



## wwPDB EM Validation Summary Report ⓘ

Dec 18, 2022 – 05:34 pm GMT

PDB ID : 7AQQ  
EMDB ID : EMD-11872  
Title : Cryo-EM structure of Arabidopsis thaliana Complex-I (membrane core)  
Authors : Klusch, N.; Kuehlbrandt, W.; Yildiz, O.  
Deposited on : 2020-10-22  
Resolution : 3.06 Å (reported)

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

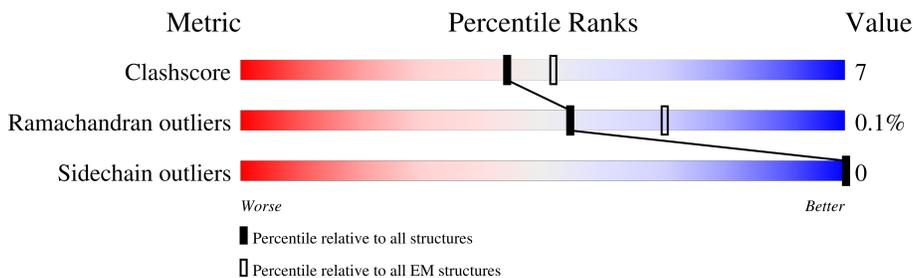
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.06 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.



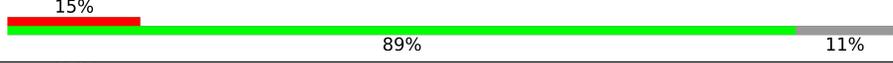
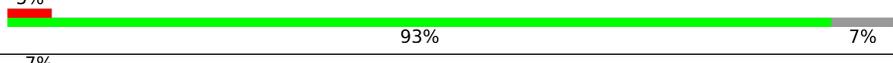
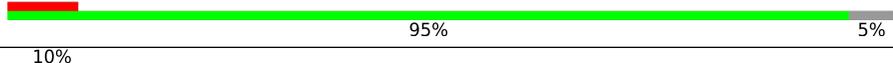
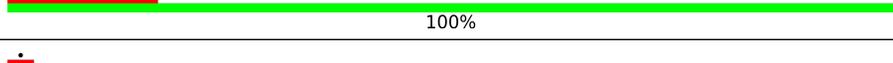
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	119	
2	H	325	
3	J	205	
4	K	100	
5	L	669	
6	M	495	
7	N	499	
8	O	159	

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Mol	Chain	Length	Quality of chain
9	X	106	
10	Z	143	
11	a	65	
12	b	65	
13	d	81	
14	e	83	
15	f	106	
16	i	98	
17	u	30	
18	v	113	
19	x	256	
20	y	278	
21	z	275	

## 2 Entry composition i

There are 30 unique types of molecules in this entry. The entry contains 23281 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 NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	92	779	553	105	117	4	0	0

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	311	2439	1659	372	393	15	0	0

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	147	1162	784	179	191	8	0	0

- Molecule 4 is a protein called NADH dehydrogenase subunit 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	K	90	707	476	109	115	7	0	0

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	L	26	208	133	37	38	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	91	PHE	SER	conflict	UNP B5TM94

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	M	262	2126	1457	319	339	11	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	326	LEU	PRO	conflict	UNP B5TM93
M	378	PHE	SER	conflict	UNP B5TM93

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	N	488	3820	2573	577	642	28	0	0

- Molecule 8 is a protein called AT3G07480.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	O	122	956	598	169	185	4	0	0

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	X	97	767	480	132	143	12	0	0

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Z	98	798	514	137	142	5	0	0

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	a	58	469	302	84	78	5	0	0

- Molecule 12 is a protein called At2g46540/F11C10.23.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	40	Total	C	N	O	S	0	0
			295	195	48	49	3		

- Molecule 13 is a protein called Excitatory amino acid transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	d	75	Total	C	N	O	S	0	0
			592	382	106	99	5		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	e	65	Total	C	N	O	S	0	0
			557	344	106	100	7		

- Molecule 15 is a protein called At4g16450.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	101	Total	C	N	O	S	0	0
			763	490	126	142	5		

- Molecule 16 is a protein called P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	i	70	Total	C	N	O	S	0	0
			614	384	116	111	3		

- Molecule 17 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	u	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 18 is a protein called Uncharacterized protein At2g27730, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	v	30	Total	C	N	O	0	0
			226	147	39	40		

- Molecule 19 is a protein called Gamma carbonic anhydrase-like 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	x	214	1659	1063	285	306	5	0	0

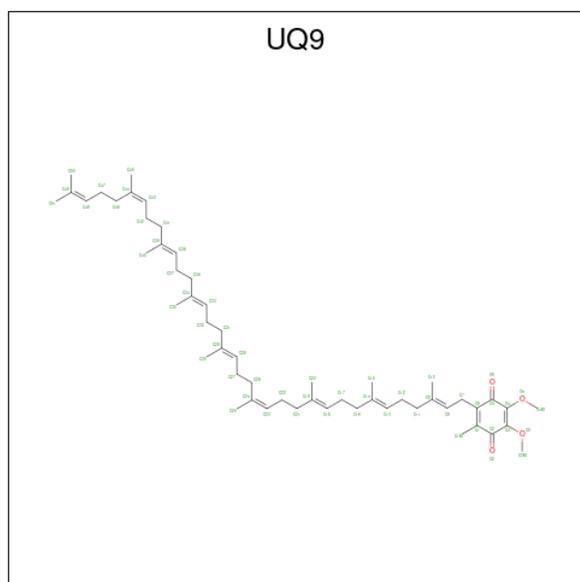
- Molecule 20 is a protein called Gamma carbonic anhydrase 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	y	268	2032	1271	363	391	7	0	0

- Molecule 21 is a protein called Gamma carbonic anhydrase 1, mitochondrial.

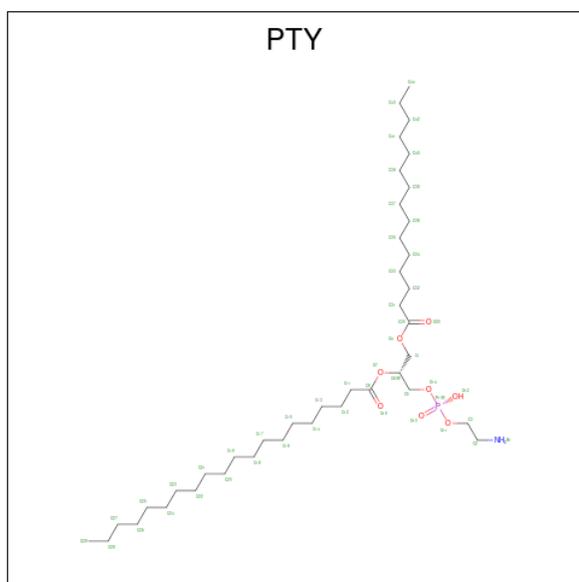
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	z	233	1772	1111	325	330	6	0	0

- Molecule 22 is Ubiquinone-9 (three-letter code: UQ9) (formula:  $C_{54}H_{82}O_4$ ).



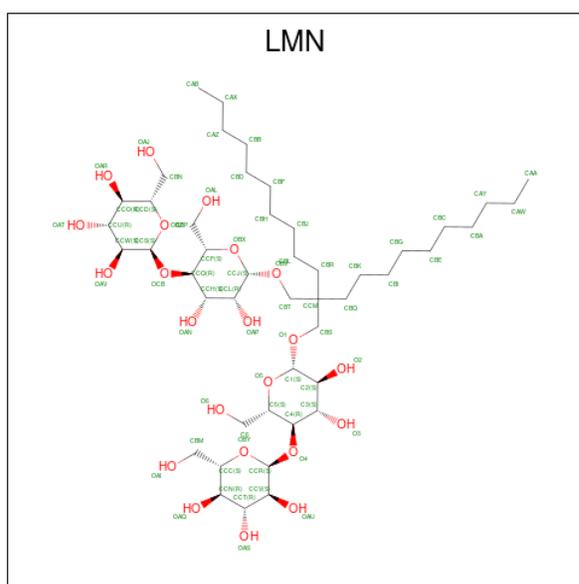
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
22	H	1	35	31	4	0

- Molecule 23 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula:  $C_{40}H_{80}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	H	1	50	40	1	8	1	0
23	N	1	50	40	1	8	1	0

- Molecule 24 is Lauryl Maltose Neopentyl Glycol (three-letter code: LMN) (formula:  $C_{47}H_{88}O_{22}$ ).

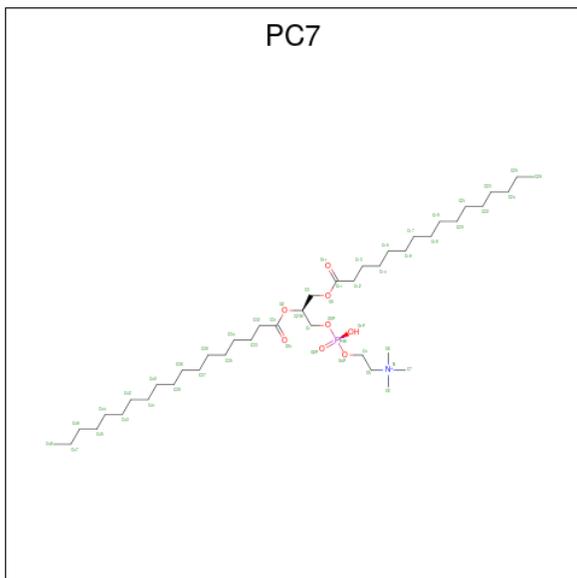


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	M	1	69	47	22	0

- Molecule 25 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
25	O	1	Total	Fe	0
			1	1	

- Molecule 26 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PC7) (formula: C<sub>42</sub>H<sub>85</sub>NO<sub>8</sub>P).

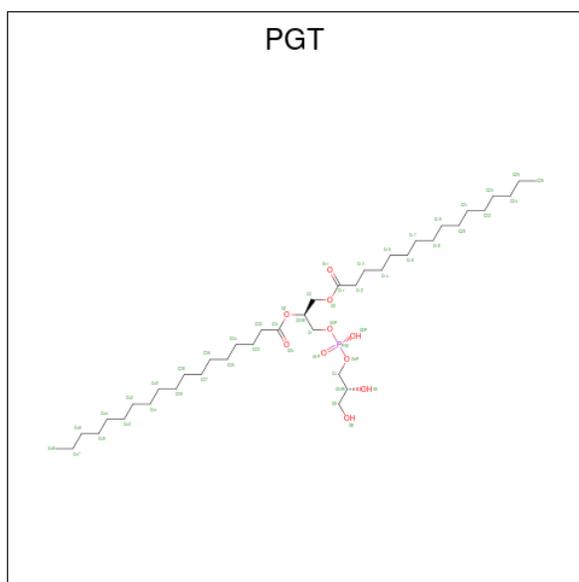


Mol	Chain	Residues	Atoms					AltConf
26	v	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

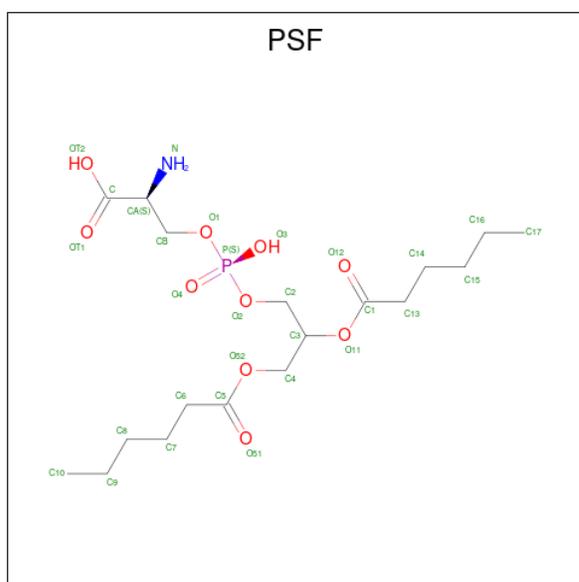
Mol	Chain	Residues	Atoms		AltConf
27	y	1	Total	Zn	0
			1	1	

- Molecule 28 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: C<sub>40</sub>H<sub>79</sub>O<sub>10</sub>P).



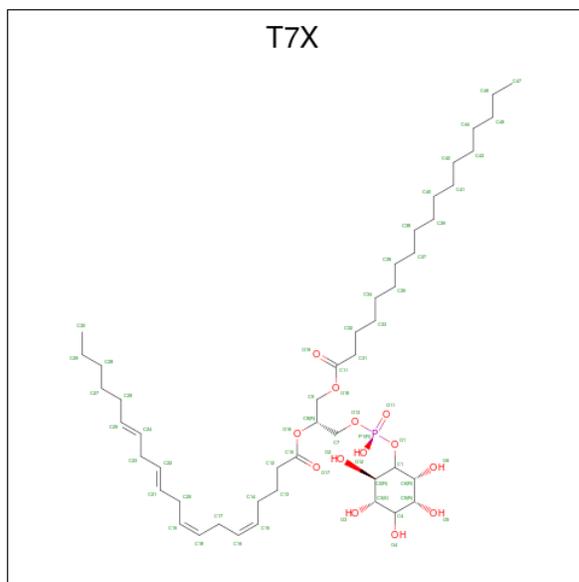
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
28	y	1	41	30	10	1	0

- Molecule 29 is 1,2-DICAPROYL-SN-PHOSPHATIDYL-L-SERINE (three-letter code: PSF) (formula:  $C_{18}H_{34}NO_{10}P$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
29	z	1	30	18	1	10	1	0

- Molecule 30 is Phosphatidylinositol (three-letter code: T7X) (formula:  $C_{47}H_{83}O_{13}P$ ).



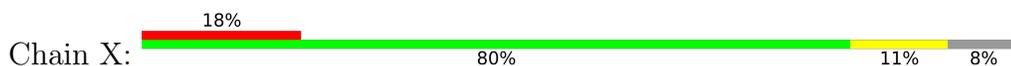
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
30	z	1	61	47	13	1	0



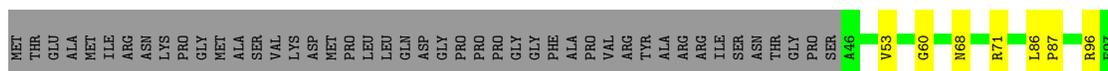




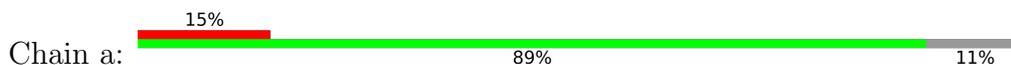
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B



- Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A



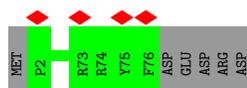
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



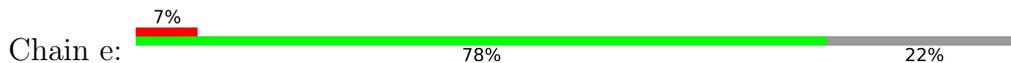
- Molecule 12: At2g46540/F11C10.23



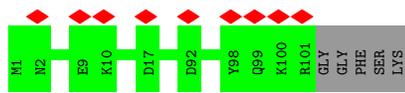
- Molecule 13: Excitatory amino acid transporter



- Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B



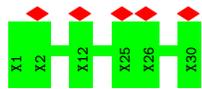
- Molecule 15: At4g16450



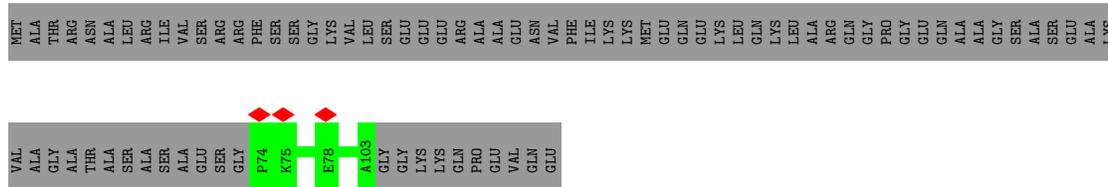
• Molecule 16: P1



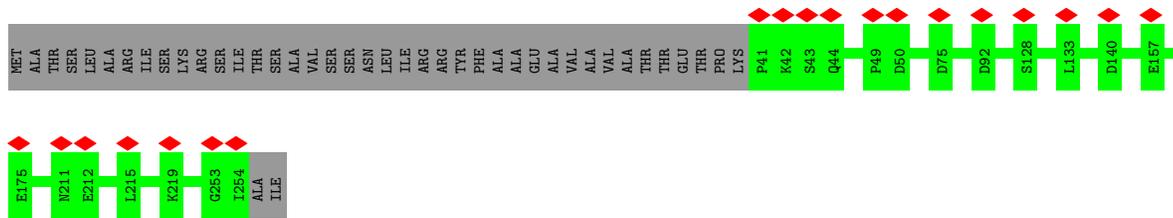
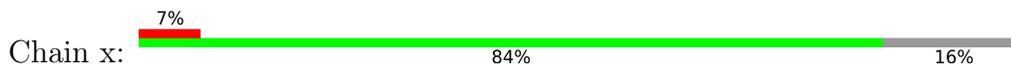
• Molecule 17: unknown



• Molecule 18: Uncharacterized protein At2g27730, mitochondrial



• Molecule 19: Gamma carbonic anhydrase-like 2, mitochondrial

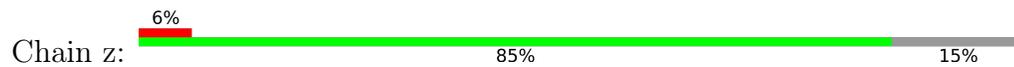


• Molecule 20: Gamma carbonic anhydrase 2, mitochondrial



VAL  
PRO  
SER  
THR  
GLN  
TYR  
PHE

- Molecule 21: Gamma carbonic anhydrase 1, mitochondrial



ASP  
LYS  
GLU  
THR  
LYS  
ARG  
PRO  
SER  
ASN  
VAL  
ASN

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	459177	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 ( $e^-/\text{\AA}^2$ )	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.056	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.013	Depositor
Map size ( $\text{\AA}$ )	502.2, 502.2, 502.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.837, 0.837, 0.837	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: ZN, PC7, FE, PTY, PGT, PSF, UQ9, T7X, LMN

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	0.28	0/807	0.44	0/1096
2	H	0.29	0/2510	0.49	0/3416
3	J	0.28	0/1187	0.47	0/1617
4	K	0.28	0/717	0.47	0/969
5	L	0.23	0/211	0.54	0/282
6	M	0.27	0/2188	0.44	0/2976
7	N	0.28	0/3924	0.46	0/5327
8	O	0.24	0/971	0.49	0/1314
9	X	0.26	0/781	0.45	0/1049
10	Z	0.28	0/820	0.51	0/1108
11	a	0.25	0/481	0.50	0/646
12	b	0.25	0/300	0.46	0/407
13	d	0.26	0/605	0.49	0/815
14	e	0.27	0/570	0.49	0/759
15	f	0.28	0/779	0.46	0/1052
16	i	0.26	0/632	0.50	0/852
18	v	0.24	0/230	0.39	0/311
19	x	0.28	0/1700	0.50	0/2320
20	y	0.27	0/2066	0.48	0/2800
21	z	0.27	0/1804	0.50	0/2441
All	All	0.27	0/23283	0.48	0/31557

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	779	0	796	22	0
2	H	2439	0	2554	39	0
3	J	1162	0	1238	26	0
4	K	707	0	771	15	0
5	L	208	0	211	8	0
6	M	2126	0	2227	33	0
7	N	3820	0	3926	66	0
8	O	956	0	968	8	0
9	X	767	0	766	8	0
10	Z	798	0	780	12	0
11	a	469	0	472	0	0
12	b	295	0	322	0	0
13	d	592	0	610	0	0
14	e	557	0	525	0	0
15	f	763	0	767	0	0
16	i	614	0	577	0	0
17	u	150	0	34	0	0
18	v	226	0	235	0	0
19	x	1659	0	1673	0	0
20	y	2032	0	2044	0	0
21	z	1772	0	1771	0	0
22	H	35	0	43	2	0
23	H	50	0	79	4	0
23	N	50	0	79	5	0
24	M	69	0	88	1	0
25	O	1	0	0	0	0
26	v	52	0	84	0	0
27	y	1	0	0	0	0
28	y	41	0	52	0	0
29	z	30	0	32	0	0
30	z	61	0	0	0	0
All	All	23281	0	23724	198	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 7.

The worst 5 of 198 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)
6:M:142:PHE:O	6:M:146:PHE:HB2	1.78	0.83
4:K:36:GLU:OE1	4:K:73:SER:OG	1.99	0.79
4:K:42:VAL:HG11	7:N:191:LEU:HG	1.66	0.76
3:J:37:THR:HG21	4:K:40:LEU:HD11	1.65	0.76
1:A:88:ILE:HD12	1:A:92:GLY:HA3	1.69	0.73

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	88/119 (74%)	86 (98%)	2 (2%)	0	100	100
2	H	307/325 (94%)	287 (94%)	19 (6%)	1 (0%)	41	70
3	J	143/205 (70%)	136 (95%)	7 (5%)	0	100	100
4	K	88/100 (88%)	86 (98%)	2 (2%)	0	100	100
5	L	24/669 (4%)	21 (88%)	3 (12%)	0	100	100
6	M	260/495 (52%)	256 (98%)	3 (1%)	1 (0%)	34	64
7	N	486/499 (97%)	475 (98%)	11 (2%)	0	100	100
8	O	120/159 (76%)	114 (95%)	6 (5%)	0	100	100
9	X	95/106 (90%)	94 (99%)	1 (1%)	0	100	100
10	Z	96/143 (67%)	91 (95%)	4 (4%)	1 (1%)	15	45
11	a	56/65 (86%)	56 (100%)	0	0	100	100
12	b	38/65 (58%)	38 (100%)	0	0	100	100
13	d	73/81 (90%)	71 (97%)	2 (3%)	0	100	100
14	e	63/83 (76%)	63 (100%)	0	0	100	100
15	f	99/106 (93%)	96 (97%)	3 (3%)	0	100	100
16	i	68/98 (69%)	66 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	v	28/113 (25%)	27 (96%)	1 (4%)	0	100	100
19	x	212/256 (83%)	207 (98%)	5 (2%)	0	100	100
20	y	266/278 (96%)	252 (95%)	14 (5%)	0	100	100
21	z	231/275 (84%)	227 (98%)	4 (2%)	0	100	100
All	All	2841/4240 (67%)	2749 (97%)	89 (3%)	3 (0%)	54	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	201	ALA
6	M	231	VAL
10	Z	120	VAL

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	83/106 (78%)	83 (100%)	0	100	100
2	H	262/272 (96%)	262 (100%)	0	100	100
3	J	131/186 (70%)	131 (100%)	0	100	100
4	K	78/86 (91%)	78 (100%)	0	100	100
5	L	21/568 (4%)	21 (100%)	0	100	100
6	M	232/434 (54%)	232 (100%)	0	100	100
7	N	406/416 (98%)	406 (100%)	0	100	100
8	O	107/141 (76%)	107 (100%)	0	100	100
9	X	87/94 (93%)	87 (100%)	0	100	100
10	Z	79/115 (69%)	79 (100%)	0	100	100
11	a	48/53 (91%)	48 (100%)	0	100	100
12	b	33/53 (62%)	33 (100%)	0	100	100
13	d	60/66 (91%)	60 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	e	60/73 (82%)	60 (100%)	0	100	100
15	f	81/84 (96%)	81 (100%)	0	100	100
16	i	64/90 (71%)	64 (100%)	0	100	100
18	v	23/84 (27%)	23 (100%)	0	100	100
19	x	183/216 (85%)	183 (100%)	0	100	100
20	y	223/232 (96%)	223 (100%)	0	100	100
21	z	188/228 (82%)	188 (100%)	0	100	100
All	All	2449/3597 (68%)	2449 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
6	M	31	ASN
7	N	53	ASN
9	X	45	ASN
19	x	116	ASN
21	z	101	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z  > 2$
26	PC7	v	201	-	51,51,51	0.95	4 (7%)	57,59,59	1.04	2 (3%)
28	PGT	y	302	-	40,40,50	1.16	3 (7%)	43,46,56	1.10	2 (4%)
29	PSF	z	301	-	28,29,29	1.18	4 (14%)	32,36,36	1.22	2 (6%)
23	PTY	N	501	-	49,49,49	0.86	4 (8%)	52,54,54	1.12	2 (3%)
24	LMN	M	501	-	72,72,72	1.65	14 (19%)	96,98,98	1.02	3 (3%)
23	PTY	H	402	-	49,49,49	0.87	4 (8%)	52,54,54	1.12	2 (3%)
22	UQ9	H	401	-	35,35,58	2.51	12 (34%)	42,45,73	1.86	12 (28%)
30	T7X	z	302	-	61,61,61	0.84	4 (6%)	71,73,73	1.07	3 (4%)

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
26	PC7	v	201	-	-	23/55/55/55	-
28	PGT	y	302	-	-	22/45/45/55	-
29	PSF	z	301	-	-	12/35/35/35	-
23	PTY	N	501	-	-	26/53/53/53	-
24	LMN	M	501	-	-	34/50/130/130	0/4/4/4
23	PTY	H	402	-	-	19/53/53/53	-
22	UQ9	H	401	-	-	8/30/54/81	0/1/1/1
30	T7X	z	302	-	-	29/56/80/80	0/1/1/1

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	H	401	UQ9	C6-C1	9.90	1.53	1.35
24	M	501	LMN	O5-C1	4.69	1.53	1.41
22	H	401	UQ9	C4-C3	4.32	1.53	1.36
24	M	501	LMN	CBS-CCM	4.16	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	501	LMN	CBT-CCM	4.07	1.62	1.53

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	H	401	UQ9	C7-C6-C5	4.75	124.20	118.48
30	z	302	T7X	O16-C10-C12	4.26	120.69	111.50
23	N	501	PTY	O7-C8-C11	4.17	120.49	111.50
28	y	302	PGT	O2-C31-C32	4.08	120.29	111.50
23	H	402	PTY	O7-C8-C11	4.07	120.27	111.50

There are no chirality outliers.

5 of 173 torsion outliers are listed below:

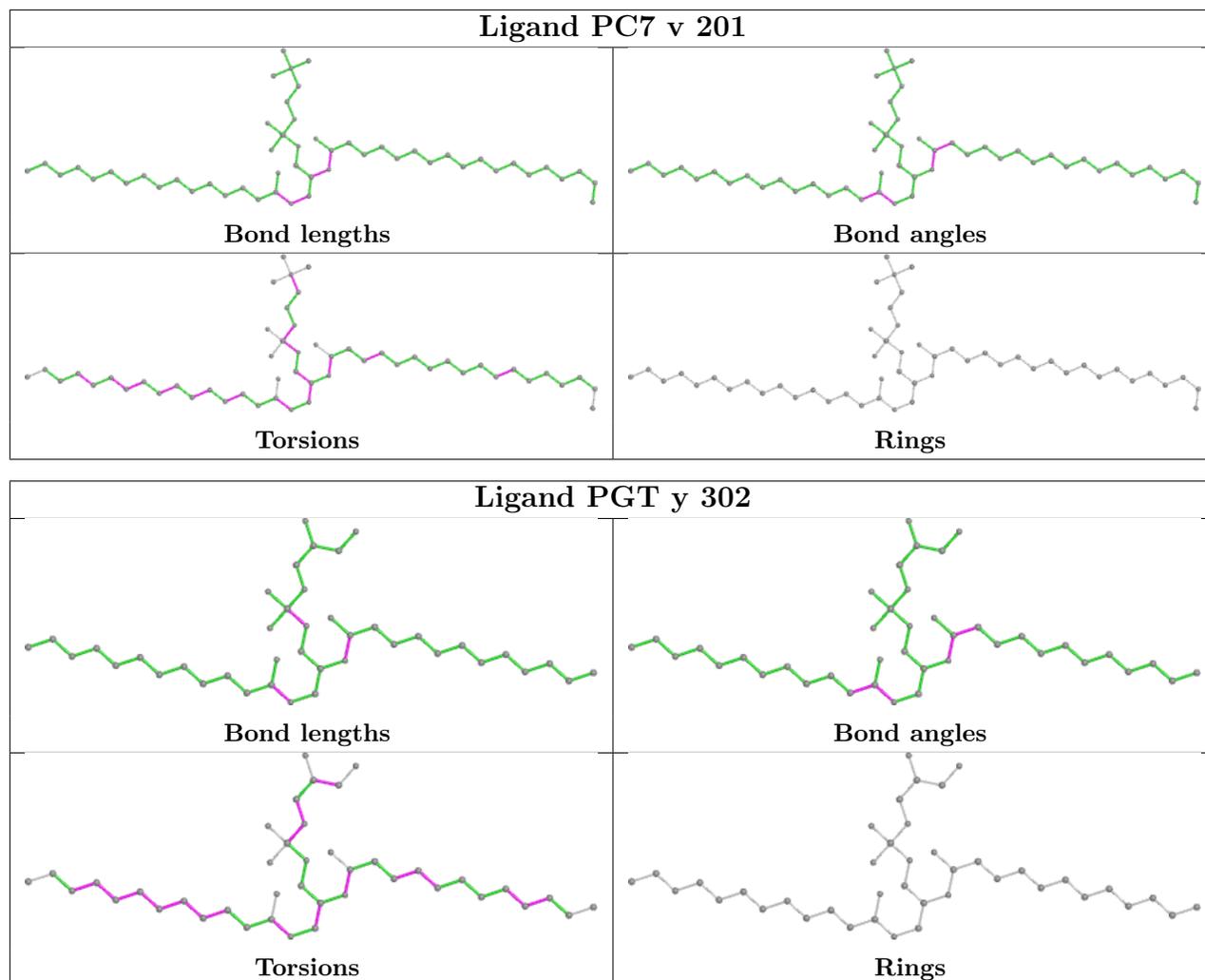
Mol	Chain	Res	Type	Atoms
22	H	401	UQ9	C9-C11-C12-C13
22	H	401	UQ9	C1-C6-C7-C8
22	H	401	UQ9	C5-C6-C7-C8
23	H	402	PTY	C5-O14-P1-O13
23	N	501	PTY	C5-C6-O7-C8

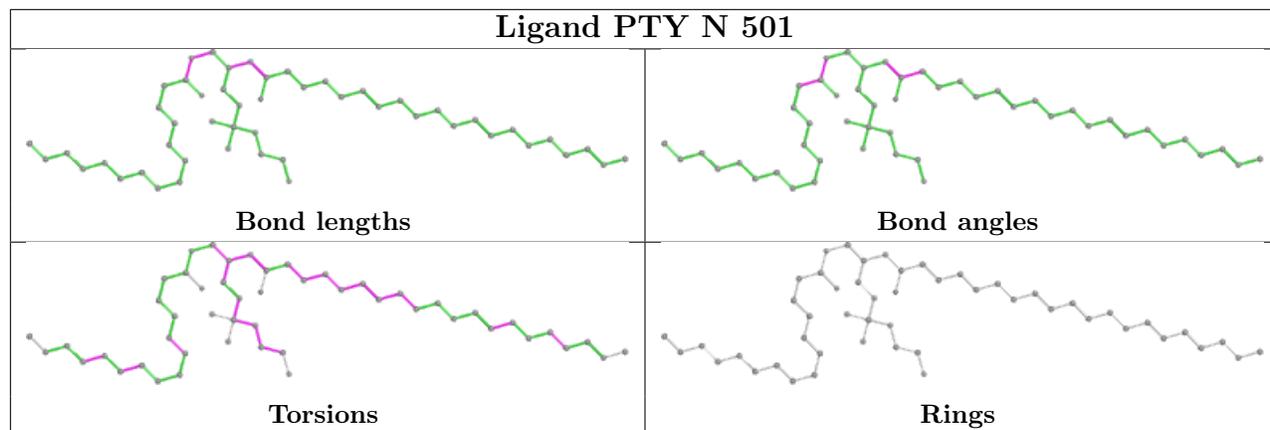
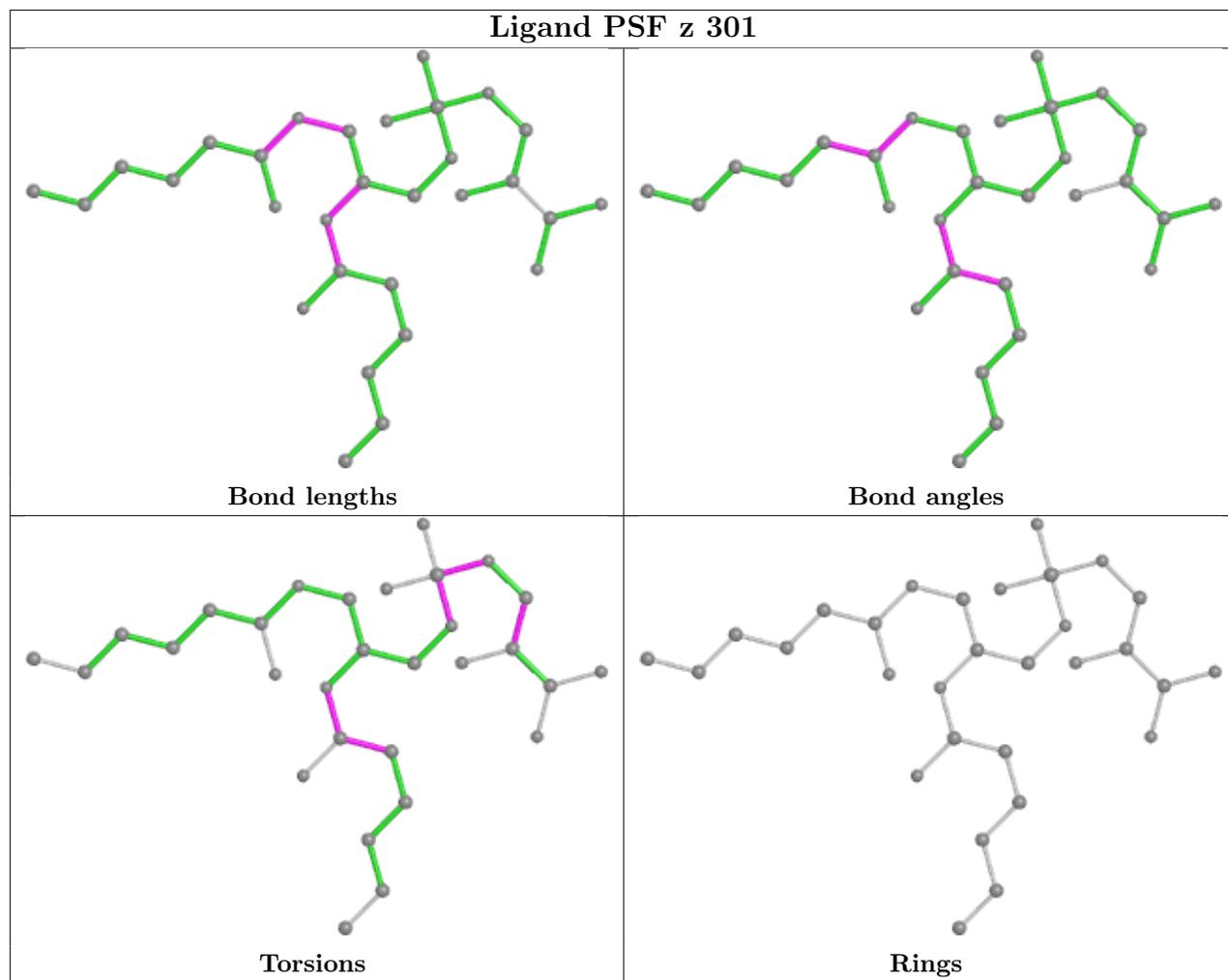
There are no ring outliers.

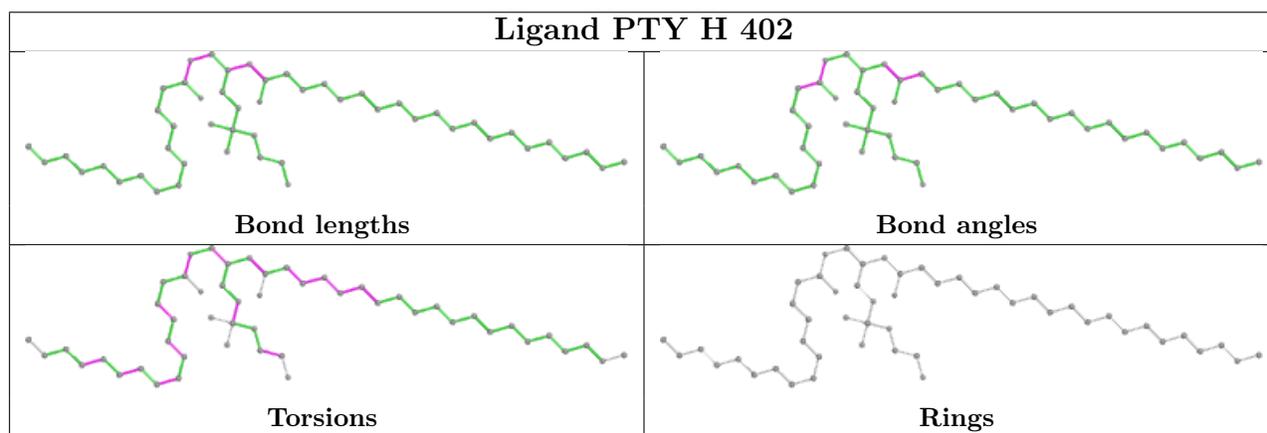
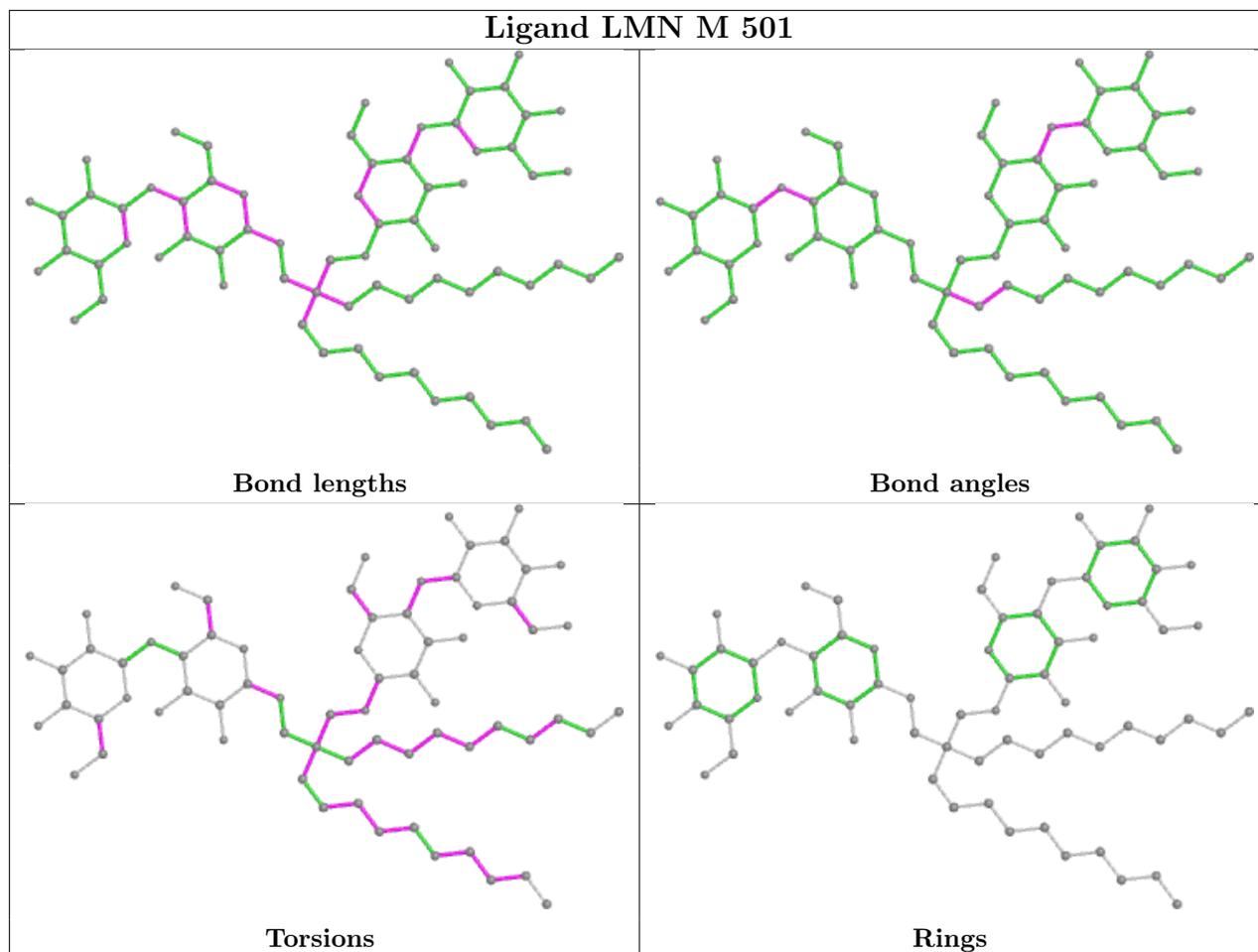
4 monomers are involved in 12 short contacts:

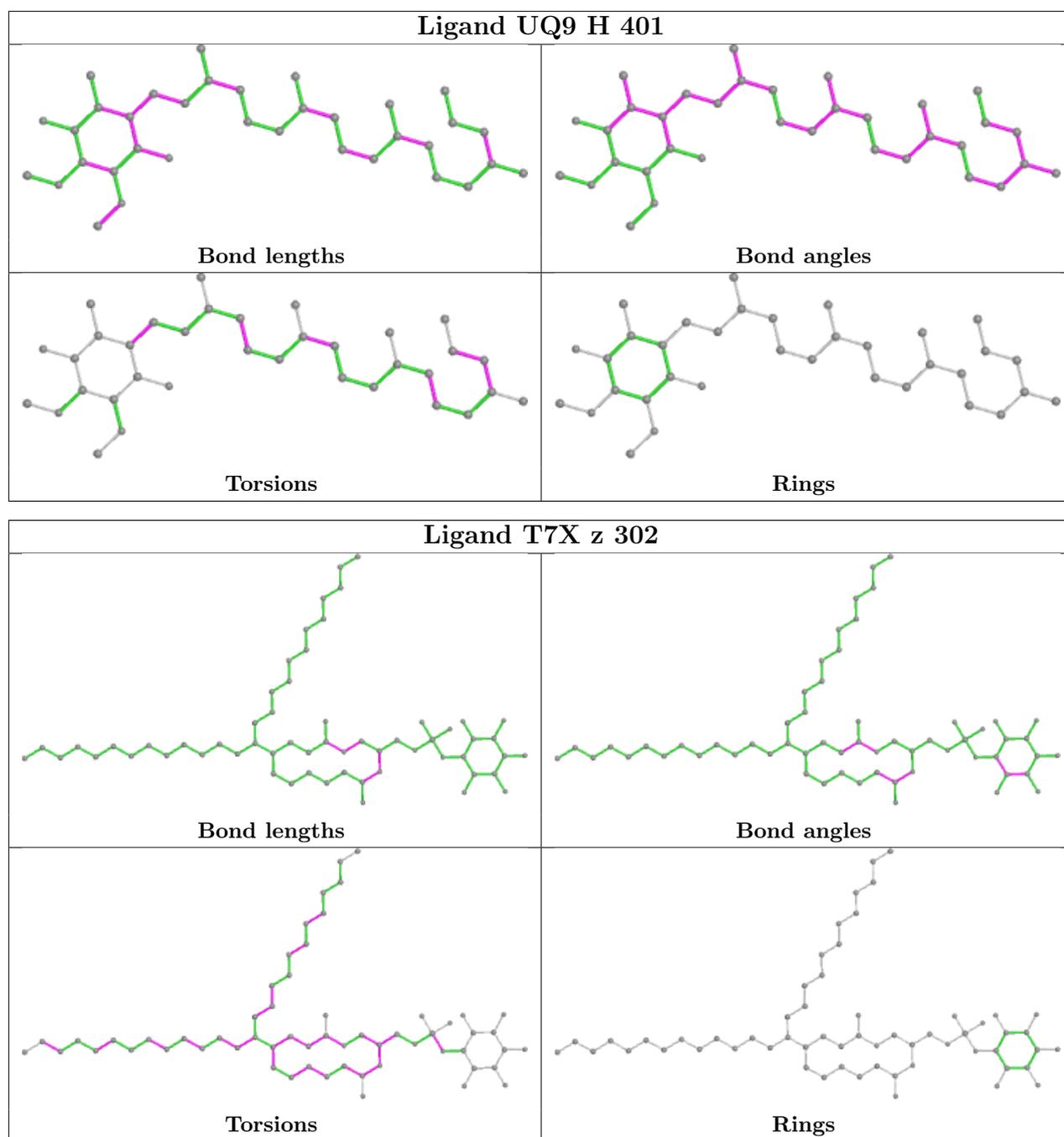
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	N	501	PTY	5	0
24	M	501	LMN	1	0
23	H	402	PTY	4	0
22	H	401	UQ9	2	0

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.

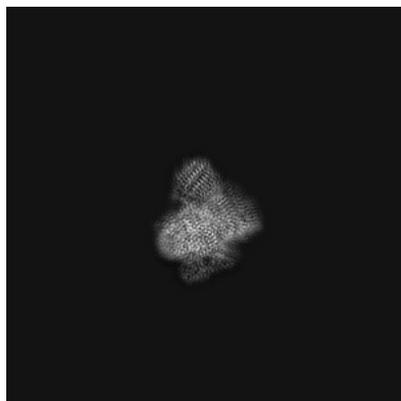
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11872. These allow visual inspection of the internal detail of the map and identification of artifacts.

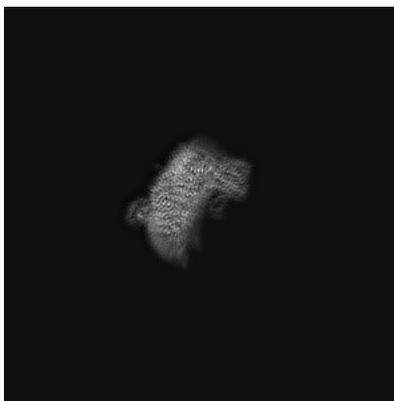
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

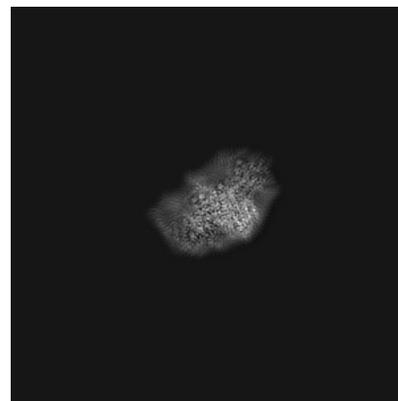
#### 6.1.1 Primary map



X

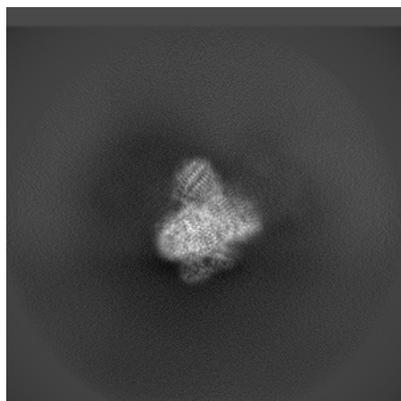


Y

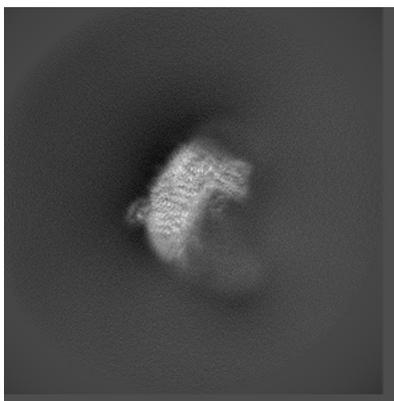


Z

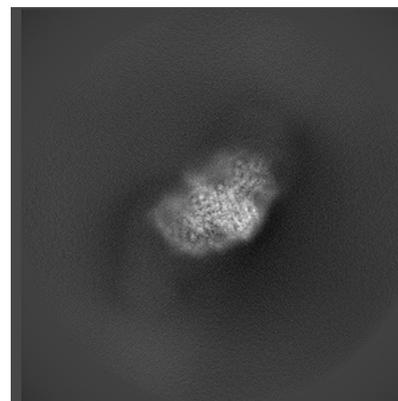
#### 6.1.2 Raw map



X



Y

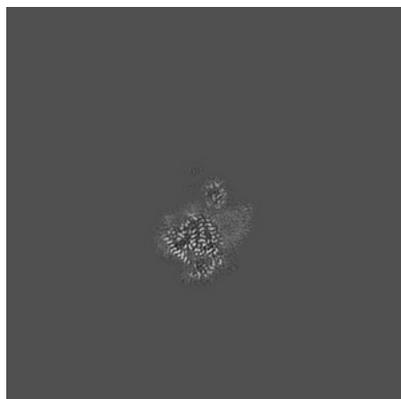


Z

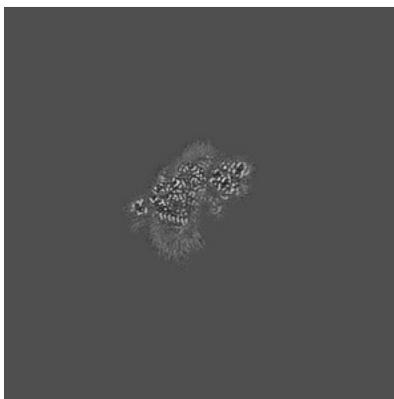
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

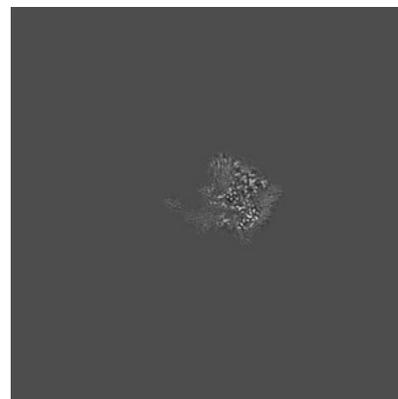
### 6.2.1 Primary map



X Index: 300

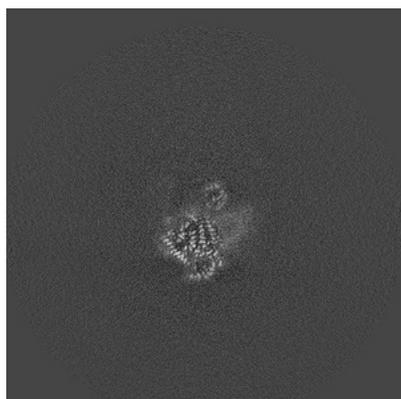


Y Index: 300

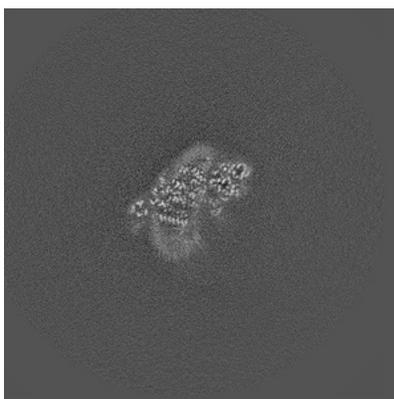


Z Index: 300

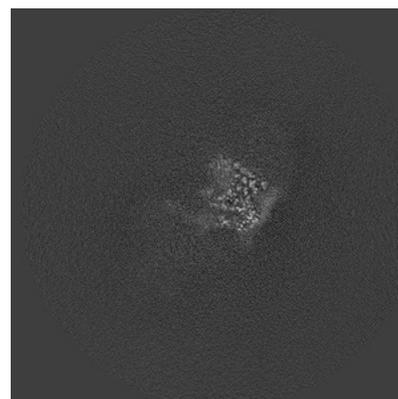
### 6.2.2 Raw map



X Index: 300



Y Index: 300

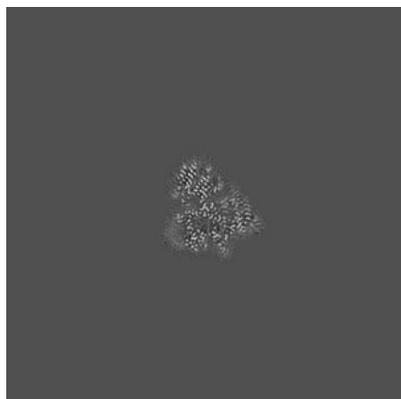


Z Index: 300

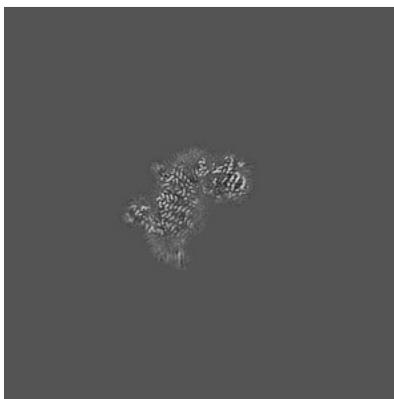
The images above show central slices of the map in three orthogonal directions.

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

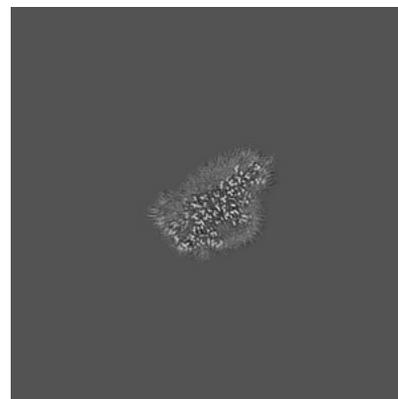
### 6.3.1 Primary map



X Index: 341

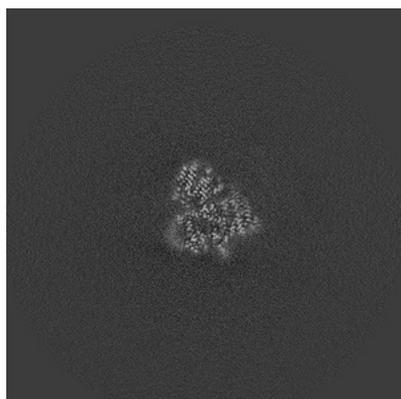


Y Index: 279

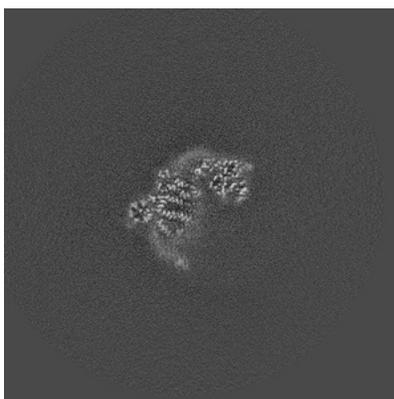


Z Index: 262

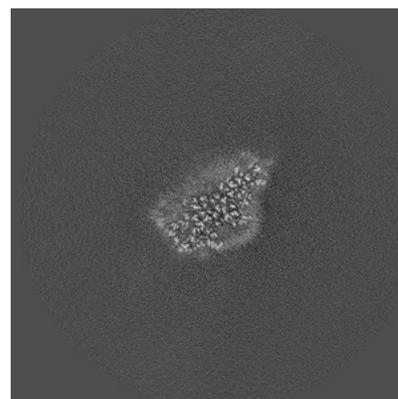
### 6.3.2 Raw map



X Index: 341



Y Index: 289

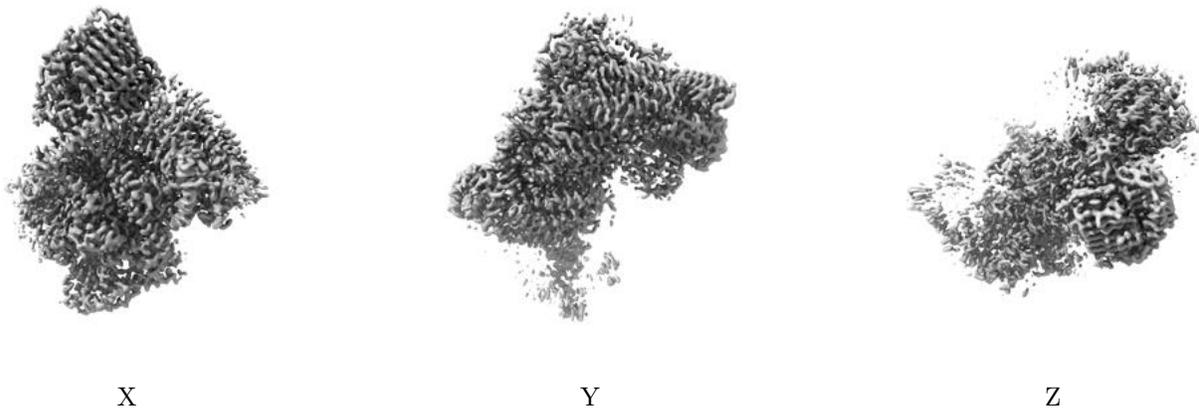


Z Index: 262

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

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

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

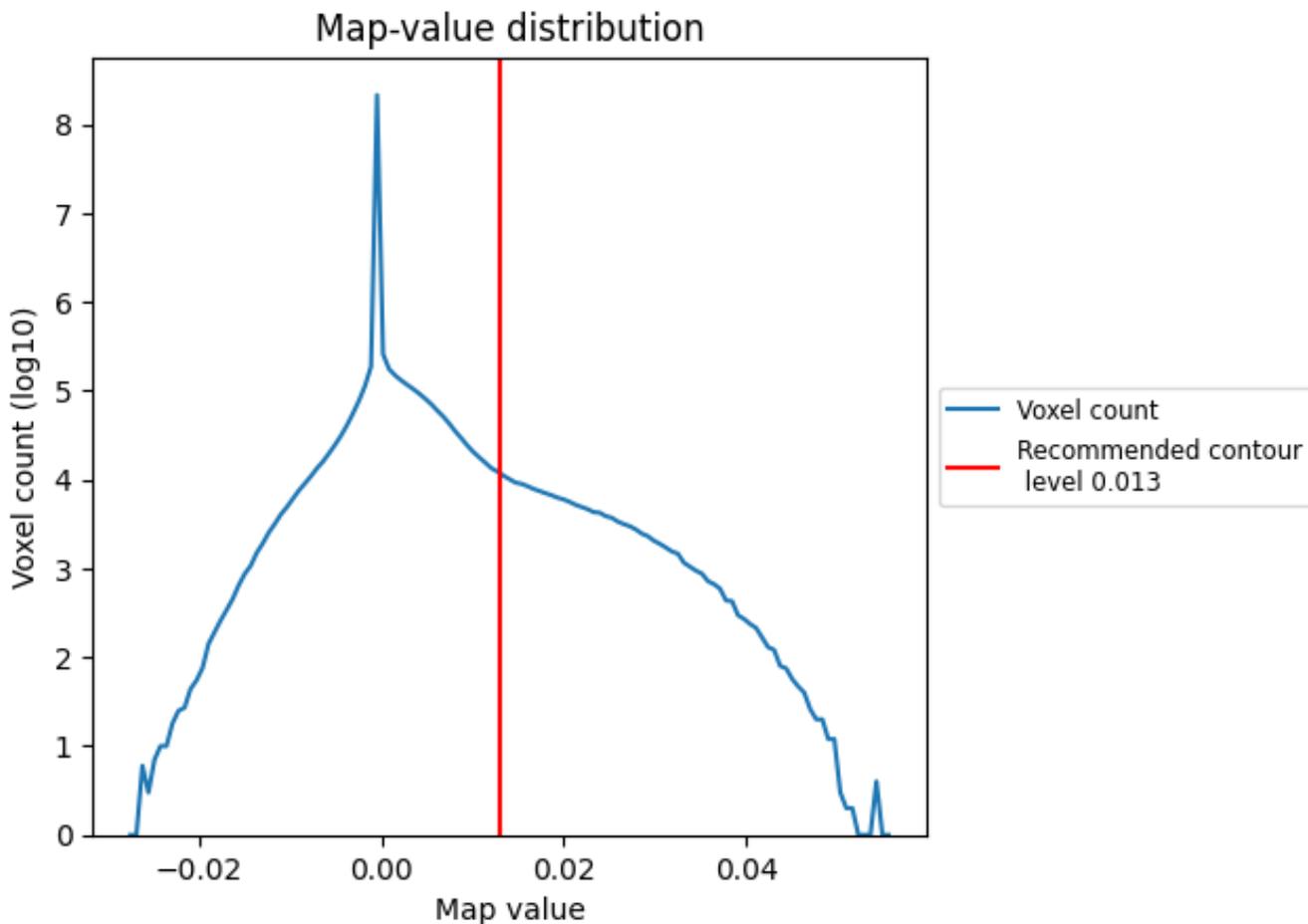
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

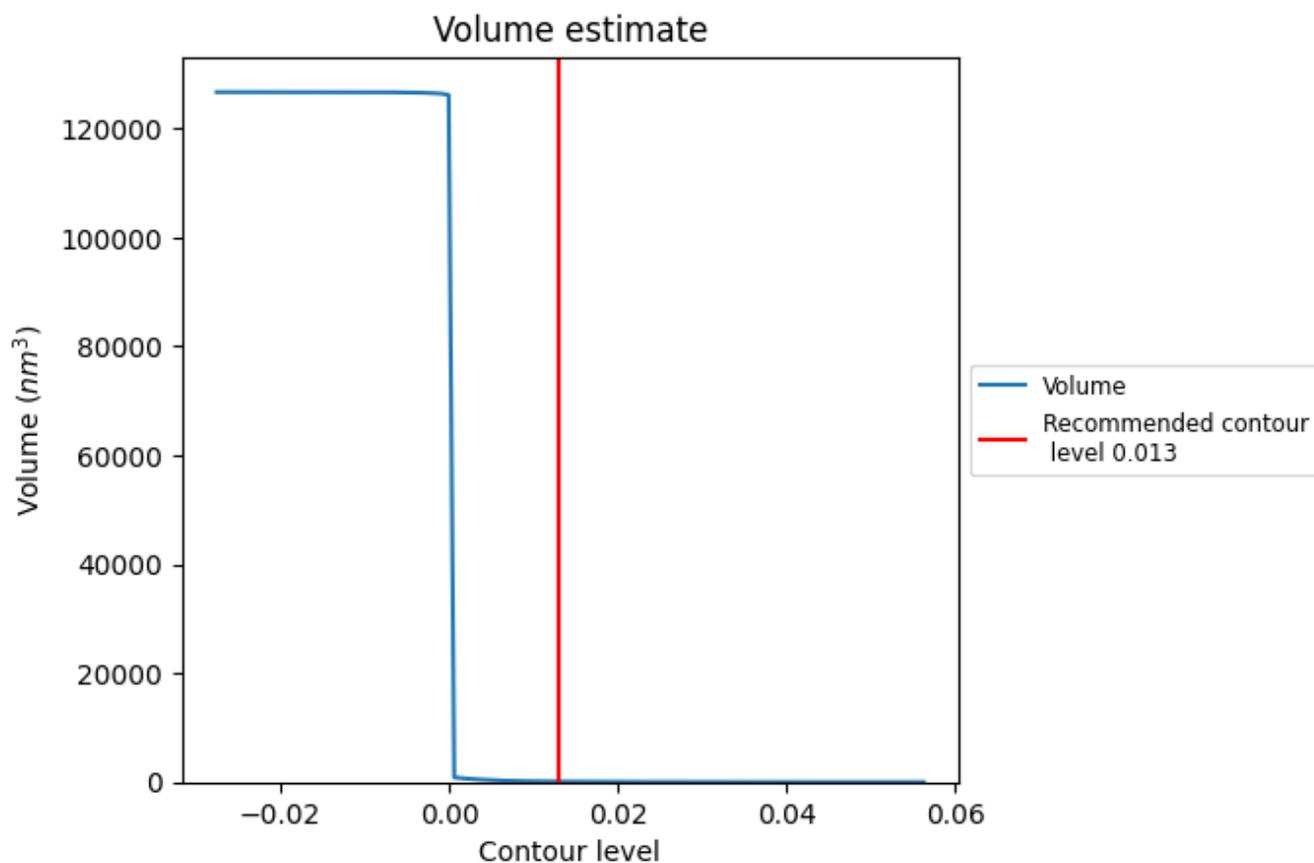
This section contains the results of statistical analysis of the map.

### 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.

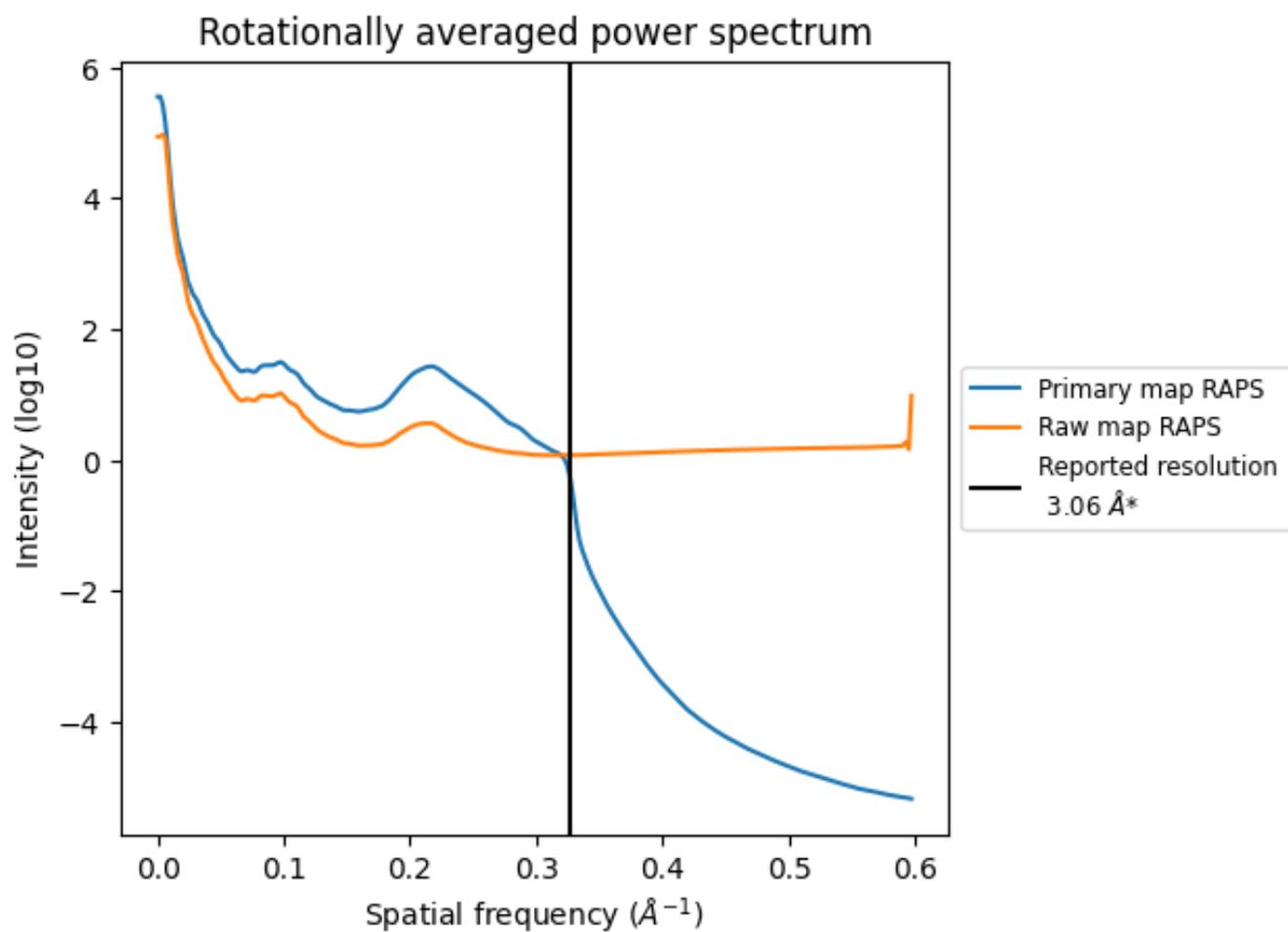
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 98  $\text{nm}^3$ ; this corresponds to an approximate mass of 89 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

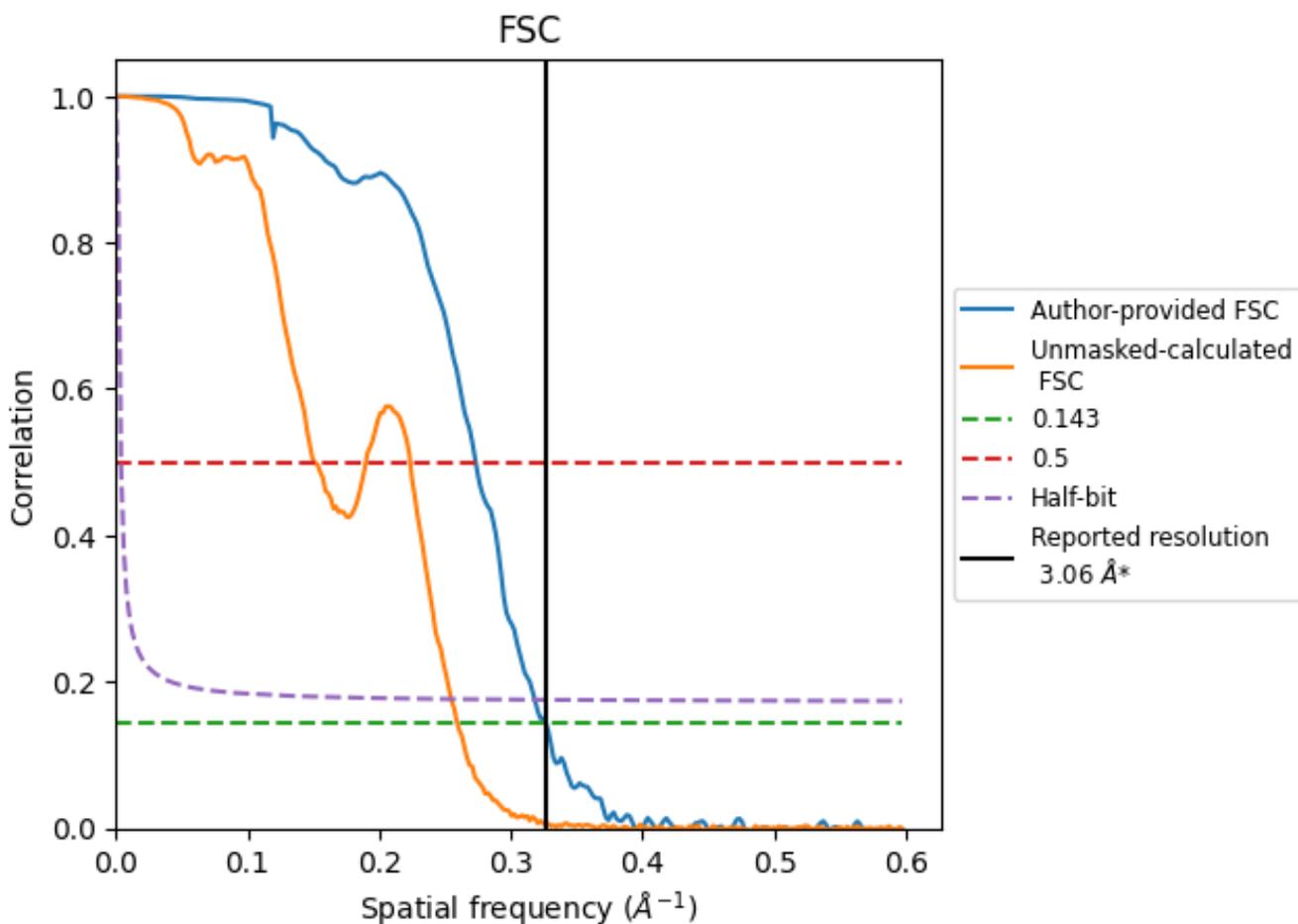


\*Reported resolution corresponds to spatial frequency of 0.327 Å<sup>-1</sup>

## 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 0.327 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

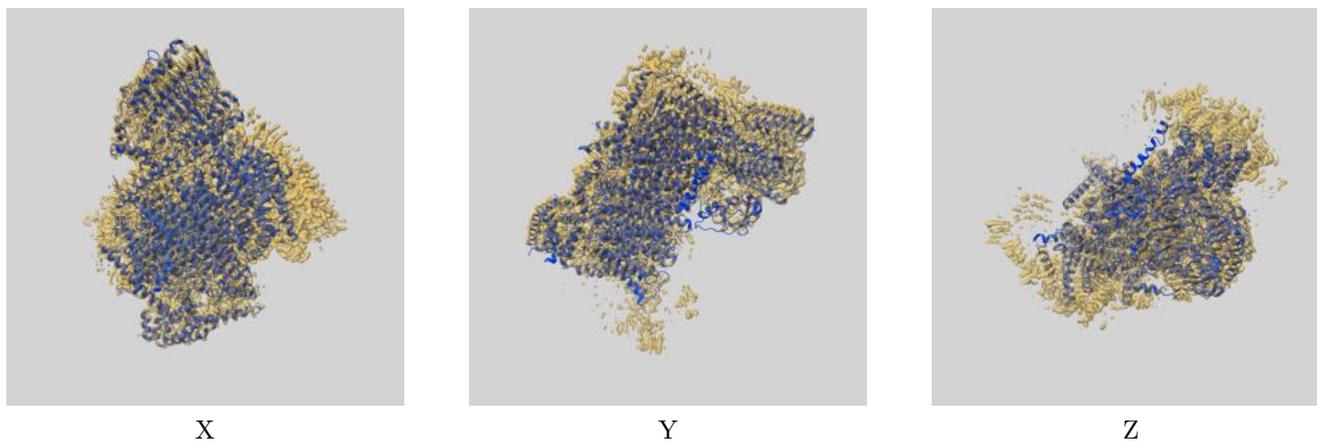
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	3.06	3.66	3.14
Unmasked-calculated*	3.85	6.62	3.93

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.85 differs from the reported value 3.06 by more than 10 %

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

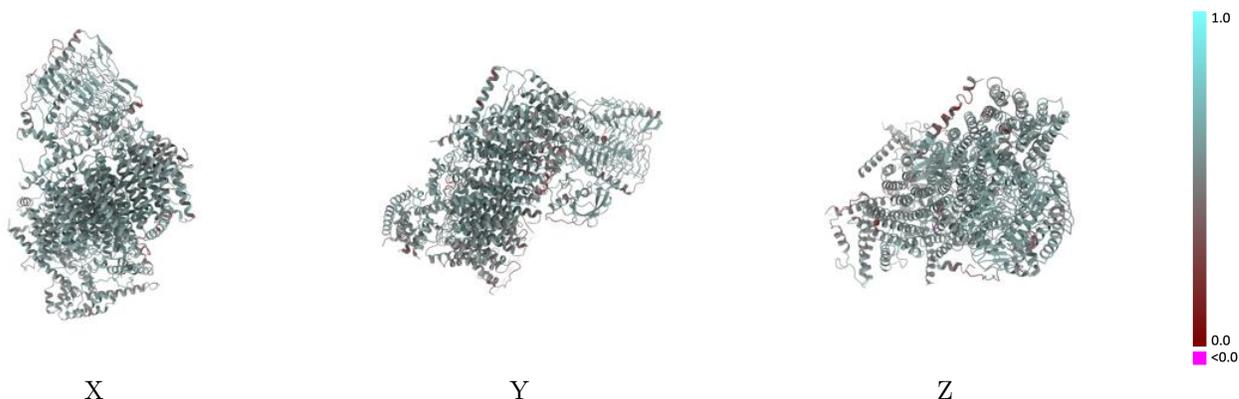
This section contains information regarding the fit between EMDB map EMD-11872 and PDB model 7AQQ. Per-residue inclusion information can be found in section [3](#) on page [12](#).

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



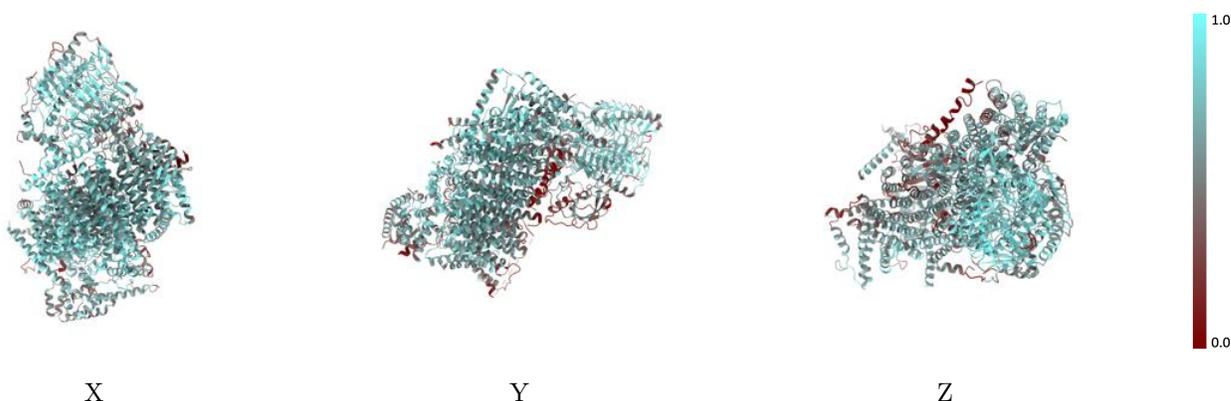
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



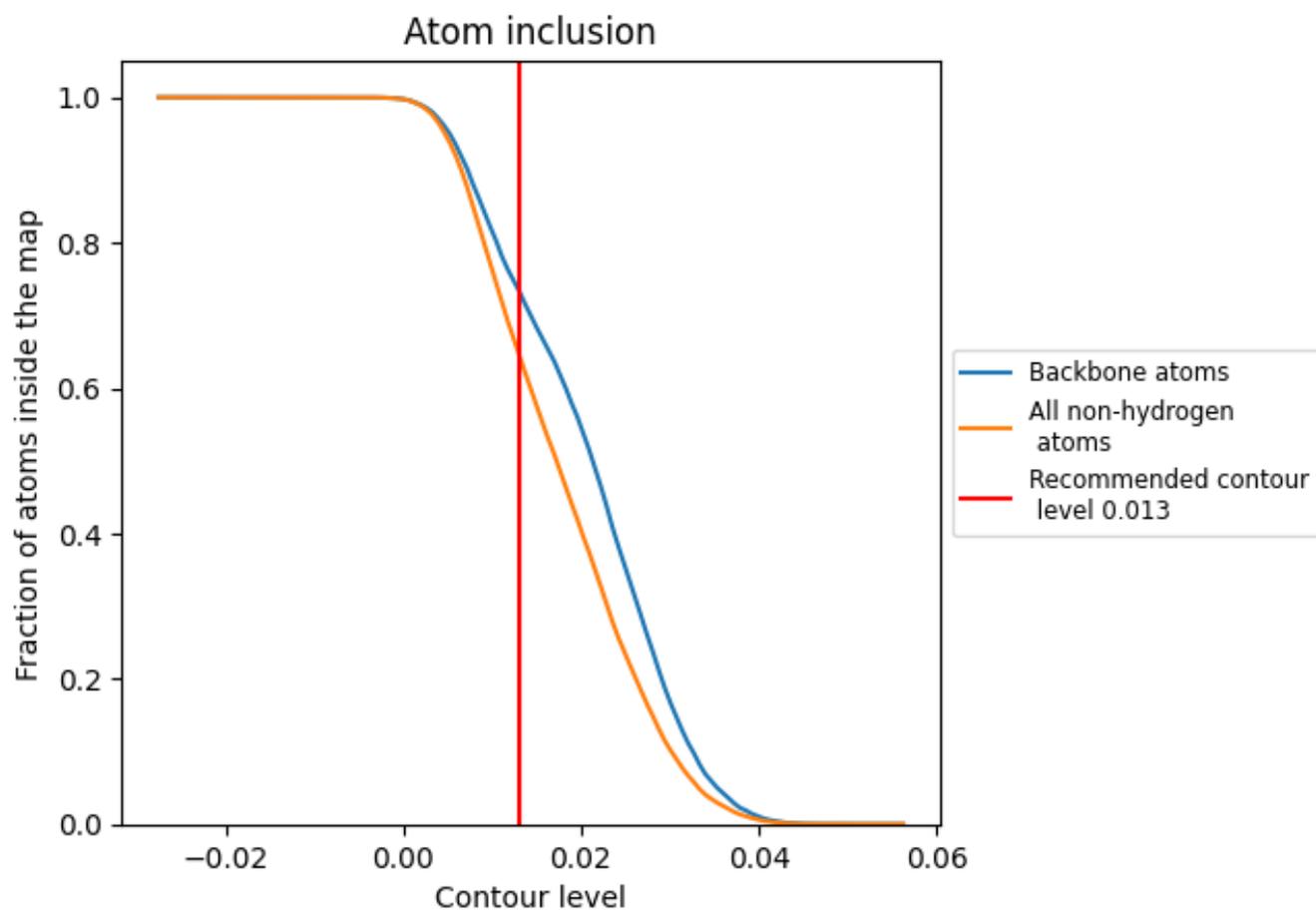
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6469	 0.5490
A	 0.6302	 0.5510
H	 0.6632	 0.5430
J	 0.6171	 0.5450
K	 0.6026	 0.5490
L	 0.0350	 0.3690
M	 0.6370	 0.5430
N	 0.6868	 0.5690
O	 0.3600	 0.5230
X	 0.5563	 0.5250
Z	 0.6628	 0.5360
a	 0.6266	 0.5220
b	 0.5876	 0.5360
d	 0.6932	 0.5550
e	 0.7313	 0.5650
f	 0.7250	 0.5740
i	 0.6983	 0.5520
u	 0.6467	 0.4880
v	 0.5751	 0.5550
x	 0.7176	 0.5670
y	 0.6616	 0.5440
z	 0.6980	 0.5610

