



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:47 PM UTC

PDB ID : 9YC6 / pdb_00009yc6
EMDB ID : EMD-72761
Title : Mutant human uPAR bound to the Fab fragment of the targeted cancer therapeutic antibody FL1
Authors : Anane, R.F.; Whisstock, J.C.; Engelholm, L.H.; Law, R.H.P.; Ploug, M.
Deposited on : 2025-09-18
Resolution : 4.80 Å(reported)
Based on initial model : 3u74

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
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

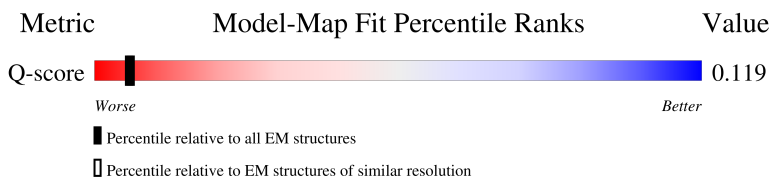
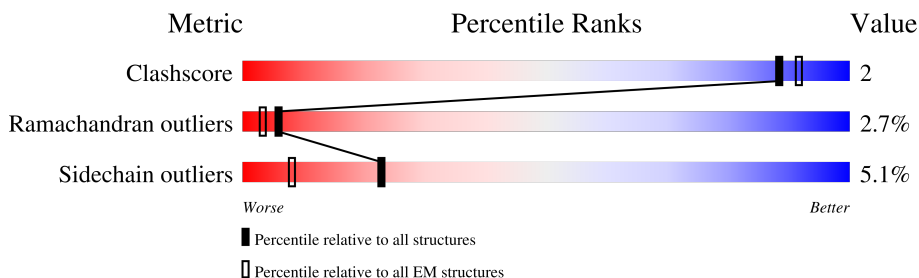
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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.



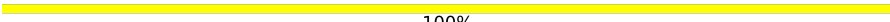
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1575 (4.30 - 5.30)

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	L	219	 81% 13% . .
2	U	283	 80% 17% . .
3	H	221	 90% 7% .
4	A	3	 100%

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Mol	Chain	Length	Quality of chain
5	B	2	 100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10788 atoms, of which 5273 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 Anti-uPAR antibody FL1 Fab light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	L	212	Total	C	H	N	O	S	0	0
			3232	1028	1593	275	330	6		

- Molecule 2 is a protein called Urokinase plasminogen activator surface receptor.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	U	283	Total	C	H	N	O	S	0	0
			4194	1298	2023	402	435	36		

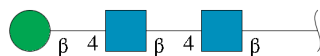
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	47	CYS	HIS	engineered mutation	UNP Q03405
U	259	CYS	ASN	engineered mutation	UNP Q03405

- Molecule 3 is a protein called Anti-uPAR antibody FL1 Fab heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	H	214	Total	C	H	N	O	S	0	0
			3175	1020	1565	261	323	6		

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



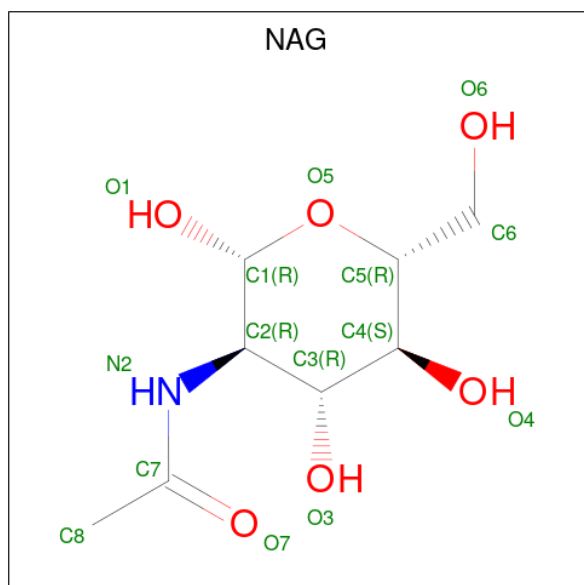
Mol	Chain	Residues	Atoms						AltConf	Trace
4	A	3	Total	C	H	N	O		0	0
			76	22	37	2	15			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	2	Total	C	H	N	O	0	0
			55	16	27	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

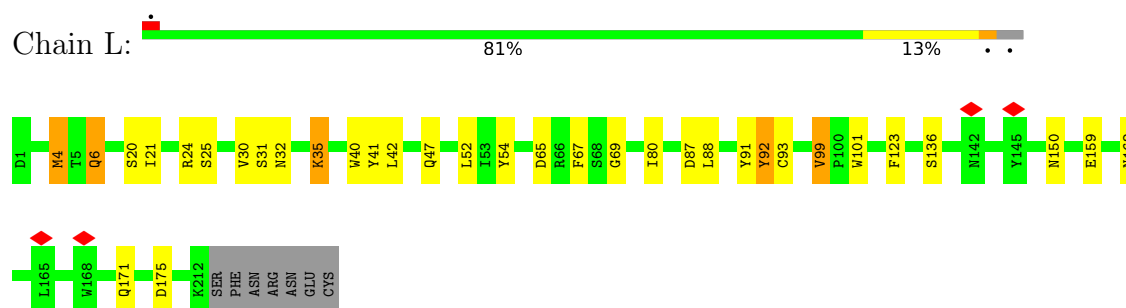


Mol	Chain	Residues	Atoms					AltConf
6	U	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	U	1	Total	C	H	N	O	0
			28	8	14	1	5	

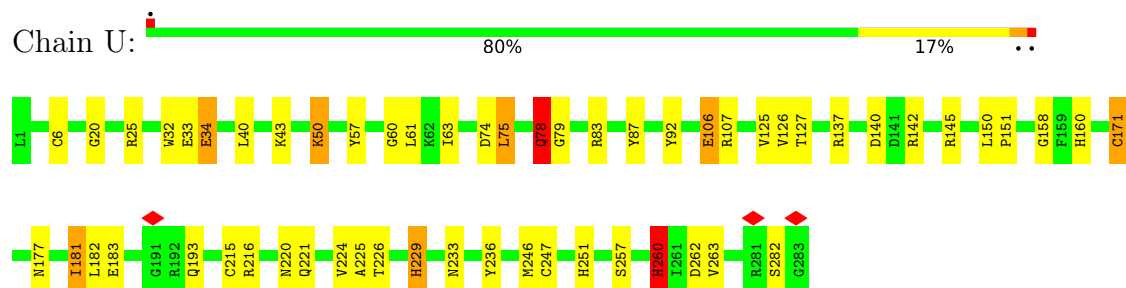
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

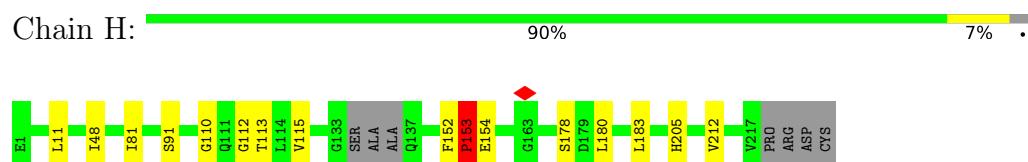
- Molecule 1: Anti-uPAR antibody FL1 Fab light chain



- Molecule 2: Urokinase plasminogen activator surface receptor



- Molecule 3: Anti-uPAR antibody FL1 Fab heavy chain



- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	86404	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF corrections were performed after 3D reconstruction to improve the final resolution	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	12.06	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.429	Depositor
Minimum map value	-0.527	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	270.0, 270.0, 270.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.75, 0.75, 0.75	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	L	0.82	0/1677	1.52	10/2277 (0.4%)
2	U	1.05	3/2206 (0.1%)	1.79	34/2970 (1.1%)
3	H	0.82	1/1652 (0.1%)	1.43	6/2262 (0.3%)
All	All	0.92	4/5535 (0.1%)	1.61	50/7509 (0.7%)

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	L	0	2
2	U	0	6
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	78	GLN	CA-C	10.82	1.57	1.52
3	H	110	GLY	N-CA	6.09	1.50	1.44
2	U	79	GLY	CA-C	5.28	1.59	1.51
2	U	142	ARG	CZ-NH2	-5.25	1.26	1.33

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	78	GLN	O-C-N	-31.72	97.36	120.83
2	U	106	GLU	CA-C-O	-10.40	109.39	120.42
2	U	87	TYR	CA-C-N	8.56	137.89	121.54
2	U	87	TYR	C-N-CA	8.56	137.89	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	60	GLY	CA-C-N	7.64	136.12	121.54
2	U	60	GLY	C-N-CA	7.64	136.12	121.54
2	U	60	GLY	O-C-N	7.45	132.38	122.70
3	H	113	THR	N-CA-C	7.34	119.29	110.19
2	U	247	CYS	N-CA-C	7.13	121.43	112.87
1	L	162	ASN	CA-CB-CG	6.92	119.53	112.60
2	U	106	GLU	CA-C-N	-6.92	109.79	122.31
2	U	106	GLU	C-N-CA	-6.92	109.79	122.31
3	H	153	PRO	CA-N-CD	-6.88	102.36	112.00
2	U	75	LEU	O-C-N	-6.57	115.09	122.91
2	U	182	LEU	CA-C-N	6.36	129.86	120.90
2	U	182	LEU	C-N-CA	6.36	129.86	120.90
1	L	101	TRP	N-CA-C	6.34	118.05	110.19
2	U	171	CYS	N-CA-C	6.29	118.64	109.07
2	U	262	ASP	CA-CB-CG	-6.26	106.34	112.60
2	U	151	PRO	N-CA-C	6.16	122.10	113.53
2	U	78	GLN	N-CA-C	5.93	117.55	108.30
1	L	6	GLN	OE1-CD-NE2	-5.93	116.67	122.60
2	U	50	LYS	N-CA-C	5.90	116.08	108.34
2	U	260	HIS	CB-CG-CD2	-5.84	123.61	131.20
2	U	158	GLY	N-CA-C	5.78	118.95	110.80
1	L	87	ASP	CA-CB-CG	5.74	118.34	112.60
1	L	67	PHE	CA-CB-CG	5.67	119.47	113.80
1	L	24	ARG	NE-CZ-NH2	5.64	124.28	119.20
2	U	282	SER	CA-C-N	5.58	131.75	121.70
2	U	282	SER	C-N-CA	5.58	131.75	121.70
1	L	47	GLN	N-CA-C	5.56	119.56	112.34
3	H	113	THR	CA-C-N	5.56	131.68	121.85
3	H	113	THR	C-N-CA	5.56	131.68	121.85
2	U	251	HIS	CB-CG-CD2	-5.54	123.99	131.20
3	H	205	HIS	N-CA-C	5.52	121.12	113.45
2	U	25	ARG	NE-CZ-NH2	5.44	124.10	119.20
2	U	140	ASP	CA-CB-CG	5.41	118.01	112.60
2	U	177	ASN	CA-CB-CG	5.39	117.99	112.60
2	U	260	HIS	CA-CB-CG	5.31	119.11	113.80
1	L	92	TYR	CA-C-N	5.28	131.63	121.54
1	L	92	TYR	C-N-CA	5.28	131.63	121.54
2	U	216	ARG	NE-CZ-NH2	5.26	123.94	119.20
2	U	107	ARG	NE-CZ-NH2	5.16	123.85	119.20
2	U	150	LEU	CA-C-N	5.13	124.75	119.05
2	U	150	LEU	C-N-CA	5.13	124.75	119.05
2	U	229	HIS	CB-CG-CD2	-5.10	124.56	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	125	VAL	N-CA-C	5.05	114.52	108.06
1	L	123	PHE	CA-CB-CG	5.03	118.83	113.80
2	U	246	MET	N-CA-C	5.01	116.83	111.36
3	H	112	GLY	N-CA-C	5.01	121.23	111.66

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	92	TYR	Sidechain
1	L	99	VAL	Peptide
2	U	236	TYR	Sidechain
2	U	74	ASP	Mainchain
2	U	75	LEU	Mainchain
2	U	78	GLN	Peptide,Mainchain
2	U	92	TYR	Sidechain

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	L	1639	1593	1593	8	0
2	U	2171	2023	2023	11	0
3	H	1610	1565	1564	2	0
4	A	39	37	34	0	0
5	B	28	27	25	0	0
6	U	28	28	26	0	0
All	All	5515	5273	5265	20	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 (20) 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:L:88:LEU:H	1:L:99:VAL:HG22	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:88:LEU:H	1:L:99:VAL:CG2	2.22	0.52
1:L:35:LYS:HE3	1:L:88:LEU:HD23	1.91	0.52
2:U:20:GLY:HA3	2:U:260:HIS:CE1	2.46	0.50
3:H:152:PHE:CG	3:H:153:PRO:HD2	2.48	0.49
1:L:32:ASN:HD22	2:U:106:GLU:HG3	1.76	0.48
1:L:80:ILE:HD12	1:L:80:ILE:H	1.78	0.48
1:L:6:GLN:OE1	1:L:99:VAL:HG21	2.14	0.47
2:U:181:ILE:H	2:U:181:ILE:HD13	1.80	0.47
2:U:233:ASN:HD21	2:U:260:HIS:CE1	2.33	0.46
2:U:32:TRP:CH2	2:U:34:GLU:HA	2.52	0.45
1:L:4:MET:HE3	1:L:25:SER:HB2	1.99	0.44
1:L:6:GLN:HE21	1:L:21:ILE:CG2	2.30	0.44
3:H:48:ILE:HG21	3:H:81:ILE:CD1	2.49	0.43
2:U:6:CYS:SG	2:U:43:LYS:HE3	2.58	0.43
2:U:32:TRP:CE3	2:U:33:GLU:HA	2.54	0.43
2:U:32:TRP:HB3	2:U:63:ILE:H	1.85	0.42
2:U:224:VAL:HG22	2:U:225:ALA:N	2.35	0.41
2:U:160:HIS:CE1	2:U:215:CYS:HA	2.56	0.41
2:U:233:ASN:ND2	2:U:260:HIS:CE1	2.89	0.41

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	L	210/219 (96%)	176 (84%)	25 (12%)	9 (4%)	2	17
2	U	281/283 (99%)	242 (86%)	33 (12%)	6 (2%)	5	29
3	H	210/221 (95%)	183 (87%)	23 (11%)	4 (2%)	6	32
All	All	701/723 (97%)	601 (86%)	81 (12%)	19 (3%)	6	25

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	153	PRO
1	L	20	SER
1	L	31	SER
1	L	42	LEU
1	L	93	CYS
2	U	257	SER
3	H	212	VAL
1	L	69	GLY
1	L	91	TYR
1	L	150	ASN
1	L	171	GLN
2	U	83	ARG
2	U	61	LEU
3	H	91	SER
3	H	178	SER
1	L	52	LEU
2	U	34	GLU
2	U	137	ARG
2	U	220	ASN

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	L	189/196 (96%)	179 (95%)	10 (5%)	20	42
2	U	250/250 (100%)	234 (94%)	16 (6%)	16	38
3	H	186/191 (97%)	180 (97%)	6 (3%)	34	55
All	All	625/637 (98%)	593 (95%)	32 (5%)	23	43

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	4	MET
1	L	30	VAL
1	L	35	LYS
1	L	40	TRP

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Mol	Chain	Res	Type
1	L	41	TYR
1	L	54	TYR
1	L	65	ASP
1	L	136	SER
1	L	159	GLU
1	L	175	ASP
2	U	40	LEU
2	U	50	LYS
2	U	57	TYR
2	U	78	GLN
2	U	126	VAL
2	U	127	THR
2	U	145	ARG
2	U	171	CYS
2	U	181	ILE
2	U	183	GLU
2	U	193	GLN
2	U	221	GLN
2	U	226	THR
2	U	229	HIS
2	U	260	HIS
2	U	263	VAL
3	H	11	LEU
3	H	115	VAL
3	H	153	PRO
3	H	154	GLU
3	H	180	LEU
3	H	183	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	32	ASN
1	L	43	GLN
1	L	142	ASN
1	L	143	ASN
1	L	166	ASN
2	U	5	GLN
2	U	128	HIS
2	U	166	HIS
2	U	229	HIS
2	U	233	ASN

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Mol	Chain	Res	Type
3	H	19	ASN
3	H	43	GLN
3	H	82	ASN
3	H	111	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

5 monosaccharides are 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$
4	NAG	A	1	4,2	14,14,15	0.87	0	17,19,21	1.51	2 (11%)
4	NAG	A	2	4	14,14,15	1.18	2 (14%)	17,19,21	0.86	1 (5%)
4	BMA	A	3	4	11,11,12	1.18	1 (9%)	15,15,17	0.92	0
5	NAG	B	1	5,2	14,14,15	1.37	3 (21%)	17,19,21	0.86	0
5	NAG	B	2	5	14,14,15	1.50	3 (21%)	17,19,21	1.68	3 (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	NAG	A	1	4,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	2	4	-	0/6/23/26	0/1/1/1
4	BMA	A	3	4	-	0/2/19/22	0/1/1/1
5	NAG	B	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	B	2	5	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2	NAG	C1-C2	3.43	1.57	1.52
5	B	1	NAG	O4-C4	2.52	1.49	1.43
5	B	2	NAG	O5-C5	2.45	1.48	1.43
5	B	1	NAG	O5-C5	2.45	1.48	1.43
4	A	2	NAG	O4-C4	2.39	1.48	1.43
4	A	2	NAG	O5-C5	2.27	1.47	1.43
5	B	2	NAG	O5-C1	2.26	1.47	1.43
5	B	1	NAG	C1-C2	2.19	1.55	1.52
4	A	3	BMA	O5-C5	2.04	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2	NAG	C1-O5-C5	4.96	118.84	112.19
4	A	1	NAG	C1-O5-C5	-4.08	106.71	112.19
5	B	2	NAG	O5-C5-C4	-2.75	104.15	110.83
4	A	1	NAG	C3-C4-C5	2.33	114.46	110.23
5	B	2	NAG	C3-C4-C5	-2.06	106.50	110.23
4	A	2	NAG	O4-C4-C5	-2.02	104.35	109.32

There are no chirality outliers.

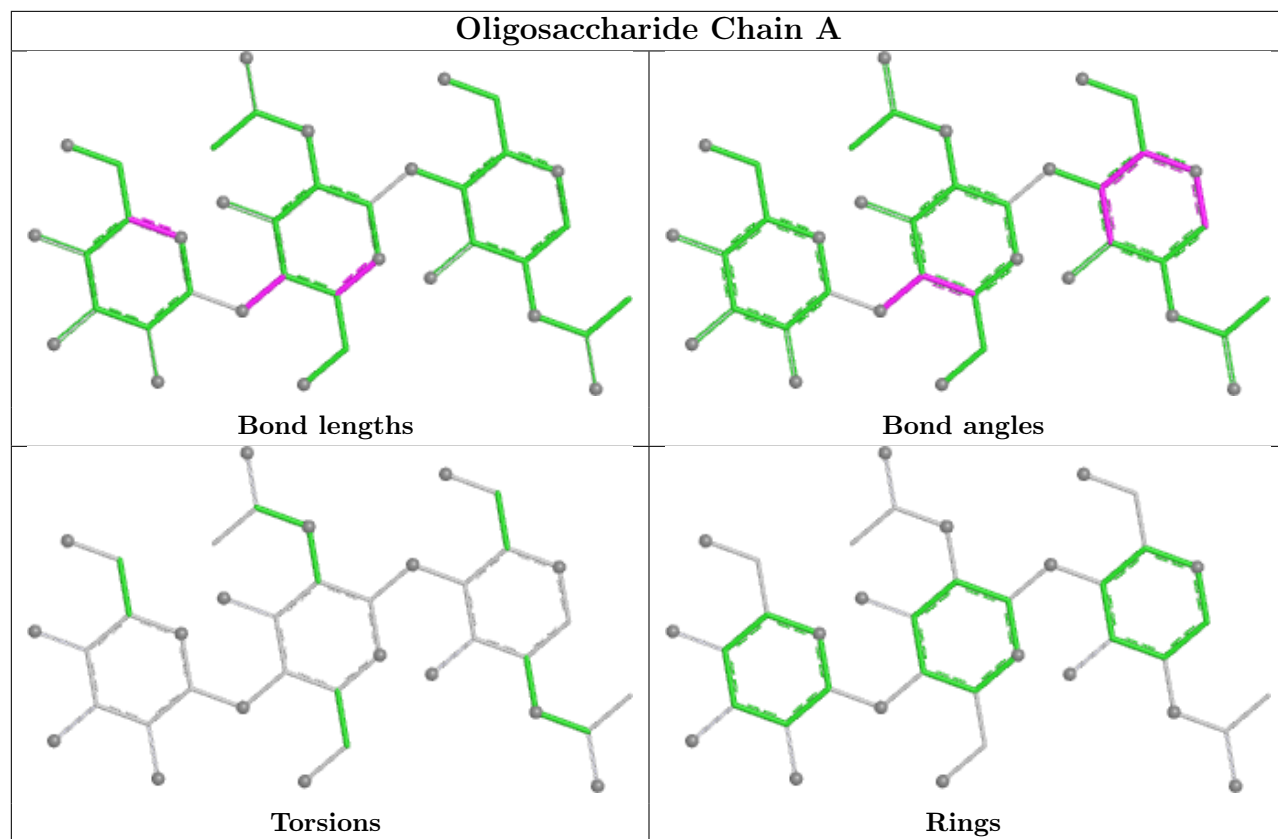
All (2) torsion outliers are listed below:

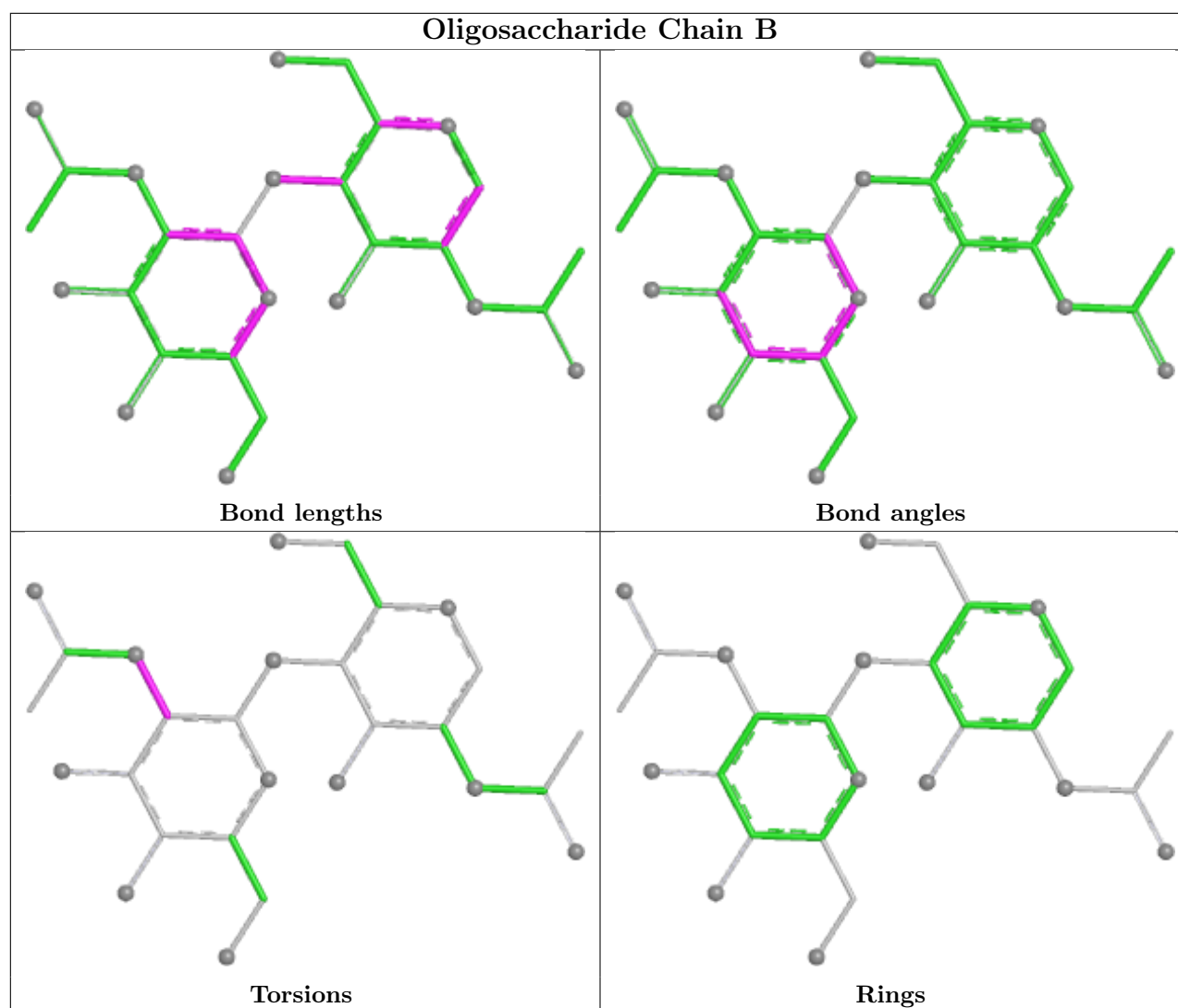
Mol	Chain	Res	Type	Atoms
5	B	2	NAG	C1-C2-N2-C7
5	B	2	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

2 ligands are 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	$\# Z > 2$
6	NAG	U	301	2	14,14,15	1.39	3 (21%)	17,19,21	0.66	0
6	NAG	U	302	2	14,14,15	1.28	1 (7%)	17,19,21	0.80	0

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
6	NAG	U	301	2	-	0/6/23/26	0/1/1/1
6	NAG	U	302	2	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	U	301	NAG	O5-C5	2.99	1.49	1.43
6	U	302	NAG	O5-C5	2.91	1.49	1.43
6	U	301	NAG	O5-C1	2.30	1.47	1.43
6	U	301	NAG	C1-C2	2.22	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	U	302	NAG	C4-C5-C6-O6
6	U	302	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

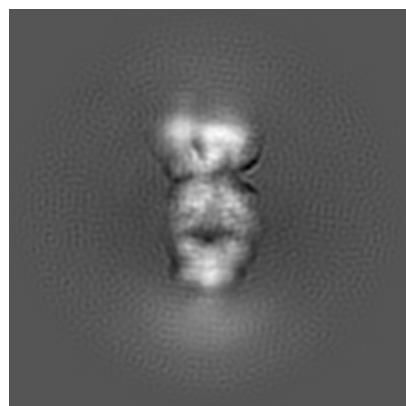
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72761. These allow visual inspection of the internal detail of the map and identification of artifacts.

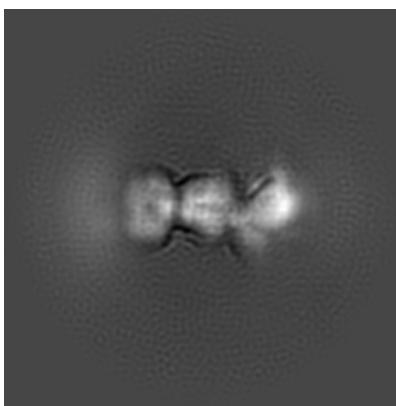
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

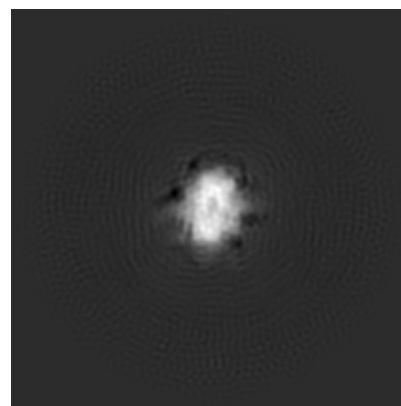
6.1.1 Primary map



X

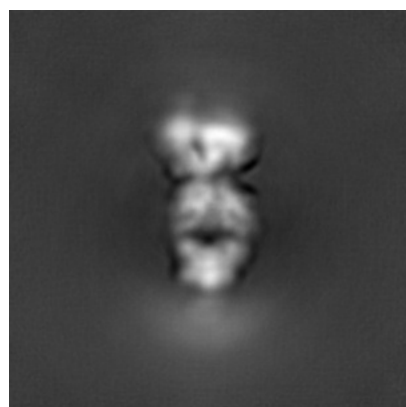


Y

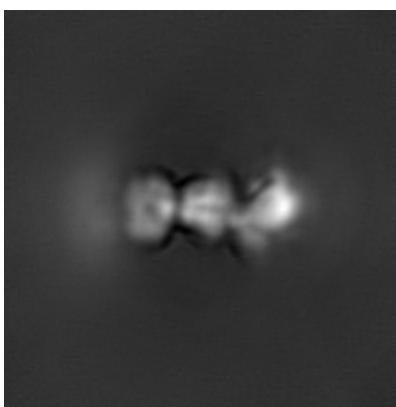


Z

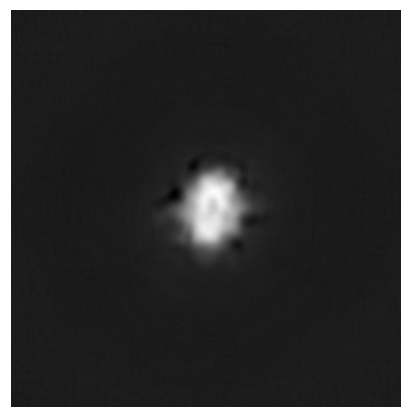
6.1.2 Raw map



X



Y

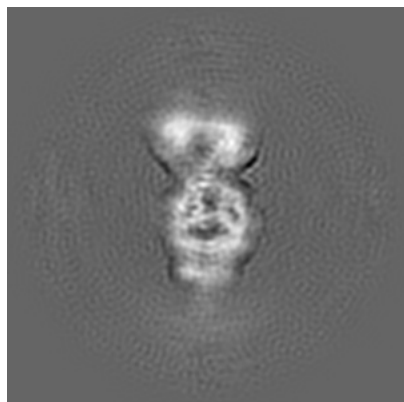


Z

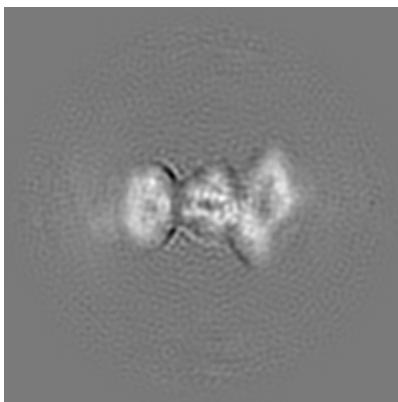
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

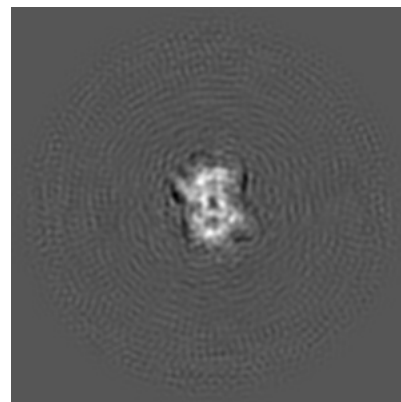
6.2.1 Primary map



X Index: 180

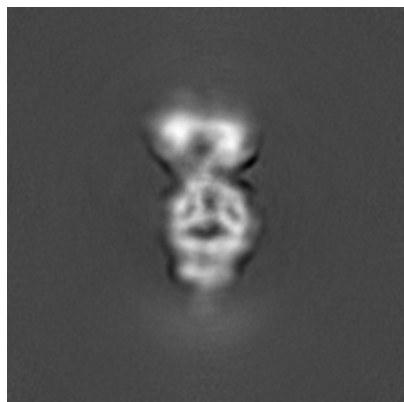


Y Index: 180

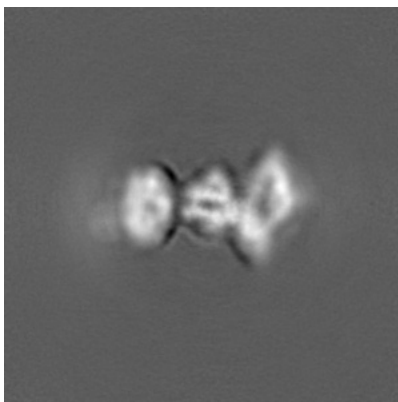


Z Index: 180

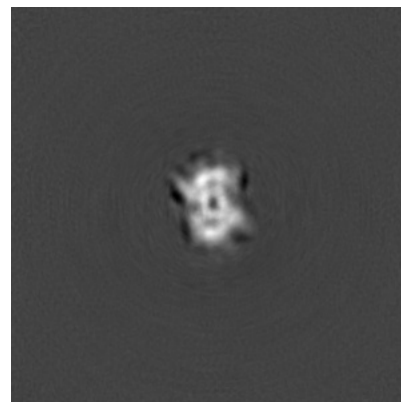
6.2.2 Raw map



X Index: 180



Y Index: 180

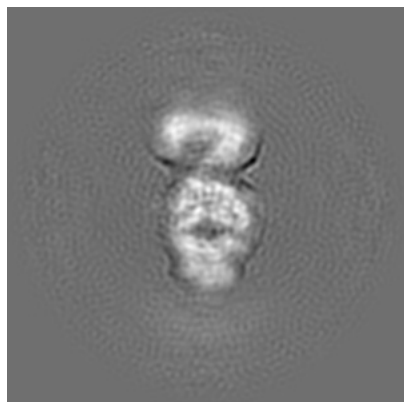


Z Index: 180

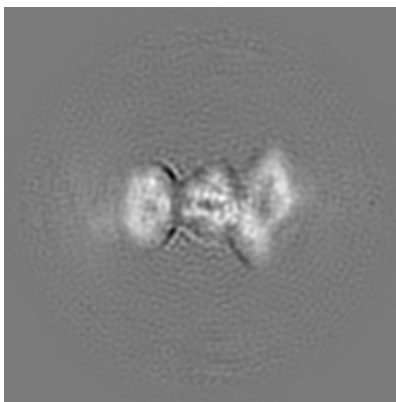
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

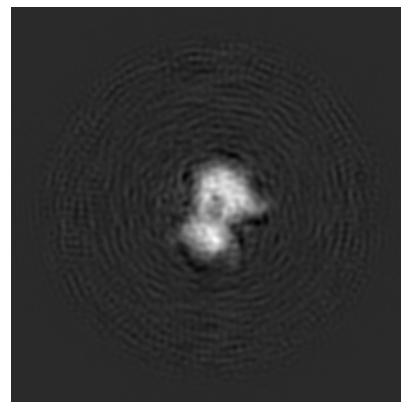
6.3.1 Primary map



X Index: 186

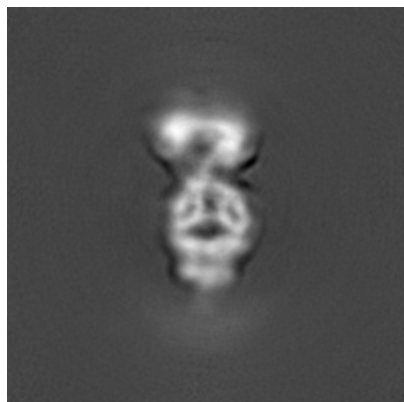


Y Index: 180

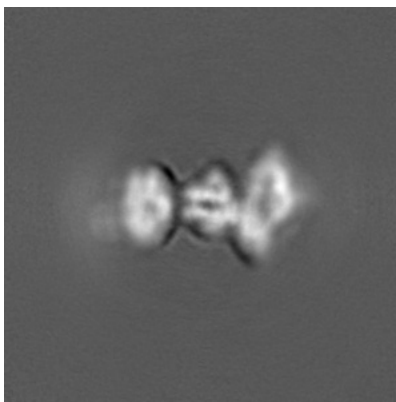


Z Index: 247

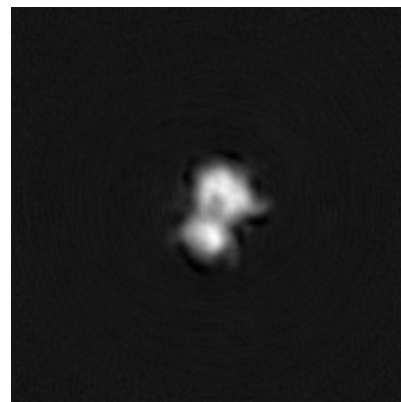
6.3.2 Raw map



X Index: 182



Y Index: 182

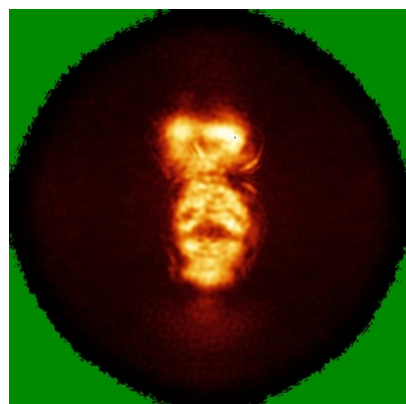


Z Index: 248

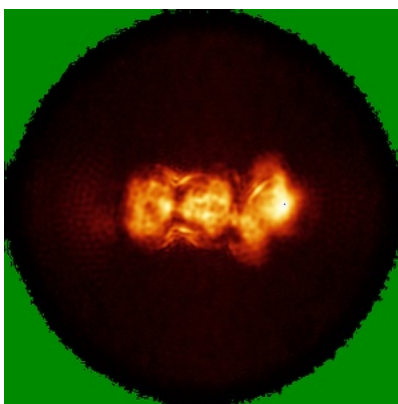
The images above show the largest variance slices of the map in three orthogonal directions.

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

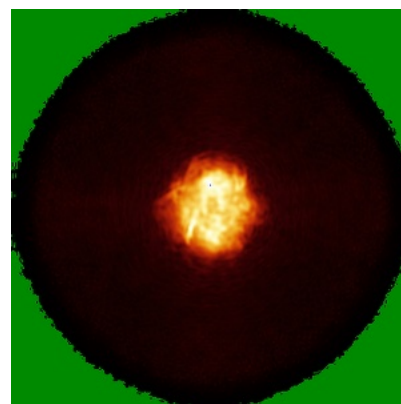
6.4.1 Primary map



X

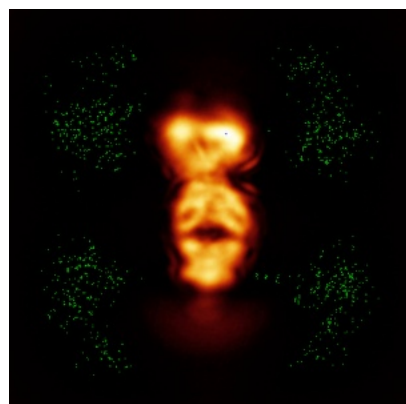


Y

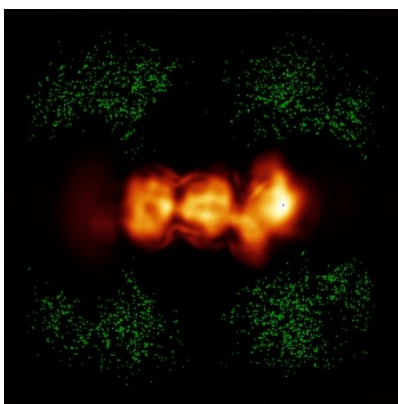


Z

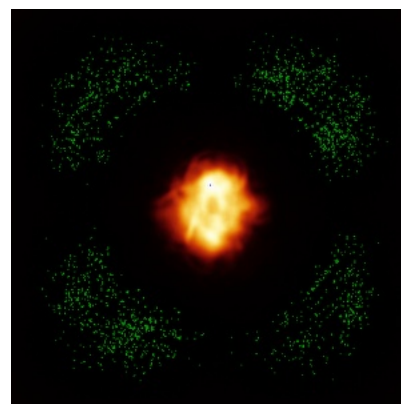
6.4.2 Raw map



X



Y

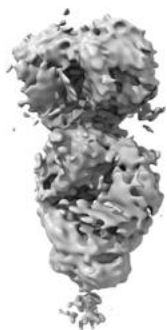


Z

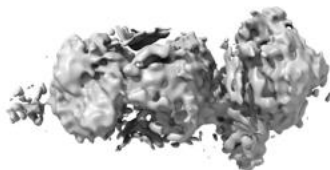
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

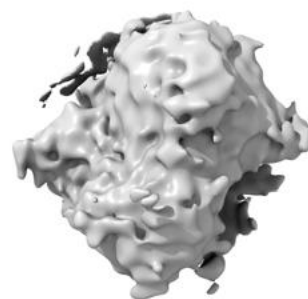
6.5.1 Primary map



X



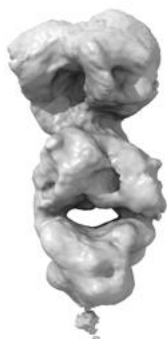
Y



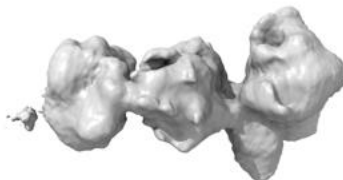
Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

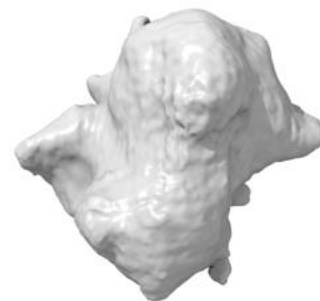
6.5.2 Raw map



X



Y



Z

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.

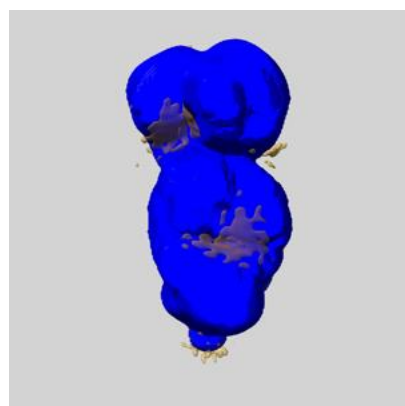
6.6 Mask visualisation [i](#)

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

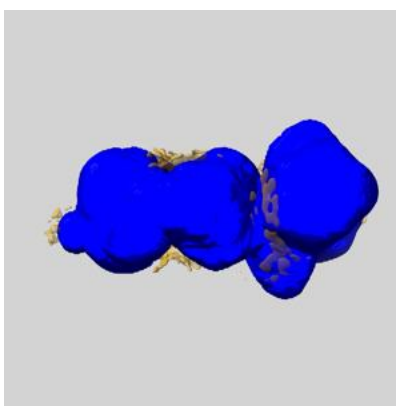
A mask typically either:

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

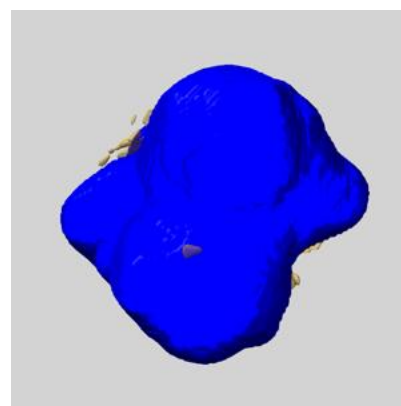
6.6.1 emd_72761_msk_1.map [i](#)



X



Y

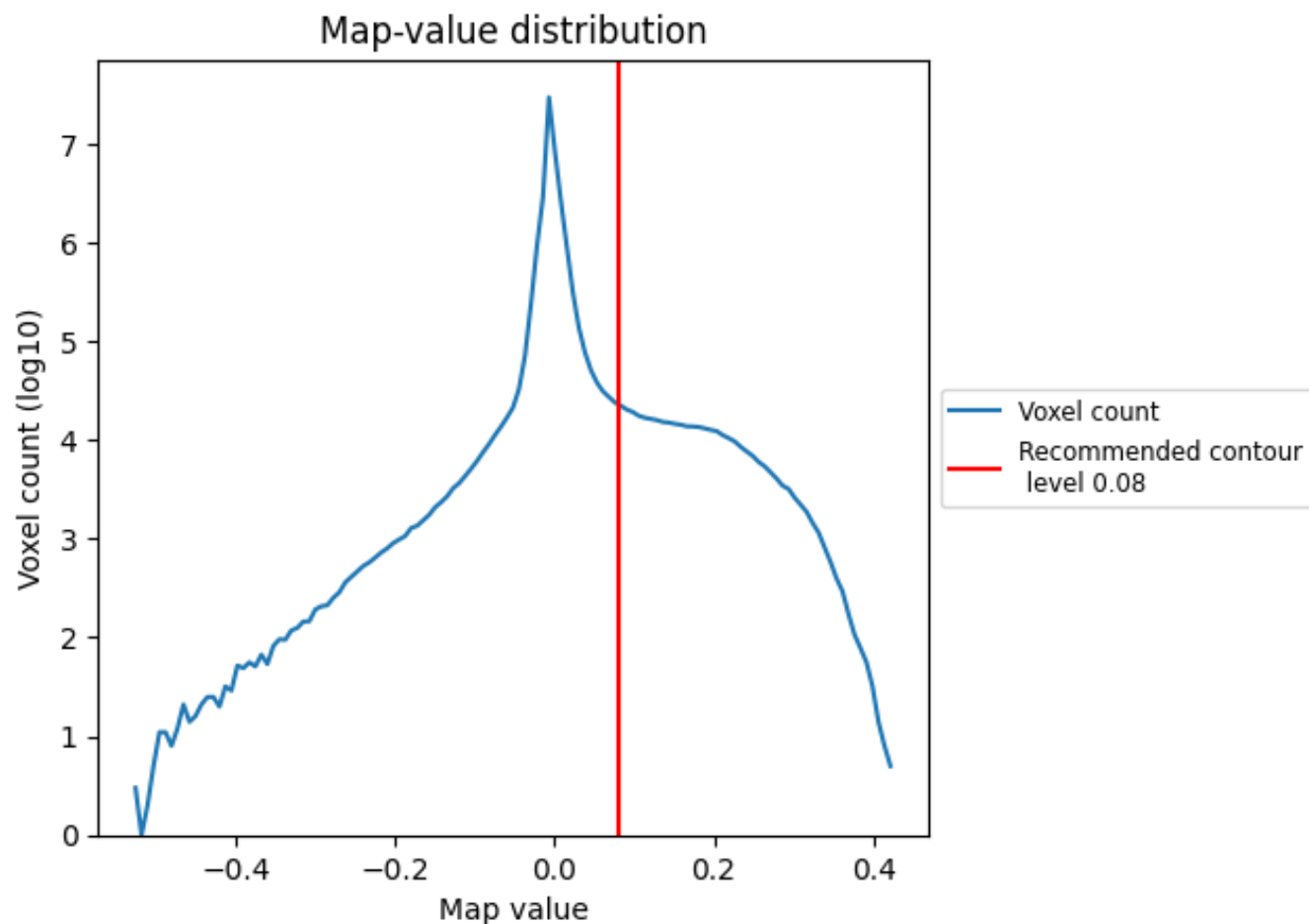


Z

7 Map analysis [i](#)

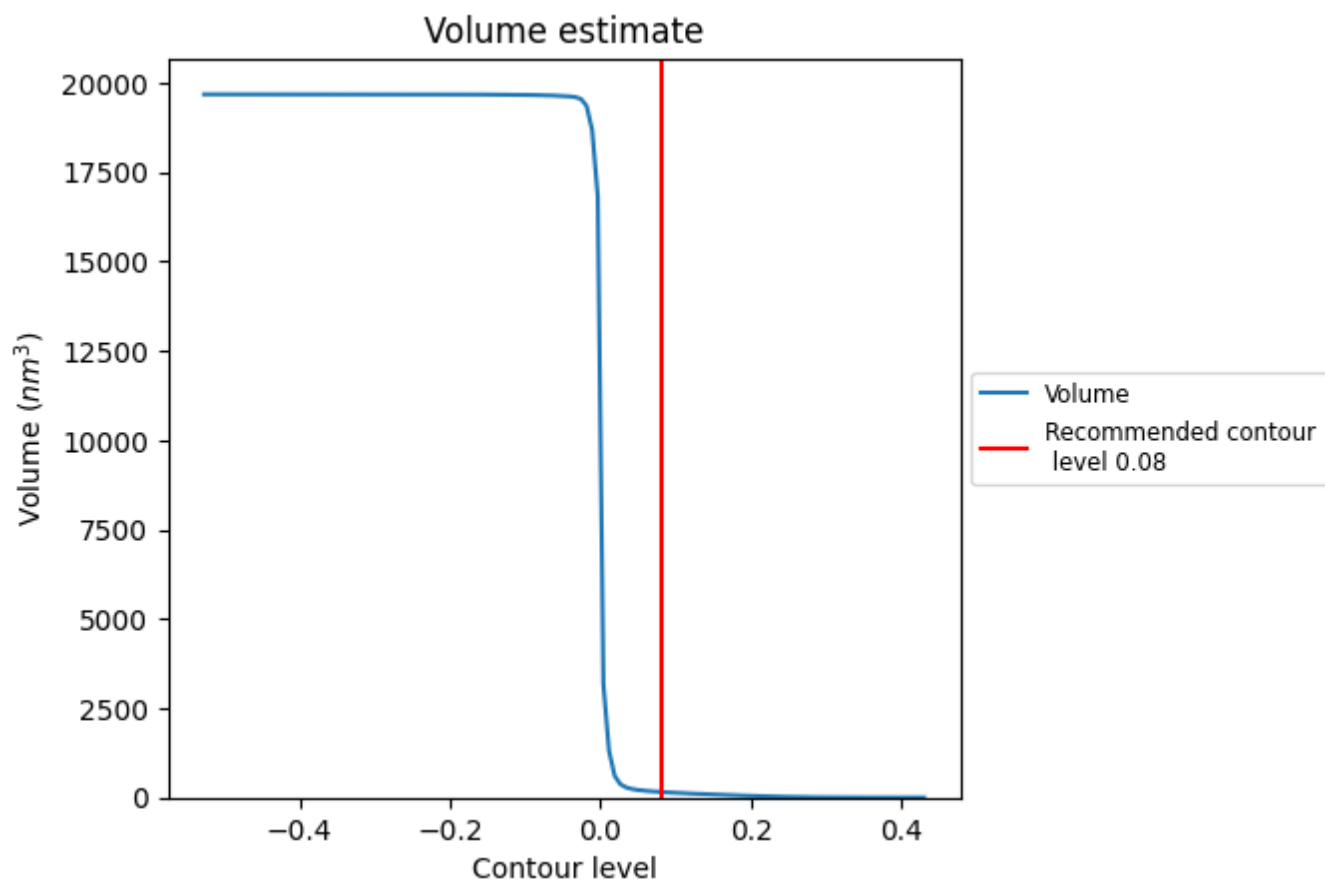
This section contains the results of statistical analysis of the map.

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.

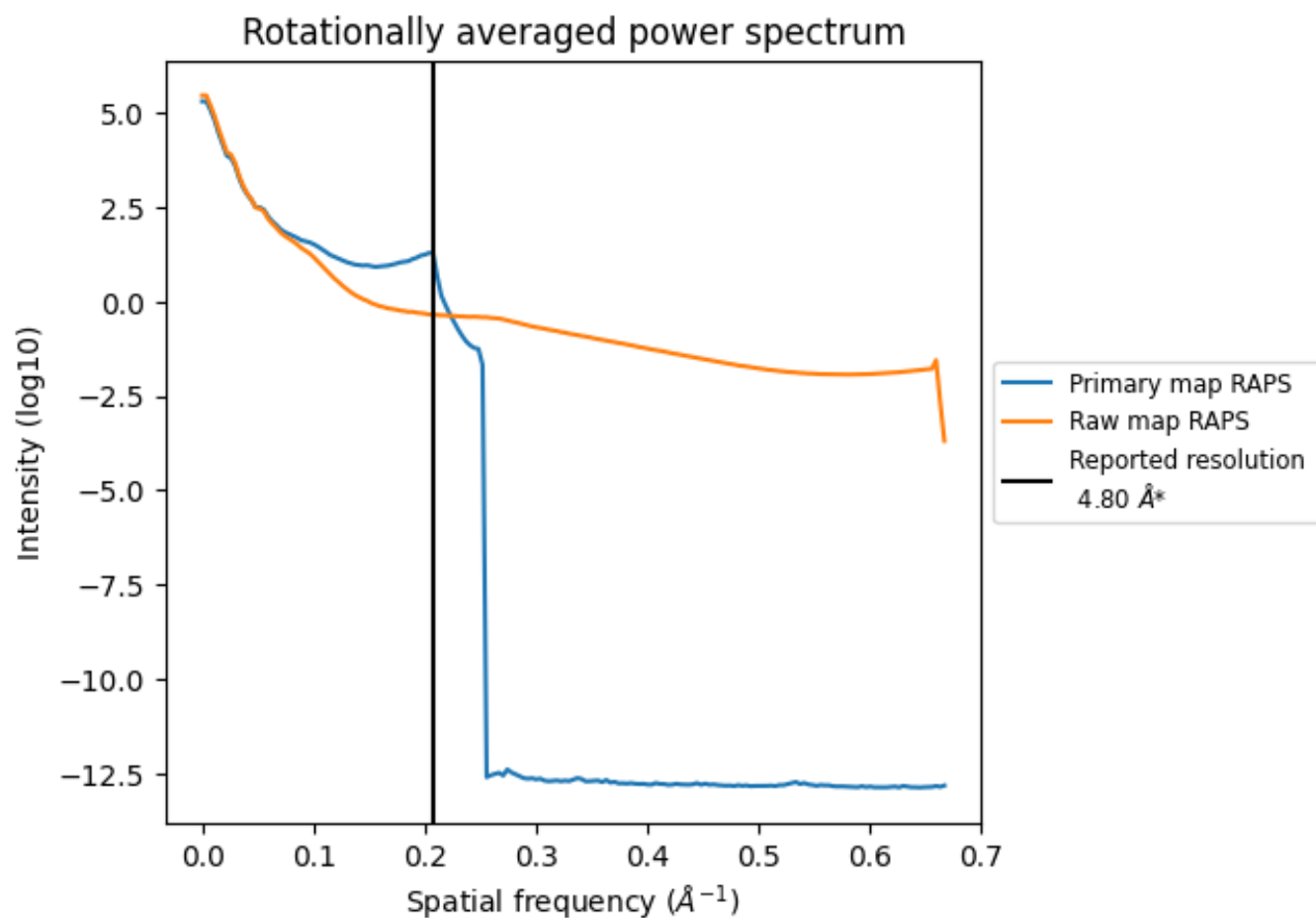
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 156 nm³; this corresponds to an approximate mass of 141 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 ⓘ

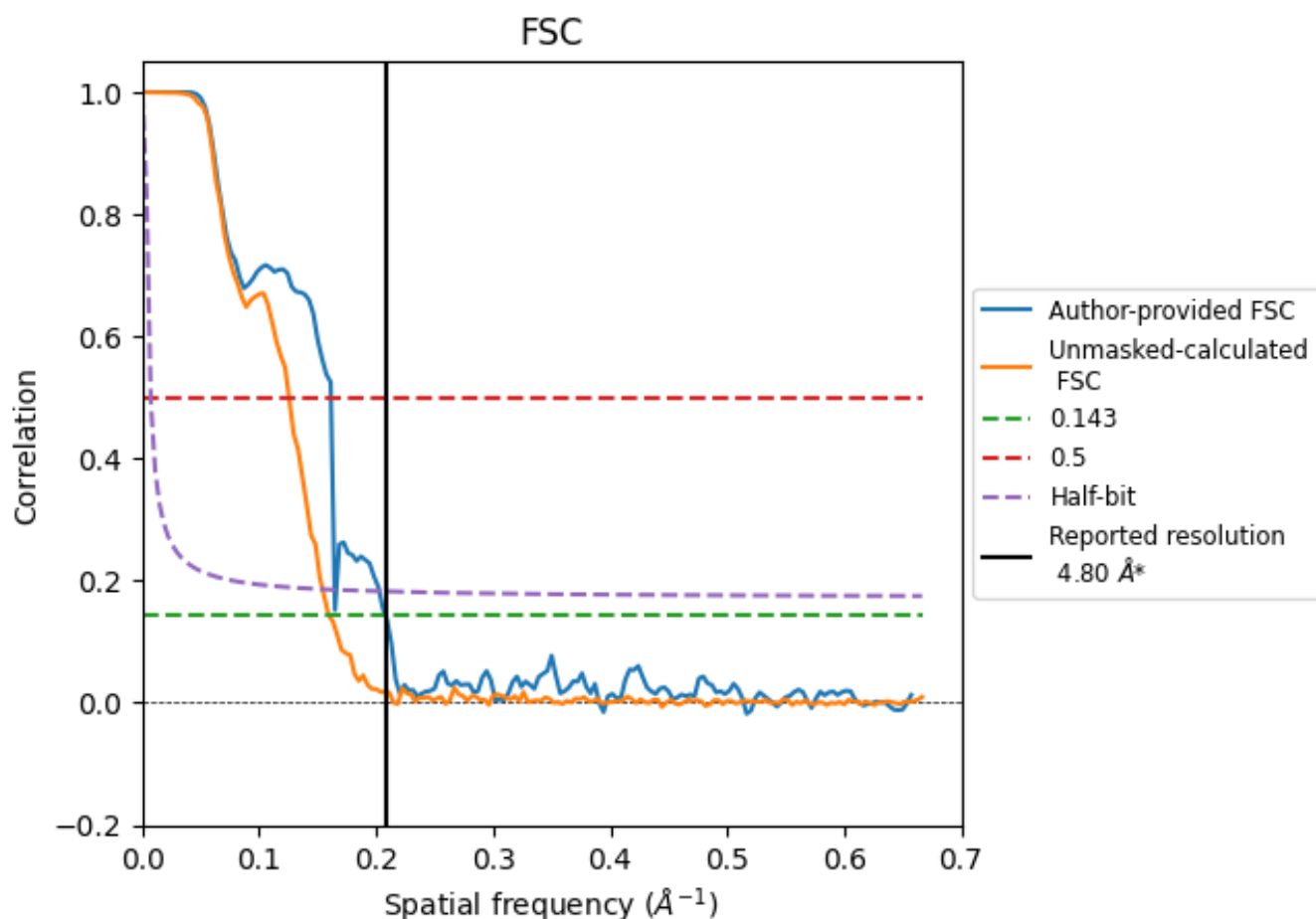


*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

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 0.208 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

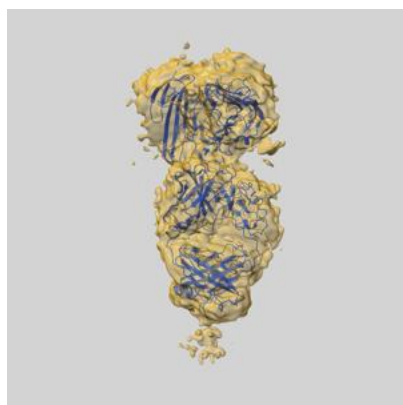
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.81	6.20	6.08
Unmasked-calculated*	6.27	7.97	6.49

*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 6.27 differs from the reported value 4.8 by more than 10 %

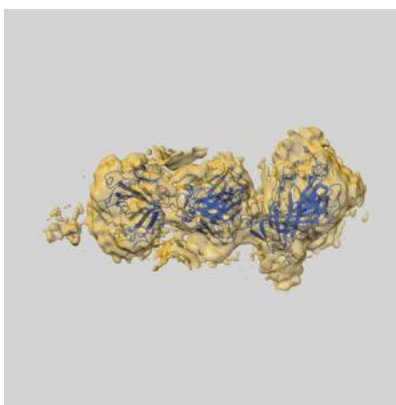
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72761 and PDB model 9YC6. Per-residue inclusion information can be found in section [3](#) on page [6](#).

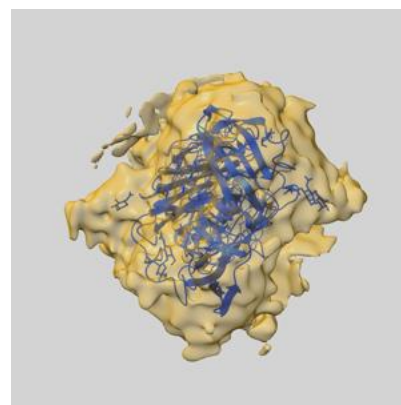
9.1 Map-model overlay [i](#)



X



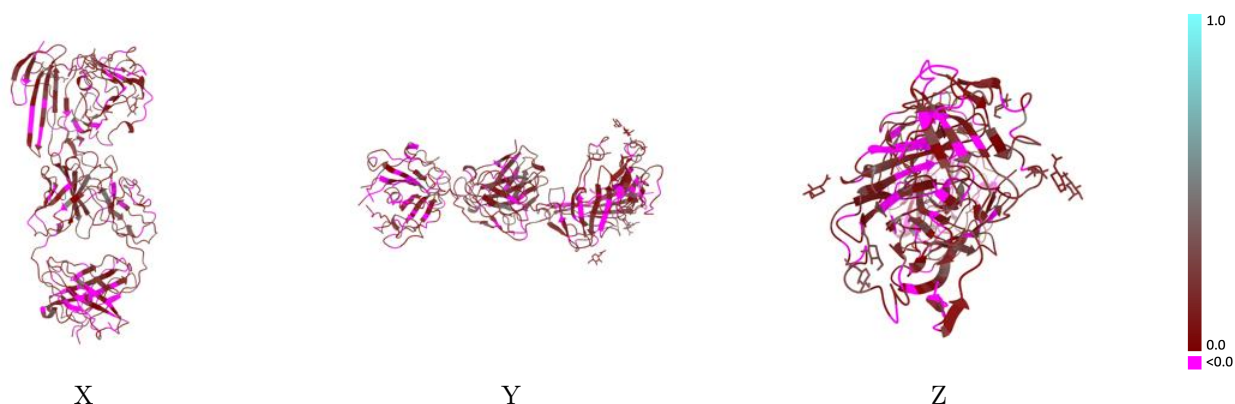
Y



Z

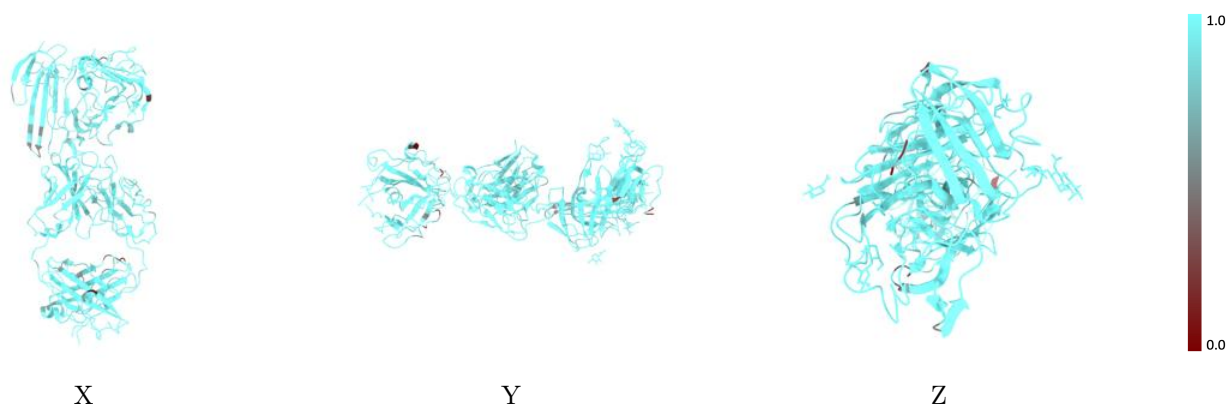
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



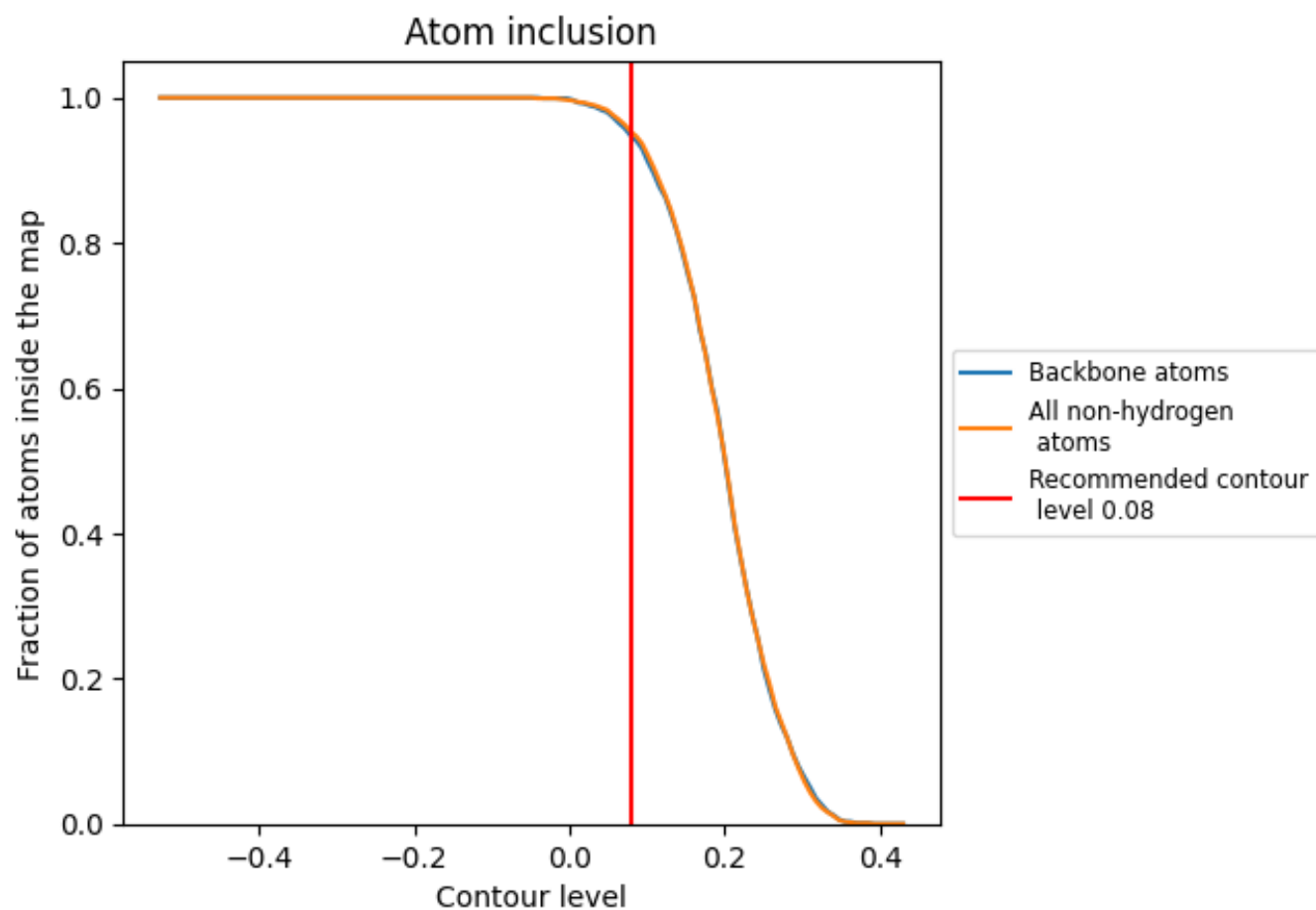
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 95% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9520	0.1190
A	1.0000	0.1810
B	1.0000	0.2900
H	0.9680	0.1370
L	0.9470	0.1110
U	0.9630	0.1090

