



## wwPDB EM Validation Summary Report ⓘ

Nov 23, 2022 – 01:20 AM EST

PDB ID : 7TKN  
EMDB ID : EMD-25975  
Title : Yeast ATP synthase State 3binding(c) with 10 mM ATP backbone model  
Authors : Guo, H.; Rubinstein, J.L.  
Deposited on : 2022-01-17  
Resolution : 7.10 Å(reported)  
Based on initial model : 2HLD

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

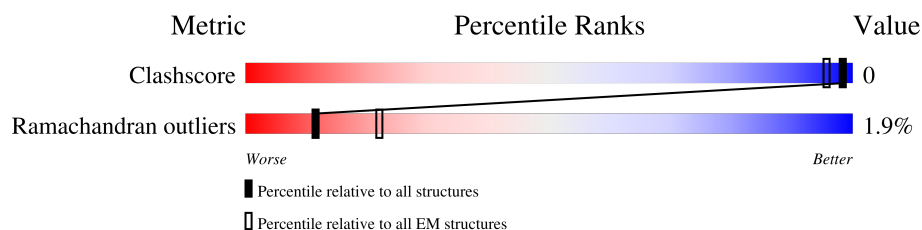
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.10 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.



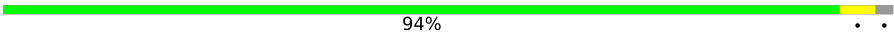
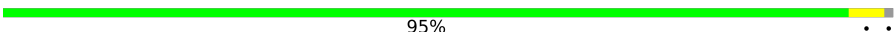
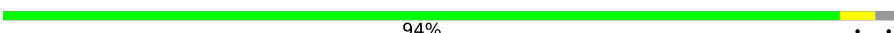
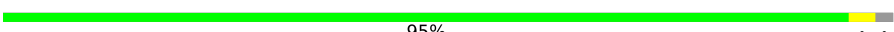








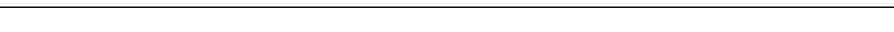



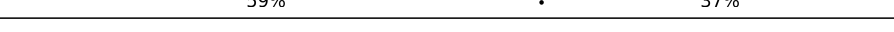
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	0	76	97% ..
1	1	76	95% . .
1	2	76	97% ..
1	3	76	93% . . .
1	4	76	93% . .
1	5	76	96% . .
1	6	76	91% 7% .
1	7	76	91% . . .
1	8	76	93% 5% .
1	9	76	93% . .

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Mol	Chain	Length	Quality of chain
2	A	510	 94% . .
2	B	510	 95% . .
2	C	510	 94% . .
3	D	478	 95% . .
3	E	478	 94% . .
3	F	478	 94% . .
4	G	278	 92% . 5%
5	H	138	 82% 5% 13%
6	I	61	 79% 21%
7	O	195	 91% 5% .
8	T	249	 88% . 10%
9	U	209	 74% 26%
10	V	173	 94% 5% .
11	W	95	 82% 7% 11%
12	X	92	 62% 5% 33%
13	Y	59	 59% . 37%
14	Z	48	 98% .

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 20225 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 ATP synthase subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	75	Total	C	N	O	0	0
			300	150	75	75		
1	1	75	Total	C	N	O	0	0
			300	150	75	75		
1	2	75	Total	C	N	O	0	0
			300	150	75	75		
1	3	74	Total	C	N	O	0	0
			296	148	74	74		
1	4	75	Total	C	N	O	0	0
			300	150	75	75		
1	5	75	Total	C	N	O	0	0
			300	150	75	75		
1	6	74	Total	C	N	O	0	0
			296	148	74	74		
1	7	73	Total	C	N	O	0	0
			292	146	73	73		
1	8	75	Total	C	N	O	0	0
			300	150	75	75		
1	9	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 2 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	A	499	Total	C	N	O	0	0
			1996	998	499	499		
2	B	507	Total	C	N	O	0	0
			2028	1014	507	507		
2	C	496	Total	C	N	O	0	0
			1984	992	496	496		

- Molecule 3 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	468	Total	C	N	O	0	0
			1872	936	468	468		
3	E	469	Total	C	N	O	0	0
			1876	938	469	469		
3	F	470	Total	C	N	O	0	0
			1880	940	470	470		

- Molecule 4 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	265	Total	C	N	O	0	0
			1059	530	265	264		

- Molecule 5 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	120	Total	C	N	O	0	0
			478	240	120	118		

- Molecule 6 is a protein called ATP synthase subunit epsilon.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	I	48	Total	C	N	O	0	0
			193	96	48	49		

- Molecule 7 is a protein called ATP synthase subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	187	Total	C	N	O	0	0
			748	374	187	187		

- Molecule 8 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	T	224	Total	C	N	O	0	0
			897	448	224	225		

- Molecule 9 is a protein called ATP synthase subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	U	155	Total	C	N	O	0	0
			620	310	155	155		

- Molecule 10 is a protein called ATP synthase subunit d.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	V	171	Total	C	N	O	0	0
			685	342	171	172		

- Molecule 11 is a protein called ATP synthase subunit f.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	W	85	Total	C	N	O	0	0
			340	170	85	85		

- Molecule 12 is a protein called ATP synthase subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	62	Total	C	N	O	0	0
			248	124	62	62		

- Molecule 13 is a protein called ATP synthase subunit J.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Y	37	Total	C	N	O	0	0
			148	74	37	37		

- Molecule 14 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	Z	48	Total	C	N	O	0	0
			193	96	48	49		

### 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. 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. 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.

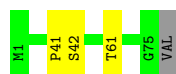
- Molecule 1: ATP synthase subunit 9

Chain 0:  97% ..



- Molecule 1: ATP synthase subunit 9

Chain 1:  95% ..



- Molecule 1: ATP synthase subunit 9

Chain 2:  97% ..



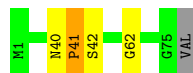
- Molecule 1: ATP synthase subunit 9

Chain 3:  93% ...



- Molecule 1: ATP synthase subunit 9

Chain 4:  93% ..



- Molecule 1: ATP synthase subunit 9

Chain 5:  96% ..



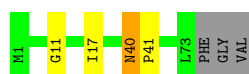
- Molecule 1: ATP synthase subunit 9

Chain 6: 91% 7% .



- Molecule 1: ATP synthase subunit 9

Chain 7: 91% . . .



- Molecule 1: ATP synthase subunit 9

Chain 8: 93% 5% .



- Molecule 1: ATP synthase subunit 9

Chain 9: 93% . .



- Molecule 2: ATP synthase subunit alpha

Chain A: 94% . .



- Molecule 2: ATP synthase subunit alpha

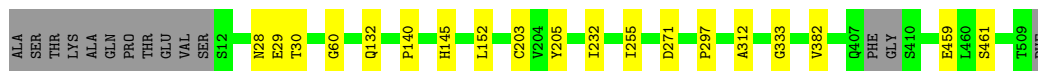
Chain B: 95% . .



- Molecule 2: ATP synthase subunit alpha

Chain C: 94% . .





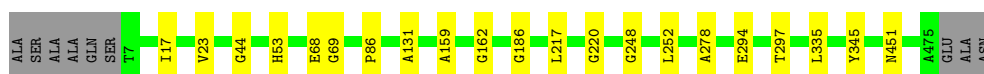
- Molecule 3: ATP synthase subunit beta

Chain D: 95%



- Molecule 3: ATP synthase subunit beta

Chain E: 94%



- Molecule 3: ATP synthase subunit beta

Chain F: 94%



- Molecule 4: ATP synthase subunit gamma

Chain G: 92%



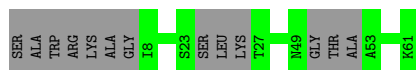
- Molecule 5: ATP synthase subunit delta

Chain H: 82%



- Molecule 6: ATP synthase subunit epsilon

Chain I: 79%

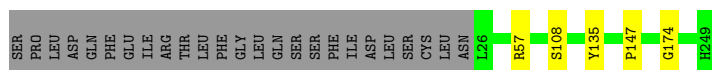


- Molecule 7: ATP synthase subunit 5

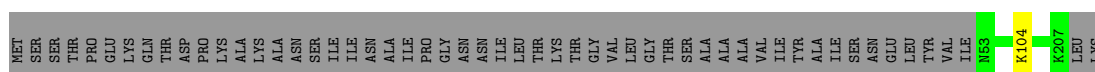
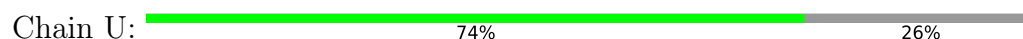
Chain O: 91%



- Molecule 8: ATP synthase subunit a



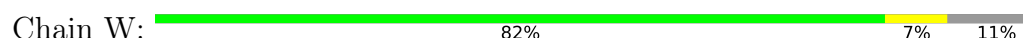
- Molecule 9: ATP synthase subunit 4



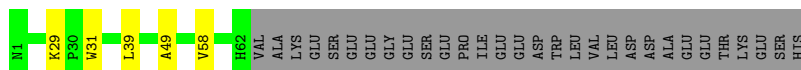
- Molecule 10: ATP synthase subunit d



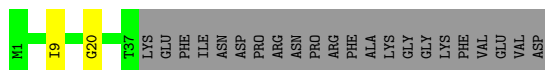
- Molecule 11: ATP synthase subunit f



- Molecule 12: ATP synthase subunit H

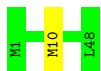


- Molecule 13: ATP synthase subunit J



- Molecule 14: ATP synthase protein 8





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	16301	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	103896	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor

## 5 Model quality [i](#)

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

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	0	1.62	1/299 (0.3%)	1.47	0/372
1	1	1.54	1/299 (0.3%)	1.52	0/372
1	2	1.46	1/299 (0.3%)	1.59	0/372
1	3	1.41	0/295	1.50	2/367 (0.5%)
1	4	1.52	1/299 (0.3%)	1.46	1/372 (0.3%)
1	5	1.47	0/299	1.45	0/372
1	6	1.56	3/295 (1.0%)	1.50	0/367
1	7	1.57	2/291 (0.7%)	1.49	1/362 (0.3%)
1	8	1.53	2/299 (0.7%)	1.52	0/372
1	9	1.55	1/295 (0.3%)	1.44	0/367
2	A	1.52	5/1994 (0.3%)	1.59	7/2489 (0.3%)
2	B	1.45	2/2027 (0.1%)	1.59	8/2532 (0.3%)
2	C	1.53	4/1982 (0.2%)	1.56	6/2474 (0.2%)
3	D	1.53	4/1871 (0.2%)	1.62	5/2337 (0.2%)
3	E	1.57	5/1875 (0.3%)	1.58	8/2342 (0.3%)
3	F	1.54	3/1879 (0.2%)	1.56	3/2347 (0.1%)
4	G	1.45	2/1057 (0.2%)	1.42	1/1318 (0.1%)
5	H	1.34	0/473	1.50	3/583 (0.5%)
6	I	1.38	0/190	1.54	0/231
7	O	1.46	0/747	1.56	0/932
8	T	1.50	2/896 (0.2%)	1.46	0/1117
9	U	1.50	0/619	1.39	1/772 (0.1%)
10	V	1.46	0/684	1.49	0/852
11	W	1.55	0/339	1.65	1/422 (0.2%)
12	X	1.54	0/247	1.58	2/307 (0.7%)
13	Y	1.55	1/147 (0.7%)	1.38	0/182
14	Z	1.50	0/192	1.49	2/237 (0.8%)
All	All	1.51	40/20189 (0.2%)	1.54	51/25169 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	4	0	1
1	5	0	1
1	6	0	1
1	7	0	1
1	9	0	1
2	A	0	1
2	B	0	1
3	E	0	1
3	F	0	1
5	H	0	2
10	V	0	1
All	All	0	12

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	69	GLY	N-CA	-6.72	1.35	1.46
3	D	188	GLY	CA-C	-6.49	1.41	1.51
2	C	203	CYS	N-CA	-6.43	1.33	1.46
3	E	162	GLY	CA-C	6.26	1.61	1.51
2	A	127	GLY	CA-C	-6.26	1.41	1.51

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	148	VAL	N-CA-C	-6.80	92.63	111.00
9	U	104	LYS	O-C-N	-6.54	112.24	122.70
14	Z	10	MET	O-C-N	6.42	132.98	122.70
2	B	233	ILE	N-CA-C	-6.42	93.67	111.00
3	E	17	ILE	N-CA-C	-6.36	93.83	111.00

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	4	40	ASN	Peptide
1	5	40	ASN	Peptide
1	6	40	ASN	Peptide
1	7	40	ASN	Peptide
1	9	40	ASN	Peptide

## 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	0	300	0	95	0	0
1	1	300	0	95	0	0
1	2	300	0	95	0	0
1	3	296	0	91	0	0
1	4	300	0	95	0	0
1	5	300	0	95	0	0
1	6	296	0	91	0	0
1	7	292	0	91	0	0
1	8	300	0	95	0	0
1	9	296	0	91	0	0
2	A	1996	0	570	0	0
2	B	2028	0	580	1	0
2	C	1984	0	567	0	0
3	D	1872	0	537	1	0
3	E	1876	0	537	0	0
3	F	1880	0	538	1	0
4	G	1059	0	277	0	0
5	H	478	0	122	0	0
6	I	193	0	43	0	0
7	O	748	0	205	0	0
8	T	897	0	248	1	0
9	U	620	0	158	0	0
10	V	685	0	173	0	0
11	W	340	0	92	1	0
12	X	248	0	61	0	0
13	Y	148	0	40	0	0
14	Z	193	0	49	0	0
All	All	20225	0	5731	4	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 0.

All (4) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:137:GLY:HA2	3:F:432:VAL:H	1.73	0.52
2:B:281:ARG:CA	2:B:296:TYR:CA	2.90	0.49
8:T:57:ARG:H	11:W:58:GLY:HA3	1.79	0.47
3:D:41:THR:C	3:D:43:GLN:H	2.24	0.41

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	0	73/76 (96%)	73 (100%)	0	0	100	100
1	1	73/76 (96%)	70 (96%)	1 (1%)	2 (3%)	5	31
1	2	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
1	3	72/76 (95%)	69 (96%)	1 (1%)	2 (3%)	5	30
1	4	73/76 (96%)	70 (96%)	1 (1%)	2 (3%)	5	31
1	5	73/76 (96%)	71 (97%)	1 (1%)	1 (1%)	11	46
1	6	72/76 (95%)	70 (97%)	1 (1%)	1 (1%)	11	46
1	7	71/76 (93%)	69 (97%)	1 (1%)	1 (1%)	11	46
1	8	73/76 (96%)	70 (96%)	1 (1%)	2 (3%)	5	31
1	9	72/76 (95%)	70 (97%)	1 (1%)	1 (1%)	11	46
2	A	495/510 (97%)	460 (93%)	30 (6%)	5 (1%)	15	54
2	B	505/510 (99%)	468 (93%)	28 (6%)	9 (2%)	8	40
2	C	492/510 (96%)	455 (92%)	28 (6%)	9 (2%)	8	40
3	D	466/478 (98%)	433 (93%)	28 (6%)	5 (1%)	14	52
3	E	467/478 (98%)	426 (91%)	34 (7%)	7 (2%)	10	46
3	F	468/478 (98%)	427 (91%)	31 (7%)	10 (2%)	7	36
4	G	261/278 (94%)	244 (94%)	11 (4%)	6 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	H	110/138 (80%)	105 (96%)	3 (3%)	2 (2%)	8	40
6	I	42/61 (69%)	41 (98%)	1 (2%)	0	100	100
7	O	185/195 (95%)	160 (86%)	15 (8%)	10 (5%)	2	19
8	T	222/249 (89%)	211 (95%)	9 (4%)	2 (1%)	17	57
9	U	153/209 (73%)	152 (99%)	1 (1%)	0	100	100
10	V	169/173 (98%)	148 (88%)	14 (8%)	7 (4%)	3	22
11	W	83/95 (87%)	65 (78%)	13 (16%)	5 (6%)	1	17
12	X	60/92 (65%)	53 (88%)	4 (7%)	3 (5%)	2	20
13	Y	35/59 (59%)	31 (89%)	3 (9%)	1 (3%)	4	29
14	Z	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
All	All	4984/5321 (94%)	4627 (93%)	264 (5%)	93 (2%)	11	38

5 of 93 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	41	PRO
1	3	41	PRO
1	4	41	PRO
1	5	41	PRO
1	6	41	PRO

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

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

### 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](#)

There are no ligands in this entry.

## 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

This section contains visualisations of the EMDB entry EMD-25975. 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

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal surface views

This section was not generated.

### 6.5 Mask visualisation

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

## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit

This section was not generated.