



Full wwPDB EM Validation Report ⓘ

May 6, 2026 – 04:06 PM EDT

PDB ID : 9NLC / pdb_00009nlc
EMDB ID : EMD-49519
Title : Cryo-EM structure of the Class 1 PI3K alpha/KRas complex on POPC/POPS nanodiscs low-pass filtered to 10 angstroms
Authors : Torosyan, H.; Natalia, J.; Verba, K.A.
Deposited on : 2025-03-03
Resolution : 10.00 Å(reported)

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

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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:

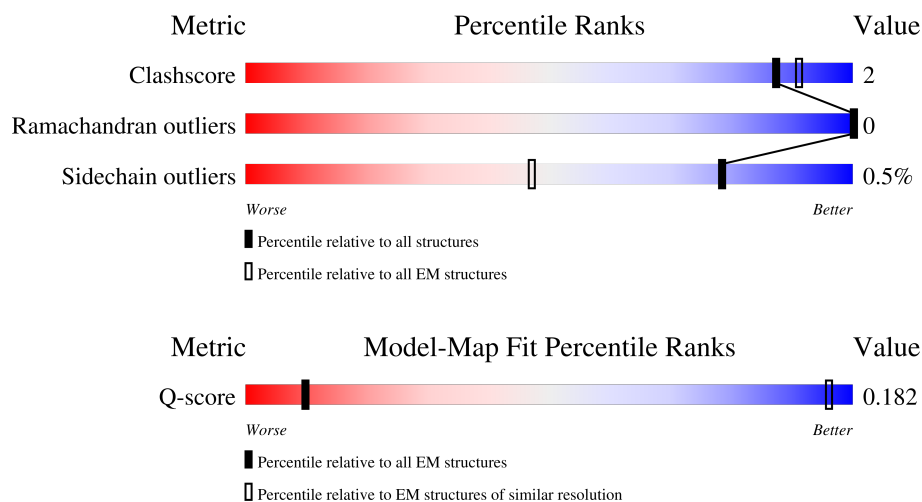
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 10.00 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	147 (9.50 - 10.50)

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	1096	
2	B	724	
3	C	189	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26015 atoms, of which 12963 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 Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit alpha isoform.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	1009	16568	5287	8301	1416	1495	69	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	expression tag	UNP P42336
A	-26	SER	-	expression tag	UNP P42336
A	-25	TYR	-	expression tag	UNP P42336
A	-24	TYR	-	expression tag	UNP P42336
A	-23	HIS	-	expression tag	UNP P42336
A	-22	HIS	-	expression tag	UNP P42336
A	-21	HIS	-	expression tag	UNP P42336
A	-20	HIS	-	expression tag	UNP P42336
A	-19	HIS	-	expression tag	UNP P42336
A	-18	HIS	-	expression tag	UNP P42336
A	-17	ASP	-	expression tag	UNP P42336
A	-16	TYR	-	expression tag	UNP P42336
A	-15	ASP	-	expression tag	UNP P42336
A	-14	ILE	-	expression tag	UNP P42336
A	-13	PRO	-	expression tag	UNP P42336
A	-12	THR	-	expression tag	UNP P42336
A	-11	THR	-	expression tag	UNP P42336
A	-10	GLU	-	expression tag	UNP P42336
A	-9	ASN	-	expression tag	UNP P42336
A	-8	LEU	-	expression tag	UNP P42336
A	-7	TYR	-	expression tag	UNP P42336
A	-6	PHE	-	expression tag	UNP P42336
A	-5	GLN	-	expression tag	UNP P42336
A	-4	GLY	-	expression tag	UNP P42336
A	-3	ALA	-	expression tag	UNP P42336
A	-2	MET	-	expression tag	UNP P42336
A	-1	GLY	-	expression tag	UNP P42336

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P42336

- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	401	Total	C	H	N	O	S	0	0
			6613	2086	3267	597	653	10		

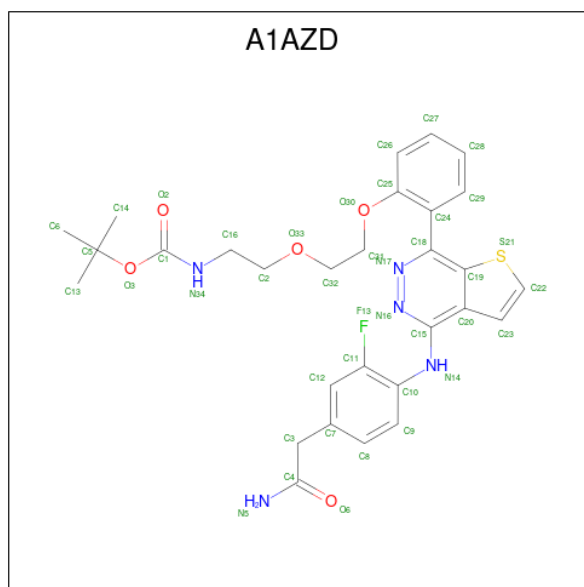
- Molecule 3 is a protein called Isoform 2B of GTPase KRas.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	171	Total	C	H	N	O	S	0	0
			2715	854	1350	235	269	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP P01116

- Molecule 4 is tert-butyl [2-(2-[[[(2P)-2-{4-[4-(2-amino-2-oxoethyl)-2-fluoroanilino]thieno[2,3-d]pyridazin-7-yl}phenyl]oxy}ethoxy)ethyl]carbamate (CCD ID: A1AZD) (formula: C₂₉H₃₂FN₅O₅S) (labeled as "Ligand of Interest" by depositor).

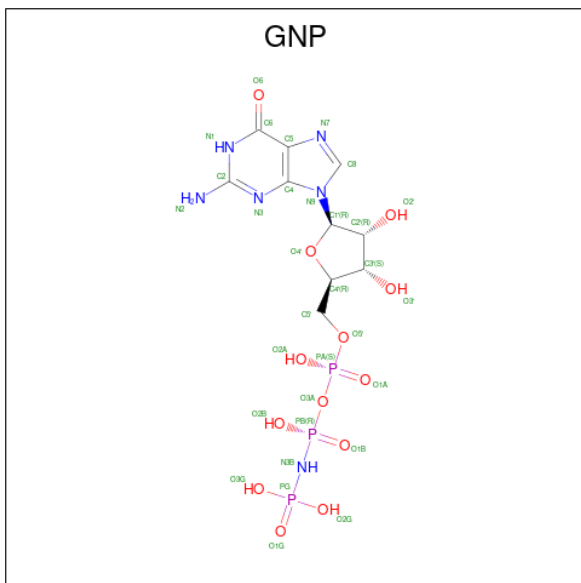


Mol	Chain	Residues	Atoms							AltConf
4	A	1	Total	C	F	H	N	O	S	0
			73	29	1	32	5	5	1	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total	Mg	0
			1	1	

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
6	C	1	Total	C	H	N	O	P	0
			45	10	13	6	13	3	



• Molecule 3: Isoform 2B of GTPase KRas

Chain C: 81% 8% • 10%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111772	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.7	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.492	Depositor
Minimum map value	-0.079	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.0105	Depositor
Map size (\AA)	366.8672, 366.8672, 366.8672	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8189, 0.8189, 0.8189	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, A1AZD, MG

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	4/8450 (0.0%)	1.16	11/11413 (0.1%)
2	B	0.81	1/3407 (0.0%)	1.10	9/4581 (0.2%)
3	C	0.88	3/1386 (0.2%)	1.23	7/1867 (0.4%)
All	All	0.78	8/13243 (0.1%)	1.16	27/17861 (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	2
2	B	0	2
3	C	0	1
All	All	0	5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	445	VAL	C-N	11.65	1.50	1.33
3	C	134	ALA	CA-CB	-9.08	1.39	1.53
3	C	130	ALA	CA-CB	-8.41	1.40	1.53
3	C	134	ALA	C-O	-8.25	1.14	1.24
1	A	821	GLU	C-O	-7.02	1.16	1.24
1	A	502	ARG	C-O	-6.37	1.10	1.23
1	A	366	PRO	N-CD	-6.05	1.39	1.47
1	A	561	ILE	C-O	-5.38	1.17	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	445	VAL	CA-C-N	-13.80	104.57	120.03
2	B	445	VAL	C-N-CA	-13.80	104.57	120.03
3	C	134	ALA	CA-C-O	-11.27	108.99	120.82
1	A	920	ASN	CA-CB-CG	8.42	121.02	112.60
2	B	445	VAL	N-CA-C	-7.47	102.86	111.00
3	C	134	ALA	O-C-N	7.36	129.65	122.07
2	B	444	ALA	N-CA-C	-5.99	104.68	112.23
1	A	230	ARG	NE-CZ-NH2	5.94	124.55	119.20
1	A	38	ARG	NE-CZ-NH2	5.89	124.50	119.20
3	C	131	GLN	CA-C-N	5.88	128.64	120.29
3	C	131	GLN	C-N-CA	5.88	128.64	120.29
2	B	586	GLN	N-CA-C	-5.87	104.96	111.36
2	B	557	ARG	NE-CZ-NH2	5.66	124.29	119.20
3	C	120	LEU	CA-C-O	-5.66	115.13	119.32
2	B	543	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	A	207	TYR	N-CA-CB	-5.54	102.28	110.37
1	A	821	GLU	CA-C-O	-5.49	115.05	120.82
1	A	917	HIS	CA-CB-CG	-5.30	108.50	113.80
2	B	499	GLN	CA-C-N	5.28	127.31	120.44
2	B	499	GLN	C-N-CA	5.28	127.31	120.44
3	C	27	HIS	CB-CG-CD2	-5.23	124.40	131.20
3	C	129	GLN	N-CA-C	-5.21	105.50	111.07
1	A	502	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	A	201	ASN	CA-C-N	5.16	131.39	121.54
1	A	201	ASN	C-N-CA	5.16	131.39	121.54
1	A	205	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	A	555	ARG	NE-CZ-NH2	5.07	123.76	119.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	TYR	Sidechain
1	A	947	TYR	Sidechain
2	B	443	GLU	Mainchain
2	B	685	TYR	Sidechain
3	C	71	TYR	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	8267	8301	8295	38	0
2	B	3346	3267	3266	9	0
3	C	1365	1350	1347	8	0
4	A	41	32	0	1	0
5	C	1	0	0	0	0
6	C	32	13	13	1	0
All	All	13052	12963	12921	51	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 (51) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:GLU:N	1:A:557:TYR:HH	1.75	0.85
1:A:915:ASP:HB3	2:B:605:ASP:H	1.66	0.60
1:A:749:GLN:OE1	1:A:763:ASN:OD1	2.18	0.60
1:A:225:ILE:HG21	1:A:243:VAL:HA	1.84	0.59
1:A:856:THR:HA	1:A:922:MET:HG2	1.86	0.58
1:A:916:ARG:HG3	1:A:954:PHE:H	1.76	0.50
1:A:603:ASP:C	1:A:603:ASP:OD1	2.54	0.50
1:A:774:SER:HB2	1:A:778:PRO:CD	2.42	0.50
1:A:951:ARG:C	1:A:953:PRO:HD3	2.37	0.50
1:A:923:VAL:HG22	1:A:929:LEU:HA	1.93	0.49
2:B:470:TYR:CE1	2:B:556:TYR:CE1	3.01	0.49
1:A:723:LYS:HE3	1:A:734:PHE:CG	2.48	0.48
1:A:922:MET:HB2	1:A:930:PHE:CE2	2.49	0.47
1:A:986:LYS:HE3	1:A:1055:MET:SD	2.55	0.47
3:C:7:VAL:HB	3:C:78:PHE:CD2	2.50	0.47
1:A:1047:HIS:CG	1:A:1051:TRP:HE1	2.32	0.46
1:A:665:HIS:CE1	1:A:669:TRP:HE1	2.33	0.46
1:A:1047:HIS:C	1:A:1048:HIS:CG	2.94	0.46
1:A:1055:MET:HA	1:A:1055:MET:HE2	1.98	0.45
3:C:113:LEU:CD2	3:C:134:ALA:HB2	2.46	0.45
3:C:15:GLY:HA2	6:C:202:GNP:H8	1.99	0.45
1:A:861:GLN:HG3	1:A:862:CYS:SG	2.57	0.44
1:A:862:CYS:CB	2:B:685:TYR:HA	2.47	0.44
1:A:859:GLN:HB3	2:B:685:TYR:CE1	2.53	0.44
2:B:508:TYR:C	2:B:508:TYR:CD1	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:GLN:CD	1:A:795:GLN:H	2.25	0.43
1:A:862:CYS:HB2	2:B:685:TYR:HA	2.00	0.43
2:B:329:GLN:O	2:B:430:LYS:NZ	2.50	0.43
3:C:113:LEU:HD23	3:C:134:ALA:HB2	2.01	0.43
1:A:767:GLU:H	1:A:767:GLU:CD	2.26	0.43
1:A:950:GLU:H	1:A:950:GLU:CD	2.26	0.43
1:A:83:PHE:O	1:A:108:ARG:NH2	2.52	0.42
1:A:287:LEU:HD21	4:A:1101:A1AZD:C27	2.49	0.42
2:B:567:LYS:HB3	2:B:568:PRO:HD3	2.01	0.42
1:A:864:GLY:HA3	1:A:880:TRP:N	2.34	0.42
3:C:72:MET:HA	3:C:78:PHE:CE2	2.54	0.42
1:A:669:TRP:CZ3	1:A:709:MET:SD	3.13	0.42
1:A:808:ARG:NH2	1:A:1008:SER:O	2.52	0.42
1:A:544:THR:HG23	1:A:547:GLU:H	1.85	0.41
1:A:591:PRO:HA	1:A:592:PRO:HD3	1.97	0.41
3:C:28:PHE:CE2	3:C:147:LYS:HD3	2.55	0.41
1:A:628:LEU:HD23	1:A:628:LEU:C	2.46	0.41
1:A:774:SER:HB2	1:A:778:PRO:HD2	2.03	0.41
3:C:28:PHE:CG	3:C:29:VAL:N	2.89	0.41
1:A:195:TRP:CZ3	1:A:206:LYS:HB3	2.56	0.41
1:A:118:GLY:HA2	1:A:123:MET:O	2.21	0.40
1:A:942:LYS:HA	1:A:947:TYR:CD2	2.57	0.40
1:A:70:PHE:CD1	1:A:99:LEU:HB3	2.56	0.40
2:B:445:VAL:O	2:B:446:GLY:C	2.63	0.40
3:C:36:ILE:HD12	3:C:64:TYR:CZ	2.56	0.40
1:A:668:PHE:CD1	1:A:668:PHE:C	3.00	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	999/1096 (91%)	970 (97%)	29 (3%)	0	100	100
2	B	399/724 (55%)	389 (98%)	10 (2%)	0	100	100
3	C	169/189 (89%)	165 (98%)	4 (2%)	0	100	100
All	All	1567/2009 (78%)	1524 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	928/999 (93%)	923 (100%)	5 (0%)	81	83
2	B	368/654 (56%)	367 (100%)	1 (0%)	86	86
3	C	151/167 (90%)	150 (99%)	1 (1%)	76	81
All	All	1447/1820 (80%)	1440 (100%)	7 (0%)	78	83

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

Mol	Chain	Res	Type
1	A	191	ILE
1	A	228	LYS
1	A	925	ASP
1	A	1042	GLN
1	A	1048	HIS
2	B	607	TYR
3	C	27	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	ASN
1	A	661	GLN
1	A	861	GLN

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Mol	Chain	Res	Type
1	A	873	ASN
1	A	918	ASN
1	A	981	GLN
1	A	1044	ASN
2	B	378	ASN
2	B	478	GLN
2	B	600	ASN
2	B	606	GLN
2	B	673	ASN
2	B	699	GLN
3	C	131	GLN
3	C	150	GLN
3	C	166	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
4	A1AZD	A	1101	-	44,44,44	0.99	3 (6%)	53,61,61	1.33	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GNP	C	202	5	34,34,34	2.03	8 (23%)	47,54,54	1.80	8 (17%)

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
4	A1AZD	A	1101	-	-	5/27/27/27	0/4/4/4
6	GNP	C	202	5	-	4/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	202	GNP	PA-O3A	-4.91	1.54	1.59
6	C	202	GNP	C5-N7	-4.26	1.30	1.39
6	C	202	GNP	PG-N3B	-4.24	1.52	1.63
6	C	202	GNP	PB-O3A	-4.20	1.53	1.59
6	C	202	GNP	PB-N3B	-3.53	1.54	1.63
6	C	202	GNP	PG-O3G	-3.36	1.47	1.56
6	C	202	GNP	PG-O2G	-3.30	1.48	1.56
4	A	1101	A1AZD	C24-C18	-3.29	1.46	1.49
6	C	202	GNP	PB-O2B	-2.94	1.49	1.56
4	A	1101	A1AZD	C20-C19	-2.26	1.37	1.41
4	A	1101	A1AZD	O3-C5	-2.04	1.44	1.48

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	202	GNP	O1B-PB-N3B	-8.01	99.97	111.77
6	C	202	GNP	O2B-PB-O3A	4.59	119.97	104.64
4	A	1101	A1AZD	C24-C18-C19	3.49	128.81	122.38
4	A	1101	A1AZD	C19-S21-C22	-3.30	86.87	91.24
4	A	1101	A1AZD	C20-C19-S21	3.16	115.90	111.64
4	A	1101	A1AZD	C25-C24-C18	-3.12	118.81	123.28
4	A	1101	A1AZD	C12-C11-C10	-2.96	120.40	123.43
6	C	202	GNP	N9-C4-N3	2.78	131.51	125.95
6	C	202	GNP	O2A-PA-O3A	2.72	114.63	107.27
6	C	202	GNP	C5-C4-N3	-2.40	124.56	128.39
4	A	1101	A1AZD	F13-C11-C10	2.37	120.54	117.59
4	A	1101	A1AZD	C19-C18-N17	-2.31	118.65	121.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	202	GNP	O1G-PG-N3B	2.27	115.11	111.77
6	C	202	GNP	O3A-PA-O1A	2.23	117.42	110.70
6	C	202	GNP	C6-C5-N7	-2.23	126.23	130.29
4	A	1101	A1AZD	C24-C18-N17	-2.17	112.48	116.34

There are no chirality outliers.

All (9) torsion outliers are listed below:

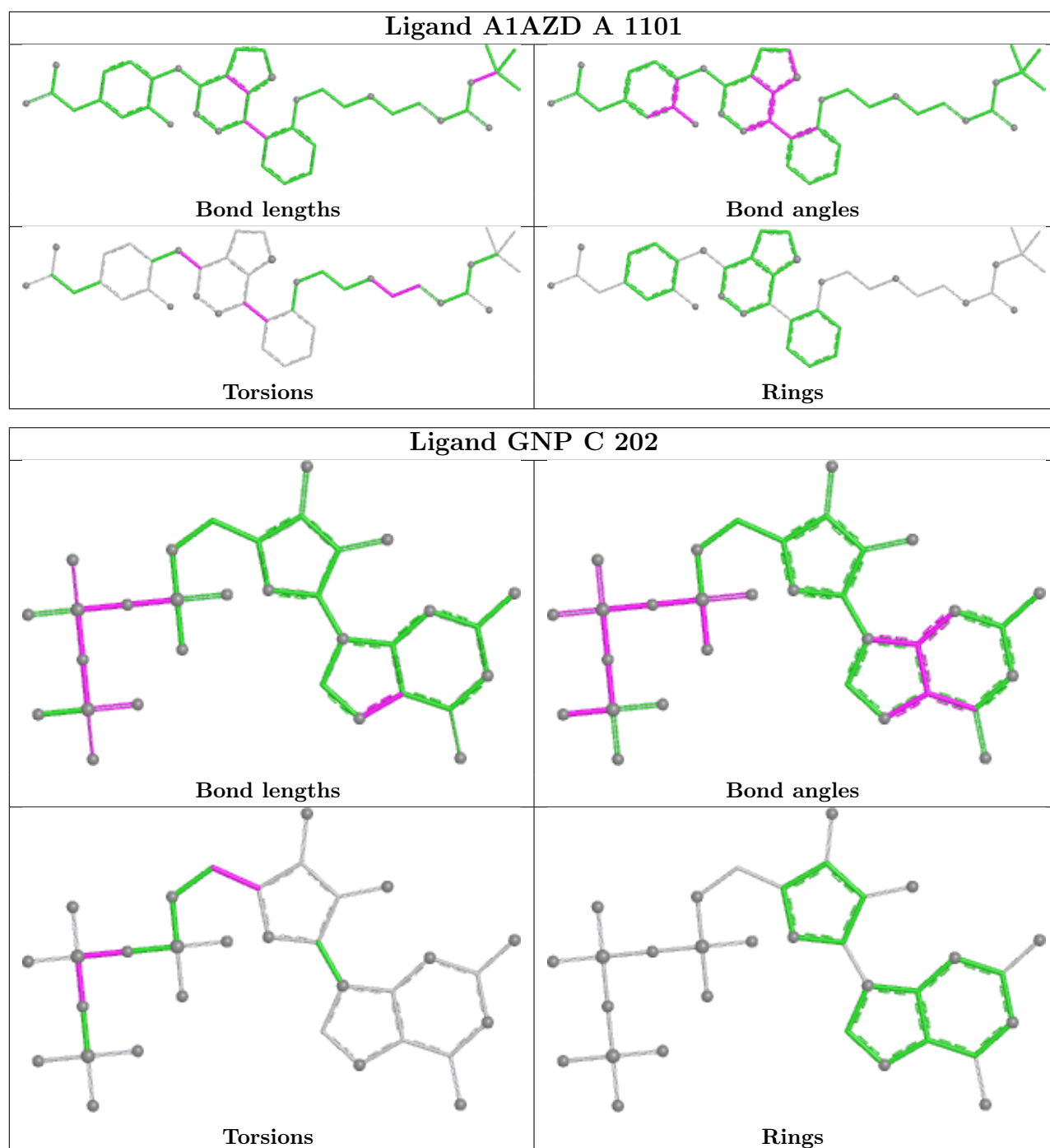
Mol	Chain	Res	Type	Atoms
6	C	202	GNP	PG-N3B-PB-O1B
6	C	202	GNP	PA-O3A-PB-O2B
6	C	202	GNP	O4'-C4'-C5'-O5'
6	C	202	GNP	C3'-C4'-C5'-O5'
4	A	1101	A1AZD	N34-C16-C2-O33
4	A	1101	A1AZD	C16-C2-O33-C32
4	A	1101	A1AZD	C20-C15-N14-C10
4	A	1101	A1AZD	C19-C18-C24-C25
4	A	1101	A1AZD	N17-C18-C24-C25

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1101	A1AZD	1	0
6	C	202	GNP	1	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.

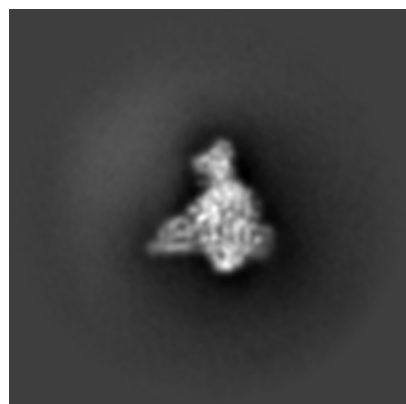
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49519. These allow visual inspection of the internal detail of the map and identification of artifacts.

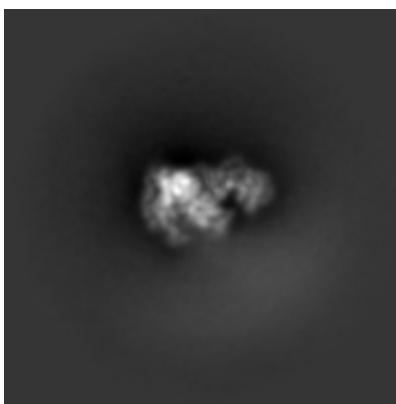
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

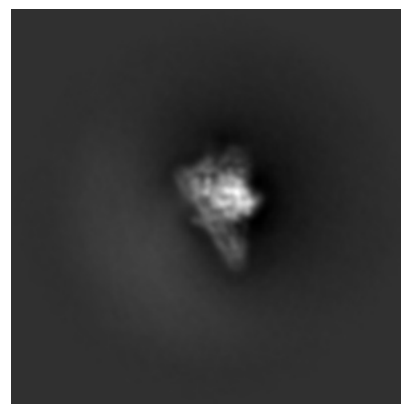
6.1.1 Primary map



X

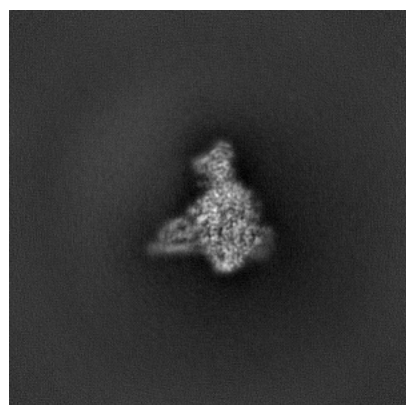


Y

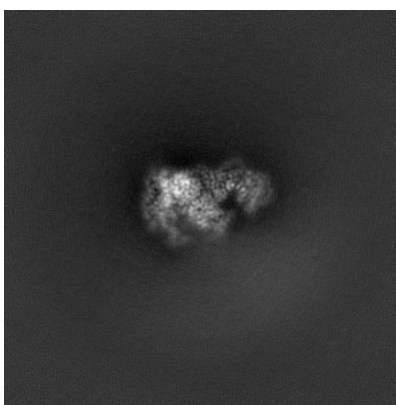


Z

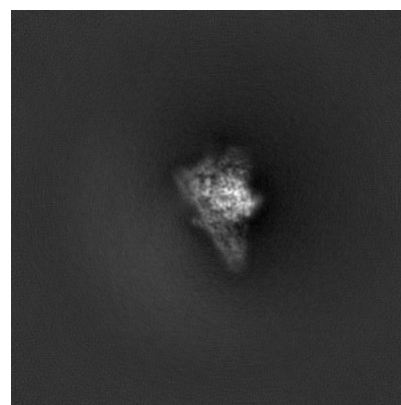
6.1.2 Raw map



X



Y

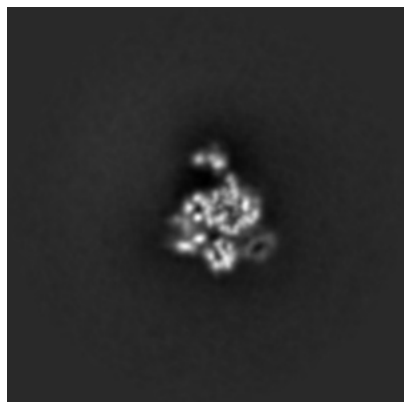


Z

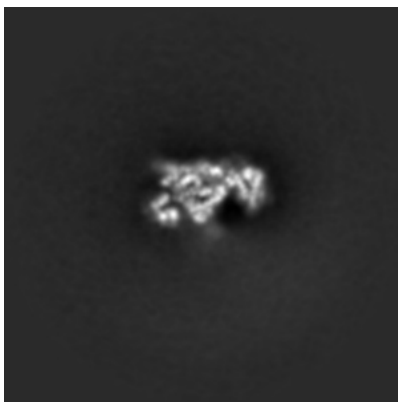
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

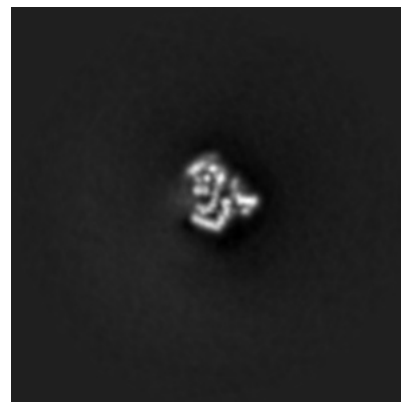
6.2.1 Primary map



X Index: 224

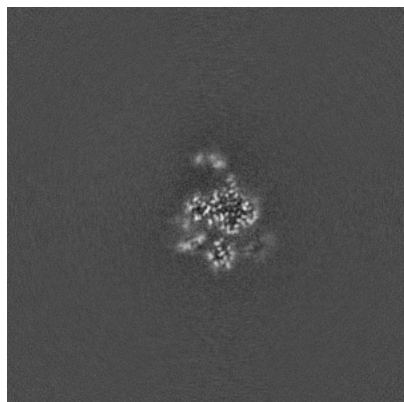


Y Index: 224

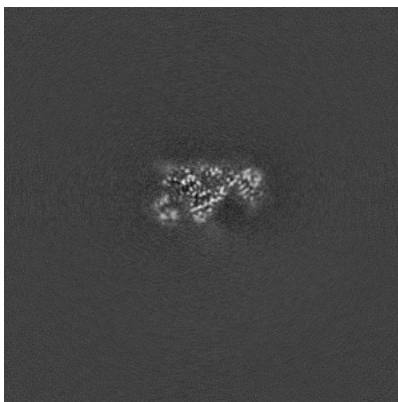


Z Index: 224

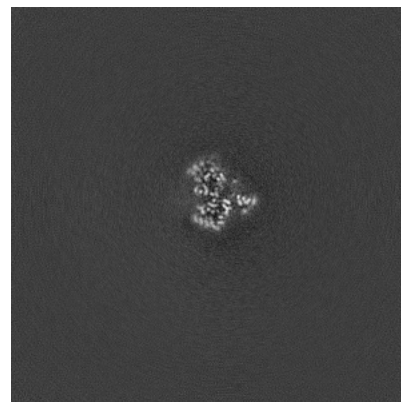
6.2.2 Raw map



X Index: 224



Y Index: 224

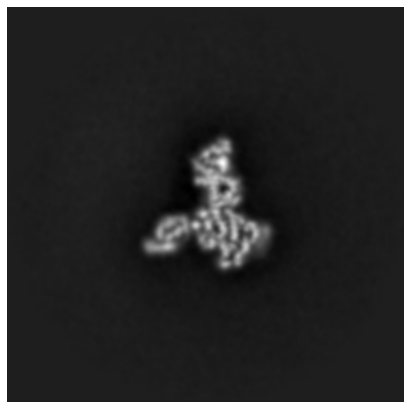


Z Index: 224

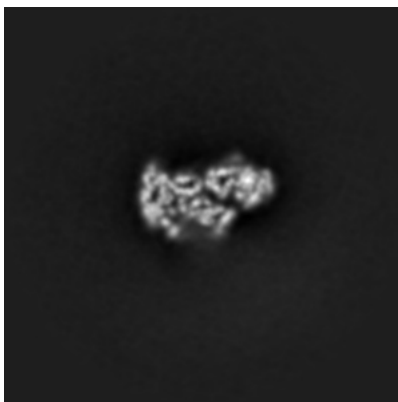
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

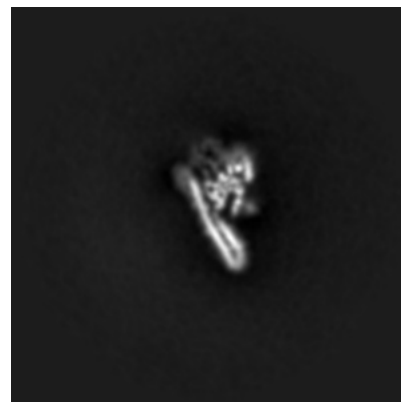
6.3.1 Primary map



X Index: 253

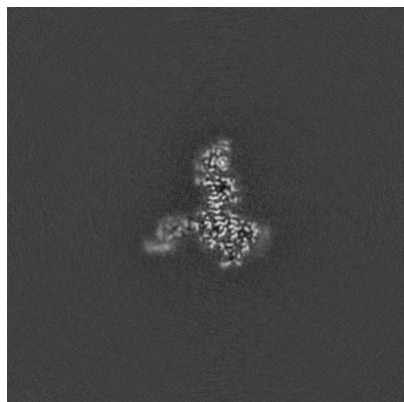


Y Index: 243

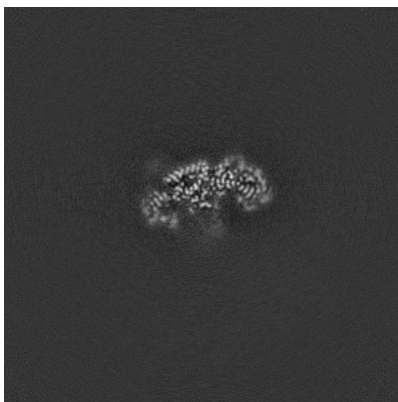


Z Index: 181

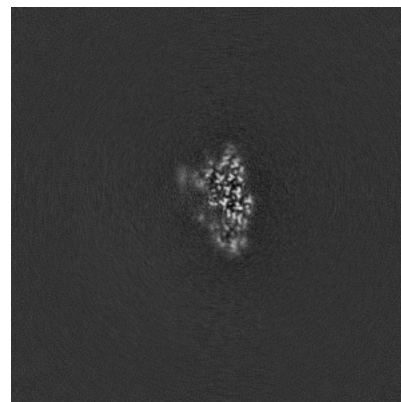
6.3.2 Raw map



X Index: 254



Y Index: 231



Z Index: 205

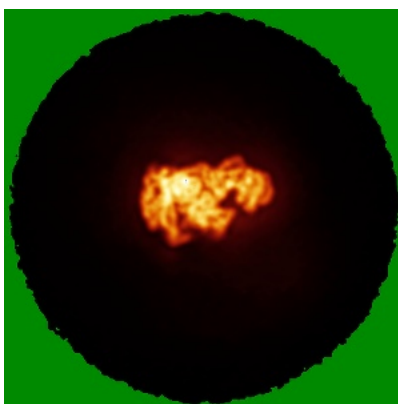
The images above show the largest variance slices of the map in three orthogonal directions.

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

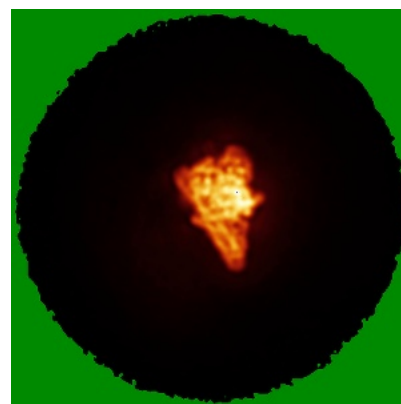
6.4.1 Primary map



X



Y

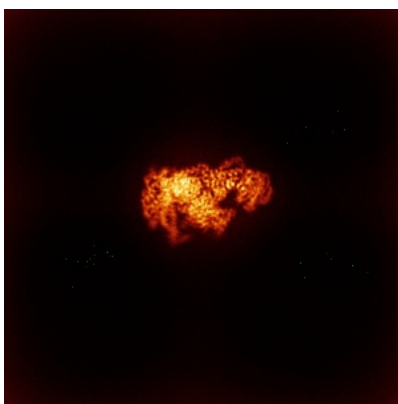


Z

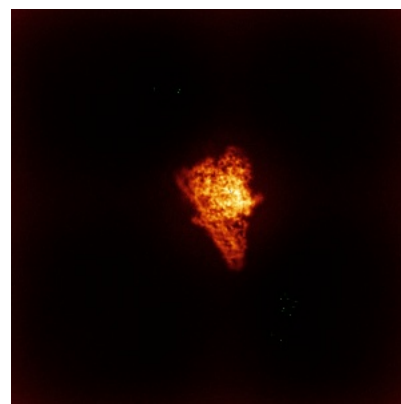
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

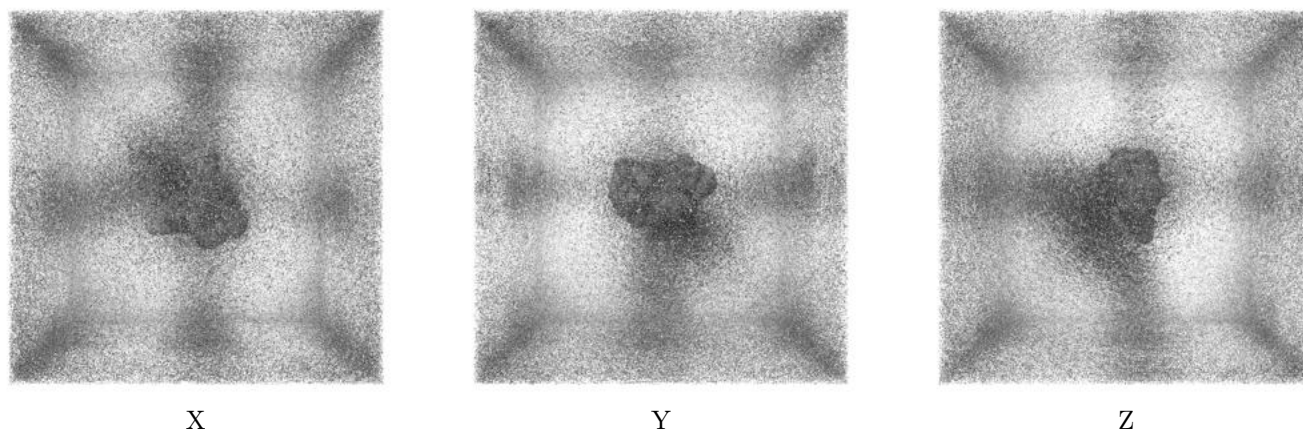
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0105. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

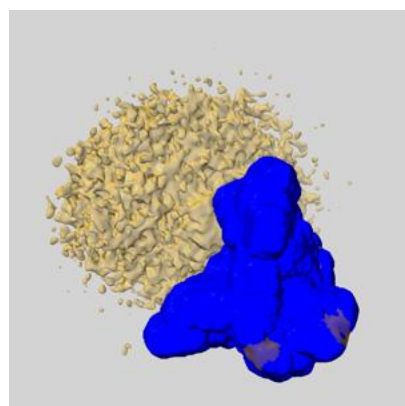
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

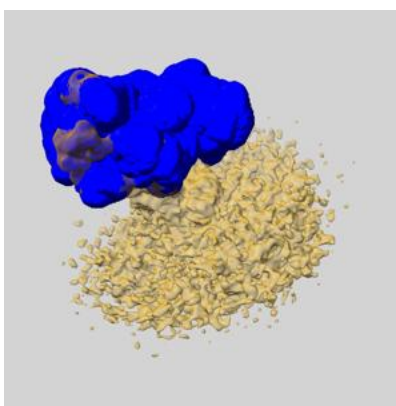
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

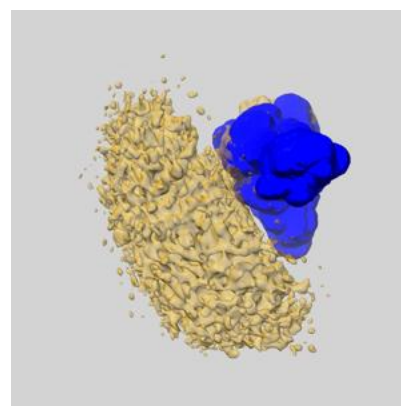
6.6.1 emd_49519_msk_1.map [i](#)



X



Y

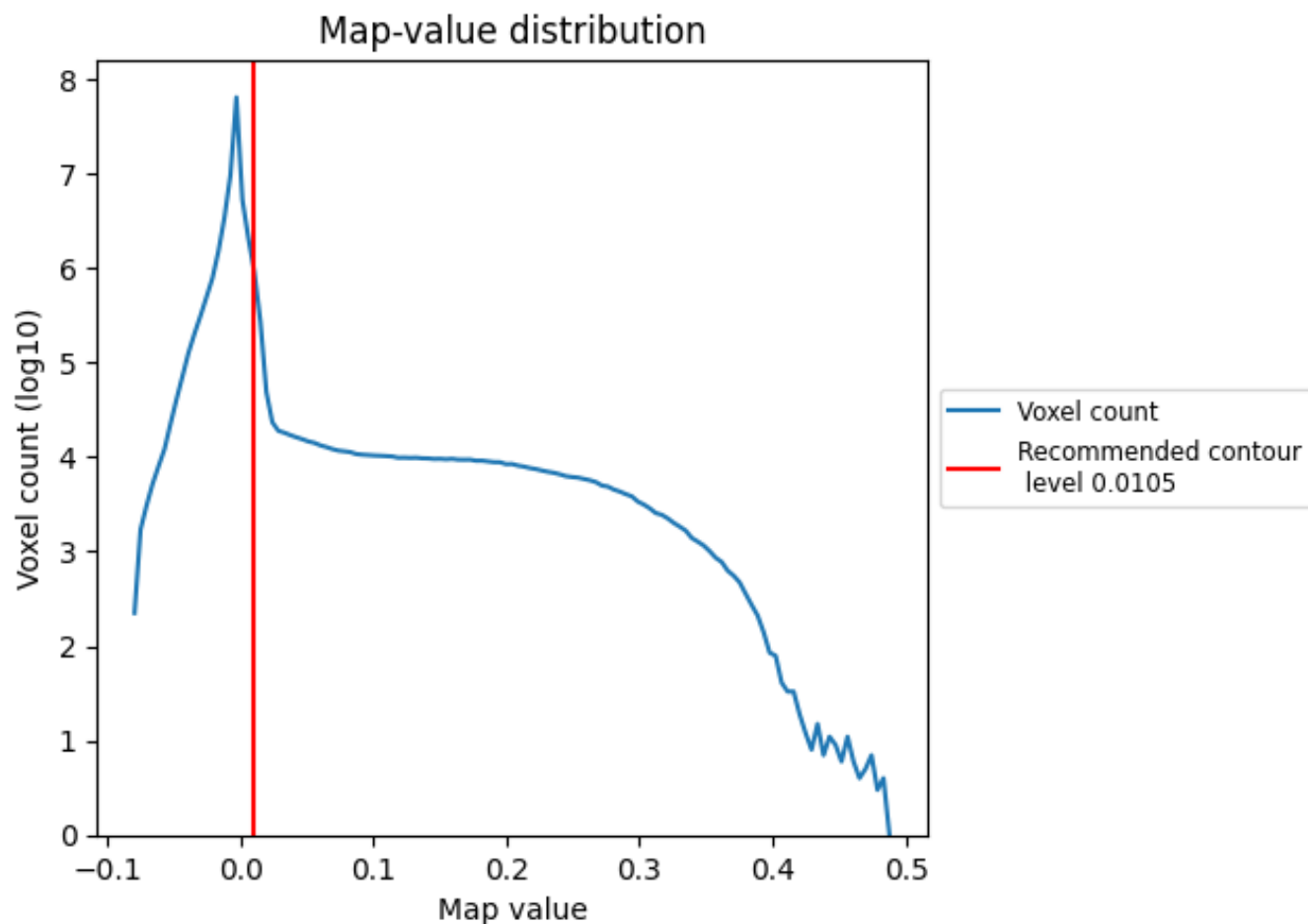


Z

7 Map analysis [i](#)

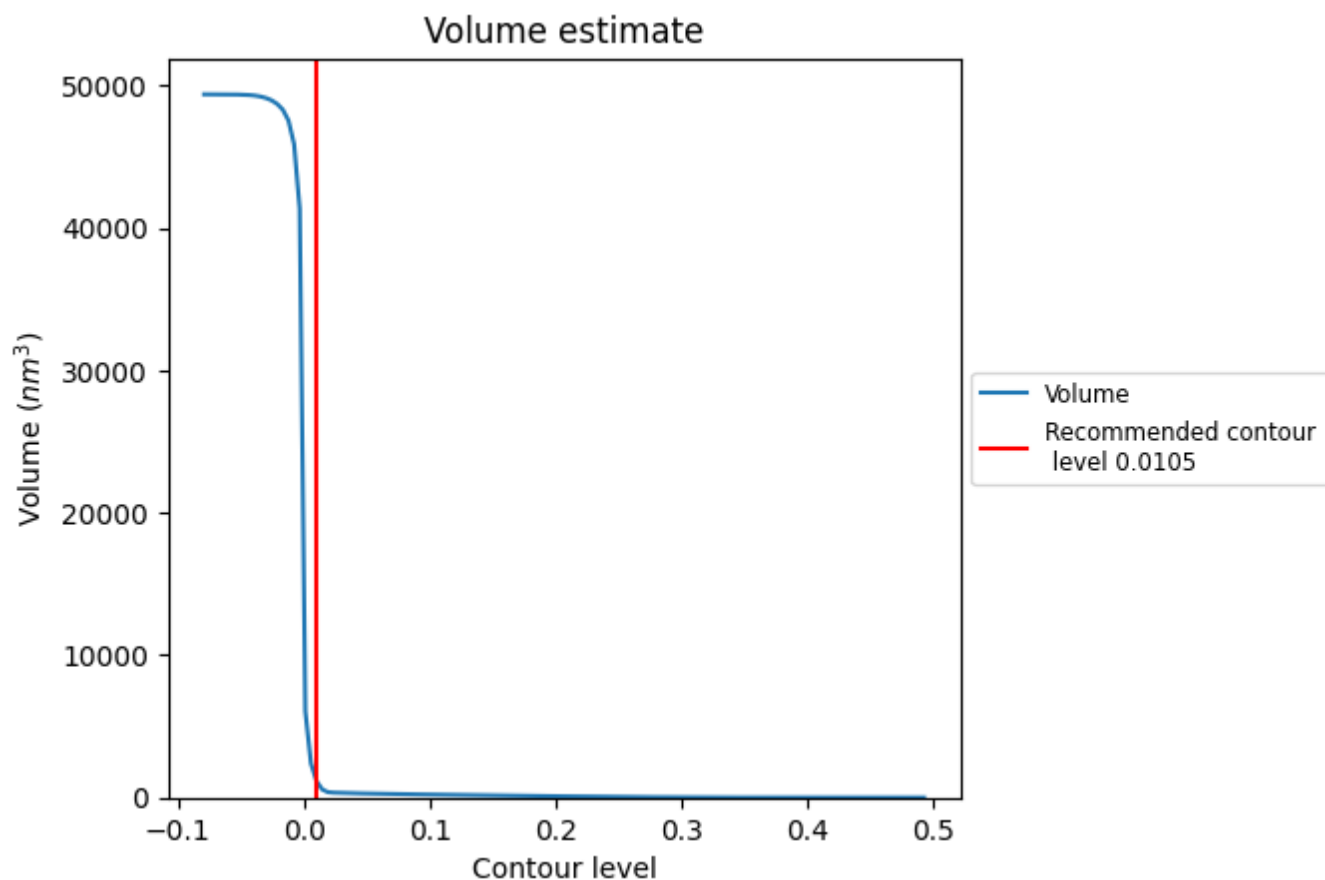
This section contains the results of statistical analysis of the map.

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.

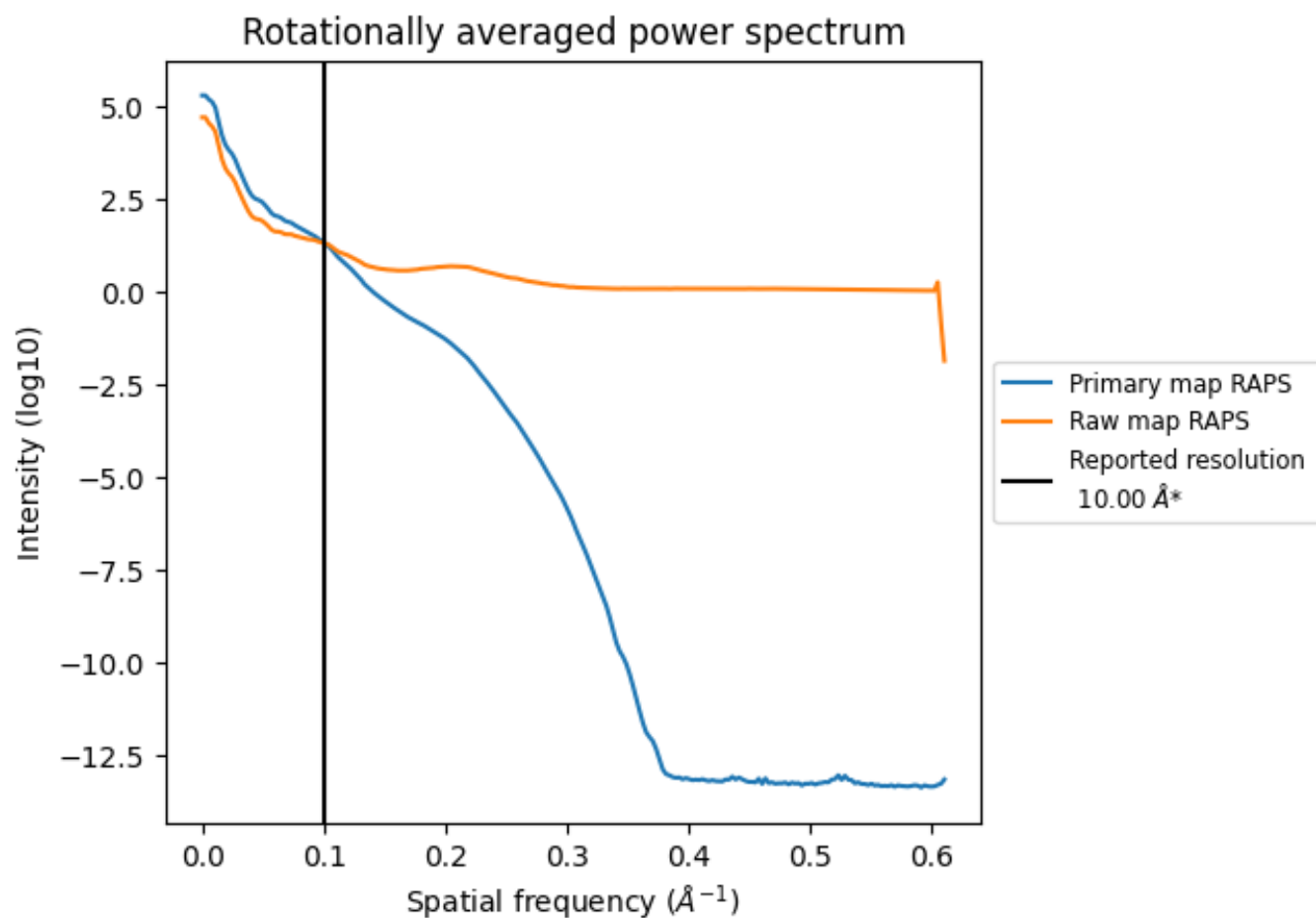
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1088 nm³; this corresponds to an approximate mass of 983 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 ⓘ

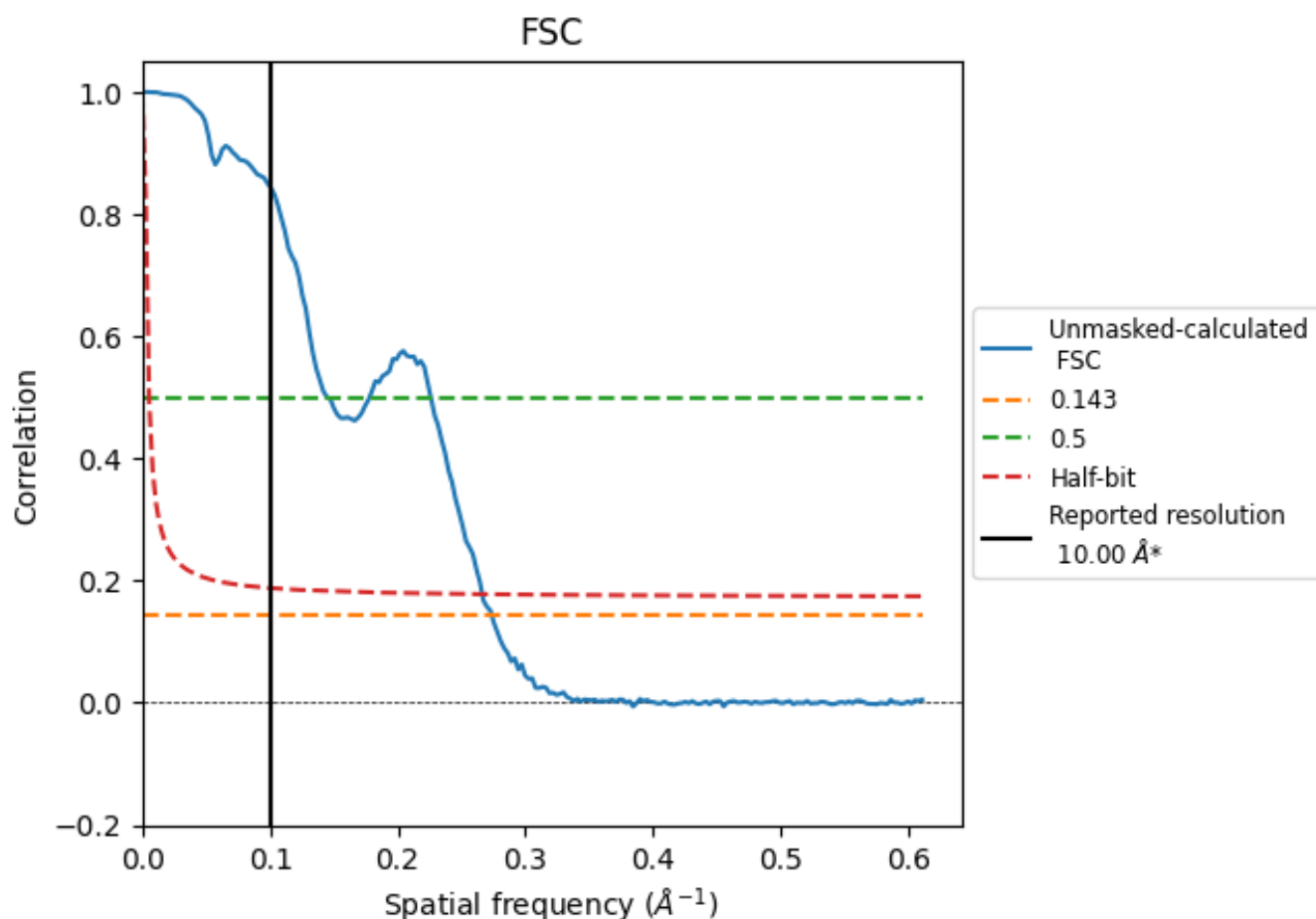


*Reported resolution corresponds to spatial frequency of 0.100 Å⁻¹

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 0.100 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.65	6.91	3.76

*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 3.65 differs from the reported value 10.0 by more than 10 %

9 Map-model fit [i](#)

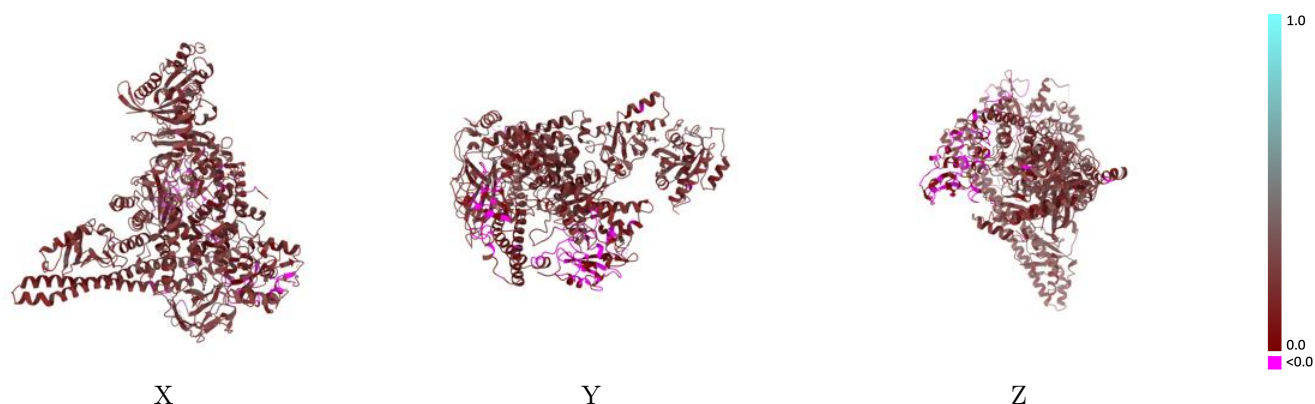
This section contains information regarding the fit between EMDB map EMD-49519 and PDB model 9NLC. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



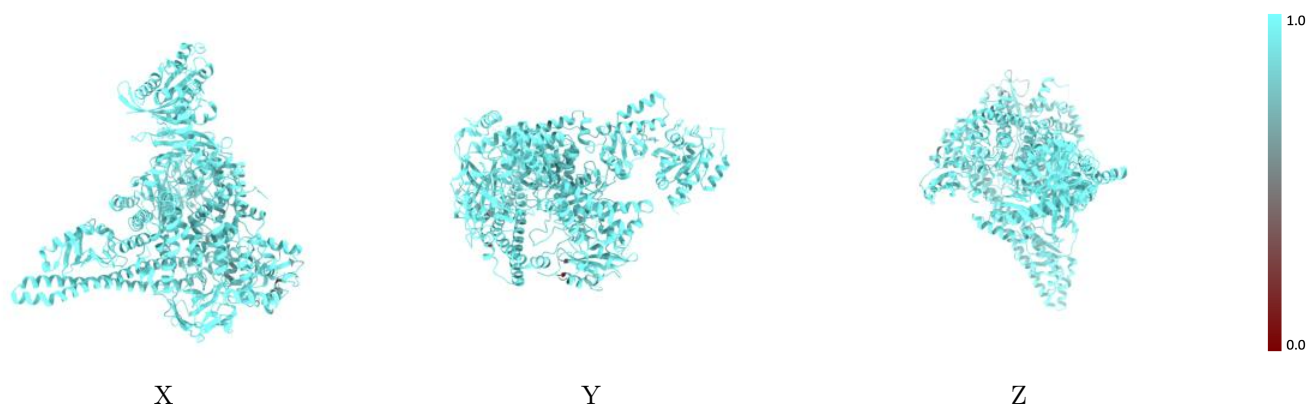
The images above show the 3D surface view of the map at the recommended contour level 0.0105 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



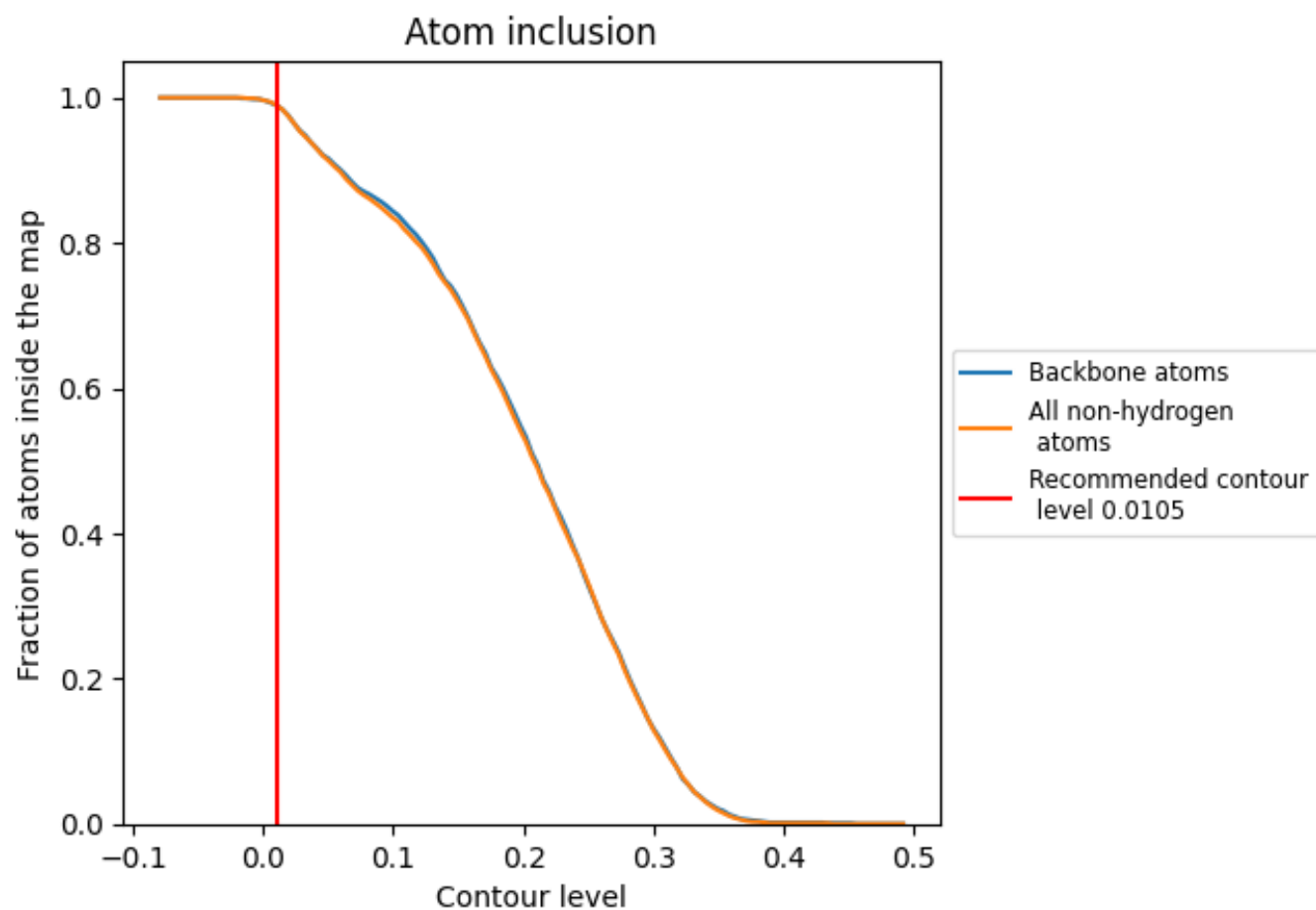
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0105).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.0105) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9890	<div></div> 0.1820
A	<div></div> 1.0000	<div></div> 0.2130
B	<div></div> 0.9660	<div></div> 0.0900
C	<div></div> 1.0000	<div></div> 0.2200

