Full wwPDB EM Map/Model Validation Report ⓘ

May 15, 2020 – 03:56 am BST

PDB ID	:	6OWO
EMDB ID	:	EMD-20215
Title	:	CRYO-EM STRUCTURE OF PHOSPHORYLATED AP-2 CORE BOUND TO NECAP
Authors	:	Partlow, E.A.; Baker, R.W.; Beacham, G.M.; Chappie, J.S.; Leschziner, A.E.; Hollopeter, G.
Deposited on	:	2019-05-10
Resolution	:	3.20 Å(reported)
Based on initial models	:	1TQZ, 2VGL

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

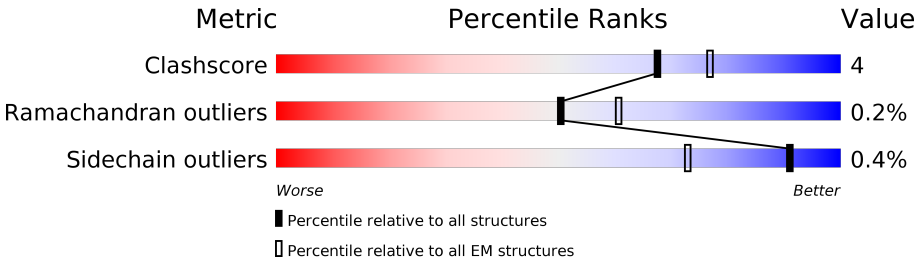
EMDB validation analysis	:	0.0.0.dev33
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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 on 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	621	83% 9% 8%
2	B	591	6% 85% 9% • 5%
3	M	435	76% 14% 9%
4	S	142	86% 13% •
5	N	266	41% 5% 54%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14276 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 AP-2 complex subunit alpha-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	569	4505	2875	776	835	19	0	0

- Molecule 2 is a protein called AP-2 complex subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	559	4443	2837	737	845	24	0	0

- Molecule 3 is a protein called AP-2 complex subunit mu.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
3	M	395	3166	2036	549	562	1	18	0	0

- Molecule 4 is a protein called AP-2 complex subunit sigma.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	S	141	1190	773	199	211	7	0	0

- Molecule 5 is a protein called Adaptin ear-binding coat-associated protein 2.

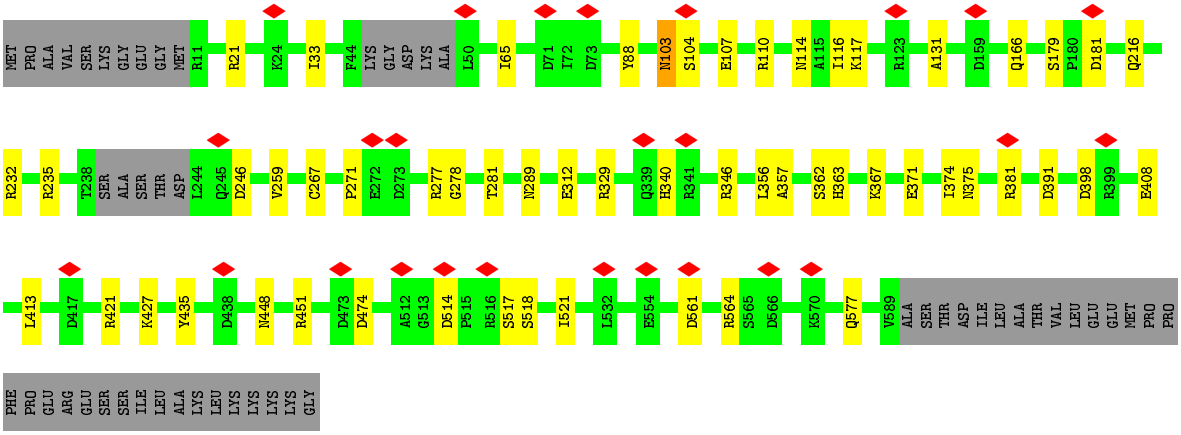
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	N	122	972	625	166	179	2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

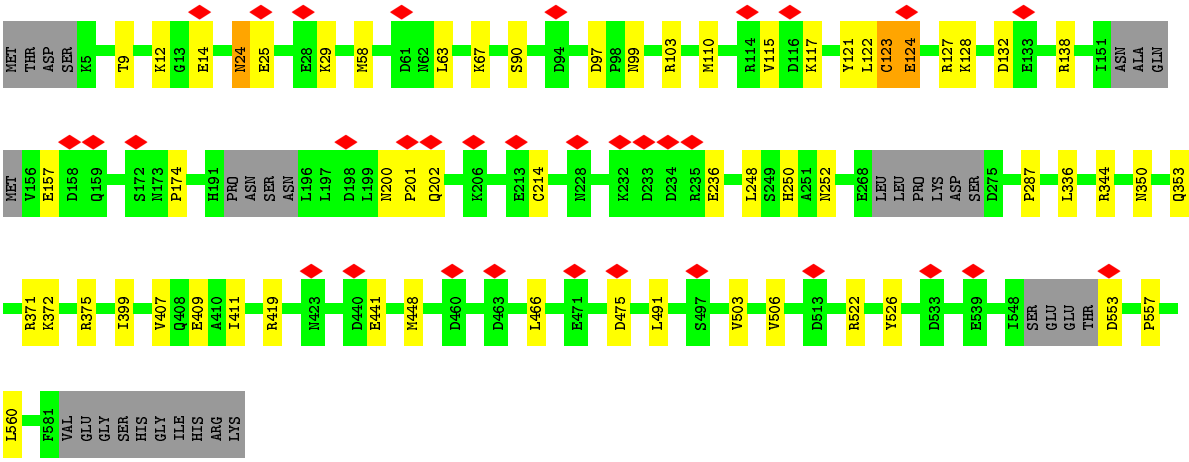
- Molecule 1: AP-2 complex subunit alpha-2

Chain A:



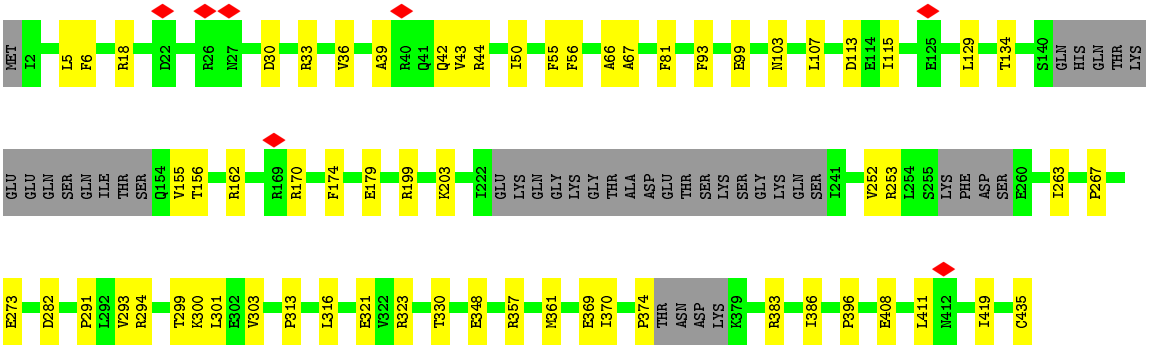
- Molecule 2: AP-2 complex subunit beta

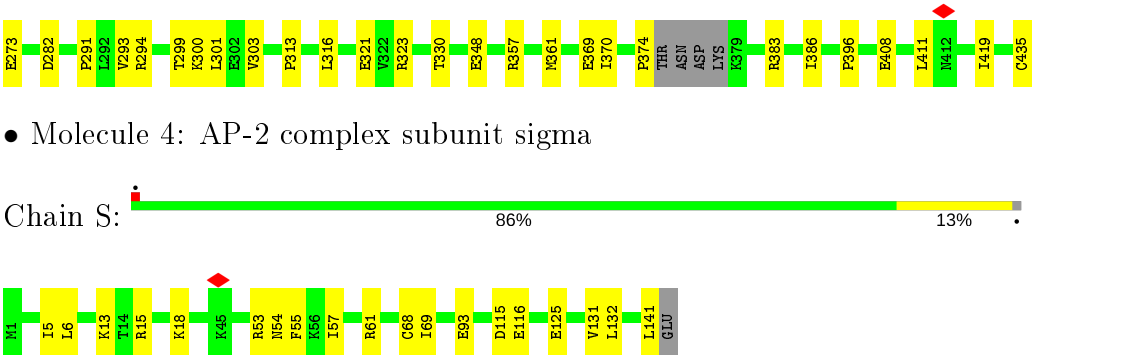
Chain B:



- Molecule 3: AP-2 complex subunit mu

Chain M:



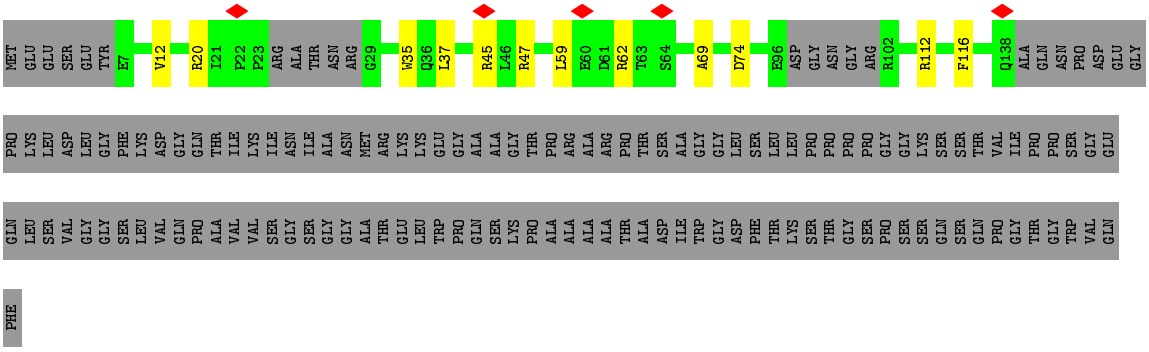


• Molecule 4: AP-2 complex subunit sigma

Chain S:

• Molecule 5: Adaptin ear-binding coat-associated protein 2

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT	Depositor
Number of particles used	71571, 71571	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	1	Depositor
Minimum defocus (nm)	600.00	Depositor
Maximum defocus (nm)	2500.00	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.175	Depositor
Minimum map value	-0.091	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	348.0, 348.0, 348.0	Depositor
Map dimensions	300, 300, 300	Depositor
Map angles (°)	90.0, 90.0, 90.0	Depositor
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.37	0/4584	0.50	0/6216
2	B	0.39	0/4509	0.55	0/6109
3	M	0.52	0/3216	0.58	1/4332 (0.0%)
4	S	0.52	0/1214	0.60	0/1638
5	N	0.44	0/996	0.63	1/1346 (0.1%)
All	All	0.43	0/14519	0.55	2/19641 (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
4	S	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	N	74	ASP	CB-CG-OD1	8.52	125.97	118.30
3	M	282	ASP	CB-CG-OD1	5.25	123.03	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	S	53	ARG	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	4505	0	4596	32	0
2	B	4443	0	4559	33	0
3	M	3166	0	3235	38	0
4	S	1190	0	1189	11	0
5	N	972	0	933	8	0
All	All	14276	0	14512	111	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 4.

All (111) 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)
4:S:57:ILE:HD11	4:S:68:CYS:HB3	1.75	0.67
3:M:199:ARG:NH1	3:M:273:GLU:OE2	2.28	0.64
3:M:156:TPO:O1P	5:N:112:ARG:NH2	2.31	0.63
3:M:253:ARG:CB	5:N:112:ARG:NH1	2.64	0.60
4:S:18:LYS:NZ	4:S:115:ASP:OD1	2.33	0.60
1:A:232:ARG:HE	1:A:235:ARG:HH21	1.48	0.60
2:B:127:ARG:NH2	2:B:157:GLU:OE2	2.35	0.59
3:M:30:ASP:OD1	3:M:33:ARG:NH1	2.35	0.59
1:A:259:VAL:HG13	1:A:312:GLU:HG3	1.84	0.59
3:M:301:LEU:HB3	3:M:370:ILE:HB	1.85	0.58
2:B:58:MET:HG2	2:B:90:SER:HB2	1.85	0.57
3:M:6:PHE:HB2	3:M:66:ALA:HB3	1.86	0.57
2:B:97:ASP:O	2:B:103:ARG:NH1	2.35	0.57
3:M:42:GLN:NE2	3:M:43:VAL:O	2.38	0.57
3:M:316:LEU:HD21	3:M:357:ARG:HD2	1.87	0.56
1:A:116:ILE:HG23	1:A:131:ALA:HB1	1.88	0.55
2:B:336:LEU:HD22	2:B:372:LYS:HD3	1.89	0.55
2:B:24:ASN:ND2	2:B:25:GLU:OE1	2.40	0.55
1:A:367:LYS:NZ	1:A:398:ASP:OD2	2.39	0.55
1:A:448:ASN:OD1	1:A:451:ARG:NH2	2.38	0.55
3:M:300:LYS:NZ	3:M:369:GLU:OE2	2.40	0.54
1:A:391:ASP:OD1	1:A:427:LYS:NZ	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:466:LEU:HD12	2:B:491:LEU:HD22	1.90	0.54
5:N:12:VAL:HG22	5:N:47:ARG:HG2	1.89	0.54
1:A:216:GLN:NE2	1:A:267:CYS:SG	2.81	0.54
2:B:63:LEU:HD22	2:B:99:ASN:HD21	1.72	0.54
1:A:107:GLU:OE2	1:A:110:ARG:NH2	2.40	0.54
4:S:93:GLU:OE1	4:S:132:LEU:CD1	2.56	0.54
3:M:321:GLU:OE2	3:M:323:ARG:NH2	2.41	0.54
2:B:375:ARG:NE	2:B:409:GLU:OE2	2.41	0.53
2:B:371:ARG:NH1	2:B:441:GLU:OE2	2.41	0.53
1:A:577:GLN:OE1	2:B:419:ARG:NH2	2.39	0.53
2:B:174:PRO:HB2	2:B:214:CYS:HB3	1.91	0.52
1:A:114:ASN:OD1	1:A:117:LYS:NZ	2.44	0.51
2:B:200:ASN:ND2	2:B:236:GLU:OE2	2.43	0.51
3:M:323:ARG:NH1	3:M:348:GLU:OE2	2.44	0.51
1:A:289:ASN:OD1	1:A:329:ARG:NH2	2.43	0.51
1:A:561:ASP:HA	1:A:564:ARG:HG2	1.92	0.51
1:A:88:TYR:HB2	4:S:141:LEU:HD22	1.93	0.50
1:A:340:HIS:O	1:A:346:ARG:NH1	2.44	0.50
1:A:413:LEU:O	1:A:421:ARG:NH1	2.40	0.50
3:M:174:PHE:HD2	3:M:203:LYS:HD2	1.77	0.50
1:A:271:PRO:HD2	1:A:277:ARG:HG2	1.95	0.49
4:S:13:LYS:HE2	4:S:15:ARG:HH12	1.77	0.49
5:N:45:ARG:NH2	5:N:62:ARG:O	2.39	0.49
1:A:33:ILE:HD12	1:A:65:ILE:HG12	1.95	0.49
3:M:93:PHE:HE1	3:M:107:LEU:HD23	1.77	0.49
3:M:253:ARG:CB	5:N:112:ARG:HH11	2.24	0.49
4:S:54:ASN:OD1	4:S:54:ASN:N	2.46	0.49
2:B:248:LEU:HD13	2:B:287:PRO:HG3	1.95	0.48
3:M:170:ARG:HH11	3:M:419:ILE:HD12	1.78	0.48
3:M:115:ILE:HD11	3:M:129:LEU:HD11	1.95	0.48
1:A:518:SER:HB3	1:A:521:ILE:HD13	1.95	0.48
3:M:36:VAL:O	3:M:44:ARG:NH1	2.33	0.48
2:B:115:VAL:HG12	2:B:117:LYS:H	1.78	0.48
1:A:21:ARG:NH2	2:B:14:GLU:OE1	2.45	0.48
1:A:514:ASP:HB3	1:A:517:SER:HB3	1.96	0.47
3:M:56:PHE:HB2	3:M:67:ALA:HB3	1.96	0.47
1:A:179:SER:OG	1:A:181:ASP:OD1	2.33	0.47
1:A:371:GLU:O	1:A:375:ASN:ND2	2.47	0.47
2:B:411:ILE:HG21	2:B:448:MET:HG2	1.97	0.47
4:S:6:LEU:HB2	4:S:68:CYS:HB2	1.97	0.47
2:B:475:ASP:O	3:M:357:ARG:NH2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:GLY:O	1:A:281:THR:OG1	2.32	0.46
3:M:39:ALA:HB1	3:M:42:GLN:HB3	1.97	0.46
3:M:99:GLU:O	3:M:103:ASN:ND2	2.48	0.46
3:M:18:ARG:NH1	3:M:113:ASP:OD1	2.49	0.46
2:B:117:LYS:NZ	2:B:121:TYR:OH	2.48	0.46
3:M:5:LEU:HD11	3:M:81:PHE:HE2	1.81	0.45
2:B:9:THR:OG1	2:B:12:LYS:O	2.33	0.45
3:M:174:PHE:HB2	3:M:203:LYS:HB3	1.99	0.45
5:N:59:LEU:HD12	5:N:69:ALA:HB3	1.98	0.45
1:A:166:GLN:NE2	4:S:125:GLU:OE1	2.48	0.45
1:A:103:ASN:HD22	1:A:104:SER:H	1.65	0.44
2:B:250:HIS:CD2	2:B:252:ASN:H	2.36	0.44
2:B:522:ARG:NH2	2:B:526:TYR:OH	2.51	0.44
2:B:67:LYS:NZ	3:M:134:THR:HG23	2.33	0.44
2:B:399:ILE:HA	2:B:407:VAL:HG22	1.99	0.43
2:B:557:PRO:HA	2:B:560:LEU:HB3	1.99	0.43
3:M:408:GLU:HG2	3:M:411:LEU:HB2	2.00	0.43
4:S:116:GLU:HG2	4:S:131:VAL:HG13	2.01	0.43
2:B:124:GLU:HG3	2:B:128:LYS:NZ	2.34	0.43
3:M:291:PRO:HB3	3:M:386:ILE:HD12	2.00	0.43
4:S:93:GLU:OE1	4:S:132:LEU:HD11	2.19	0.43
1:A:246:ASP:N	1:A:246:ASP:OD1	2.46	0.43
2:B:201:PRO:HB2	2:B:202:GLN:OE1	2.19	0.42
1:A:474:ASP:OD1	1:A:474:ASP:N	2.51	0.42
3:M:179:GLU:HG3	3:M:396:PRO:HD2	2.01	0.42
2:B:110:MET:HB3	2:B:122:LEU:HD11	2.02	0.42
2:B:132:ASP:O	2:B:138:ARG:NH1	2.41	0.41
2:B:344:ARG:NH2	2:B:553:ASP:O	2.48	0.41
5:N:112:ARG:O	5:N:116:PHE:N	2.54	0.41
1:A:374:ILE:HD13	1:A:408:GLU:HG3	2.02	0.41
2:B:350:ASN:HB2	2:B:353:GLN:HE21	1.85	0.41
5:N:35:TRP:HB2	5:N:37:LEU:HD23	2.03	0.41
2:B:67:LYS:HZ3	3:M:134:THR:HG23	1.85	0.41
3:M:162:ARG:NH1	3:M:267:PRO:O	2.54	0.41
4:S:5:ILE:HG12	4:S:69:ILE:HG12	2.02	0.41
1:A:357:ALA:O	1:A:363:HIS:ND1	2.50	0.41
2:B:123:CYS:SG	2:B:124:GLU:N	2.94	0.41
1:A:356:LEU:O	1:A:362:SER:OG	2.39	0.40
1:A:435:TYR:OH	3:M:294:ARG:NH1	2.53	0.40
3:M:293:VAL:HG22	3:M:303:VAL:HG13	2.03	0.40
2:B:503:VAL:HA	2:B:506:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:330:THR:HG23	3:M:370:ILE:HG23	2.04	0.40
3:M:50:ILE:HD11	3:M:55:PHE:HE2	1.85	0.40
3:M:313:PRO:HG3	3:M:361:MET:HB2	2.02	0.40
1:A:181:ASP:OD1	1:A:181:ASP:N	2.55	0.40
3:M:252:VAL:HG13	3:M:263:ILE:HG23	2.02	0.40
3:M:299:THR:HG22	3:M:374:PRO:HG3	2.04	0.40
3:M:383:ARG:HB3	3:M:435:CYS:HB3	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	563/621 (91%)	558 (99%)	5 (1%)	0	100	100
2	B	549/591 (93%)	528 (96%)	19 (4%)	2 (0%)	34	69
3	M	384/435 (88%)	363 (94%)	20 (5%)	1 (0%)	41	74
4	S	139/142 (98%)	131 (94%)	8 (6%)	0	100	100
5	N	116/266 (44%)	109 (94%)	7 (6%)	0	100	100
All	All	1751/2055 (85%)	1689 (96%)	59 (3%)	3 (0%)	50	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	123	CYS
3	M	155	VAL
2	B	124	GLU

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	500/543 (92%)	498 (100%)	2 (0%)	91 95
2	B	502/532 (94%)	500 (100%)	2 (0%)	91 95
3	M	346/386 (90%)	346 (100%)	0	100 100
4	S	130/131 (99%)	128 (98%)	2 (2%)	65 85
5	N	101/212 (48%)	100 (99%)	1 (1%)	76 90
All	All	1579/1804 (88%)	1572 (100%)	7 (0%)	91 95

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	381	ARG
2	B	24	ASN
2	B	29	LYS
4	S	55	PHE
4	S	61	ARG
5	N	20	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	216	GLN
1	A	307	ASN
1	A	524	ASN
2	B	99	ASN
2	B	179	ASN
2	B	252	ASN
2	B	500	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

1 non-standard protein/DNA/RNA residue 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	$\#\|Z\| > 2$
3	TPO	M	156	3	8,10,11	1.67	1 (12%)	10,14,16	1.28	1 (10%)

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
3	TPO	M	156	3	-	1/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	156	TPO	P-O1P	3.46	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	156	TPO	CG2-CB-CA	-2.78	107.69	113.16

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	156	TPO	CG2-CB-OG1-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	156	TPO	1	0

5.5 Carbohydrates (i)

There are no carbohydrates 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.

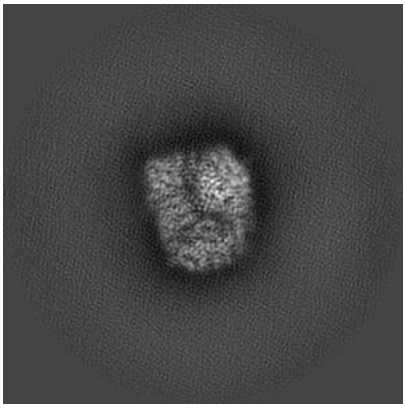
5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

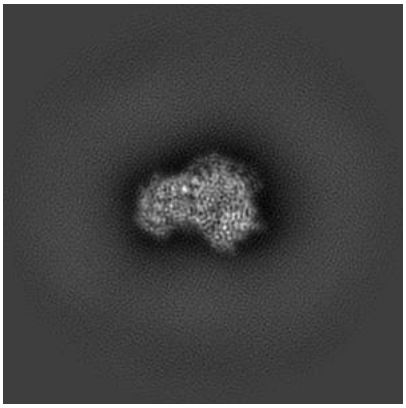
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20215. These are intended to permit visual inspection of the internal detail of the map and identification of artifacts.

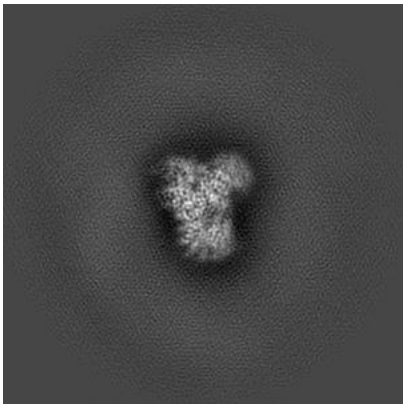
6.1 Orthogonal projections



X



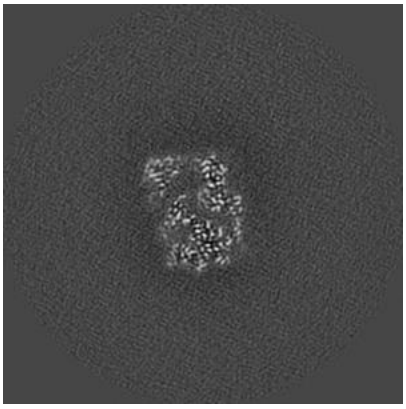
Y



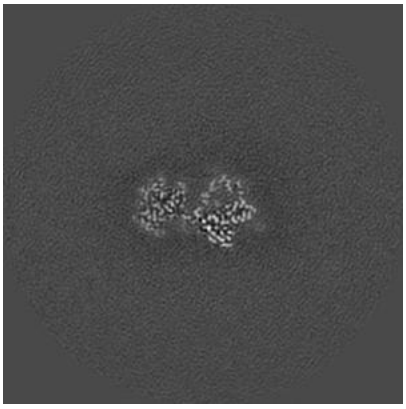
Z

The images above show the map projected in three orthogonal projections, in greyscale.

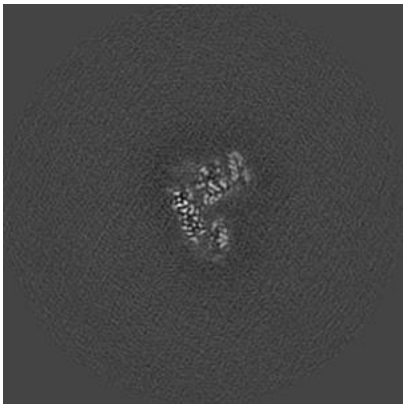
6.2 Central slices



X



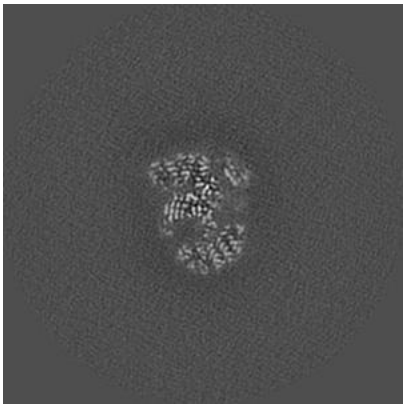
Y



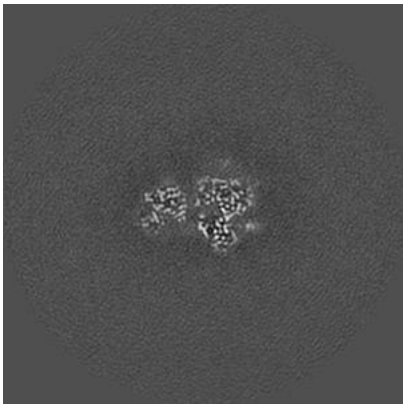
Z

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

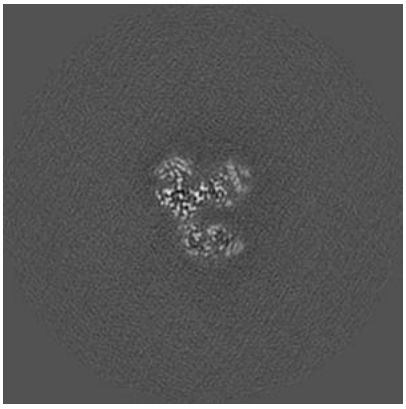
6.3 Largest variance slices (i)



X Index: 139



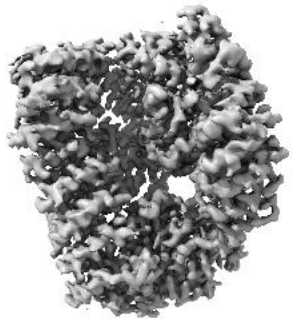
Y Index: 157



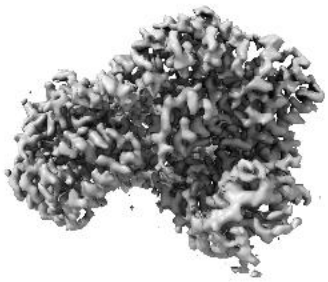
Z Index: 165

The images above show the highest variance slices of the map in three orthogonal directions, in greyscale.

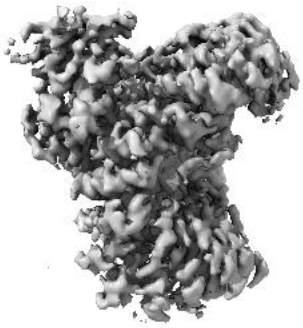
6.4 Orthogonal surface views (i)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. This in conjunction with the slice images can indicate whether an appropriate contour level has been selected.

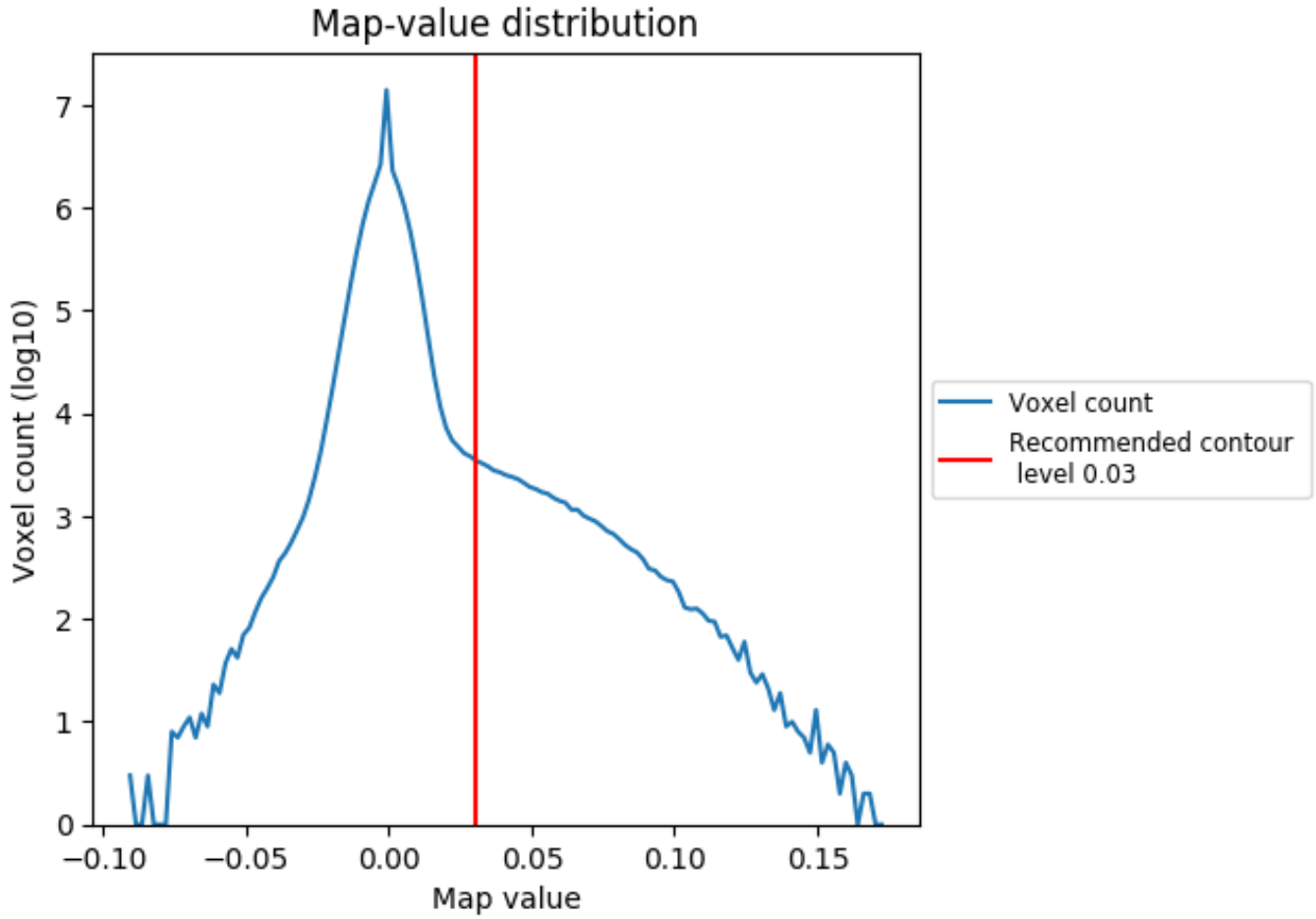
6.5 Mask visualisation (i)

This section was not generated. No masks were provided.

7 Map analysis

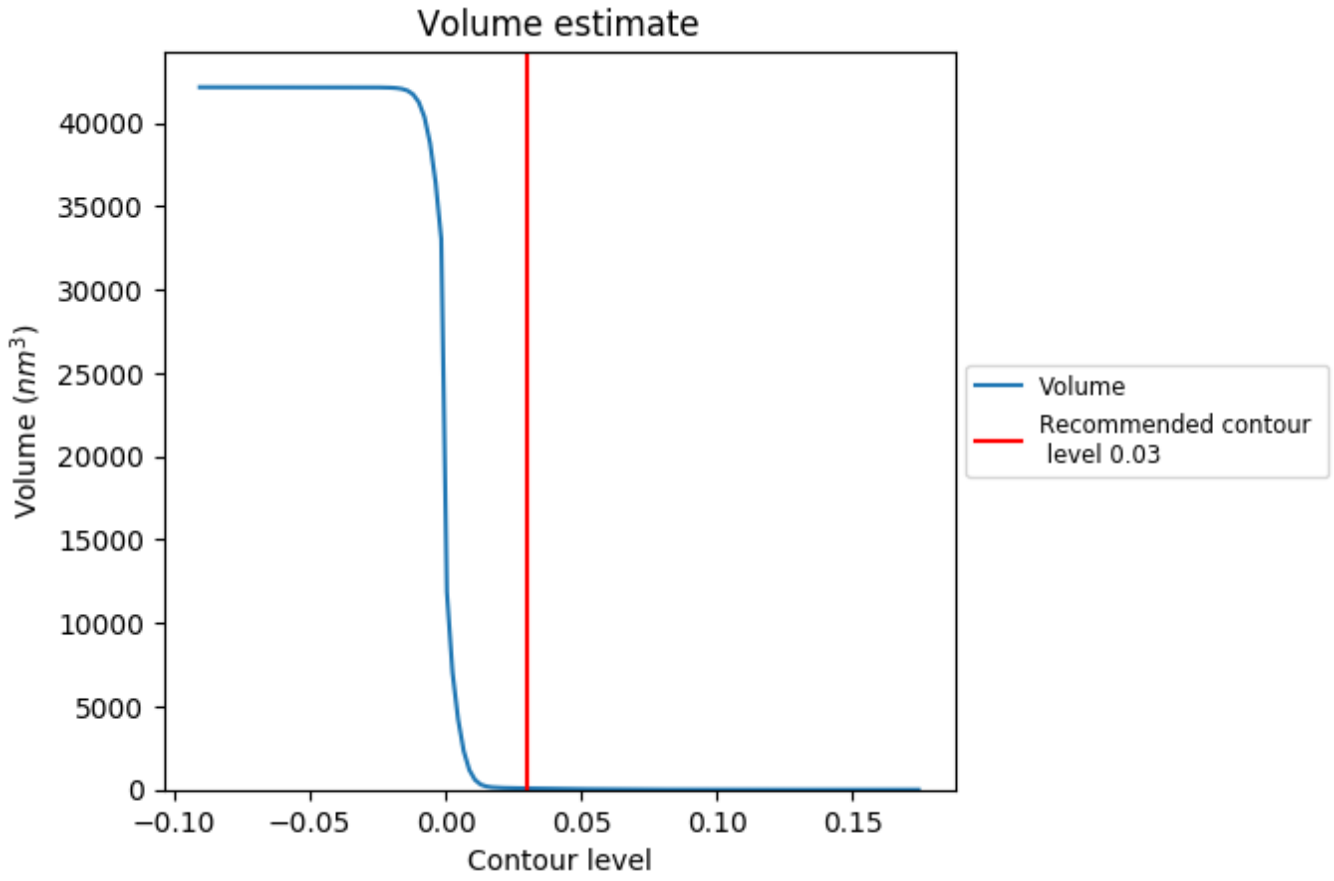
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

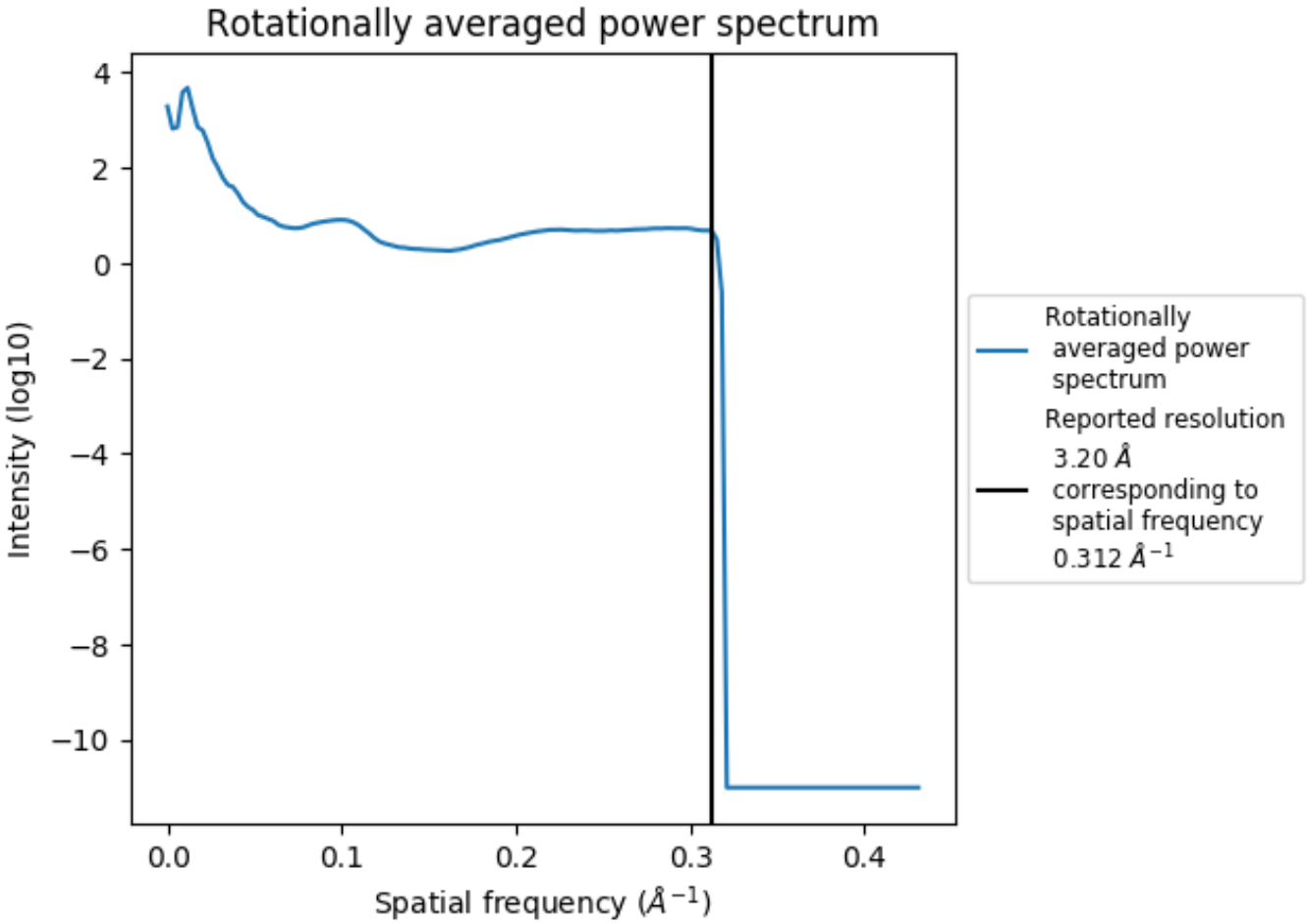
7.2 Volume estimate



The volume at the recommended contour level is 77 nm^3; this corresponds to an approximate mass of 70 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)



8 Fourier-Shell correlation

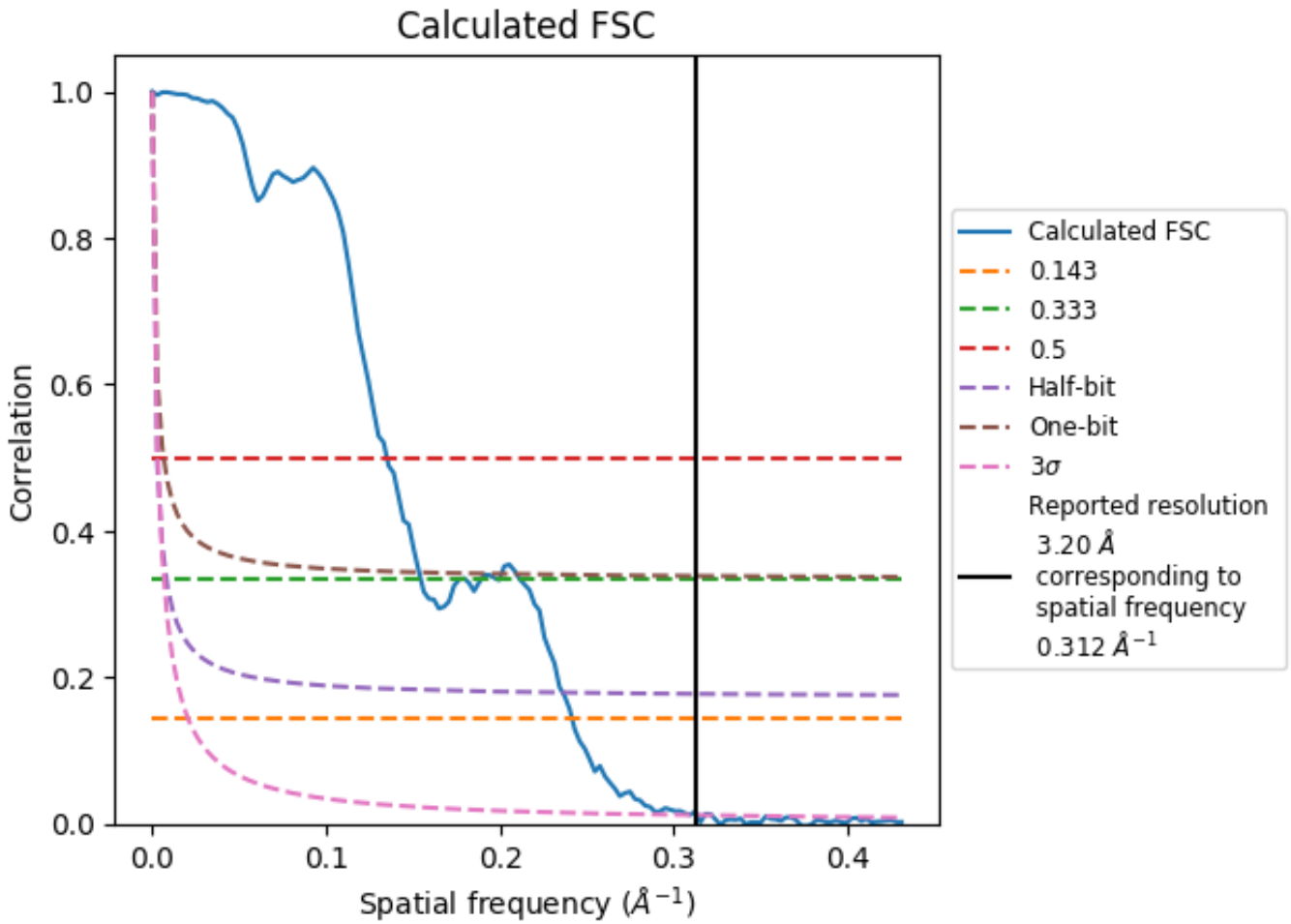
Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution for single-particle and subtomogram-averaging methods. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. Curves are displayed for 3σ, 1-bit and 1/2-bit in addition to lines showing the 0.143 gold standard cut-off, 0.333 cut-off and legacy 0.5 cut-off.

8.1 Resolution estimates

These are global values for the map.

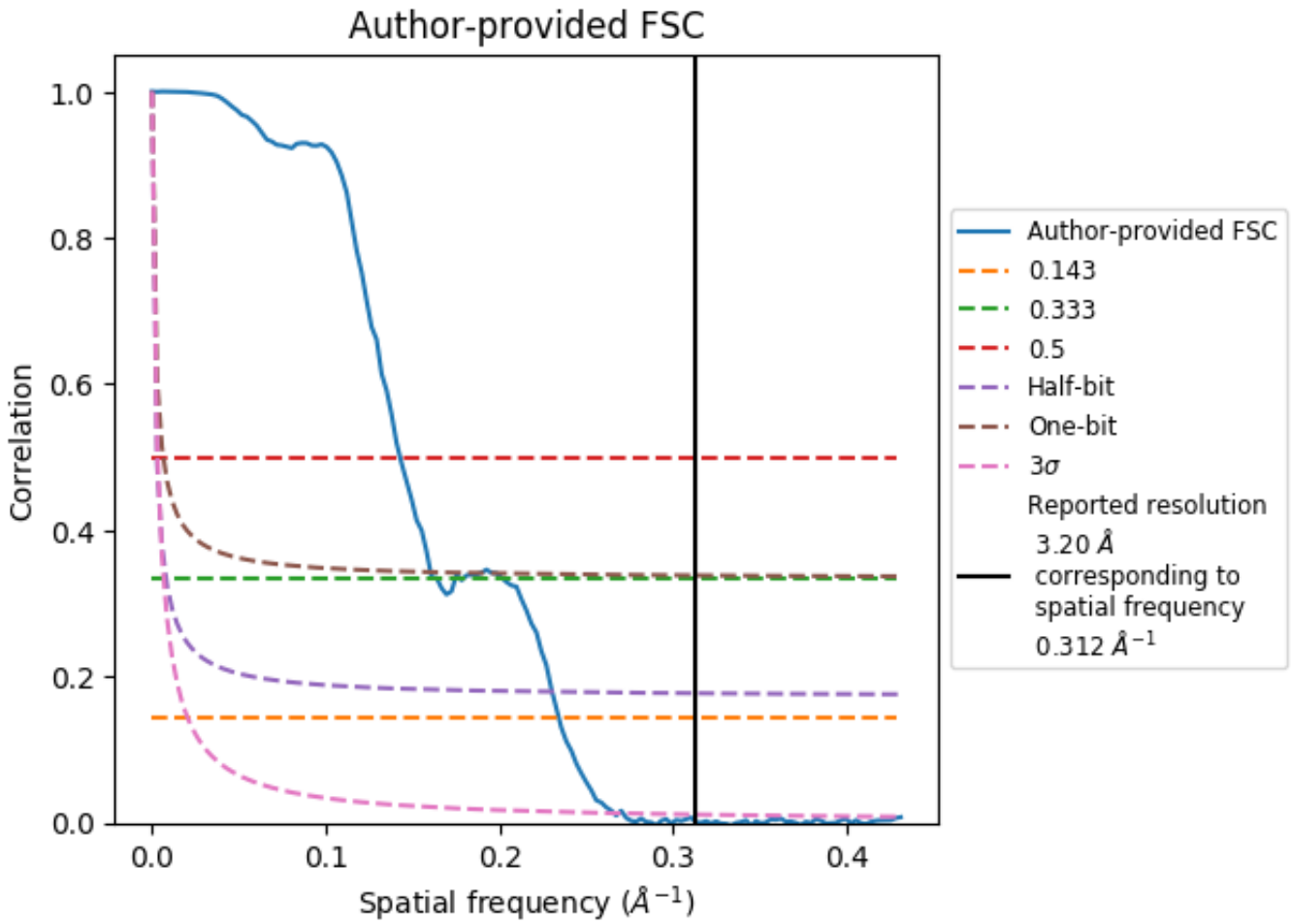
Source	Criterion	Resolution estimate (Å)
Reported value	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	3.20
Calculated FSC	FSC 0.5 CUT-OFF	7.41
Calculated FSC	FSC 1 BIT CUT-OFF	6.64
Calculated FSC	FSC 0.33 CUT-OFF	6.47
Calculated FSC	FSC 1/2 BIT CUT-OFF	4.29
Calculated FSC	FSC 0.143 CUT-OFF	4.14
Calculated FSC	FSC 3 SIGMA CUT-OFF	3.22
Author-provided FSC	FSC 0.5 CUT-OFF	7.15
Author-provided FSC	FSC 1 BIT CUT-OFF	6.35
Author-provided FSC	FSC 0.33 CUT-OFF	6.20
Author-provided FSC	FSC 1/2 BIT CUT-OFF	4.40
Author-provided FSC	FSC 0.143 CUT-OFF	4.32
Author-provided FSC	FSC 3 SIGMA CUT-OFF	3.80

8.2 Calculated FSC



This FSC information has been calculated from the half-maps provided by the depositor. As we request un-masked, un-processed half-maps the curve may be significantly different to the author-provided FSC.

8.3 Author-provided FSC (i)

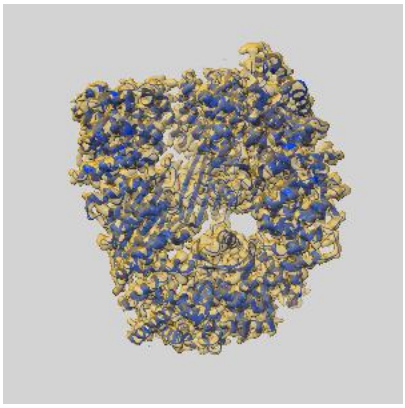


This FSC information was provided by the depositor.

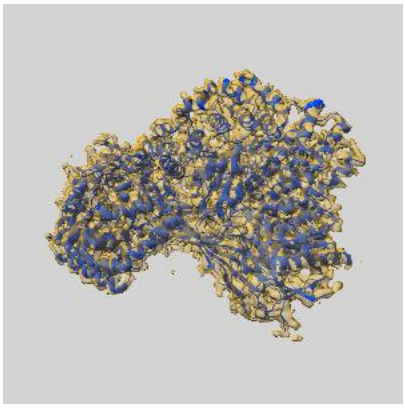
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20215 and PDB model 6OWO. Per-residue inclusion information can be found in section 3 on page 4.

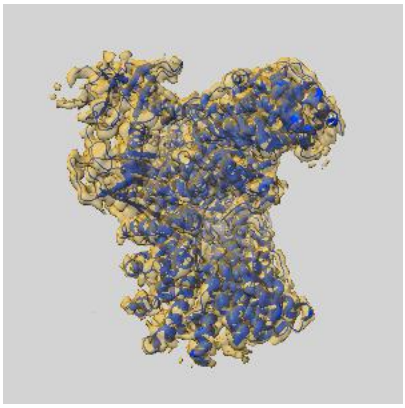
9.1 Map-model overlay



X



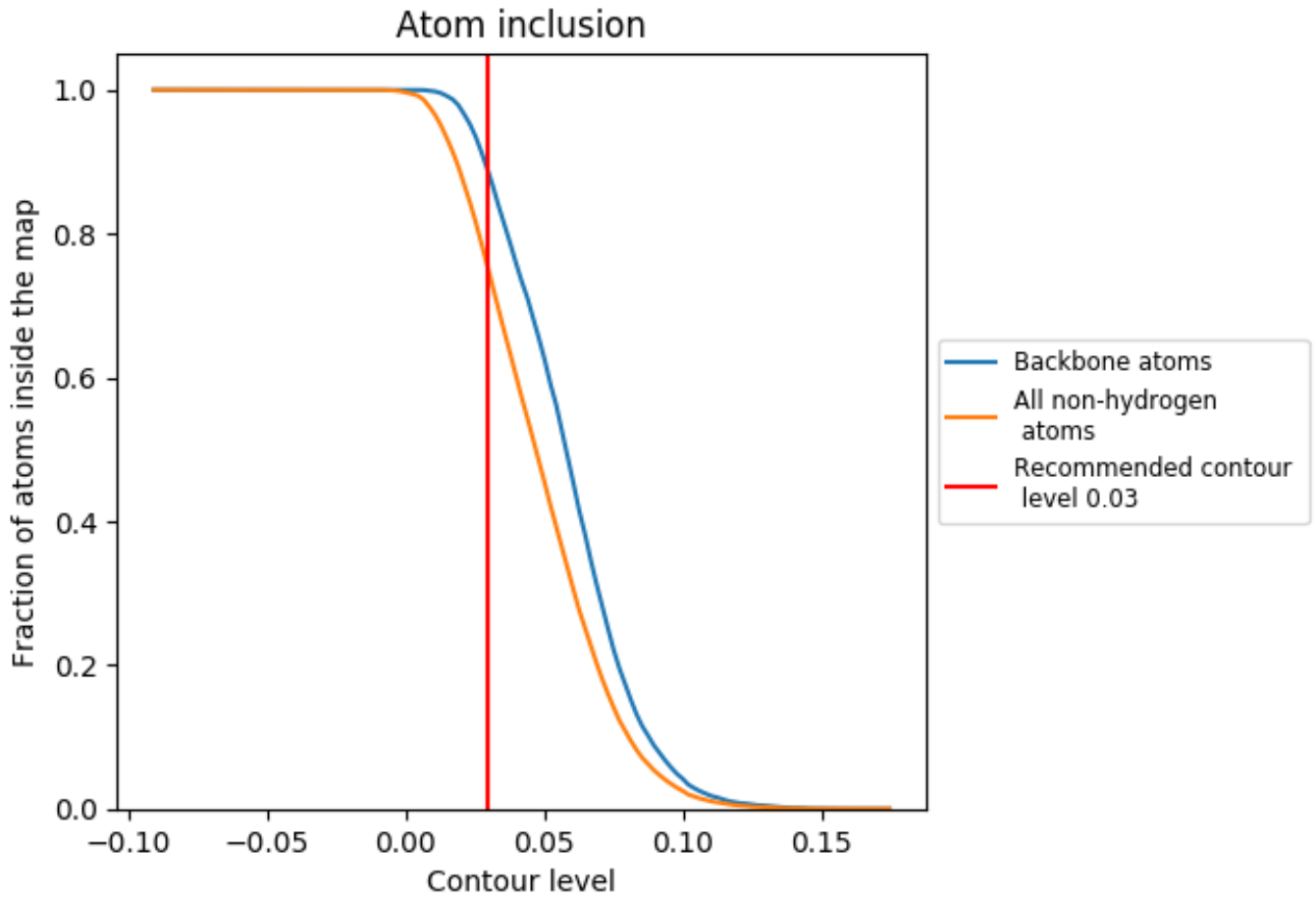
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.