



## wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 06:06 AM UTC

PDB ID : 7VCF / pdb\_00007vcf  
EMDB ID : EMD-31890  
Title : Cryo-EM structure of Chlamydomonas TOC-TIC supercomplex  
Authors : Wu, J.; Yan, Z.; Jin, Z.; Zhang, Y.  
Deposited on : 2021-09-02  
Resolution : 2.50 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:

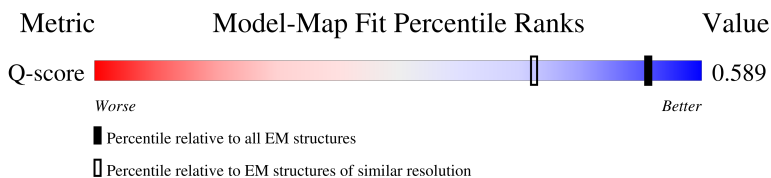
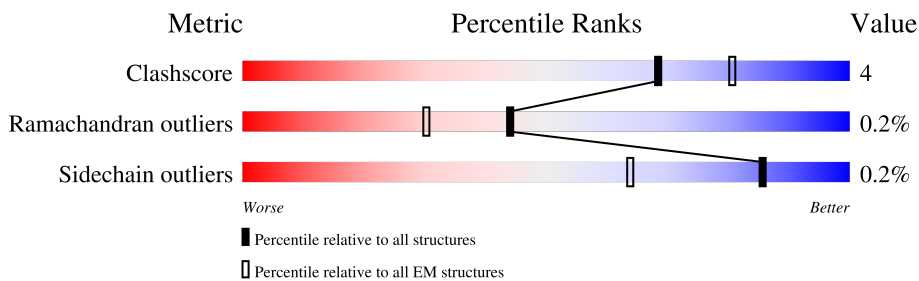
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 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.





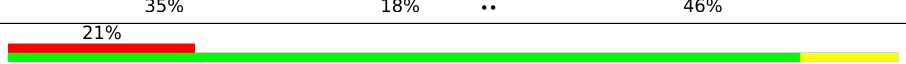
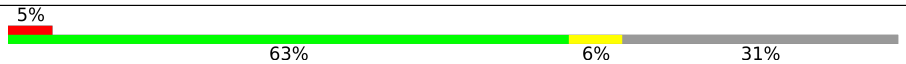

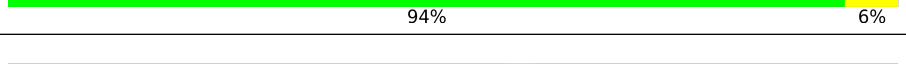
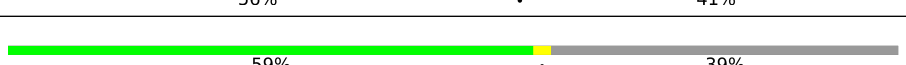




Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 ( 2.00 - 3.00 )

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	1995	
2	B	798	
3	C	477	
4	D	124	

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Mol	Chain	Length	Quality of chain
5	F	967	
6	G	397	
7	H	187	
8	I	363	
9	K	98	
10	M	127	
11	N	18	
12	O	329	
13	Q	244	
14	T	955	
15	W	532	

## 2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 39626 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 Tic214.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
1	A	1496	12577	8149	2237	2163	1	27	0	0

- Molecule 2 is a protein called Toc75.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
2	B	651	5142	3233	890	1000	2	17	0	0

- Molecule 3 is a protein called Toc52.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
3	C	217	1728	1089	315	317	1	6	0	0

- Molecule 4 is a protein called Tic13.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
4	D	69	529	333	100	96	0	0

- Molecule 5 is a protein called Toc120.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
5	F	402	3139	1994	522	606	1	16	0	0

- Molecule 6 is a protein called Toc34.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
6	G	70	612	383	124	104	1	0	0

- Molecule 7 is a protein called YlmG.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
7	H	101	861	576	126	149	3	7	0	0

- Molecule 8 is a protein called Toc39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	363	2751	1728	497	522	4	0	0

- Molecule 9 is a protein called Toc10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K	68	549	343	103	101	2	0	0

- Molecule 10 is a protein called Tic12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	M	115	939	611	168	154	6	0	0

- Molecule 11 is a protein called Unknown fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	N	18	155	108	21	25	1	0	0

- Molecule 12 is a protein called Tic35.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	O	195	1572	1008	278	286	0	0

- Molecule 13 is a protein called Tic56.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Q	149	1244	805	222	208	9	0	0

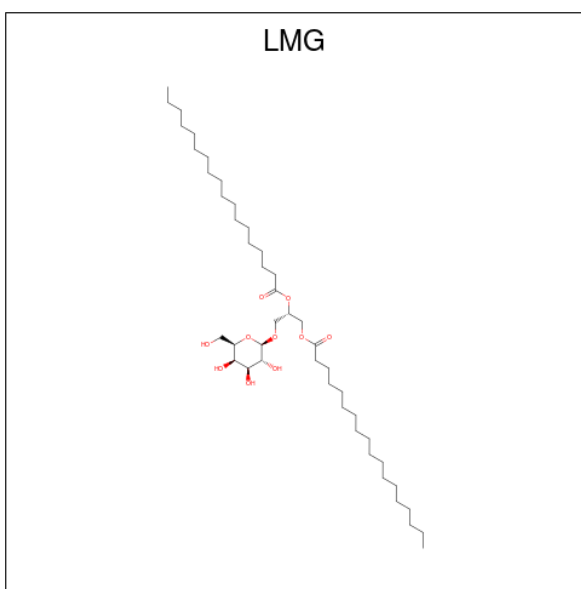
- Molecule 14 is a protein called Tic100.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
14	T	763	6185	3812	1060	1263	19	31	0	0

- Molecule 15 is a protein called Tic20-Venus-Flag.

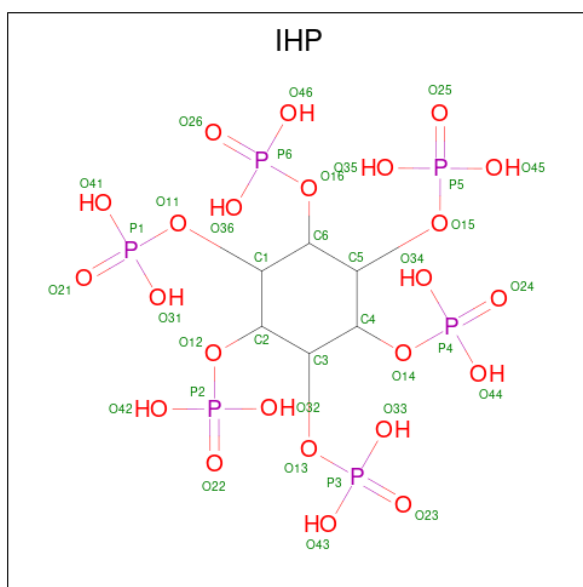
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	W	164	1398	955	205	226	12	0	0

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
16	A	1	49	39	10	0
16	A	1	46	36	10	0
16	A	1	55	45	10	0
16	A	1	55	45	10	0

- Molecule 17 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula:  $C_6H_{18}O_{24}P_6$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
17	A	1	36	6	24	6	0

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
18	F	1	1	1	0
18	T	1	1	1	0

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
19	A	1	1	1	0
19	O	1	1	1	0













## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	595638	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	82000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	12.516	Depositor
Minimum map value	-2.213	Depositor
Average map value	0.037	Depositor
Map value standard deviation	0.144	Depositor
Recommended contour level	0.5	Depositor
Map size ( $\text{\AA}$ )	417.40802, 417.40802, 417.40802	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.087, 1.087, 1.087	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: IHP, SEP, TPO, LMG, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.32	0/12854	0.62	3/17304 (0.0%)
2	B	0.24	0/5233	0.57	4/7079 (0.1%)
3	C	0.30	0/1752	0.61	0/2369
4	D	0.20	0/544	0.53	0/742
5	F	0.32	1/3216 (0.0%)	0.64	2/4370 (0.0%)
6	G	0.35	0/628	0.68	1/847 (0.1%)
7	H	0.52	0/857	0.67	1/1163 (0.1%)
8	I	0.19	0/2804	0.52	0/3810
9	K	0.24	0/562	0.51	0/755
10	M	0.26	0/976	0.51	0/1327
11	N	0.25	0/161	0.53	0/218
12	O	0.23	0/1610	0.47	0/2182
13	Q	0.29	0/1282	0.59	0/1742
14	T	0.29	0/6112	0.58	3/8228 (0.0%)
15	W	0.33	0/1455	0.57	0/1991
All	All	0.30	1/40046 (0.0%)	0.59	14/54127 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	839	LEU	N-CA	5.43	1.50	1.46

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	ASN	N-CA-C	6.31	123.75	109.81
14	T	544	PRO	CA-C-N	5.86	132.74	121.54
14	T	544	PRO	C-N-CA	5.86	132.74	121.54
1	A	1790	VAL	N-CA-C	-5.73	103.77	111.44
5	F	695	GLY	N-CA-C	5.49	120.91	112.51

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12577	0	12986	121	0
2	B	5142	0	4967	47	0
3	C	1728	0	1712	13	0
4	D	529	0	515	7	0
5	F	3139	0	2945	29	0
6	G	612	0	594	2	0
7	H	861	0	827	44	0
8	I	2751	0	2758	25	0
9	K	549	0	526	5	0
10	M	939	0	904	8	0
11	N	155	0	144	1	0
12	O	1572	0	1547	8	0
13	Q	1244	0	1263	4	0
14	T	6185	0	5745	34	0
15	W	1398	0	1362	19	0
16	A	205	0	305	5	0
17	A	36	0	6	1	0
18	F	1	0	0	0	0
18	T	1	0	0	0	0
19	A	1	0	0	0	0
19	O	1	0	0	0	0
All	All	39626	0	39106	294	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 4.

The worst 5 of 294 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:1721:TYR:CD1	1:A:1724:LEU:HD12	1.45	1.47
1:A:1721:TYR:CD1	1:A:1724:LEU:CD1	2.27	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1721:TYR:HD1	1:A:1724:LEU:CD1	1.59	1.14
7:H:110:ASP:O	7:H:116:TRP:HD1	1.42	1.01
5:F:690:SER:HB3	5:F:695:GLY:HA2	1.46	0.97

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	1465/1995 (73%)	1372 (94%)	90 (6%)	3 (0%)	43	63
2	B	645/798 (81%)	593 (92%)	52 (8%)	0	100	100
3	C	214/477 (45%)	205 (96%)	9 (4%)	0	100	100
4	D	67/124 (54%)	60 (90%)	7 (10%)	0	100	100
5	F	399/967 (41%)	370 (93%)	28 (7%)	1 (0%)	36	55
6	G	68/397 (17%)	65 (96%)	3 (4%)	0	100	100
7	H	94/187 (50%)	84 (89%)	8 (8%)	2 (2%)	5	9
8	I	361/363 (99%)	348 (96%)	13 (4%)	0	100	100
9	K	66/98 (67%)	63 (96%)	3 (4%)	0	100	100
10	M	113/127 (89%)	108 (96%)	5 (4%)	0	100	100
11	N	16/18 (89%)	14 (88%)	2 (12%)	0	100	100
12	O	193/329 (59%)	185 (96%)	8 (4%)	0	100	100
13	Q	147/244 (60%)	142 (97%)	5 (3%)	0	100	100
14	T	736/955 (77%)	707 (96%)	29 (4%)	0	100	100
15	W	162/532 (30%)	159 (98%)	1 (1%)	2 (1%)	10	20
All	All	4746/7611 (62%)	4475 (94%)	263 (6%)	8 (0%)	44	63

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	TYR
1	A	352	GLN
7	H	114	GLN
15	W	257	LEU
5	F	837	ASP

### 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	1391/1847 (75%)	1390 (100%)	1 (0%)	88	96
2	B	548/651 (84%)	548 (100%)	0	100	100
3	C	172/372 (46%)	172 (100%)	0	100	100
4	D	53/97 (55%)	53 (100%)	0	100	100
5	F	321/712 (45%)	317 (99%)	4 (1%)	63	83
6	G	61/336 (18%)	61 (100%)	0	100	100
7	H	88/155 (57%)	86 (98%)	2 (2%)	44	72
8	I	287/287 (100%)	287 (100%)	0	100	100
9	K	54/71 (76%)	54 (100%)	0	100	100
10	M	95/106 (90%)	95 (100%)	0	100	100
11	N	14/14 (100%)	14 (100%)	0	100	100
12	O	155/245 (63%)	155 (100%)	0	100	100
13	Q	135/213 (63%)	135 (100%)	0	100	100
14	T	613/736 (83%)	613 (100%)	0	100	100
15	W	149/457 (33%)	148 (99%)	1 (1%)	76	89
All	All	4136/6299 (66%)	4128 (100%)	8 (0%)	85	95

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	W	256	GLN
7	H	140	GLN

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Mol	Chain	Res	Type
5	F	838	TRP
5	F	836	TYR
7	H	114	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	850	GLN
8	I	90	HIS
5	F	867	ASN
7	H	140	GLN
9	K	54	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](#)

27 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	SEP	T	251	14	8,9,10	1.53	1 (12%)	7,12,14	0.92	0
14	TPO	T	708	18,14	8,10,11	0.99	0	10,14,16	1.80	1 (10%)
14	SEP	T	706	14	8,9,10	1.52	1 (12%)	7,12,14	1.70	1 (14%)
14	TPO	T	239	14	8,10,11	1.53	2 (25%)	10,14,16	1.71	2 (20%)
7	TPO	H	177	7	8,10,11	1.78	3 (37%)	10,14,16	1.47	2 (20%)
14	TPO	T	523	14	8,10,11	1.05	0	10,14,16	1.71	1 (10%)
14	TPO	T	712	18,14	8,10,11	1.04	0	10,14,16	1.82	1 (10%)
2	SEP	B	344	2	8,9,10	1.61	1 (12%)	7,12,14	1.49	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	TPO	T	249	14	8,10,11	1.59	2 (25%)	10,14,16	1.91	1 (10%)
5	TPO	F	564	5	8,10,11	1.58	1 (12%)	10,14,16	1.91	1 (10%)
14	SEP	T	173	14	8,9,10	1.43	1 (12%)	7,12,14	1.10	0
14	SEP	T	212	14	8,9,10	1.55	1 (12%)	7,12,14	1.43	1 (14%)
14	SEP	T	229	14	8,9,10	1.49	1 (12%)	7,12,14	1.30	1 (14%)
14	TPO	T	168	14	8,10,11	1.00	0	10,14,16	1.95	1 (10%)
14	SEP	T	514	14	8,9,10	1.51	1 (12%)	7,12,14	1.06	1 (14%)
14	SEP	T	42	14	8,9,10	1.47	1 (12%)	7,12,14	1.02	0
2	SEP	B	339	2	8,9,10	1.53	1 (12%)	7,12,14	1.02	1 (14%)
1	TPO	A	1795	1	8,10,11	1.61	2 (25%)	10,14,16	1.62	1 (10%)
7	TPO	H	178	7	8,10,11	1.33	2 (25%)	10,14,16	1.64	1 (10%)
14	SEP	T	244	14	8,9,10	1.39	1 (12%)	7,12,14	1.10	0
14	TPO	T	77	14	8,10,11	1.01	0	10,14,16	1.85	1 (10%)
14	SEP	T	714	14	8,9,10	1.47	1 (12%)	7,12,14	1.83	1 (14%)
7	TPO	H	176	7	8,10,11	1.49	1 (12%)	10,14,16	1.64	1 (10%)
14	SEP	T	537	14	8,9,10	1.55	1 (12%)	7,12,14	1.40	1 (14%)
14	SEP	T	505	14	8,9,10	1.59	1 (12%)	7,12,14	1.04	0
14	TPO	T	510	14	8,10,11	0.98	0	10,14,16	1.88	1 (10%)
3	TPO	C	328	3	8,10,11	1.53	2 (25%)	10,14,16	1.72	1 (10%)

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	SEP	T	251	14	-	0/6/8/10	-
14	TPO	T	708	18,14	-	3/9/11/13	-
14	SEP	T	706	14	-	5/6/8/10	-
14	TPO	T	239	14	-	1/9/11/13	-
7	TPO	H	177	7	-	2/9/11/13	-
14	TPO	T	523	14	-	1/9/11/13	-
14	TPO	T	712	18,14	-	0/9/11/13	-
2	SEP	B	344	2	-	3/6/8/10	-
14	TPO	T	249	14	-	2/9/11/13	-
5	TPO	F	564	5	-	3/9/11/13	-
14	SEP	T	173	14	-	5/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	SEP	T	212	14	-	0/6/8/10	-
14	SEP	T	229	14	-	2/6/8/10	-
14	TPO	T	168	14	-	1/9/11/13	-
14	SEP	T	514	14	-	3/6/8/10	-
14	SEP	T	42	14	-	0/6/8/10	-
2	SEP	B	339	2	-	2/6/8/10	-
1	TPO	A	1795	1	-	3/9/11/13	-
7	TPO	H	178	7	-	4/9/11/13	-
14	SEP	T	244	14	-	2/6/8/10	-
14	TPO	T	77	14	-	2/9/11/13	-
14	SEP	T	714	14	-	6/6/8/10	-
7	TPO	H	176	7	-	2/9/11/13	-
14	SEP	T	537	14	-	1/6/8/10	-
14	SEP	T	505	14	-	0/6/8/10	-
14	TPO	T	510	14	-	2/9/11/13	-
3	TPO	C	328	3	-	1/9/11/13	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	505	SEP	P-O1P	3.50	1.61	1.50
2	B	344	SEP	P-O1P	3.50	1.61	1.50
14	T	212	SEP	P-O1P	3.40	1.61	1.50
14	T	537	SEP	P-O1P	3.40	1.61	1.50
14	T	706	SEP	P-O1P	3.39	1.61	1.50

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	168	TPO	P-OG1-CB	-5.78	107.61	123.33
14	T	249	TPO	P-OG1-CB	-5.42	108.60	123.33
14	T	77	TPO	P-OG1-CB	-5.41	108.62	123.33
5	F	564	TPO	P-OG1-CB	-5.24	109.10	123.33
14	T	510	TPO	P-OG1-CB	-5.22	109.14	123.33

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1795	TPO	N-CA-CB-OG1
1	A	1795	TPO	O-C-CA-CB
2	B	344	SEP	CB-OG-P-O2P
2	B	344	SEP	CB-OG-P-O3P
3	C	328	TPO	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	177	TPO	1	0
5	F	564	TPO	1	0
2	B	339	SEP	1	0
14	T	77	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z  > 2$
16	LMG	A	2004	-	55,55,55	0.85	4 (7%)	63,63,63	1.39	9 (14%)
17	IHP	A	2005	-	36,36,36	0.94	0	60,60,60	1.65	11 (18%)
16	LMG	A	2002	-	46,46,55	0.86	1 (2%)	54,54,63	1.30	4 (7%)
16	LMG	A	2001	-	49,49,55	0.81	2 (4%)	57,57,63	1.34	7 (12%)
16	LMG	A	2003	-	55,55,55	0.84	3 (5%)	63,63,63	1.40	8 (12%)

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
16	LMG	A	2004	-	-	23/50/70/70	0/1/1/1
17	IHP	A	2005	-	-	5/30/54/54	0/1/1/1
16	LMG	A	2002	-	-	15/41/61/70	0/1/1/1
16	LMG	A	2001	-	-	22/44/64/70	0/1/1/1
16	LMG	A	2003	-	-	18/50/70/70	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	2003	LMG	O7-C8	-2.61	1.40	1.46
16	A	2004	LMG	C4-C5	2.58	1.58	1.53
16	A	2002	LMG	O7-C8	-2.53	1.40	1.46
16	A	2003	LMG	O1-C7	-2.50	1.39	1.43
16	A	2001	LMG	O7-C8	-2.43	1.40	1.46

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	2005	IHP	O12-C2-C1	4.18	117.65	108.76
17	A	2005	IHP	C6-C1-C2	3.86	118.90	110.43
17	A	2005	IHP	O14-C4-C3	3.59	116.41	108.76
16	A	2004	LMG	O1-C7-C8	-3.38	102.59	110.82
17	A	2005	IHP	C6-C5-C4	3.33	117.74	110.43

There are no chirality outliers.

5 of 83 torsion outliers are listed below:

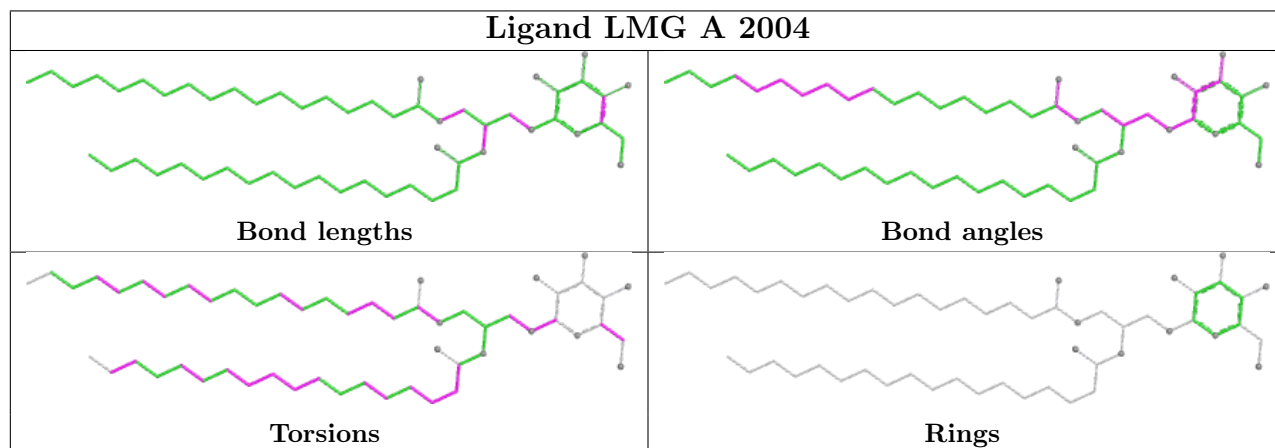
Mol	Chain	Res	Type	Atoms
16	A	2004	LMG	O6-C1-O1-C7
16	A	2001	LMG	O10-C28-O8-C9
16	A	2004	LMG	O6-C5-C6-O5
16	A	2001	LMG	O6-C5-C6-O5
16	A	2002	LMG	O6-C5-C6-O5

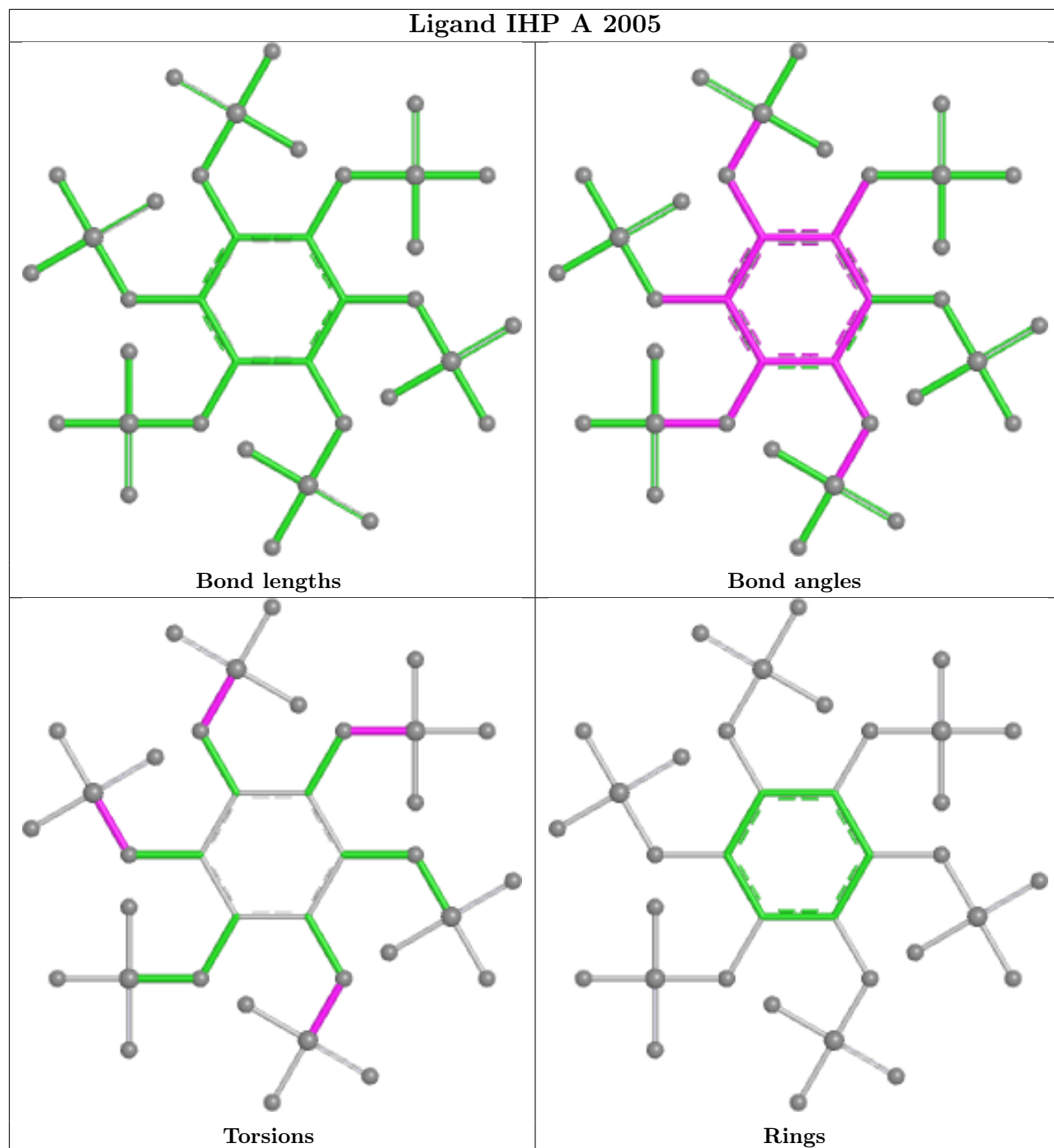
There are no ring outliers.

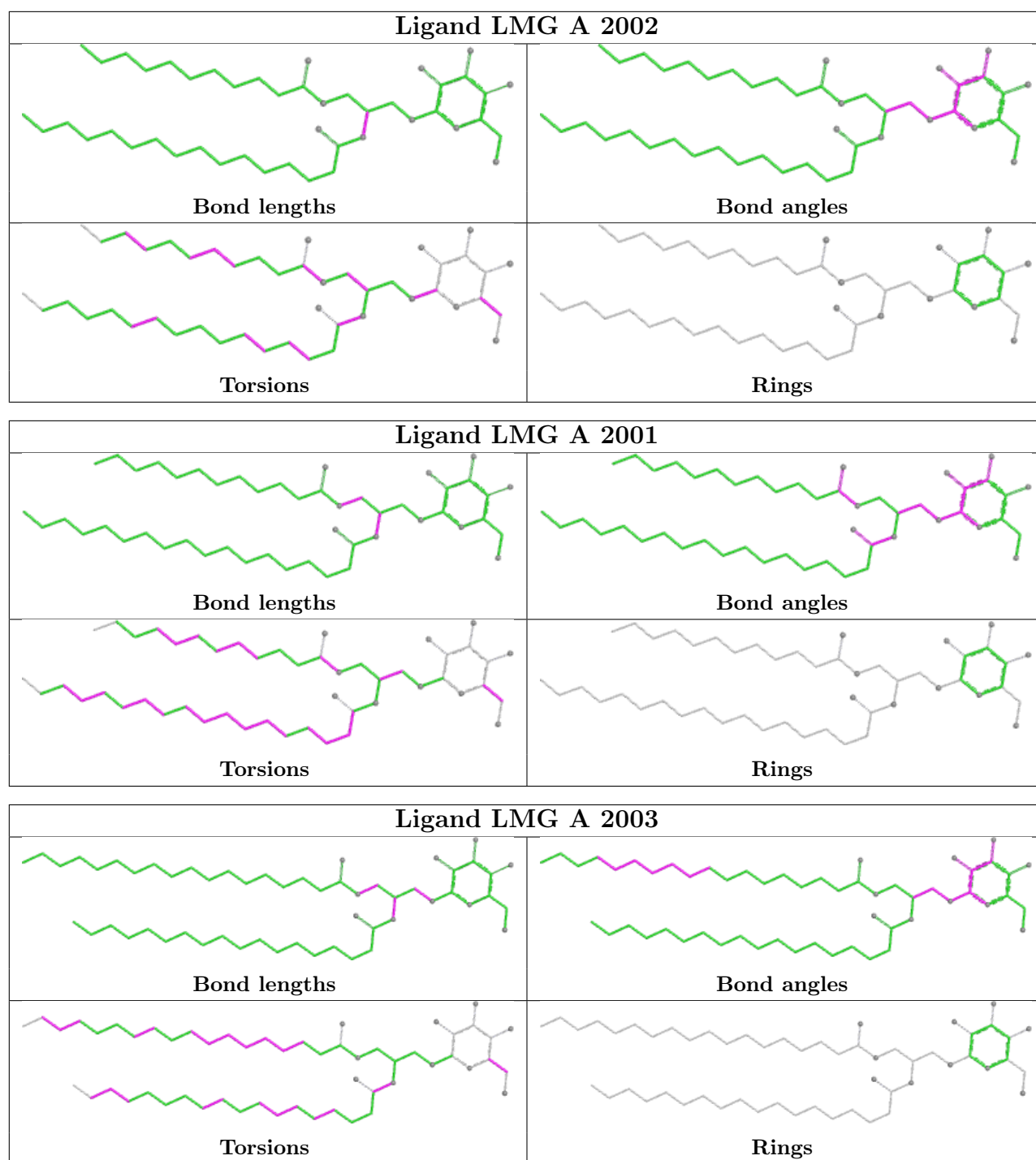
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	2004	LMG	3	0
17	A	2005	IHP	1	0
16	A	2002	LMG	1	0
16	A	2001	LMG	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.

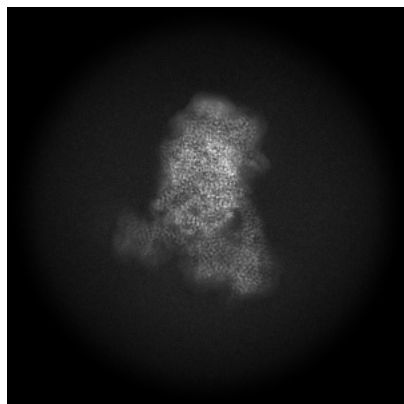
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31890. These allow visual inspection of the internal detail of the map and identification of artifacts.

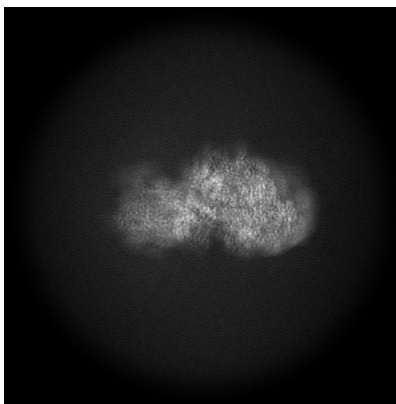
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

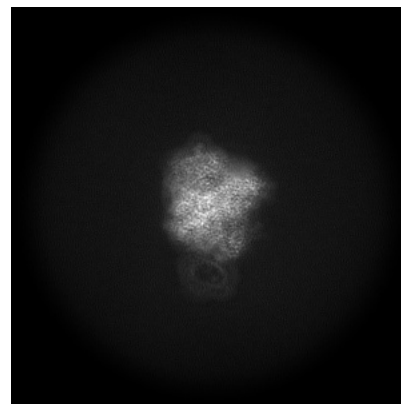
#### 6.1.1 Primary map



X

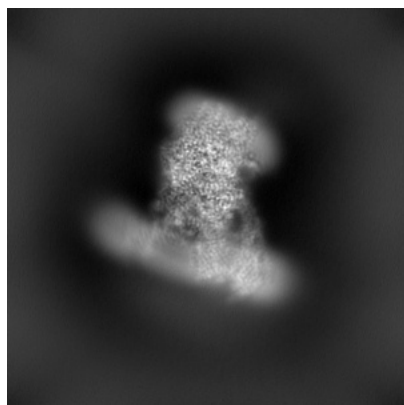


Y

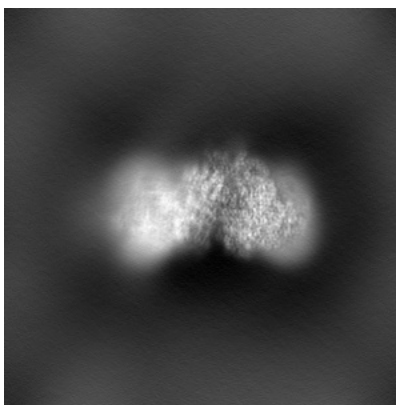


Z

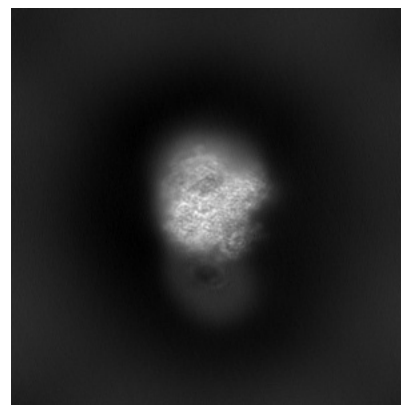
#### 6.1.2 Raw map



X



Y

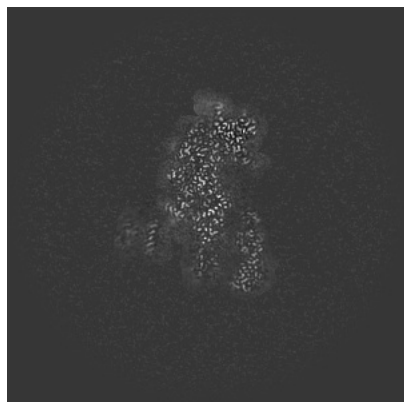


Z

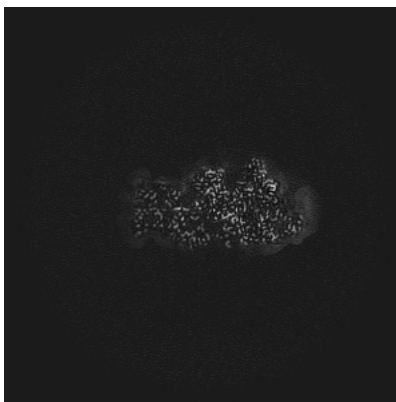
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

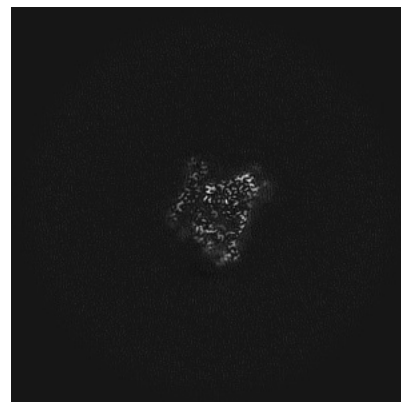
### 6.2.1 Primary map



X Index: 192

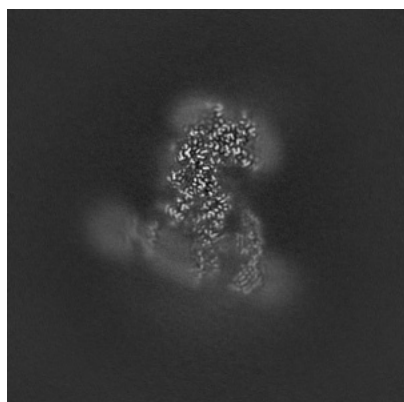


Y Index: 192

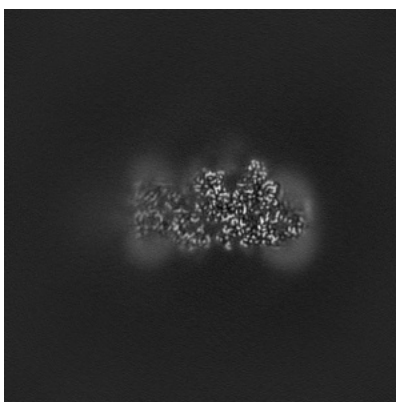


Z Index: 192

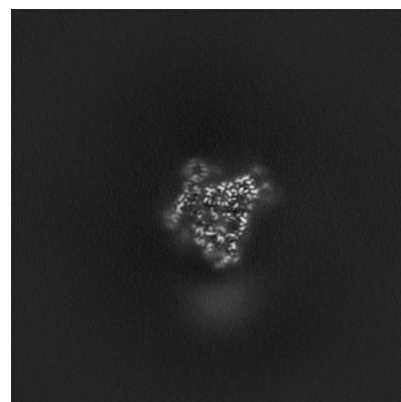
### 6.2.2 Raw map



X Index: 192



Y Index: 192

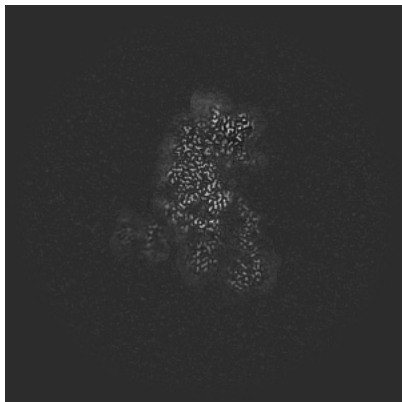


Z Index: 192

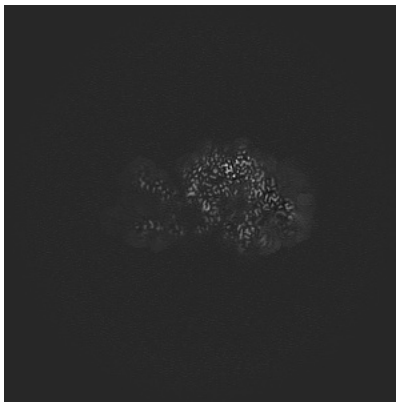
The images above show central slices of the map in three orthogonal directions.

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

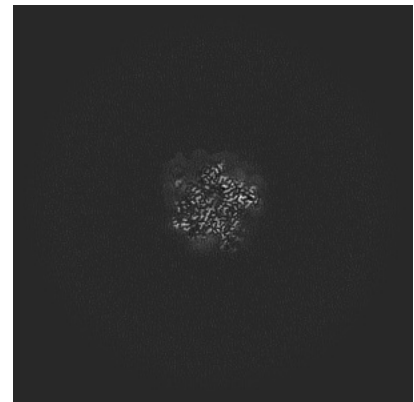
### 6.3.1 Primary map



X Index: 188

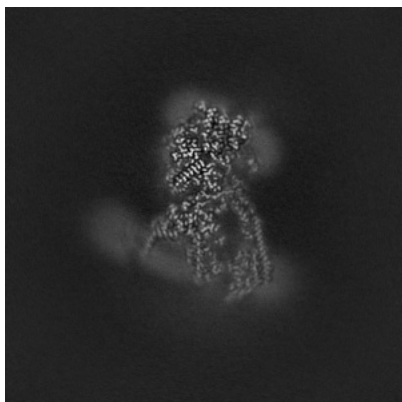


Y Index: 210

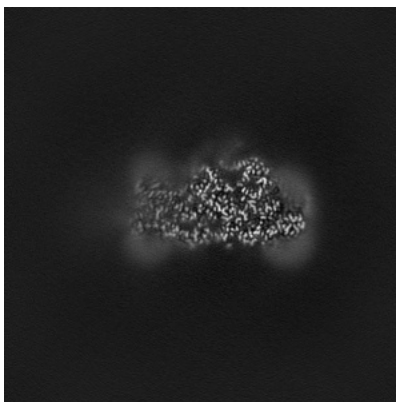


Z Index: 246

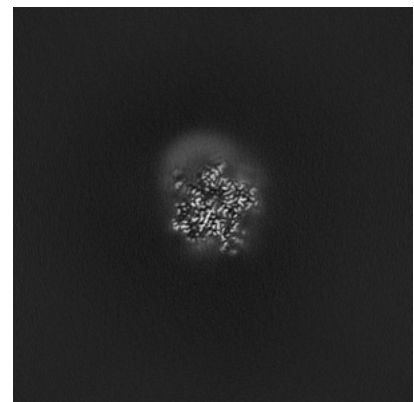
### 6.3.2 Raw map



X Index: 180



Y Index: 196



Z Index: 246

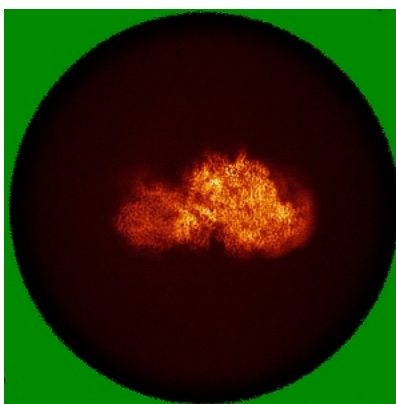
The images above show the largest variance slices of the map in three orthogonal directions.

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

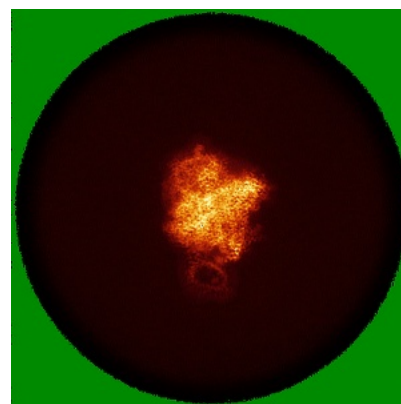
### 6.4.1 Primary map



X

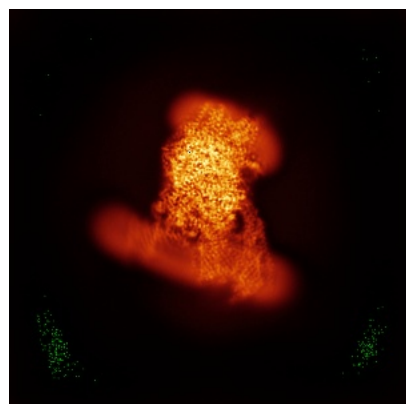


Y

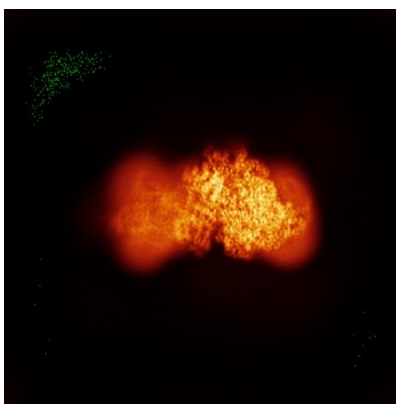


Z

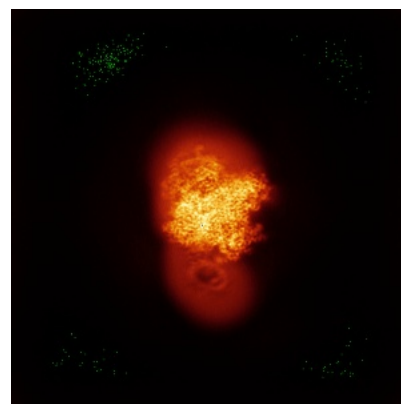
### 6.4.2 Raw map



X



Y

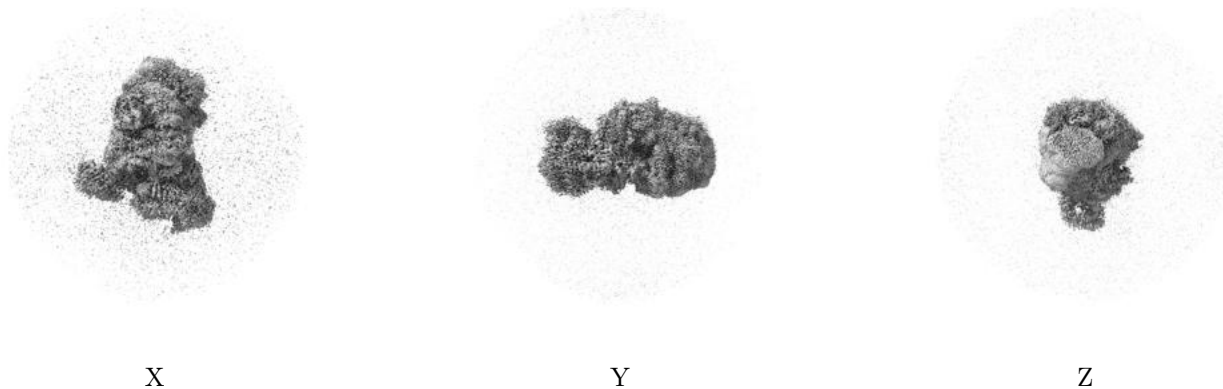


Z

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.

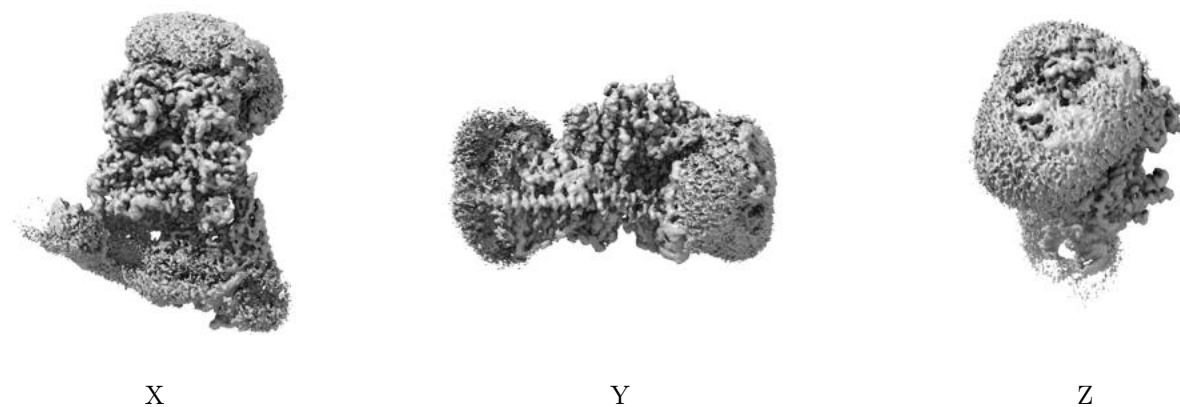
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

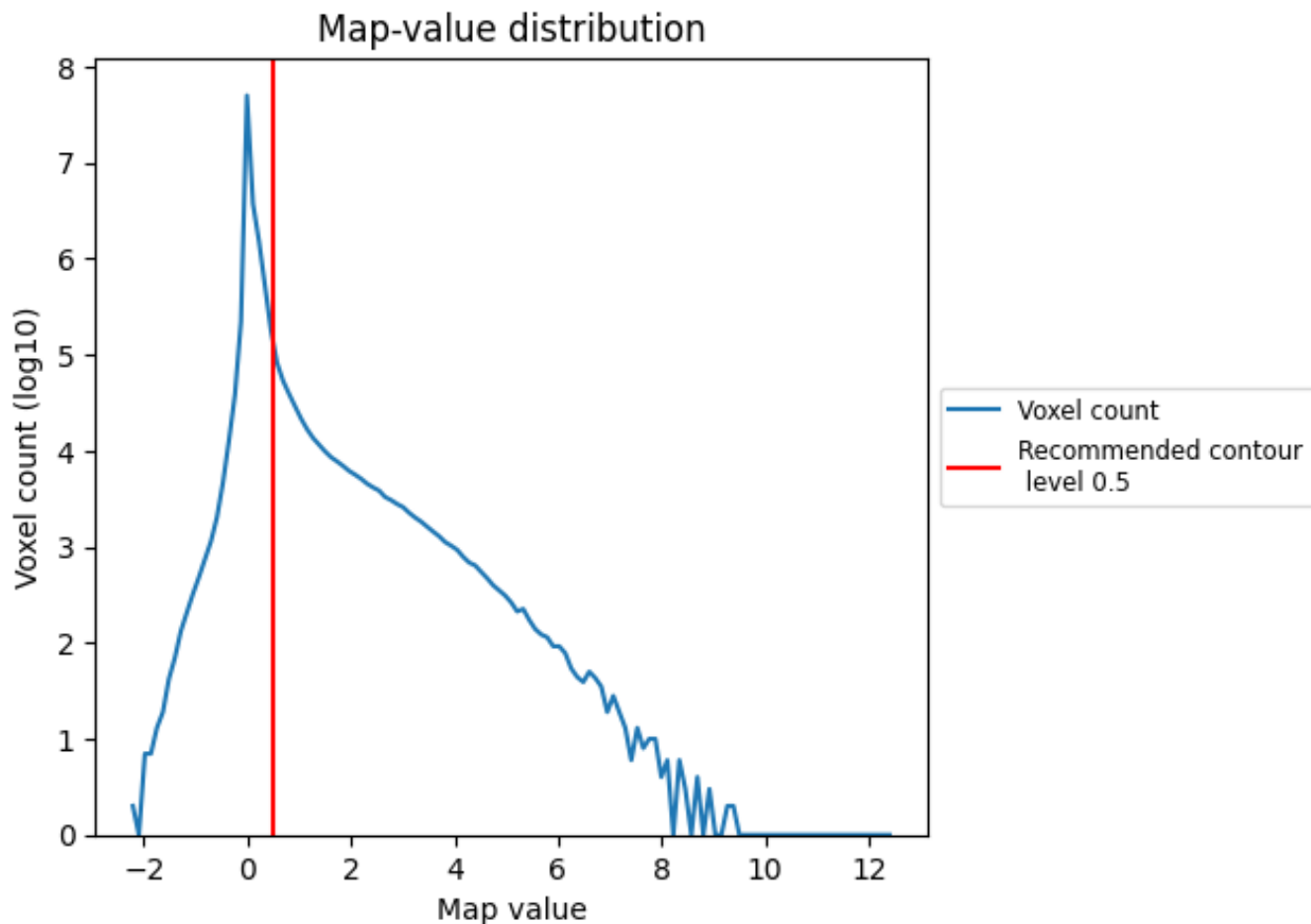
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

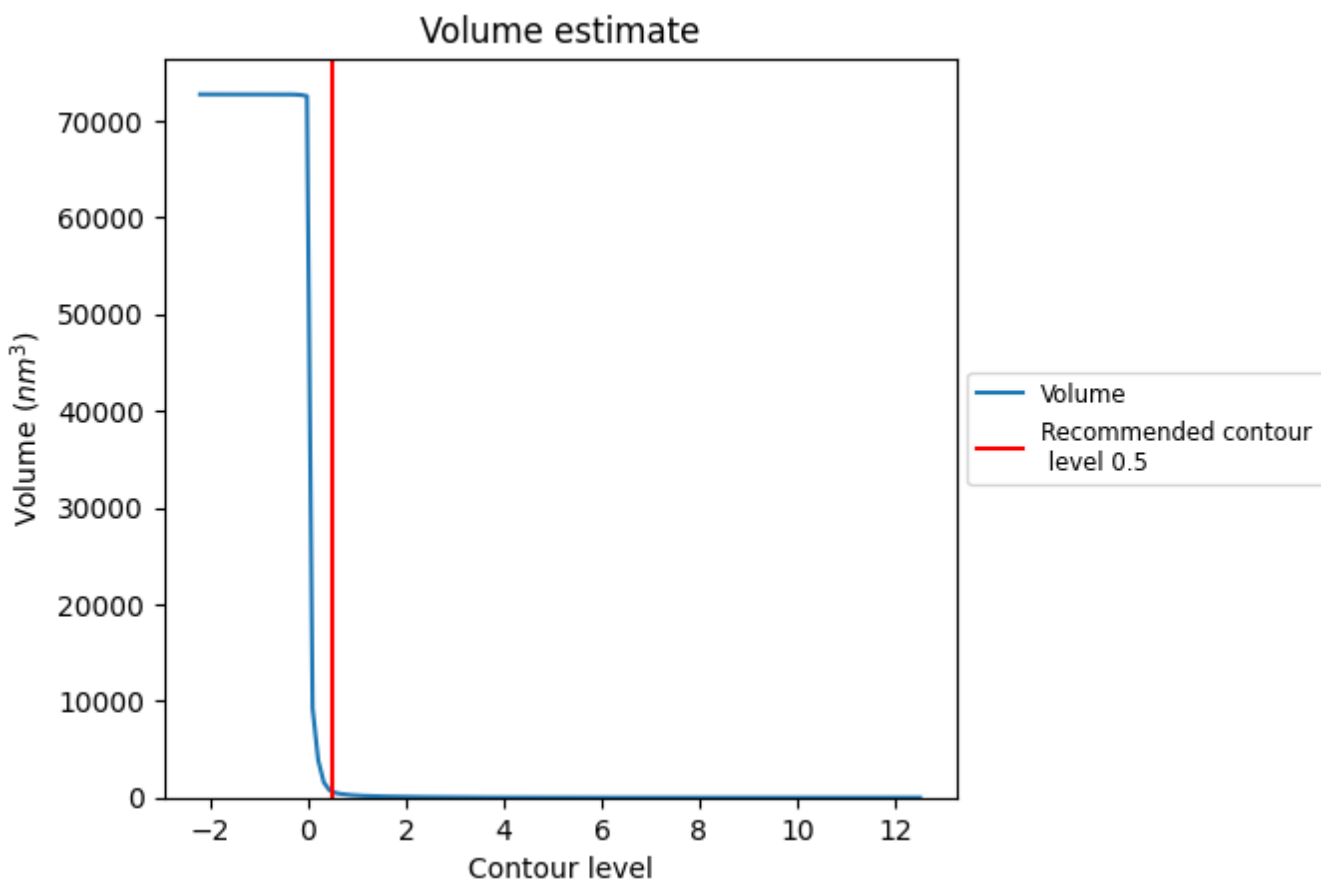
This section contains the results of statistical analysis of the map.

### 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.

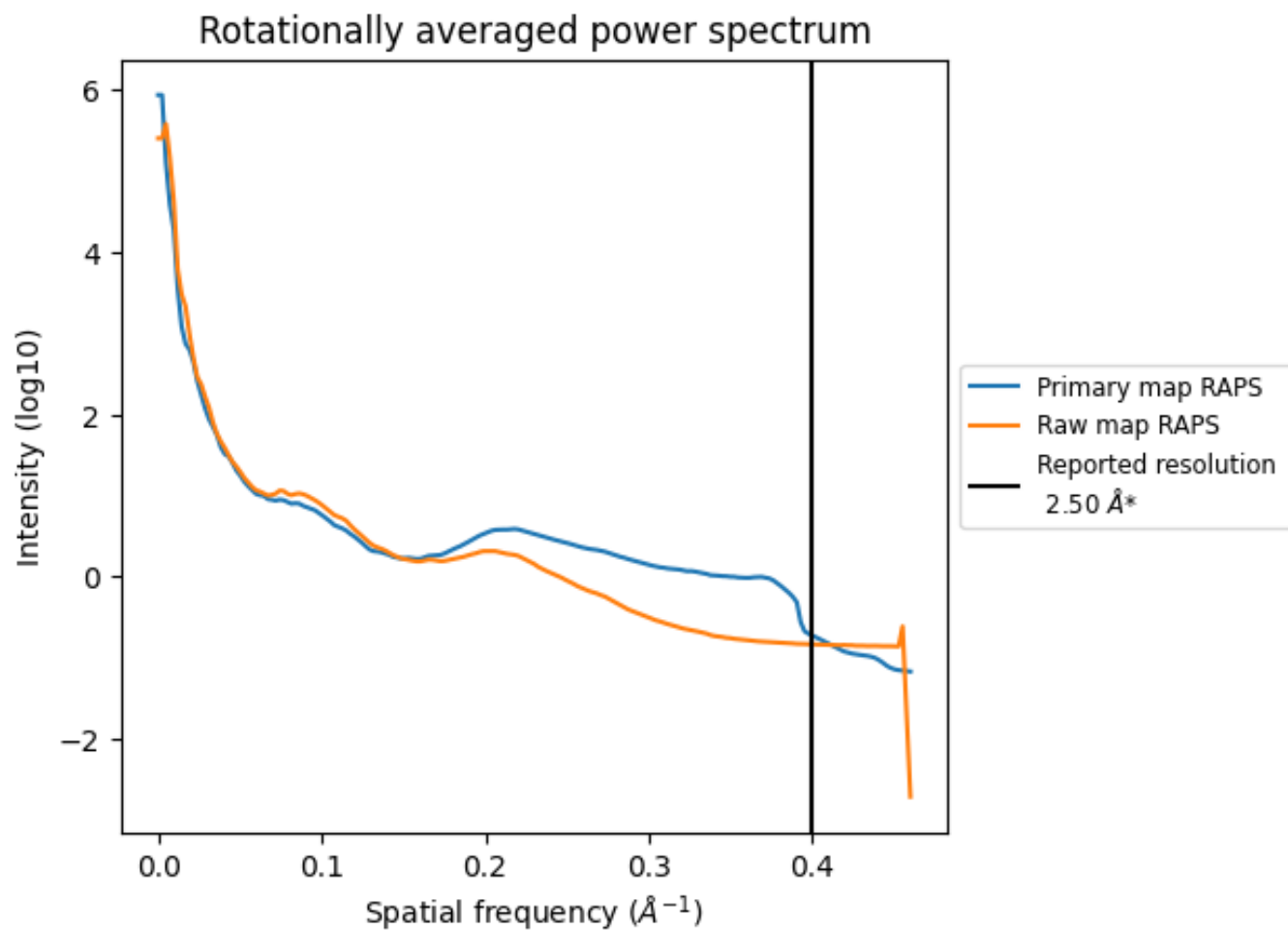
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 608  $\text{nm}^3$ ; this corresponds to an approximate mass of 549 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

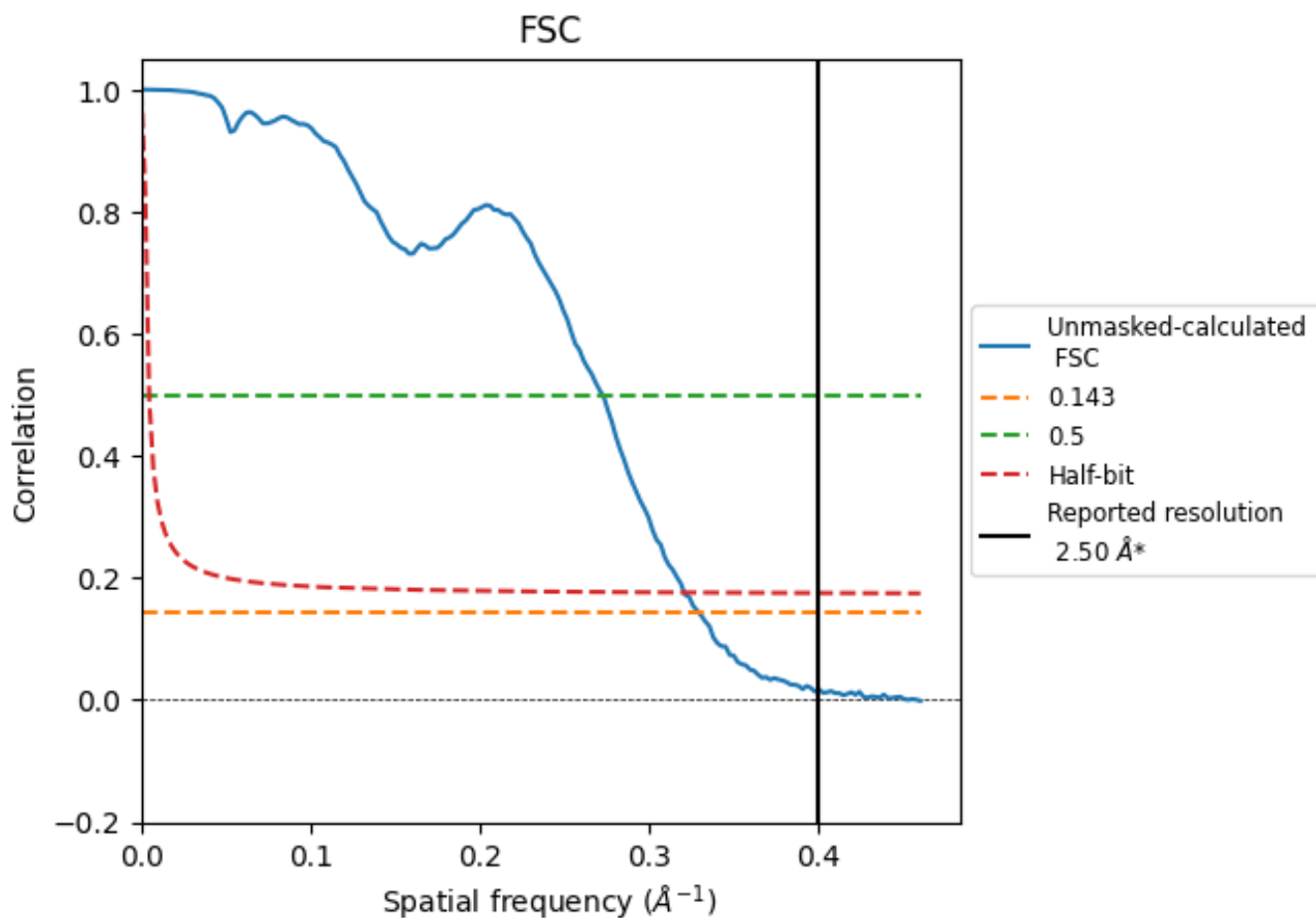


\*Reported resolution corresponds to spatial frequency of 0.400 Å<sup>-1</sup>

## 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  $0.400 \text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

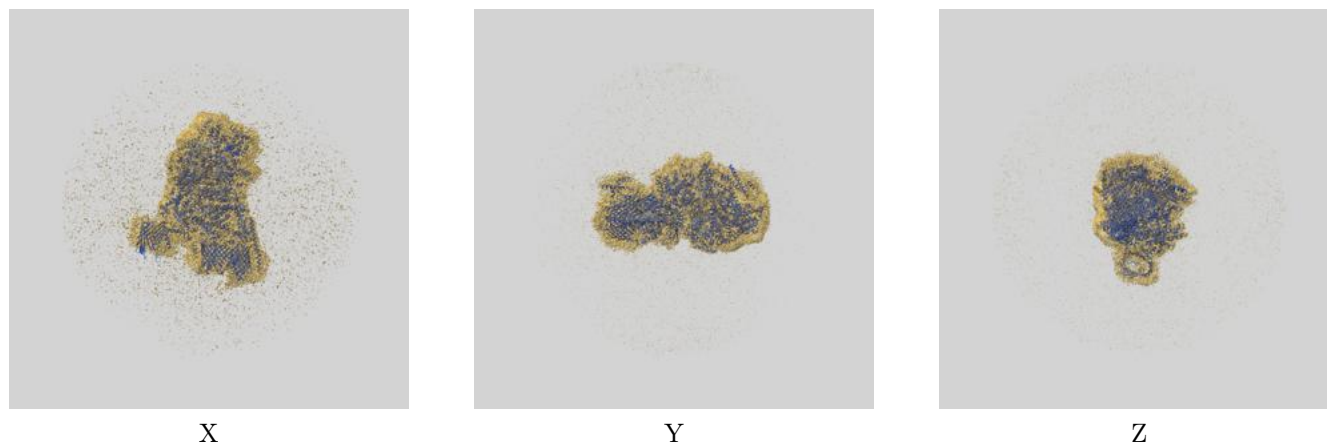
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.04	3.67	3.12

\*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 3.04 differs from the reported value 2.5 by more than 10 %

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

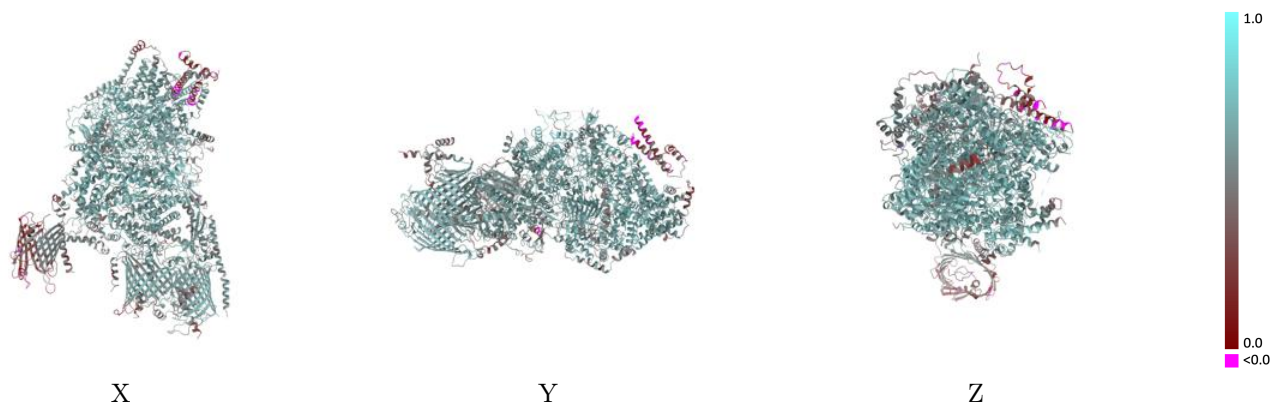
This section contains information regarding the fit between EMDB map EMD-31890 and PDB model 7VCF. Per-residue inclusion information can be found in section 3 on page 8.

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



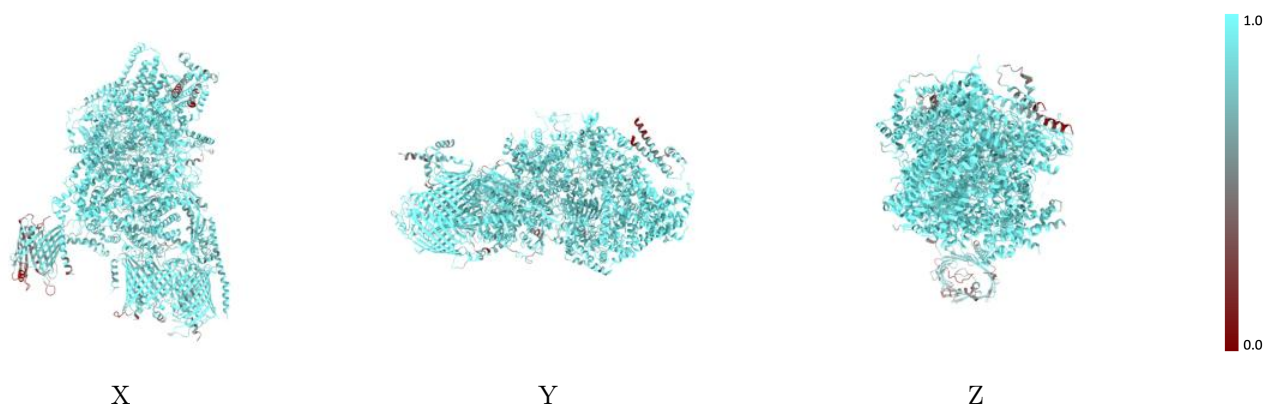
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



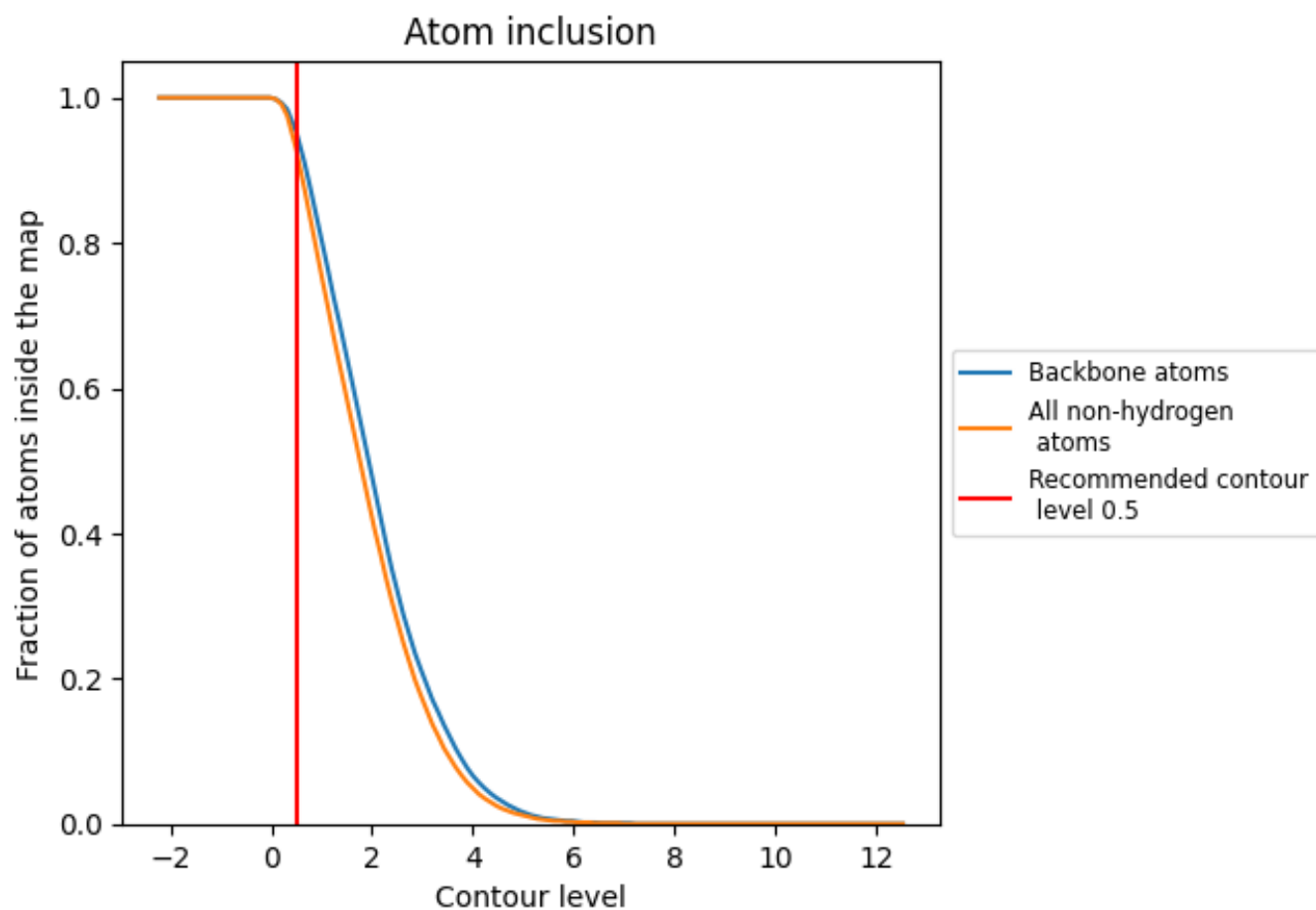
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 93% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9280	 0.5890
A	 0.9840	 0.6200
B	 0.9190	 0.5700
C	 0.9490	 0.5900
D	 0.8830	 0.5100
F	 0.9070	 0.5620
G	 0.9210	 0.5650
H	 0.6730	 0.2740
I	 0.6840	 0.3860
K	 0.8230	 0.5110
M	 0.9920	 0.6910
N	 0.8810	 0.4330
O	 0.9250	 0.6000
Q	 0.9620	 0.6730
T	 0.9650	 0.6620
W	 0.9850	 0.6350

