Full wwPDB EM Validation Report (i)

Nov 16, 2022 – 01:36 PM JST

PDB ID	:	7C81
EMDB ID	:	EMD-30304
Title	:	E30 F-particle in complex with 6C5
Authors	:	Wang, K.; Zheng, B.; Zhang, L.; Cui, L.; Su, X.; Zhang, Q.; Guo, Y.; Zhu, L.; Zhu, F.; Rao, Z.; Wang, X.
Deposited on	:	2020-05-28
Resolution	:	3.10 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 (1)) were used in the production of this report:

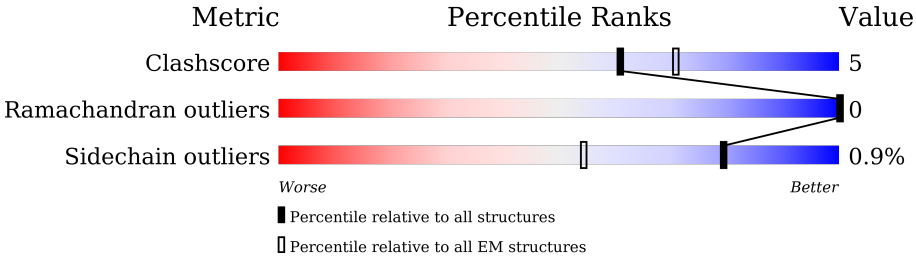
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.10 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	292	84% 11% 5%
2	B	261	89% 7% •
3	C	238	87% 13%
4	D	69	77% 7% 16%
5	L	213	95% 84% 15%
6	H	216	88% 85% 13% •

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9514 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	276	2211	1397	391	412	11	0	0

- Molecule 2 is a protein called VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	251	1949	1233	334	366	16	0	0

- Molecule 3 is a protein called VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	238	1836	1167	301	354	14	0	0

- Molecule 4 is a protein called VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	58	464	296	77	90	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MYR	-	acetylation	UNP Q33C85

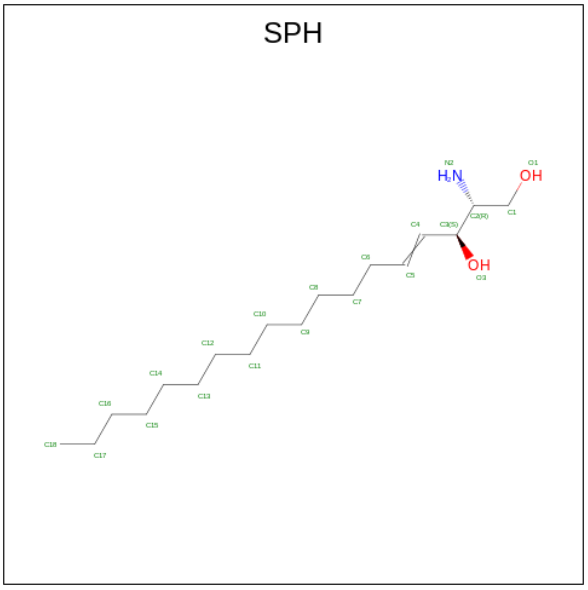
- Molecule 5 is a protein called Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L	213	1543	943	268	323	9	0	0

- Molecule 6 is a protein called Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	212	1490	931	251	303	5	0	0

- Molecule 7 is SPHINGOSINE (three-letter code: SPH) (formula: $C_{18}H_{37}NO_2$).



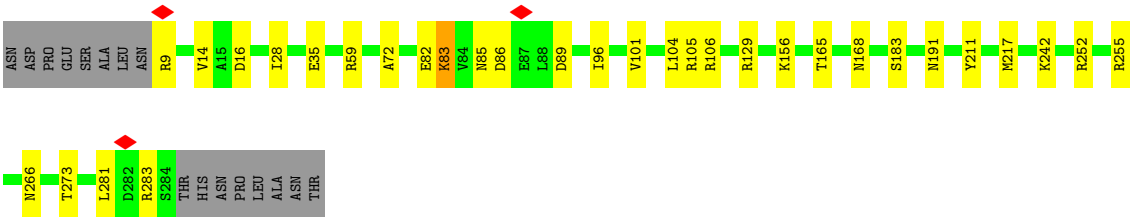
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	A	1	21	18	1	2	0

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:

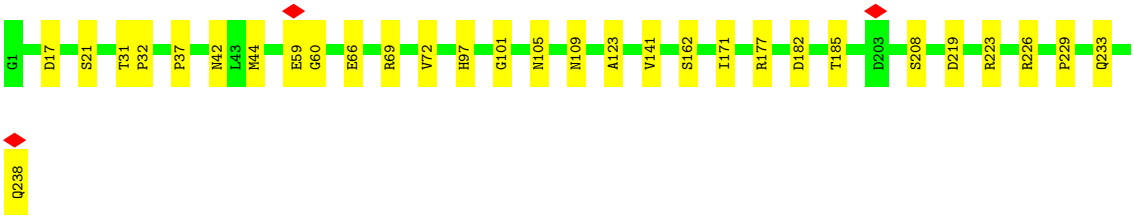


- Molecule 2: VP2

Chain B:

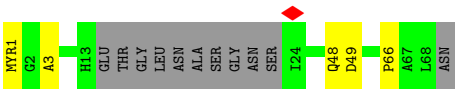
- Molecule 3: VP3

Chain C:



- Molecule 4: VP4

Chain D:



- Molecule 5: Light chain

Chain L: 95% 84% 15%

D1 I2 E3 L4 T5 Q6 S7 P8 A9 I10 M11 S12 A13 S14 P15 G16 E17 K18 V19 T20 M21 T22 C23 S24 A25 S26 S27 S28 L29 R30 Y31 M32 H33 W34 Y35 Q36 Q37 K38 S39 G40 T41 S42 P43 K44 R45 W46 I47 Y48 D49 T50 Y51 N52 L53 A54 S55 G56 V57 P58 V59 R60

F61 S62 G63 S64 G65 S66 G67 T68 S69 Y70 S71 L72 T73 I74 S75 S76 M77 E78 A79 E80 D81 A82 A83 T84 Y85 Y86 C87 Q88 Q89 W90 S91 S92 N93 P94 P95 T96 F97 G98 A99 G100 T101 K102 L103 E104 L105 K106 R107 A108 D109 A110 A111 P112 T113 V114 S115 I116 F117 P118 P119 S120

S121 E122 Q123 L124 T125 S126 G127 G128 A129 S130 V131 V132 C133 F134 L135 N136 N137 F138 Y139 P140 K141 D142 I143 N144 V145 K146 W147 K148 I149 D150 G151 S152 E153 R154 Q155 N156 G157 V158 L159 N160 S161 W162 T163 D164 Q165 D166 S167 K168 D169 S170 T171 Y172 S173 M174 S175 S176 T177 L178 T179 L180

T181 K182 D183 E184 Y185 E186 R187 H188 N189 S190 Y191 T192 C193 E194 A195 T196 H197 K198 T199 S200 T201 S202 P203 I204 V205 K206 S207 F208 N209 R210 N211 E212 C213

- Molecule 6: Heavy chain

Chain H: 88% 85% 13%

Q1 V2 Q3 L4 Q5 Q6 S7 G8 S9 E10 L11 V12 R13 P14 G15 A16 S17 V18 K19 L20 S21 C22 R23 A24 S25 G26 Y27 T28 F29 T30 W33 M34 H35 W36 V37 K38 Q39 R40 P41 G42 Q43 G44 L45 E46 W47 I48 G49 Y52 Y60 D61 E62 R63 F64 K65 S66 K67 A68

T69 L70 T71 V72 D73 T74 S75 S76 S77 T78 A79 Y80 M81 Q82 L83 S84 S85 L86 T87 S88 E89 D90 S91 A92 V93 Y94 Y95 C96 T97 R98 D99 L100 R101 G102 F103 A104 Y105 W106 G107 Q108 G109 T110 T111 V112 T113 V114 S115 S116 P117 K118 T119 T120 P121 P122 S123 V124 Y125 P126 L127 A128

P129 A130 ALA ALA SER THR A135 A136 S137 M138 V139 T140 L141 G142 C143 L144 V145 K146 G147 Y148 F149 P150 E151 P152 V153 T154 V155 T156 W157 N158 S159 G160 S161 L162 S163 S164 G165 V166 H167 T168 F169 P170 A171 V172 L173 Q174 S175 D176 L177 Y178 T179 L180 S181 S182 S183 V184 T185 V186 P187 S188

S189 T190 W191 P192 S193 E194 T195 V196 T197 C198 N199 V200 A201 H202 P203 A204 S205 S206 T207 K208 V209 D210 K211 K212 I213 V214 P215 R216

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	10127	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.194	Depositor
Minimum map value	-0.114	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	475.2, 475.2, 475.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.35	0/2274	0.51	0/3102
2	B	0.34	0/2004	0.54	1/2737 (0.0%)
3	C	0.35	0/1886	0.51	0/2580
4	D	0.29	0/457	0.47	0/618
5	L	0.28	0/1575	0.58	2/2142 (0.1%)
6	H	0.28	0/1528	0.61	1/2103 (0.0%)
All	All	0.32	0/9724	0.54	4/13282 (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
5	L	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	138	ASP	CB-CG-OD1	6.59	124.23	118.30
5	L	91	SER	C-N-CA	5.80	136.19	121.70
6	H	27	TYR	C-N-CA	5.54	135.55	121.70
5	L	91	SER	CB-CA-C	5.03	119.65	110.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	L	51	TYR	Peptide
5	L	91	SER	Peptide
5	L	94	PRO	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	2211	0	2135	24	0
2	B	1949	0	1862	12	0
3	C	1836	0	1775	23	0
4	D	464	0	467	4	0
5	L	1543	0	1389	18	0
6	H	1490	0	1329	19	0
7	A	21	0	35	2	0
All	All	9514	0	8992	85	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 5.

All (85) 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)
6:H:33:TRP:NE1	6:H:52:TYR:CE2	2.44	0.85
6:H:33:TRP:CE2	6:H:52:TYR:CD2	2.71	0.79
6:H:33:TRP:CE2	6:H:52:TYR:HD2	2.02	0.77
6:H:33:TRP:NE1	6:H:52:TYR:HE2	1.87	0.70
2:B:27:GLU:HB2	2:B:196:ASN:HB2	1.77	0.67
5:L:116:ILE:HG13	5:L:133:CYS:HB3	1.77	0.66
6:H:33:TRP:NE1	6:H:52:TYR:CD2	2.65	0.65
1:A:59:ARG:HD3	4:D:48:GLN:HE22	1.62	0.65
3:C:101:GLY:O	3:C:105:ASN:ND2	2.35	0.59
1:A:191:ASN:ND2	3:C:32:PRO:O	2.35	0.59
6:H:127:LEU:HD11	6:H:144:LEU:HG	1.86	0.57
1:A:273:THR:HA	3:C:97:HIS:HD2	1.70	0.56
5:L:19:VAL:HB	5:L:74:ILE:HB	1.87	0.56
6:H:33:TRP:CD1	6:H:52:TYR:HE2	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ARG:NH2	2:B:128:PRO:O	2.38	0.55
1:A:242:LYS:NZ	3:C:17:ASP:O	2.39	0.55
5:L:107:ARG:NH1	5:L:169:ASP:O	2.38	0.55
6:H:211:LYS:HZ3	6:H:213:ILE:HA	1.72	0.55
6:H:121:PRO:HB3	6:H:207:THR:HG21	1.88	0.55
1:A:86:ASP:N	1:A:86:ASP:OD1	2.40	0.55
1:A:106:ARG:NH1	1:A:255:ARG:O	2.40	0.54
1:A:105:ARG:NH2	1:A:211:TYR:OH	2.41	0.53
6:H:33:TRP:CD1	6:H:52:TYR:CE2	2.97	0.53
6:H:126:PRO:HG3	6:H:211:LYS:HE3	1.91	0.53
1:A:165:THR:OG1	1:A:168:ASN:O	2.28	0.52
2:B:193:ARG:NH1	3:C:123:ALA:O	2.43	0.52
1:A:72:ALA:HB3	1:A:104:LEU:HD22	1.91	0.51
3:C:66:GLU:OE1	3:C:69:ARG:NH1	2.43	0.51
5:L:184:GLU:HA	5:L:187:ARG:HE	1.76	0.50
5:L:194:GLU:HG2	5:L:205:VAL:HG22	1.93	0.50
3:C:109:ASN:HD22	3:C:223:ARG:HE	1.60	0.50
6:H:39:GLN:NE2	6:H:95:TYR:OH	2.45	0.50
1:A:9:ARG:NH2	1:A:16:ASP:OD1	2.42	0.50
5:L:184:GLU:HG3	5:L:187:ARG:HH21	1.77	0.50
6:H:67:LYS:O	6:H:84:SER:N	2.45	0.50
6:H:151:GLU:HG2	6:H:152:PRO:HD3	1.94	0.49
3:C:105:ASN:O	3:C:226:ARG:NH1	2.45	0.49
1:A:82:GLU:O	1:A:129:ARG:NH2	2.42	0.49
3:C:219:ASP:OD1	3:C:219:ASP:N	2.47	0.48
4:D:49:ASP:N	4:D:49:ASP:OD1	2.44	0.48
1:A:101:VAL:HA	3:C:233:GLN:HE22	1.80	0.47
1:A:217:MET:HG3	7:A:500:SPH:H5	1.97	0.47
1:A:266:ASN:HB3	2:B:137:THR:HG22	1.97	0.47
6:H:62:GLU:HA	6:H:65:LYS:HE2	1.97	0.47
5:L:60:ARG:NH2	5:L:80:GLU:OE2	2.48	0.46
3:C:72:VAL:HG23	3:C:208:SER:HB3	1.97	0.46
1:A:281:LEU:HB3	3:C:141:VAL:HG21	1.98	0.46
6:H:171:ALA:HB2	6:H:180:LEU:HD23	1.97	0.46
5:L:96:THR:OG1	5:L:97:PHE:N	2.49	0.46
2:B:37:VAL:HG21	3:C:37:PRO:HB3	1.98	0.46
3:C:171:ILE:O	3:C:177:ARG:NH2	2.46	0.46
5:L:35:TYR:HD1	5:L:45:ARG:HA	1.80	0.45
3:C:182:ASP:OD1	3:C:185:THR:OG1	2.34	0.45
1:A:183:SER:OG	3:C:21:SER:OG	2.33	0.44
5:L:60:ARG:H	5:L:60:ARG:HG2	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:177:ARG:HG2	3:C:185:THR:HB	1.98	0.44
1:A:85:ASN:N	1:A:85:ASN:OD1	2.51	0.44
2:B:156:SER:OG	2:B:158:LYS:O	2.34	0.44
1:A:9:ARG:NH2	1:A:14:VAL:O	2.39	0.44
4:D:1:MYR:O1	4:D:3:ALA:N	2.49	0.44
1:A:28:ILE:HD11	4:D:66:PRO:HG3	1.98	0.43
3:C:42:ASN:HD22	3:C:44:MET:HB2	1.82	0.43
5:L:142:ASP:OD1	5:L:142:ASP:N	2.52	0.43
2:B:119:GLN:HE21	2:B:230:GLU:HG3	1.84	0.43
1:A:83:LYS:HG3	1:A:89:ASP:OD1	2.19	0.43
2:B:105:GLY:O	2:B:248:MET:N	2.48	0.43
5:L:166:ASP:HB3	5:L:170:SER:H	1.84	0.43
6:H:3:GLN:O	6:H:25:SER:N	2.40	0.42
5:L:42:SER:H	6:H:108:GLN:HE22	1.67	0.42
2:B:91:LEU:O	2:B:95:ASN:ND2	2.40	0.42
5:L:1:ASP:HA	5:L:2:ILE:HA	1.66	0.42
1:A:283:ARG:HD2	1:A:283:ARG:HA	1.85	0.42
5:L:186:GLU:HG3	5:L:210:ARG:HH12	1.85	0.42
3:C:226:ARG:HH12	3:C:229:PRO:HD3	1.84	0.42
5:L:112:PRO:HB3	5:L:138:PHE:HB3	2.01	0.41
6:H:9:SER:H	6:H:112:VAL:HG22	1.85	0.41
2:B:226:PHE:O	3:C:69:ARG:NE	2.45	0.41
3:C:59:GLU:HA	3:C:60:GLY:HA2	1.74	0.41
2:B:189:TRP:O	2:B:195:ASN:ND2	2.51	0.41
5:L:63:GLY:HA2	5:L:72:LEU:HA	2.02	0.41
1:A:35:GLU:OE2	3:C:162:SER:OG	2.32	0.40
2:B:158:LYS:NZ	2:B:159:LYS:O	2.41	0.40
3:C:31:THR:HA	3:C:32:PRO:HD3	1.98	0.40
5:L:6:GLN:NE2	5:L:100:GLY:O	2.55	0.40
1:A:96:ILE:HD13	7:A:500:SPH:H102	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	274/292 (94%)	265 (97%)	9 (3%)	0	100	100
2	B	249/261 (95%)	237 (95%)	12 (5%)	0	100	100
3	C	236/238 (99%)	230 (98%)	6 (2%)	0	100	100
4	D	53/69 (77%)	51 (96%)	2 (4%)	0	100	100
5	L	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
6	H	208/216 (96%)	187 (90%)	21 (10%)	0	100	100
All	All	1231/1289 (96%)	1168 (95%)	63 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	244/258 (95%)	242 (99%)	2 (1%)	81	92
2	B	211/221 (96%)	209 (99%)	2 (1%)	78	91
3	C	207/207 (100%)	206 (100%)	1 (0%)	88	94
4	D	51/59 (86%)	51 (100%)	0	100	100
5	L	161/188 (86%)	160 (99%)	1 (1%)	86	94
6	H	151/187 (81%)	148 (98%)	3 (2%)	55	80
All	All	1025/1120 (92%)	1016 (99%)	9 (1%)	79	91

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	LYS
1	A	156	LYS
2	B	138	ASP
2	B	256	ARG

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Mol	Chain	Res	Type
3	C	238	GLN
5	L	44	LYS
6	H	73	ASP
6	H	87	THR
6	H	106	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	277	ASN
2	B	111	GLN
3	C	42	ASN
3	C	75	GLN
3	C	97	HIS
3	C	109	ASN
3	C	195	GLN
4	D	48	GLN
6	H	39	GLN
6	H	108	GLN
6	H	174	GLN

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)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	SPH	A	500	-	19,20,20	0.90	1 (5%)	18,21,21	1.09	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SPH	A	500	-	-	13/21/21/21	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	500	SPH	C4-C5	3.61	1.47	1.31

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	500	SPH	C3-C4-C5	-2.97	118.17	124.79
7	A	500	SPH	O3-C3-C2	2.56	111.38	107.31

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	500	SPH	O1-C1-C2-N2
7	A	500	SPH	O1-C1-C2-C3
7	A	500	SPH	C1-C2-C3-O3
7	A	500	SPH	C1-C2-C3-C4
7	A	500	SPH	N2-C2-C3-O3
7	A	500	SPH	N2-C2-C3-C4
7	A	500	SPH	C9-C10-C11-C12
7	A	500	SPH	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	500	SPH	C13-C14-C15-C16
7	A	500	SPH	C10-C11-C12-C13
7	A	500	SPH	C11-C10-C9-C8
7	A	500	SPH	C7-C8-C9-C10
7	A	500	SPH	C6-C7-C8-C9

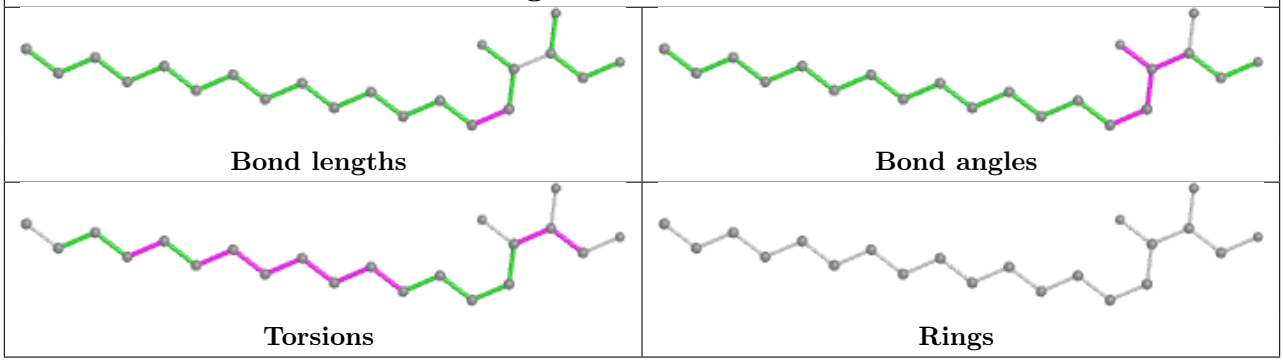
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	500	SPH	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SPH A 500



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.

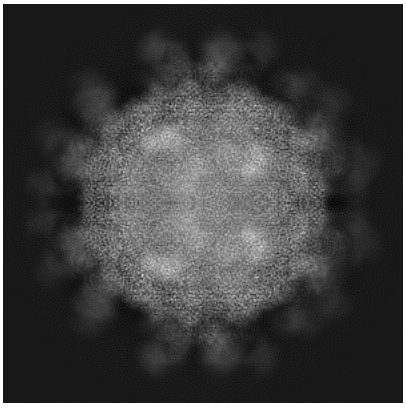
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30304. These allow visual inspection of the internal detail of the map and identification of artifacts.

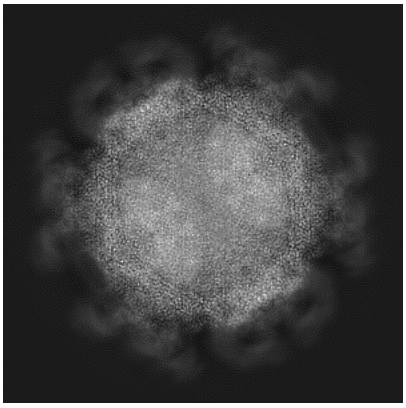
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

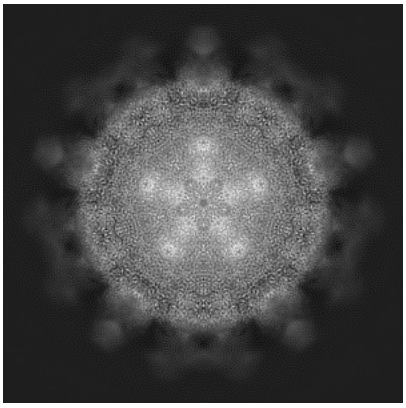
6.1.1 Primary map



X



Y

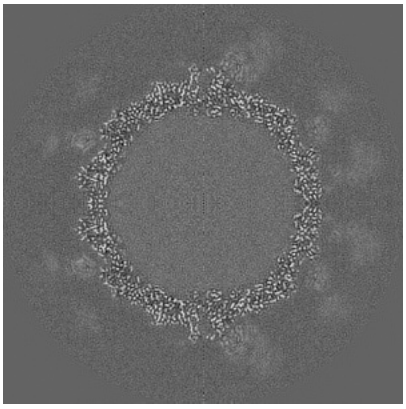


Z

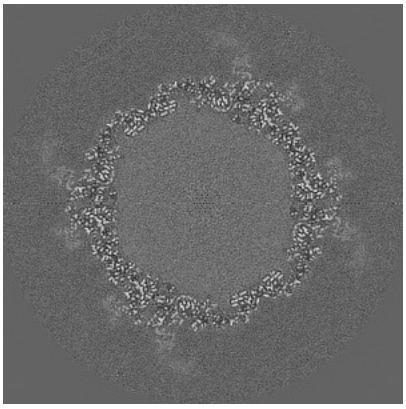
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

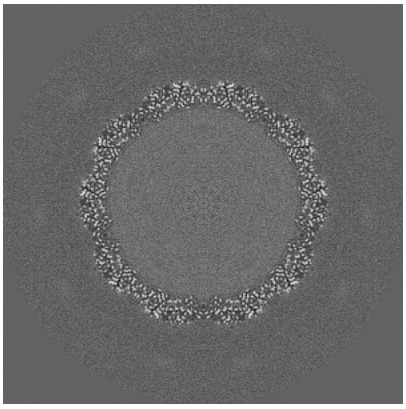
6.2.1 Primary map



X Index: 180



Y Index: 180

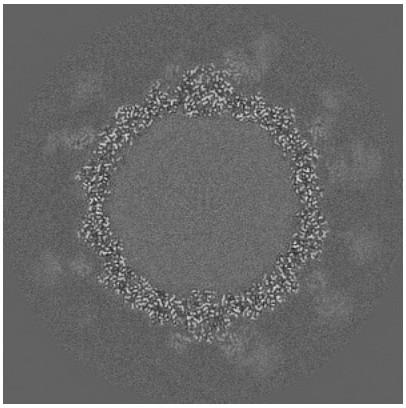


Z Index: 180

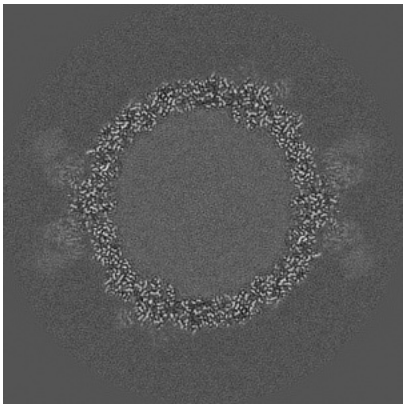
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

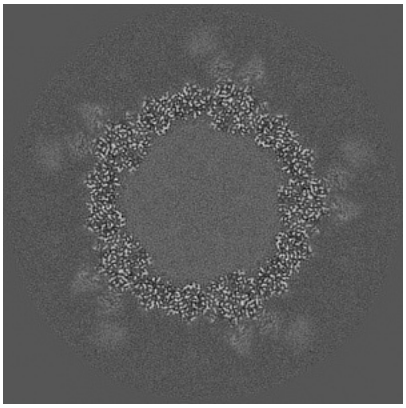
6.3.1 Primary map



X Index: 185



Y Index: 191



Z Index: 220

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

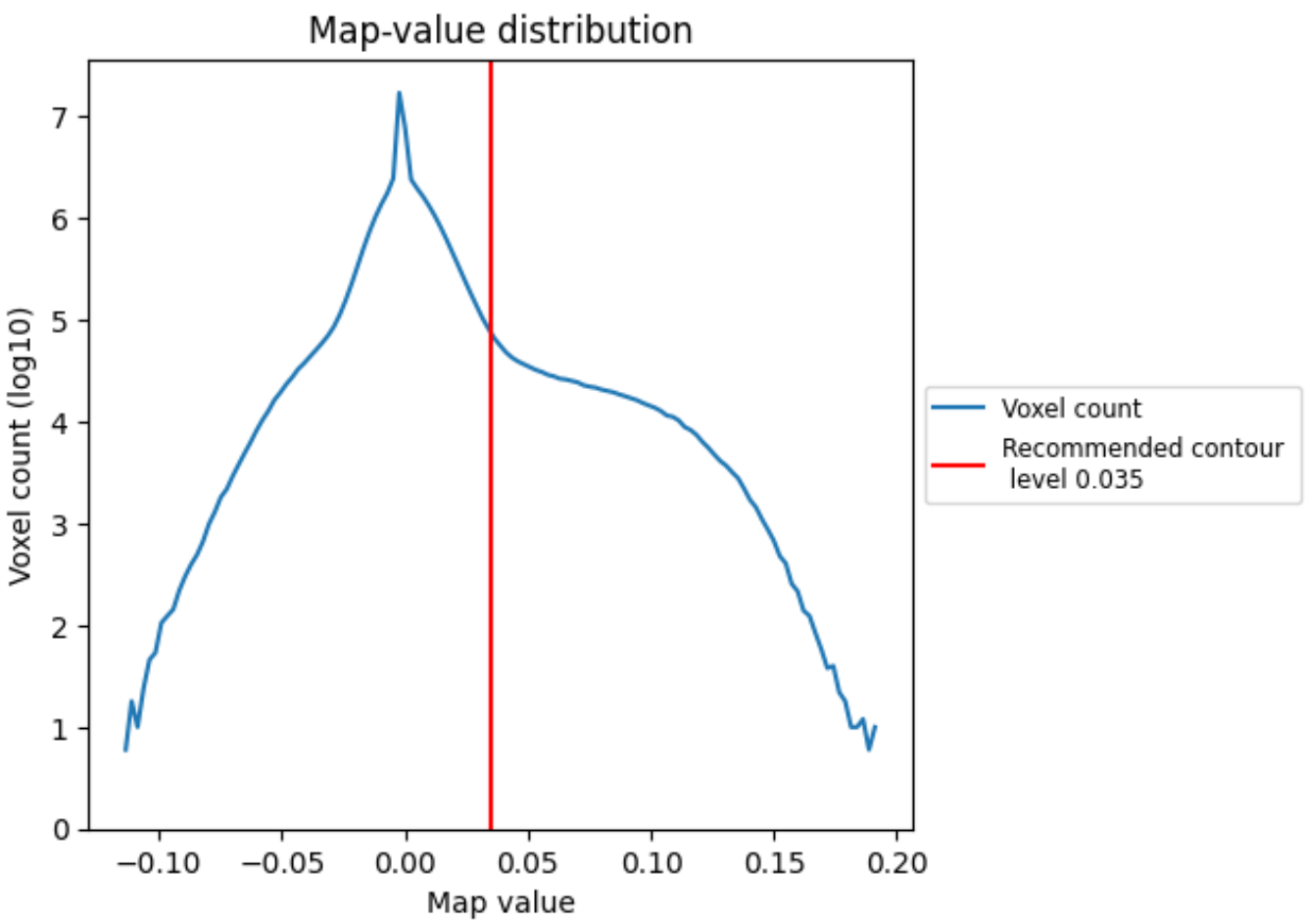
6.5 Mask visualisation (i)

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

7 Map analysis (i)

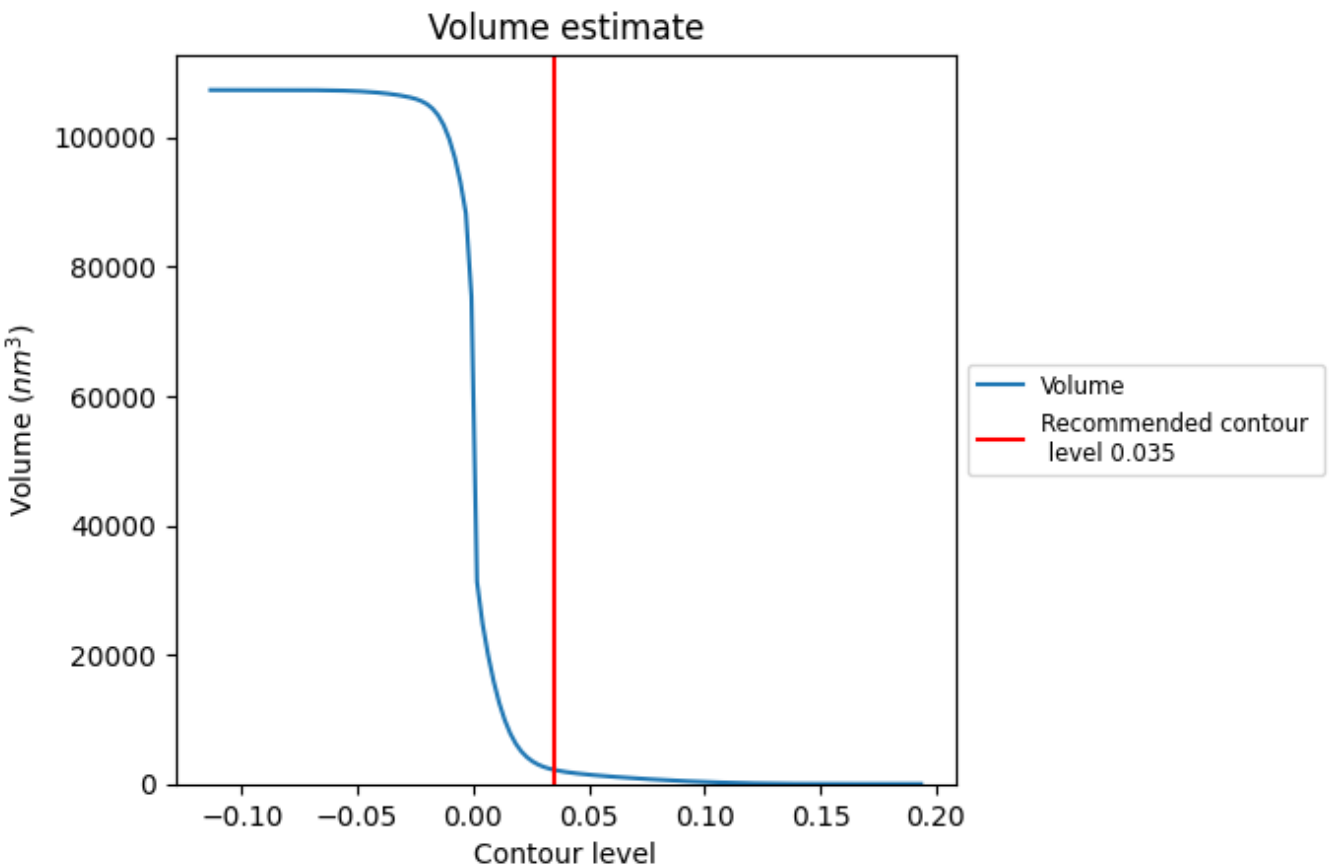
This section contains the results of statistical analysis of the map.

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.

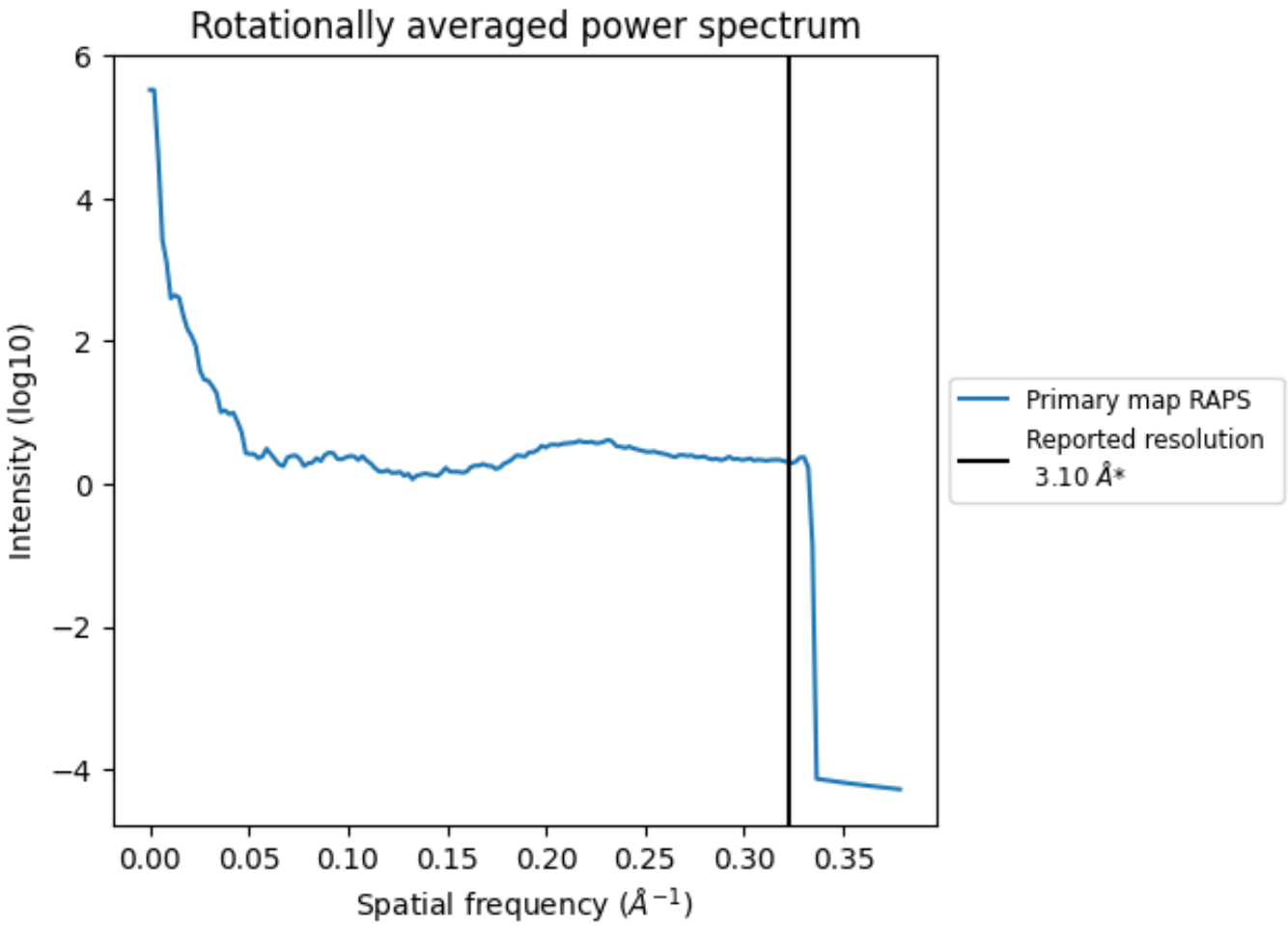
7.2 Volume estimate (i)



The volume at the recommended contour level is 2178 nm^3; this corresponds to an approximate mass of 1967 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 0.323 Å^{-1}

8 Fourier-Shell correlation (i)

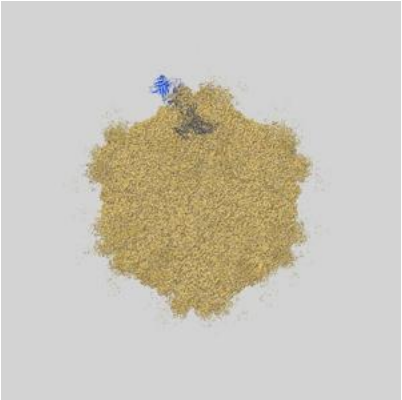
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

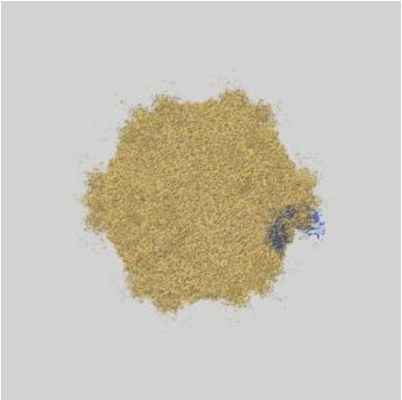
This section contains information regarding the fit between EMDB map EMD-30304 and PDB model 7C81. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

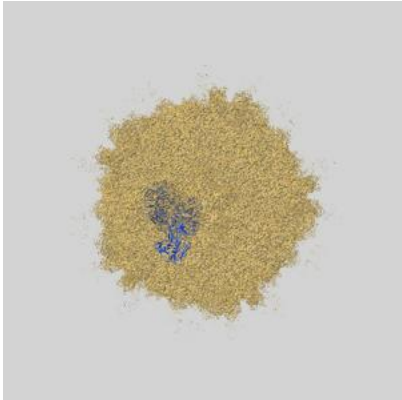
9.1.1 Map-model overlay (i)



X

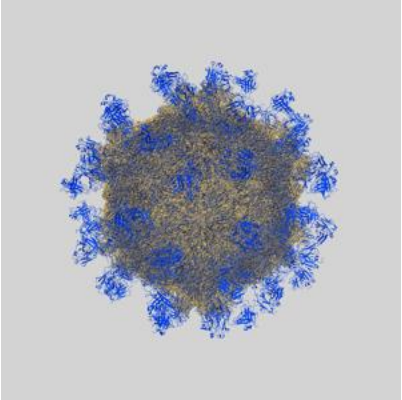


Y

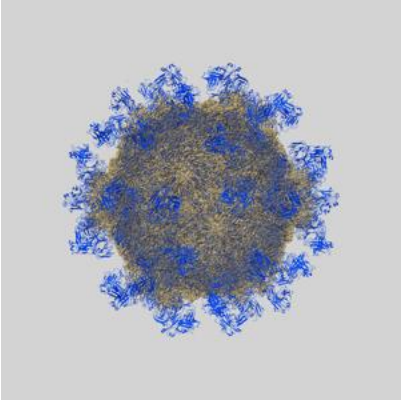


Z

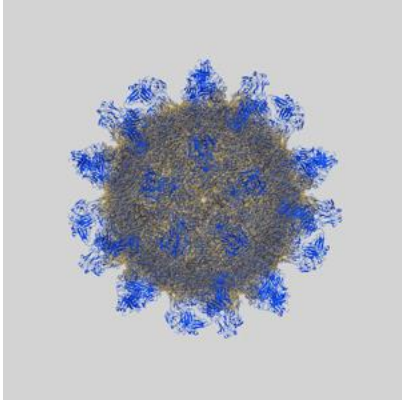
9.1.2 Map-model assembly overlay (i)



X



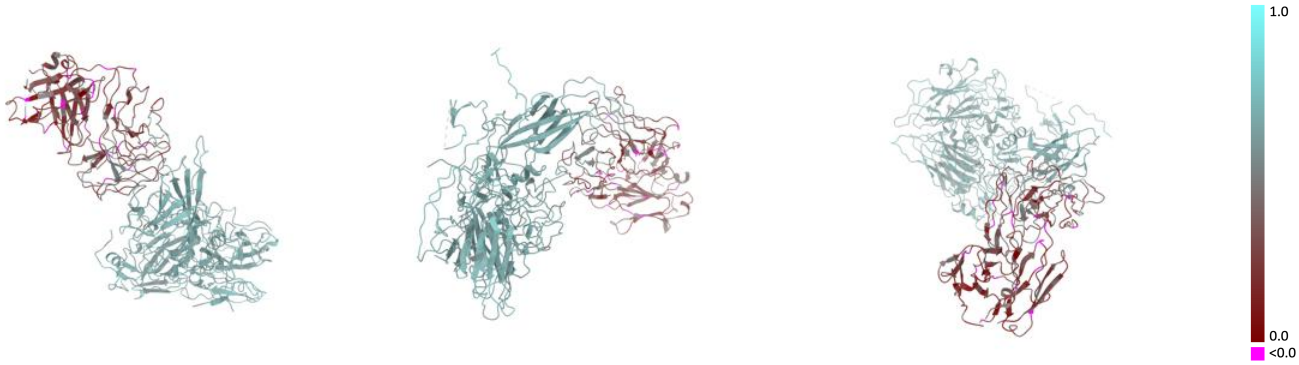
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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.

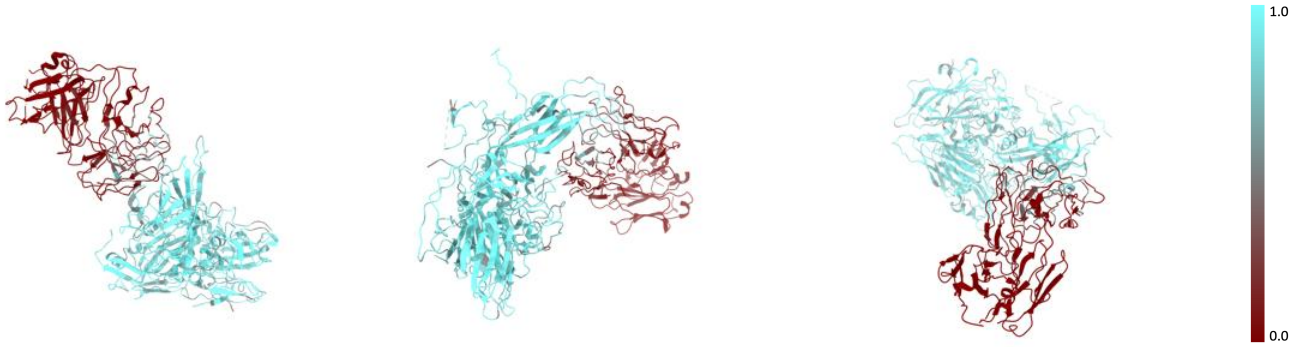
9.2 Q-score mapped to coordinate model (i)



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.

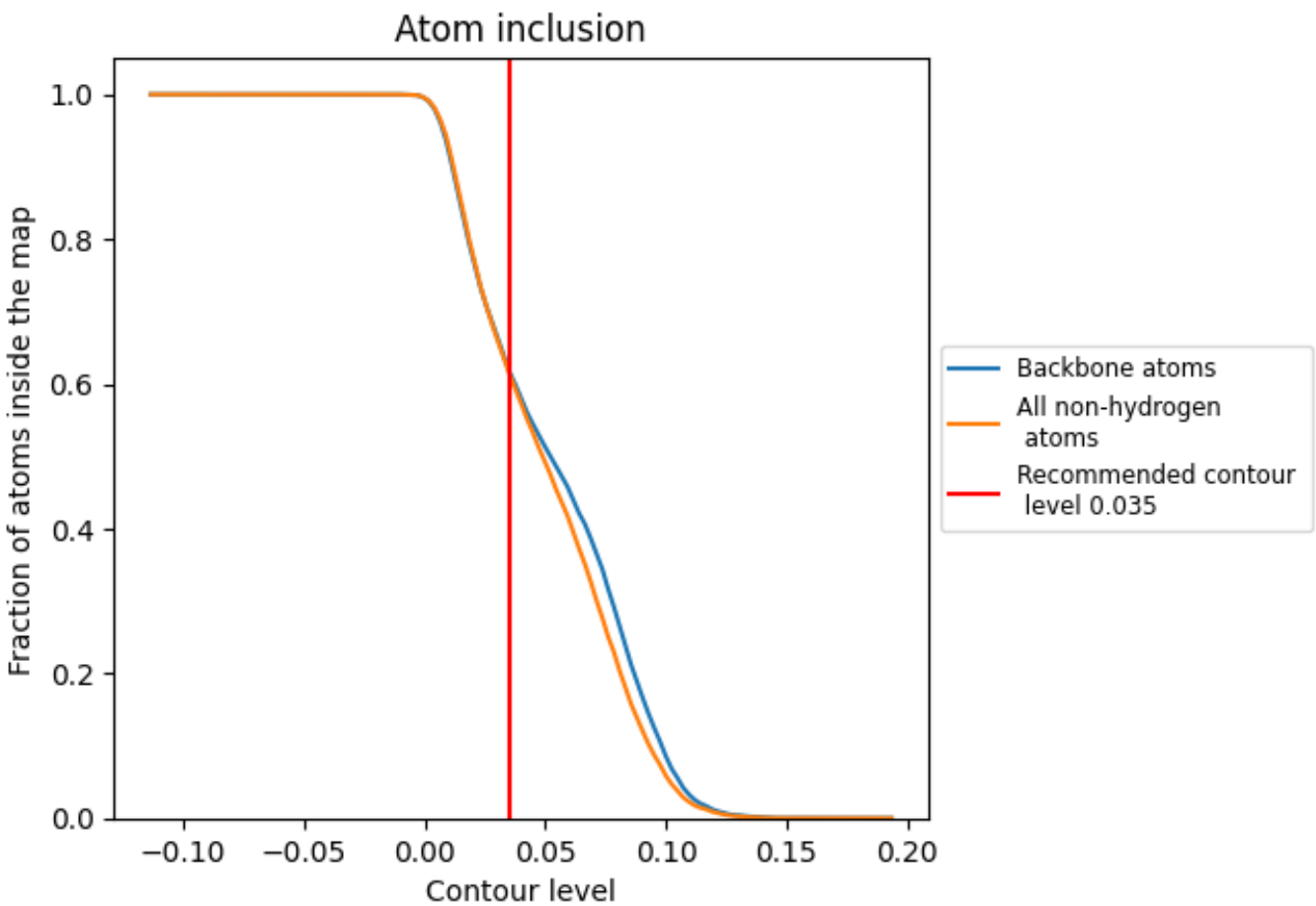
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 62% of all backbone atoms, 61% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6148	0.5170
A	0.8509	0.6210
B	0.8936	0.6270
C	0.8721	0.6240
D	0.7669	0.6160
H	0.1110	0.2870
L	0.0593	0.2900