



## wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 04:46 am GMT

PDB ID : 8C8Q  
EMDB ID : EMD-16491  
Title : Cytochrome c oxidase from Schizosaccharomyces pombe  
Authors : Moe, A.; Adelroth, P.; Brzezinski, P.; Nasvik Ojemyr, L.  
Deposited on : 2023-01-20  
Resolution : 3.36 Å(reported)

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We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

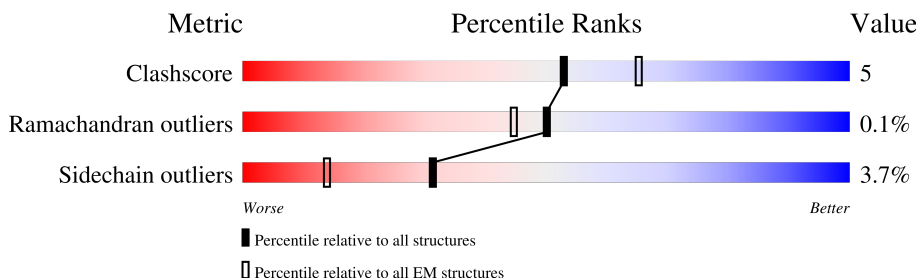
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.36 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



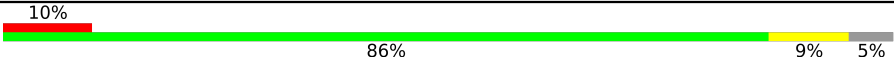

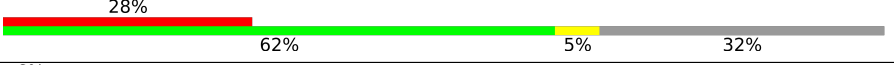


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	538	
2	B	248	
3	C	269	
4	D	159	
5	E	228	
6	F	140	
7	G	59	
8	H	66	

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Mol	Chain	Length	Quality of chain
9	I	58	
10	J	86	
11	K	130	
12	L	242	
13	M	26	

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 14787 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	537	Total	C	N	O	S	0	0
			4212	2827	652	711	22		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	TYR	-	insertion	UNP P07657

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	238	Total	C	N	O	S	0	0
			1902	1242	297	354	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	268	Total	C	N	O	S	0	0
			2156	1452	332	365	7		

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	121	Total	C	N	O	S	0	0
			922	573	160	182	7		

- Molecule 5 is a protein called Cytochrome c oxidase polypeptide 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	145	Total	C	N	O	S	0	0
			1146	728	202	212	4		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	187	GLU	-	expression tag	UNP O74988
E	188	ASN	-	expression tag	UNP O74988
E	189	LEU	-	expression tag	UNP O74988
E	190	TYR	-	expression tag	UNP O74988
E	191	PHE	-	expression tag	UNP O74988
E	192	GLN	-	expression tag	UNP O74988
E	193	GLY	-	expression tag	UNP O74988
E	194	GLY	-	expression tag	UNP O74988
E	195	GLY	-	expression tag	UNP O74988
E	196	GLY	-	expression tag	UNP O74988
E	197	GLY	-	expression tag	UNP O74988
E	198	GLY	-	expression tag	UNP O74988
E	199	SER	-	expression tag	UNP O74988
E	200	ALA	-	expression tag	UNP O74988
E	201	TRP	-	expression tag	UNP O74988
E	202	SER	-	expression tag	UNP O74988
E	203	HIS	-	expression tag	UNP O74988
E	204	PRO	-	expression tag	UNP O74988
E	205	GLN	-	expression tag	UNP O74988
E	206	PHE	-	expression tag	UNP O74988
E	207	GLU	-	expression tag	UNP O74988
E	208	LYS	-	expression tag	UNP O74988
E	209	GLY	-	expression tag	UNP O74988
E	210	GLY	-	expression tag	UNP O74988
E	211	GLY	-	expression tag	UNP O74988
E	212	SER	-	expression tag	UNP O74988
E	213	GLY	-	expression tag	UNP O74988
E	214	GLY	-	expression tag	UNP O74988
E	215	GLY	-	expression tag	UNP O74988
E	216	SER	-	expression tag	UNP O74988
E	217	GLY	-	expression tag	UNP O74988
E	218	GLY	-	expression tag	UNP O74988
E	219	SER	-	expression tag	UNP O74988
E	220	ALA	-	expression tag	UNP O74988
E	221	TRP	-	expression tag	UNP O74988
E	222	SER	-	expression tag	UNP O74988
E	223	HIS	-	expression tag	UNP O74988
E	224	PRO	-	expression tag	UNP O74988
E	225	GLN	-	expression tag	UNP O74988
E	226	PHE	-	expression tag	UNP O74988
E	227	GLU	-	expression tag	UNP O74988
E	228	LYS	-	expression tag	UNP O74988

- Molecule 6 is a protein called Cytochrome c oxidase subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	100	Total	C	N	O	S	0	0
			813	520	137	154	2		

- Molecule 7 is a protein called Cytochrome c oxidase subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	57	Total	C	N	O	S	0	0
			457	301	78	77	1		

- Molecule 8 is a protein called Cytochrome c oxidase polypeptide VIII, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	45	Total	C	N	O	S	0	0
			363	249	57	57			

- Molecule 9 is a protein called Cytochrome c oxidase subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	55	Total	C	N	O	S	0	0
			445	292	77	73	3		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	75	Total	C	N	O	S	0	0
			636	411	107	113	5		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	88	Total	C	N	O	S	0	0
			741	480	124	136	1		

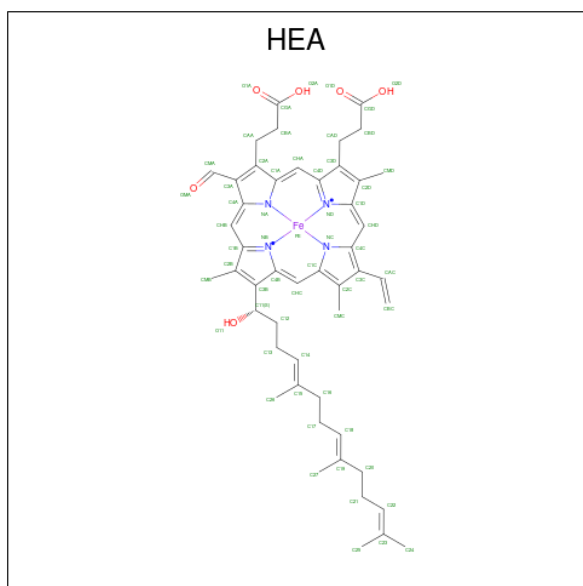
- Molecule 12 is a protein called Respiratory supercomplex factor 2 homolog C1565.01.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	69	Total	C	N	O	S	0	0
			550	356	95	97	2		

- Molecule 13 is a protein called Unknown polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	26	Total	C	N	O	0	0
			130	78	26	26		

- Molecule 14 is HEME-A (three-letter code: HEA) (formula:  $C_{49}H_{56}FeN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	Cu	0
			1	1	

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

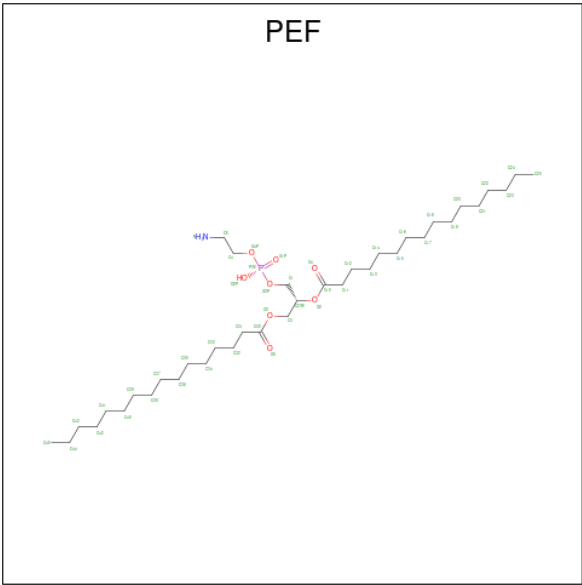
Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	Mg	0
			1	1	

- Molecule 17 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

of Interest" by depositor).

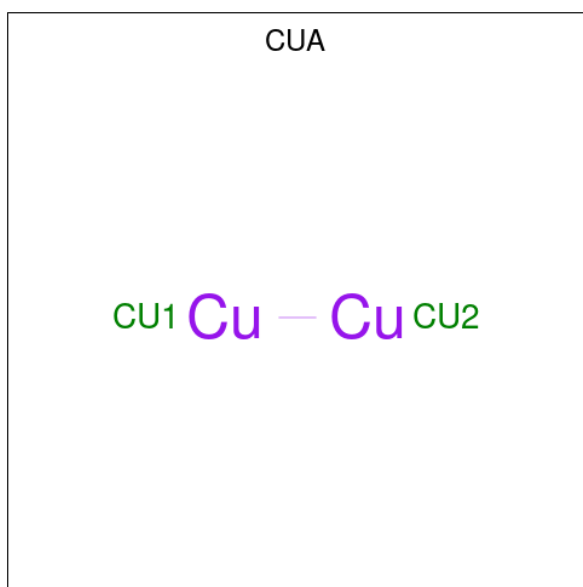
Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	Ca	0
			1	1	

- Molecule 18 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: C<sub>37</sub>H<sub>74</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
18	B	1	Total	C	N	O	P	0
			47	37	1	8	1	
18	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
18	C	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 19 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
19	B	1	Total 2	Cu 2	0

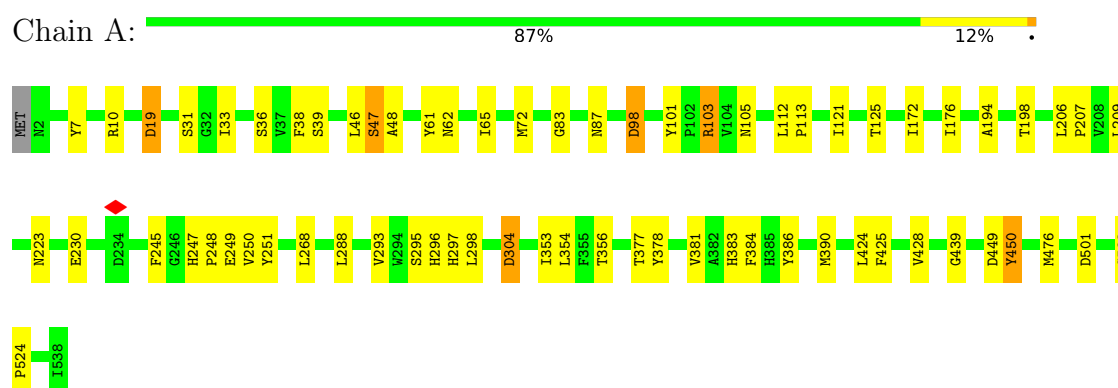
- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
20	D	1	Total 1	Zn 1	0

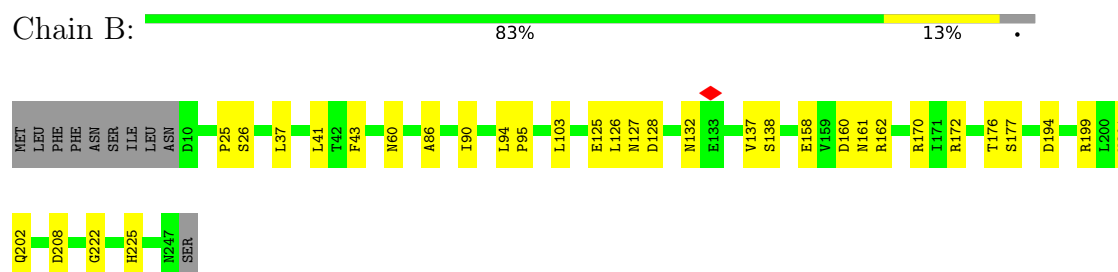
### 3 Residue-property plots [i](#)

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.

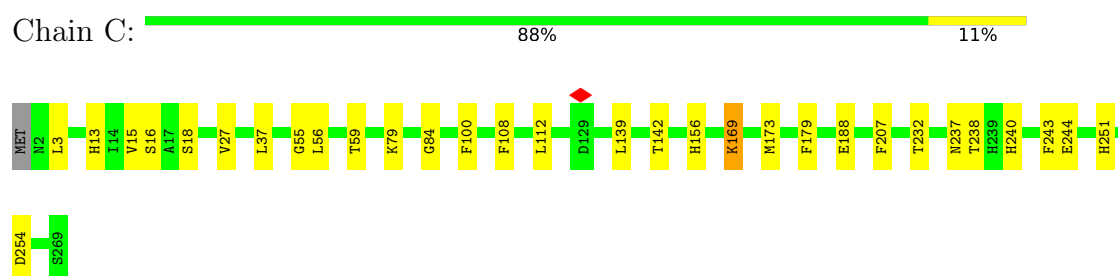
#### • Molecule 1: Cytochrome c oxidase subunit 1



#### • Molecule 2: Cytochrome c oxidase subunit 2

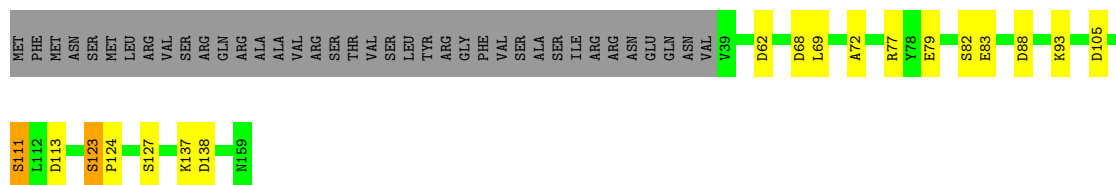


#### • Molecule 3: Cytochrome c oxidase subunit 3



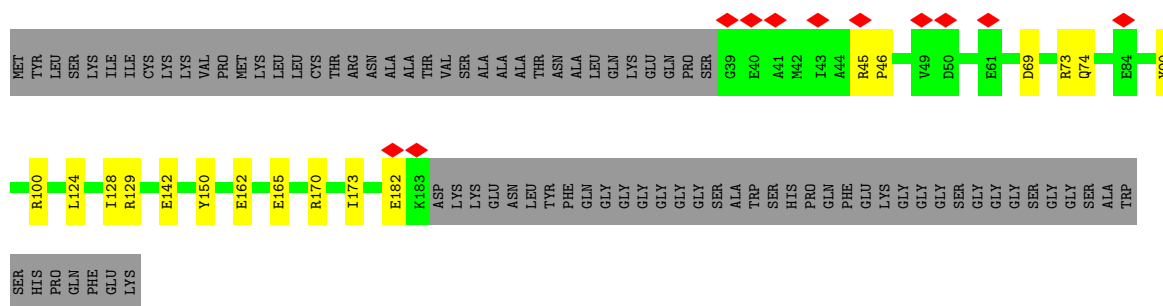
#### • Molecule 4: Cytochrome c oxidase subunit 4, mitochondrial

Chain D:  65% 10% 24%



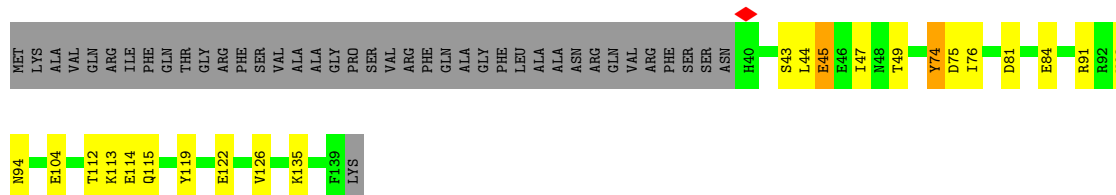
- Molecule 5: Cytochrome c oxidase polypeptide 5, mitochondrial

Chain E:  5% 56% 7% 36%



- Molecule 6: Cytochrome c oxidase subunit 6, mitochondrial

Chain F:  56% 14% 29%



- Molecule 7: Cytochrome c oxidase subunit 7

Chain G:  90% 7% 3%

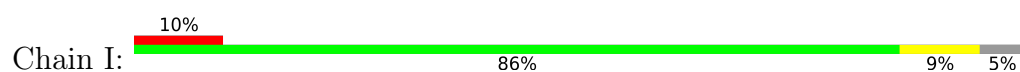


- Molecule 8: Cytochrome c oxidase polypeptide VIII, mitochondrial

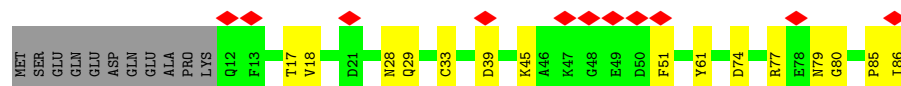
Chain H:  56% 11% 32%



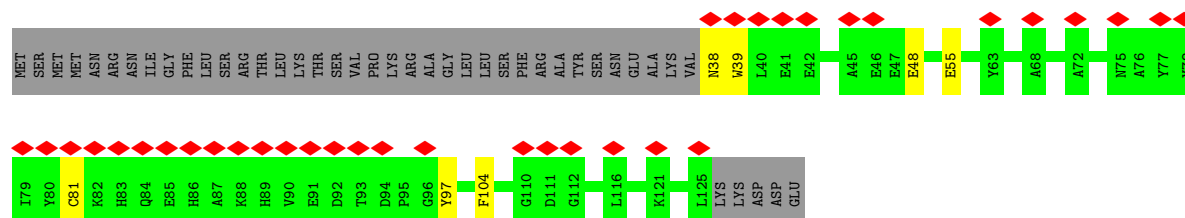
- Molecule 9: Cytochrome c oxidase subunit 9, mitochondrial



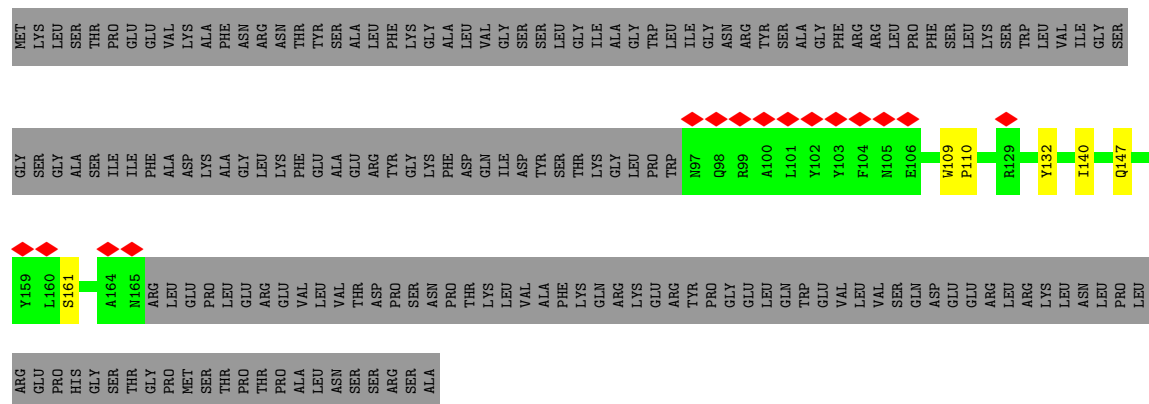
- Molecule 10: Cytochrome c oxidase subunit 12, mitochondrial



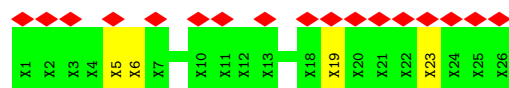
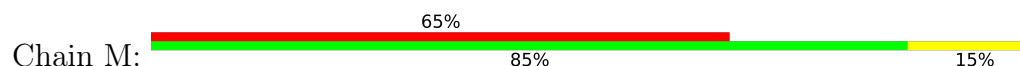
- Molecule 11: Cytochrome c oxidase subunit 13, mitochondrial



- Molecule 12: Respiratory supercomplex factor 2 homolog C1565.01



- Molecule 13: Unknown polypeptide



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	127659	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.105	Depositor
Minimum map value	-1.370	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.084	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	220.5952, 220.5952, 220.5952	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8617, 0.8617, 0.8617	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CUA, HEA, CA, MG, CU, ZN, PEF

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	0.29	0/4353	0.44	0/5950
2	B	0.26	0/1953	0.44	0/2668
3	C	0.28	0/2237	0.42	0/3057
4	D	0.26	0/940	0.52	0/1270
5	E	0.25	0/1173	0.48	0/1580
6	F	0.29	0/828	0.47	0/1119
7	G	0.29	0/469	0.46	0/633
8	H	0.29	0/377	0.51	0/514
9	I	0.29	0/458	0.47	0/618
10	J	0.26	0/660	0.45	0/893
11	K	0.26	0/767	0.43	0/1039
12	L	0.25	0/563	0.48	0/767
All	All	0.28	0/14778	0.45	0/20108

There are no bond length outliers.

There are no bond angle outliers.

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	4212	0	4233	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1902	0	1874	17	0
3	C	2156	0	2101	22	0
4	D	922	0	907	12	0
5	E	1146	0	1140	9	0
6	F	813	0	805	14	0
7	G	457	0	467	2	0
8	H	363	0	379	7	0
9	I	445	0	444	2	0
10	J	636	0	575	8	0
11	K	741	0	689	4	0
12	L	550	0	554	4	0
13	M	130	0	29	2	0
14	A	120	0	108	4	0
15	A	1	0	0	0	0
16	A	1	0	0	0	0
17	A	1	0	0	0	0
18	A	47	0	73	0	0
18	B	47	0	73	0	0
18	C	94	0	146	0	0
19	B	2	0	0	0	0
20	D	1	0	0	0	0
All	All	14787	0	14597	149	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 5.

The worst 5 of 149 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:247:HIS:NE2	1:A:251:TYR:CE2	2.05	1.23
1:A:390:MET:HE1	1:A:428:VAL:HB	1.30	1.09
1:A:247:HIS:NE2	1:A:251:TYR:HE2	1.57	0.99
1:A:247:HIS:CD2	1:A:251:TYR:CE2	2.56	0.94
1:A:377:THR:HG22	1:A:378:TYR:H	1.30	0.93

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	535/538 (99%)	509 (95%)	26 (5%)	0	100	100
2	B	236/248 (95%)	222 (94%)	14 (6%)	0	100	100
3	C	266/269 (99%)	252 (95%)	14 (5%)	0	100	100
4	D	119/159 (75%)	112 (94%)	7 (6%)	0	100	100
5	E	143/228 (63%)	132 (92%)	11 (8%)	0	100	100
6	F	98/140 (70%)	92 (94%)	5 (5%)	1 (1%)	13	39
7	G	55/59 (93%)	54 (98%)	1 (2%)	0	100	100
8	H	43/66 (65%)	35 (81%)	7 (16%)	1 (2%)	5	23
9	I	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
10	J	73/86 (85%)	68 (93%)	5 (7%)	0	100	100
11	K	86/130 (66%)	80 (93%)	6 (7%)	0	100	100
12	L	67/242 (28%)	66 (98%)	1 (2%)	0	100	100
All	All	1774/2223 (80%)	1674 (94%)	98 (6%)	2 (0%)	50	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	43	SER
8	H	38	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	452/453 (100%)	437 (97%)	15 (3%)	33	59
2	B	213/223 (96%)	207 (97%)	6 (3%)	38	63
3	C	226/227 (100%)	220 (97%)	6 (3%)	40	64
4	D	101/135 (75%)	95 (94%)	6 (6%)	16	42
5	E	119/180 (66%)	115 (97%)	4 (3%)	32	58
6	F	90/121 (74%)	85 (94%)	5 (6%)	17	44
7	G	47/49 (96%)	44 (94%)	3 (6%)	14	40
8	H	41/59 (70%)	40 (98%)	1 (2%)	44	67
9	I	44/46 (96%)	42 (96%)	2 (4%)	23	50
10	J	67/77 (87%)	63 (94%)	4 (6%)	16	42
11	K	76/113 (67%)	74 (97%)	2 (3%)	41	65
12	L	57/203 (28%)	55 (96%)	2 (4%)	31	57
All	All	1533/1886 (81%)	1477 (96%)	56 (4%)	31	55

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	88	ASP
12	L	161	SER
5	E	74	GLN
12	L	132	TYR
10	J	39	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	526	HIS

### 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	$\# Z  > 2$
14	HEA	A	601	1	57,67,67	2.12	17 (29%)	61,103,103	2.32	23 (37%)
18	PEF	B	301	-	46,46,46	0.96	2 (4%)	49,51,51	1.02	3 (6%)
19	CUA	B	302	2	0,1,1	-	-	-	-	-
18	PEF	C	302	-	46,46,46	0.95	2 (4%)	49,51,51	0.91	2 (4%)
18	PEF	C	301	-	46,46,46	0.95	2 (4%)	49,51,51	1.01	3 (6%)
18	PEF	A	606	-	46,46,46	0.95	2 (4%)	49,51,51	0.99	3 (6%)
14	HEA	A	602	1	57,67,67	2.10	18 (31%)	61,103,103	2.32	25 (40%)

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
14	HEA	A	601	1	-	4/32/76/76	-
18	PEF	B	301	-	-	10/50/50/50	-
18	PEF	C	302	-	-	8/50/50/50	-
18	PEF	C	301	-	-	9/50/50/50	-
18	PEF	A	606	-	-	16/50/50/50	-
14	HEA	A	602	1	-	4/32/76/76	-

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	C3B-C2B	5.72	1.47	1.34
14	A	602	HEA	C3B-C2B	5.42	1.46	1.34
14	A	601	HEA	C3A-C2A	5.31	1.47	1.40
14	A	602	HEA	C3A-C2A	5.30	1.47	1.40
14	A	601	HEA	C3C-C2C	5.10	1.47	1.40

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602	HEA	C3D-C4D-ND	6.43	116.58	110.36
14	A	601	HEA	C3D-C4D-ND	6.17	116.33	110.36
14	A	601	HEA	C2B-C1B-NB	5.50	116.47	109.88
14	A	601	HEA	C2D-C1D-ND	5.41	116.25	109.84
14	A	602	HEA	C2B-C1B-NB	5.41	116.36	109.88

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	606	PEF	O2-C2-C3-O3
18	A	606	PEF	C1-O3P-P-O1P
18	B	301	PEF	C1-O3P-P-O1P
18	B	301	PEF	C1-O3P-P-O2P
18	B	301	PEF	C4-O4P-P-O2P

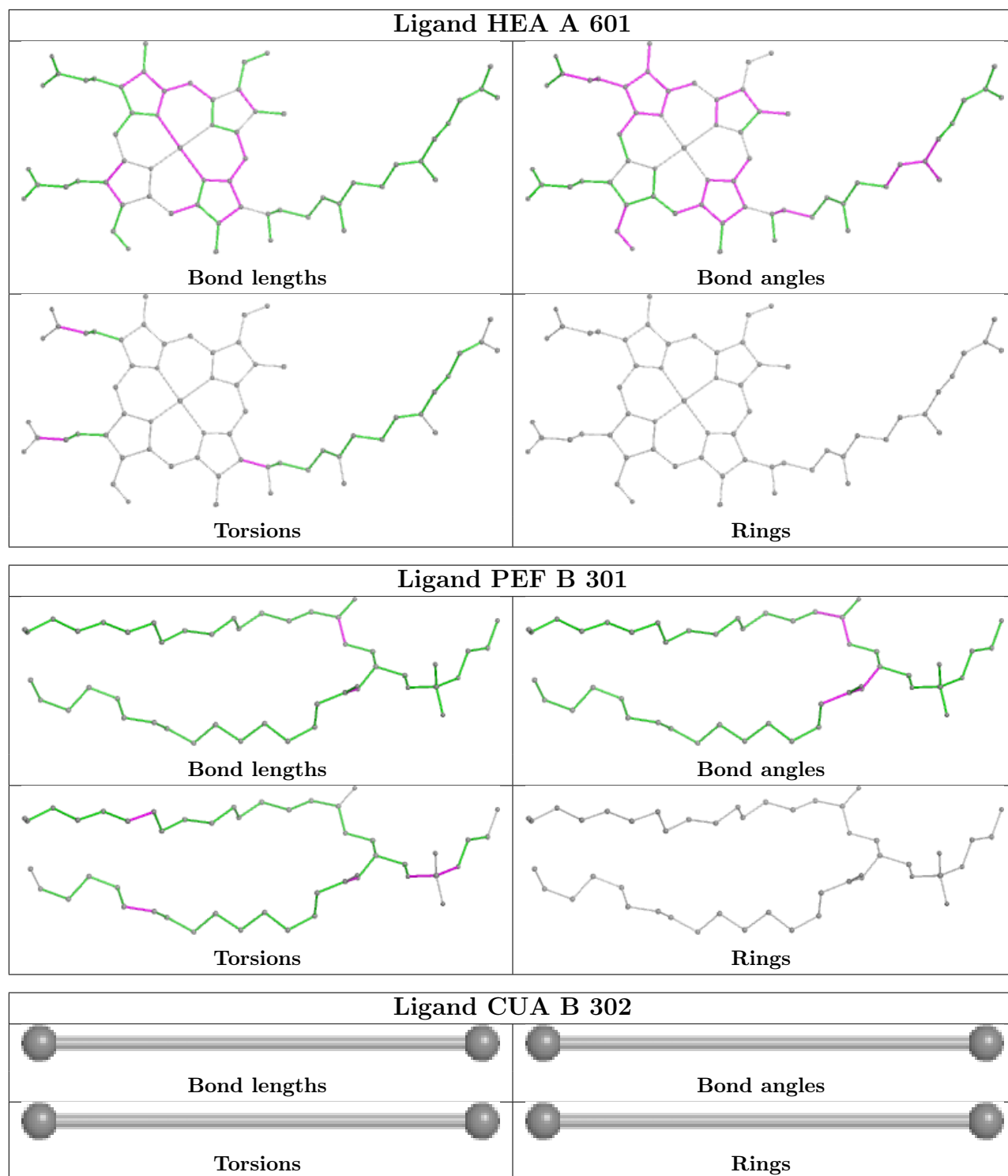
There are no ring outliers.

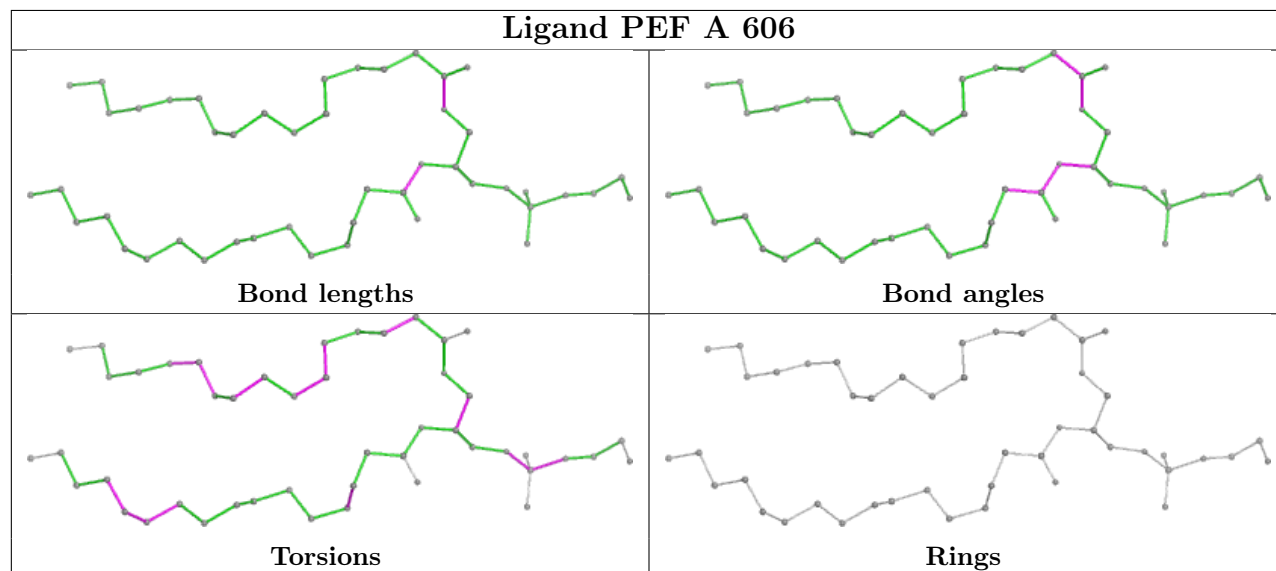
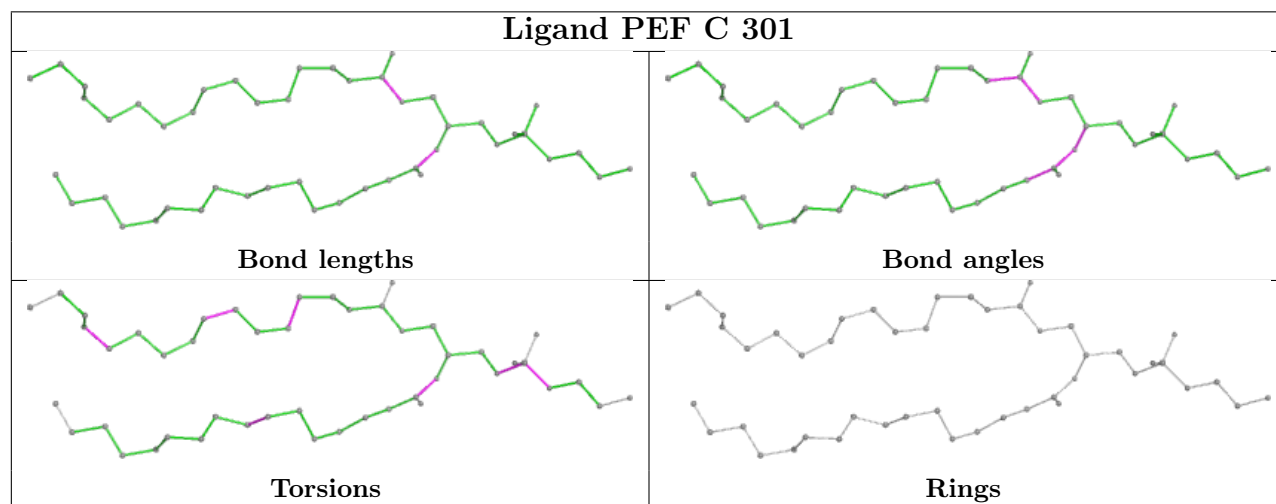
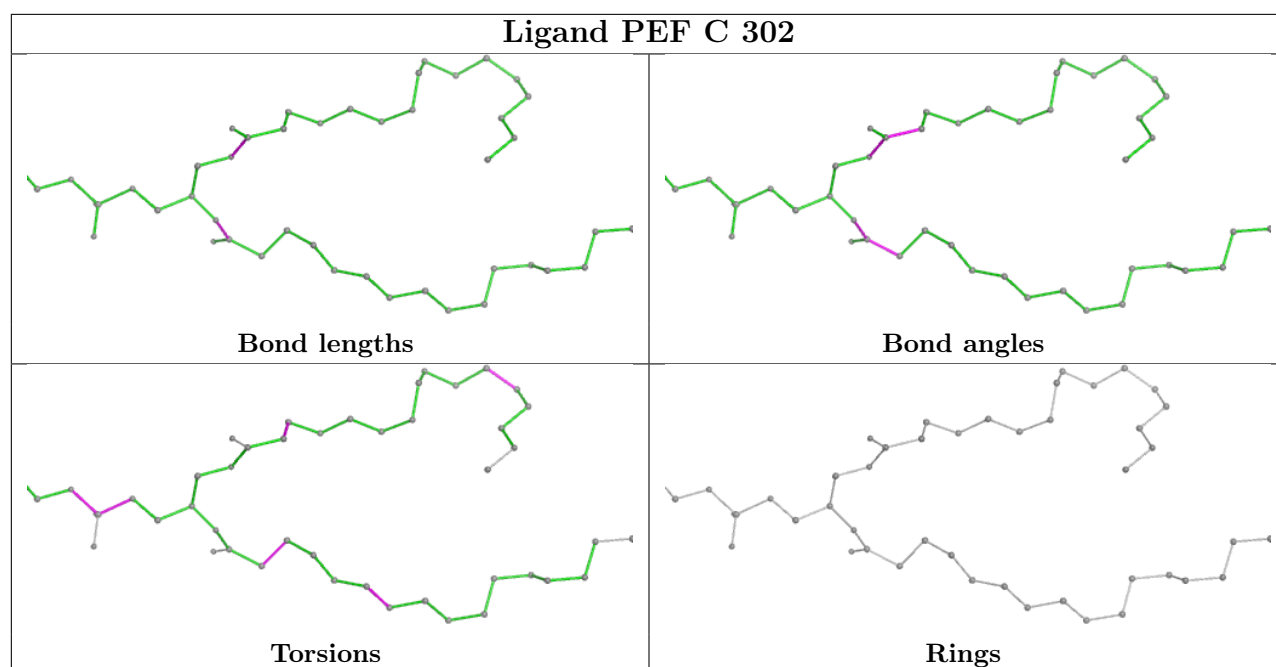
2 monomers are involved in 4 short contacts:

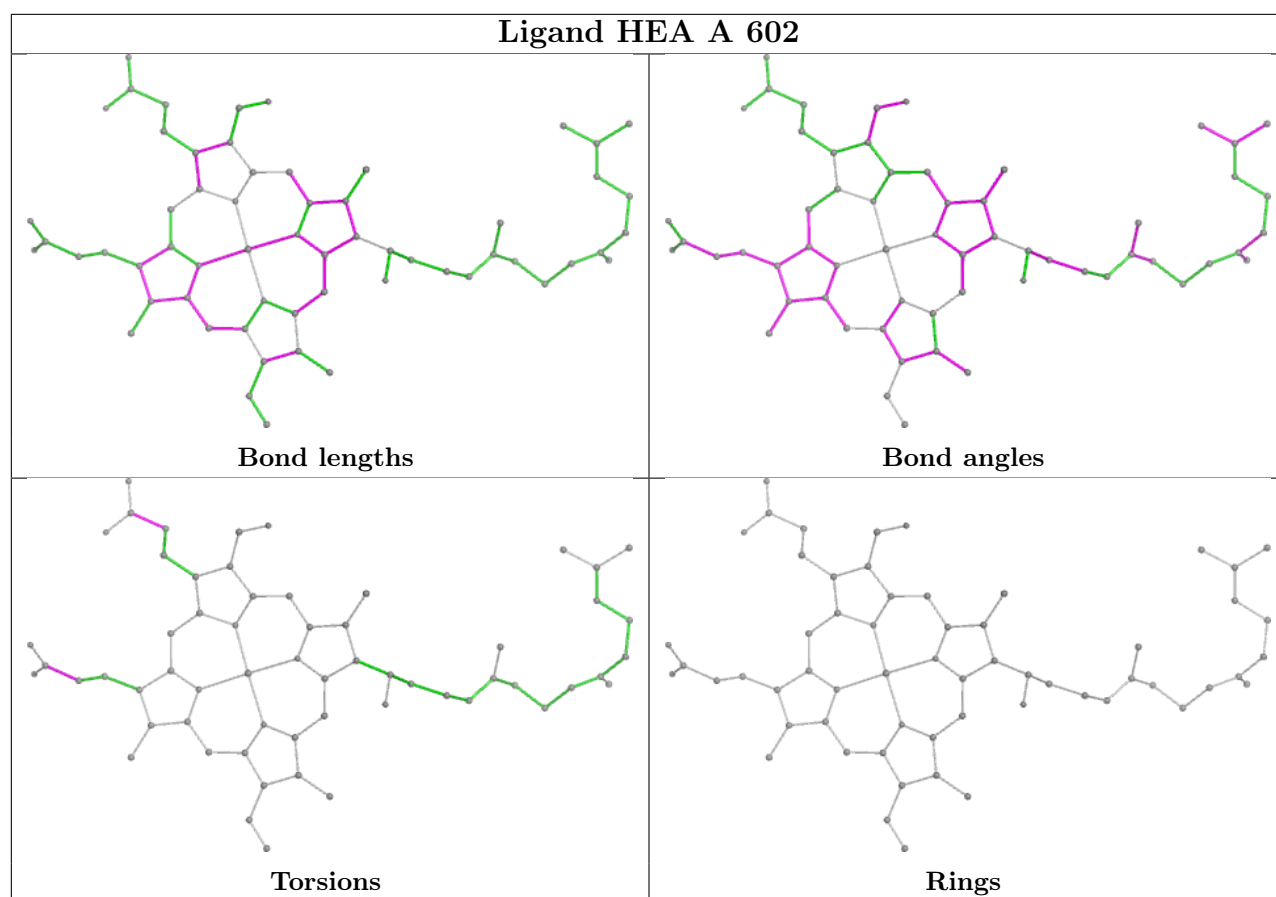
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	601	HEA	3	0
14	A	602	HEA	1	0

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.

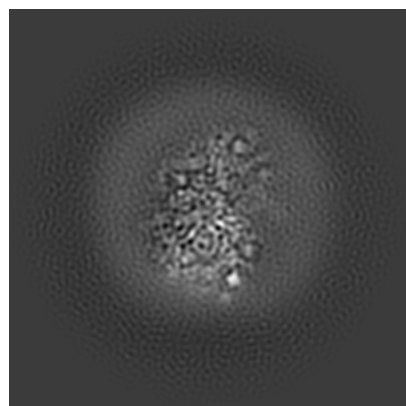
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16491. These allow visual inspection of the internal detail of the map and identification of artifacts.

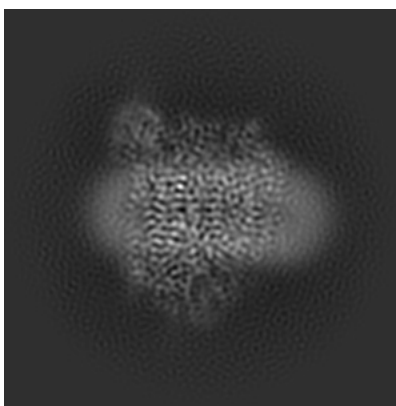
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

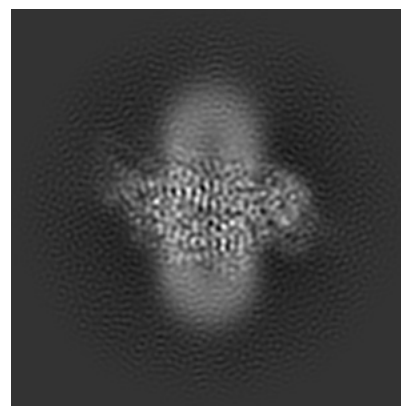
#### 6.1.1 Primary map



X

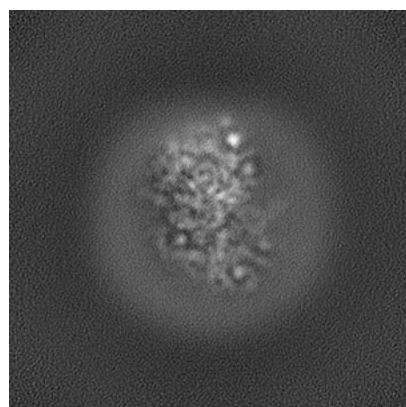


Y

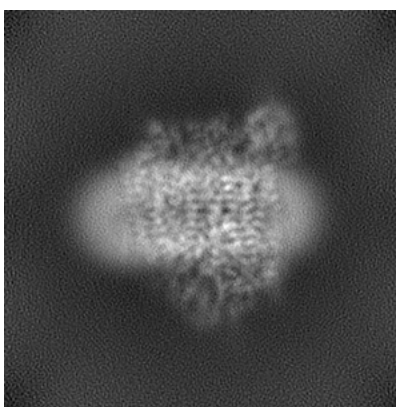


Z

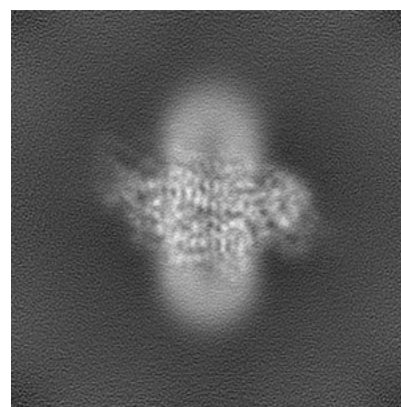
#### 6.1.2 Raw map



X



Y

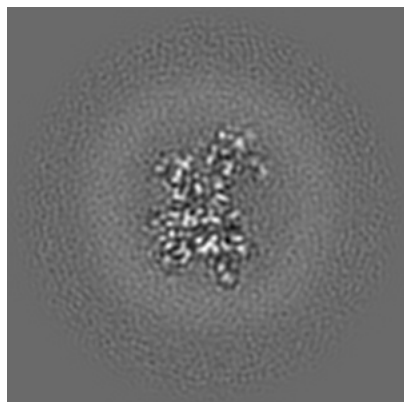


Z

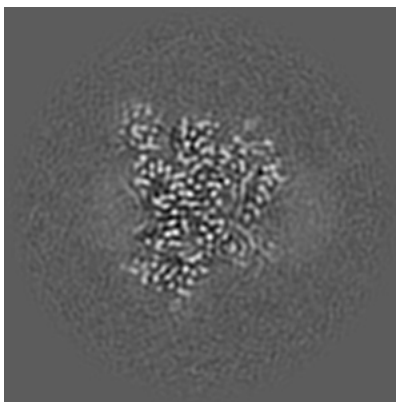
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

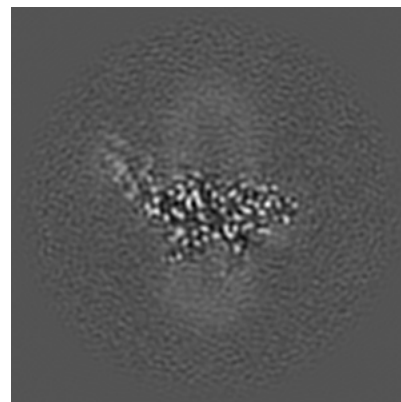
### 6.2.1 Primary map



X Index: 128

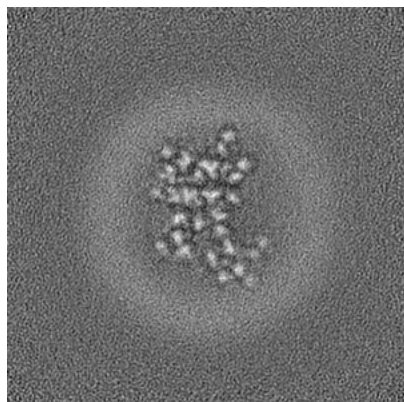


Y Index: 128

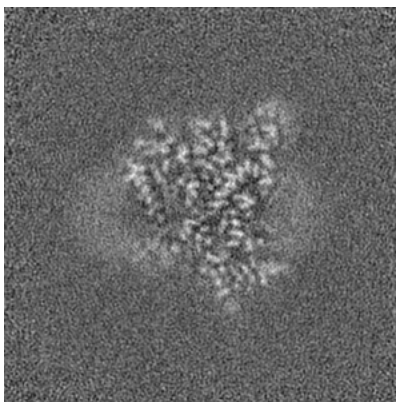


Z Index: 128

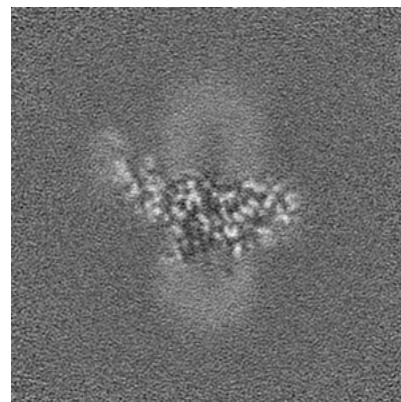
### 6.2.2 Raw map



X Index: 128



Y Index: 128

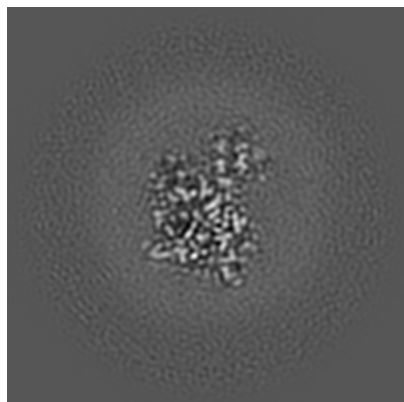


Z Index: 128

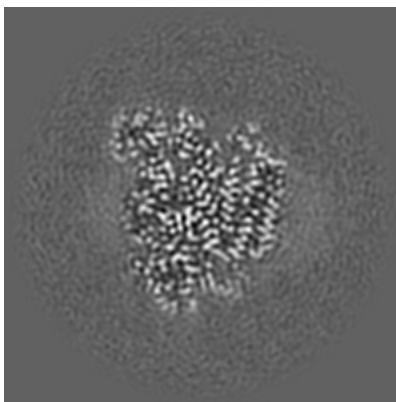
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

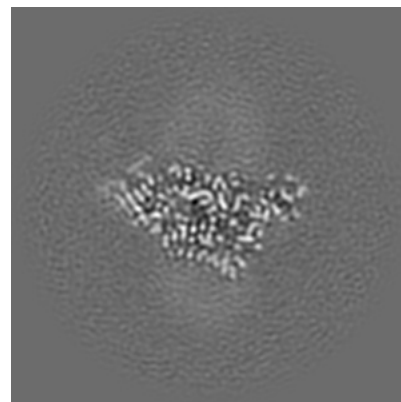
### 6.3.1 Primary map



X Index: 113

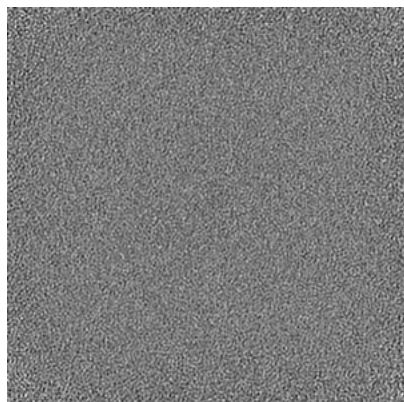


Y Index: 136

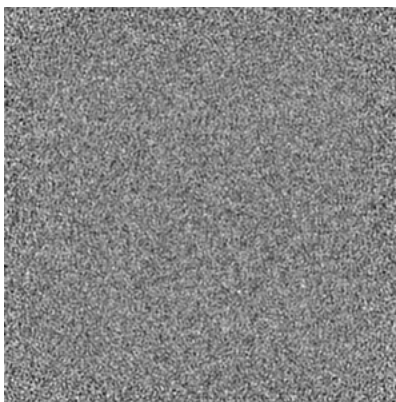


Z Index: 118

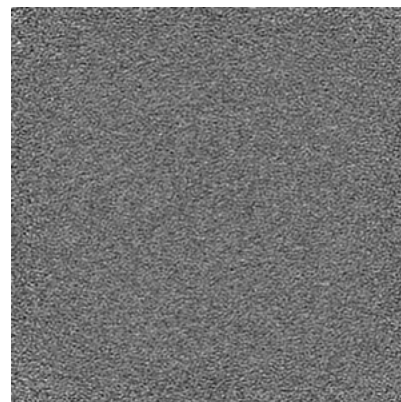
### 6.3.2 Raw map



X Index: 0



Y Index: 0

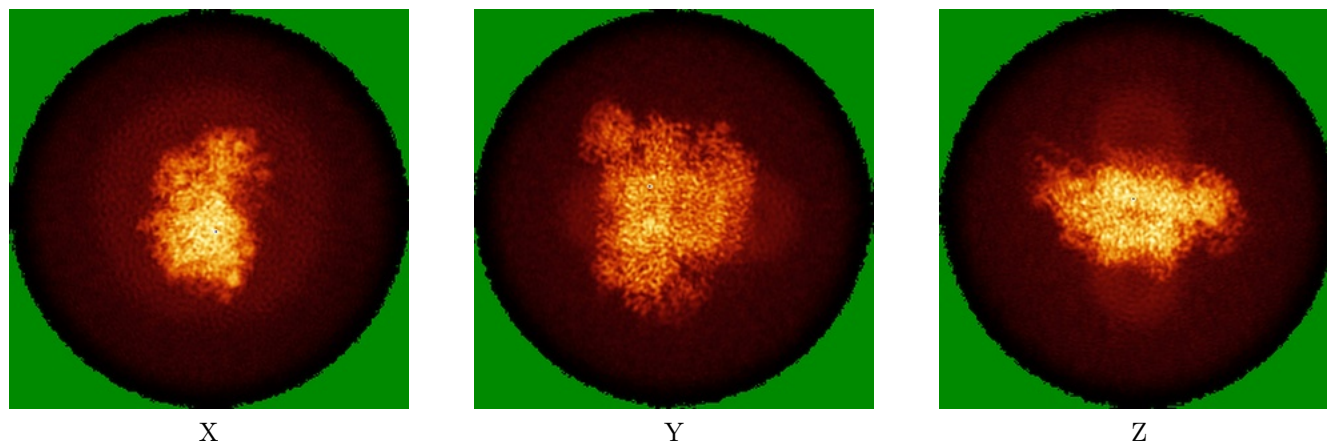


Z Index: 0

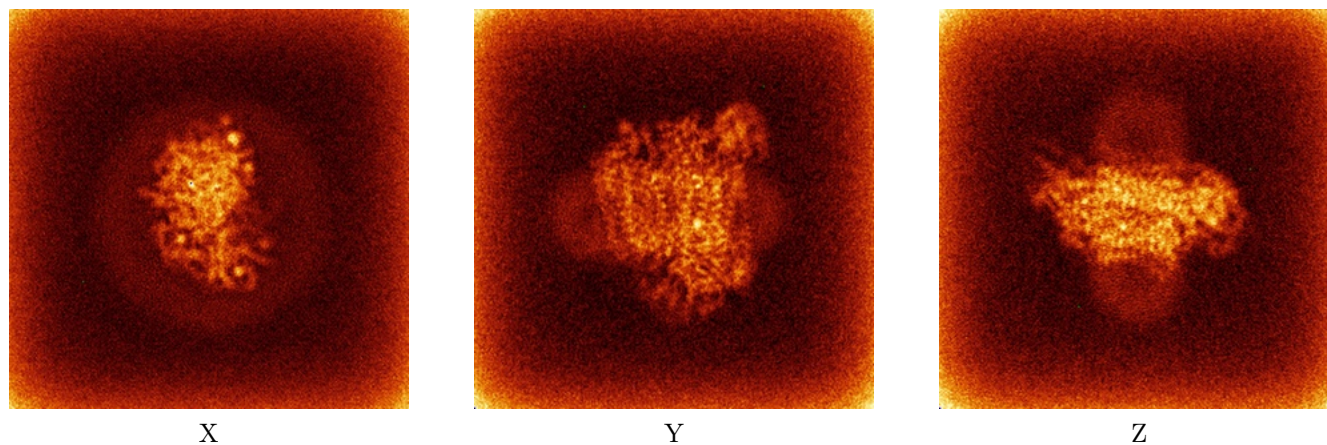
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



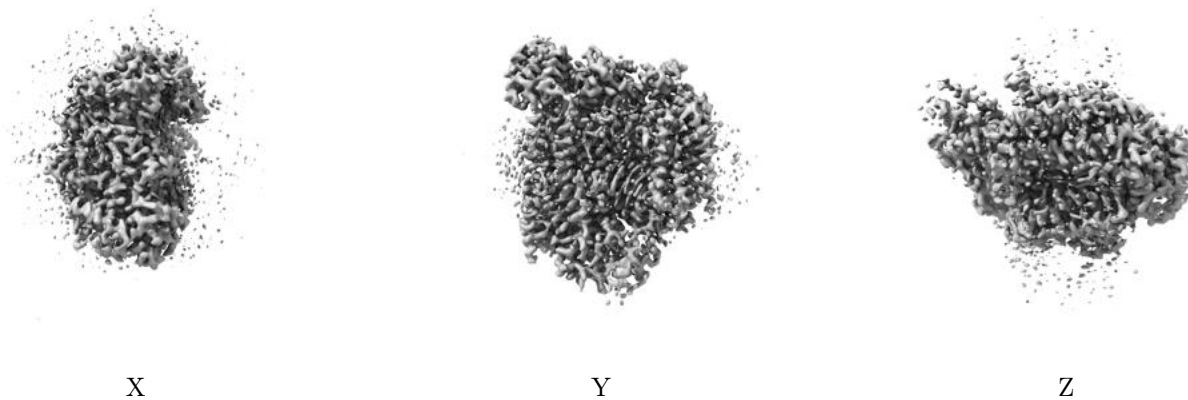
### 6.4.2 Raw map



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

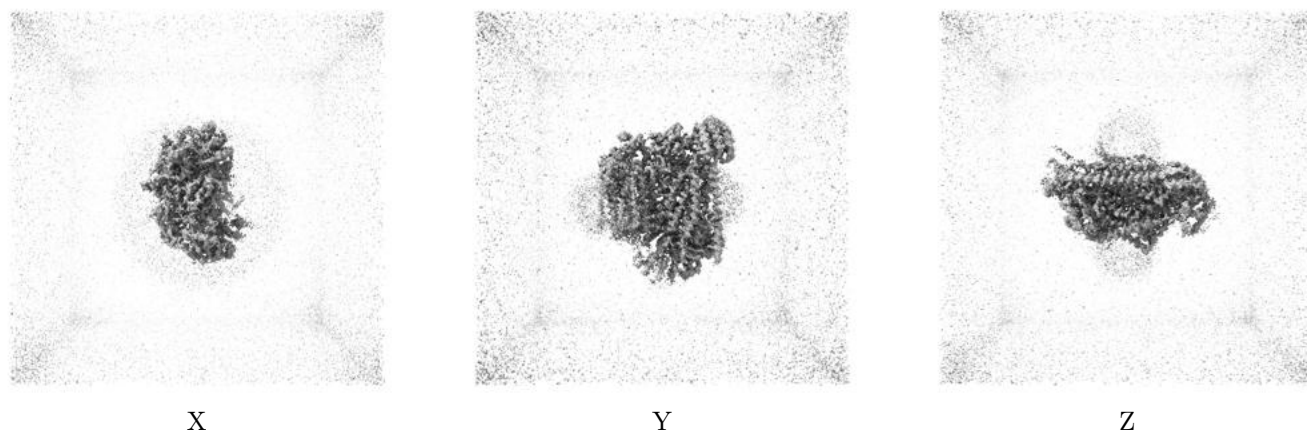
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

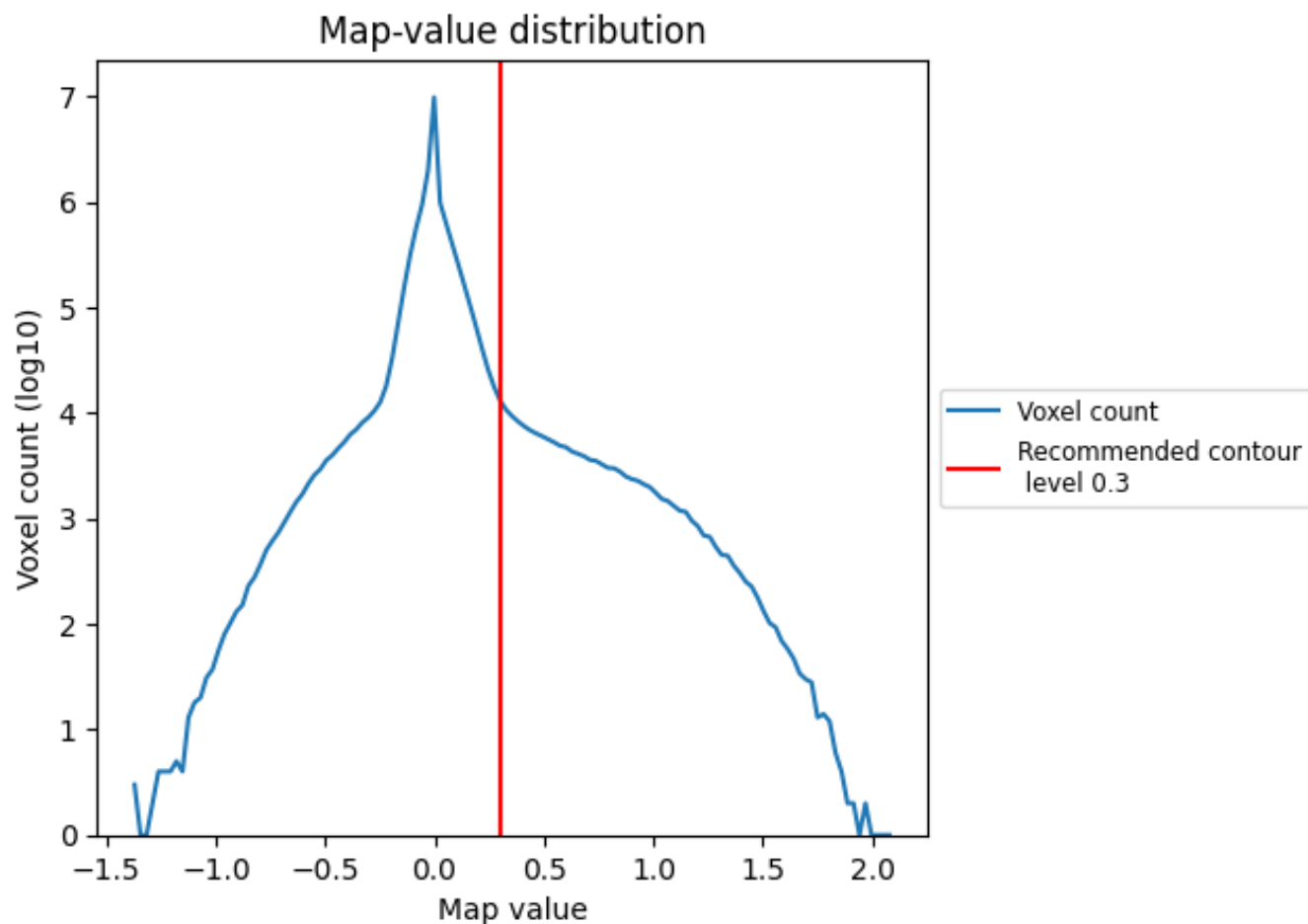
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

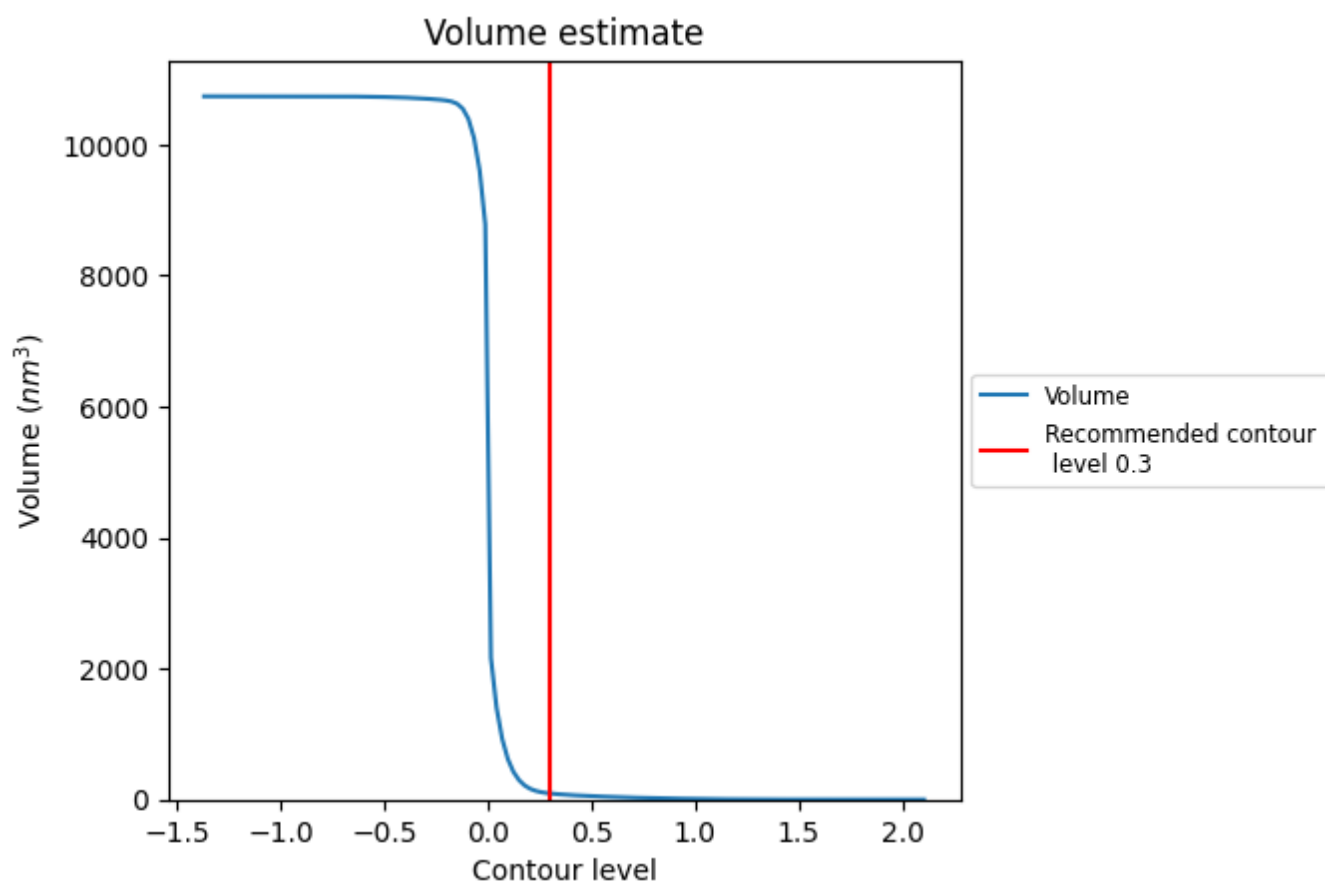
This section contains the results of statistical analysis of the map.

### 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.

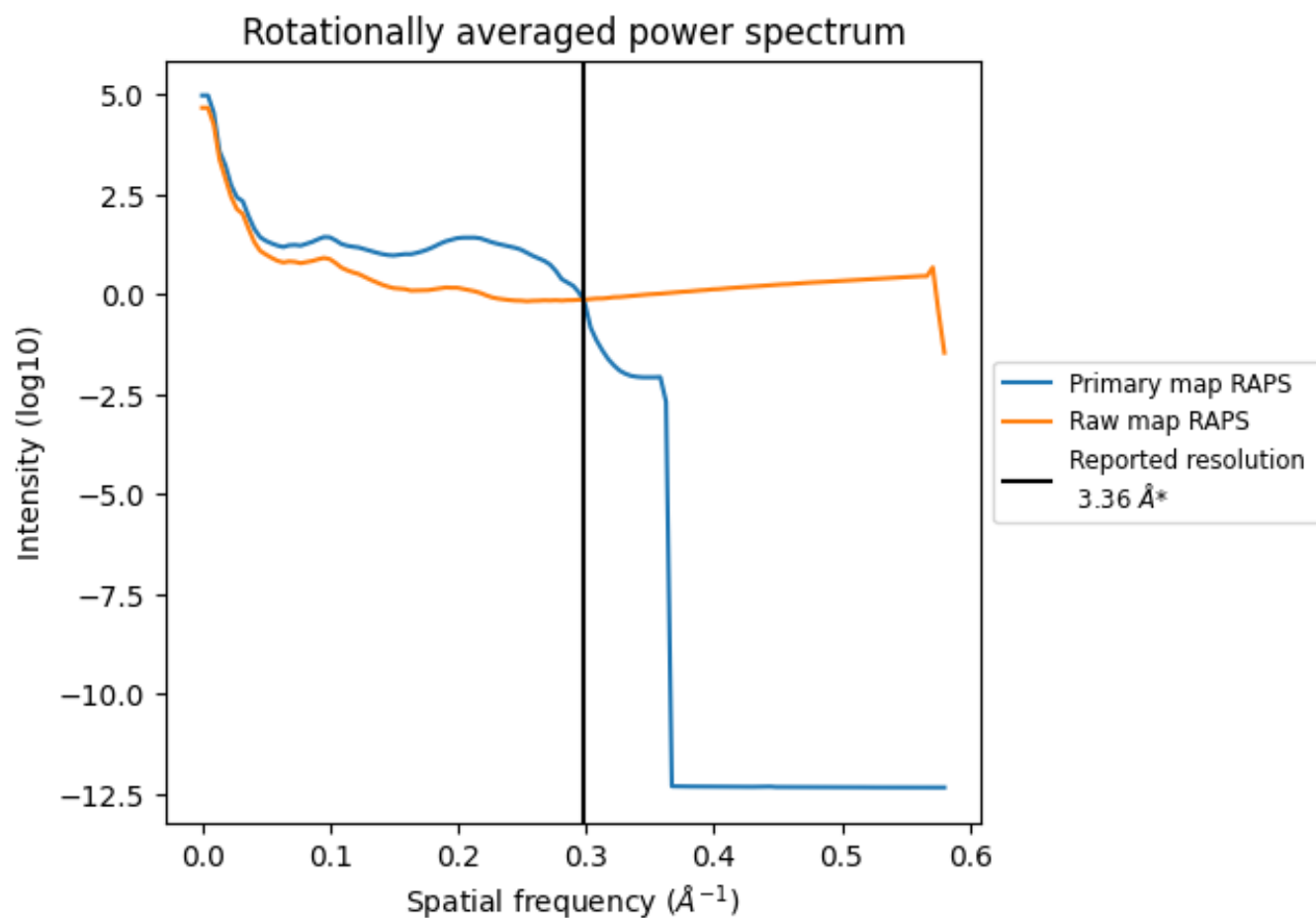
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 94  $\text{nm}^3$ ; this corresponds to an approximate mass of 85 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 ⓘ

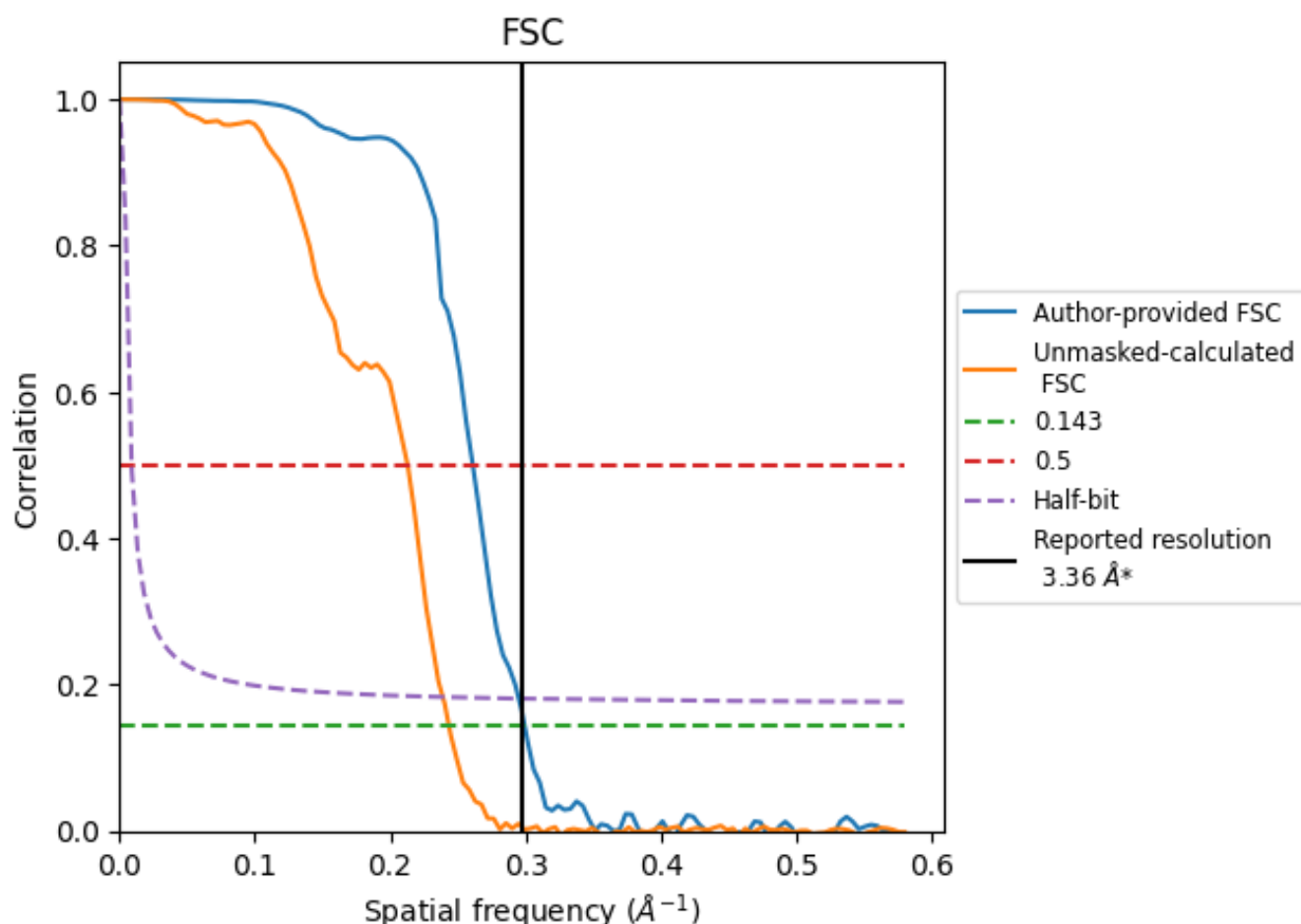


\*Reported resolution corresponds to spatial frequency of 0.298 Å<sup>-1</sup>

## 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 0.298  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

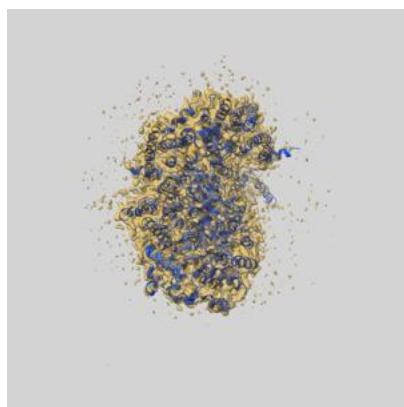
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.36	-	-
Author-provided FSC curve	3.34	3.83	3.39
Unmasked-calculated*	4.11	4.70	4.19

\*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 4.11 differs from the reported value 3.36 by more than 10 %

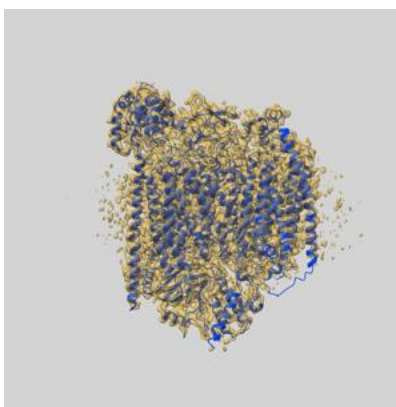
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16491 and PDB model 8C8Q. Per-residue inclusion information can be found in section [3](#) on page [10](#).

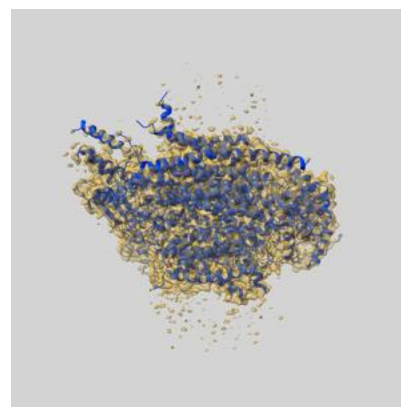
### 9.1 Map-model overlay [i](#)



X



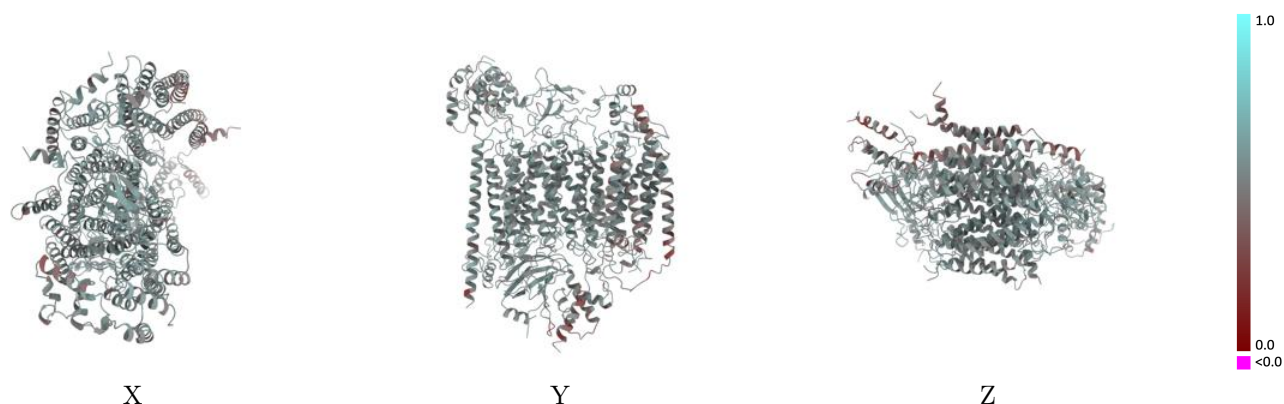
Y



Z

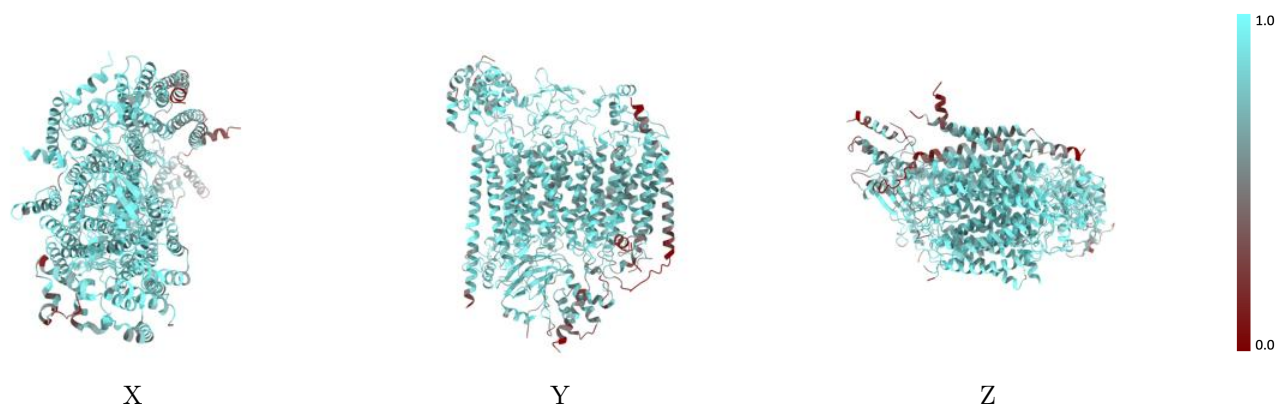
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



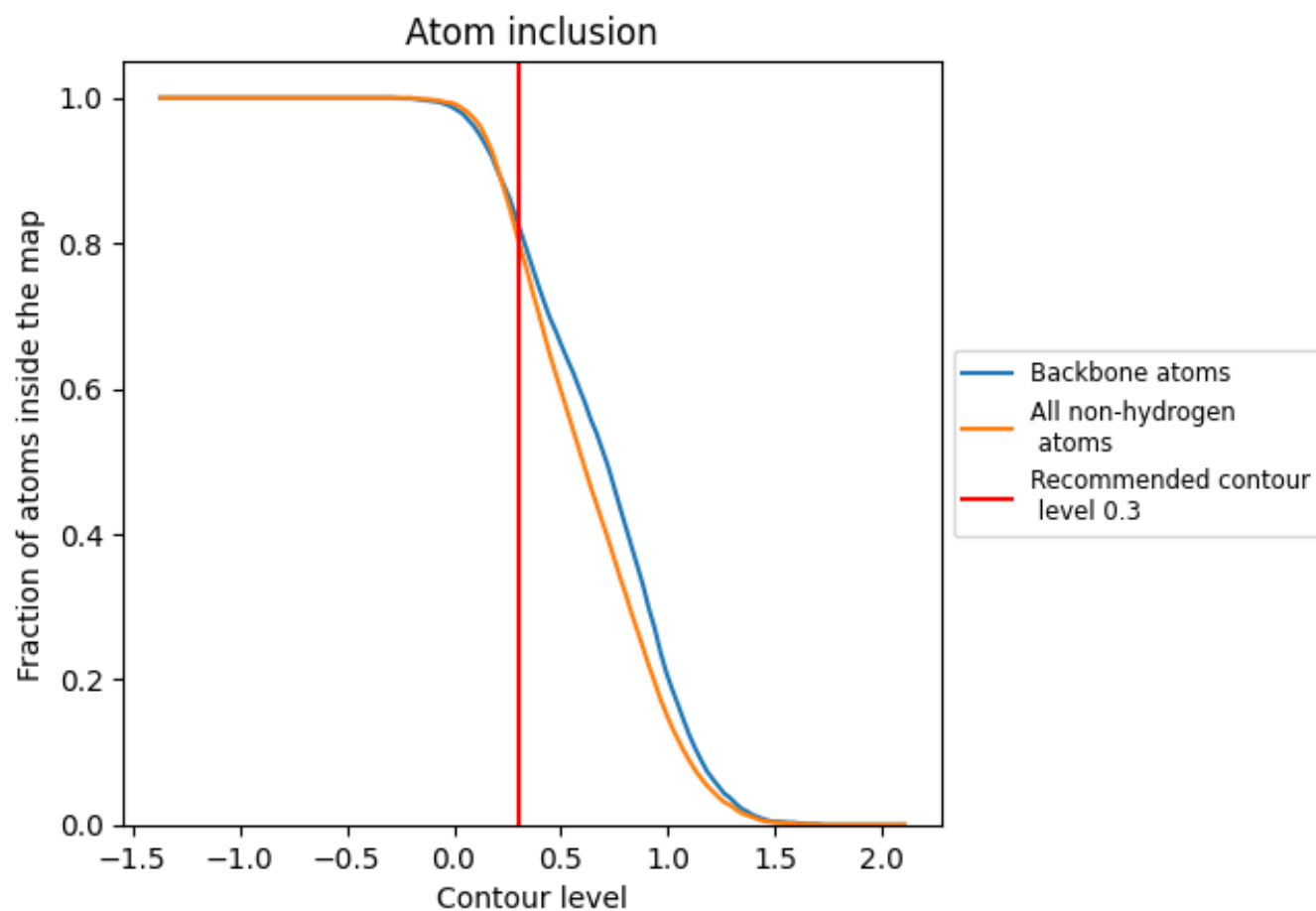
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).





























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 80% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8050	 0.5250
A	 0.8880	 0.5460
B	 0.8470	 0.5390
C	 0.8500	 0.5350
D	 0.8260	 0.5390
E	 0.7620	 0.5190
F	 0.8020	 0.5200
G	 0.8450	 0.5170
H	 0.8160	 0.5080
I	 0.7730	 0.5160
J	 0.6660	 0.5040
K	 0.4640	 0.4490
L	 0.5580	 0.4530
M	 0.4000	 0.4230

