



wwPDB EM Validation Summary Report ⓘ

Oct 1, 2026 – 04:57 PM EDT

PDB ID : 9ZAK / pdb_00009zak
EMDB ID : EMD-73966
Title : Cryo-EM structure of Leishmania tarentolae respiratory complex IV (cytochrome c oxidase dimer)
Authors : Liao, Y.T.; Chao, L.
Deposited on : 2025-11-19
Resolution : 3.21 Å(reported)
Based on initial model : .

This is a wwPDB EM Validation Summary 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:

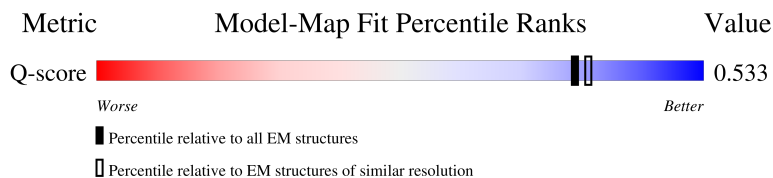
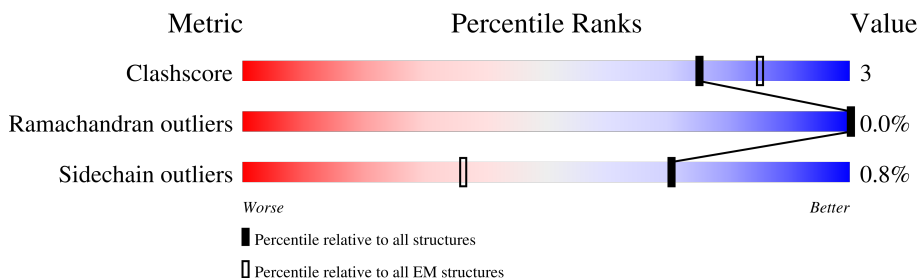
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.2
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.51

1 Overall quality at a glance

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

The reported resolution of this entry is 3.21 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.



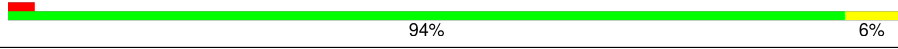
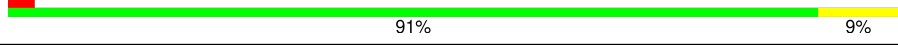
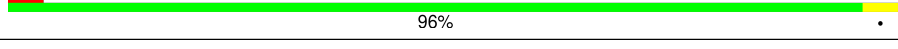
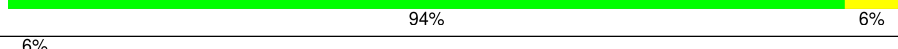
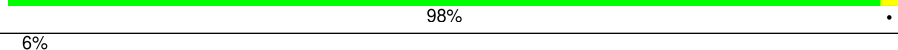
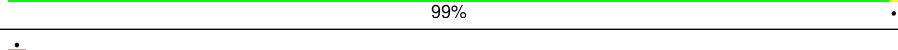
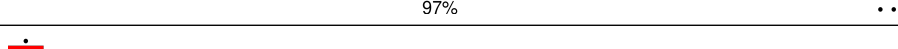
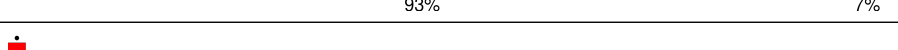
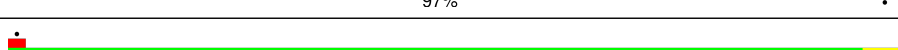
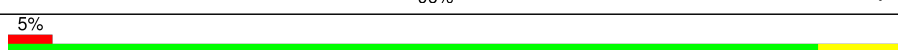
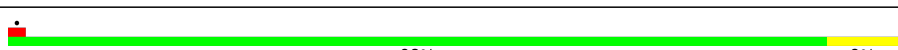
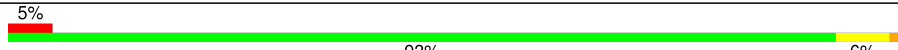
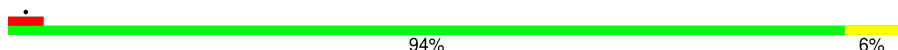
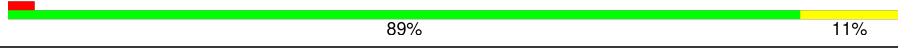
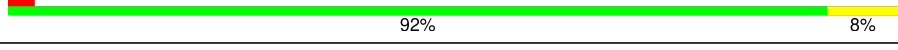
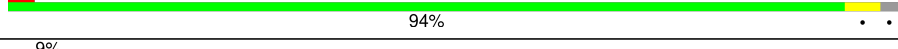
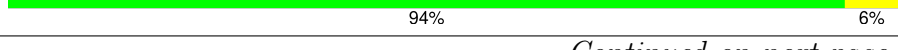
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14613 (2.71 - 3.71)

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	223	5% 93% 7%
1	a	223	5% 94% 5%
2	B	179	9% 97% .
2	b	179	9% 93% 7%

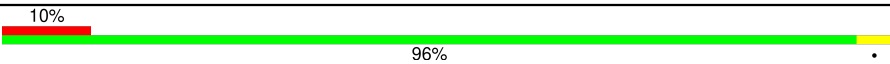
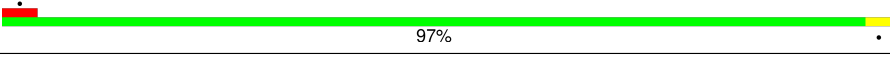
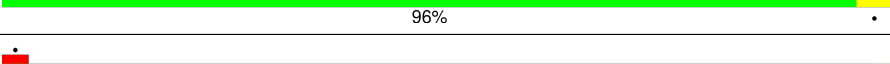
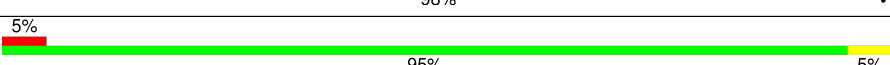
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Mol	Chain	Length	Quality of chain
3	C	210	
3	c	210	
4	D	157	
4	d	157	
5	E	200	
5	e	200	
6	F	127	
6	f	127	
7	G	107	
7	g	107	
8	H	165	
8	h	165	
9	K	202	
9	k	202	
10	L	95	
10	l	95	
11	M	110	
11	m	110	
12	N	549	
12	n	549	
13	O	287	
13	o	287	
14	P	93	
14	p	93	
15	Q	82	

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Mol	Chain	Length	Quality of chain
15	q	82	
16	R	311	
16	r	311	
17	S	128	
17	s	128	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	HEA	n	602	-	-	X	-

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 53313 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 P27 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	223	Total	C	N	O	S	0	0
			1830	1182	322	318	8		
1	a	223	Total	C	N	O	S	0	0
			1830	1182	322	318	8		

- Molecule 2 is a protein called Cytochrome c oxidase subunit V, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	179	Total	C	N	O	S	0	0
			1431	911	242	271	7		
2	b	179	Total	C	N	O	S	0	0
			1431	911	242	271	7		

- Molecule 3 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	210	Total	C	N	O	S	0	0
			1689	1142	250	280	17		
3	c	210	Total	C	N	O	S	0	0
			1689	1142	250	280	17		

- Molecule 4 is a protein called Cytochrome C oxidase subunit VI, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	157	Total	C	N	O	S	0	0
			1362	879	239	234	10		
4	d	157	Total	C	N	O	S	0	0
			1362	879	239	234	10		

- Molecule 5 is a protein called Hypothetical protein, conserved, LtaP04.0630.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	200	Total	C	N	O	S	0	0
			1639	1053	277	292	17		
5	e	200	Total	C	N	O	S	0	0
			1639	1053	277	292	17		

- Molecule 6 is a protein called Cytochrome c oxidase VIII, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	127	Total	C	N	O	S	0	0
			1094	718	183	183	10		
6	f	127	Total	C	N	O	S	0	0
			1094	718	183	183	10		

- Molecule 7 is a protein called Hypothetical protein, conserved, LtaP09.0030.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	107	Total	C	N	O	S	0	0
			872	555	163	145	9		
7	g	107	Total	C	N	O	S	0	0
			872	555	163	145	9		

- Molecule 8 is a protein called Cytochrome c oxidase VII, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	165	Total	C	N	O	S	0	0
			1355	889	226	233	7		
8	h	165	Total	C	N	O	S	0	0
			1355	889	226	233	7		

- Molecule 9 is a protein called Cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	202	Total	C	N	O	S	0	0
			1670	1062	278	318	12		
9	k	202	Total	C	N	O	S	0	0
			1670	1062	278	318	12		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	95	Total	C	N	O	S	0	0
			824	530	147	145	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	95	Total	C	N	O	S	0	0
			824	530	147	145	2		

- Molecule 11 is a protein called Cytochrome c oxidase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	110	Total	C	N	O	S	0	0
			850	551	142	151	6		
11	m	110	Total	C	N	O	S	0	0
			850	551	142	151	6		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	549	Total	C	N	O	S	0	0
			4475	3097	637	694	47		
12	n	549	Total	C	N	O	S	0	0
			4475	3097	637	694	47		

- Molecule 13 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	287	Total	C	N	O	S	0	0
			2422	1713	329	351	29		
13	o	287	Total	C	N	O	S	0	0
			2422	1713	329	351	29		

- Molecule 14 is a protein called Hypothetical protein, conserved, LtaP33.2260.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	93	Total	C	N	O	S	0	0
			738	466	122	143	7		
14	p	91	Total	C	N	O	S	0	0
			723	458	119	139	7		

- Molecule 15 is a protein called Hypothetical protein, conserved, LtaP36.1760.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	82	Total	C	N	O	S	0	0
			687	452	113	118	4		
15	q	82	Total	C	N	O	S	0	0
			687	452	113	118	4		

- Molecule 16 is a protein called Cytochrome c oxidase subunit iv.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	311	Total	C	N	O	S	0	0
			2529	1576	449	495	9		
16	r	311	Total	C	N	O	S	0	0
			2529	1576	449	495	9		

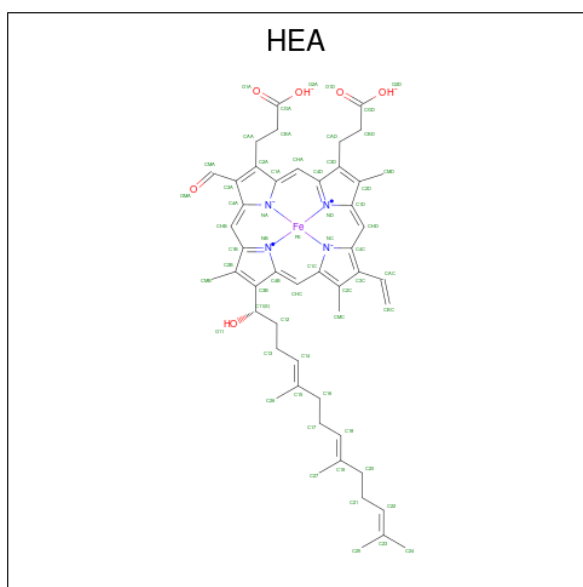
- Molecule 17 is a protein called Cytochrome c oxidase assembly factor like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	128	Total	C	N	O	S	0	0
			1076	706	195	170	5		
17	s	128	Total	C	N	O	S	0	0
			1076	706	195	170	5		

- Molecule 18 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
18	N	1	Total	Cu	0
			1	1	
18	n	1	Total	Cu	0
			1	1	

- Molecule 19 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).

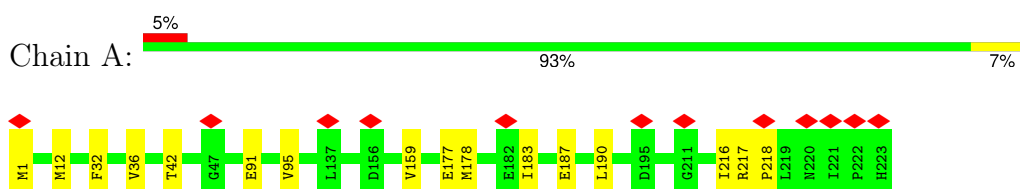


Mol	Chain	Residues	Atoms					AltConf
19	N	1	Total 60	C 49	Fe 1	N 4	O 6	0
19	N	1	Total 60	C 49	Fe 1	N 4	O 6	0
19	n	1	Total 60	C 49	Fe 1	N 4	O 6	0
19	n	1	Total 60	C 49	Fe 1	N 4	O 6	0

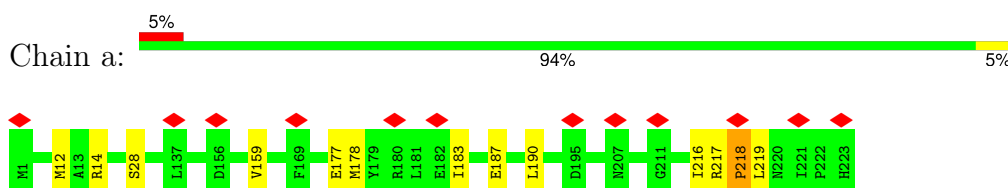
3 Residue-property plots

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.

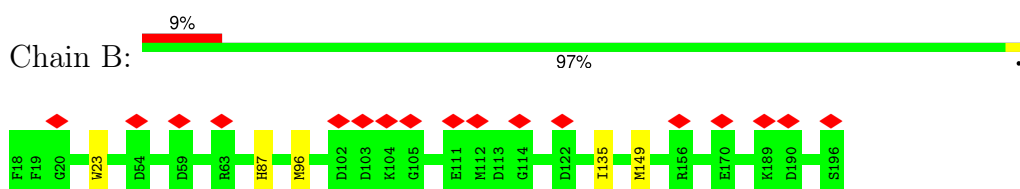
- Molecule 1: P27 protein



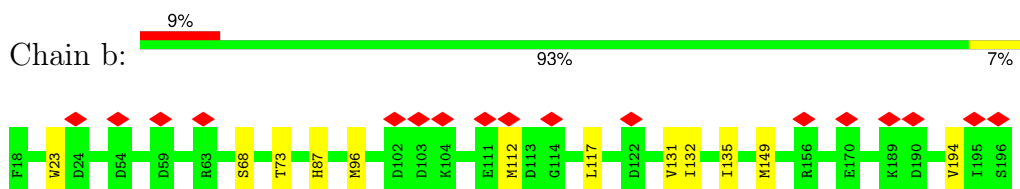
- Molecule 1: P27 protein



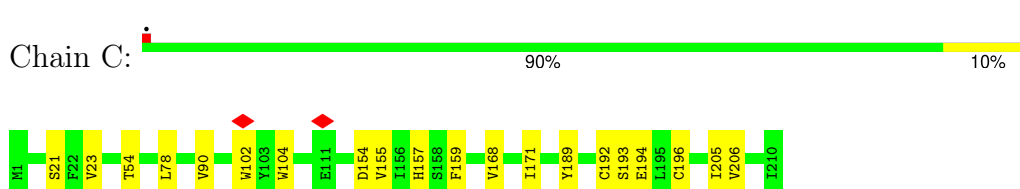
- Molecule 2: Cytochrome c oxidase subunit V, putative



- Molecule 2: Cytochrome c oxidase subunit V, putative



- Molecule 3: Cytochrome c oxidase subunit 2

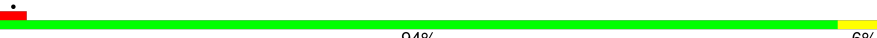


- Molecule 3: Cytochrome c oxidase subunit 2

Chain c:  89% 10%



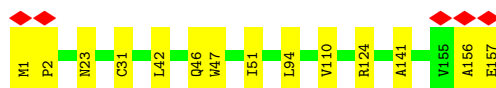
- Molecule 4: Cytochrome C oxidase subunit VI, putative

Chain D:  94% 6%



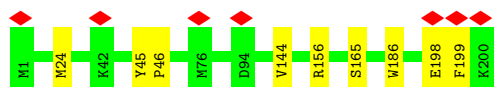
- Molecule 4: Cytochrome C oxidase subunit VI, putative

Chain d:  91% 9%



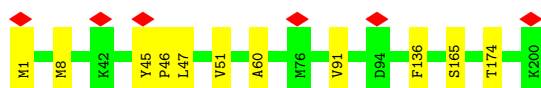
- Molecule 5: Hypothetical protein, conserved, LtaP04.0630

Chain E:  96%



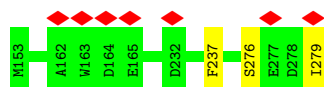
- Molecule 5: Hypothetical protein, conserved, LtaP04.0630

Chain e:  94% 6%



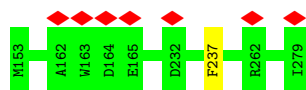
- Molecule 6: Cytochrome c oxidase VIII, putative

Chain F:  6% 98%

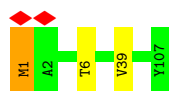


- Molecule 6: Cytochrome c oxidase VIII, putative

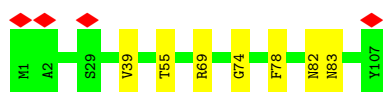
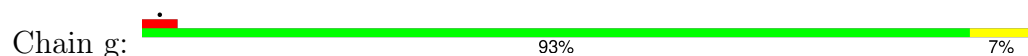
Chain f:  6% 99%



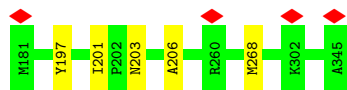
- Molecule 7: Hypothetical protein, conserved, LtaP09.0030



- Molecule 7: Hypothetical protein, conserved, LtaP09.0030



- Molecule 8: Cytochrome c oxidase VII, putative



- Molecule 8: Cytochrome c oxidase VII, putative



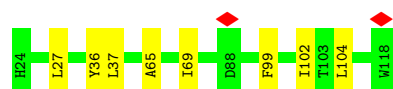
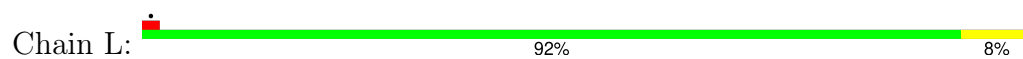
- Molecule 9: Cytochrome-c oxidase



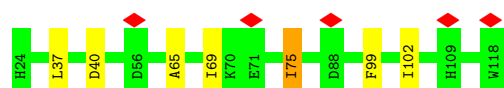
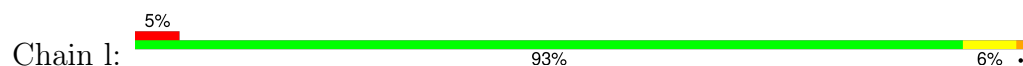
- Molecule 9: Cytochrome-c oxidase



- Molecule 10: Cytochrome c oxidase subunit 10



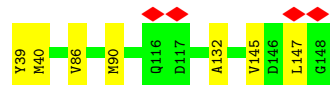
- Molecule 10: Cytochrome c oxidase subunit 10



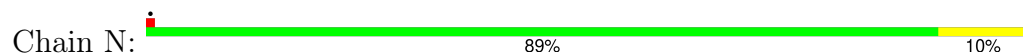
- Molecule 11: Cytochrome c oxidase subunit I



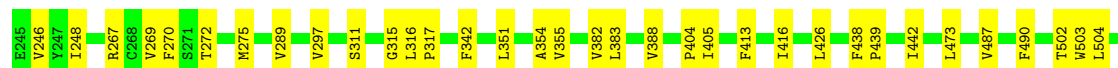
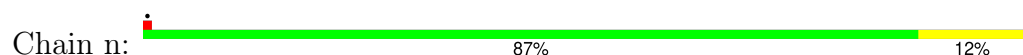
- Molecule 11: Cytochrome c oxidase subunit I

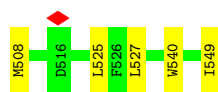


- Molecule 12: Cytochrome c oxidase subunit 1

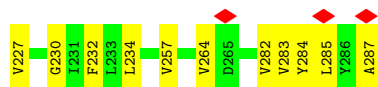
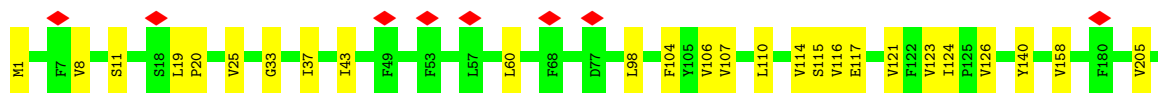
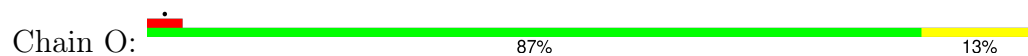


- Molecule 12: Cytochrome c oxidase subunit 1

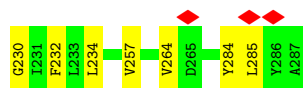
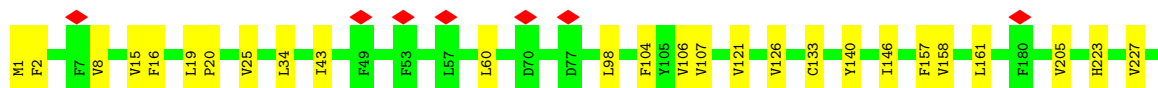
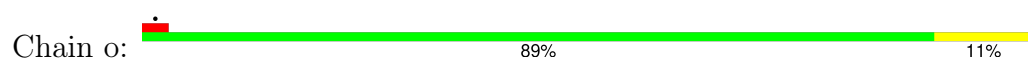




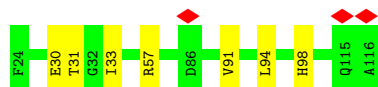
- Molecule 13: Cytochrome c oxidase subunit 3



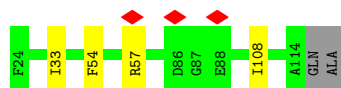
- Molecule 13: Cytochrome c oxidase subunit 3



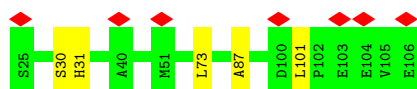
- Molecule 14: Hypothetical protein, conserved, LtaP33.2260



- Molecule 14: Hypothetical protein, conserved, LtaP33.2260



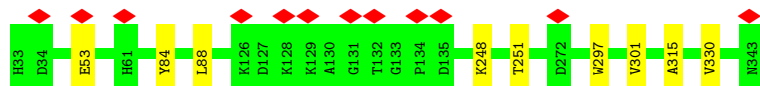
- Molecule 15: Hypothetical protein, conserved, LtaP36.1760



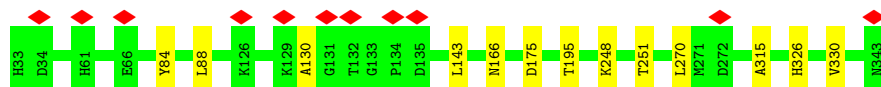
- Molecule 15: Hypothetical protein, conserved, LtaP36.1760



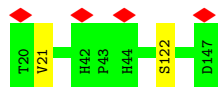
- Molecule 16: Cytochrome c oxidase subunit iv



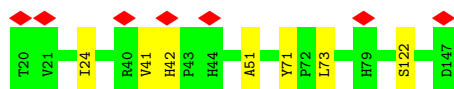
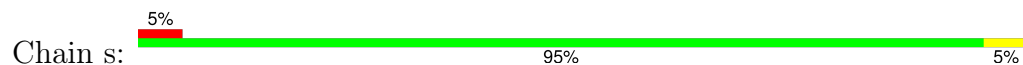
- Molecule 16: Cytochrome c oxidase subunit iv



- Molecule 17: Cytochrome c oxidase assembly factor like protein



- Molecule 17: Cytochrome c oxidase assembly factor like protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	5392	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 ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.289	Depositor
Minimum map value	-0.134	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0728	Depositor
Map size (Å)	471.04, 471.04, 471.04	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.736, 0.736, 0.736	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.16	0/1884	0.29	0/2560
1	a	0.16	0/1884	0.30	0/2560
2	B	0.16	0/1463	0.28	0/1978
2	b	0.16	0/1463	0.29	0/1978
3	C	0.19	0/1737	0.33	0/2365
3	c	0.25	0/1737	0.49	4/2365 (0.2%)
4	D	0.17	0/1412	0.29	0/1905
4	d	0.17	0/1412	0.31	0/1905
5	E	0.17	0/1681	0.32	0/2263
5	e	0.17	0/1681	0.30	0/2263
6	F	0.15	0/1138	0.28	0/1539
6	f	0.15	0/1138	0.30	0/1539
7	G	0.17	0/902	0.29	0/1213
7	g	0.17	0/902	0.29	0/1213
8	H	0.16	0/1407	0.30	0/1917
8	h	0.15	0/1407	0.28	0/1917
9	K	0.18	0/1731	0.34	0/2365
9	k	0.18	0/1731	0.32	0/2365
10	L	0.17	0/853	0.29	0/1154
10	l	0.17	0/853	0.28	0/1154
11	M	0.17	0/880	0.32	0/1193
11	m	0.17	0/880	0.31	0/1193
12	N	0.19	0/4637	0.35	0/6310
12	n	0.19	0/4637	0.35	0/6310
13	O	0.18	0/2515	0.35	0/3421
13	o	0.18	0/2515	0.35	0/3421
14	P	0.16	0/749	0.25	0/1008
14	p	0.17	0/734	0.31	0/989
15	Q	0.16	0/711	0.34	0/961
15	q	0.16	0/711	0.35	0/961
16	R	0.16	0/2578	0.28	0/3481
16	r	0.15	0/2578	0.29	0/3481

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	S	0.18	0/1124	0.35	0/1526
17	s	0.17	0/1124	0.36	0/1526
All	All	0.17	0/54789	0.32	4/74299 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	195	LEU	N-CA-C	-8.85	96.64	110.36
3	c	194	GLU	N-CA-C	7.05	120.17	108.96
3	c	192	CYS	N-CA-C	5.96	119.68	108.65
3	c	195	LEU	CA-C-O	-5.78	114.83	121.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1830	0	1821	10	0
1	a	1830	0	1821	10	0
2	B	1431	0	1421	4	0
2	b	1431	0	1421	11	0
3	C	1689	0	1716	12	0
3	c	1689	0	1716	19	0
4	D	1362	0	1295	10	0
4	d	1362	0	1295	12	0
5	E	1639	0	1629	7	0
5	e	1639	0	1629	9	0
6	F	1094	0	1028	2	0
6	f	1094	0	1028	1	0
7	G	872	0	835	5	0
7	g	872	0	835	4	0
8	H	1355	0	1308	3	0
8	h	1355	0	1308	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	K	1670	0	1526	14	0
9	k	1670	0	1526	10	0
10	L	824	0	777	6	0
10	l	824	0	777	3	0
11	M	850	0	799	6	0
11	m	850	0	799	4	0
12	N	4475	0	4495	55	0
12	n	4475	0	4495	62	0
13	O	2422	0	2421	24	0
13	o	2422	0	2421	24	0
14	P	738	0	724	5	0
14	p	723	0	711	3	0
15	Q	687	0	656	5	0
15	q	687	0	656	4	0
16	R	2529	0	2453	6	0
16	r	2529	0	2453	9	0
17	S	1076	0	1023	1	0
17	s	1076	0	1023	7	0
18	N	1	0	0	0	0
18	n	1	0	0	0	0
19	N	120	0	108	18	0
19	n	120	0	108	33	0
All	All	53313	0	52057	321	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 3.

The worst 5 of 321 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:c:155:VAL:HG21	3:c:195:LEU:HD13	1.43	0.96
19:N:603:HEA:HHA	19:N:603:HEA:HBD1	1.56	0.87
3:c:26:VAL:HG11	19:n:603:HEA:H271	1.60	0.81
13:O:158:VAL:HG21	7:g:39:VAL:HG23	1.63	0.80
4:d:47:TRP:CZ2	4:d:51:ILE:HD11	2.18	0.79

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	221/223 (99%)	212 (96%)	9 (4%)	0	100	100
1	a	221/223 (99%)	211 (96%)	9 (4%)	1 (0%)	24	58
2	B	177/179 (99%)	175 (99%)	2 (1%)	0	100	100
2	b	177/179 (99%)	174 (98%)	3 (2%)	0	100	100
3	C	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
3	c	208/210 (99%)	202 (97%)	6 (3%)	0	100	100
4	D	155/157 (99%)	150 (97%)	5 (3%)	0	100	100
4	d	155/157 (99%)	147 (95%)	8 (5%)	0	100	100
5	E	198/200 (99%)	188 (95%)	10 (5%)	0	100	100
5	e	198/200 (99%)	194 (98%)	4 (2%)	0	100	100
6	F	125/127 (98%)	122 (98%)	3 (2%)	0	100	100
6	f	125/127 (98%)	125 (100%)	0	0	100	100
7	G	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
7	g	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
8	H	163/165 (99%)	155 (95%)	8 (5%)	0	100	100
8	h	163/165 (99%)	156 (96%)	7 (4%)	0	100	100
9	K	200/202 (99%)	192 (96%)	8 (4%)	0	100	100
9	k	200/202 (99%)	190 (95%)	10 (5%)	0	100	100
10	L	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
10	l	93/95 (98%)	91 (98%)	2 (2%)	0	100	100
11	M	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
11	m	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
12	N	547/549 (100%)	518 (95%)	29 (5%)	0	100	100
12	n	547/549 (100%)	520 (95%)	27 (5%)	0	100	100
13	O	285/287 (99%)	275 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	285/287 (99%)	276 (97%)	9 (3%)	0	100	100
14	P	91/93 (98%)	91 (100%)	0	0	100	100
14	p	89/93 (96%)	88 (99%)	1 (1%)	0	100	100
15	Q	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
15	q	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
16	R	309/311 (99%)	304 (98%)	5 (2%)	0	100	100
16	r	309/311 (99%)	305 (99%)	4 (1%)	0	100	100
17	S	126/128 (98%)	116 (92%)	9 (7%)	1 (1%)	16	48
17	s	126/128 (98%)	117 (93%)	9 (7%)	0	100	100
All	All	6380/6450 (99%)	6144 (96%)	234 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	S	21	VAL
1	a	218	PRO

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	197/197 (100%)	194 (98%)	3 (2%)	57	74
1	a	197/197 (100%)	197 (100%)	0	100	100
2	B	156/156 (100%)	155 (99%)	1 (1%)	78	83
2	b	156/156 (100%)	155 (99%)	1 (1%)	78	83
3	C	192/192 (100%)	186 (97%)	6 (3%)	35	63
3	c	192/192 (100%)	187 (97%)	5 (3%)	40	66
4	D	141/141 (100%)	141 (100%)	0	100	100
4	d	141/141 (100%)	141 (100%)	0	100	100
5	E	178/178 (100%)	177 (99%)	1 (1%)	78	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	178/178 (100%)	178 (100%)	0	100	100
6	F	113/113 (100%)	113 (100%)	0	100	100
6	f	113/113 (100%)	113 (100%)	0	100	100
7	G	88/88 (100%)	87 (99%)	1 (1%)	65	77
7	g	88/88 (100%)	86 (98%)	2 (2%)	44	68
8	H	139/139 (100%)	138 (99%)	1 (1%)	76	81
8	h	139/139 (100%)	138 (99%)	1 (1%)	76	81
9	K	182/182 (100%)	181 (100%)	1 (0%)	81	84
9	k	182/182 (100%)	182 (100%)	0	100	100
10	L	87/87 (100%)	86 (99%)	1 (1%)	65	77
10	l	87/87 (100%)	85 (98%)	2 (2%)	44	68
11	M	82/82 (100%)	82 (100%)	0	100	100
11	m	82/82 (100%)	81 (99%)	1 (1%)	63	77
12	N	487/487 (100%)	482 (99%)	5 (1%)	68	78
12	n	487/487 (100%)	481 (99%)	6 (1%)	63	77
13	O	270/270 (100%)	269 (100%)	1 (0%)	84	85
13	o	270/270 (100%)	268 (99%)	2 (1%)	76	81
14	P	80/80 (100%)	79 (99%)	1 (1%)	61	75
14	p	79/80 (99%)	79 (100%)	0	100	100
15	Q	70/70 (100%)	70 (100%)	0	100	100
15	q	70/70 (100%)	70 (100%)	0	100	100
16	R	266/266 (100%)	266 (100%)	0	100	100
16	r	266/266 (100%)	265 (100%)	1 (0%)	84	85
17	S	109/109 (100%)	109 (100%)	0	100	100
17	s	109/109 (100%)	109 (100%)	0	100	100
All	All	5673/5674 (100%)	5630 (99%)	43 (1%)	70	80

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	g	55	THR
12	n	131	LEU
7	g	69	ARG

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Mol	Chain	Res	Type
10	l	75	ILE
12	n	297	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
17	S	98	ASN
16	r	166	ASN
3	c	200	HIS
12	n	397	HIS
3	c	133	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
19	HEA	n	602	12	67,67,67	1.17	6 (8%)	81,103,103	1.40	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	HEA	N	602	-	67,67,67	1.16	6 (8%)	81,103,103	1.36	13 (16%)
19	HEA	N	603	12	67,67,67	1.16	7 (10%)	81,103,103	1.41	17 (20%)
19	HEA	n	603	-	67,67,67	1.17	6 (8%)	81,103,103	1.40	14 (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
19	HEA	n	602	12	-	17/36/76/76	-
19	HEA	N	602	-	-	16/36/76/76	-
19	HEA	N	603	12	-	16/36/76/76	-
19	HEA	n	603	-	-	14/36/76/76	-

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	N	602	HEA	CMA-C3A	-3.96	1.36	1.45
19	n	603	HEA	CMA-C3A	-3.92	1.36	1.45
19	N	603	HEA	CMA-C3A	-3.87	1.36	1.45
19	n	602	HEA	CMA-C3A	-3.87	1.36	1.45
19	n	602	HEA	C4C-NC	-2.57	1.34	1.39

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	N	602	HEA	CMD-C2D-C1D	3.55	130.59	125.03
19	n	603	HEA	CMD-C2D-C1D	3.46	130.43	125.03
19	n	602	HEA	CMD-C2D-C1D	3.33	130.24	125.03
19	N	603	HEA	CMD-C2D-C1D	3.31	130.20	125.03
19	n	603	HEA	CHB-C4A-NA	-3.11	121.07	124.45

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	N	602	HEA	C1A-C2A-CAA-CBA
19	N	602	HEA	C3A-C2A-CAA-CBA
19	N	602	HEA	C3B-C11-C12-C13

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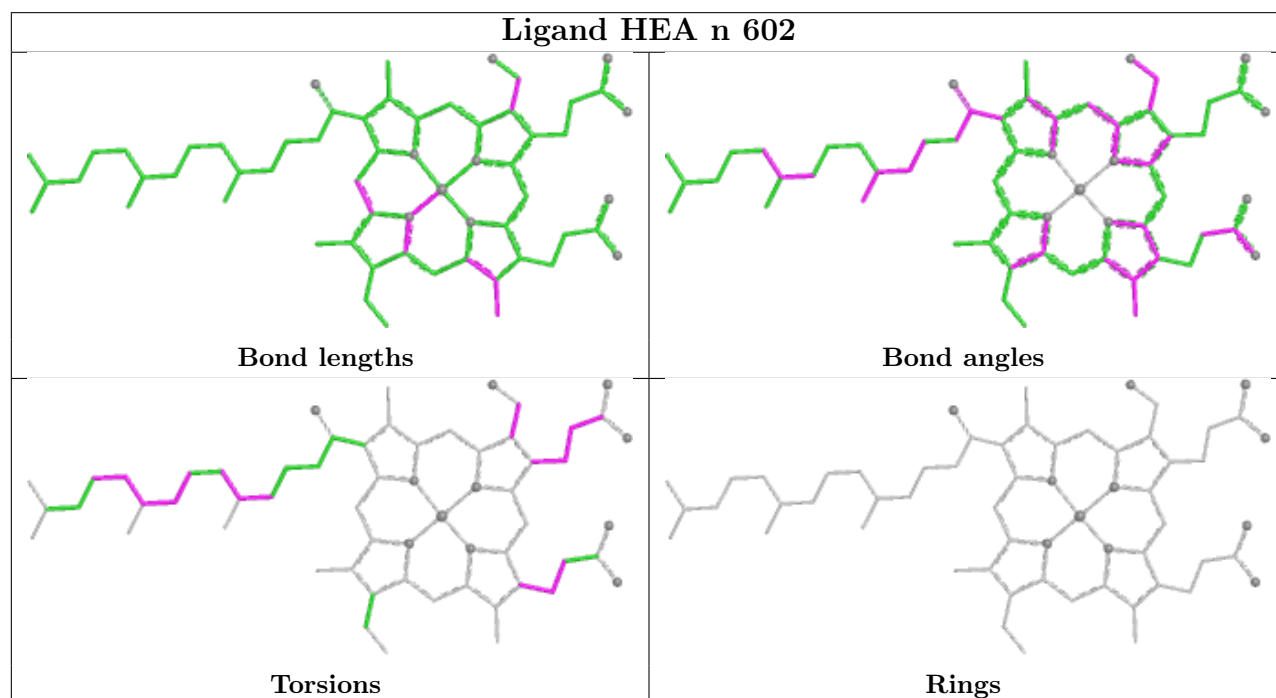
Mol	Chain	Res	Type	Atoms
19	N	602	HEA	O11-C11-C12-C13
19	N	602	HEA	C15-C16-C17-C18

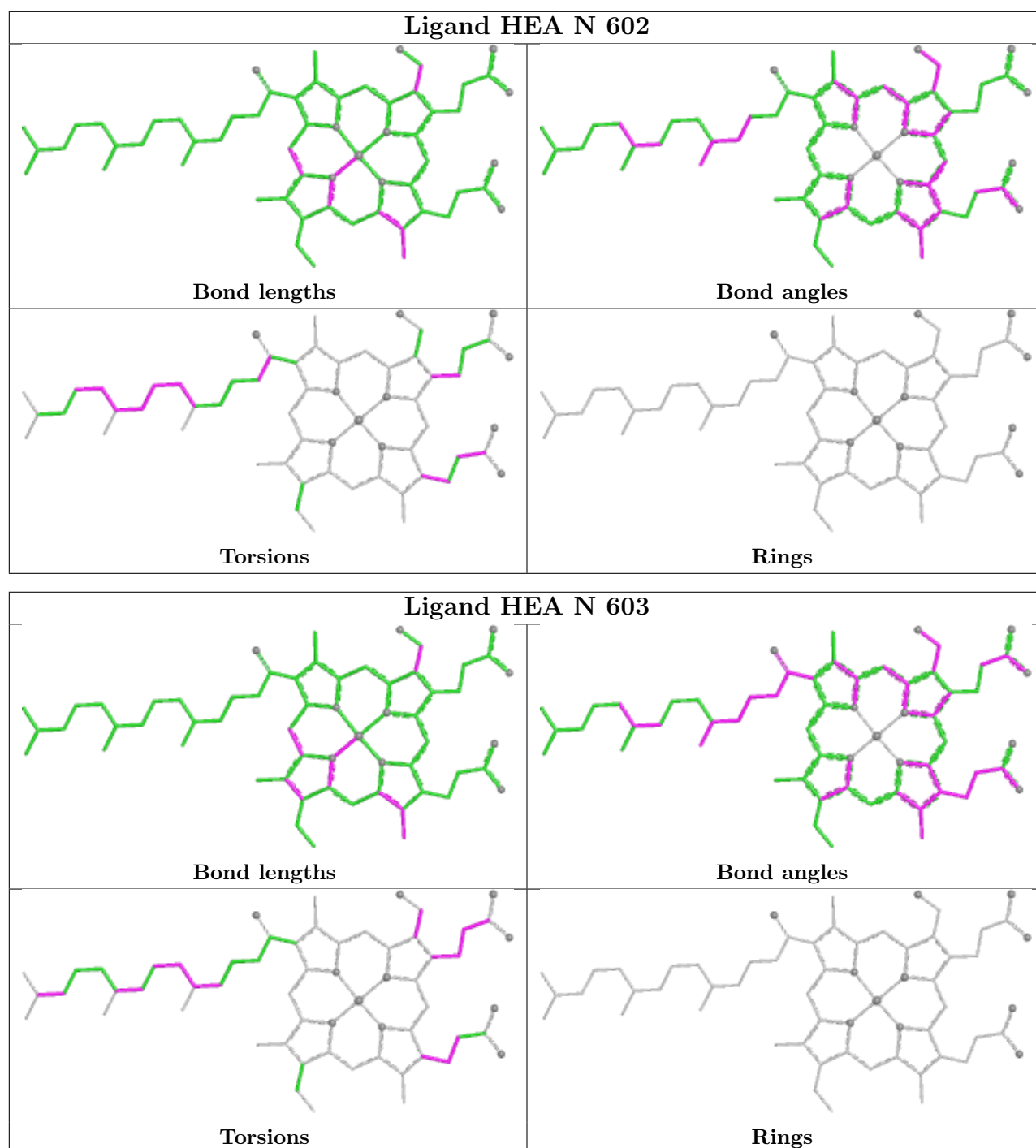
There are no ring outliers.

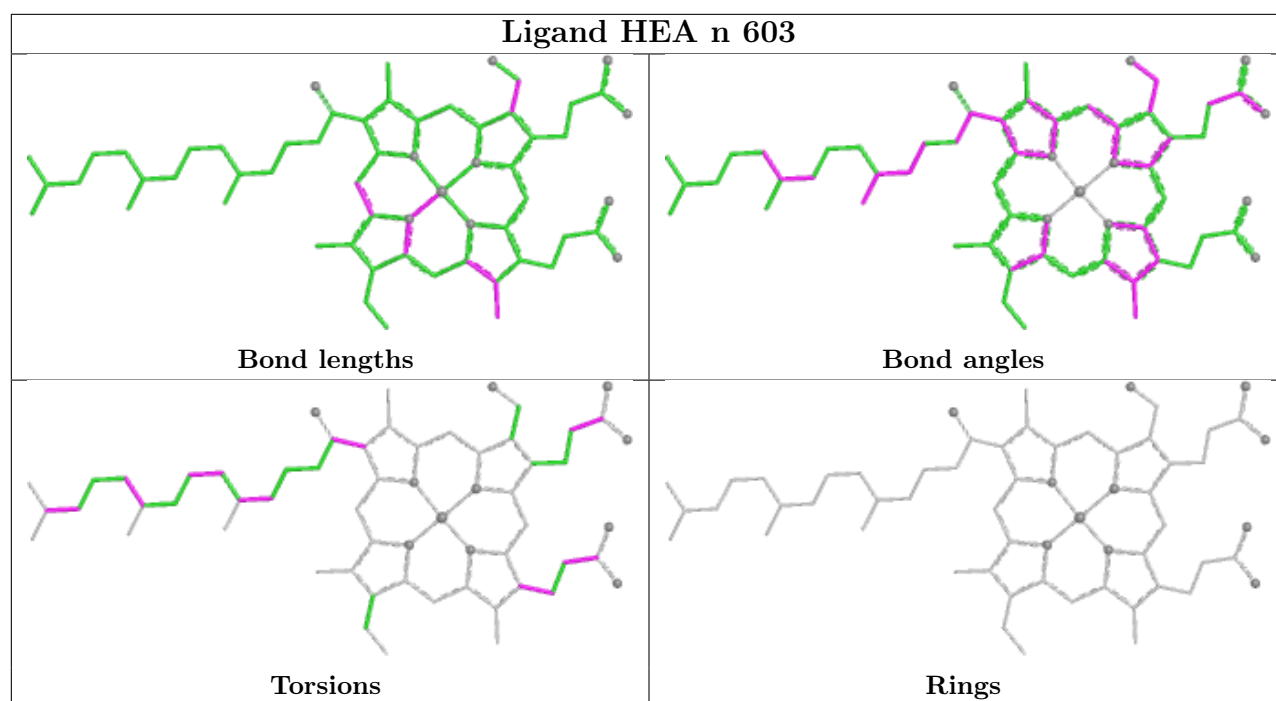
4 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	n	602	HEA	21	0
19	N	602	HEA	2	0
19	N	603	HEA	16	0
19	n	603	HEA	12	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.

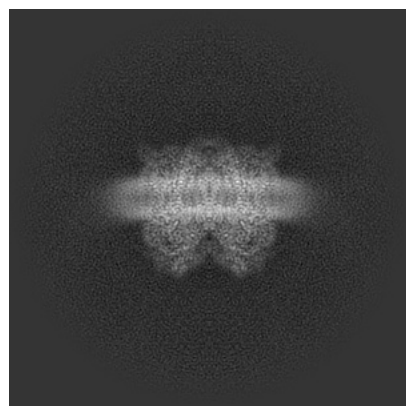
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73966. These allow visual inspection of the internal detail of the map and identification of artifacts.

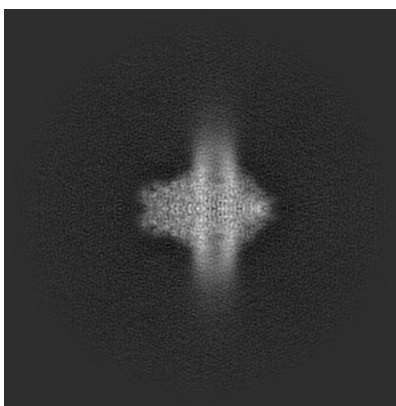
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

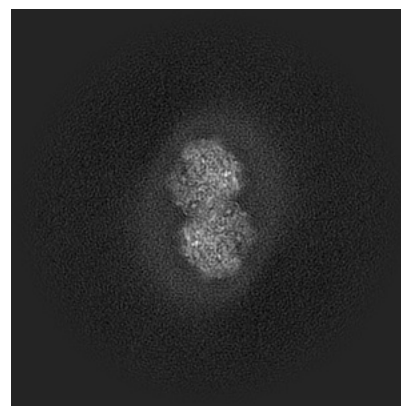
6.1.1 Primary map



X

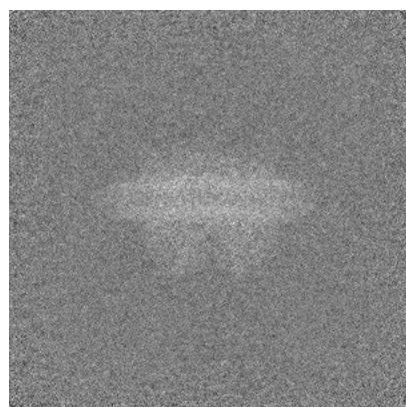


Y

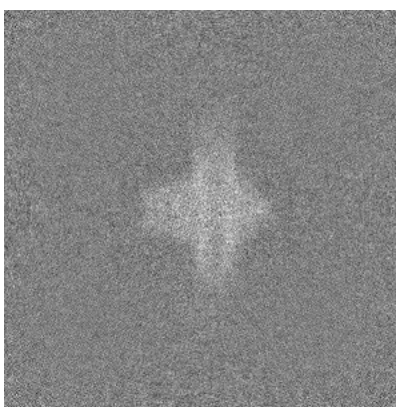


Z

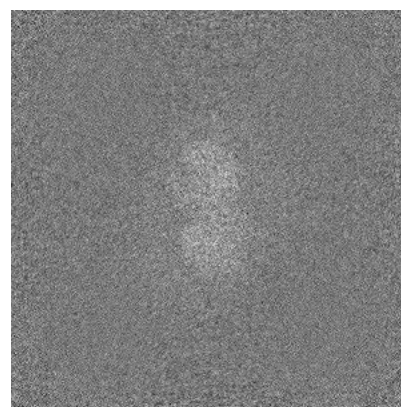
6.1.2 Raw map



X



Y

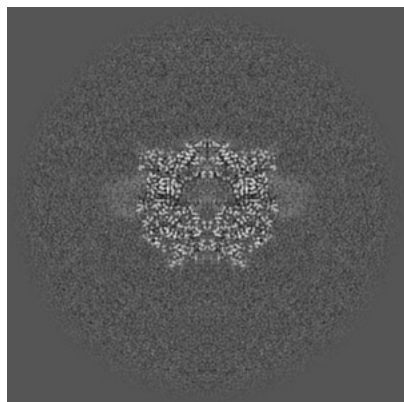


Z

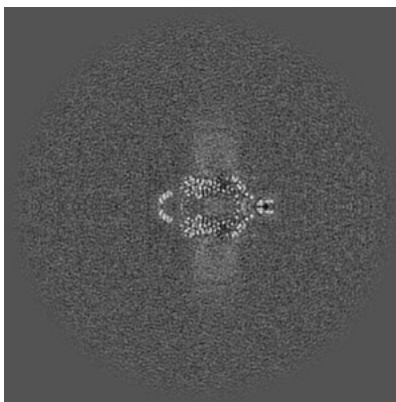
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

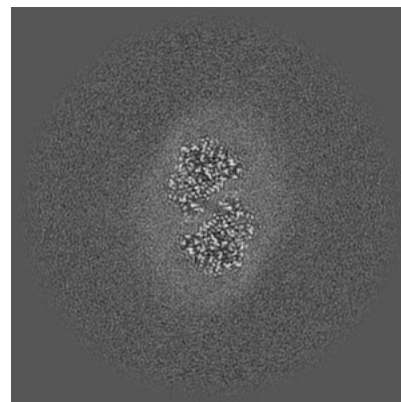
6.2.1 Primary map



X Index: 320

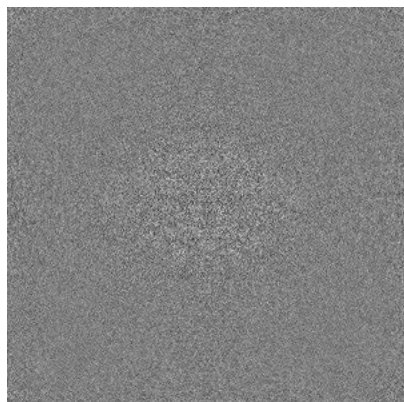


Y Index: 320

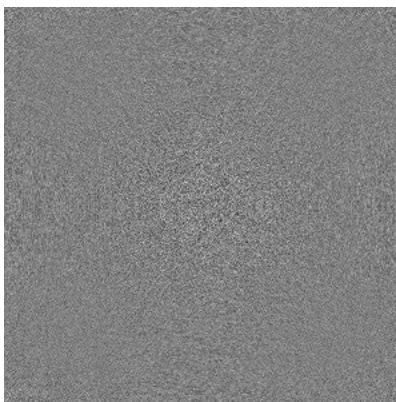


Z Index: 320

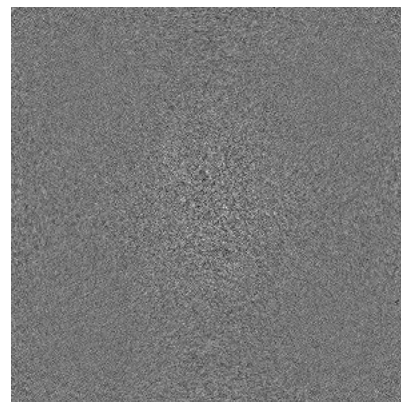
6.2.2 Raw map



X Index: 320



Y Index: 320

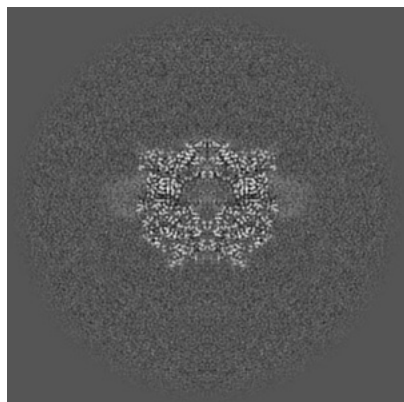


Z Index: 320

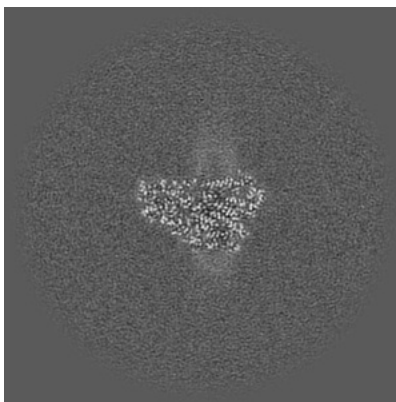
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

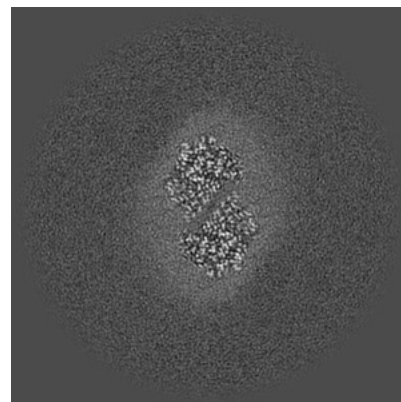
6.3.1 Primary map



X Index: 320

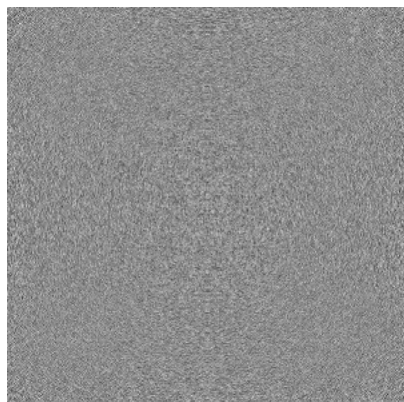


Y Index: 365

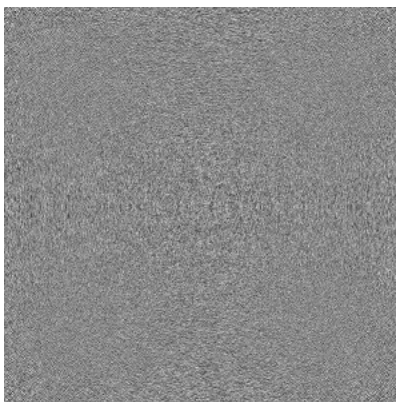


Z Index: 316

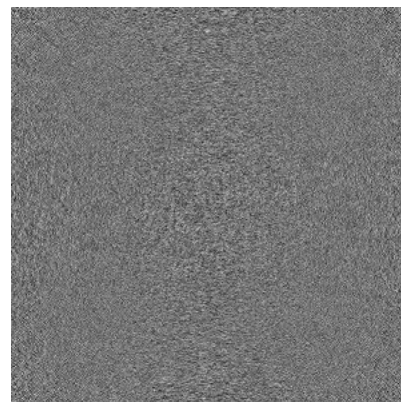
6.3.2 Raw map



X Index: 0



Y Index: 0

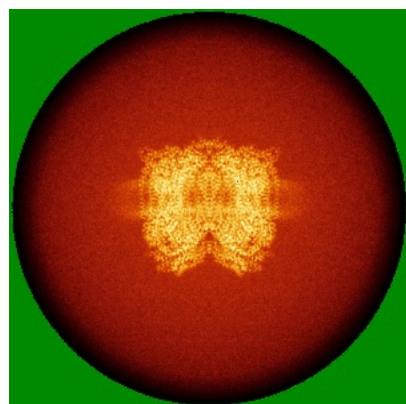


Z Index: 1

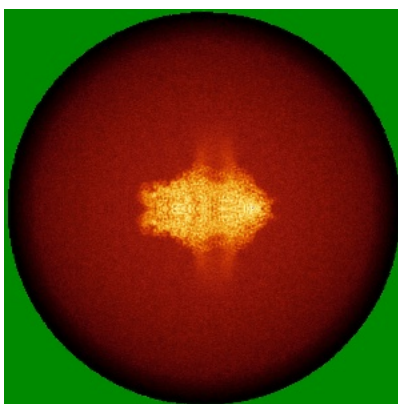
The images above show the largest variance slices of the map in three orthogonal directions.

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

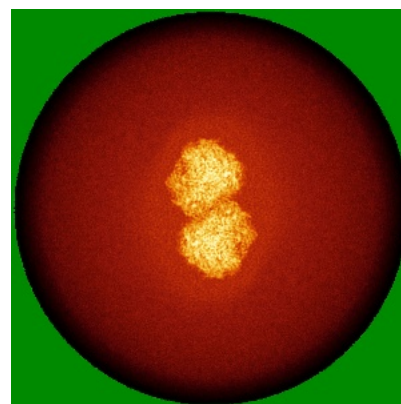
6.4.1 Primary map



X

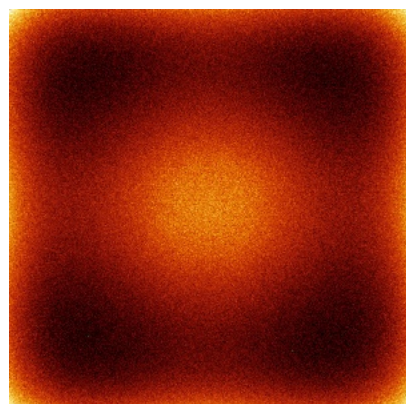


Y

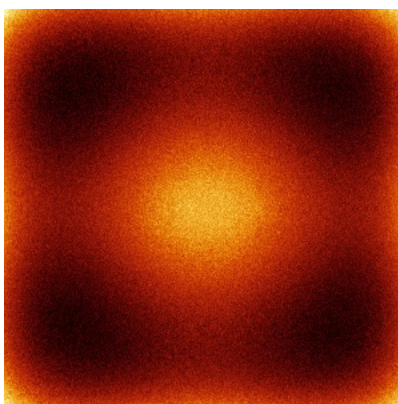


Z

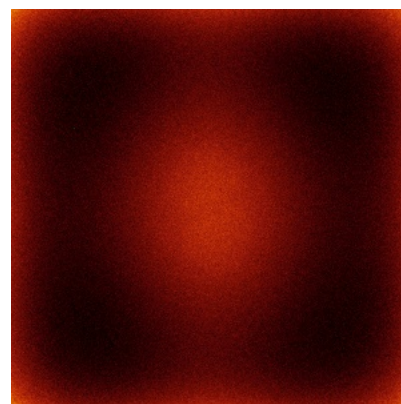
6.4.2 Raw map



X



Y

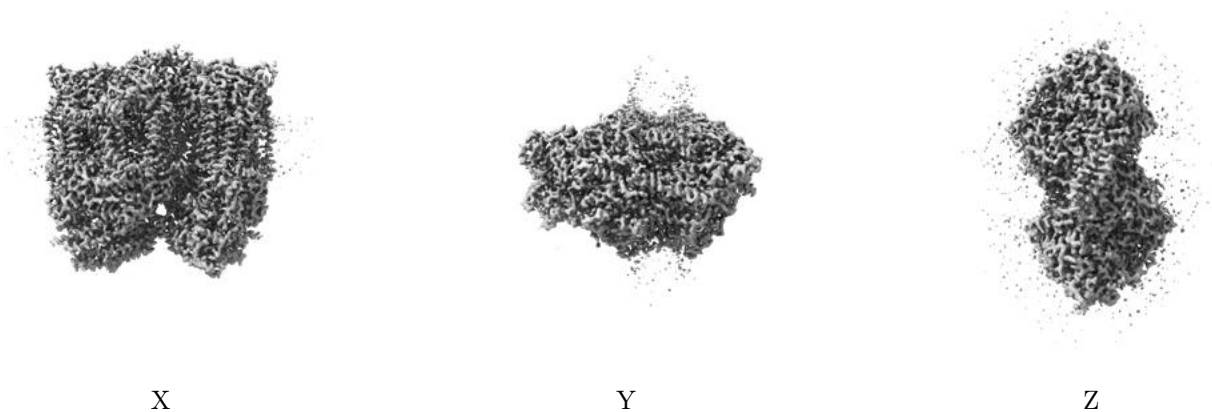


Z

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.

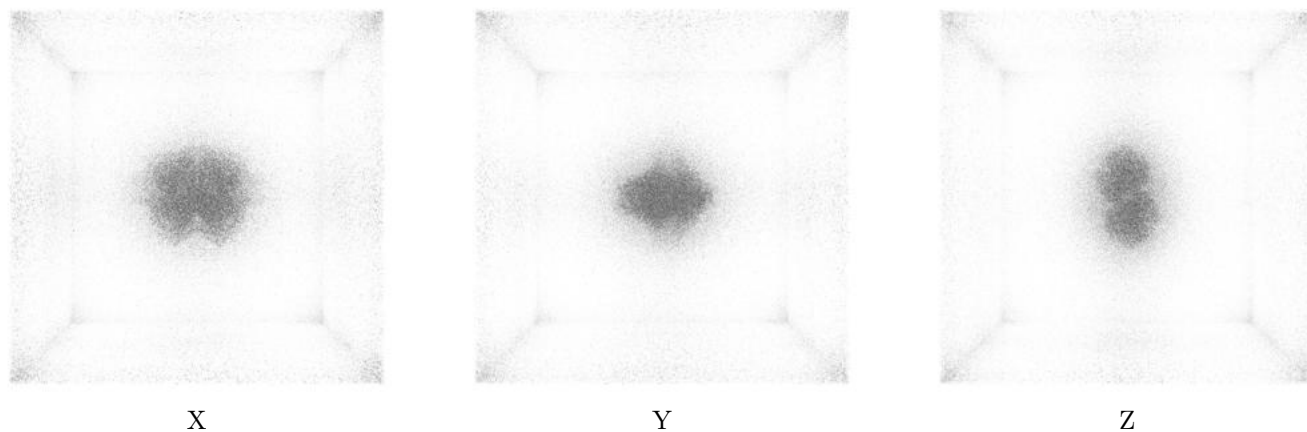
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0728. 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.

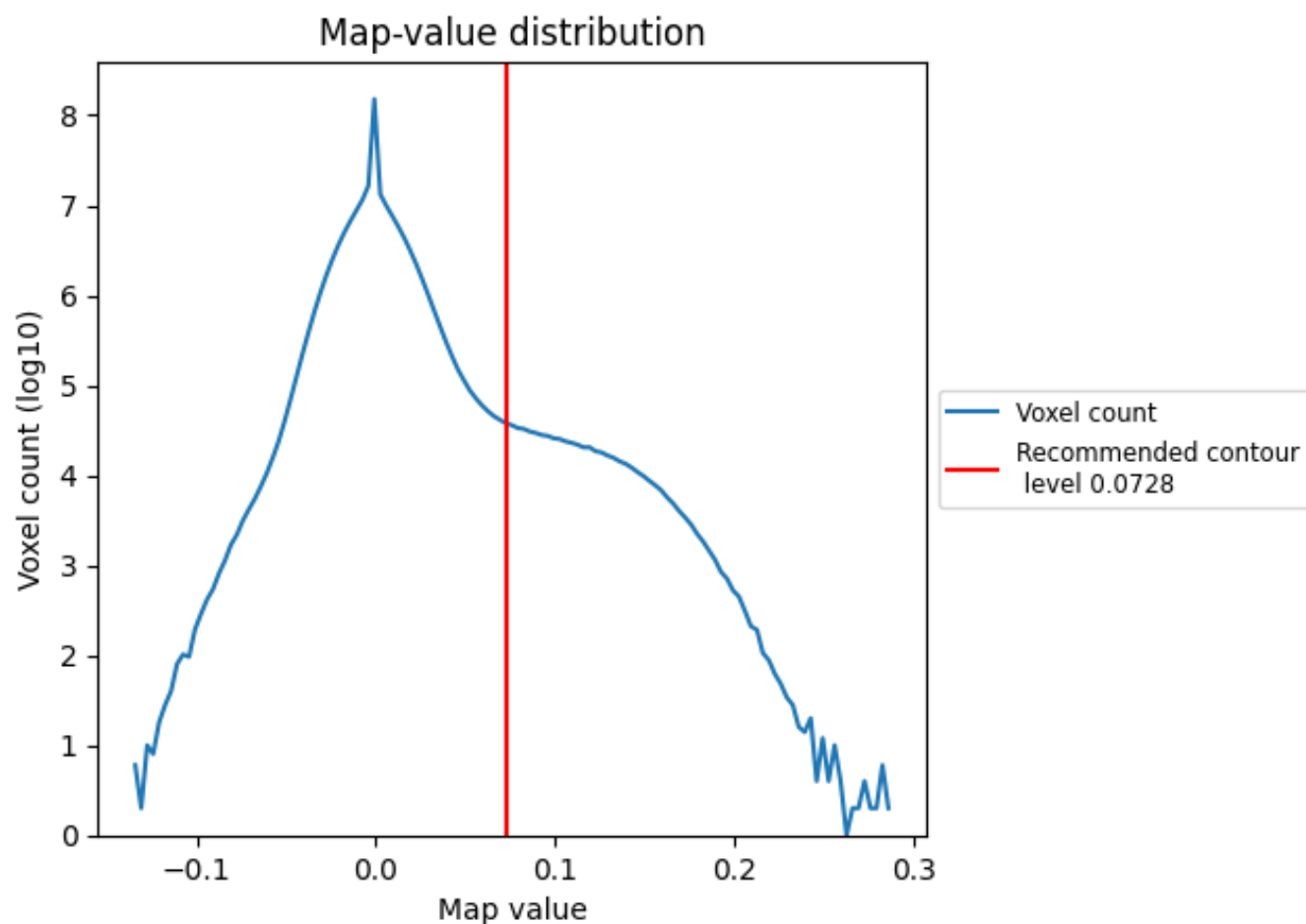
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

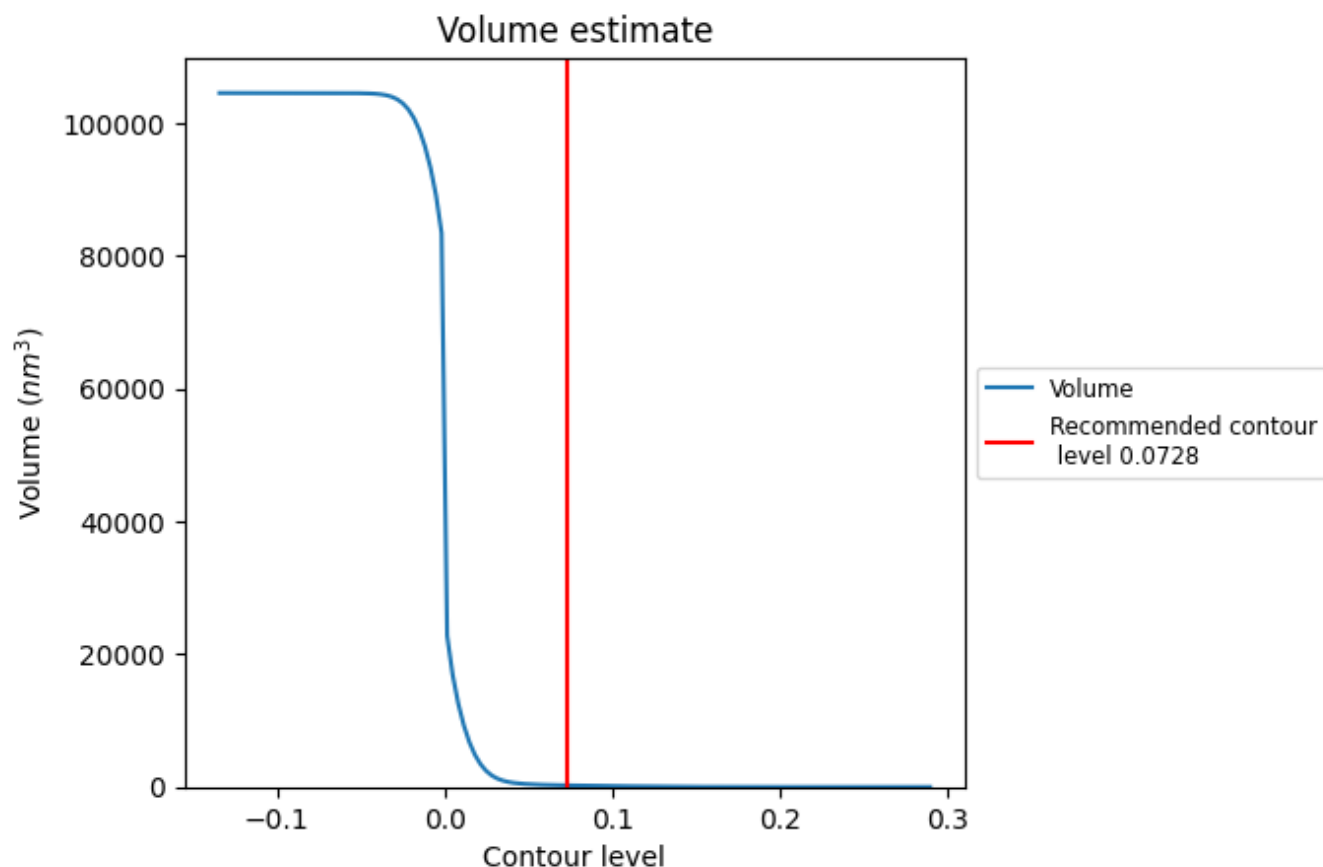
This section contains the results of statistical analysis of the map.

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.

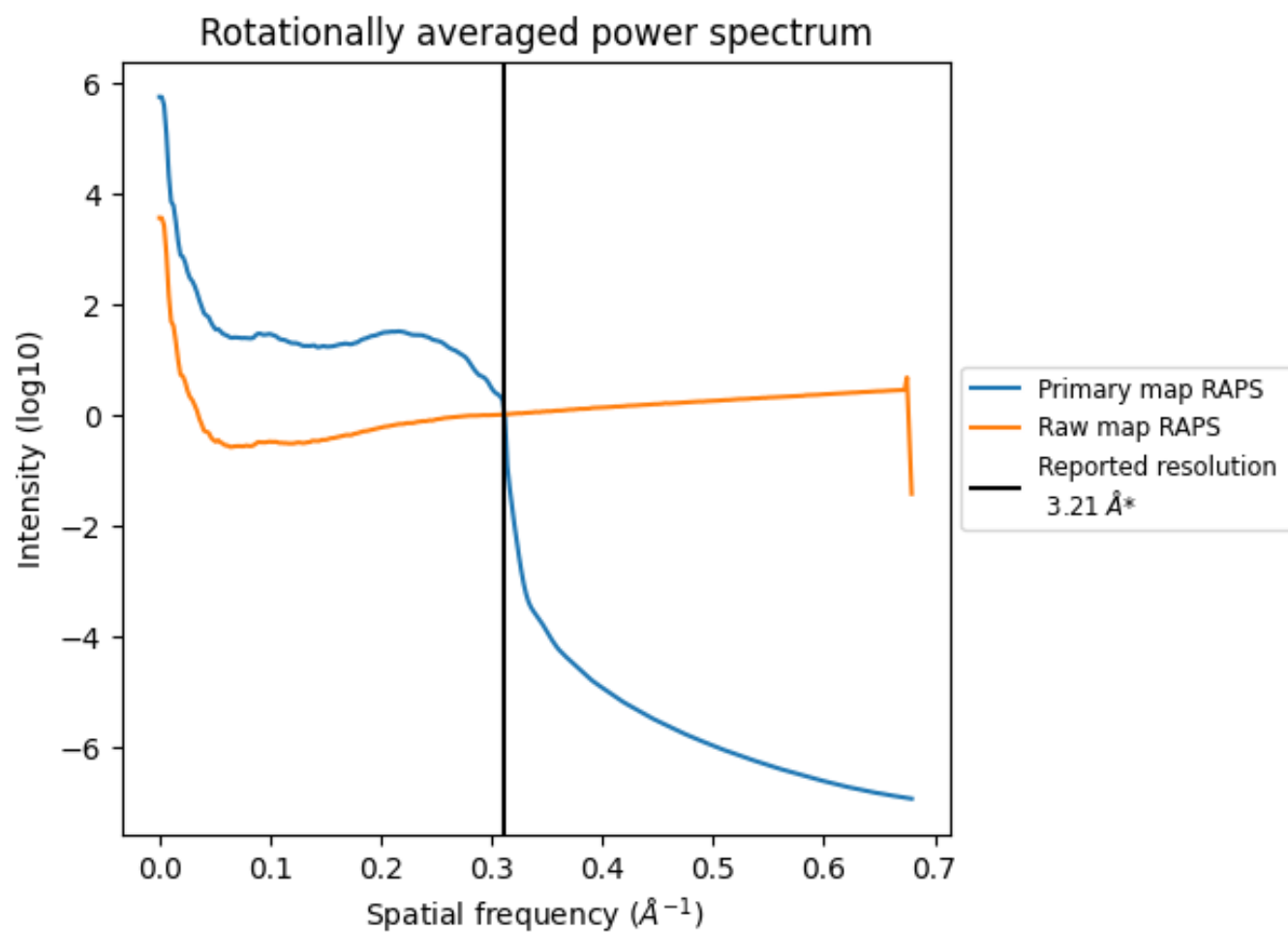
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 238 nm^3 ; this corresponds to an approximate mass of 215 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 ⓘ

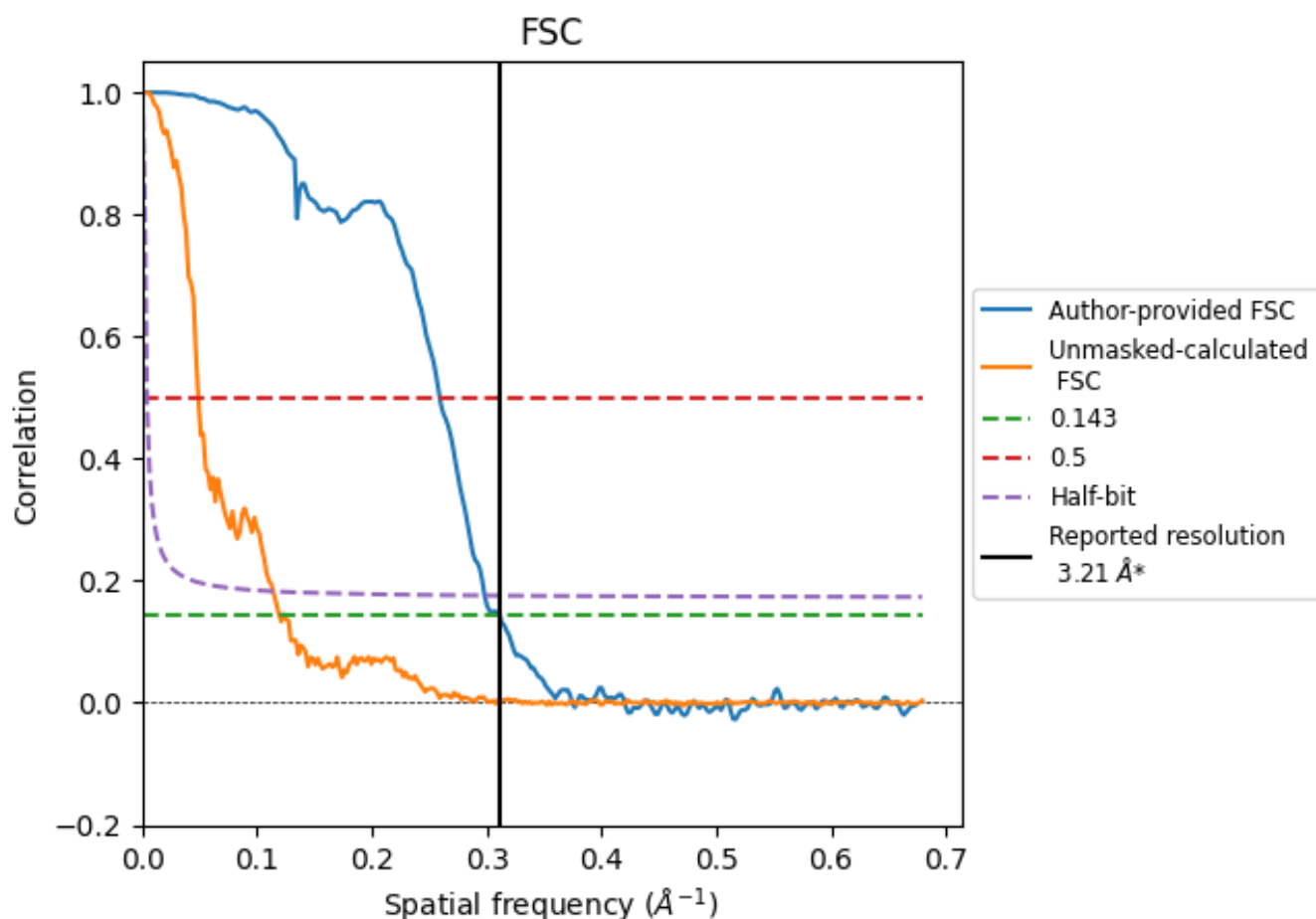


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

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 $0.312 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

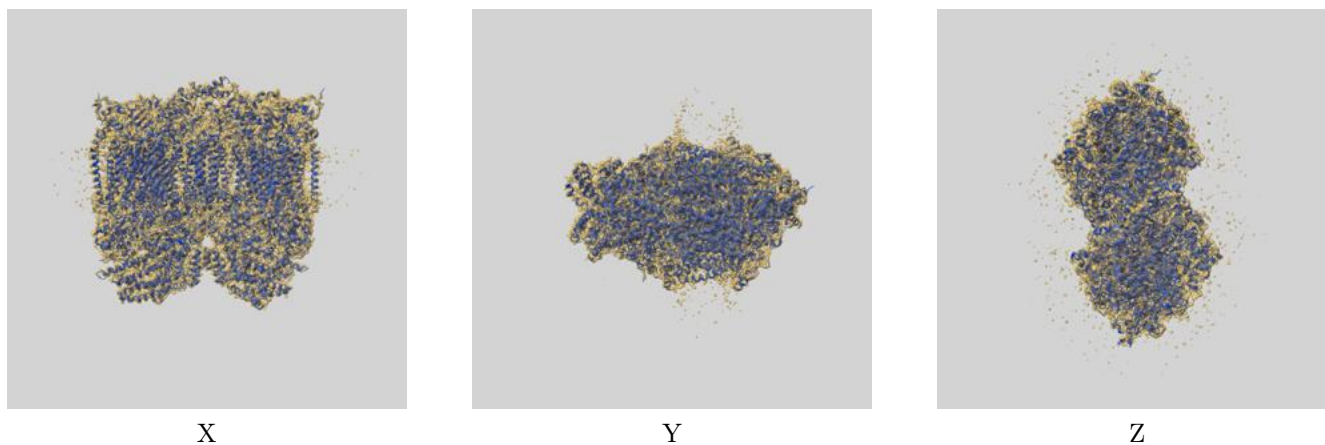
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.21	-	-
Author-provided FSC curve	3.21	3.86	3.35
Unmasked-calculated*	8.38	20.49	8.77

*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 8.38 differs from the reported value 3.21 by more than 10 %

9 Map-model fit [i](#)

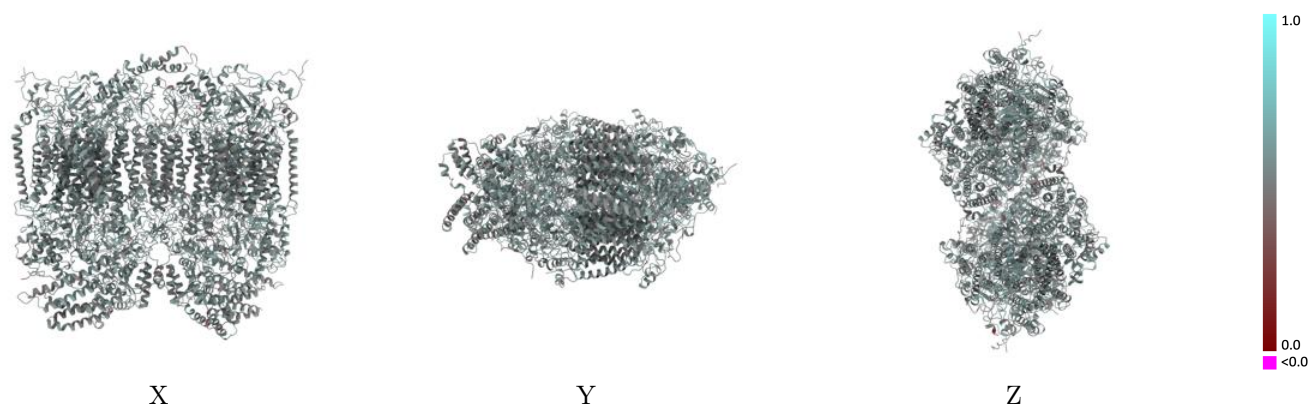
This section contains information regarding the fit between EMDB map EMD-73966 and PDB model 9ZAK. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



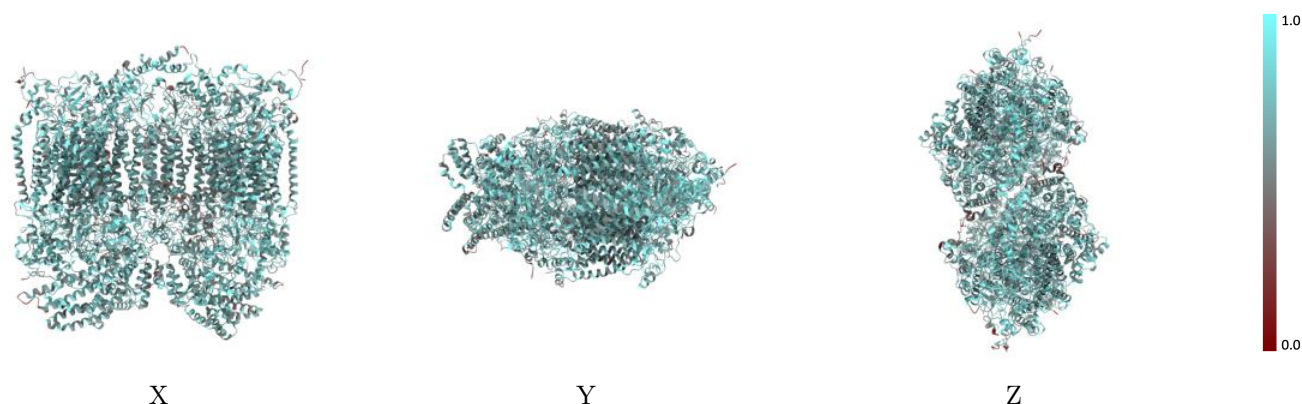
The images above show the 3D surface view of the map at the recommended contour level 0.0728 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



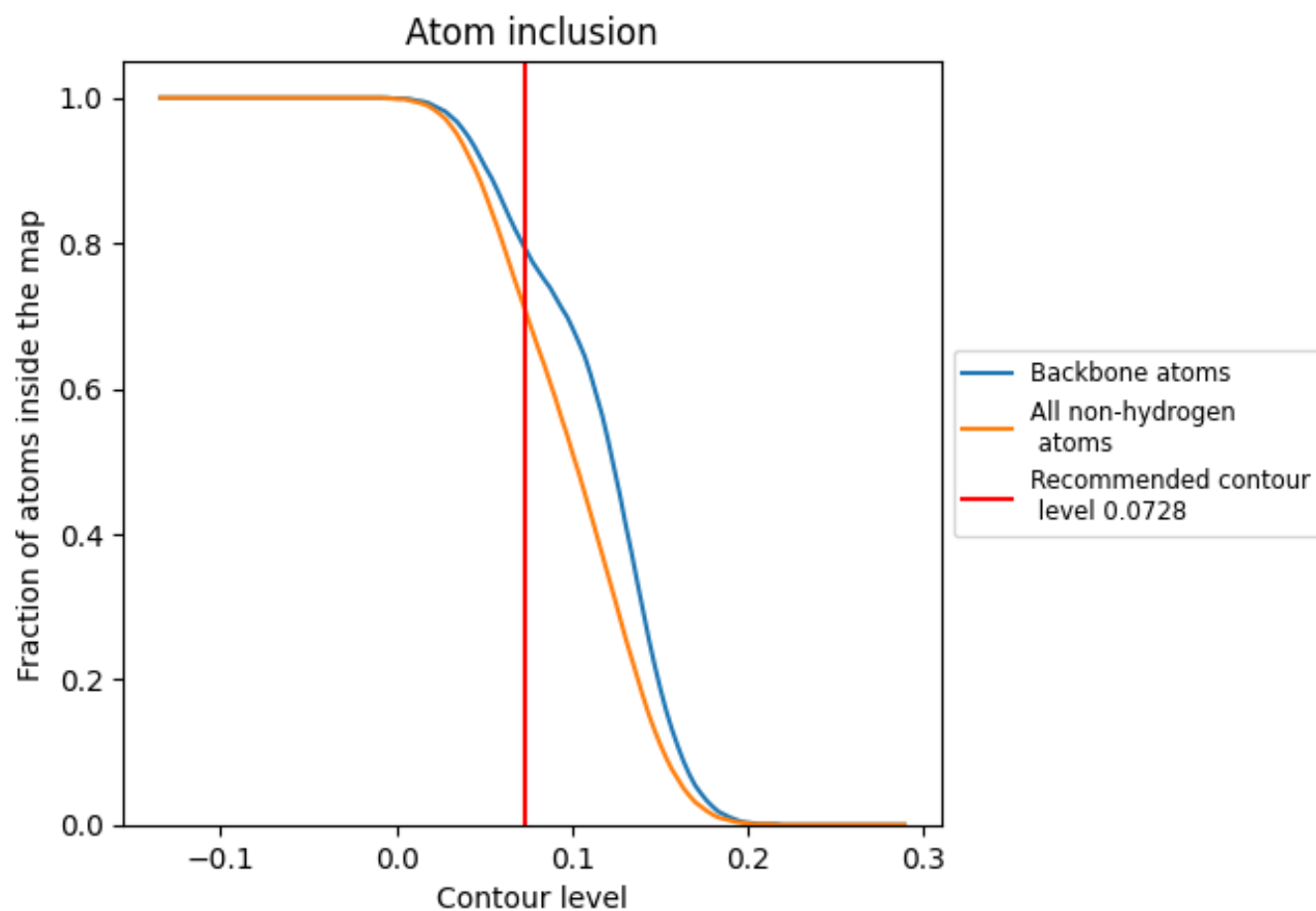
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0728).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 71% 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 (0.0728) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7120	 0.5330
A	 0.6890	 0.5330
B	 0.6840	 0.5290
C	 0.7150	 0.5330
D	 0.7450	 0.5410
E	 0.7210	 0.5290
F	 0.7090	 0.5260
G	 0.7430	 0.5380
H	 0.7260	 0.5360
K	 0.7320	 0.5450
L	 0.7540	 0.5260
M	 0.7040	 0.5250
N	 0.7300	 0.5400
O	 0.6760	 0.5280
P	 0.6680	 0.5250
Q	 0.6870	 0.5260
R	 0.6920	 0.5270
S	 0.7290	 0.5410
a	 0.6990	 0.5360
b	 0.6860	 0.5290
c	 0.7180	 0.5310
d	 0.7430	 0.5410
e	 0.7200	 0.5310
f	 0.7110	 0.5300
g	 0.7320	 0.5360
h	 0.7240	 0.5350
k	 0.7280	 0.5440
l	 0.7500	 0.5320
m	 0.6990	 0.5270
n	 0.7280	 0.5390
o	 0.6780	 0.5300
p	 0.6810	 0.5280
q	 0.6900	 0.5230
r	 0.6900	 0.5250
s	 0.7220	 0.5380

