



## Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 04:30 PM EST

PDB ID : 7K25  
EMDB ID : EMD-22643  
Title : Murine polyomavirus hexavalent capsomer, subparticle reconstruction  
Authors : Goetschius, D.J.; Hafenstein, S.L.  
Deposited on : 2020-09-08  
Resolution : 2.90 Å(reported)  
Based on initial models : 1SIE, 3GK8

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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

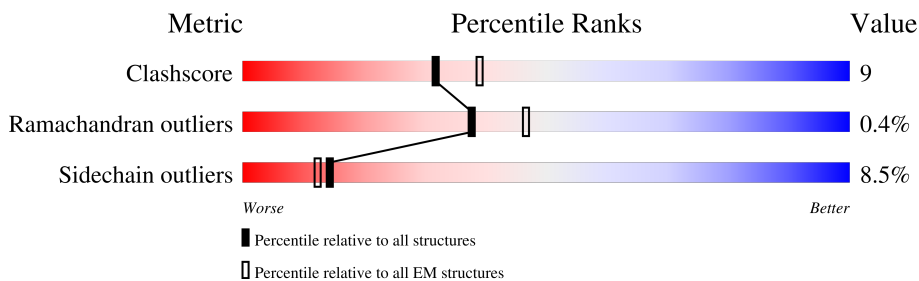
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 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	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  $\geq 3$ , 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	383	
1	B	383	
1	C	383	
1	D	383	
1	E	383	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14005 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

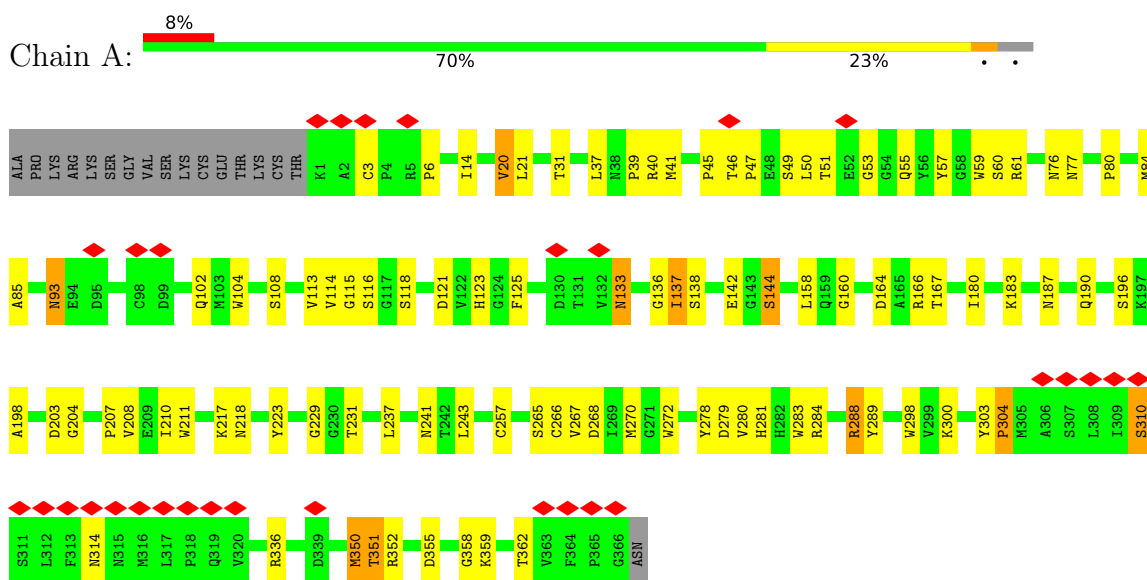
- Molecule 1 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	366	Total 2854	C 1807	N 479	O 552	S 16	0	0
1	B	367	Total 2862	C 1811	N 481	O 554	S 16	0	0
1	C	357	Total 2789	C 1764	N 468	O 541	S 16	0	0
1	D	340	Total 2650	C 1677	N 445	O 513	S 15	0	0
1	E	366	Total 2850	C 1804	N 479	O 551	S 16	0	0

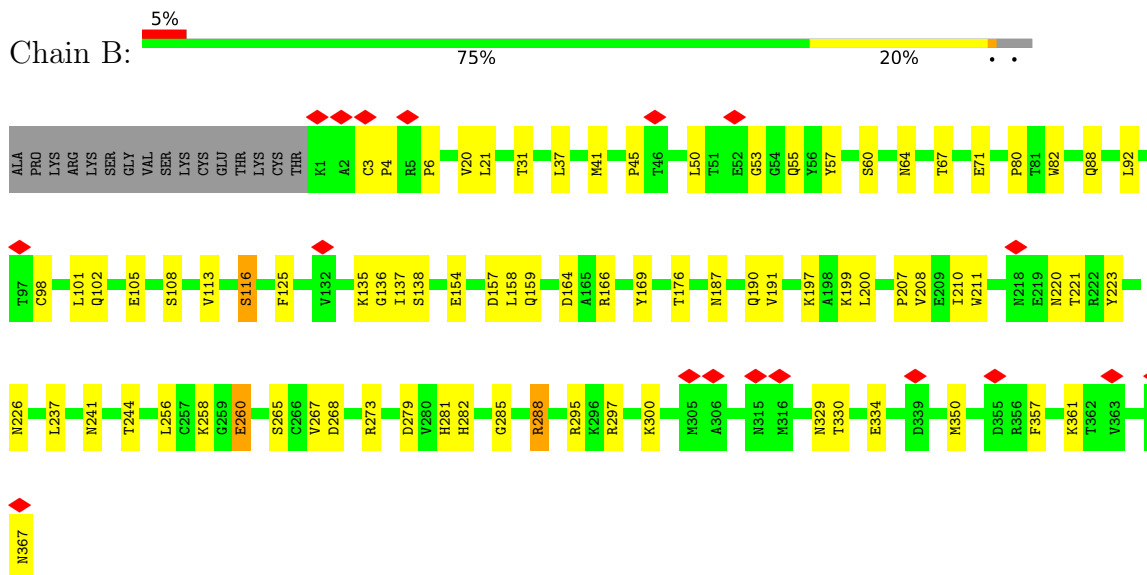
### 3 Residue-property plots

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.

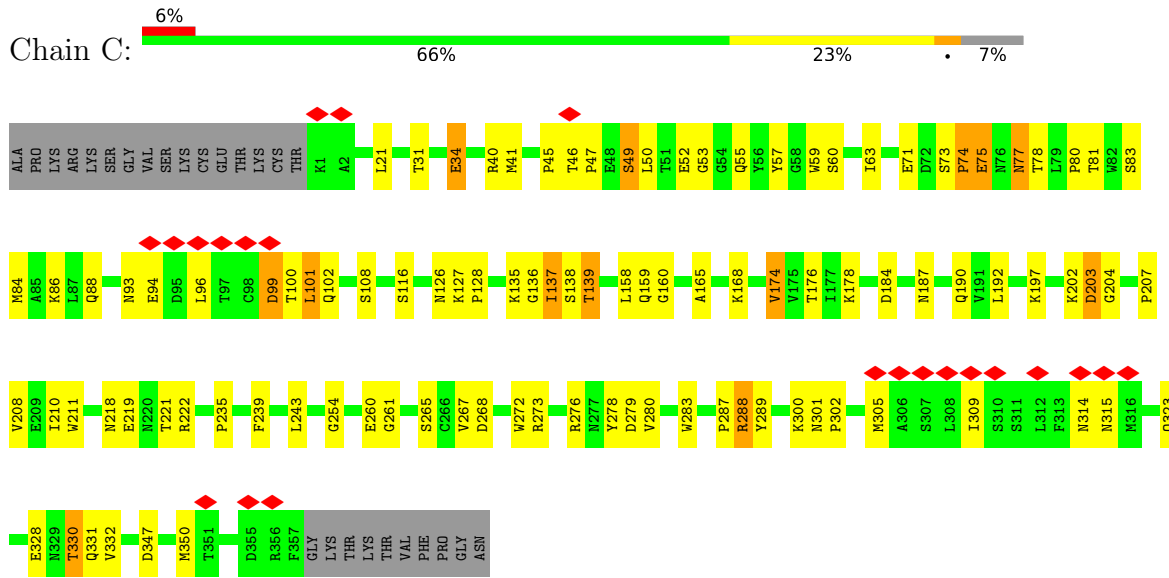
- Molecule 1: Capsid protein VP1



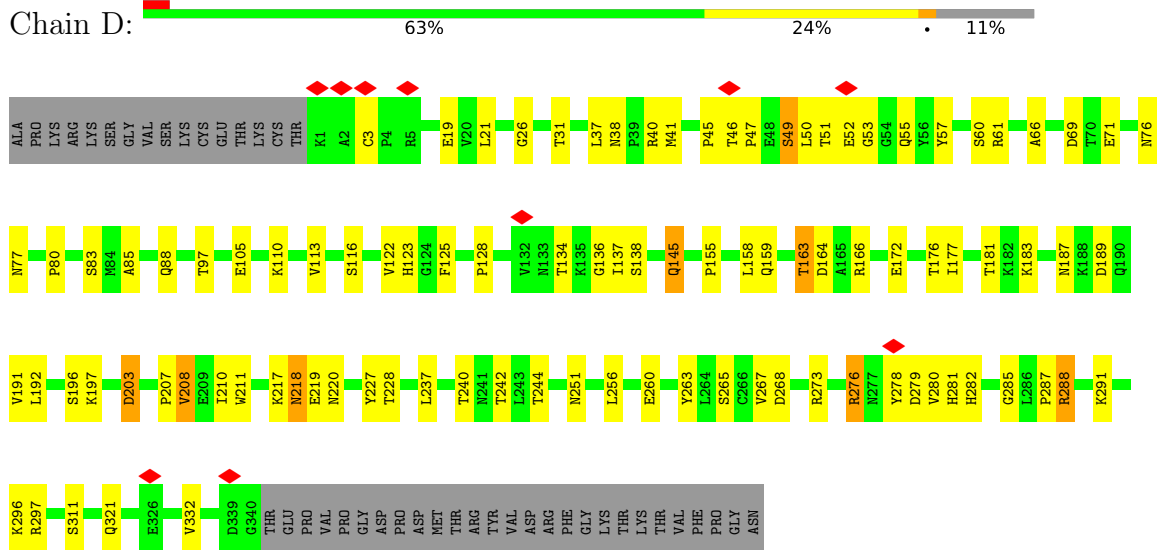
- Molecule 1: Capsid protein VP1



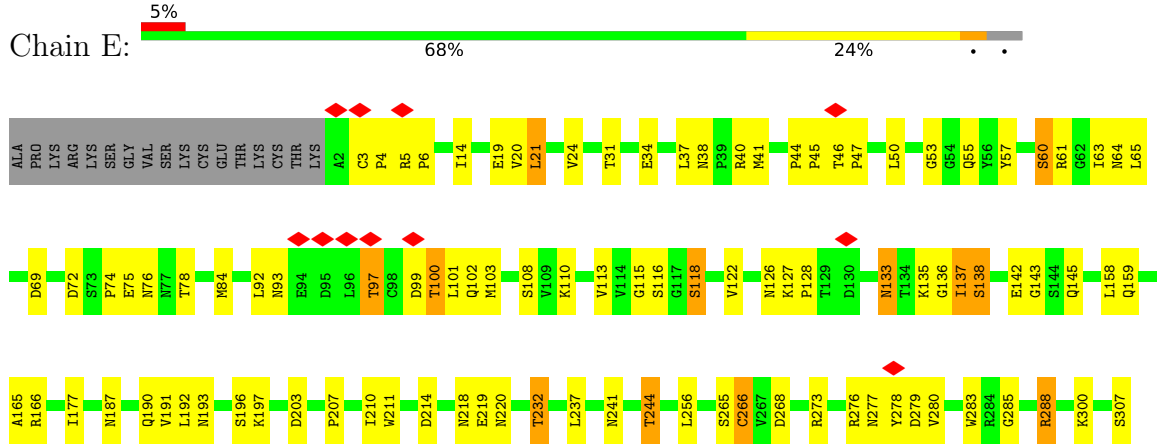
- Molecule 1: Capsid protein VP1

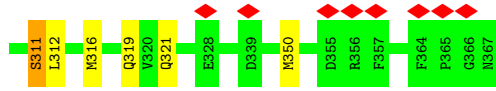


• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	929940	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 ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	30.467	Depositor
Minimum map value	-23.311	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.0	Depositor
Map size (Å)	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	0.43	0/2925	0.54	0/3988
1	B	0.44	0/2933	0.54	0/3999
1	C	0.45	0/2858	0.56	0/3898
1	D	0.47	0/2714	0.56	0/3700
1	E	0.44	0/2921	0.56	0/3984
All	All	0.45	0/14351	0.55	0/19569

There are no bond length outliers.

There are no bond angle outliers.

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	2854	0	2821	59	0
1	B	2862	0	2827	52	0
1	C	2789	0	2750	58	0
1	D	2650	0	2623	58	0
1	E	2850	0	2809	83	0
All	All	14005	0	13830	264	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 9.

All (264) 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:154:GLU:HB3	1:B:258:LYS:HE2	1.20	1.15
1:B:154:GLU:HB3	1:B:258:LYS:CE	1.91	1.00
1:A:298:TRP:CZ2	1:E:4:PRO:HG2	1.99	0.97
1:B:154:GLU:CB	1:B:258:LYS:HE2	2.01	0.89
1:B:154:GLU:OE1	1:B:258:LYS:NZ	2.08	0.86
1:E:99:ASP:O	1:E:300:LYS:HE2	1.77	0.84
1:D:50:LEU:HA	1:D:55:GLN:HG2	1.61	0.82
1:E:97:THR:HG21	1:E:101:LEU:HD12	1.62	0.81
1:A:50:LEU:HA	1:A:55:GLN:HG2	1.64	0.78
1:C:165:ALA:H	1:C:190:GLN:HE21	1.29	0.77
1:D:240:THR:HG1	1:D:242:THR:HG1	1.29	0.77
1:B:50:LEU:HA	1:B:55:GLN:HG2	1.67	0.76
1:D:159:GLN:OE1	1:D:197:LYS:NZ	2.20	0.75
1:D:38:ASN:H	1:D:40:ARG:HH21	1.35	0.74
1:E:50:LEU:HA	1:E:55:GLN:HG2	1.69	0.73
1:C:55:GLN:HG3	1:D:187:ASN:HB3	1.68	0.72
1:C:71:GLU:OE1	1:C:168:LYS:NZ	2.24	0.71
1:E:38:ASN:H	1:E:40:ARG:HH21	1.39	0.71
1:C:159:GLN:OE1	1:C:197:LYS:NZ	2.24	0.70
1:A:55:GLN:HG3	1:B:187:ASN:HB3	1.73	0.70
1:B:88:GLN:HE22	1:B:260:GLU:HB2	1.56	0.70
1:A:40:ARG:NH1	1:A:203:ASP:OD2	2.26	0.69
1:C:40:ARG:NH1	1:C:203:ASP:OD2	2.25	0.68
1:D:49:SER:HB2	1:D:52:GLU:HG2	1.76	0.68
1:E:126:ASN:HD21	1:E:273:ARG:HD2	1.57	0.67
1:C:50:LEU:HA	1:C:55:GLN:HG2	1.75	0.67
1:E:97:THR:HG21	1:E:101:LEU:HA	1.76	0.66
1:E:159:GLN:NE2	1:E:193:ASN:O	2.27	0.66
1:E:268:ASP:OD1	1:E:288:ARG:NH1	2.28	0.65
1:B:164:ASP:HA	1:B:190:GLN:HE21	1.61	0.65
1:A:278:TYR:HB3	1:E:135:LYS:HD3	1.78	0.65
1:D:321:GLN:OE1	1:D:321:GLN:N	2.29	0.64
1:E:100:THR:HG23	1:E:300:LYS:HE3	1.80	0.64
1:B:92:LEU:HB3	1:B:102:GLN:HG3	1.79	0.64
1:D:207:PRO:HG2	1:D:210:ILE:HD12	1.80	0.64
1:A:39:PRO:HD2	1:B:191:VAL:HG13	1.79	0.63
1:C:45:PRO:HB3	1:C:57:TYR:CZ	2.34	0.63
1:D:268:ASP:OD1	1:D:288:ARG:NH1	2.31	0.63
1:A:298:TRP:CE2	1:E:4:PRO:HG2	2.33	0.63
1:E:60:SER:HB3	1:E:283:TRP:HB2	1.81	0.62
1:B:135:LYS:HD3	1:C:278:TYR:HB3	1.80	0.62
1:D:191:VAL:HG23	1:D:192:LEU:H	1.64	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:LYS:O	1:C:139:THR:OG1	2.14	0.62
1:B:207:PRO:HG2	1:B:210:ILE:HD12	1.80	0.62
1:B:208:VAL:HG21	1:B:267:VAL:HG21	1.81	0.62
1:A:113:VAL:HB	1:A:237:LEU:HD21	1.80	0.62
1:A:237:LEU:HD13	1:A:270:MET:HE1	1.80	0.61
1:E:191:VAL:HG23	1:E:192:LEU:H	1.65	0.61
1:D:208:VAL:HG21	1:D:267:VAL:HG21	1.82	0.61
1:C:101:LEU:HD22	1:C:302:PRO:HD2	1.82	0.61
1:A:115:GLY:O	1:A:118:SER:OG	2.16	0.61
1:C:176:THR:HG22	1:C:178:LYS:H	1.64	0.61
1:E:64:ASN:HD21	1:E:75:GLU:HB2	1.66	0.61
1:B:279:ASP:O	1:B:281:HIS:ND1	2.32	0.60
1:D:55:GLN:HG3	1:E:187:ASN:HB3	1.84	0.60
1:A:208:VAL:HG11	1:A:267:VAL:HG21	1.82	0.60
1:B:45:PRO:HB3	1:B:57:TYR:CZ	2.37	0.60
1:B:6:PRO:HG2	1:C:300:LYS:HE3	1.84	0.60
1:E:113:VAL:HB	1:E:237:LEU:HD21	1.84	0.59
1:C:278:TYR:O	1:C:280:VAL:N	2.35	0.59
1:E:93:ASN:HD22	1:E:102:GLN:HB3	1.67	0.59
1:A:187:ASN:HD22	1:E:55:GLN:HE21	1.50	0.59
1:D:137:ILE:HG22	1:E:63:ILE:HG21	1.85	0.58
1:C:268:ASP:OD1	1:C:288:ARG:NH1	2.36	0.58
1:C:305:MET:O	1:C:309:ILE:HG13	2.05	0.57
1:D:145:GLN:HG3	1:D:228:THR:HB	1.87	0.57
1:C:21:LEU:HD21	1:C:31:THR:HG21	1.86	0.57
1:B:113:VAL:HB	1:B:237:LEU:HD21	1.86	0.57
1:C:208:VAL:HG11	1:C:267:VAL:HG21	1.87	0.56
1:A:187:ASN:HB3	1:E:55:GLN:HG3	1.87	0.56
1:E:21:LEU:HD11	1:E:31:THR:HG21	1.87	0.56
1:A:121:ASP:OD1	1:A:123:HIS:NE2	2.39	0.56
1:D:88:GLN:HE22	1:D:260:GLU:HB2	1.71	0.56
1:A:41:MET:HB2	1:A:80:PRO:HB3	1.88	0.55
1:A:223:TYR:CE2	1:E:241:ASN:HB2	2.41	0.55
1:D:69:ASP:O	1:D:166:ARG:NH2	2.31	0.55
1:E:143:GLY:O	1:E:145:GLN:NE2	2.40	0.55
1:D:113:VAL:HB	1:D:237:LEU:HD21	1.89	0.55
1:E:278:TYR:O	1:E:280:VAL:N	2.40	0.55
1:A:144:SER:HB2	1:A:229:GLY:HA2	1.88	0.54
1:A:21:LEU:HD21	1:A:31:THR:HG21	1.89	0.54
1:A:278:TYR:O	1:A:280:VAL:N	2.41	0.54
1:D:21:LEU:HD21	1:D:31:THR:HG21	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ASP:O	1:E:136:GLY:HA2	2.07	0.54
1:E:128:PRO:HD3	1:E:276:ARG:HG3	1.89	0.54
1:E:115:GLY:O	1:E:118:SER:HB3	2.08	0.54
1:D:41:MET:HB2	1:D:80:PRO:HB3	1.90	0.53
1:D:41:MET:SD	1:D:285:GLY:HA3	2.48	0.53
1:B:88:GLN:NE2	1:B:260:GLU:HB2	2.23	0.53
1:C:88:GLN:HE22	1:C:260:GLU:HB2	1.74	0.53
1:A:190:GLN:NE2	1:E:57:TYR:O	2.42	0.53
1:A:203:ASP:OD1	1:A:204:GLY:N	2.42	0.53
1:B:55:GLN:HG3	1:C:187:ASN:HB3	1.90	0.53
1:D:45:PRO:HB3	1:D:57:TYR:CZ	2.44	0.52
1:A:37:LEU:HD21	1:A:85:ALA:HB2	1.92	0.52
1:B:154:GLU:CG	1:B:258:LYS:HE2	2.39	0.52
1:B:67:THR:OG1	1:B:71:GLU:OE2	2.24	0.52
1:E:127:LYS:NZ	1:E:279:ASP:OD2	2.42	0.52
1:C:137:ILE:HG12	1:D:281:HIS:CG	2.45	0.52
1:E:100:THR:HG23	1:E:300:LYS:CE	2.40	0.52
1:A:158:LEU:HD13	1:A:211:TRP:HB3	1.90	0.51
1:B:350:MET:HE2	1:B:361:LYS:HE3	1.92	0.51
1:D:37:LEU:HD21	1:D:85:ALA:HB2	1.91	0.51
1:E:158:LEU:HD13	1:E:211:TRP:HB3	1.91	0.51
1:A:45:PRO:HB3	1:A:57:TYR:CZ	2.44	0.51
1:A:137:ILE:HG12	1:B:281:HIS:CD2	2.46	0.51
1:A:180:ILE:HD13	1:A:198:ALA:HB2	1.92	0.51
1:A:350:MET:SD	1:A:352:ARG:NH2	2.83	0.51
1:E:5:ARG:CG	1:E:6:PRO:HD2	2.41	0.51
1:E:38:ASN:H	1:E:40:ARG:NH2	2.08	0.51
1:E:5:ARG:HG2	1:E:6:PRO:HD2	1.92	0.51
1:A:217:LYS:HA	1:E:34:GLU:OE2	2.11	0.51
1:C:46:THR:OG1	1:C:47:PRO:HD3	2.10	0.51
1:D:137:ILE:HA	1:E:65:LEU:HD11	1.93	0.51
1:C:99:ASP:O	1:C:301:ASN:N	2.43	0.50
1:E:37:LEU:HD23	1:E:266:CYS:HB3	1.94	0.50
1:A:268:ASP:OD1	1:A:288:ARG:NH1	2.44	0.50
1:A:50:LEU:HD23	1:B:166:ARG:HG2	1.93	0.50
1:B:136:GLY:HA2	1:C:279:ASP:O	2.11	0.50
1:B:158:LEU:HD11	1:B:200:LEU:HD13	1.92	0.50
1:C:330:THR:HG22	1:C:332:VAL:H	1.76	0.50
1:A:46:THR:HB	1:A:47:PRO:HD3	1.94	0.50
1:C:128:PRO:HD3	1:C:276:ARG:HD3	1.93	0.50
1:D:26:GLY:O	1:D:296:LYS:NZ	2.33	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:TRP:CE2	1:E:4:PRO:CB	2.95	0.50
1:D:110:LYS:HB2	1:D:291:LYS:HB3	1.93	0.50
1:A:14:ILE:HG12	1:A:20:VAL:HG22	1.94	0.49
1:C:84:MET:HG3	1:C:203:ASP:HB2	1.92	0.49
1:C:235:PRO:HB2	1:D:227:TYR:HE2	1.76	0.49
1:D:189:ASP:OD1	1:D:196:SER:OG	2.22	0.49
1:B:41:MET:SD	1:B:80:PRO:HB3	2.53	0.49
1:B:268:ASP:OD1	1:B:288:ARG:NH1	2.45	0.49
1:E:84:MET:HG3	1:E:203:ASP:HB2	1.94	0.49
1:E:207:PRO:HG2	1:E:210:ILE:HD12	1.94	0.49
1:A:310:SER:O	1:A:310:SER:OG	2.28	0.49
1:E:110:LYS:HG3	1:E:244:THR:HG23	1.93	0.49
1:A:298:TRP:CD2	1:E:4:PRO:HB2	2.48	0.49
1:C:88:GLN:NE2	1:C:260:GLU:HB2	2.28	0.49
1:C:135:LYS:HD3	1:D:278:TYR:HB3	1.94	0.49
1:A:53:GLY:C	1:A:55:GLN:H	2.15	0.49
1:E:74:PRO:O	1:E:78:THR:OG1	2.31	0.49
1:B:220:ASN:ND2	1:B:256:LEU:O	2.39	0.48
1:C:41:MET:HB2	1:C:80:PRO:HB3	1.95	0.48
1:C:53:GLY:C	1:C:55:GLN:H	2.15	0.48
1:E:40:ARG:HH11	1:E:203:ASP:CG	2.16	0.48
1:B:53:GLY:C	1:B:55:GLN:H	2.15	0.48
1:D:158:LEU:HD13	1:D:211:TRP:HB3	1.95	0.48
1:D:287:PRO:HG3	1:E:191:VAL:O	2.14	0.48
1:C:174:VAL:HG22	1:C:207:PRO:HD3	1.95	0.48
1:C:222:ARG:HH21	1:C:254:GLY:HA2	1.79	0.48
1:C:137:ILE:HD13	1:C:137:ILE:HA	1.65	0.47
1:D:53:GLY:C	1:D:55:GLN:H	2.16	0.47
1:E:165:ALA:H	1:E:190:GLN:HE21	1.62	0.47
1:E:312:LEU:O	1:E:316:MET:HG2	2.14	0.47
1:C:207:PRO:HG2	1:C:210:ILE:HD12	1.96	0.47
1:B:158:LEU:HD13	1:B:211:TRP:HB3	1.96	0.47
1:B:105:GLU:OE1	1:B:295:ARG:NE	2.40	0.47
1:B:116:SER:OG	1:B:237:LEU:HD23	2.14	0.47
1:E:133:ASN:N	1:E:133:ASN:OD1	2.47	0.47
1:D:55:GLN:HE21	1:E:187:ASN:HB2	1.80	0.46
1:B:282:HIS:CD2	1:B:282:HIS:H	2.33	0.46
1:E:53:GLY:C	1:E:55:GLN:H	2.18	0.46
1:A:93:ASN:HD22	1:A:102:GLN:H	1.64	0.46
1:E:19:GLU:HG3	1:E:20:VAL:N	2.31	0.45
1:A:6:PRO:HG2	1:B:300:LYS:HG3	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:GLN:NE2	1:B:260:GLU:CB	2.79	0.45
1:B:4:PRO:O	1:C:100:THR:HG21	2.17	0.45
1:E:21:LEU:HD12	1:E:21:LEU:HA	1.83	0.45
1:E:177:ILE:HG12	1:E:196:SER:HB2	1.98	0.45
1:E:307:SER:O	1:E:311:SER:OG	2.30	0.45
1:A:137:ILE:HG12	1:B:281:HIS:CG	2.52	0.45
1:C:160:GLY:HA2	1:C:210:ILE:O	2.17	0.45
1:D:163:THR:O	1:D:164:ASP:C	2.54	0.45
1:C:158:LEU:HD13	1:C:211:TRP:HB3	1.99	0.45
1:D:77:ASN:ND2	1:D:77:ASN:H	2.14	0.45
1:A:303:TYR:N	1:A:304:PRO:HD2	2.32	0.45
1:E:64:ASN:ND2	1:E:75:GLU:HB2	2.30	0.45
1:B:282:HIS:CD2	1:B:282:HIS:N	2.85	0.44
1:A:281:HIS:CG	1:E:137:ILE:HG12	2.52	0.44
1:B:105:GLU:OE2	1:B:297:ARG:NE	2.51	0.44
1:E:122:VAL:O	1:E:138:SER:HB3	2.18	0.44
1:E:97:THR:CG2	1:E:101:LEU:HA	2.44	0.44
1:A:136:GLY:HA2	1:B:279:ASP:O	2.18	0.44
1:A:207:PRO:HG2	1:A:210:ILE:HD12	2.00	0.44
1:B:41:MET:HE3	1:B:285:GLY:HA3	2.00	0.44
1:C:41:MET:HE3	1:C:41:MET:HB3	1.77	0.44
1:C:74:PRO:O	1:C:75:GLU:HG2	2.18	0.44
1:E:61:ARG:HD2	1:E:61:ARG:HA	1.60	0.44
1:A:61:ARG:HB2	1:A:77:ASN:HD22	1.83	0.44
1:C:41:MET:HE2	1:C:80:PRO:HB3	1.98	0.44
1:D:278:TYR:O	1:D:280:VAL:N	2.48	0.44
1:E:14:ILE:HG23	1:E:20:VAL:HG13	1.98	0.44
1:E:45:PRO:HB3	1:E:57:TYR:CZ	2.51	0.44
1:A:298:TRP:CE2	1:E:4:PRO:CG	3.00	0.44
1:B:329:ASN:OD1	1:B:329:ASN:N	2.42	0.44
1:D:46:THR:HB	1:D:47:PRO:HD3	2.00	0.44
1:A:187:ASN:HD22	1:E:55:GLN:NE2	2.16	0.43
1:E:126:ASN:ND2	1:E:273:ARG:HD2	2.29	0.43
1:A:164:ASP:HB3	1:A:167:THR:OG1	2.18	0.43
1:C:278:TYR:O	1:C:280:VAL:HG23	2.18	0.43
1:C:81:THR:OG1	1:C:204:GLY:HA2	2.18	0.43
1:D:61:ARG:O	1:D:282:HIS:NE2	2.52	0.43
1:C:55:GLN:HG3	1:D:187:ASN:CB	2.43	0.43
1:C:63:ILE:HD13	1:C:78:THR:HG23	1.99	0.43
1:A:352:ARG:HD3	1:A:359:LYS:HD3	2.01	0.43
1:B:241:ASN:ND2	1:C:221:THR:O	2.48	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:MET:HE3	1:D:80:PRO:HB3	2.01	0.43
1:D:155:PRO:HD3	1:D:263:TYR:CZ	2.53	0.43
1:E:41:MET:SD	1:E:285:GLY:HA3	2.59	0.43
1:D:66:ALA:HB1	1:D:71:GLU:O	2.19	0.43
1:B:157:ASP:OD1	1:B:199:LYS:HD3	2.19	0.43
1:D:176:THR:HG22	1:D:177:ILE:N	2.33	0.43
1:E:46:THR:OG1	1:E:47:PRO:HD3	2.19	0.43
1:C:86:LYS:HE3	1:C:261:GLY:HA3	2.00	0.43
1:A:231:THR:HA	1:A:272:TRP:HZ3	1.84	0.42
1:E:220:ASN:ND2	1:E:256:LEU:O	2.46	0.42
1:A:104:TRP:HB2	1:A:257:CYS:HB2	2.01	0.42
1:E:277:ASN:HD22	1:E:277:ASN:HA	1.75	0.42
1:B:21:LEU:HD21	1:B:31:THR:HG21	2.01	0.42
1:E:103:MET:SD	1:E:256:LEU:HB3	2.59	0.42
1:A:298:TRP:CE2	1:E:4:PRO:HB2	2.55	0.42
1:D:61:ARG:HD2	1:D:61:ARG:HA	1.67	0.42
1:E:93:ASN:ND2	1:E:101:LEU:HG	2.34	0.42
1:B:159:GLN:OE1	1:B:197:LYS:HE2	2.19	0.42
1:C:287:PRO:HG3	1:D:191:VAL:O	2.20	0.42
1:E:44:PRO:HB2	1:E:46:THR:HG23	2.01	0.42
1:A:351:THR:HG23	1:A:362:THR:HB	2.02	0.42
1:B:82:TRP:HB2	1:B:200:LEU:HD11	2.01	0.42
1:D:128:PRO:HG2	1:D:134:THR:HG23	2.01	0.42
1:B:154:GLU:HB3	1:B:258:LYS:HE3	1.94	0.42
1:C:126:ASN:HB2	1:C:138:SER:OG	2.20	0.42
1:D:219:GLU:HG3	1:D:220:ASN:H	1.85	0.42
1:A:59:TRP:CZ3	1:A:284:ARG:HB2	2.55	0.41
1:C:77:ASN:H	1:C:77:ASN:ND2	2.17	0.41
1:D:105:GLU:HB2	1:D:256:LEU:HD23	2.02	0.41
1:D:136:GLY:HA2	1:E:279:ASP:O	2.20	0.41
1:E:142:GLU:HB3	1:E:232:THR:O	2.19	0.41
1:E:159:GLN:HE21	1:E:197:LYS:NZ	2.18	0.41
1:A:133:ASN:OD1	1:A:133:ASN:N	2.54	0.41
1:A:241:ASN:HB2	1:B:223:TYR:CE2	2.55	0.41
1:C:93:ASN:ND2	1:C:102:GLN:O	2.52	0.41
1:D:128:PRO:HD3	1:D:276:ARG:HG3	2.03	0.41
1:A:160:GLY:HA2	1:A:210:ILE:O	2.19	0.41
1:A:355:ASP:N	1:A:358:GLY:O	2.45	0.41
1:A:142:GLU:O	1:A:272:TRP:N	2.40	0.41
1:C:323:GLN:NE2	1:C:331:GLN:HE22	2.17	0.41
1:D:218:ASN:OD1	1:D:218:ASN:N	2.53	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:TYR:CB	1:B:176:THR:HG21	2.51	0.41
1:C:34:GLU:HG2	1:C:289:TYR:HE1	1.86	0.41
1:D:122:VAL:O	1:D:138:SER:HB3	2.20	0.41
1:D:123:HIS:HD2	1:E:72:ASP:OD2	2.04	0.41
1:D:181:THR:O	1:D:181:THR:OG1	2.38	0.41
1:E:159:GLN:HB2	1:E:214:ASP:HB2	2.03	0.41
1:C:49:SER:O	1:C:55:GLN:NE2	2.53	0.41
1:B:279:ASP:HB3	1:B:281:HIS:HE1	1.86	0.40
1:E:92:LEU:HD13	1:E:102:GLN:HG2	2.02	0.40
1:E:93:ASN:ND2	1:E:102:GLN:N	2.69	0.40
1:C:136:GLY:HA2	1:D:279:ASP:O	2.21	0.40
1:C:323:GLN:HE21	1:C:331:GLN:HE22	1.69	0.40
1:D:55:GLN:HG3	1:E:187:ASN:CB	2.51	0.40
1:E:3:CYS:HB2	1:E:4:PRO:CD	2.51	0.40
1:C:34:GLU:CD	1:D:217:LYS:HA	2.42	0.40
1:C:347:ASP:HB3	1:C:350:MET:HB2	2.02	0.40
1:D:50:LEU:HD22	1:E:166:ARG:HG3	2.03	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	364/383 (95%)	326 (90%)	37 (10%)	1 (0%)	41	71
1	B	365/383 (95%)	338 (93%)	26 (7%)	1 (0%)	41	71
1	C	355/383 (93%)	330 (93%)	23 (6%)	2 (1%)	25	58
1	D	338/383 (88%)	303 (90%)	32 (10%)	3 (1%)	17	48
1	E	364/383 (95%)	322 (88%)	41 (11%)	1 (0%)	41	71
All	All	1786/1915 (93%)	1619 (91%)	159 (9%)	8 (0%)	38	66

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	74	PRO
1	D	203	ASP
1	B	260	GLU
1	C	75	GLU
1	D	76	ASN
1	D	163	THR
1	E	76	ASN
1	A	76	ASN

### 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	322/337 (96%)	290 (90%)	32 (10%)	8	24
1	B	323/337 (96%)	301 (93%)	22 (7%)	16	42
1	C	315/337 (94%)	281 (89%)	34 (11%)	6	20
1	D	299/337 (89%)	275 (92%)	24 (8%)	12	33
1	E	321/337 (95%)	298 (93%)	23 (7%)	14	39
All	All	1580/1685 (94%)	1445 (92%)	135 (8%)	14	31

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	CYS
1	A	20	VAL
1	A	49	SER
1	A	51	THR
1	A	60	SER
1	A	84	MET
1	A	93	ASN
1	A	108	SER
1	A	114	VAL
1	A	116	SER

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	125	PHE
1	A	133	ASN
1	A	137	ILE
1	A	138	SER
1	A	144	SER
1	A	166	ARG
1	A	183	LYS
1	A	196	SER
1	A	218	ASN
1	A	243	LEU
1	A	265	SER
1	A	266	CYS
1	A	283	TRP
1	A	288	ARG
1	A	289	TYR
1	A	300	LYS
1	A	304	PRO
1	A	310	SER
1	A	314	ASN
1	A	336	ARG
1	A	350	MET
1	A	351	THR
1	B	3	CYS
1	B	20	VAL
1	B	37	LEU
1	B	60	SER
1	B	64	ASN
1	B	98	CYS
1	B	101	LEU
1	B	108	SER
1	B	116	SER
1	B	125	PHE
1	B	137	ILE
1	B	138	SER
1	B	221	THR
1	B	226	ASN
1	B	244	THR
1	B	265	SER
1	B	273	ARG
1	B	288	ARG
1	B	330	THR
1	B	334	GLU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	357	PHE
1	B	367	ASN
1	C	34	GLU
1	C	49	SER
1	C	52	GLU
1	C	59	TRP
1	C	60	SER
1	C	73	SER
1	C	77	ASN
1	C	83	SER
1	C	94	GLU
1	C	96	LEU
1	C	99	ASP
1	C	101	LEU
1	C	108	SER
1	C	116	SER
1	C	137	ILE
1	C	139	THR
1	C	174	VAL
1	C	184	ASP
1	C	192	LEU
1	C	202	LYS
1	C	203	ASP
1	C	218	ASN
1	C	219	GLU
1	C	239	PHE
1	C	243	LEU
1	C	265	SER
1	C	272	TRP
1	C	273	ARG
1	C	283	TRP
1	C	288	ARG
1	C	314	ASN
1	C	315	ASN
1	C	328	GLU
1	C	330	THR
1	D	3	CYS
1	D	19	GLU
1	D	49	SER
1	D	51	THR
1	D	60	SER
1	D	83	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	97	THR
1	D	116	SER
1	D	125	PHE
1	D	145	GLN
1	D	172	GLU
1	D	183	LYS
1	D	203	ASP
1	D	208	VAL
1	D	218	ASN
1	D	244	THR
1	D	251	ASN
1	D	265	SER
1	D	273	ARG
1	D	276	ARG
1	D	288	ARG
1	D	297	ARG
1	D	311	SER
1	D	332	VAL
1	E	21	LEU
1	E	24	VAL
1	E	60	SER
1	E	69	ASP
1	E	97	THR
1	E	100	THR
1	E	108	SER
1	E	116	SER
1	E	118	SER
1	E	133	ASN
1	E	137	ILE
1	E	138	SER
1	E	218	ASN
1	E	219	GLU
1	E	232	THR
1	E	244	THR
1	E	265	SER
1	E	266	CYS
1	E	288	ARG
1	E	311	SER
1	E	319	GLN
1	E	321	GLN
1	E	350	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	93	ASN
1	A	102	GLN
1	A	126	ASN
1	A	147	HIS
1	A	187	ASN
1	A	190	GLN
1	B	64	ASN
1	B	123	HIS
1	B	126	ASN
1	B	147	HIS
1	B	190	GLN
1	B	282	HIS
1	B	323	GLN
1	B	331	GLN
1	C	38	ASN
1	C	88	GLN
1	C	126	ASN
1	C	190	GLN
1	C	282	HIS
1	C	314	ASN
1	C	323	GLN
1	C	331	GLN
1	D	55	GLN
1	D	88	GLN
1	D	147	HIS
1	D	301	ASN
1	D	331	GLN
1	E	93	ASN
1	E	126	ASN
1	E	159	GLN
1	E	190	GLN
1	E	277	ASN
1	E	282	HIS
1	E	314	ASN
1	E	315	ASN
1	E	323	GLN
1	E	331	GLN

### 5.3.3 RNA

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.

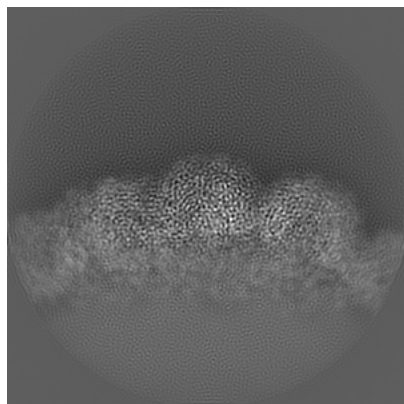
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22643. These allow visual inspection of the internal detail of the map and identification of artifacts.

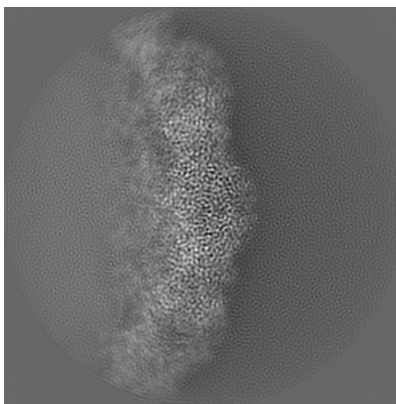
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

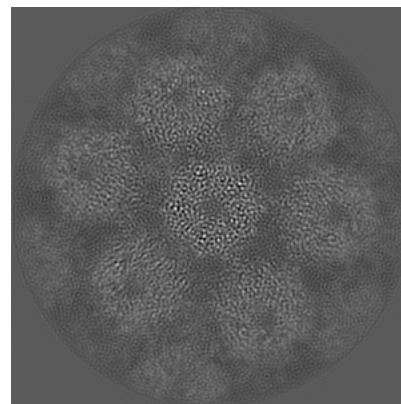
#### 6.1.1 Primary map



X

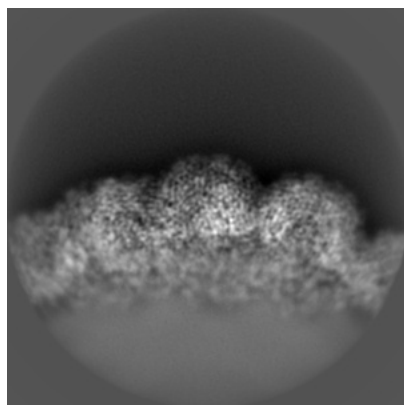


Y

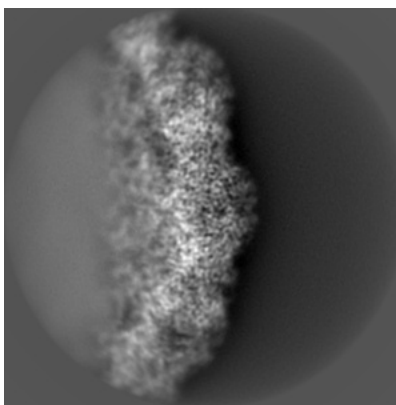


Z

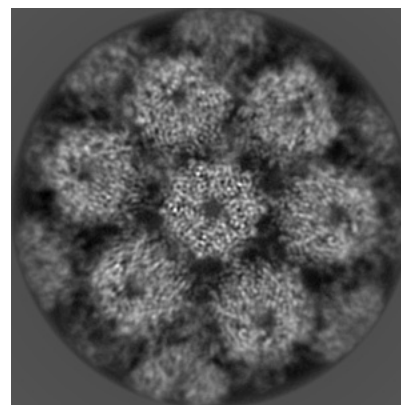
#### 6.1.2 Raw map



X



Y

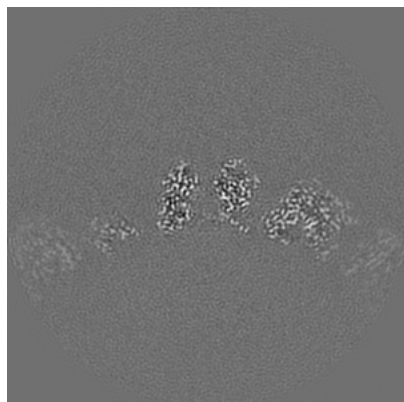


Z

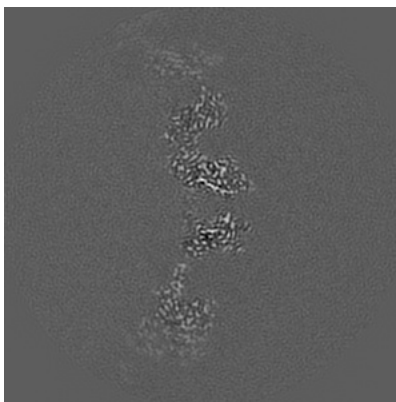
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

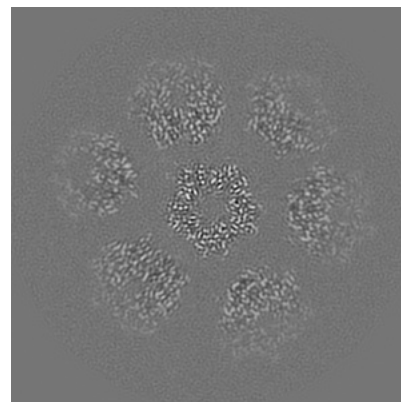
### 6.2.1 Primary map



X Index: 150

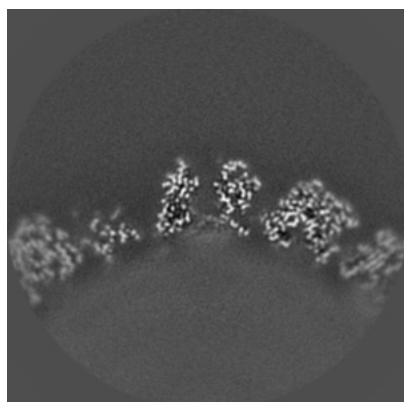


Y Index: 150

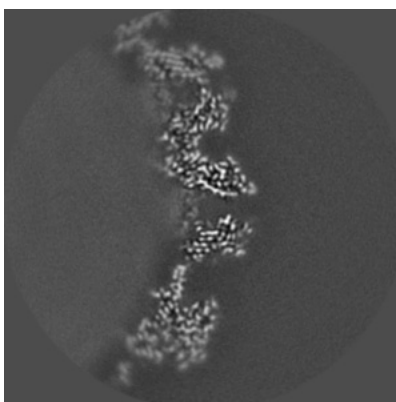


Z Index: 150

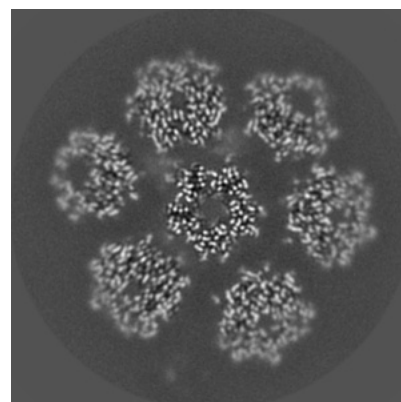
### 6.2.2 Raw map



X Index: 150



Y Index: 150

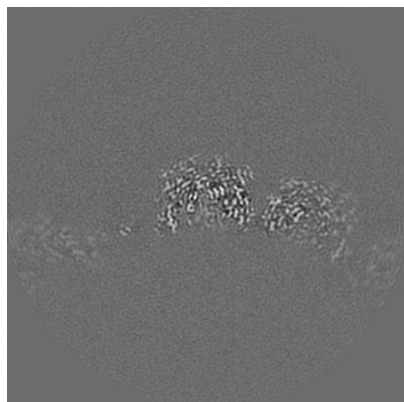


Z Index: 150

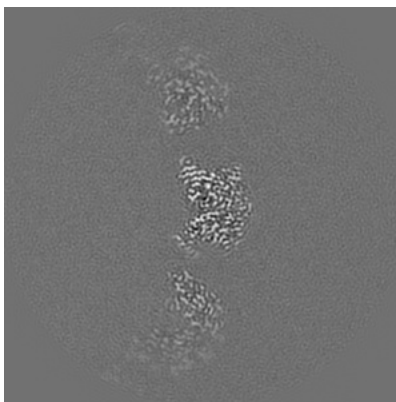
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

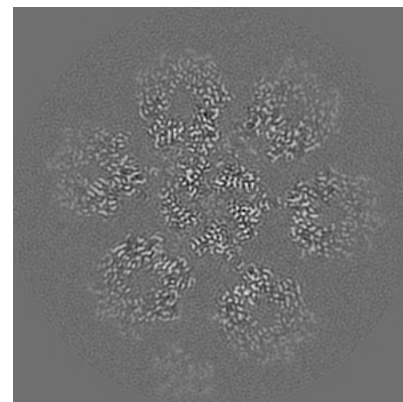
### 6.3.1 Primary map



X Index: 139

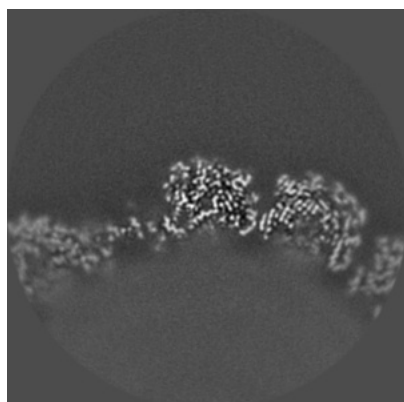


Y Index: 167

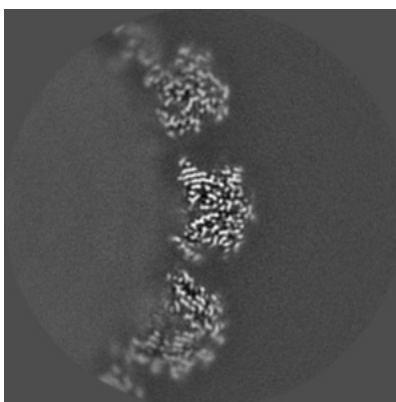


Z Index: 141

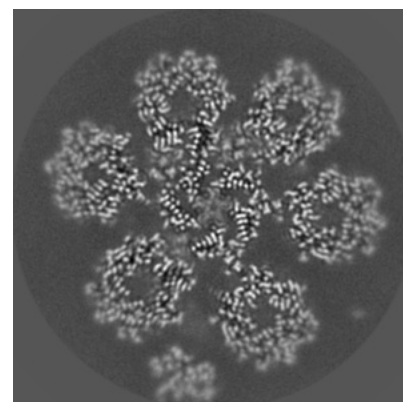
### 6.3.2 Raw map



X Index: 135



Y Index: 167



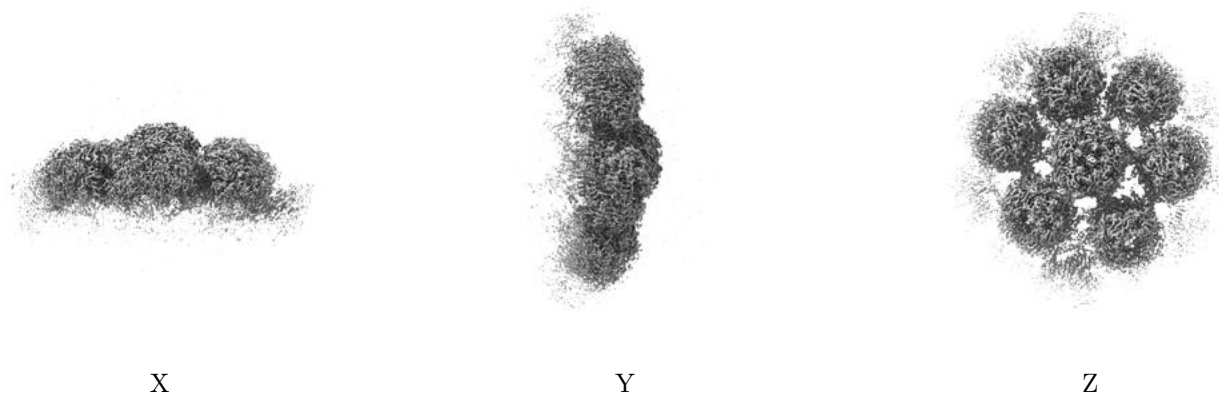
Z Index: 140

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



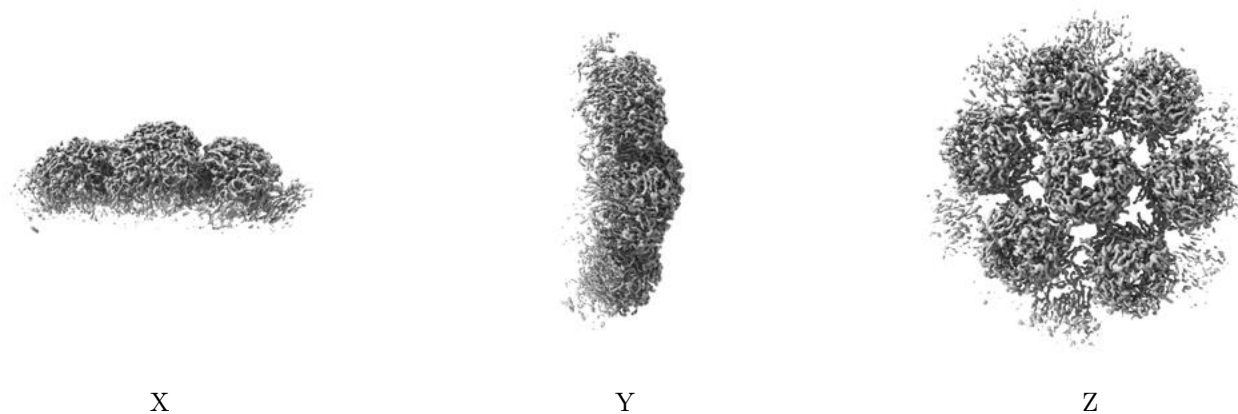
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

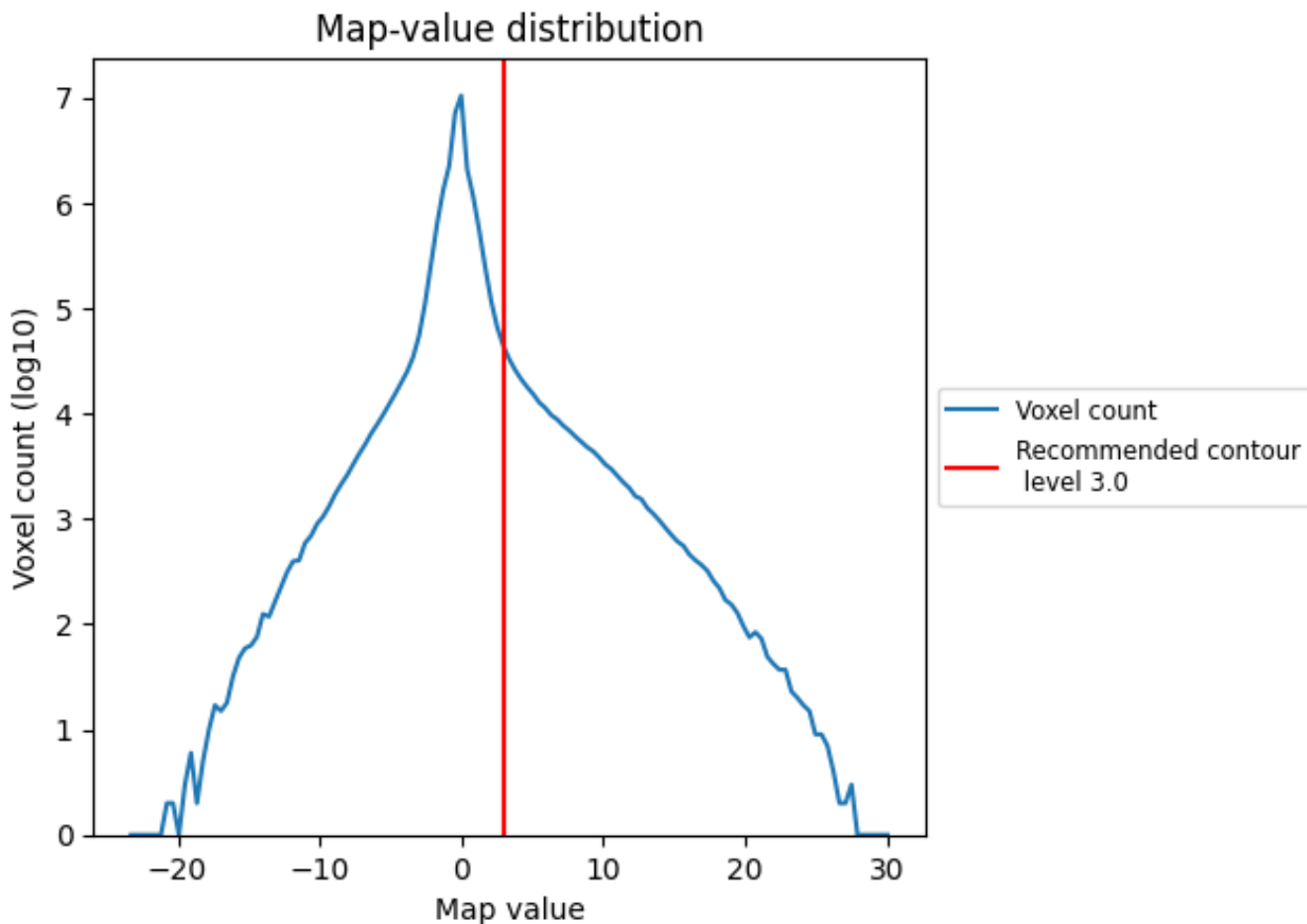
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

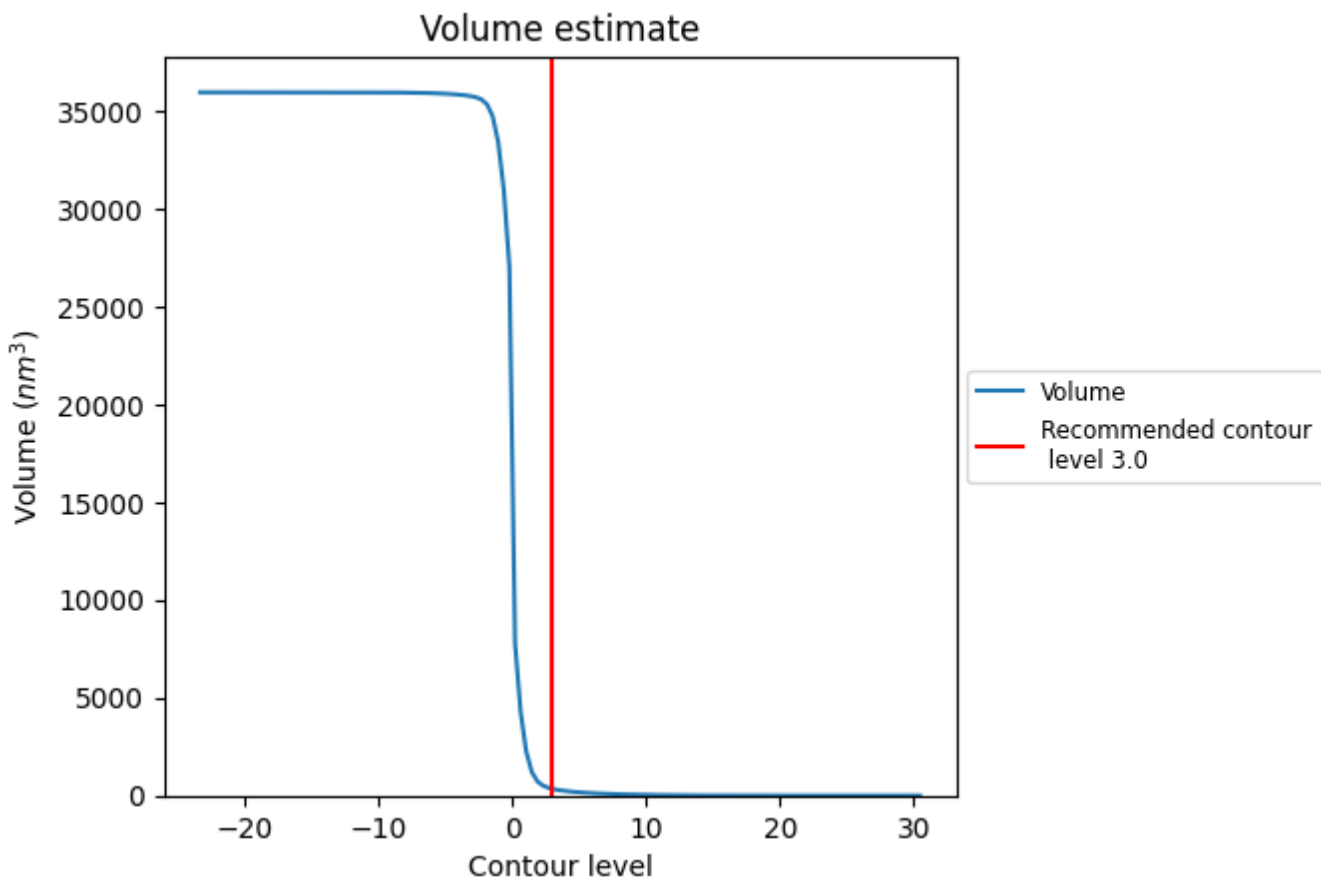
This section contains the results of statistical analysis of the map.

### 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.

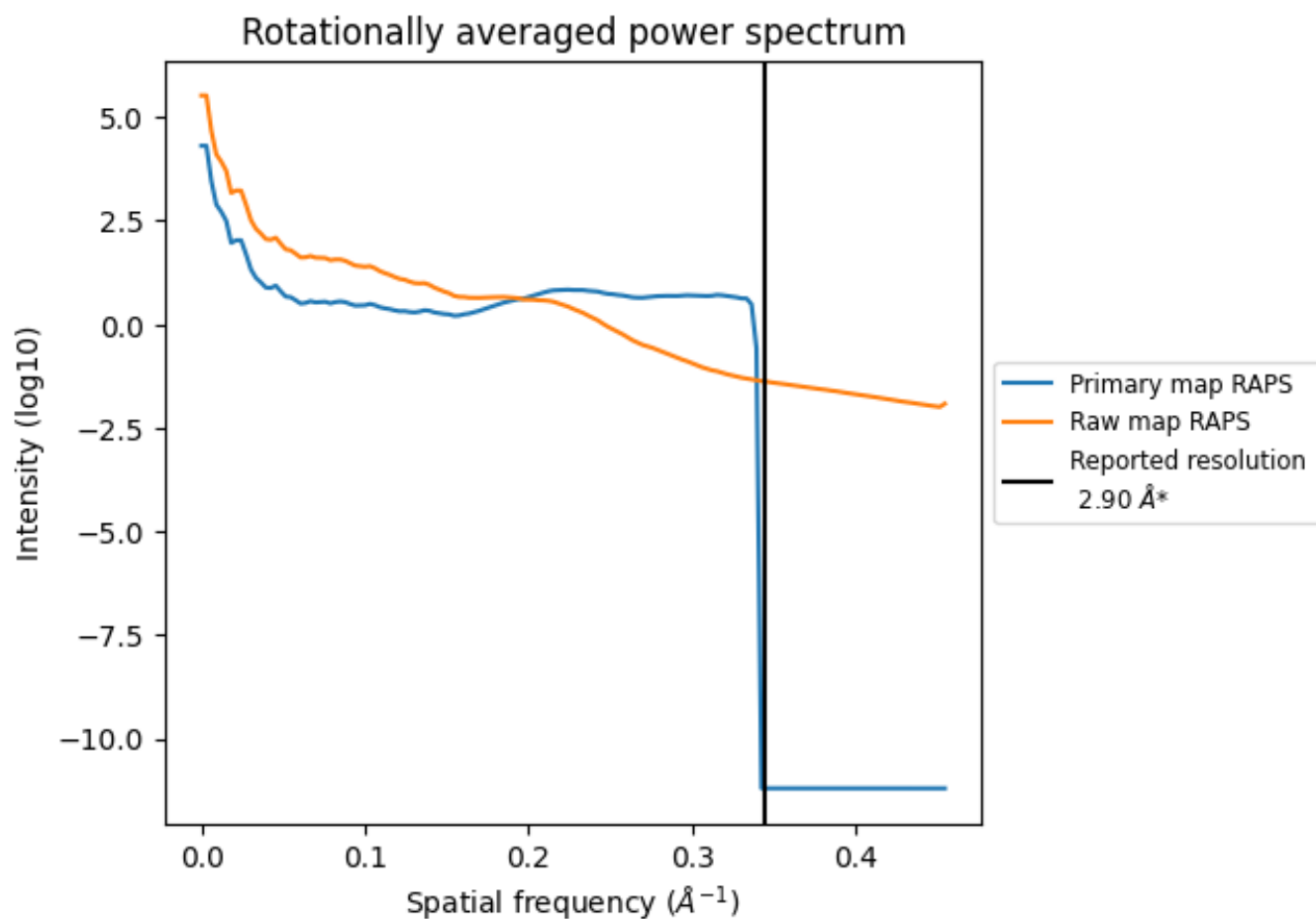
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 346 nm<sup>3</sup>; this corresponds to an approximate mass of 313 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](#)

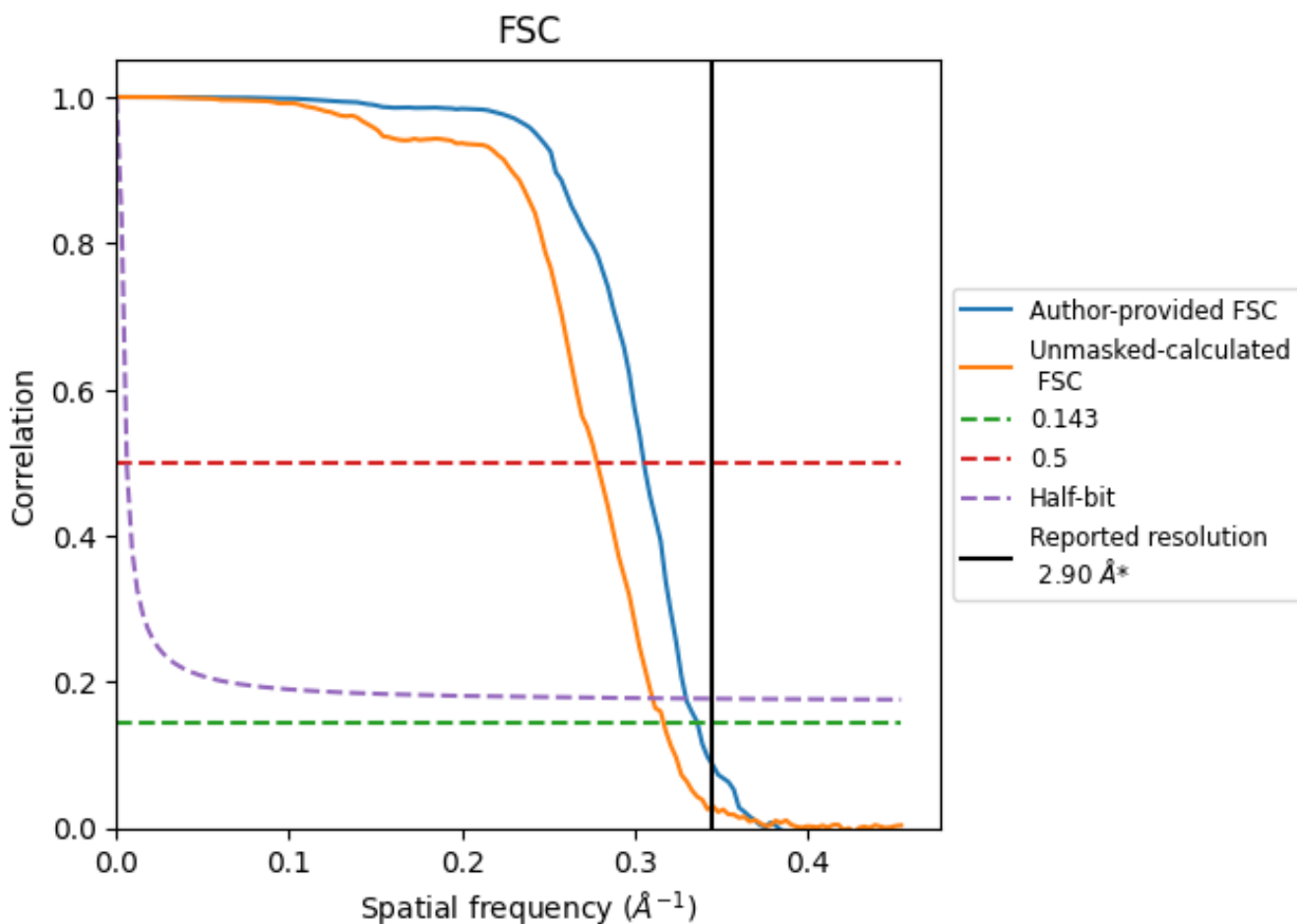


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 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 0.345 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

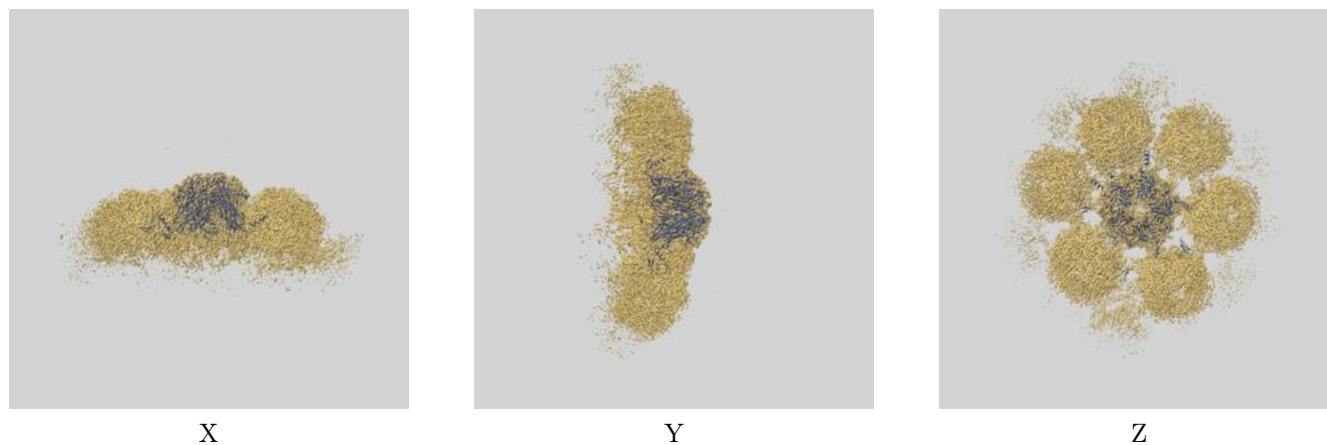
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.97	3.27	3.03
Unmasked-calculated*	3.15	3.59	3.22

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

## 9 Map-model fit [i](#)

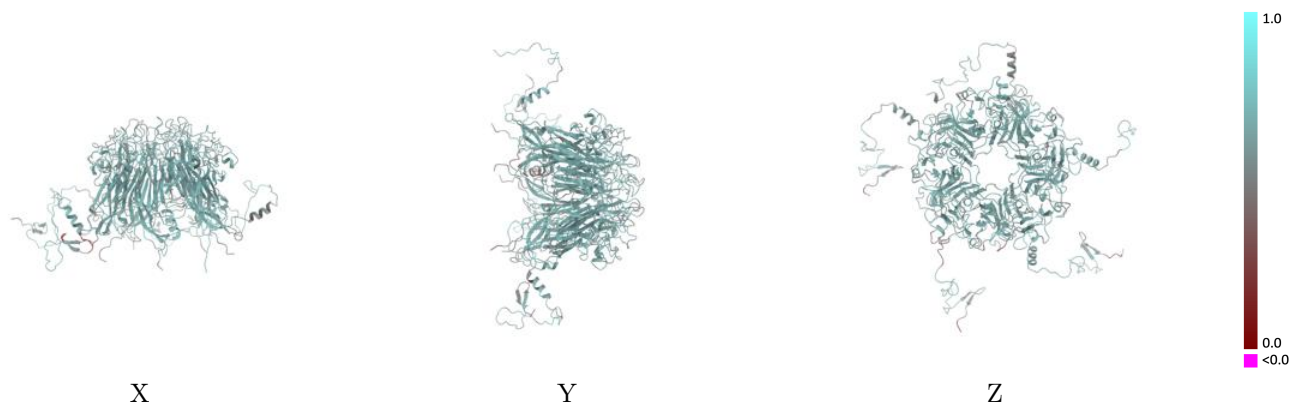
This section contains information regarding the fit between EMDB map EMD-22643 and PDB model 7K25. Per-residue inclusion information can be found in section [3](#) on page [4](#).

### 9.1 Map-model overlay [i](#)



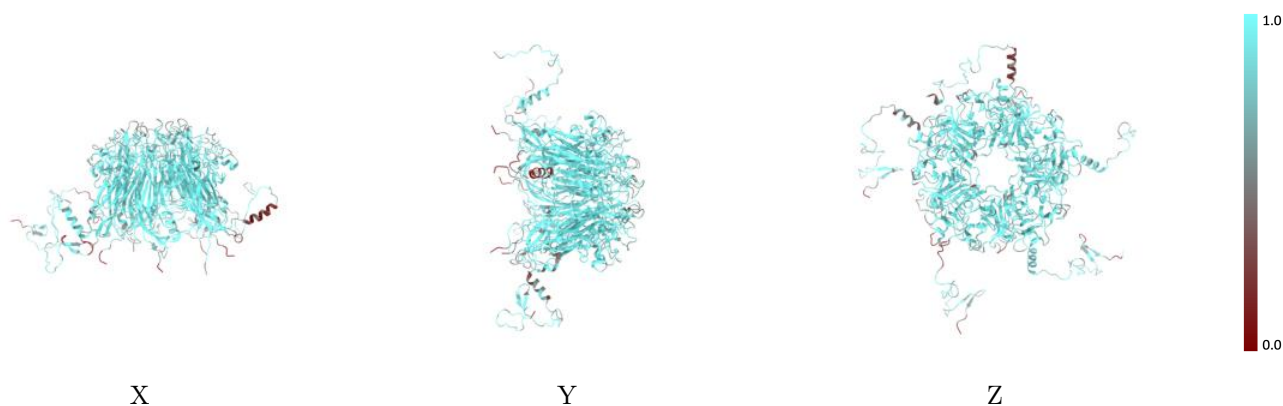
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

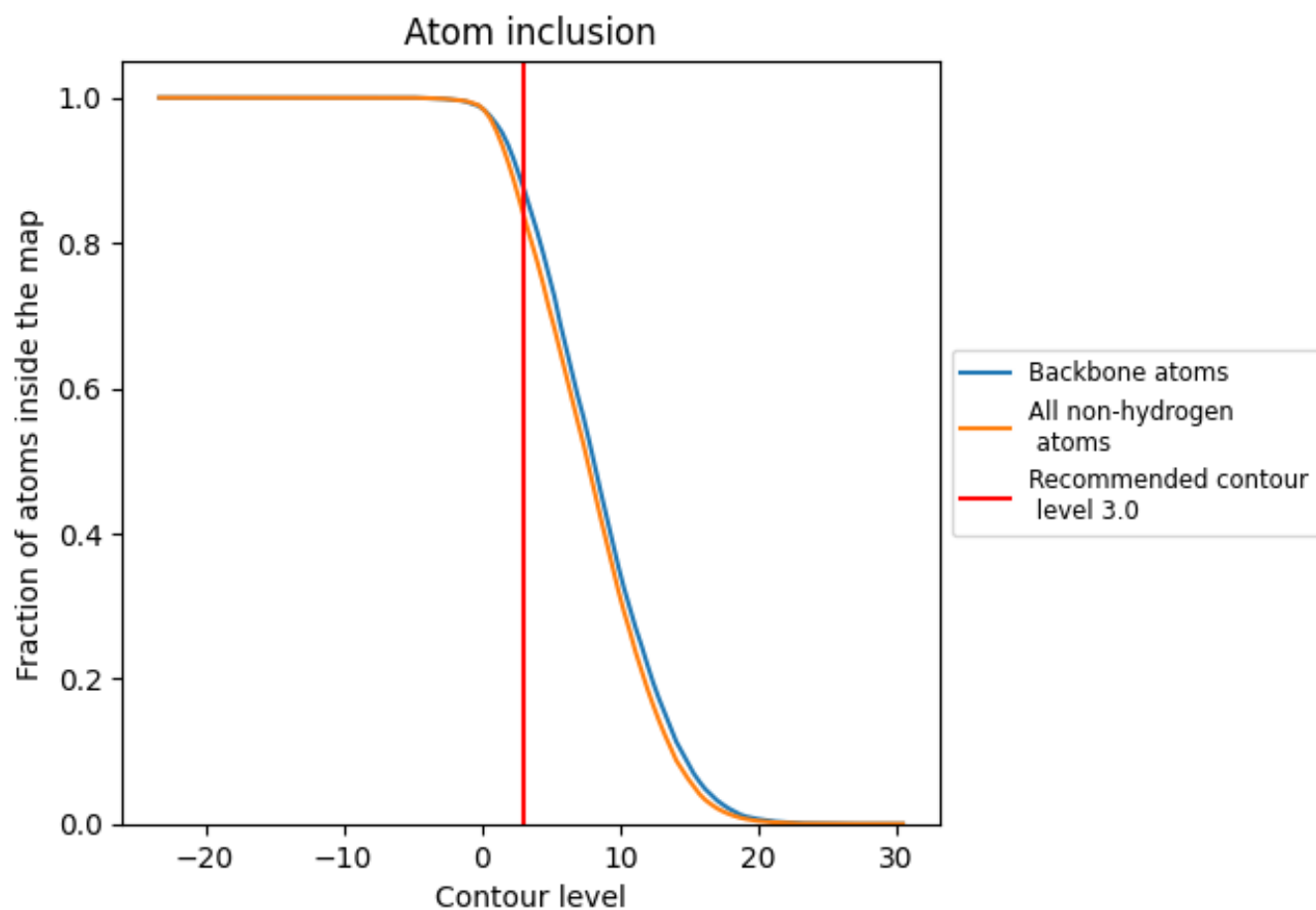
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (3.0).















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 84% 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 (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8400	 0.6100
A	 0.8122	 0.6000
B	 0.8401	 0.6100
C	 0.8384	 0.6160
D	 0.8742	 0.6230
E	 0.8376	 0.6030

