



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 10:24 AM UTC

PDB ID : 7QO1 / pdb_00007qo1
EMDB ID : EMD-14080
Title : complex of DNA ligase I and FEN1 on PCNA and DNA
Authors : Blair, K.; Tehseen, M.; Raducanu, V.S.; Shahid, T.; Lancey, C.; Cruehet, R.;
Hamdan, S.; De Biasio, A.
Deposited on : 2021-12-23
Resolution : 4.40 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

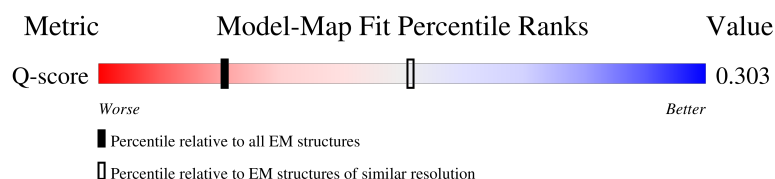
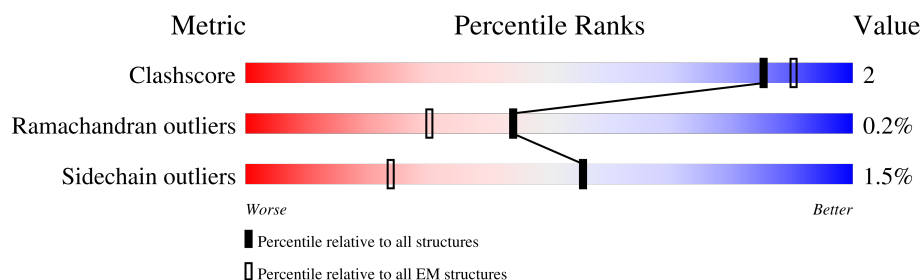
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	760	
2	B	264	
2	F	264	
2	G	264	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	19	47% 37% 16%
4	I	13	31% 31% 31% 8%
5	J	32	6% 59% 34% • •
6	Y	380	24% 74% 5% 21%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 14179 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 DNA ligase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	640	Total	C	N	O	S	0	0
			4960	3146	865	933	16		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	160	CYS	-	expression tag	UNP P18858

- Molecule 2 is a protein called Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	255	Total	C	N	O	S	0	0
			1930	1214	317	383	16		
2	F	252	Total	C	N	O	S	0	0
			1925	1211	315	383	16		
2	G	246	Total	C	N	O	S	0	0
			1873	1182	304	371	16		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P12004
B	-1	PRO	-	expression tag	UNP P12004
B	0	HIS	-	expression tag	UNP P12004
F	-2	GLY	-	expression tag	UNP P12004
F	-1	PRO	-	expression tag	UNP P12004
F	0	HIS	-	expression tag	UNP P12004
G	-2	GLY	-	expression tag	UNP P12004
G	-1	PRO	-	expression tag	UNP P12004
G	0	HIS	-	expression tag	UNP P12004

- Molecule 3 is a DNA chain called Oligo19ddC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	19	Total	C	N	O	P	0	0
			387	185	64	119	19		

- Molecule 4 is a DNA chain called Oligo13P.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	12	Total	C	N	O	P	0	0
			248	117	48	71	12		

- Molecule 5 is a DNA chain called Oligo32.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	31	Total	C	N	O	P	0	0
			635	300	123	181	31		

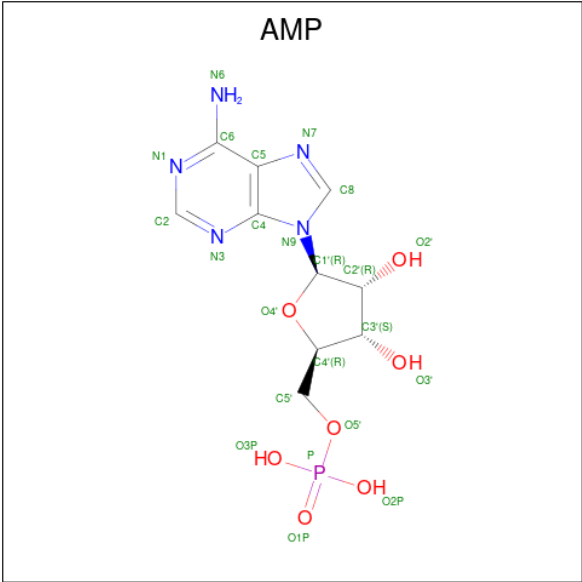
- Molecule 6 is a protein called Flap endonuclease 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Y	301	Total	C	N	O	S	0	0
			2198	1380	378	427	13		

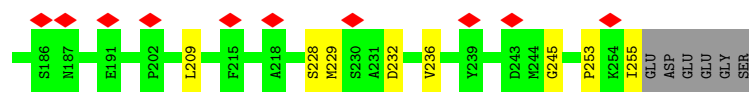
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	181	ALA	ASP	engineered mutation	UNP P39748

- Molecule 7 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P) (labeled as "Ligand of Interest" by depositor).

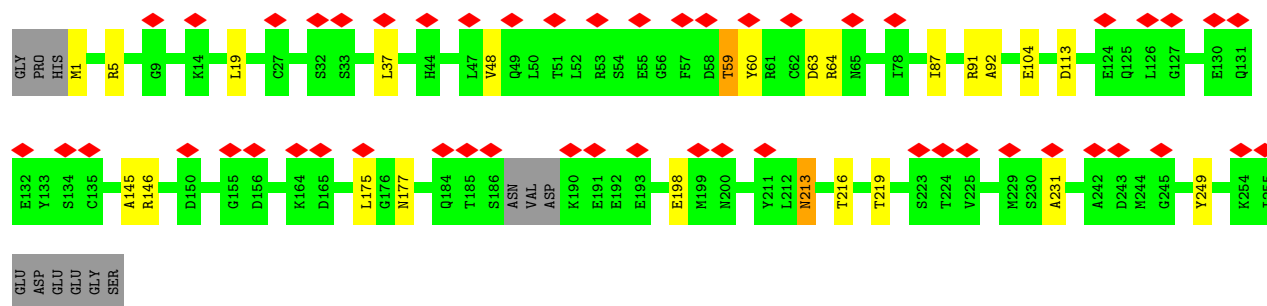


Mol	Chain	Residues	Atoms					AltConf
7	I	1	Total	C	N	O	P	0
			23	10	5	7	1	



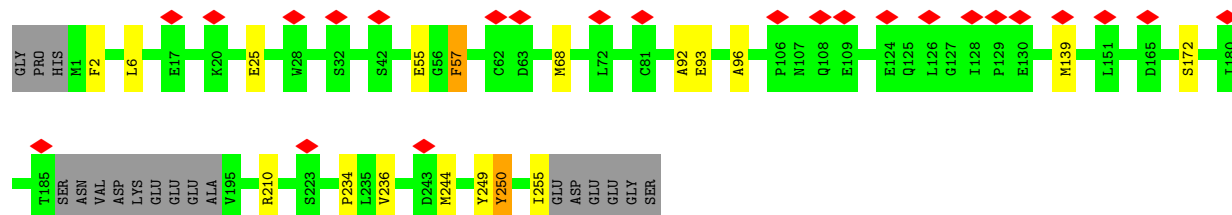
- Molecule 2: Proliferating cell nuclear antigen

Chain F: 19% 86% 8% 5%



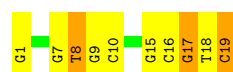
- Molecule 2: Proliferating cell nuclear antigen

Chain G: 9% 86% 6% 7%



- Molecule 3: Oligo19ddC

Chain H: 47% 37% 16%



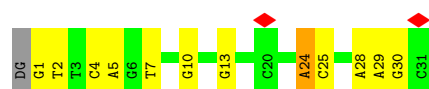
- Molecule 4: Oligo13P

Chain I: 31% 31% 31% 8%

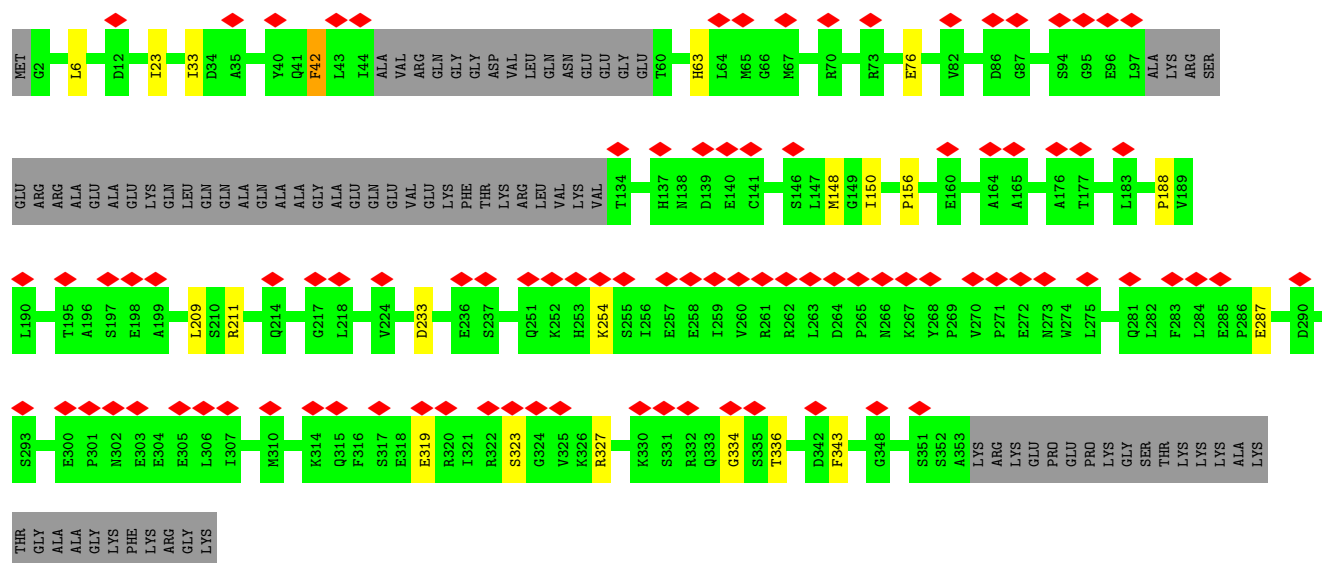


- Molecule 5: Oligo32

Chain J: 6% 59% 34% 1%



Chain Y:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99243	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	18	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.038	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	215.43, 215.43, 215.43	wwPDB
Map dimensions	258, 258, 258	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.75	0/5059	1.30	14/6859 (0.2%)
2	B	0.66	0/1956	1.25	7/2649 (0.3%)
2	F	0.68	0/1950	1.21	3/2635 (0.1%)
2	G	0.65	0/1898	1.23	4/2567 (0.2%)
3	H	0.79	1/411 (0.2%)	1.25	0/633
4	I	0.70	0/278	1.21	1/427 (0.2%)
5	J	0.68	0/713	1.26	0/1097
6	Y	0.73	0/2235	1.30	6/3027 (0.2%)
All	All	0.71	1/14500 (0.0%)	1.27	35/19894 (0.2%)

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
1	A	0	5
2	F	0	3
2	G	0	2
3	H	0	4
4	I	0	4
5	J	0	5
All	All	0	23

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	17	DG	O3'-P	-8.51	1.48	1.61

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Y	42	PHE	CA-CB-CG	7.23	121.03	113.80
2	G	57	PHE	CA-CB-CG	6.63	120.43	113.80
1	A	678	ARG	NE-CZ-NH2	6.56	125.11	119.20
4	I	20	DG	P-O3'-C3'	-6.52	110.42	120.20
2	B	146	ARG	NE-CZ-NH2	6.21	124.79	119.20
1	A	585	LYS	CA-C-N	6.14	131.52	122.99
1	A	585	LYS	C-N-CA	6.14	131.52	122.99
2	G	139	MET	N-CA-C	6.04	113.65	108.22
1	A	774	ARG	NE-CZ-NH2	5.94	124.54	119.20
2	G	172	SER	CA-C-N	5.82	127.35	122.17
2	G	172	SER	C-N-CA	5.82	127.35	122.17
2	B	91	ARG	NE-CZ-NH2	5.73	124.36	119.20
2	B	245	GLY	N-CA-C	5.67	118.79	110.80
2	B	44	HIS	CA-C-N	5.62	128.99	122.35
2	B	44	HIS	C-N-CA	5.62	128.99	122.35
6	Y	233	ASP	CA-CB-CG	5.55	118.15	112.60
2	F	213	ASN	CA-CB-CG	5.54	118.14	112.60
6	Y	211	ARG	NE-CZ-NH2	5.54	124.19	119.20
2	F	113	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	871	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	A	877	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	A	738	ARG	NE-CZ-NH2	5.37	124.03	119.20
6	Y	23	ILE	N-CA-C	5.34	115.97	110.36
2	F	91	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	A	647	ASP	CA-CB-CG	5.23	117.83	112.60
6	Y	323	SER	CA-C-N	5.17	125.67	119.94
6	Y	323	SER	C-N-CA	5.17	125.67	119.94
1	A	801	SER	CA-C-N	5.16	127.15	120.44
1	A	801	SER	C-N-CA	5.16	127.15	120.44
2	B	173	GLY	CA-C-N	5.15	127.44	120.38
2	B	173	GLY	C-N-CA	5.15	127.44	120.38
1	A	791	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	A	839	SER	N-CA-C	5.12	118.79	112.54
1	A	874	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A	274	HIS	CB-CG-CD2	-5.06	124.62	131.20

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	567	TYR	Sidechain
1	A	664	TYR	Sidechain
1	A	768	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	874	ARG	Sidechain
1	A	877	ARG	Sidechain
2	F	146	ARG	Sidechain
2	F	249	TYR	Sidechain
2	F	60	TYR	Sidechain
2	G	249	TYR	Sidechain
2	G	250	TYR	Sidechain
3	H	1	DG	Sidechain
3	H	15	DG	Sidechain
3	H	16	DC	Sidechain
3	H	8	DT	Sidechain
4	I	27	DT	Sidechain
4	I	29	DA	Sidechain
4	I	30	DA	Sidechain
4	I	31	DC	Sidechain
5	J	10	DG	Sidechain
5	J	13	DG	Sidechain
5	J	2	DT	Sidechain
5	J	24	DA	Sidechain
5	J	30	DG	Sidechain

5.2 Too-close contacts

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	4960	0	4994	14	0
2	B	1930	0	1913	9	0
2	F	1925	0	1923	10	0
2	G	1873	0	1875	7	0
3	H	387	0	215	9	0
4	I	248	0	135	9	0
5	J	635	0	346	9	0
6	Y	2198	0	2050	8	0
7	I	23	0	12	3	0
All	All	14179	0	13463	61	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 2.

All (61) 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)
3:H:8:DT:H3	5:J:24:DA:H61	1.23	0.86
1:A:635:PHE:CE1	3:H:19:DOC:H4'	2.34	0.61
3:H:7:DG:H1	5:J:25:DC:H42	1.52	0.57
2:F:175:LEU:H	2:F:175:LEU:HD23	1.70	0.56
3:H:17:DG:H2''	3:H:18:DT:O5'	2.08	0.54
3:H:8:DT:H3	5:J:24:DA:N6	1.99	0.53
4:I:25:DA:H61	5:J:7:DT:H3	1.56	0.53
1:A:566:GLU:HB2	1:A:723:MET:HB3	1.91	0.52
3:H:19:DOC:N4	4:I:20:DG:C8	2.77	0.52
2:G:93:GLU:HB3	2:G:96:ALA:HB2	1.91	0.51
2:B:158:VAL:HG13	2:B:209:LEU:HD21	1.92	0.51
2:G:6:LEU:HD13	2:G:244:MET:HE1	1.91	0.51
1:A:336:ASN:HB2	1:A:450:LEU:HD13	1.93	0.50
6:Y:334:GLY:O	6:Y:336:THR:HG23	2.12	0.50
2:B:133:TYR:CG	2:B:228:SER:HB3	2.48	0.49
4:I:20:DG:P	7:I:100:AMP:H4'	2.53	0.49
2:F:87:ILE:HB	2:F:104:GLU:HB2	1.95	0.48
2:G:255:ILE:O	6:Y:336:THR:HG22	2.13	0.48
2:F:5:ARG:HB3	2:F:59:THR:HB	1.95	0.48
6:Y:188:PRO:HA	6:Y:209:LEU:HB3	1.95	0.47
2:B:1:MET:HA	2:B:93:GLU:HA	1.95	0.47
1:A:540:LEU:HD21	1:A:663:ILE:HG21	1.97	0.47
3:H:8:DT:O2	5:J:24:DA:N1	2.48	0.47
6:Y:76:GLU:HG3	6:Y:327:ARG:HH11	1.80	0.47
2:B:253:PRO:HB2	2:B:255:ILE:HG23	1.97	0.46
4:I:31:DC:C4	5:J:1:DG:O6	2.69	0.46
1:A:744:LYS:NZ	7:I:100:AMP:O3P	2.34	0.46
2:F:213:ASN:O	2:F:216:THR:HG22	2.16	0.46
2:F:63:ASP:CG	2:F:64:ARG:HE	2.24	0.45
1:A:392:LEU:HD21	2:B:45:VAL:HG22	1.99	0.45
2:F:145:ALA:HB2	2:F:219:THR:HG21	1.99	0.45
6:Y:42:PHE:HB3	6:Y:63:HIS:HA	1.98	0.45
2:F:1:MET:HA	2:F:92:ALA:O	2.16	0.45
4:I:31:DC:C2	5:J:1:DG:N1	2.85	0.44
2:F:19:LEU:HD11	2:F:48:VAL:HG21	1.99	0.44
2:B:158:VAL:CG1	2:B:209:LEU:HD21	2.48	0.44
1:A:744:LYS:HZ2	7:I:100:AMP:P	2.40	0.43
1:A:860:GLY:HA2	1:A:864:SER:HA	2.00	0.43
6:Y:148:MET:HG3	6:Y:150:ILE:HG12	2.01	0.43
5:J:28:DA:C6	5:J:29:DA:C6	3.07	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:MET:HA	2:B:229:MET:HE3	2.00	0.43
6:Y:156:PRO:HB2	6:Y:287:GLU:HG3	2.00	0.43
2:G:2:PHE:HB3	2:G:92:ALA:HB3	2.00	0.42
2:B:228:SER:HB2	2:B:236:VAL:HB	2.01	0.42
2:G:236:VAL:HG22	2:G:250:TYR:CE2	2.54	0.42
1:A:291:ALA:O	1:A:295:THR:HG23	2.19	0.42
1:A:295:THR:HG21	1:A:315:LEU:HG	2.01	0.42
1:A:636:GLN:HA	1:A:639:THR:HG22	2.02	0.42
3:H:19:DOC:C4	4:I:20:DG:C8	3.02	0.42
2:F:216:THR:O	2:F:219:THR:HG23	2.19	0.42
5:J:4:DC:H2''	5:J:5:DA:H5'	2.01	0.42
3:H:9:DG:H2''	3:H:10:DC:H5'	2.02	0.42
1:A:616:PHE:CD1	1:A:618:LEU:HD23	2.56	0.41
1:A:783:TYR:CD1	1:A:885:GLU:HA	2.56	0.41
2:B:87:ILE:HB	2:B:104:GLU:HB2	2.02	0.41
2:G:68:MET:HE2	2:G:68:MET:HA	2.03	0.41
2:G:234:PRO:HD3	6:Y:343:PHE:CD2	2.56	0.40
4:I:21:DT:H2''	4:I:22:DC:C6	2.56	0.40
2:F:37:LEU:C	2:F:37:LEU:HD23	2.47	0.40
4:I:29:DA:C5	4:I:30:DA:C6	3.10	0.40
1:A:744:LYS:NZ	4:I:21:DT:OP1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	638/760 (84%)	597 (94%)	41 (6%)	0	100	100
2	B	253/264 (96%)	244 (96%)	9 (4%)	0	100	100
2	F	248/264 (94%)	235 (95%)	12 (5%)	1 (0%)	30	66
2	G	242/264 (92%)	234 (97%)	7 (3%)	1 (0%)	30	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Y	295/380 (78%)	275 (93%)	19 (6%)	1 (0%)	36	71
All	All	1676/1932 (87%)	1585 (95%)	88 (5%)	3 (0%)	44	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	231	ALA
2	G	210	ARG
6	Y	254	LYS

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	533/647 (82%)	524 (98%)	9 (2%)	53	67
2	B	214/230 (93%)	211 (99%)	3 (1%)	59	71
2	F	216/230 (94%)	213 (99%)	3 (1%)	59	71
2	G	211/230 (92%)	208 (99%)	3 (1%)	59	71
6	Y	217/321 (68%)	214 (99%)	3 (1%)	59	71
All	All	1391/1658 (84%)	1370 (98%)	21 (2%)	55	70

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	GLU
1	A	331	LEU
1	A	342	GLN
1	A	365	GLN
1	A	498	GLU
1	A	522	GLU
1	A	549	ARG
1	A	618	LEU
1	A	692	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	61	ARG
2	B	110	LYS
2	B	232	ASP
2	F	59	THR
2	F	177	ASN
2	F	198	GLU
2	G	25	GLU
2	G	55	GLU
2	G	57	PHE
6	Y	6	LEU
6	Y	33	ILE
6	Y	319	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	ASN
1	A	465	GLN
1	A	499	GLN
1	A	636	GLN
1	A	713	GLN
2	B	65	ASN
2	F	44	HIS
2	F	179	ASN
2	G	125	GLN
2	G	177	ASN
2	G	246	HIS
6	Y	21	ASN
6	Y	41	GLN
6	Y	63	HIS
6	Y	222	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	DOC	H	19	3,5	16,19,20	4.44	12 (75%)	20,26,29	1.37	1 (5%)

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	DOC	H	19	3,5	-	2/7/18/19	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	19	DOC	O4'-C4'	8.46	1.61	1.44
3	H	19	DOC	O4'-C1'	-6.64	1.27	1.42
3	H	19	DOC	C2-N3	6.53	1.49	1.36
3	H	19	DOC	C6-C5	6.08	1.49	1.35
3	H	19	DOC	C4-N3	5.18	1.44	1.34
3	H	19	DOC	C4-N4	4.78	1.45	1.33
3	H	19	DOC	C2-N1	4.39	1.49	1.40
3	H	19	DOC	C3'-C4'	-3.84	1.32	1.52
3	H	19	DOC	C6-N1	3.09	1.45	1.38
3	H	19	DOC	C2'-C1'	2.90	1.58	1.52
3	H	19	DOC	O2-C2	-2.72	1.18	1.23
3	H	19	DOC	C5-C4	2.65	1.49	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	19	DOC	C4'-O4'-C1'	-4.68	105.39	109.81

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	19	DOC	O4'-C4'-C5'-O5'
3	H	19	DOC	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	19	DOC	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	AMP	I	100	4	25,25,25	1.71	7 (28%)	37,38,38	2.55	12 (32%)

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	AMP	I	100	4	-	1/10/26/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	100	AMP	C5-N7	-3.98	1.31	1.39
7	I	100	AMP	C6-N6	3.80	1.43	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	100	AMP	C4-N9	-2.98	1.31	1.37
7	I	100	AMP	P-O1P	-2.64	1.42	1.50
7	I	100	AMP	C2-N1	2.64	1.38	1.33
7	I	100	AMP	C5-C6	-2.18	1.34	1.41
7	I	100	AMP	C8-N7	2.12	1.35	1.31

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	100	AMP	C1'-N9-C8	-6.50	112.68	127.09
7	I	100	AMP	N3-C2-N1	-5.48	120.29	128.58
7	I	100	AMP	N6-C6-N1	-5.15	106.91	118.38
7	I	100	AMP	C4-N9-C1'	4.90	138.09	126.63
7	I	100	AMP	N9-C8-N7	-4.83	107.08	113.94
7	I	100	AMP	C5-C4-N3	-4.53	120.48	126.72
7	I	100	AMP	C5-C6-N6	4.05	133.32	123.29
7	I	100	AMP	C4-N9-C8	3.33	109.24	105.74
7	I	100	AMP	C2-N3-C4	3.17	119.56	111.83
7	I	100	AMP	N3-C4-N9	3.07	132.39	127.17
7	I	100	AMP	C5-N7-C8	3.02	108.19	103.45
7	I	100	AMP	C6-C5-C4	2.05	119.98	117.18

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	100	AMP	C4'-C5'-O5'-P

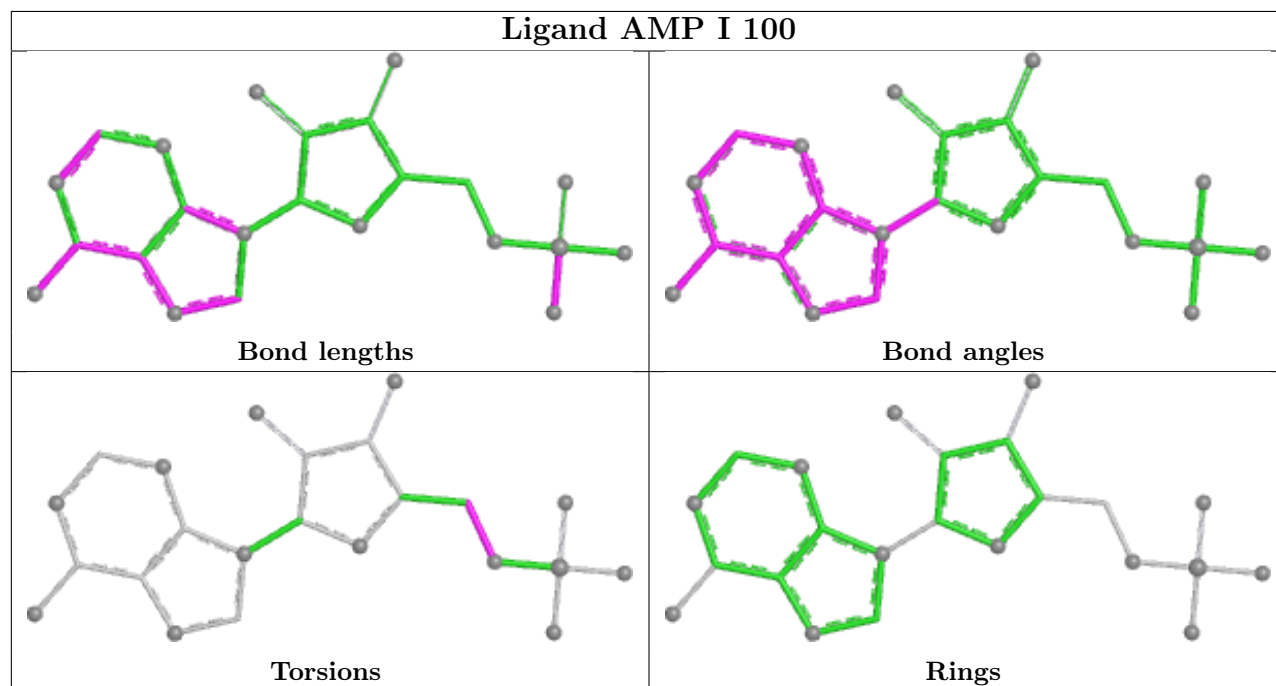
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	100	AMP	3	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 than 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.



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.

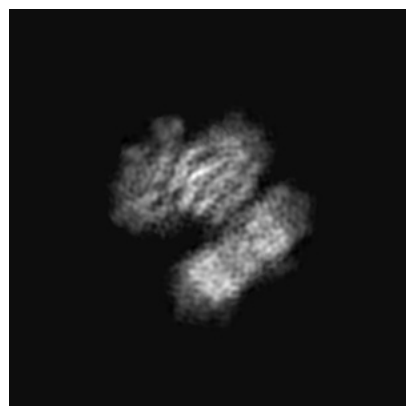
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14080. These allow visual inspection of the internal detail of the map and identification of artifacts.

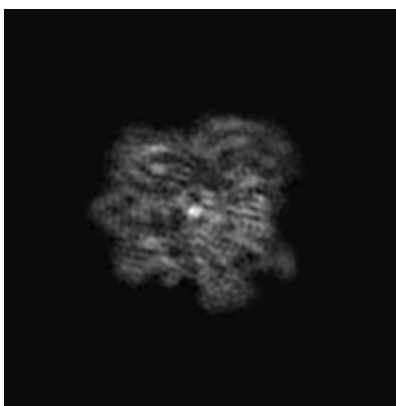
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

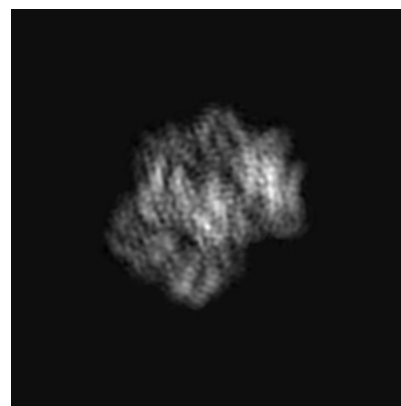
6.1.1 Primary map



X

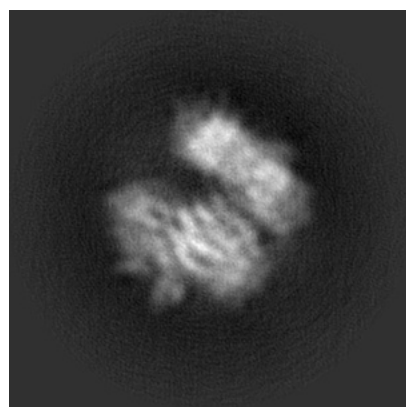


Y

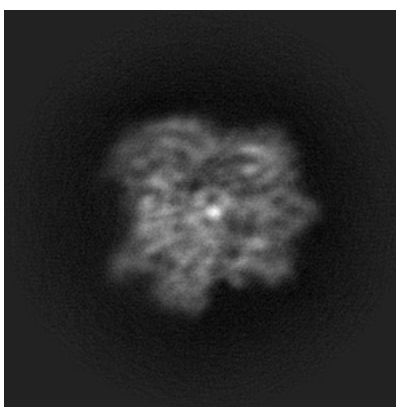


Z

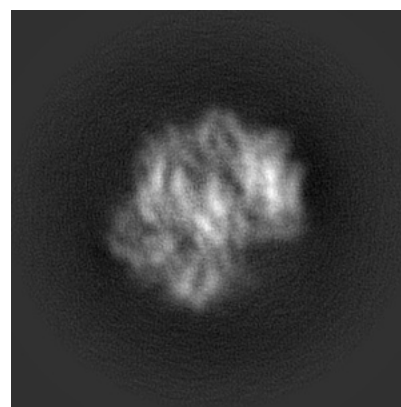
6.1.2 Raw map



X



Y

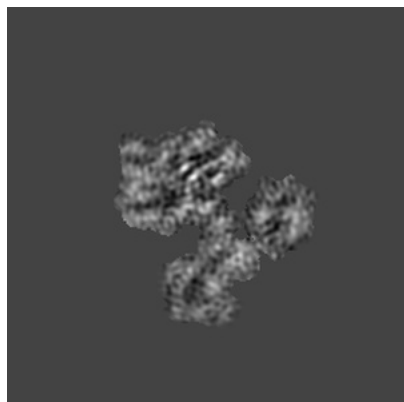


Z

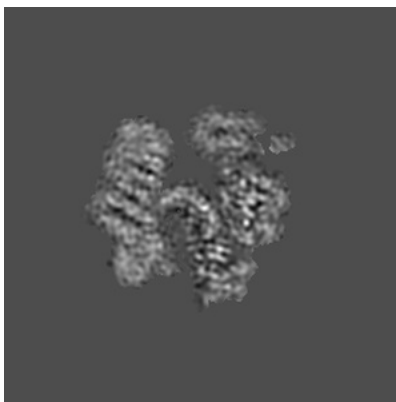
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

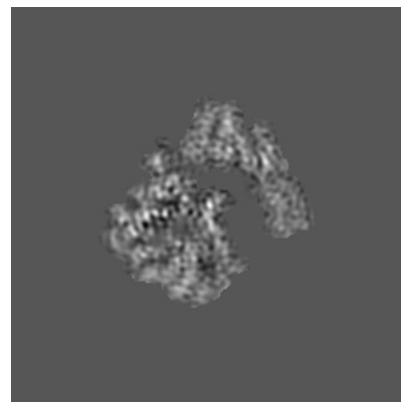
6.2.1 Primary map



X Index: 129

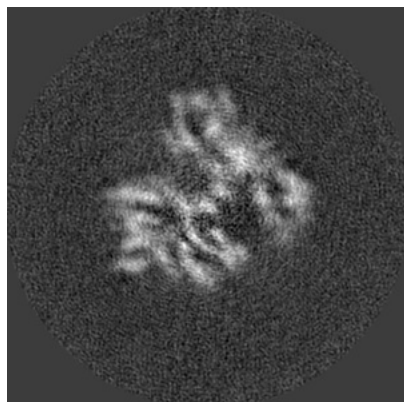


Y Index: 129

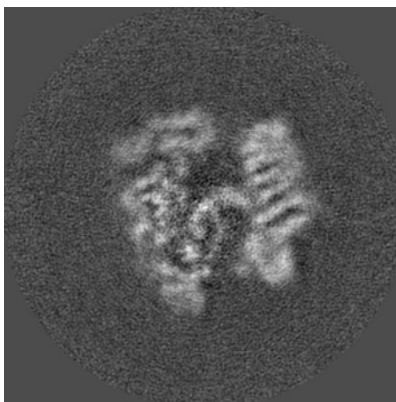


Z Index: 129

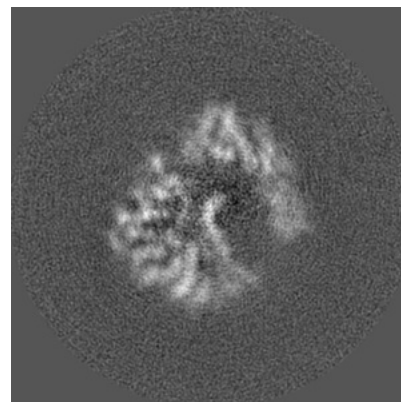
6.2.2 Raw map



X Index: 129



Y Index: 129

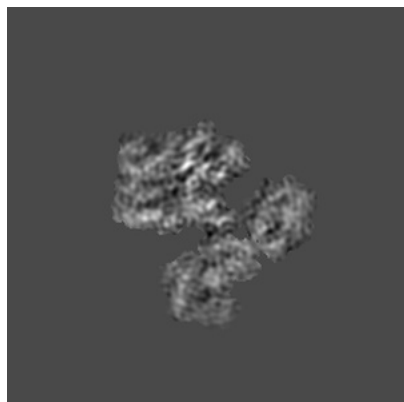


Z Index: 129

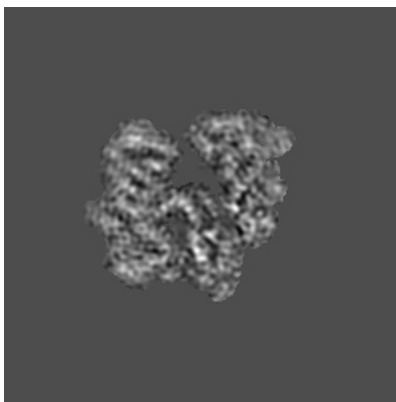
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

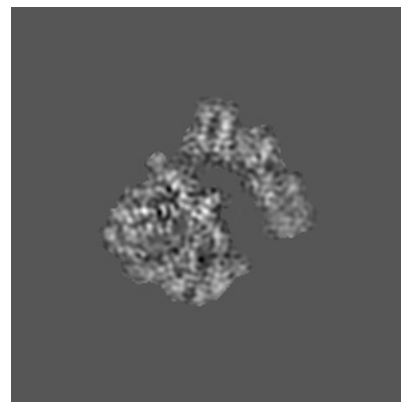
6.3.1 Primary map



X Index: 127

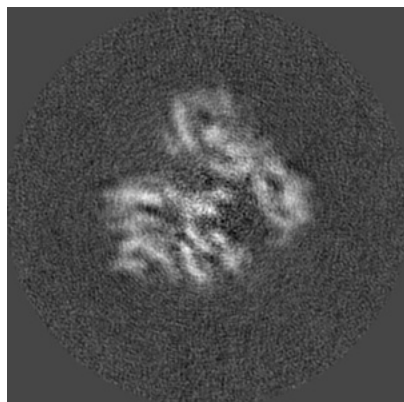


Y Index: 136

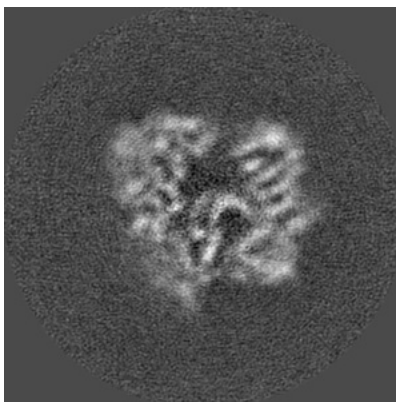


Z Index: 132

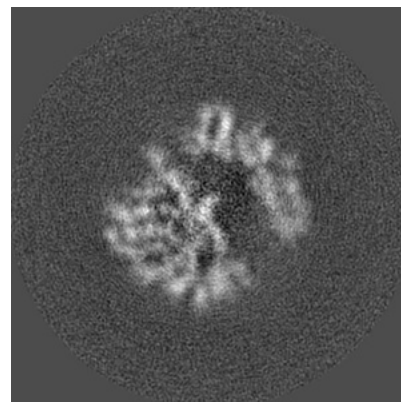
6.3.2 Raw map



X Index: 127



Y Index: 135

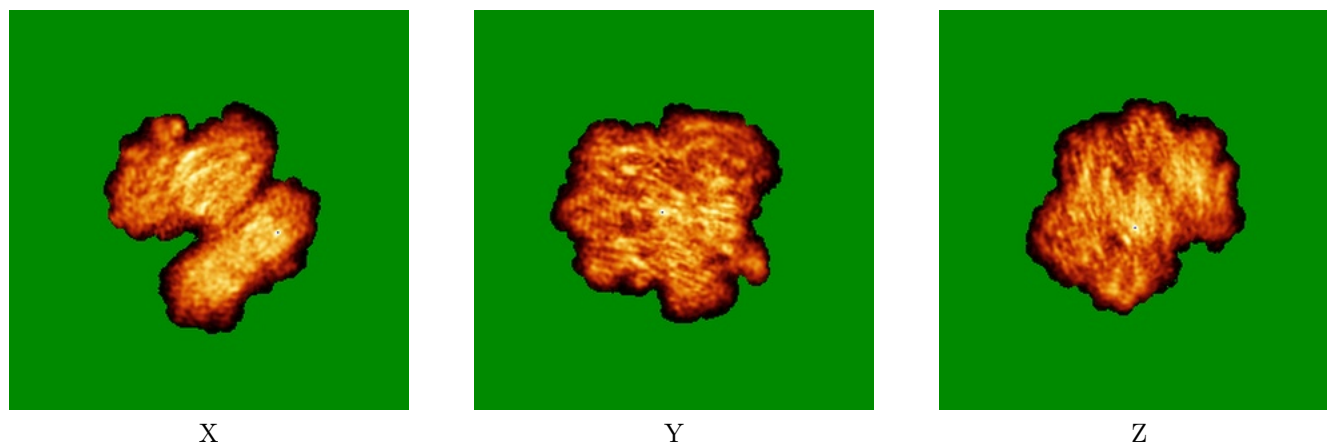


Z Index: 125

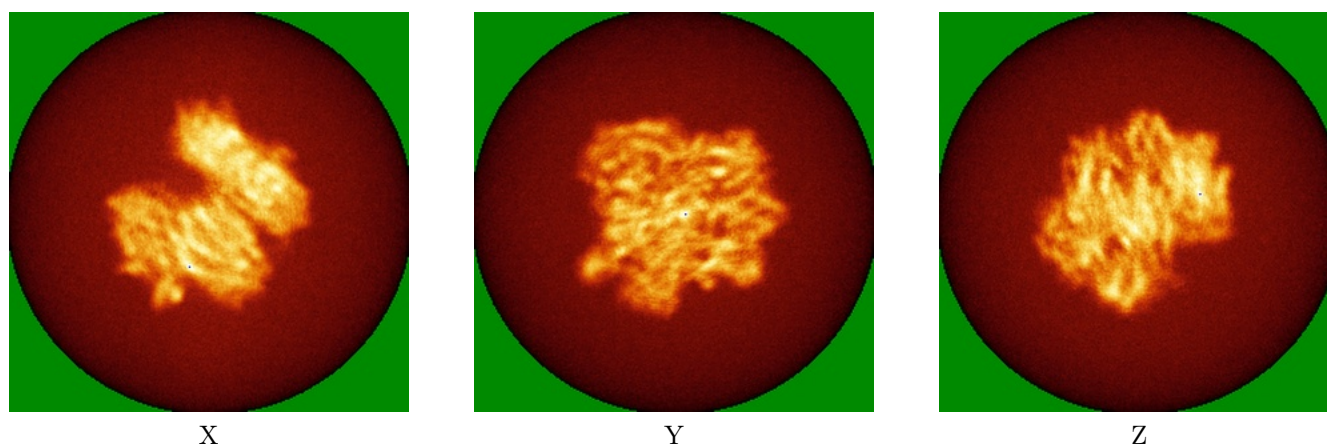
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

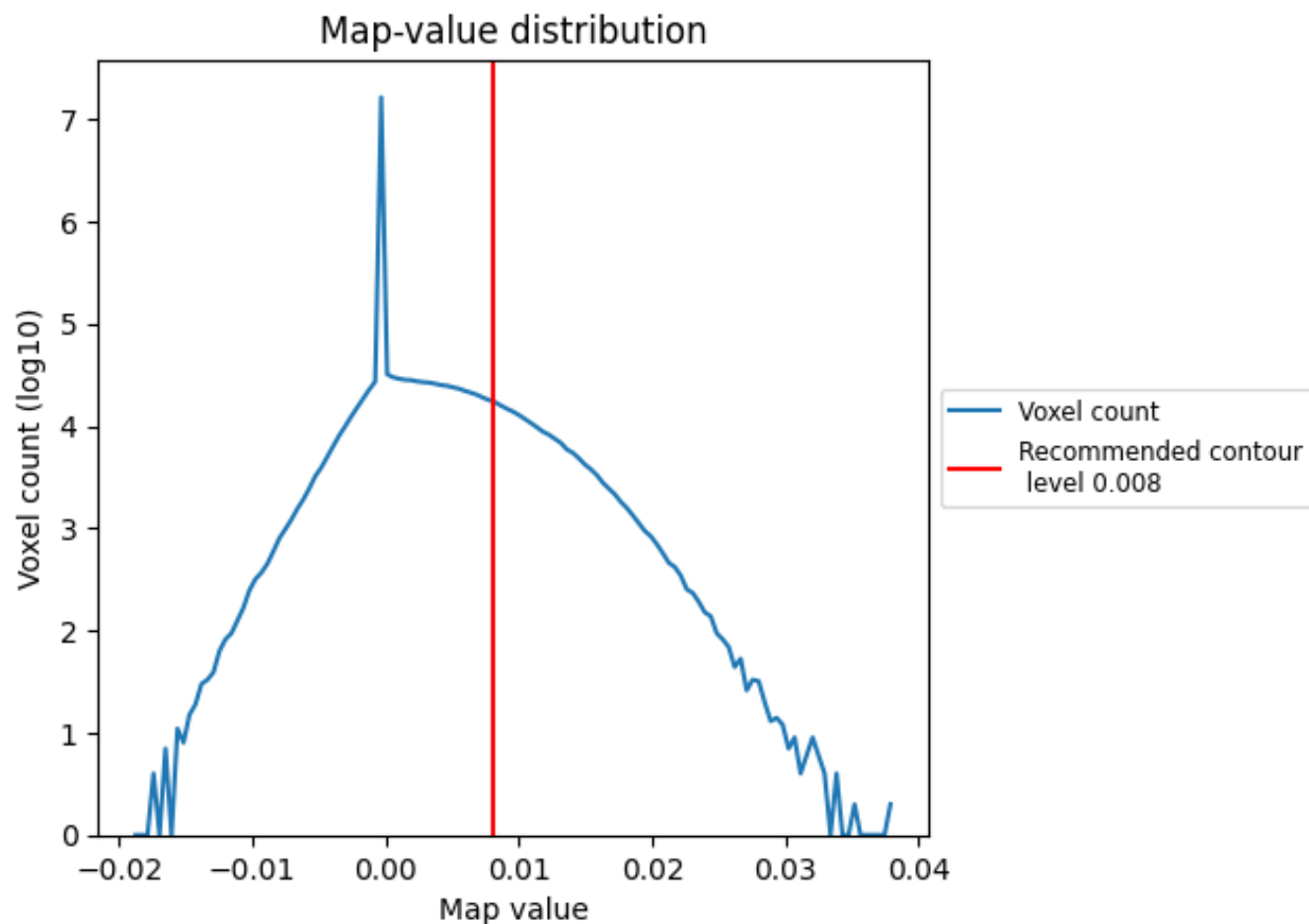
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

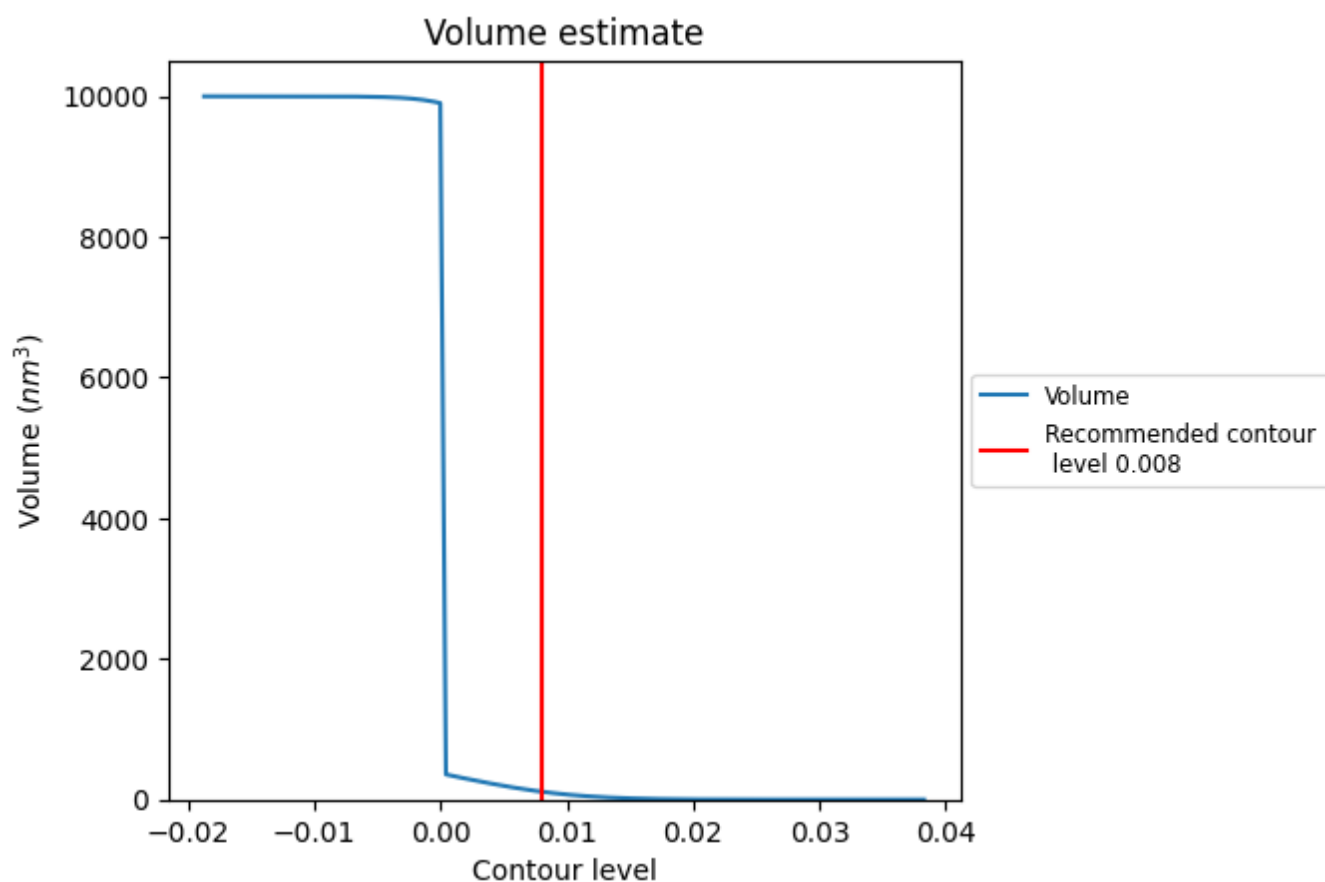
This section contains the results of statistical analysis of the map.

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.

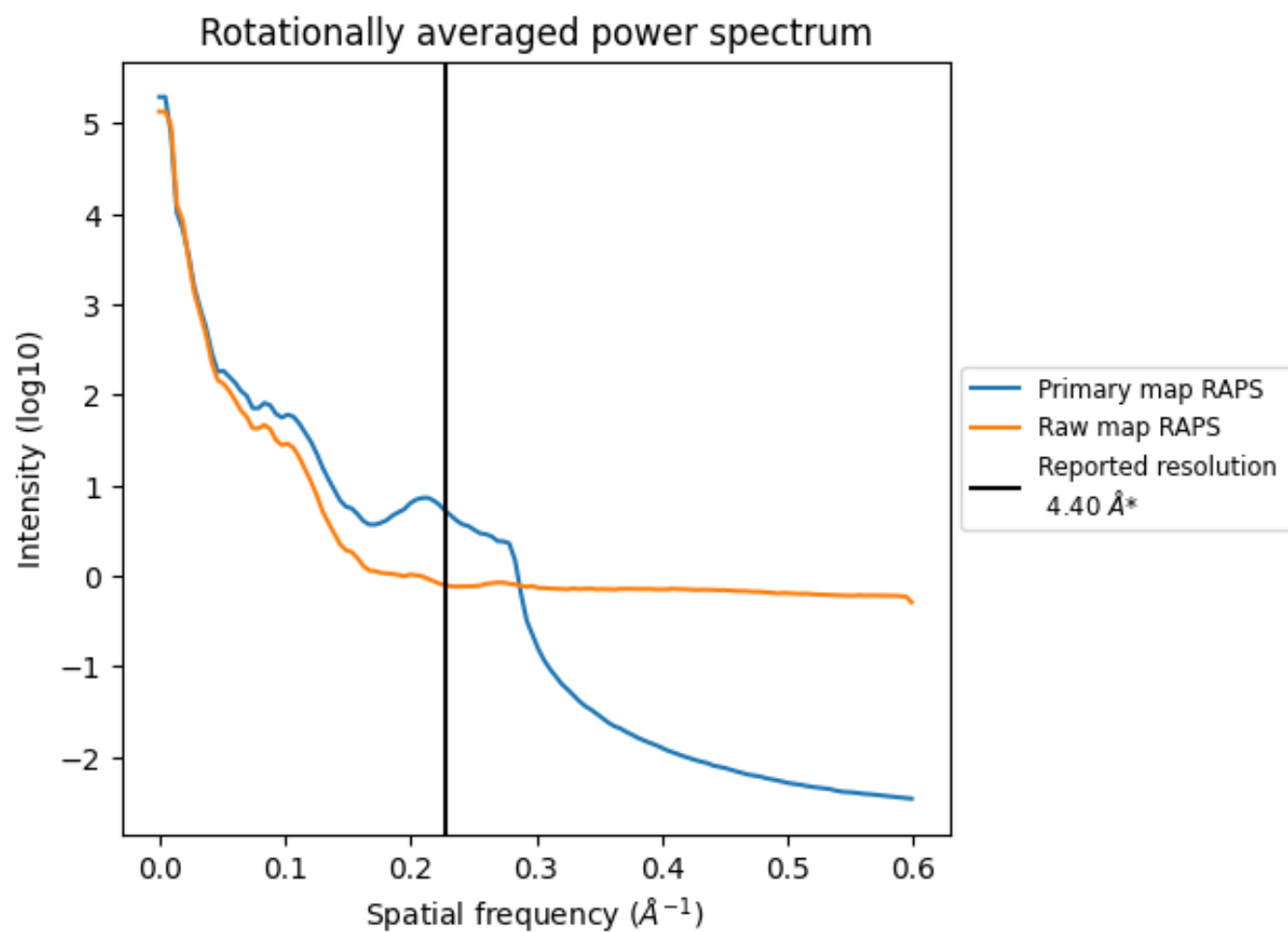
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 112 nm³; this corresponds to an approximate mass of 101 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](#)

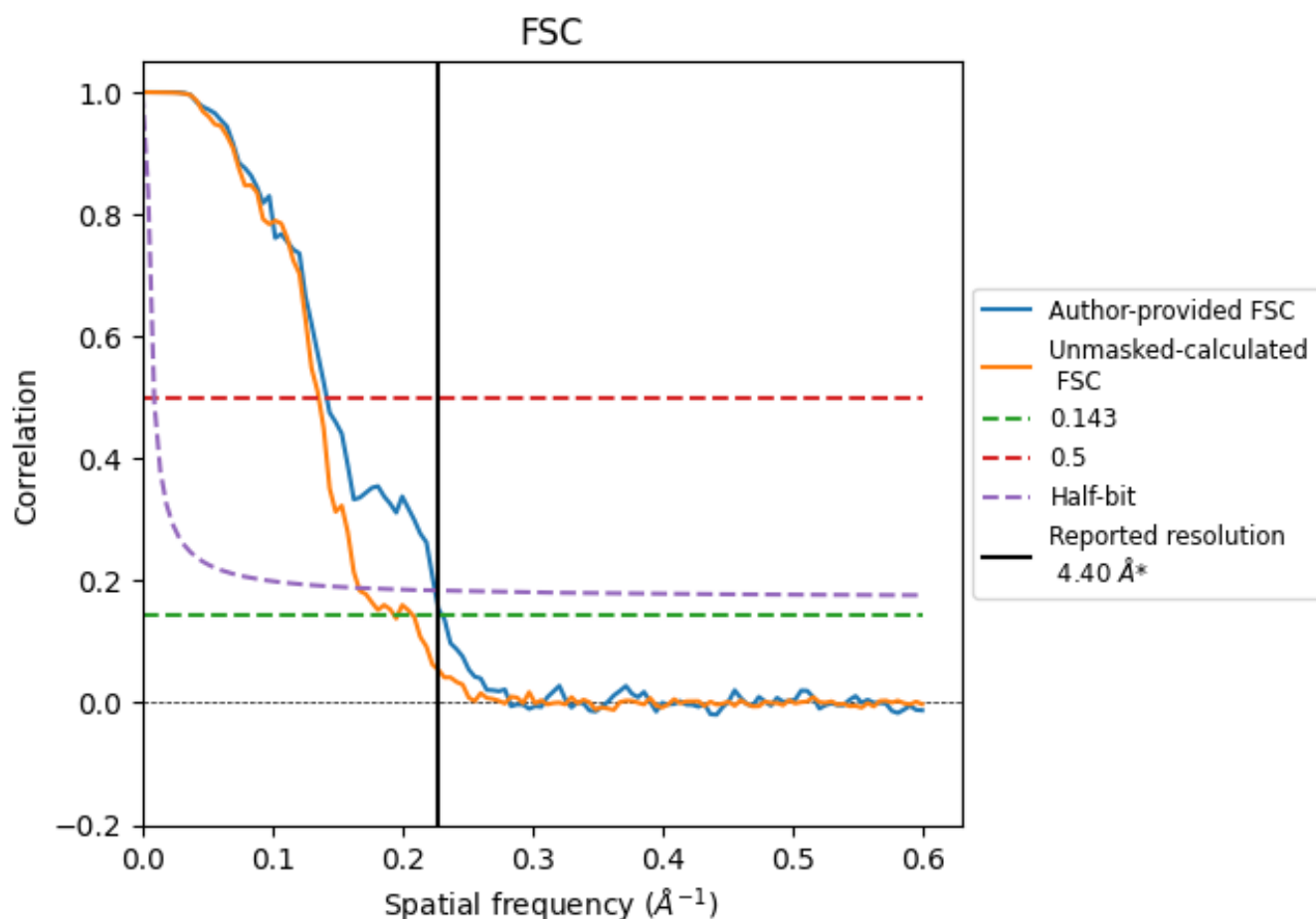


*Reported resolution corresponds to spatial frequency of 0.227 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.227 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

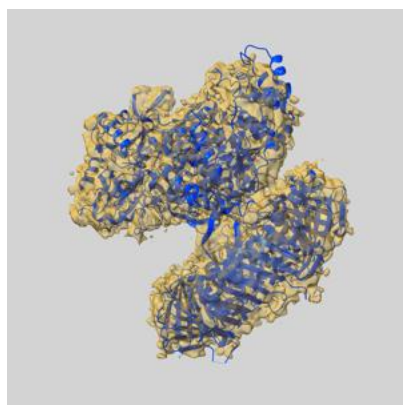
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.34	7.06	4.45
Unmasked-calculated*	5.17	7.39	6.01

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.17 differs from the reported value 4.4 by more than 10 %

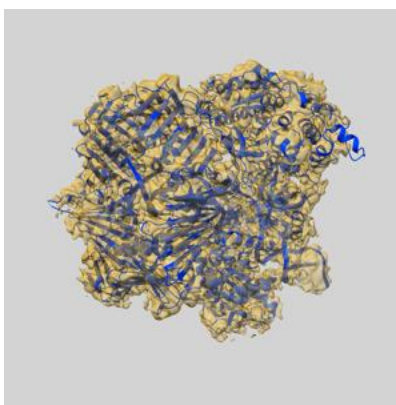
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14080 and PDB model 7QO1. Per-residue inclusion information can be found in section [3](#) on page [7](#).

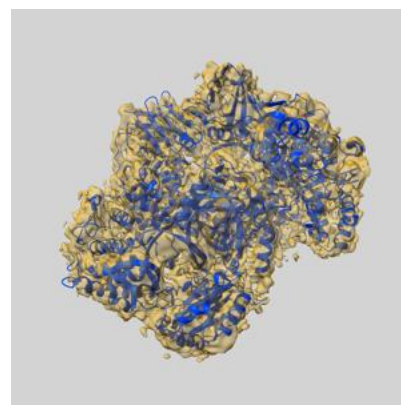
9.1 Map-model overlay [i](#)



X



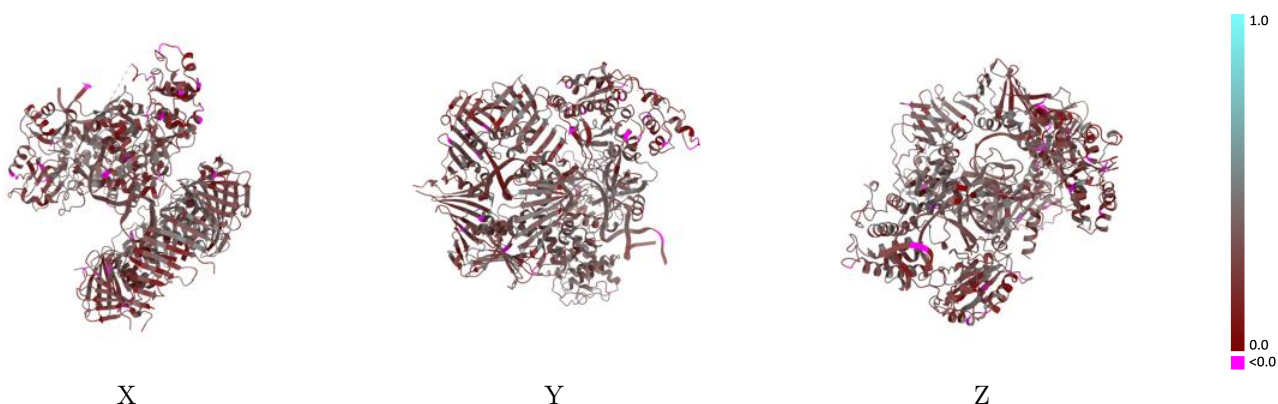
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)

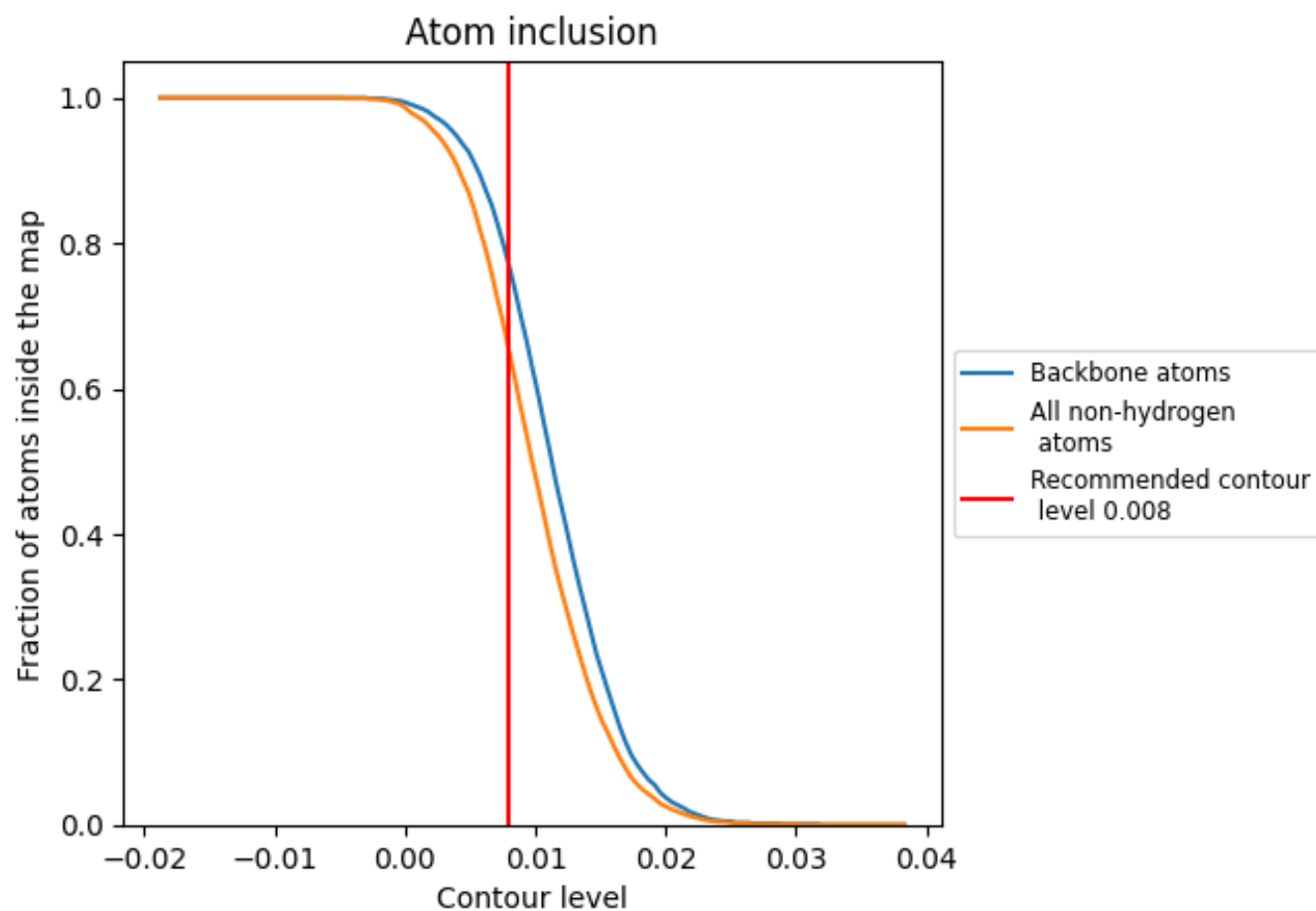


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6500	0.3030
A	0.6290	0.3240
B	0.6930	0.3160
F	0.6290	0.2660
G	0.7090	0.3350
H	0.7310	0.2750
I	0.7900	0.2780
J	0.7500	0.2810
Y	0.5660	0.2620

1.0

0.0

<0.0