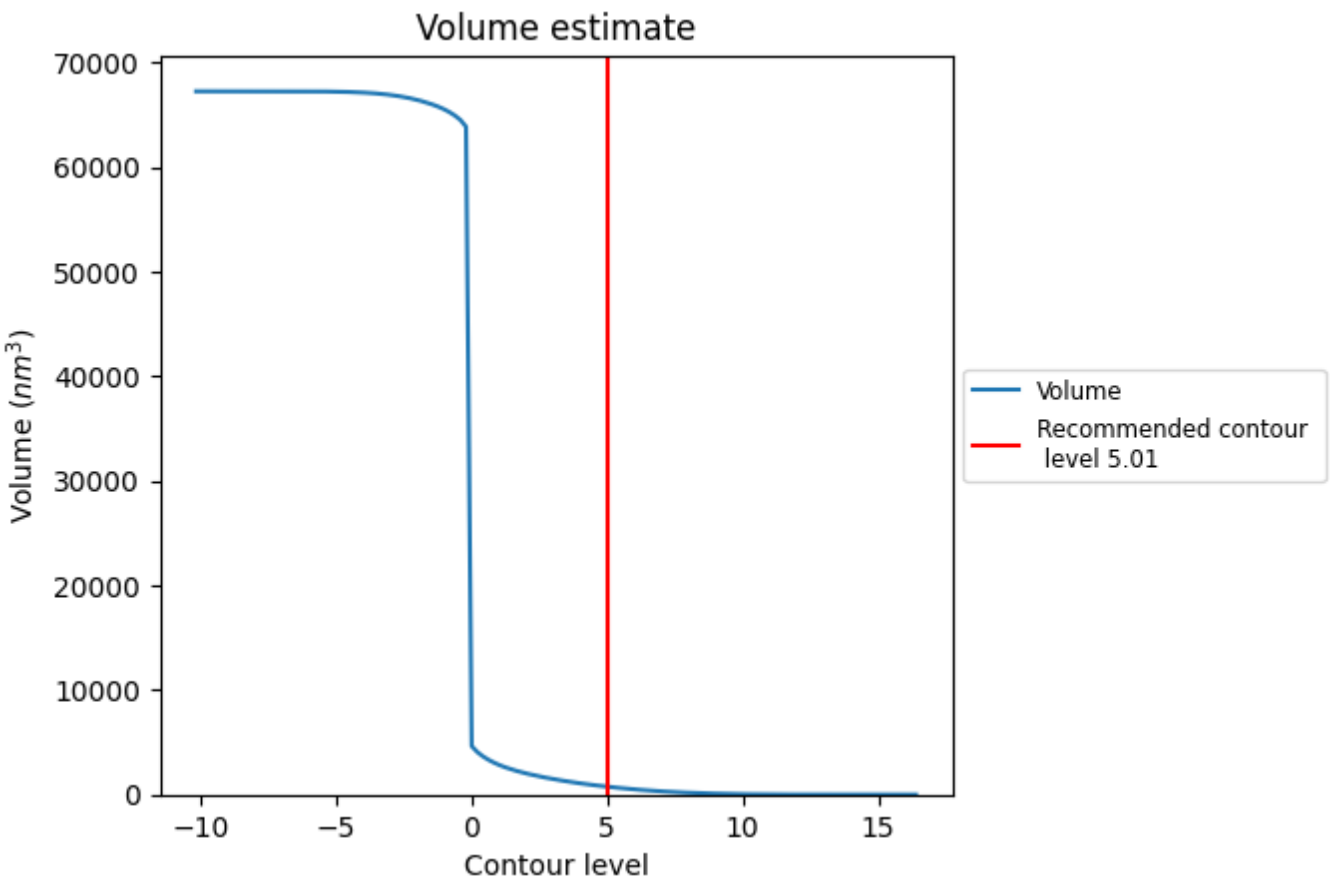
This section contains the results of statistical analysis of the map.

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.

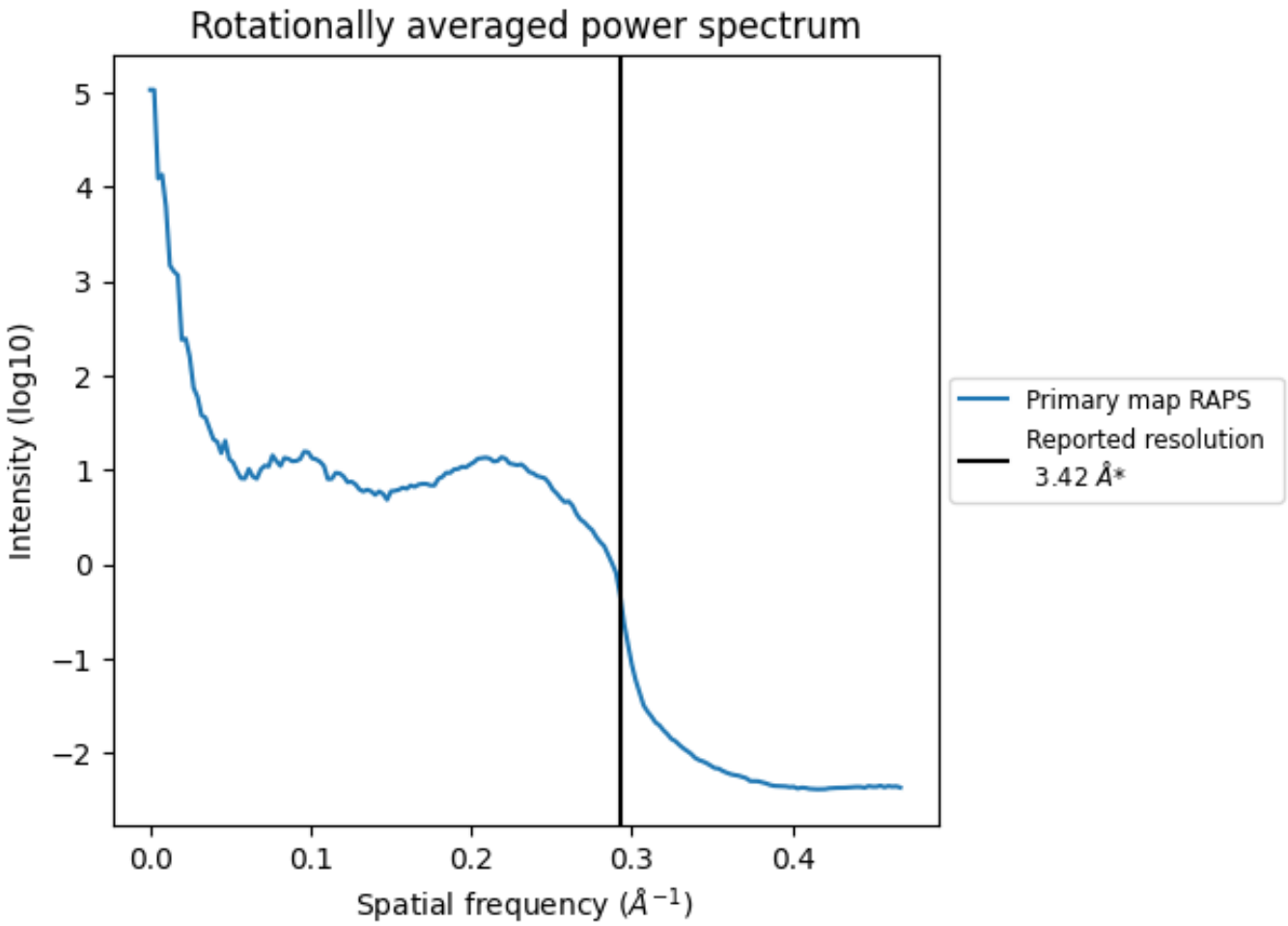
7.2 Volume estimate (i)



The volume at the recommended contour level is 754 nm^3; this corresponds to an approximate mass of 681 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)

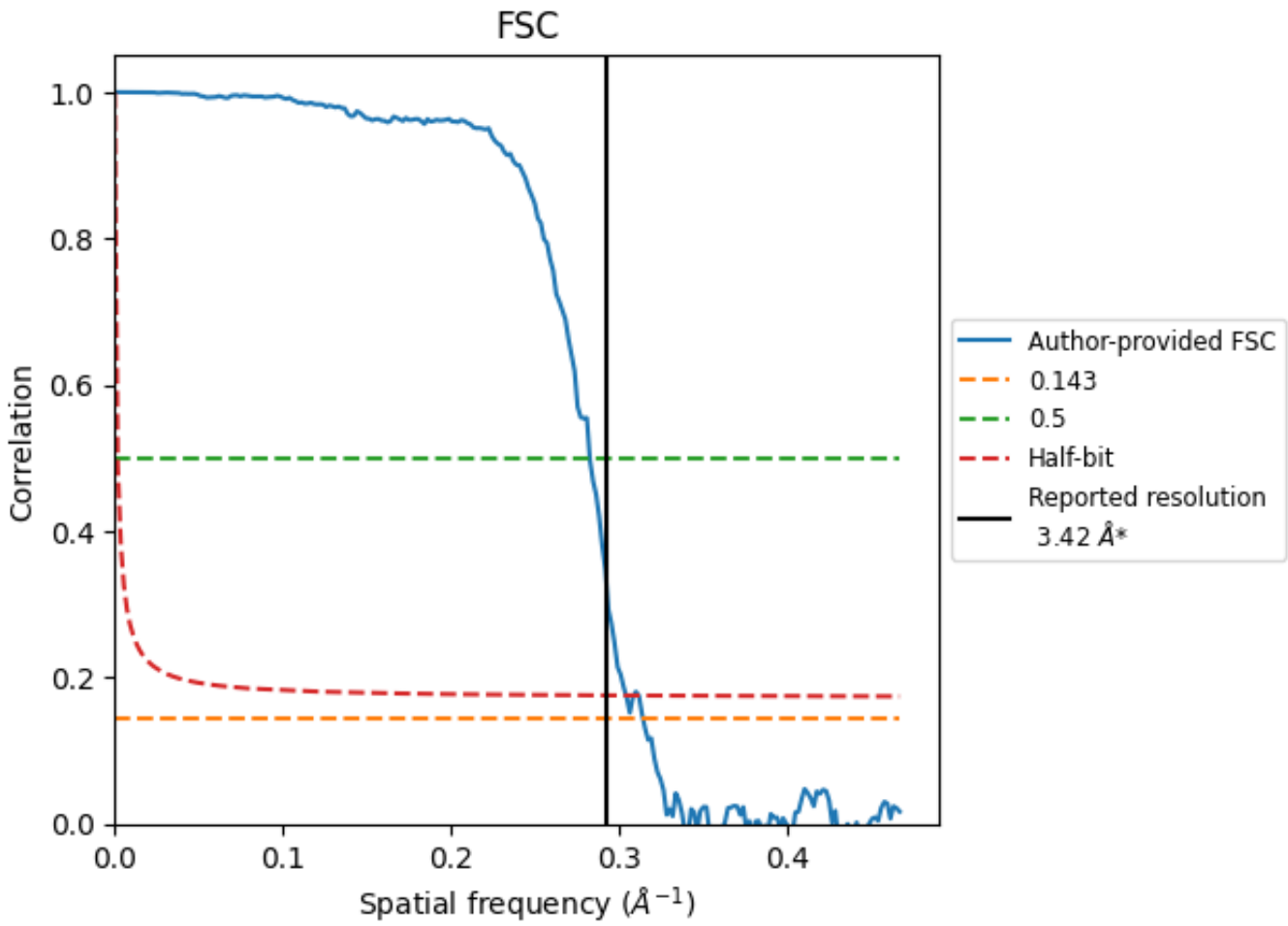


*Reported resolution corresponds to spatial frequency of 0.292 Å^{-1}

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 0.292 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.18	3.54	3.29
Unmasked-calculated*	-	-	-

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

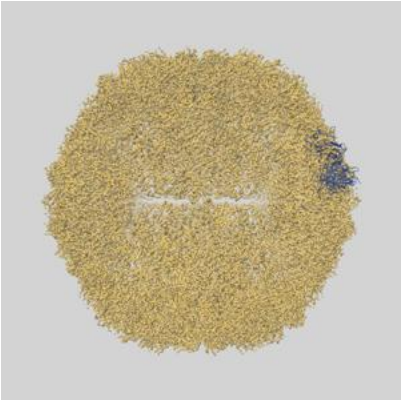
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4064 and PDB model 5LK8. Per-residue inclusion information can be found in section 3 on page 4.

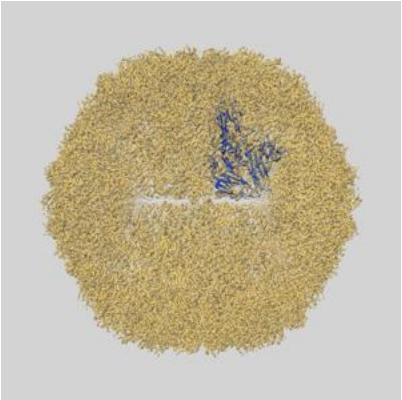
9.1 Map-model overlays

9.1.1 Map-model overlay (i)

X

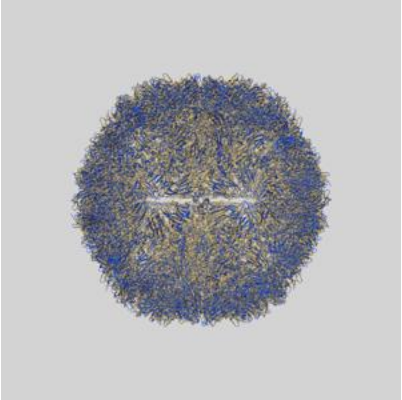


Y

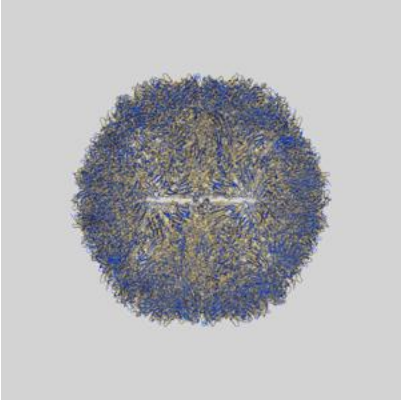


Z

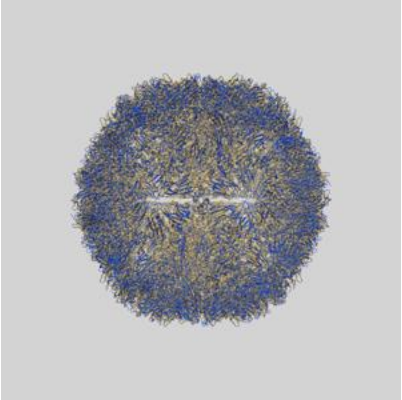
9.1.2 Map-model assembly overlay (i)



X



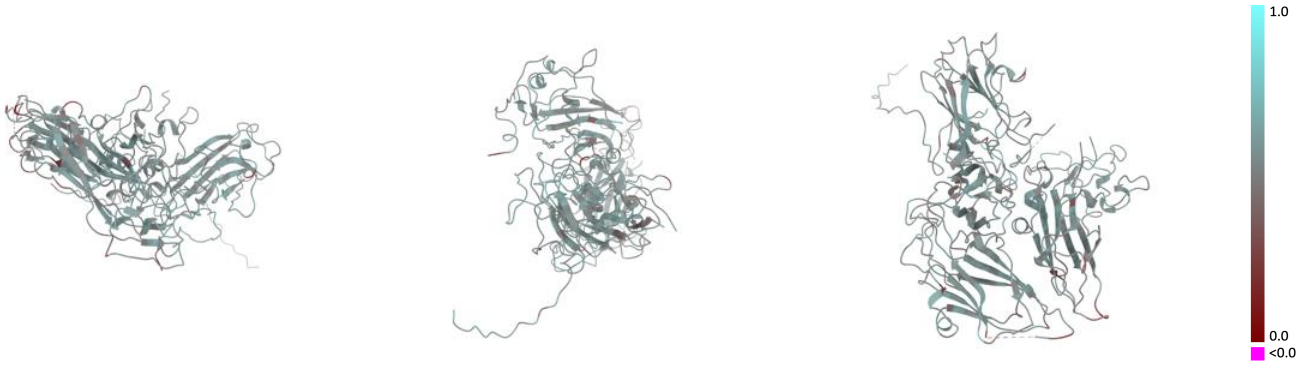
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.01 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.

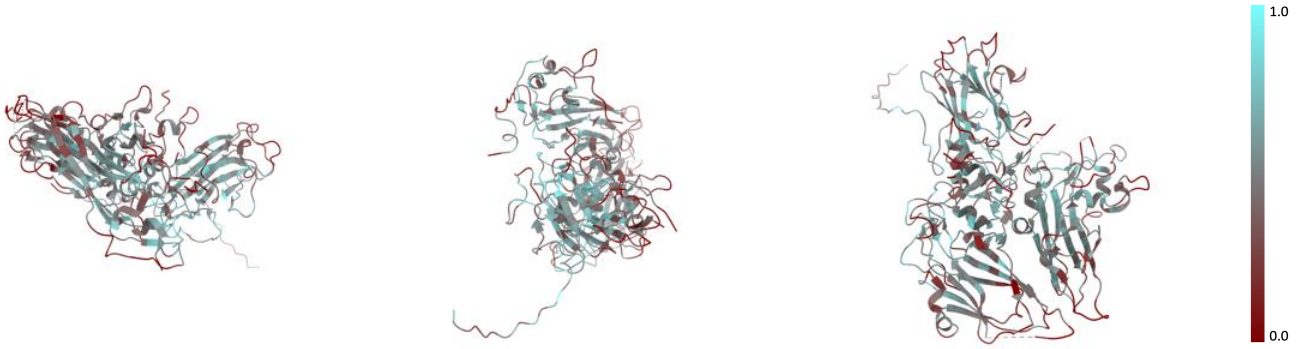
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

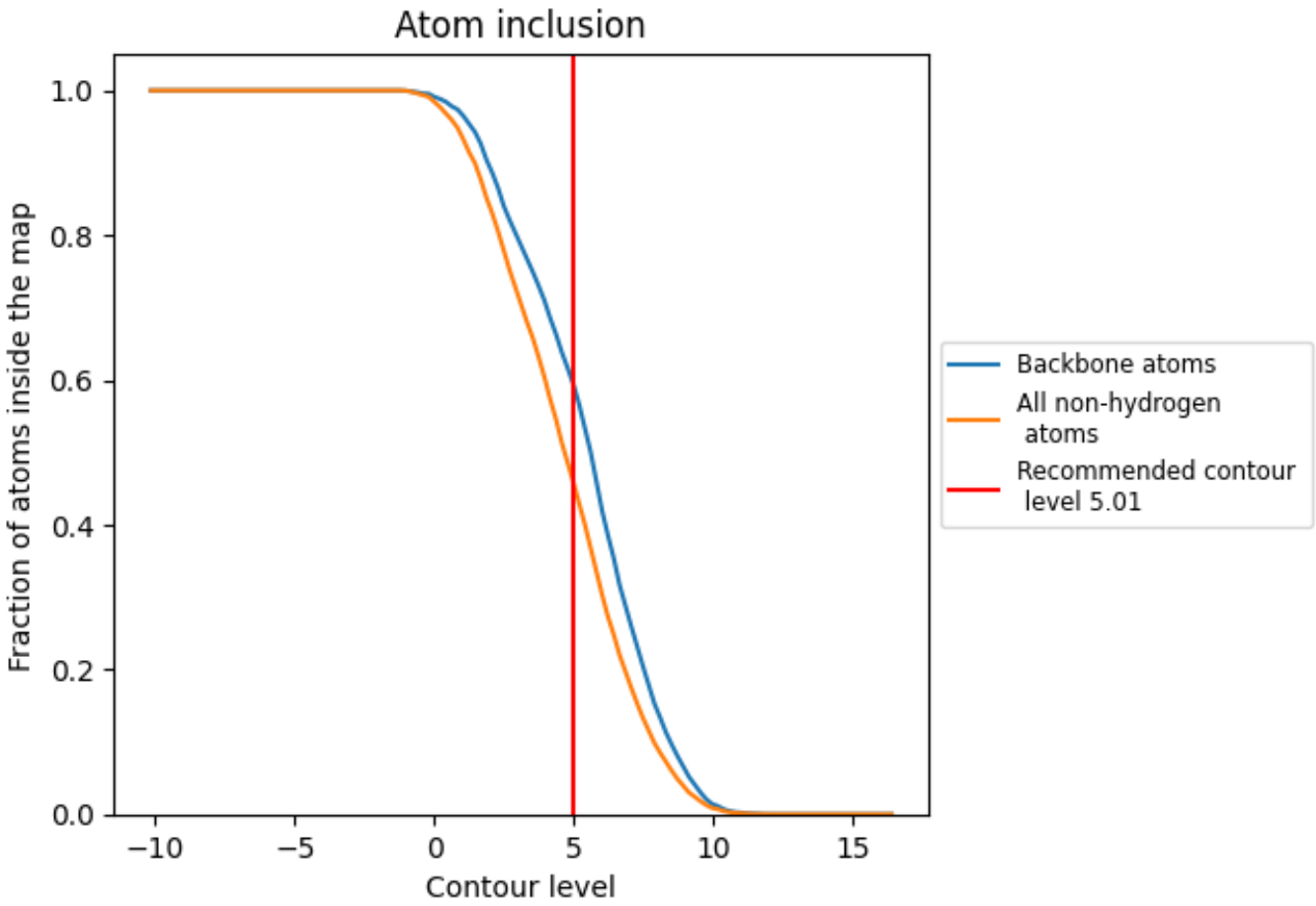
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (5.01).

9.4 Atom inclusion (i)



At the recommended contour level, 59% of all backbone atoms, 46% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (5.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4563	0.5270
A	0.4786	0.5340
B	0.4447	0.5240
C	0.4465	0.5240