Full wwPDB EM Validation Report (i)

Feb 13, 2024 – 06:40 AM EST

PDB ID	:	3J22
EMDB ID	:	EMD-5465
Title	:	The Enterovirus 71 A-particle
Authors	:	Shingler, K.L.
Deposited on	:	2012-08-13
Resolution	:	6.30 Å(reported)
Based on initial model	:	3VBU

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:

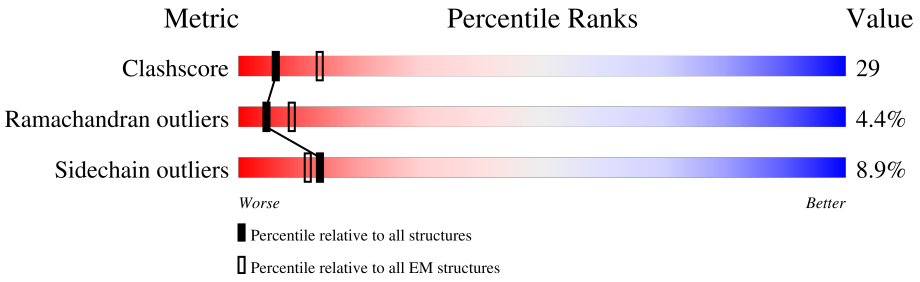
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 6.30 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	225	44% 44% 9%
2	B	237	16% 48% 46% 5%
3	C	239	55% 37% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5397 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	218	1724	1107	290	316	11	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	MET	CYS	SEE REMARK 999	UNP B2ZUN0

- Molecule 2 is a protein called capsid protein VP0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	237	1834	1179	301	346	8	0	0

- Molecule 3 is a protein called capsid protein VP3.

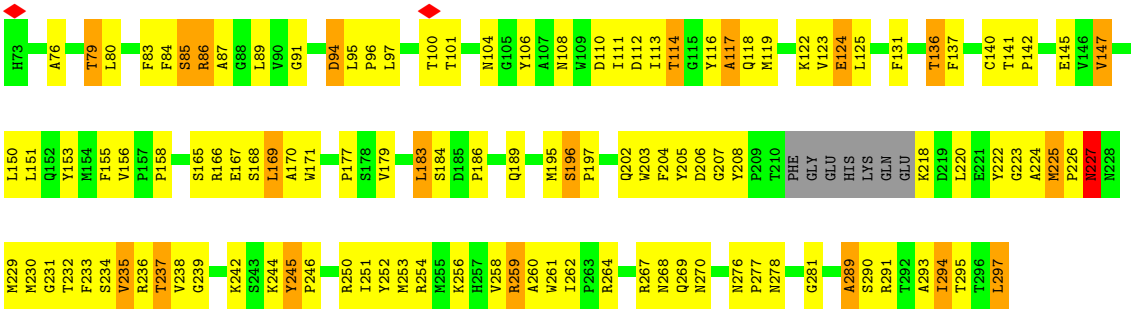
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	239	1839	1182	306	340	11	0	0

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.

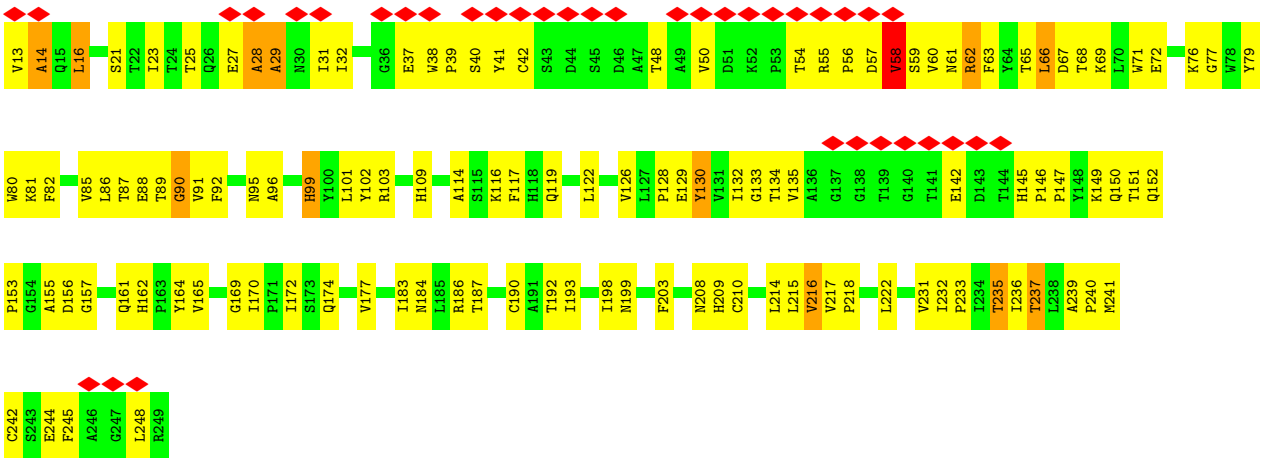
- Molecule 1: capsid protein VP1

Chain A:



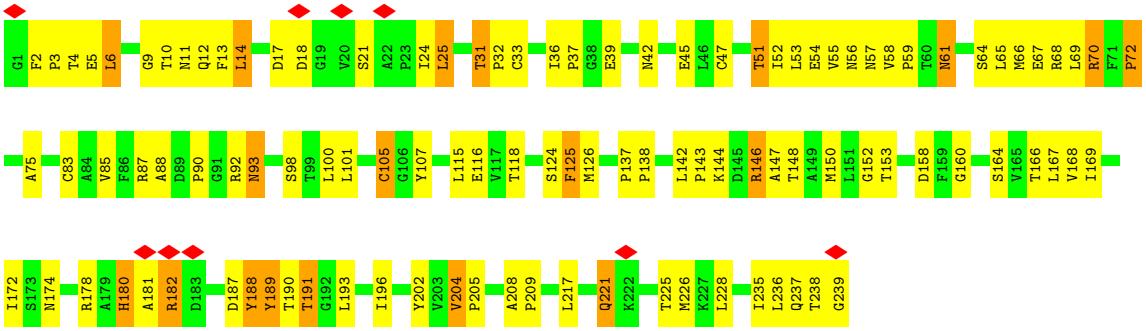
- Molecule 2: capsid protein VP0

Chain B:



- Molecule 3: capsid protein VP3

Chain C:


G1 F2 P3 T4 E5 L6 G9 T10 N11 Q12 F13 L14 D17 D18 G19 V20 S21 A22 P23 I24 L25 T31 P32 C33 I36 P37 G38 E39 N42 E45 L46 C47 T51 I52 L53 E54 V55 N56 N57 V58 P59 T60 N61 S64 L65 M66 E67 R68 L69 R70 F71 P72
A75 C83 A84 V85 F86 R87 A88 D89 P90 G91 R92 N93 S98 T99 L100 L101 C105 G106 Y107 L115 E116 V117 T118 S124 F125 M126 P137 P138 L142 P143 K144 D145 R146 A147 T148 A149 M150 L151 G152 T153 D158 F159 G160 S164 V165 T166 L167 V168 I169
I172 S173 N174 R178 A179 H180 A181 R182 D183 D187 Y188 Y189 T190 T191 G192 L193 I196 Y202 V203 V204 P205 A208 P209 L217 Q221 K222 T225 M226 K227 L228 I235 L236 Q237 T238 G239

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	11436	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	auto3DEM	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	15	Depositor
Minimum defocus (nm)	1730	Depositor
Maximum defocus (nm)	4280	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	6.560	Depositor
Minimum map value	-4.726	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.0	Depositor
Map size (Å)	445.77, 445.77, 445.77	wwPDB
Map dimensions	351, 351, 351	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.27, 1.27, 1.27	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	0.53	0/1776	0.78	0/2419
2	B	0.56	0/1889	0.75	1/2592 (0.0%)
3	C	0.50	0/1891	0.73	0/2586
All	All	0.53	0/5556	0.75	1/7597 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	248	LEU	CA-CB-CG	5.64	128.28	115.30

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	1724	0	1688	118	0
2	B	1834	0	1774	123	0
3	C	1839	0	1814	123	0
All	All	5397	0	5276	312	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 29.

All (312) 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:281:GLY:HA3	2:B:135:VAL:HG13	1.14	1.09
1:A:229:MET:HE2	1:A:231:GLY:H	1.16	1.07
1:A:156:VAL:HG22	1:A:232:THR:HB	1.42	0.99
2:B:134:THR:HG23	2:B:146:PRO:HG3	1.47	0.96
2:B:164:TYR:HA	3:C:66:MET:HE3	1.49	0.94
2:B:87:THR:HG22	2:B:96:ALA:HB1	1.51	0.92
2:B:55:ARG:HG2	2:B:244:GLU:HG2	1.56	0.87
1:A:76:ALA:O	1:A:79:THR:HG23	1.73	0.86
1:A:197:PRO:HA	3:C:31:THR:HG21	1.57	0.85
3:C:9:GLY:O	3:C:12:GLN:HG2	1.78	0.83
3:C:66:MET:HE1	3:C:69:LEU:HD11	1.58	0.83
2:B:59:SER:O	2:B:62:ARG:HG2	1.78	0.83
2:B:99:HIS:CD2	2:B:245:PHE:HB3	2.16	0.81
1:A:281:GLY:HA3	2:B:135:VAL:CG1	2.07	0.80
1:A:281:GLY:CA	2:B:135:VAL:HG13	2.04	0.79
2:B:56:PRO:HB3	2:B:60:VAL:HG21	1.63	0.78
1:A:112:ASP:OD1	1:A:114:THR:HG22	1.82	0.78
1:A:294:ILE:HD12	3:C:56:ASN:HA	1.67	0.77
2:B:103:ARG:HG2	2:B:244:GLU:HB2	1.67	0.76
2:B:16:LEU:HD21	2:B:25:THR:CG2	2.16	0.76
2:B:95:ASN:O	2:B:99:HIS:HB2	1.85	0.76
1:A:229:MET:HE2	1:A:231:GLY:N	1.98	0.76
1:A:117:ALA:HB1	3:C:236:LEU:HB3	1.67	0.74
2:B:134:THR:HG22	2:B:150:GLN:HE22	1.53	0.74
2:B:198:ILE:HG12	3:C:37:PRO:HG2	1.67	0.74
2:B:87:THR:HG22	2:B:96:ALA:CB	2.18	0.73
3:C:188:TYR:O	3:C:189:TYR:HD2	1.72	0.73
3:C:142:LEU:HD23	3:C:143:PRO:O	1.91	0.70
2:B:122:LEU:HD23	2:B:218:PRO:HA	1.72	0.70
3:C:180:HIS:CD2	3:C:181:ALA:H	2.09	0.70
3:C:92:ARG:HD3	3:C:188:TYR:HD2	1.58	0.68
3:C:10:THR:HG22	3:C:11:ASN:ND2	2.09	0.68
3:C:6:LEU:HD13	3:C:10:THR:HG21	1.74	0.68
3:C:92:ARG:HH22	3:C:191:THR:CG2	2.06	0.68
1:A:276:ASN:HB2	1:A:277:PRO:HD2	1.75	0.68
3:C:178:ARG:HH12	3:C:187:ASP:HB3	1.59	0.67
2:B:54:THR:O	2:B:56:PRO:HD3	1.95	0.67
1:A:80:LEU:HD21	1:A:260:ALA:HB3	1.75	0.66
3:C:42:ASN:O	3:C:45:GLU:HG3	1.95	0.66
3:C:58:VAL:HG23	3:C:59:PRO:HD3	1.78	0.66
2:B:119:GLN:NE2	3:C:209:PRO:HB2	2.11	0.65
1:A:270:ASN:HA	3:C:235:ILE:HG23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:TYR:HA	3:C:66:MET:CE	2.24	0.65
2:B:23:ILE:HG21	2:B:237:THR:HG21	1.79	0.65
3:C:66:MET:HE1	3:C:69:LEU:CD1	2.25	0.65
1:A:171:TRP:CH2	1:A:234:SER:HB3	2.32	0.64
3:C:158:ASP:C	3:C:160:GLY:H	1.99	0.64
2:B:21:SER:HB2	2:B:63:PHE:HB2	1.79	0.64
1:A:254:ARG:NH2	1:A:256:LYS:HD3	2.13	0.64
1:A:267:ARG:HD2	2:B:169:GLY:O	1.97	0.64
2:B:164:TYR:HD1	3:C:66:MET:HE2	1.63	0.64
2:B:132:ILE:O	2:B:146:PRO:HG2	1.98	0.63
2:B:31:ILE:HG22	2:B:192:THR:HB	1.80	0.63
3:C:6:LEU:CD1	3:C:10:THR:HG21	2.28	0.63
1:A:165:SER:HB2	1:A:167:GLU:OE2	1.99	0.62
3:C:188:TYR:O	3:C:189:TYR:CD2	2.52	0.62
1:A:294:ILE:HD12	3:C:56:ASN:CA	2.29	0.62
1:A:153:TYR:HD1	1:A:235:VAL:HG13	1.65	0.62
1:A:156:VAL:HG23	1:A:156:VAL:O	2.00	0.62
2:B:79:TYR:CB	2:B:215:LEU:HD12	2.30	0.61
1:A:206:ASP:OD1	2:B:81:LYS:HD2	2.01	0.61
3:C:2:PHE:CD1	3:C:3:PRO:HD2	2.35	0.61
1:A:150:LEU:O	1:A:151:LEU:HD23	2.01	0.61
2:B:48:THR:HG22	2:B:48:THR:O	2.00	0.61
1:A:294:ILE:HD11	3:C:55:VAL:HG12	1.82	0.61
1:A:104:ASN:O	1:A:166:ARG:HD2	2.01	0.60
2:B:69:LYS:HE3	2:B:156:ASP:O	2.02	0.60
2:B:32:ILE:HB	2:B:193:ILE:HG12	1.83	0.60
3:C:118:THR:HG23	3:C:166:THR:OG1	2.01	0.60
3:C:167:LEU:HD12	3:C:168:VAL:N	2.17	0.59
1:A:141:THR:HB	1:A:142:PRO:HD2	1.84	0.59
3:C:180:HIS:CG	3:C:181:ALA:H	2.19	0.59
1:A:226:PRO:HG2	1:A:227:ASN:OD1	2.02	0.59
2:B:79:TYR:HB3	2:B:215:LEU:HD12	1.85	0.58
1:A:136:THR:HG23	1:A:189:GLN:HG3	1.85	0.58
1:A:156:VAL:O	1:A:156:VAL:CG2	2.50	0.58
2:B:56:PRO:HB3	2:B:60:VAL:CG2	2.30	0.58
1:A:250:ARG:HH21	1:A:250:ARG:HG3	1.69	0.58
3:C:90:PRO:CG	3:C:115:LEU:HD11	2.34	0.58
3:C:92:ARG:HH22	3:C:191:THR:HG21	1.68	0.58
3:C:4:THR:HG22	3:C:5:GLU:H	1.68	0.58
2:B:153:PRO:HB2	2:B:157:GLY:O	2.04	0.57
2:B:27:GLU:O	2:B:28:ALA:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLY:HA3	2:B:208:ASN:O	2.04	0.57
3:C:105:CYS:HA	3:C:226:MET:HE2	1.87	0.57
1:A:156:VAL:CG2	1:A:232:THR:HB	2.25	0.56
2:B:231:VAL:O	2:B:232:ILE:HD13	2.05	0.56
1:A:94:ASP:C	1:A:96:PRO:HD3	2.24	0.56
2:B:149:LYS:H	2:B:149:LYS:HD2	1.70	0.56
2:B:184:ASN:HB3	2:B:187:THR:OG1	2.05	0.56
1:A:259:ARG:HG2	3:C:39:GLU:OE1	2.06	0.56
2:B:198:ILE:HG12	3:C:37:PRO:CG	2.35	0.56
2:B:177:VAL:HG22	2:B:177:VAL:O	2.04	0.56
1:A:277:PRO:HG2	2:B:133:GLY:HA3	1.88	0.56
2:B:149:LYS:HD2	2:B:149:LYS:N	2.20	0.56
3:C:6:LEU:HD13	3:C:10:THR:CG2	2.36	0.56
1:A:291:ARG:HD2	1:A:293:ALA:O	2.05	0.56
2:B:79:TYR:HA	2:B:214:LEU:O	2.06	0.56
3:C:92:ARG:NH2	3:C:191:THR:CG2	2.68	0.55
1:A:114:THR:HG23	3:C:237:GLN:HG2	1.89	0.55
1:A:290:SER:OG	3:C:68:ARG:NH2	2.39	0.55
2:B:174:GLN:HA	3:C:51:THR:HG22	1.89	0.55
3:C:4:THR:HG22	3:C:5:GLU:N	2.21	0.55
3:C:167:LEU:HD12	3:C:168:VAL:H	1.71	0.55
1:A:117:ALA:HB1	3:C:236:LEU:HD23	1.89	0.55
2:B:92:PHE:CE1	2:B:245:PHE:HZ	2.25	0.55
1:A:295:THR:HA	3:C:85:VAL:HG12	1.89	0.54
3:C:146:ARG:O	3:C:146:ARG:HG2	2.06	0.54
3:C:88:ALA:HB1	3:C:172:ILE:HG21	1.89	0.54
2:B:41:TYR:CD1	2:B:55:ARG:HD3	2.43	0.54
1:A:202:GLN:HG2	1:A:225:MET:HG2	1.89	0.53
2:B:130:TYR:HE1	2:B:215:LEU:CD1	2.20	0.53
1:A:208:TYR:CE1	1:A:222:TYR:HB2	2.44	0.53
2:B:71:TRP:CE2	2:B:222:LEU:HB2	2.44	0.53
1:A:224:ALA:O	1:A:226:PRO:HD3	2.09	0.53
2:B:82:PHE:O	2:B:210:CYS:HA	2.09	0.53
1:A:111:ILE:HD11	1:A:233:PHE:CE2	2.44	0.52
1:A:276:ASN:OD1	1:A:278:ASN:HB2	2.10	0.52
2:B:236:ILE:N	2:B:236:ILE:HD12	2.24	0.52
3:C:174:ASN:OD1	3:C:174:ASN:O	2.27	0.52
2:B:122:LEU:HB2	2:B:183:ILE:HB	1.92	0.52
3:C:83:CYS:HB3	3:C:196:ILE:HG22	1.90	0.52
1:A:84:PHE:O	1:A:85:SER:O	2.28	0.52
1:A:276:ASN:CB	1:A:277:PRO:HD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:THR:HG23	2:B:146:PRO:CG	2.29	0.52
3:C:90:PRO:HD2	3:C:188:TYR:OH	2.09	0.52
3:C:115:LEU:HB2	3:C:169:ILE:HB	1.92	0.52
1:A:155:PHE:O	1:A:177:PRO:HD2	2.10	0.52
1:A:245:TYR:CD1	1:A:245:TYR:N	2.78	0.52
1:A:254:ARG:NH1	3:C:18:ASP:HA	2.25	0.52
3:C:150:MET:O	3:C:150:MET:SD	2.67	0.51
1:A:140:CYS:HA	1:A:183:LEU:HD21	1.92	0.51
2:B:114:ALA:HB2	2:B:232:ILE:HD12	1.92	0.51
3:C:178:ARG:HH12	3:C:187:ASP:CB	2.23	0.51
3:C:158:ASP:C	3:C:160:GLY:N	2.64	0.51
1:A:104:ASN:HA	1:A:242:LYS:NZ	2.25	0.51
1:A:222:TYR:CE1	2:B:151:THR:HG23	2.45	0.51
3:C:178:ARG:NH1	3:C:187:ASP:HB3	2.25	0.51
2:B:119:GLN:HB3	3:C:124:SER:HA	1.92	0.50
1:A:220:LEU:HD23	2:B:145:HIS:HD2	1.77	0.50
2:B:16:LEU:HD21	2:B:25:THR:HG22	1.92	0.50
3:C:56:ASN:OD1	3:C:58:VAL:HG22	2.12	0.50
1:A:153:TYR:CD1	1:A:235:VAL:HG13	2.46	0.50
2:B:184:ASN:OD1	2:B:186:ARG:HG2	2.12	0.50
3:C:188:TYR:O	3:C:189:TYR:HB3	2.11	0.50
3:C:105:CYS:SG	3:C:226:MET:HE1	2.52	0.50
1:A:123:VAL:HB	1:A:203:TRP:NE1	2.26	0.50
2:B:80:TRP:HZ3	2:B:216:VAL:CG1	2.25	0.50
3:C:61:ASN:ND2	3:C:64:SER:OG	2.44	0.49
2:B:161:GLN:O	2:B:162:HIS:HD2	1.95	0.49
3:C:105:CYS:HA	3:C:226:MET:CE	2.42	0.49
2:B:103:ARG:HD2	2:B:203:PHE:CE2	2.48	0.49
1:A:245:TYR:HB3	1:A:246:PRO:HD2	1.95	0.49
2:B:165:VAL:HA	2:B:170:ILE:O	2.12	0.49
2:B:172:ILE:C	2:B:174:GLN:H	2.14	0.49
1:A:123:VAL:HB	1:A:203:TRP:HE1	1.77	0.49
1:A:261:TRP:CD1	3:C:39:GLU:HB2	2.48	0.49
1:A:250:ARG:HG3	1:A:250:ARG:NH2	2.27	0.48
2:B:56:PRO:HB3	2:B:60:VAL:CB	2.44	0.48
2:B:116:LYS:HD3	3:C:125:PHE:CE1	2.48	0.48
2:B:130:TYR:HE1	2:B:215:LEU:HD11	1.78	0.48
2:B:65:THR:OG1	2:B:237:THR:HG23	2.13	0.48
3:C:54:GLU:HG2	3:C:69:LEU:HD23	1.96	0.48
1:A:229:MET:CE	1:A:230:MET:H	2.27	0.48
3:C:182:ARG:HH21	3:C:182:ARG:HG3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:PHE:O	1:A:86:ARG:NH2	2.47	0.48
2:B:38:TRP:O	2:B:40:SER:N	2.46	0.48
2:B:41:TYR:CE1	2:B:55:ARG:HD3	2.49	0.48
3:C:236:LEU:N	3:C:236:LEU:HD12	2.29	0.47
1:A:116:TYR:CE2	1:A:118:GLN:HG3	2.48	0.47
2:B:28:ALA:O	2:B:29:ALA:O	2.33	0.47
2:B:99:HIS:HD2	2:B:245:PHE:HB3	1.70	0.47
3:C:51:THR:HG21	3:C:100:LEU:HB2	1.95	0.47
2:B:172:ILE:HG21	3:C:66:MET:CE	2.44	0.47
3:C:144:LYS:HD3	3:C:148:THR:HG21	1.97	0.47
2:B:109:HIS:CE1	2:B:190:CYS:HB2	2.49	0.47
2:B:85:VAL:HG23	2:B:155:ALA:HA	1.96	0.47
2:B:164:TYR:CD1	3:C:66:MET:HE2	2.48	0.47
3:C:182:ARG:HG3	3:C:182:ARG:NH2	2.29	0.47
2:B:71:TRP:HD1	2:B:72:GLU:N	2.13	0.47
3:C:105:CYS:SG	3:C:226:MET:CE	3.02	0.47
3:C:126:MET:HE2	3:C:205:PRO:HG3	1.96	0.47
3:C:14:LEU:HB3	3:C:17:ASP:HB2	1.96	0.46
1:A:205:TYR:O	1:A:223:GLY:HA2	2.15	0.46
1:A:137:PHE:N	1:A:137:PHE:CD2	2.82	0.46
1:A:95:LEU:N	1:A:96:PRO:HD3	2.29	0.46
1:A:104:ASN:HB2	1:A:106:TYR:CD1	2.50	0.46
1:A:238:VAL:CG1	1:A:239:GLY:N	2.78	0.46
2:B:56:PRO:HG2	2:B:245:PHE:CD2	2.51	0.46
3:C:51:THR:HG21	3:C:100:LEU:CB	2.46	0.46
3:C:56:ASN:O	3:C:59:PRO:HD2	2.15	0.46
2:B:103:ARG:HG3	2:B:103:ARG:HH11	1.80	0.46
1:A:220:LEU:HA	2:B:145:HIS:CD2	2.50	0.46
3:C:90:PRO:HG2	3:C:115:LEU:HD11	1.98	0.46
2:B:66:LEU:HD23	2:B:66:LEU:N	2.31	0.46
3:C:67:GLU:HG2	3:C:70:ARG:NH1	2.31	0.46
3:C:187:ASP:O	3:C:188:TYR:O	2.34	0.46
2:B:86:LEU:C	2:B:88:GLU:H	2.19	0.45
2:B:77:GLY:HA2	2:B:218:PRO:HD3	1.98	0.45
2:B:119:GLN:HB3	3:C:124:SER:CA	2.46	0.45
1:A:136:THR:HG21	3:C:13:PHE:CD2	2.52	0.45
3:C:75:ALA:HA	3:C:202:TYR:HB3	1.97	0.45
1:A:179:VAL:HG22	1:A:179:VAL:O	2.15	0.45
1:A:261:TRP:CD1	3:C:36:ILE:HB	2.52	0.45
1:A:85:SER:O	1:A:86:ARG:HB2	2.17	0.45
1:A:254:ARG:HH21	1:A:256:LYS:HB3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:GLU:OE2	3:C:37:PRO:HA	2.16	0.45
3:C:24:ILE:HG23	3:C:25:LEU:HD22	1.99	0.45
1:A:123:VAL:C	1:A:125:LEU:H	2.21	0.45
2:B:13:VAL:HG22	2:B:14:ALA:N	2.32	0.45
2:B:13:VAL:O	2:B:14:ALA:HB2	2.17	0.45
3:C:58:VAL:HG23	3:C:59:PRO:CD	2.46	0.45
3:C:92:ARG:HD3	3:C:188:TYR:CD2	2.45	0.45
1:A:104:ASN:HB2	1:A:106:TYR:CE1	2.51	0.45
1:A:117:ALA:CB	3:C:236:LEU:HD23	2.45	0.45
2:B:129:GLU:OE2	2:B:209:HIS:NE2	2.50	0.45
1:A:226:PRO:HG2	1:A:227:ASN:H	1.82	0.44
1:A:291:ARG:O	3:C:58:VAL:HG12	2.17	0.44
2:B:116:LYS:HB3	3:C:125:PHE:CD1	2.52	0.44
2:B:119:GLN:HB3	3:C:124:SER:N	2.32	0.44
1:A:114:THR:HG21	3:C:237:GLN:HE21	1.82	0.44
2:B:79:TYR:HB2	2:B:215:LEU:HD12	1.98	0.44
2:B:161:GLN:O	2:B:162:HIS:CD2	2.71	0.44
3:C:31:THR:HA	3:C:32:PRO:HD3	1.85	0.44
3:C:54:GLU:HG3	3:C:98:SER:CB	2.48	0.44
1:A:277:PRO:O	1:A:278:ASN:C	2.56	0.44
2:B:164:TYR:HD1	3:C:66:MET:CE	2.28	0.44
3:C:65:LEU:O	3:C:68:ARG:HG3	2.17	0.44
1:A:195:MET:O	1:A:196:SER:O	2.35	0.44
1:A:244:LYS:HB2	1:A:245:TYR:CE1	2.53	0.44
2:B:82:PHE:O	2:B:210:CYS:CA	2.66	0.44
1:A:87:ALA:HB1	1:A:252:TYR:HB3	1.99	0.44
1:A:291:ARG:HG3	3:C:58:VAL:HG12	2.00	0.44
2:B:151:THR:HG22	2:B:152:GLN:NE2	2.32	0.44
1:A:136:THR:HG21	3:C:13:PHE:CE2	2.52	0.44
1:A:113:ILE:HG22	1:A:253:MET:SD	2.58	0.44
1:A:140:CYS:HB2	1:A:145:GLU:O	2.18	0.44
2:B:101:LEU:HB3	2:B:203:PHE:HD1	1.83	0.44
1:A:197:PRO:CG	1:A:227:ASN:HB3	2.48	0.43
1:A:229:MET:HE2	1:A:230:MET:N	2.33	0.43
1:A:270:ASN:HA	3:C:235:ILE:CG2	2.46	0.43
1:A:297:LEU:HD12	1:A:297:LEU:H	1.83	0.43
1:A:168:SER:C	1:A:170:ALA:H	2.22	0.43
2:B:57:ASP:O	2:B:58:VAL:O	2.36	0.43
1:A:89:LEU:HD11	1:A:91:GLY:O	2.18	0.43
3:C:56:ASN:O	3:C:68:ARG:HA	2.19	0.43
3:C:193:LEU:HA	3:C:193:LEU:HD23	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:204:VAL:HG22	3:C:208:ALA:HB3	2.00	0.43
2:B:71:TRP:HD1	2:B:72:GLU:H	1.65	0.43
1:A:131:PHE:HB3	1:A:258:VAL:HG22	2.01	0.43
1:A:169:LEU:HD12	1:A:169:LEU:N	2.34	0.43
3:C:180:HIS:CG	3:C:181:ALA:N	2.87	0.43
1:A:112:ASP:CG	1:A:114:THR:HG22	2.39	0.43
1:A:276:ASN:HB2	1:A:277:PRO:CD	2.48	0.43
1:A:218:LYS:NZ	1:A:220:LEU:HD23	2.34	0.43
2:B:91:VAL:HG22	2:B:91:VAL:O	2.19	0.43
1:A:158:PRO:HB3	1:A:229:MET:CG	2.49	0.42
2:B:241:MET:O	2:B:242:CYS:C	2.57	0.42
2:B:21:SER:CB	2:B:63:PHE:HB2	2.46	0.42
2:B:174:GLN:O	2:B:177:VAL:HG12	2.18	0.42
3:C:47:CYS:HB3	3:C:101:LEU:CD1	2.49	0.42
3:C:147:ALA:O	3:C:150:MET:HB3	2.19	0.42
2:B:86:LEU:C	2:B:88:GLU:N	2.72	0.42
1:A:86:ARG:NH1	1:A:86:ARG:HG3	2.35	0.42
1:A:229:MET:HE3	1:A:230:MET:H	1.84	0.42
3:C:178:ARG:HD3	3:C:180:HIS:HB3	2.01	0.42
2:B:239:ALA:HA	2:B:240:PRO:HD3	1.80	0.42
3:C:54:GLU:OE2	3:C:68:ARG:NH1	2.49	0.42
3:C:138:PRO:HB3	3:C:190:THR:HA	2.01	0.42
2:B:117:PHE:CE2	3:C:126:MET:HG3	2.54	0.42
2:B:172:ILE:HG21	3:C:66:MET:HE3	2.00	0.42
2:B:232:ILE:HA	2:B:233:PRO:HD2	1.90	0.42
3:C:93:ASN:N	3:C:93:ASN:HD22	2.16	0.42
1:A:123:VAL:HG23	1:A:124:GLU:N	2.34	0.42
1:A:147:VAL:HG11	1:A:245:TYR:CD2	2.55	0.42
2:B:27:GLU:O	2:B:28:ALA:CB	2.67	0.42
2:B:122:LEU:CD2	2:B:218:PRO:HA	2.45	0.42
3:C:52:ILE:HA	3:C:217:LEU:HD23	2.02	0.42
3:C:158:ASP:OD1	3:C:160:GLY:CA	2.68	0.42
2:B:172:ILE:C	2:B:174:GLN:N	2.72	0.41
2:B:13:VAL:N	2:B:27:GLU:HG3	2.35	0.41
3:C:172:ILE:O	3:C:172:ILE:HD12	2.20	0.41
3:C:238:THR:O	3:C:239:GLY:O	2.39	0.41
1:A:86:ARG:HG3	1:A:86:ARG:HH11	1.84	0.41
1:A:277:PRO:HG2	2:B:133:GLY:CA	2.51	0.41
2:B:61:ASN:OD1	2:B:240:PRO:HB2	2.20	0.41
2:B:57:ASP:O	2:B:58:VAL:C	2.58	0.41
2:B:89:THR:HG22	2:B:90:GLY:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:152:GLY:O	3:C:153:THR:C	2.57	0.41
3:C:188:TYR:O	3:C:189:TYR:CB	2.68	0.41
1:A:104:ASN:HA	1:A:242:LYS:HZ1	1.85	0.41
1:A:108:ASN:ND2	1:A:234:SER:OG	2.54	0.41
1:A:113:ILE:O	1:A:119:MET:HG2	2.21	0.41
1:A:122:LYS:HG2	3:C:107:TYR:CE1	2.56	0.41
1:A:289:ALA:HB3	3:C:93:ASN:HB3	2.02	0.41
1:A:268:ASN:ND2	1:A:269:GLN:HE21	2.19	0.41
2:B:217:VAL:HA	2:B:218:PRO:HD3	1.88	0.41
3:C:54:GLU:OE2	3:C:68:ARG:HD3	2.21	0.41
1:A:293:ALA:C	1:A:295:THR:H	2.24	0.40
1:A:204:PHE:CE1	1:A:264:ARG:HD3	2.56	0.40
2:B:128:PRO:O	2:B:129:GLU:C	2.59	0.40
3:C:178:ARG:NH1	3:C:187:ASP:CB	2.84	0.40
1:A:166:ARG:HH21	1:A:237:THR:HG23	1.85	0.40
2:B:68:THR:OG1	2:B:235:THR:HG23	2.20	0.40
2:B:86:LEU:HD23	2:B:89:THR:HB	2.03	0.40
2:B:199:ASN:OD1	2:B:209:HIS:CE1	2.75	0.40
1:A:97:LEU:HD11	1:A:246:PRO:HD3	2.03	0.40
2:B:28:ALA:C	2:B:29:ALA:O	2.60	0.40
2:B:132:ILE:HG21	2:B:150:GLN:HE21	1.86	0.40
1:A:89:LEU:HD12	1:A:251:ILE:O	2.22	0.40
1:A:171:TRP:CE2	1:A:236:ARG:HD2	2.57	0.40
2:B:68:THR:HG21	2:B:233:PRO:HB2	2.04	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	214/225 (95%)	188 (88%)	15 (7%)	11 (5%)	2 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	235/237 (99%)	196 (83%)	31 (13%)	8 (3%)	3 26
3	C	237/239 (99%)	202 (85%)	24 (10%)	11 (5%)	2 21
All	All	686/701 (98%)	586 (85%)	70 (10%)	30 (4%)	4 22

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	SER
2	B	28	ALA
2	B	29	ALA
2	B	58	VAL
3	C	93	ASN
3	C	188	TYR
1	A	86	ARG
1	A	196	SER
1	A	227	ASN
2	B	14	ALA
2	B	90	GLY
3	C	180	HIS
3	C	182	ARG
3	C	189	TYR
1	A	124	GLU
1	A	289	ALA
2	B	39	PRO
3	C	221	GLN
1	A	117	ALA
1	A	169	LEU
3	C	72	PRO
3	C	137	PRO
2	B	67	ASP
3	C	57	ASN
3	C	105	CYS
3	C	191	THR
1	A	186	PRO
1	A	294	ILE
2	B	147	PRO
1	A	262	ILE

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	187/193 (97%)	170 (91%)	17 (9%)	9 30
2	B	201/201 (100%)	186 (92%)	15 (8%)	13 38
3	C	199/199 (100%)	179 (90%)	20 (10%)	7 25
All	All	587/593 (99%)	535 (91%)	52 (9%)	13 30

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	THR
1	A	94	ASP
1	A	100	THR
1	A	101	THR
1	A	110	ASP
1	A	114	THR
1	A	136	THR
1	A	147	VAL
1	A	183	LEU
1	A	184	SER
1	A	225	MET
1	A	227	ASN
1	A	235	VAL
1	A	237	THR
1	A	245	TYR
1	A	259	ARG
1	A	297	LEU
2	B	16	LEU
2	B	42	CYS
2	B	50	VAL
2	B	58	VAL
2	B	62	ARG
2	B	66	LEU
2	B	76	LYS
2	B	99	HIS
2	B	102	TYR

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Mol	Chain	Res	Type
2	B	126	VAL
2	B	130	TYR
2	B	142	GLU
2	B	216	VAL
2	B	235	THR
2	B	237	THR
3	C	6	LEU
3	C	14	LEU
3	C	21	SER
3	C	25	LEU
3	C	31	THR
3	C	33	CYS
3	C	51	THR
3	C	53	LEU
3	C	61	ASN
3	C	70	ARG
3	C	72	PRO
3	C	87	ARG
3	C	116	GLU
3	C	125	PHE
3	C	146	ARG
3	C	164	SER
3	C	204	VAL
3	C	221	GLN
3	C	225	THR
3	C	228	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	152	GLN
1	A	228	ASN
1	A	269	GLN
2	B	99	HIS
2	B	111	GLN
2	B	119	GLN
2	B	145	HIS
2	B	150	GLN
2	B	162	HIS
2	B	208	ASN
3	C	48	GLN

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Mol	Chain	Res	Type
3	C	61	ASN
3	C	93	ASN
3	C	154	HIS
3	C	174	ASN
3	C	180	HIS

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.

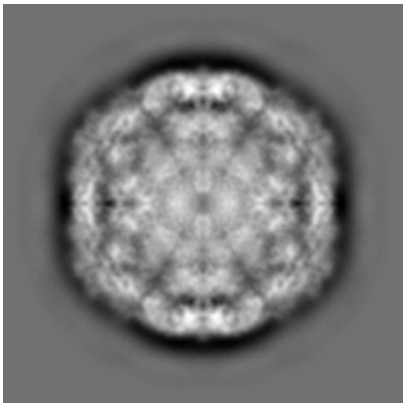
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-5465. These allow visual inspection of the internal detail of the map and identification of artifacts.

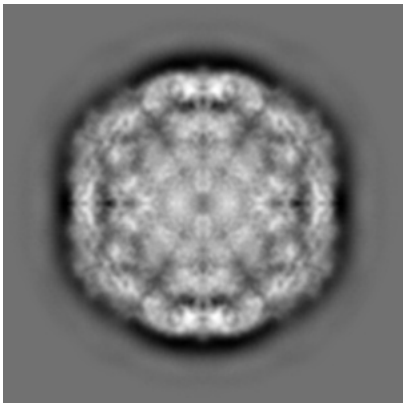
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

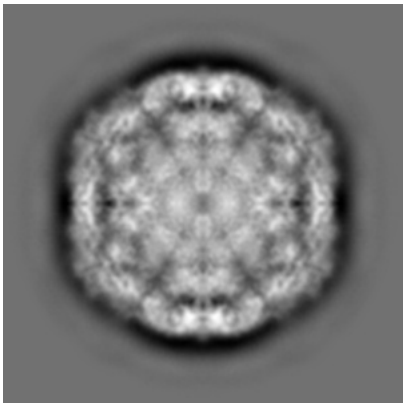
6.1.1 Primary map



X



Y

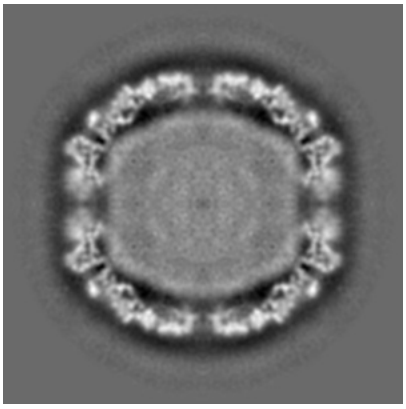


Z

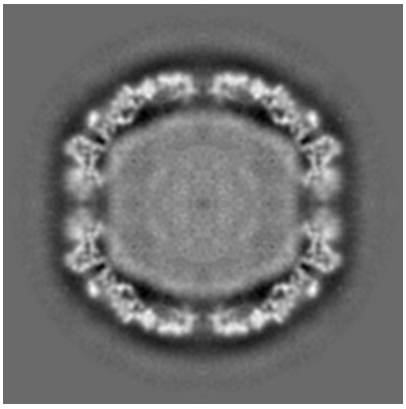
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

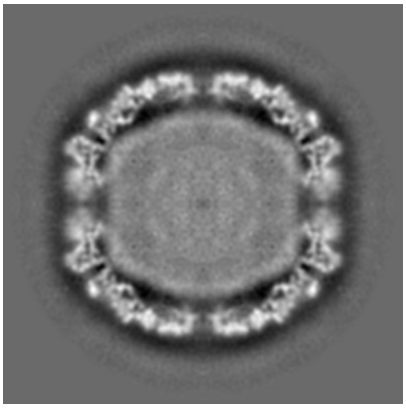
6.2.1 Primary map



X Index: 175



Y Index: 175

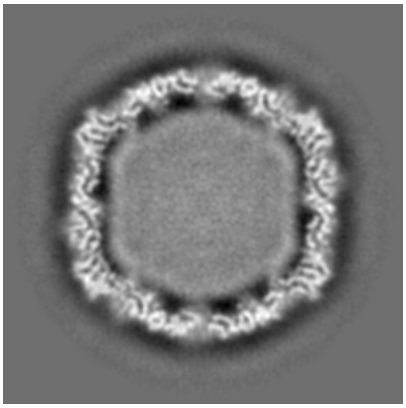


Z Index: 175

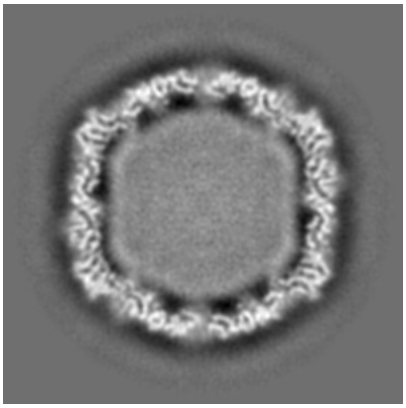
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

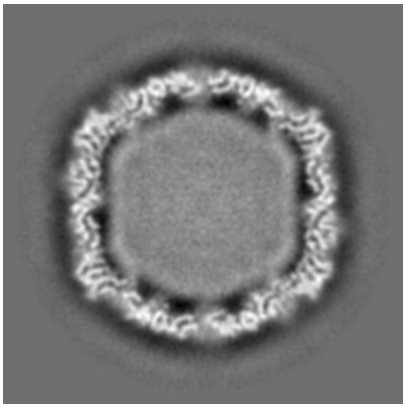
6.3.1 Primary map



X Index: 189



Y Index: 189

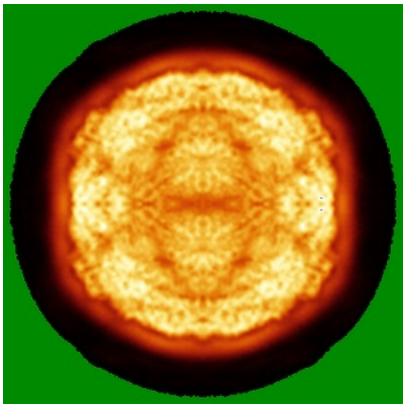


Z Index: 161

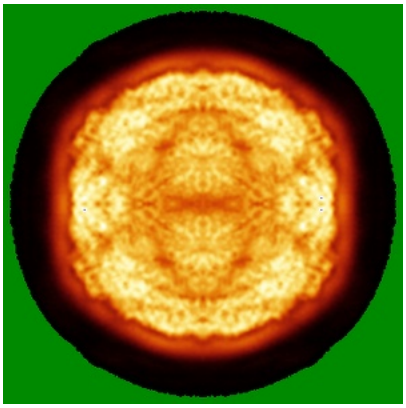
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

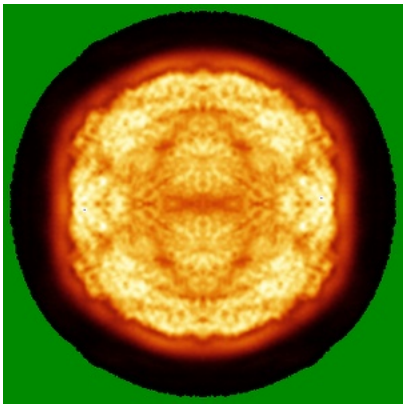
6.4.1 Primary map



X



Y

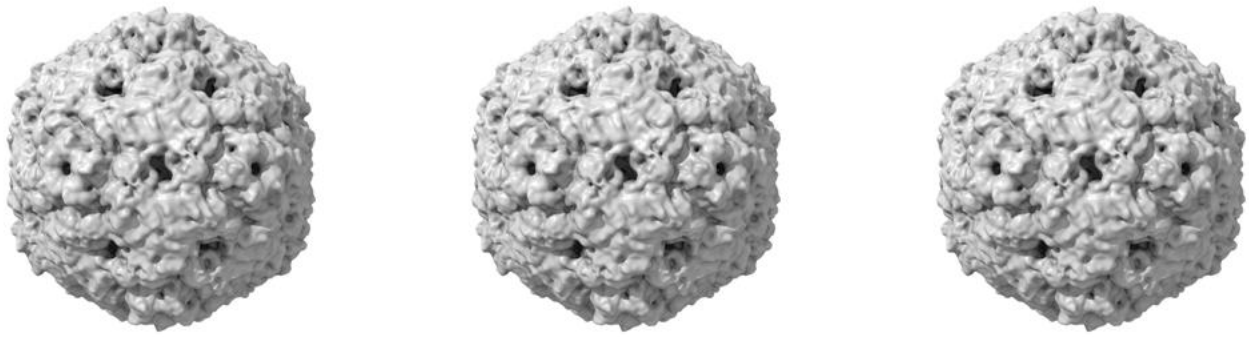


Z

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 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

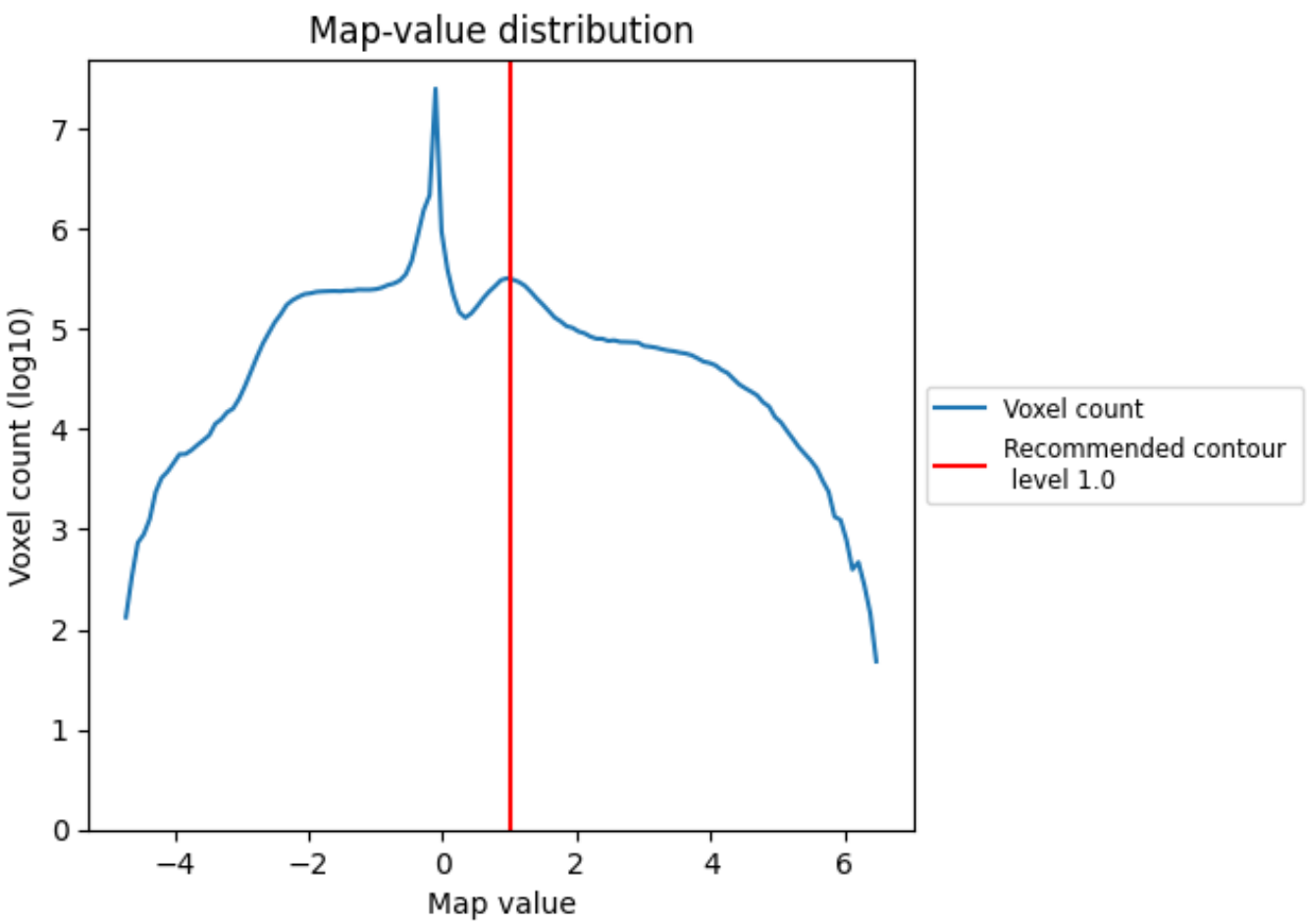
6.6 Mask visualisation (i)

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

7 Map analysis (i)

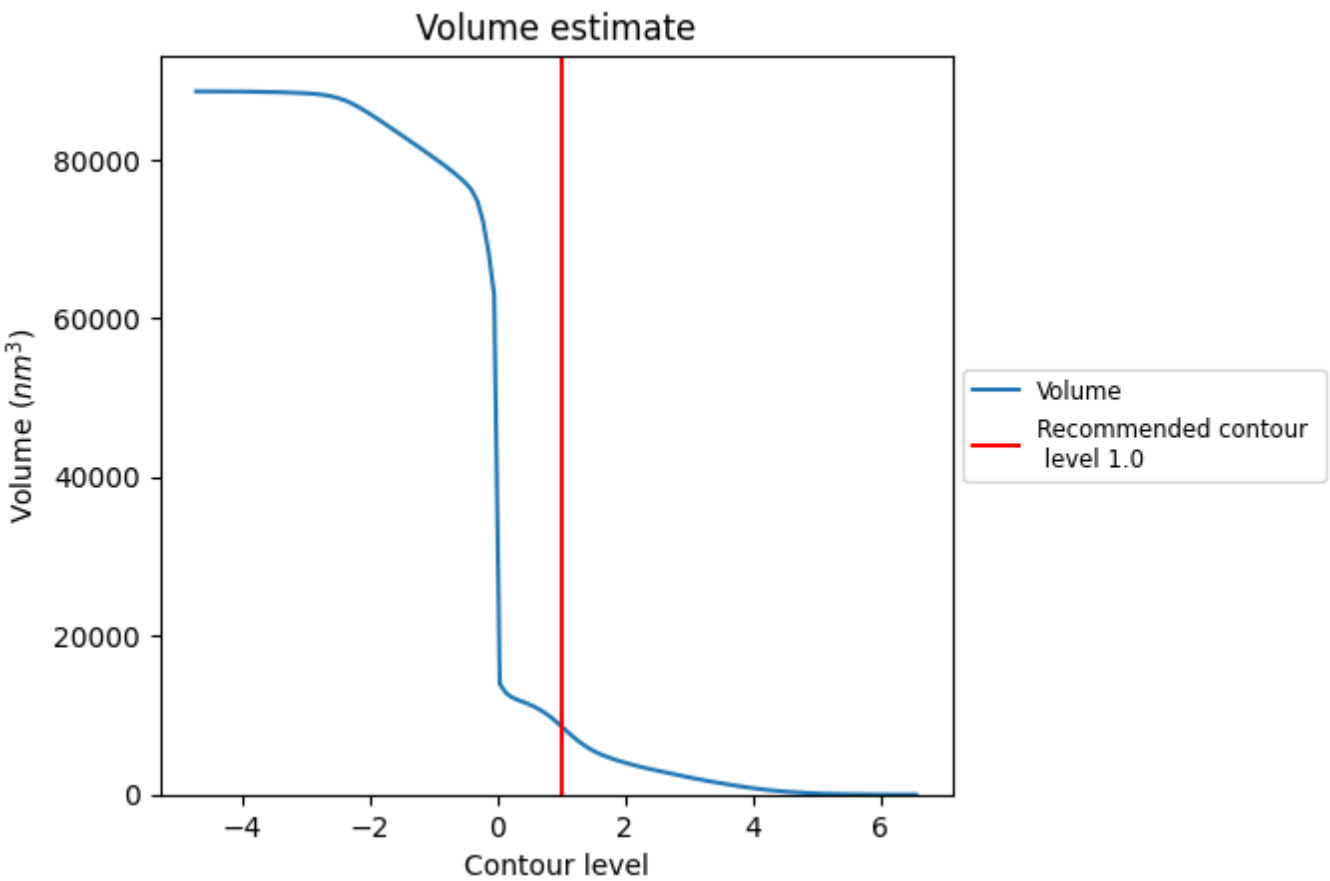
This section contains the results of statistical analysis of the map.

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.

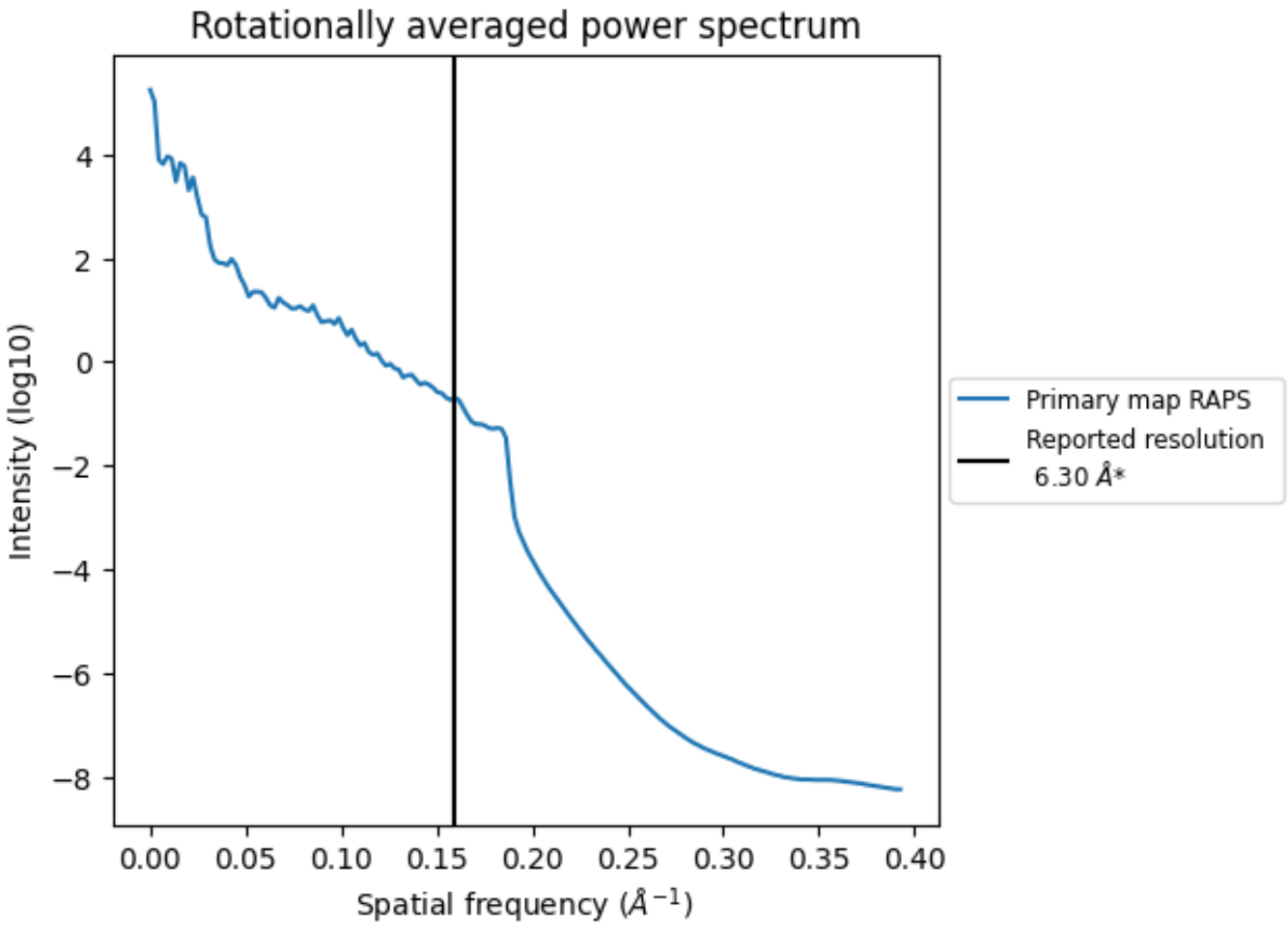
7.2 Volume estimate (i)



The volume at the recommended contour level is 8595 nm^3; this corresponds to an approximate mass of 7764 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 0.159 Å^{-1}

8 Fourier-Shell correlation (i)

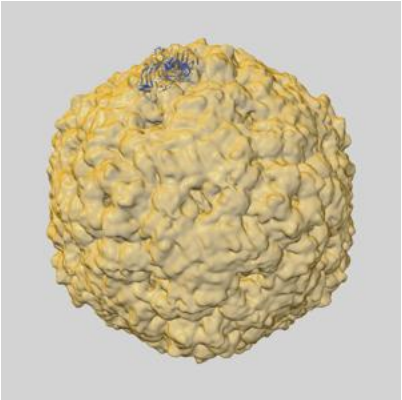
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

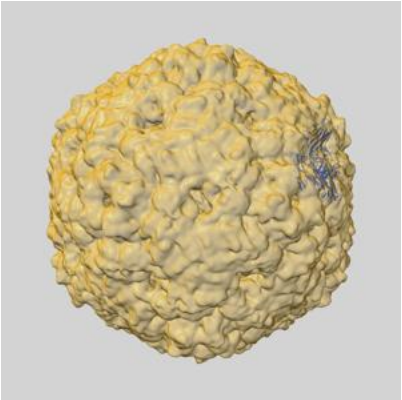
This section contains information regarding the fit between EMDB map EMD-5465 and PDB model 3J22. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

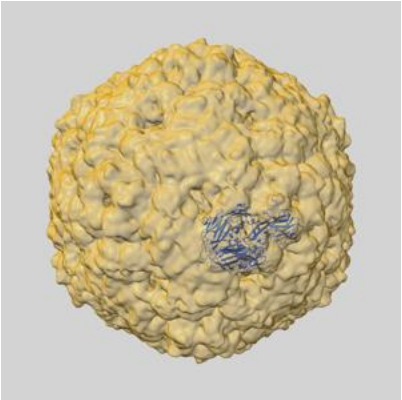
9.1.1 Map-model overlay (i)



X

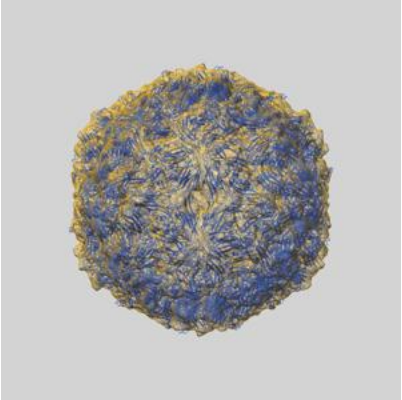


Y

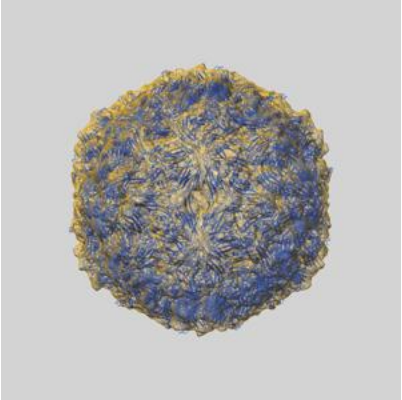


Z

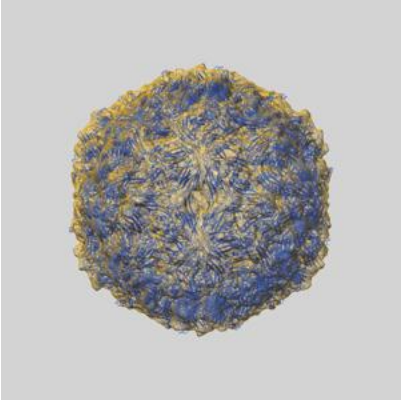
9.1.2 Map-model assembly overlay (i)



X



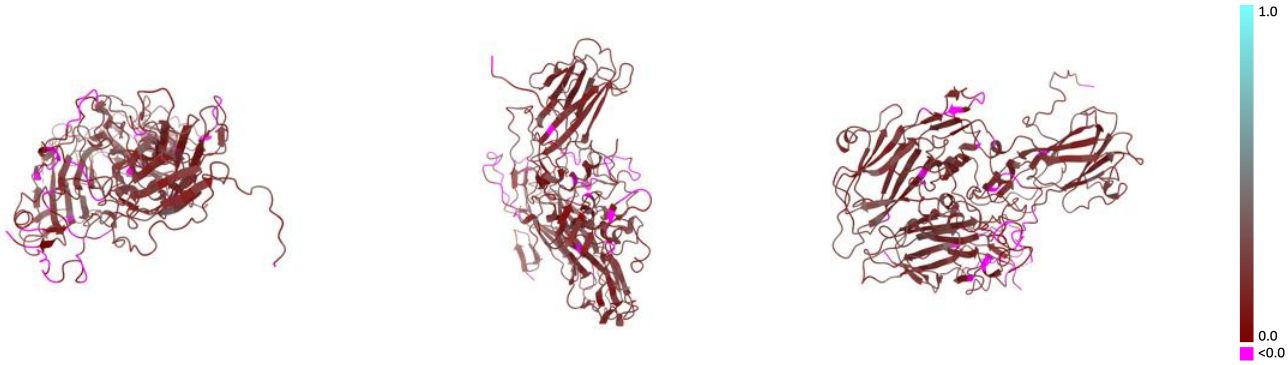
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 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.

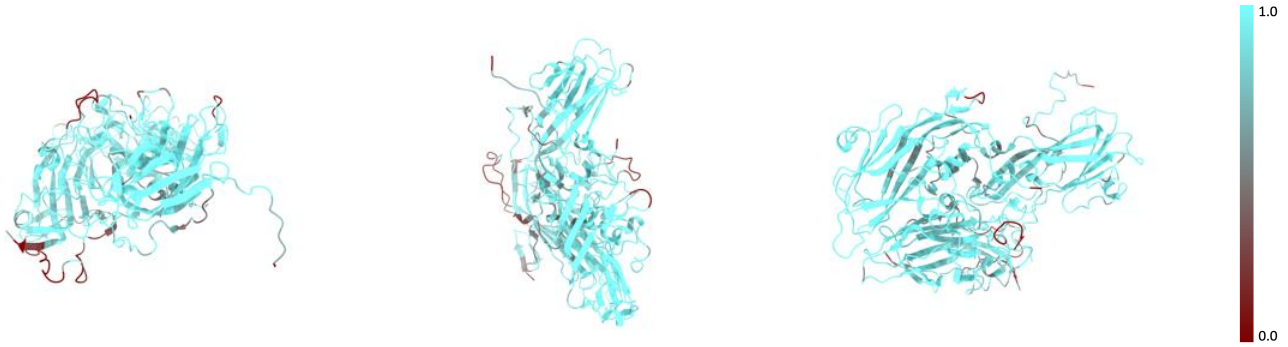
9.2 Q-score mapped to coordinate model (i)



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.

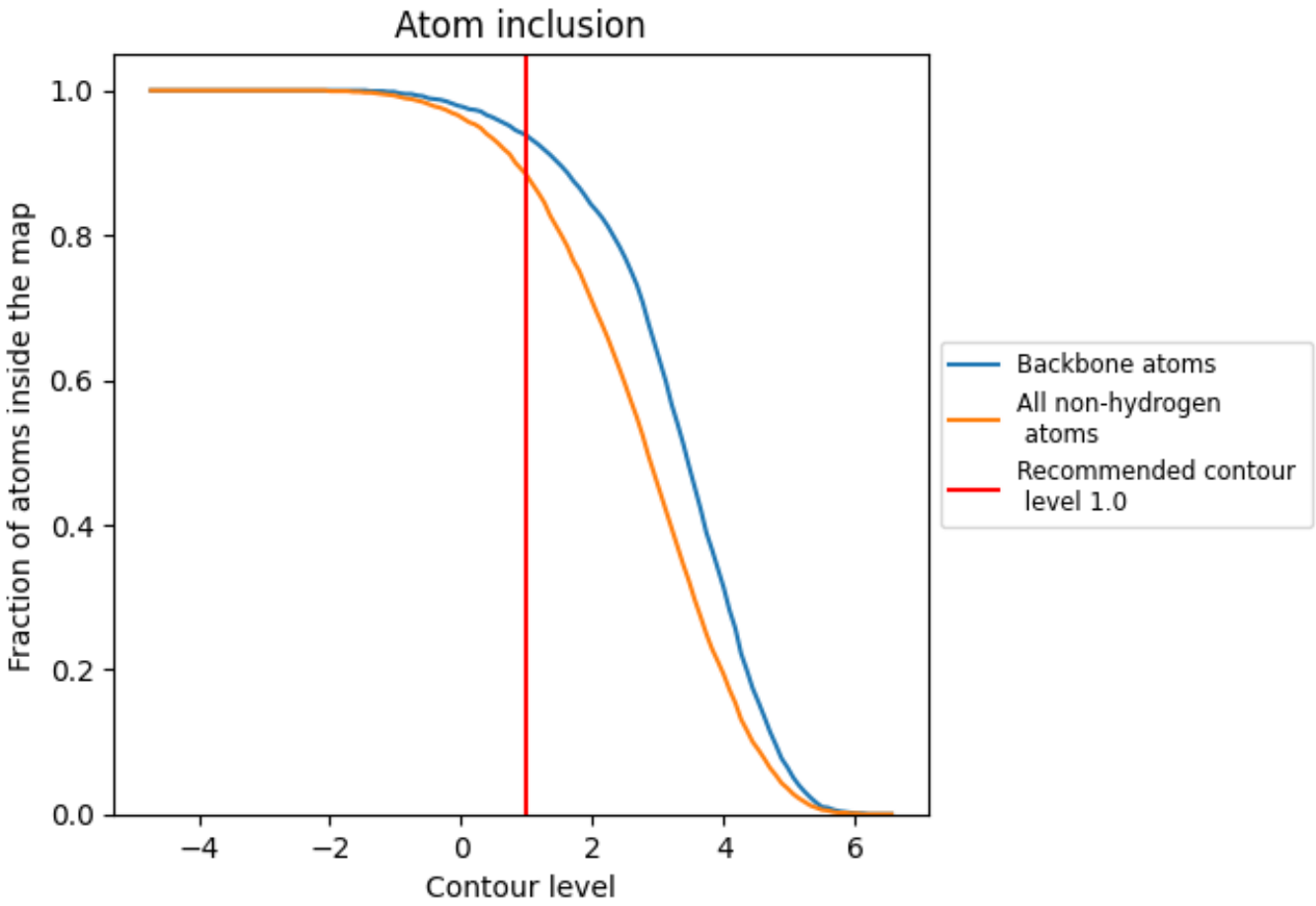
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.0).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 88% 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 (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8830	0.1690
A	0.9350	0.1820
B	0.8150	0.1450
C	0.9030	0.1820