



# Full wwPDB EM Validation Report ⓘ

Oct 22, 2024 – 02:34 AM JST

PDB ID : 8WA1  
EMDB ID : EMD-37388  
Title : The cryo-EM structure of the Nicotiana tabacum PEP-PAP-TEC2  
Authors : Wu, X.X.; Zhang, Y.  
Deposited on : 2023-09-06  
Resolution : 2.80 Å(reported)

This is a Full wwPDB EM Validation 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.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

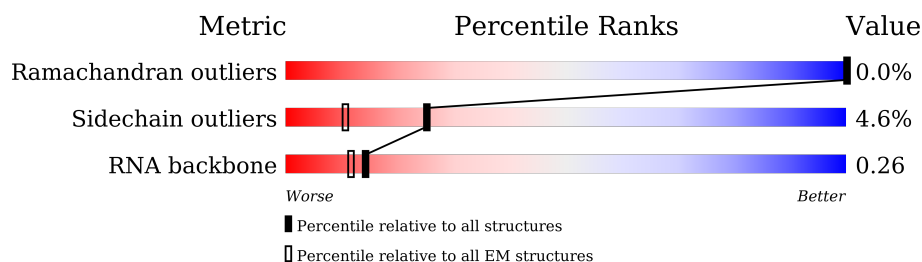
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 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.





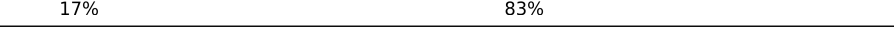
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	337	83% 15%
1	a	337	86% 10%
2	B	1070	90% 7%
3	C	688	90% 5% 5%
4	D	892	68% 28%
5	E	860	79% 19%
6	F	682	78% 20%
7	G	266	79% 18%

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Mol	Chain	Length	Quality of chain
8	H	531	
9	I	486	
10	J	507	
11	K	331	
12	L	303	
13	M	178	
13	m	178	
14	N	770	
15	O	167	
16	P	143	
17	Q	24	
18	R	24	
19	S	27	
20	c	1388	
21	i	648	

## 2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 62699 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	288	Total	C	N	O	S	0	0
			2190	1392	378	409	11		
1	a	303	Total	C	N	O	S	0	0
			2358	1508	405	434	11		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	998	Total	C	N	O	S	0	0
			7604	4823	1367	1391	23		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	653	Total	C	N	O	S	0	0
			4899	3131	873	875	20		

- Molecule 4 is a protein called PAP1(pTAC3).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	645	Total	C	N	O	S	0	0
			5063	3202	885	950	26		

- Molecule 5 is a protein called Pentatricopeptide repeat-containing protein At1g74850, chloroplastic-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	700	Total	C	N	O	S	0	0
			4563	2840	829	872	22		

- Molecule 6 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	544	Total	C	N	O	S	0	0
			4259	2692	763	785	19		

- Molecule 7 is a protein called superoxide dismutase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	218	Total	C	N	O	S	0	0
			1742	1134	291	310	7		

- Molecule 8 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 12-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	260	Total	C	N	O	S	0	0
			2110	1338	371	393	8		

- Molecule 9 is a protein called Fructokinase-like 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	376	Total	C	N	O	S	0	0
			2946	1886	519	528	13		

- Molecule 10 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 14-like isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	421	Total	C	N	O	S	0	0
			3410	2184	577	627	22		

- Molecule 11 is a protein called PAP8(pTAC6).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	204	Total	C	N	O	S	0	0
			1705	1077	298	322	8		

- Molecule 12 is a protein called superoxide dismutase.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	229	Total	C	N	O	S	0	0
			1776	1141	306	324	5		

- Molecule 13 is a protein called Thioredoxin-like protein CITRX1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	116	Total	C	N	O	S	0	0
			935	598	150	180	7		
13	m	109	Total	C	N	O	S	0	0
			855	548	136	164	7		

- Molecule 14 is a protein called UDP-N-acetylmuramoyl-L-alanyl-D-glutamate--2, 6-diaminopimelate ligase-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	537	Total	C	N	O	S	0	0
			2995	1825	582	582	6		

- Molecule 15 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 7-like isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	97	Total	C	N	O	S	0	0
			780	490	140	146	4		

- Molecule 16 is a protein called PAP13(pTAC18).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	102	Total	C	N	O	S	0	0
			843	547	142	151	3		

- Molecule 17 is a DNA chain called DNA (24-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	4	Total	C	N	O	P	0	0
			82	40	11	27	4		

- Molecule 18 is a DNA chain called DNA (24-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	14	Total	C	N	O	P	0	0
			285	136	53	82	14		

- Molecule 19 is a RNA chain called RNA (27-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	9	Total	C	N	O	P	0	0
			192	86	35	62	9		

- Molecule 20 is a protein called DNA-directed RNA polymerase subunit beta”.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	c	1176	Total	C	N	O	S	0	0
			8166	5119	1500	1517	30		

- Molecule 21 is a protein called Fructokinase-like 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	i	375	Total	C	N	O	S	0	0
			2937	1873	500	548	16		

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
22	B	1	Total	Zn	0
			1	1	

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
23	C	1	Total	Mg	0
			1	1	

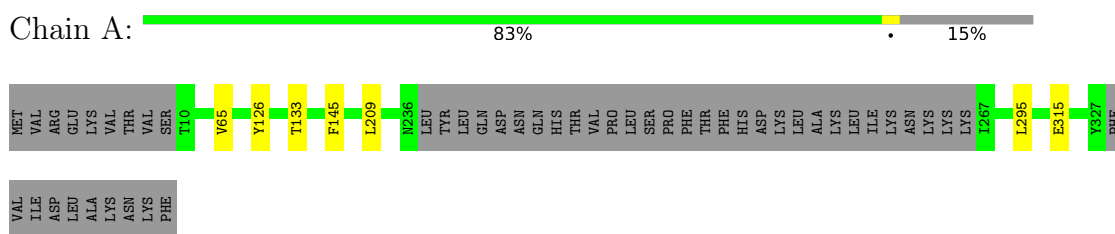
- Molecule 24 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
24	G	1	Total	Fe	0
			1	1	
24	L	1	Total	Fe	0
			1	1	

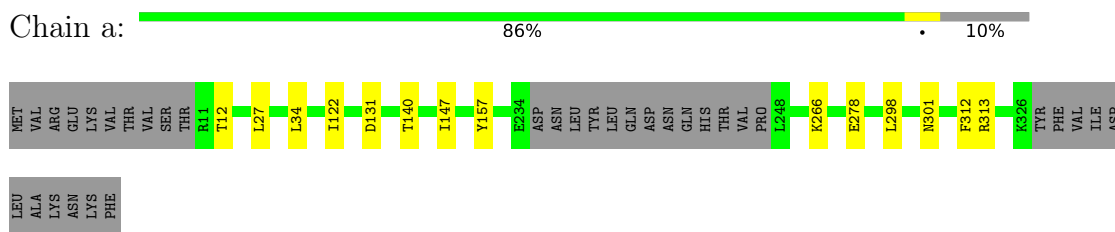
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

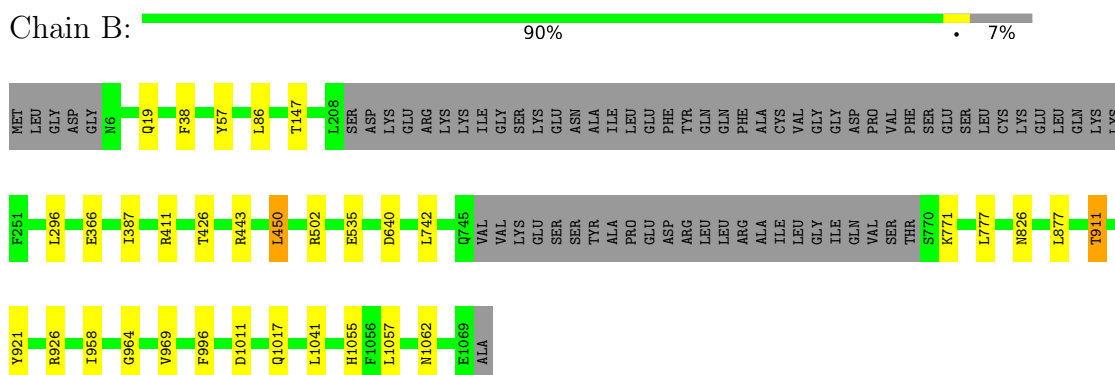
- Molecule 1: DNA-directed RNA polymerase subunit alpha



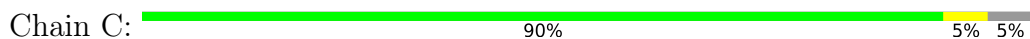
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 2: DNA-directed RNA polymerase subunit beta



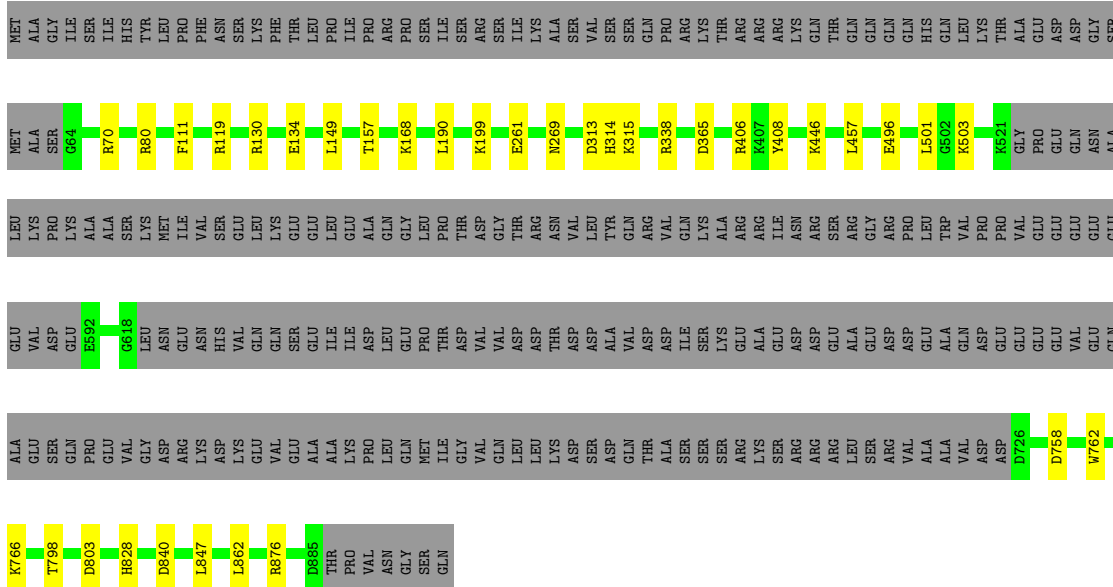
- Molecule 3: DNA-directed RNA polymerase subunit gamma



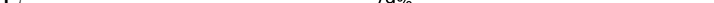


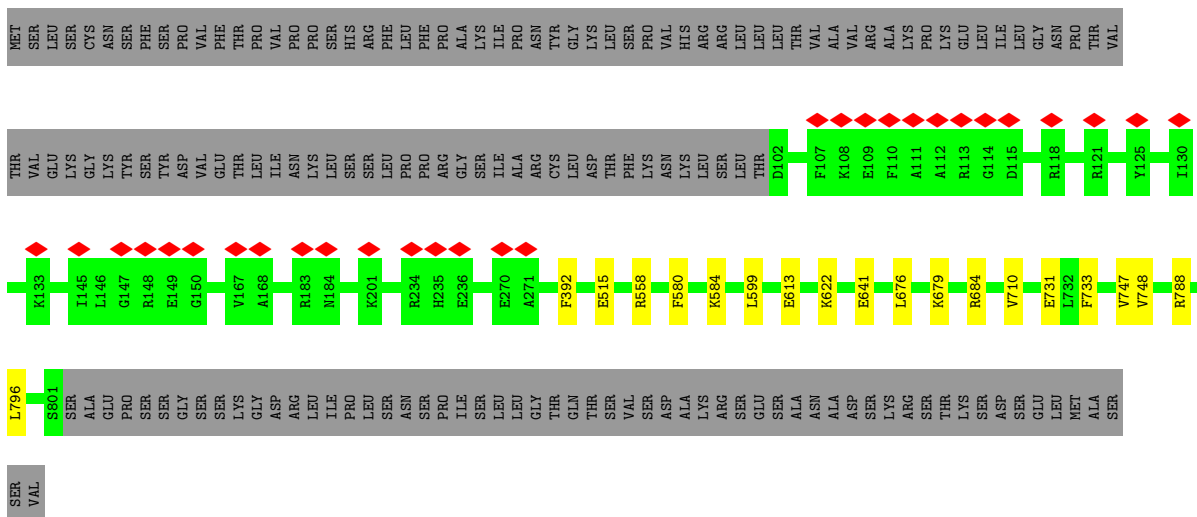
- Molecule 4: PAP1(pTAC3)

Chain D:  68% . 28%



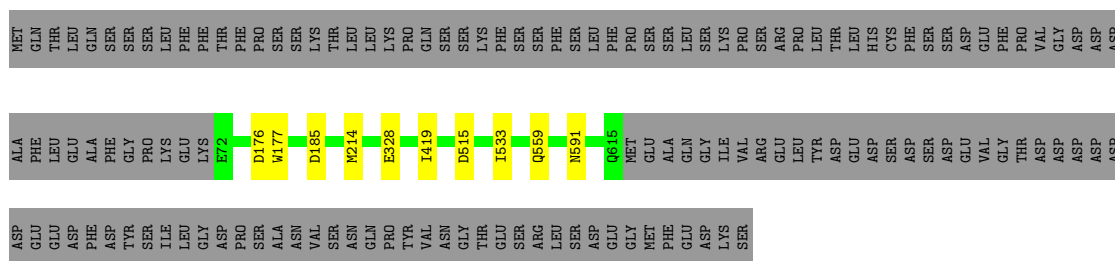
- Molecule 5: Pentatricopeptide repeat-containing protein At1g74850, chloroplastic-like

Chain E:  79% 19%



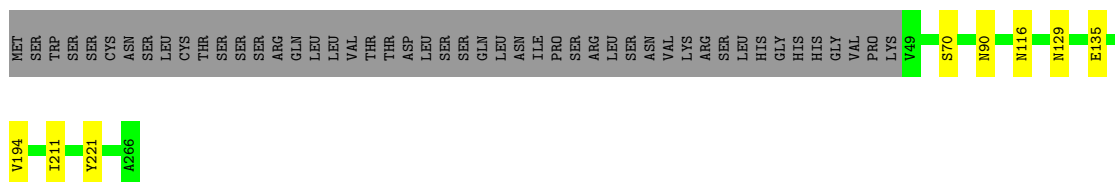
- Molecule 6: Protein PLASTID TRANSCRIPTIONALLY ACTIVE 10-like

Chain F:  78% 20%



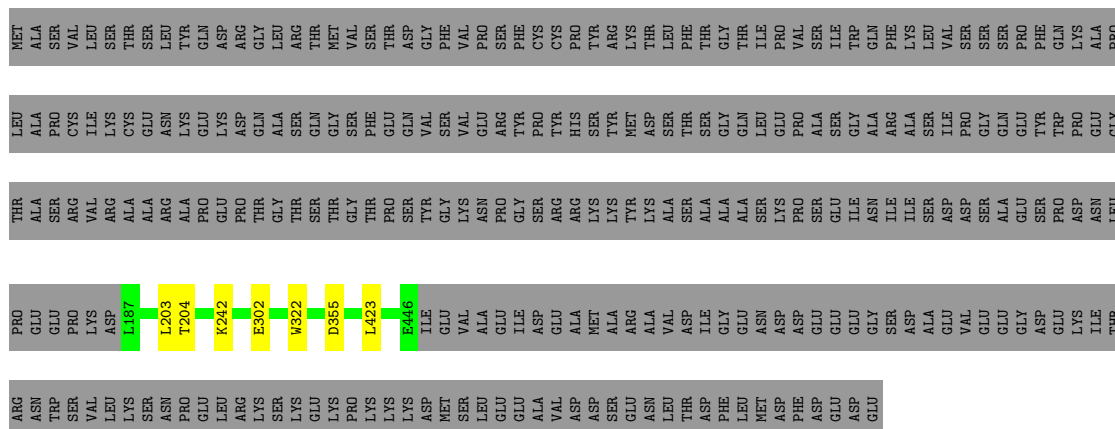
- Molecule 7: superoxide dismutase

Chain G: 79% 18%



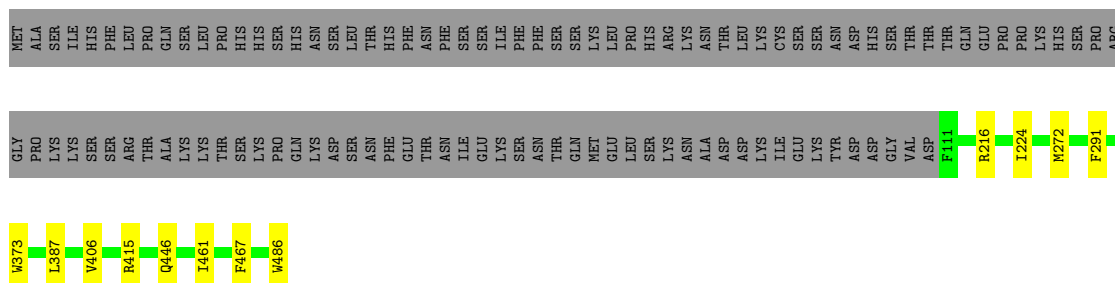
- Molecule 8: Protein PLASTID TRANSCRIPTIONALLY ACTIVE 12-like

Chain H: 48% 51%



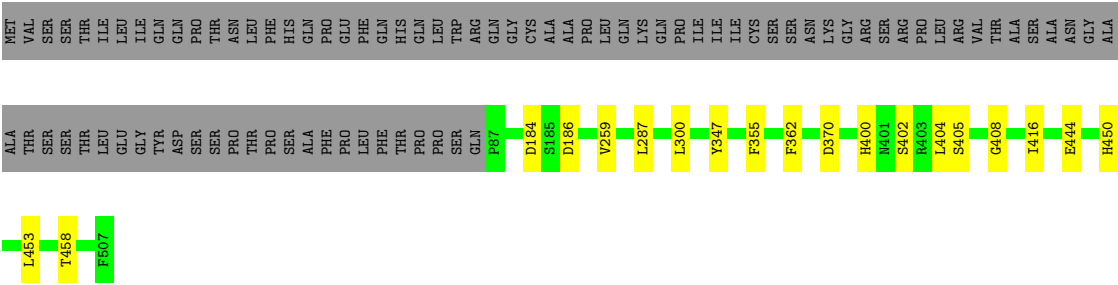
- Molecule 9: Fructokinase-like 1, chloroplastic

Chain I: 75% 23%

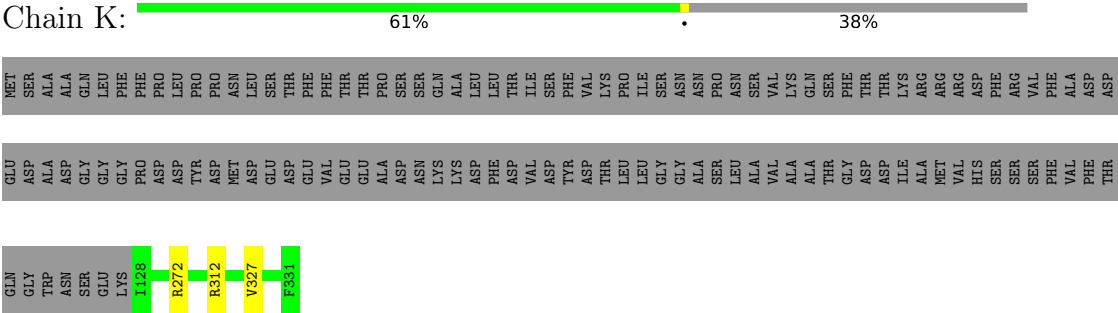


- Molecule 10: Protein PLASTID TRANSCRIPTIONALLY ACTIVE 14-like isoform X2

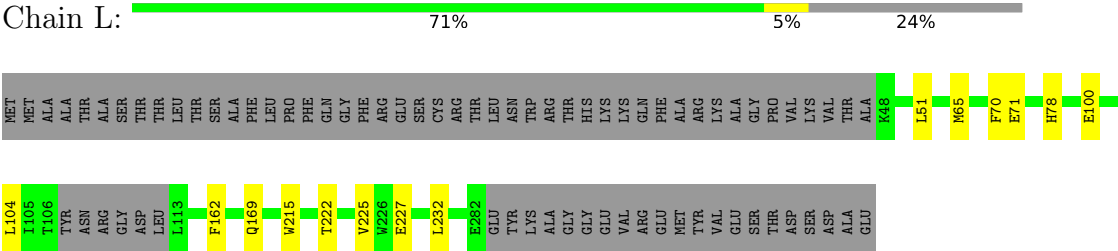
Chain J: 79% 17%



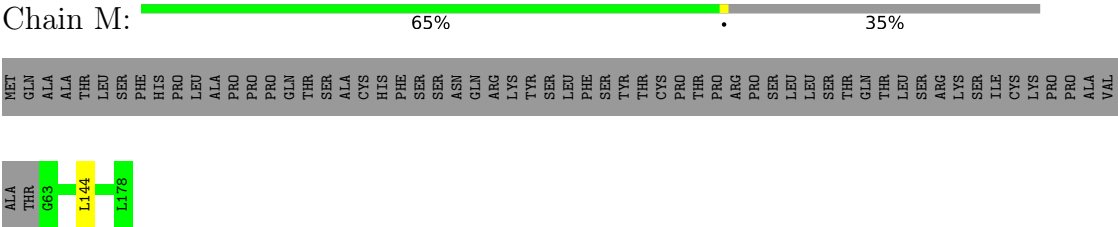
• Molecule 11: PAP8(pTAC6)



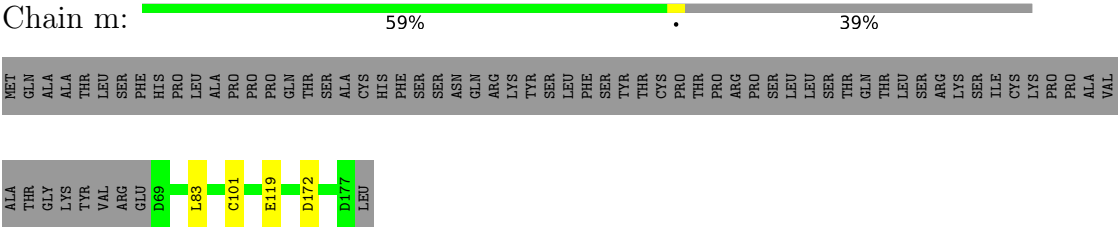
• Molecule 12: superoxide dismutase



• Molecule 13: Thioredoxin-like protein CITRX1, chloroplastic



• Molecule 13: Thioredoxin-like protein CITRX1, chloroplastic







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88607	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 ( $e^-/\text{\AA}^2$ )	57.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.362	Depositor
Minimum map value	-0.380	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	464.8, 464.8, 464.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, MG, ZN

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	0/2227	0.43	0/3019
1	a	0.24	0/2403	0.41	0/3256
2	B	0.40	0/7751	0.51	3/10510 (0.0%)
3	C	0.32	0/4998	0.45	1/6792 (0.0%)
4	D	0.26	0/5161	0.42	0/6986
5	E	0.24	0/4633	0.39	0/6321
6	F	0.26	0/4366	0.40	0/5918
7	G	0.38	0/1793	0.50	0/2437
8	H	0.29	0/2167	0.38	0/2942
9	I	0.26	0/3021	0.41	0/4092
10	J	0.26	0/3498	0.40	0/4742
11	K	0.25	0/1747	0.40	0/2362
12	L	0.41	0/1828	0.55	0/2488
13	M	0.41	0/951	0.50	0/1286
13	m	0.34	0/869	0.45	0/1179
14	N	0.26	0/3024	0.45	0/4180
15	O	0.25	0/793	0.36	0/1065
16	P	0.23	0/870	0.40	0/1182
17	Q	0.32	0/90	0.73	0/137
18	R	0.35	0/319	0.70	0/489
19	S	0.27	0/214	0.65	0/331
20	c	0.29	0/8294	0.44	0/11306
21	i	0.26	0/3009	0.44	0/4078
All	All	0.30	0/64026	0.44	4/87098 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	964	GLY	N-CA-C	9.52	136.91	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	911	THR	N-CA-C	-7.00	92.10	111.00
3	C	394	GLY	N-CA-C	-6.14	97.75	113.10
2	B	450	LEU	CA-CB-CG	5.19	127.23	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	284/337 (84%)	276 (97%)	8 (3%)	0	100	100
1	a	299/337 (89%)	291 (97%)	8 (3%)	0	100	100
2	B	992/1070 (93%)	973 (98%)	19 (2%)	0	100	100
3	C	647/688 (94%)	629 (97%)	18 (3%)	0	100	100
4	D	639/892 (72%)	627 (98%)	12 (2%)	0	100	100
5	E	698/860 (81%)	691 (99%)	7 (1%)	0	100	100
6	F	542/682 (80%)	532 (98%)	10 (2%)	0	100	100
7	G	216/266 (81%)	207 (96%)	9 (4%)	0	100	100
8	H	258/531 (49%)	256 (99%)	2 (1%)	0	100	100
9	I	374/486 (77%)	365 (98%)	9 (2%)	0	100	100
10	J	419/507 (83%)	412 (98%)	6 (1%)	1 (0%)	44	73
11	K	202/331 (61%)	200 (99%)	2 (1%)	0	100	100
12	L	225/303 (74%)	215 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	114/178 (64%)	112 (98%)	2 (2%)	0	100	100
13	m	107/178 (60%)	107 (100%)	0	0	100	100
14	N	535/770 (70%)	523 (98%)	12 (2%)	0	100	100
15	O	95/167 (57%)	93 (98%)	2 (2%)	0	100	100
16	P	100/143 (70%)	100 (100%)	0	0	100	100
20	c	1162/1388 (84%)	1129 (97%)	33 (3%)	0	100	100
21	i	373/648 (58%)	360 (96%)	13 (4%)	0	100	100
All	All	8281/10762 (77%)	8098 (98%)	182 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	408	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	226/308 (73%)	219 (97%)	7 (3%)	35	69
1	a	256/308 (83%)	242 (94%)	14 (6%)	18	47
2	B	767/924 (83%)	735 (96%)	32 (4%)	25	58
3	C	465/612 (76%)	432 (93%)	33 (7%)	12	35
4	D	523/770 (68%)	488 (93%)	35 (7%)	13	38
5	E	308/741 (42%)	289 (94%)	19 (6%)	15	43
6	F	401/615 (65%)	391 (98%)	10 (2%)	42	75
7	G	176/232 (76%)	168 (96%)	8 (4%)	23	55
8	H	212/472 (45%)	205 (97%)	7 (3%)	33	67
9	I	298/437 (68%)	286 (96%)	12 (4%)	27	60
10	J	368/449 (82%)	350 (95%)	18 (5%)	21	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	192/301 (64%)	189 (98%)	3 (2%)	58	85
12	L	167/258 (65%)	153 (92%)	14 (8%)	9	28
13	M	103/160 (64%)	102 (99%)	1 (1%)	73	91
13	m	93/160 (58%)	89 (96%)	4 (4%)	25	57
14	N	99/659 (15%)	89 (90%)	10 (10%)	6	20
15	O	79/144 (55%)	75 (95%)	4 (5%)	20	51
16	P	82/129 (64%)	78 (95%)	4 (5%)	21	52
20	c	697/1238 (56%)	666 (96%)	31 (4%)	24	56
21	i	316/567 (56%)	311 (98%)	5 (2%)	58	85
All	All	5828/9484 (62%)	5557 (95%)	271 (5%)	25	55

All (271) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	A	126	TYR
1	A	133	THR
1	A	145	PHE
1	A	209	LEU
1	A	295	LEU
1	A	315	GLU
2	B	19	GLN
2	B	38	PHE
2	B	57	TYR
2	B	86	LEU
2	B	147	THR
2	B	296	LEU
2	B	366	GLU
2	B	387	ILE
2	B	411	ARG
2	B	426	THR
2	B	443	ARG
2	B	450	LEU
2	B	502	ARG
2	B	535	GLU
2	B	640	ASP
2	B	742	LEU
2	B	771	LYS
2	B	777	LEU

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Mol	Chain	Res	Type
2	B	826	ASN
2	B	877	LEU
2	B	911	THR
2	B	921	TYR
2	B	926	ARG
2	B	958	ILE
2	B	969	VAL
2	B	996	PHE
2	B	1011	ASP
2	B	1017	GLN
2	B	1041	LEU
2	B	1055	HIS
2	B	1057	LEU
2	B	1062	ASN
3	C	22	VAL
3	C	27	ILE
3	C	62	LEU
3	C	99	VAL
3	C	102	VAL
3	C	111	MET
3	C	126	LEU
3	C	129	LEU
3	C	142	LYS
3	C	261	PHE
3	C	272	VAL
3	C	302	LEU
3	C	313	LEU
3	C	329	MET
3	C	370	LYS
3	C	371	GLU
3	C	373	ARG
3	C	376	GLU
3	C	382	ARG
3	C	393	VAL
3	C	407	GLU
3	C	459	LEU
3	C	461	ARG
3	C	474	GLN
3	C	521	PHE
3	C	524	MET
3	C	539	THR
3	C	542	MET

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Mol	Chain	Res	Type
3	C	614	TRP
3	C	632	TYR
3	C	652	LYS
3	C	672	GLU
3	C	680	PHE
4	D	70	ARG
4	D	80	ARG
4	D	111	PHE
4	D	119	ARG
4	D	130	ARG
4	D	134	GLU
4	D	149	LEU
4	D	157	THR
4	D	168	LYS
4	D	190	LEU
4	D	199	LYS
4	D	261	GLU
4	D	269	ASN
4	D	313	ASP
4	D	314	HIS
4	D	315	LYS
4	D	338	ARG
4	D	365	ASP
4	D	406	ARG
4	D	408	TYR
4	D	446	LYS
4	D	457	LEU
4	D	496	GLU
4	D	501	LEU
4	D	503	LYS
4	D	758	ASP
4	D	762	TRP
4	D	766	LYS
4	D	798	THR
4	D	803	ASP
4	D	828	HIS
4	D	840	ASP
4	D	847	LEU
4	D	862	LEU
4	D	876	ARG
5	E	392	PHE
5	E	515	GLU

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Mol	Chain	Res	Type
5	E	558	ARG
5	E	580	PHE
5	E	584	LYS
5	E	599	LEU
5	E	613	GLU
5	E	622	LYS
5	E	641	GLU
5	E	676	LEU
5	E	679	LYS
5	E	684	ARG
5	E	710	VAL
5	E	731	GLU
5	E	733	PHE
5	E	747	VAL
5	E	748	VAL
5	E	788	ARG
5	E	796	LEU
6	F	176	ASP
6	F	177	TRP
6	F	185	ASP
6	F	214	MET
6	F	328	GLU
6	F	419	ILE
6	F	515	ASP
6	F	533	ILE
6	F	559	GLN
6	F	591	ASN
7	G	70	SER
7	G	90	ASN
7	G	116	ASN
7	G	129	ASN
7	G	135	GLU
7	G	194	VAL
7	G	211	ILE
7	G	221	TYR
8	H	203	LEU
8	H	204	THR
8	H	242	LYS
8	H	302	GLU
8	H	322	TRP
8	H	355	ASP
8	H	423	LEU

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Mol	Chain	Res	Type
9	I	216	ARG
9	I	224	ILE
9	I	272	MET
9	I	291	PHE
9	I	373	TRP
9	I	387	LEU
9	I	406	VAL
9	I	415	ARG
9	I	446	GLN
9	I	461	ILE
9	I	467	PHE
9	I	486	TRP
10	J	184	ASP
10	J	186	ASP
10	J	259	VAL
10	J	287	LEU
10	J	300	LEU
10	J	347	TYR
10	J	355	PHE
10	J	362	PHE
10	J	370	ASP
10	J	400	HIS
10	J	402	SER
10	J	404	LEU
10	J	405	SER
10	J	416	ILE
10	J	444	GLU
10	J	450	HIS
10	J	453	LEU
10	J	458	THR
11	K	272	ARG
11	K	312	ARG
11	K	327	VAL
12	L	51	LEU
12	L	65	MET
12	L	70	PHE
12	L	71	GLU
12	L	78	HIS
12	L	100	GLU
12	L	104	LEU
12	L	162	PHE
12	L	169	GLN

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Mol	Chain	Res	Type
12	L	215	TRP
12	L	222	THR
12	L	225	VAL
12	L	227	GLU
12	L	232	LEU
13	M	144	LEU
14	N	588	PHE
14	N	596	HIS
14	N	608	VAL
14	N	633	ILE
14	N	651	ASN
14	N	654	THR
14	N	672	MET
14	N	687	LEU
14	N	759	THR
14	N	762	PHE
15	O	78	ARG
15	O	102	GLU
15	O	147	LYS
15	O	150	LEU
16	P	45	GLU
16	P	74	THR
16	P	91	ILE
16	P	95	GLU
1	a	12	THR
1	a	27	LEU
1	a	34	LEU
1	a	122	ILE
1	a	131	ASP
1	a	140	THR
1	a	147	ILE
1	a	157	TYR
1	a	266	LYS
1	a	278	GLU
1	a	298	LEU
1	a	301	ASN
1	a	312	PHE
1	a	313	ARG
20	c	8	VAL
20	c	21	ARG
20	c	40	ASP
20	c	65	ILE

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Mol	Chain	Res	Type
20	c	94	VAL
20	c	102	GLU
20	c	114	GLU
20	c	157	GLN
20	c	191	ASP
20	c	211	GLN
20	c	312	VAL
20	c	320	ILE
20	c	372	THR
20	c	397	ASN
20	c	422	GLU
20	c	480	ARG
20	c	569	LYS
20	c	571	ARG
20	c	1010	GLN
20	c	1022	LYS
20	c	1038	ASP
20	c	1067	ILE
20	c	1128	THR
20	c	1129	LEU
20	c	1146	LEU
20	c	1153	LEU
20	c	1173	ASN
20	c	1182	ILE
20	c	1233	LEU
20	c	1270	VAL
20	c	1290	PHE
21	i	308	ARG
21	i	392	ARG
21	i	561	THR
21	i	564	MET
21	i	596	LEU
13	m	83	LEU
13	m	101	CYS
13	m	119	GLU
13	m	172	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (147) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	85	HIS

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Mol	Chain	Res	Type
1	A	150	GLN
1	A	196	GLN
1	A	276	GLN
2	B	6	ASN
2	B	124	ASN
2	B	128	GLN
2	B	267	ASN
2	B	372	HIS
2	B	386	GLN
2	B	446	HIS
2	B	495	GLN
2	B	522	GLN
2	B	549	GLN
2	B	600	ASN
2	B	621	HIS
2	B	622	GLN
2	B	636	GLN
2	B	719	ASN
2	B	910	GLN
2	B	934	ASN
2	B	938	GLN
2	B	953	GLN
2	B	1017	GLN
2	B	1055	HIS
2	B	1062	ASN
2	B	1064	GLN
3	C	80	ASN
3	C	110	GLN
3	C	331	GLN
3	C	336	GLN
3	C	449	GLN
3	C	453	GLN
3	C	471	GLN
3	C	474	GLN
3	C	513	GLN
3	C	523	HIS
3	C	553	ASN
3	C	566	ASN
4	D	83	ASN
4	D	109	HIS
4	D	175	GLN
4	D	194	ASN

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Mol	Chain	Res	Type
4	D	227	ASN
4	D	269	ASN
4	D	359	ASN
4	D	420	GLN
4	D	778	GLN
4	D	822	ASN
4	D	882	GLN
5	E	526	ASN
5	E	579	GLN
5	E	616	ASN
5	E	645	GLN
5	E	792	GLN
6	F	128	ASN
6	F	148	GLN
6	F	196	HIS
6	F	278	GLN
6	F	288	HIS
6	F	301	HIS
6	F	317	HIS
6	F	324	HIS
6	F	366	HIS
6	F	402	ASN
6	F	484	GLN
6	F	487	ASN
6	F	518	HIS
7	G	81	HIS
7	G	90	ASN
7	G	92	GLN
7	G	116	ASN
7	G	129	ASN
7	G	253	GLN
8	H	195	GLN
8	H	247	GLN
8	H	271	GLN
8	H	300	GLN
8	H	320	GLN
8	H	332	GLN
8	H	353	GLN
8	H	418	ASN
9	I	139	GLN
9	I	193	GLN
9	I	200	ASN

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Mol	Chain	Res	Type
9	I	263	ASN
9	I	317	GLN
9	I	336	HIS
9	I	346	GLN
9	I	440	GLN
10	J	180	ASN
10	J	243	GLN
10	J	244	GLN
10	J	254	ASN
10	J	281	GLN
10	J	288	GLN
10	J	313	GLN
10	J	319	HIS
10	J	381	HIS
10	J	400	HIS
10	J	446	GLN
10	J	496	GLN
11	K	139	HIS
12	L	77	HIS
12	L	78	HIS
12	L	84	ASN
12	L	86	ASN
12	L	88	GLN
12	L	121	GLN
12	L	149	ASN
13	M	109	GLN
15	O	61	GLN
15	O	99	GLN
15	O	116	HIS
15	O	120	ASN
16	P	104	GLN
16	P	132	GLN
1	a	119	GLN
1	a	187	HIS
1	a	196	GLN
1	a	231	HIS
1	a	285	ASN
1	a	301	ASN
20	c	41	GLN
20	c	73	GLN
20	c	126	ASN
20	c	145	GLN

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Mol	Chain	Res	Type
20	c	157	GLN
20	c	397	ASN
20	c	449	HIS
20	c	456	HIS
20	c	464	ASN
20	c	497	GLN
20	c	924	GLN
20	c	1001	ASN
20	c	1007	ASN
20	c	1095	GLN
20	c	1207	GLN
20	c	1212	GLN
21	i	287	GLN
21	i	361	ASN
21	i	473	GLN
21	i	546	ASN
21	i	584	HIS
21	i	607	GLN
13	m	140	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	S	8/27 (29%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

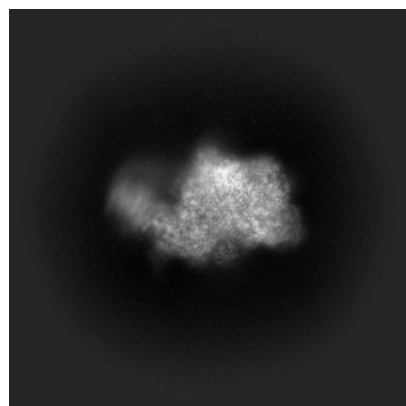
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37388. These allow visual inspection of the internal detail of the map and identification of artifacts.

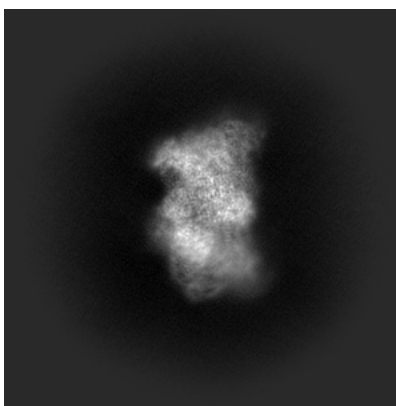
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

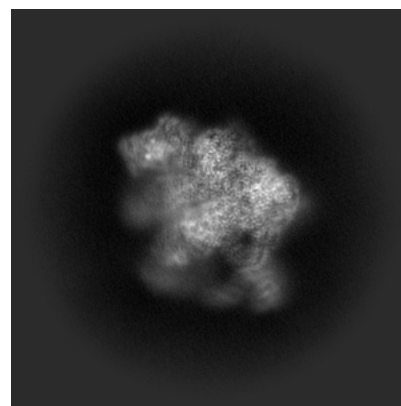
#### 6.1.1 Primary map



X

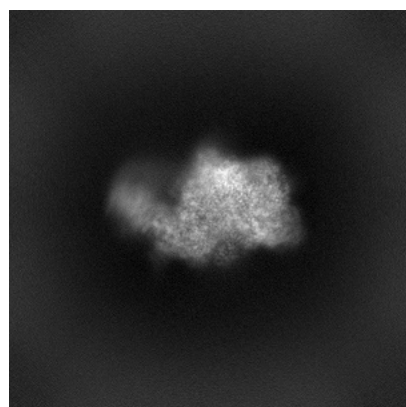


Y

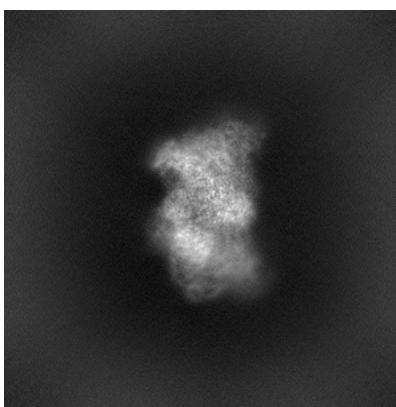


Z

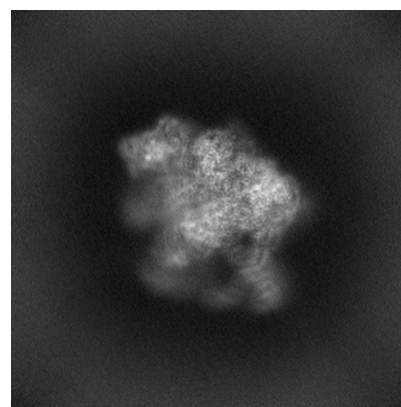
#### 6.1.2 Raw map



X



Y

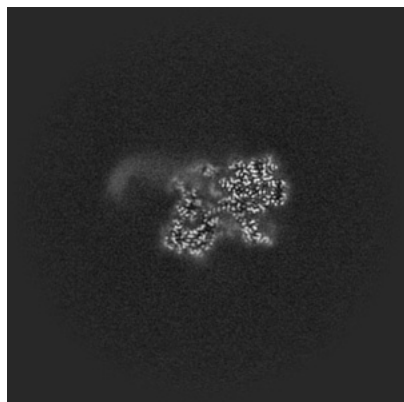


Z

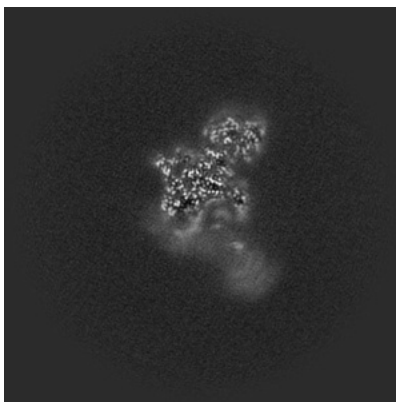
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

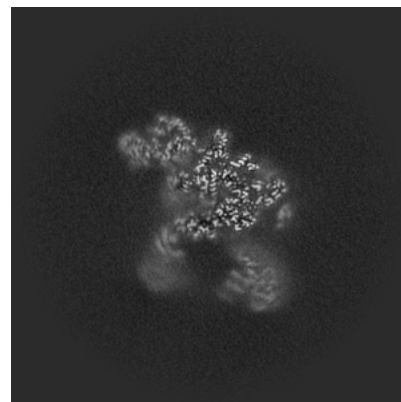
### 6.2.1 Primary map



X Index: 280

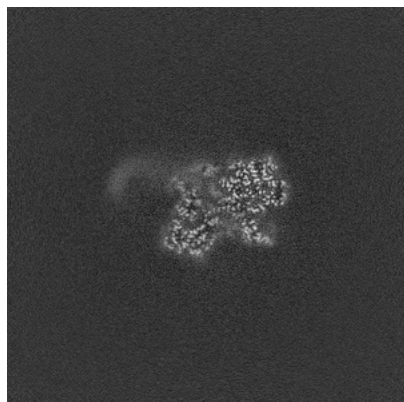


Y Index: 280

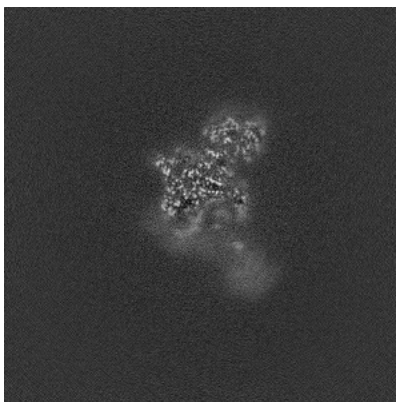


Z Index: 280

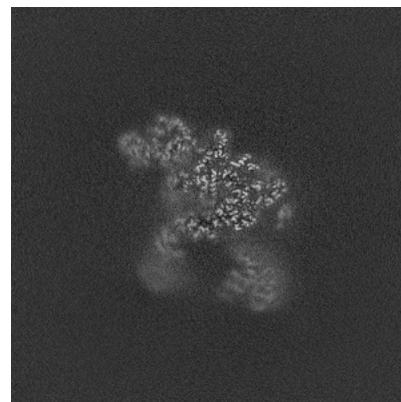
### 6.2.2 Raw map



X Index: 280



Y Index: 280

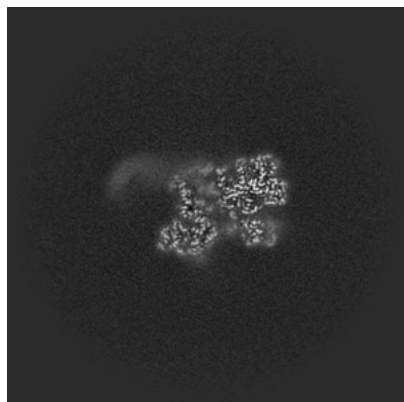


Z Index: 280

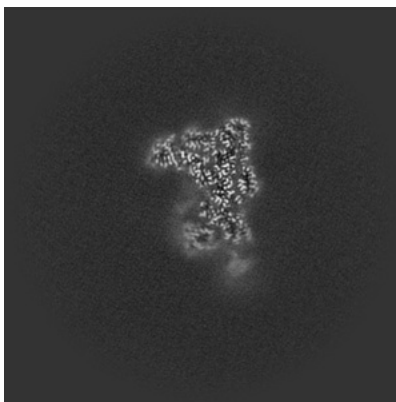
The images above show central slices of the map in three orthogonal directions.

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

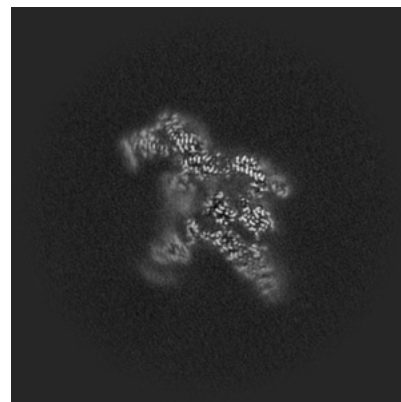
### 6.3.1 Primary map



X Index: 274

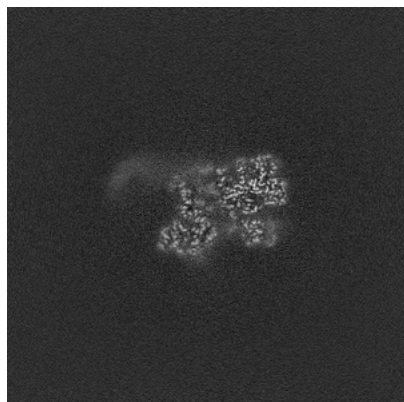


Y Index: 307

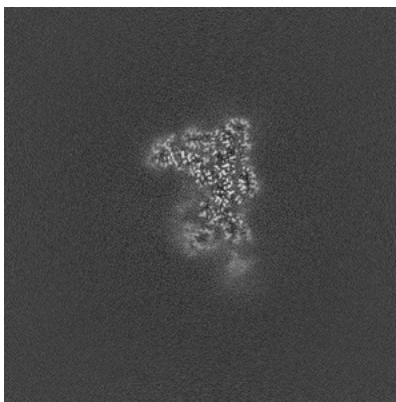


Z Index: 256

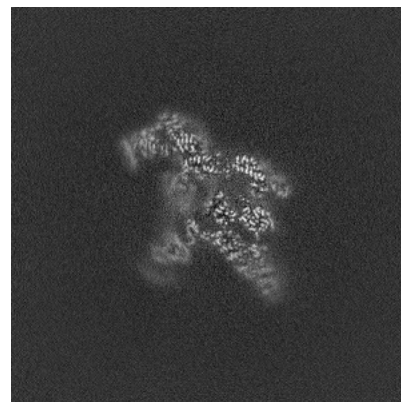
### 6.3.2 Raw map



X Index: 274



Y Index: 307



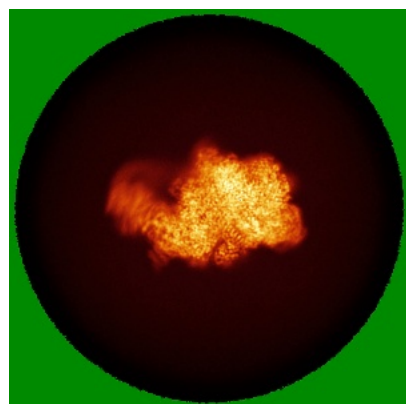
Z Index: 256

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

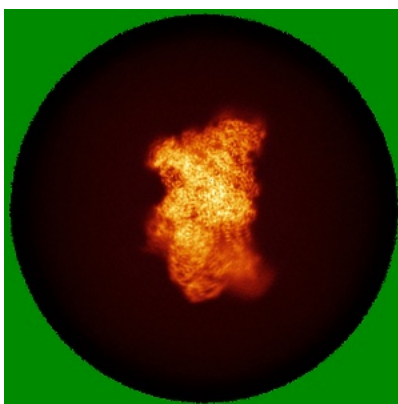


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

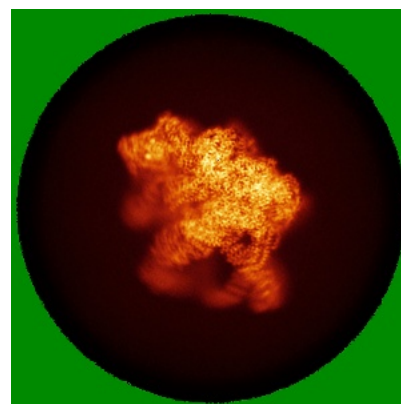
### 6.4.1 Primary map



X

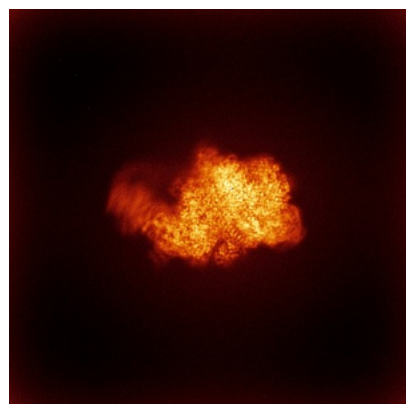


Y

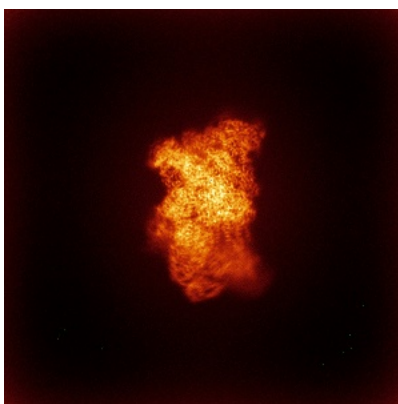


Z

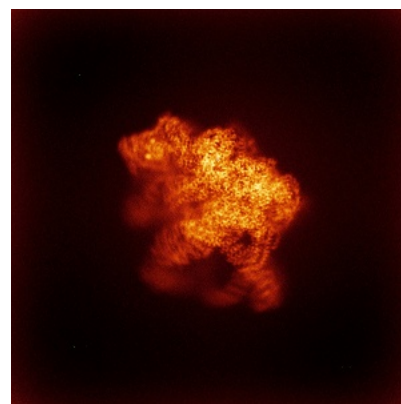
### 6.4.2 Raw map



X



Y

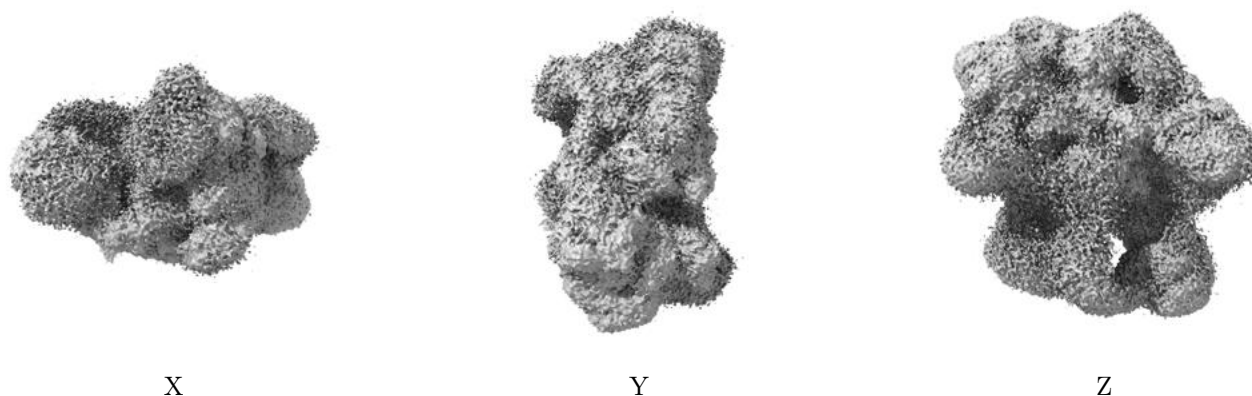


Z

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.

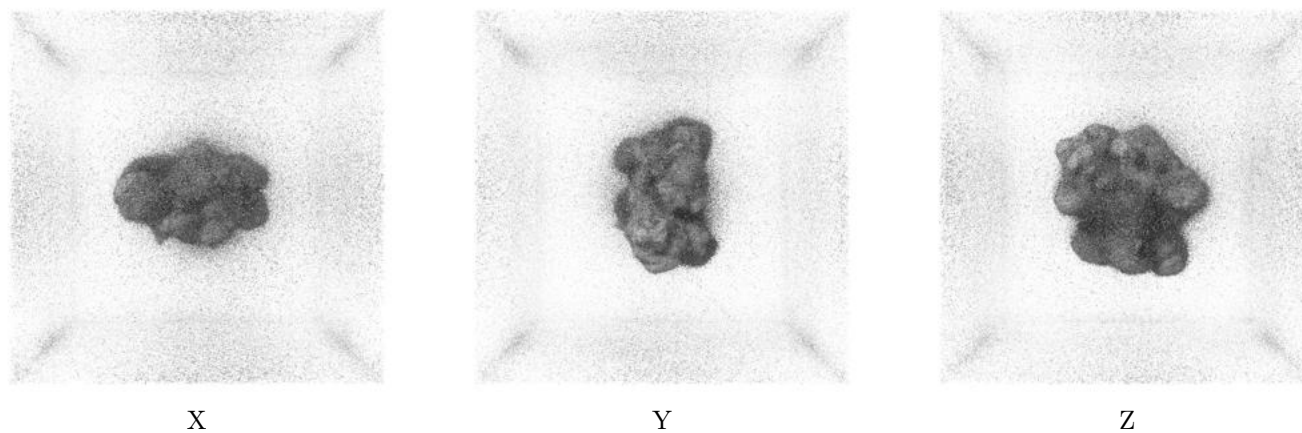
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

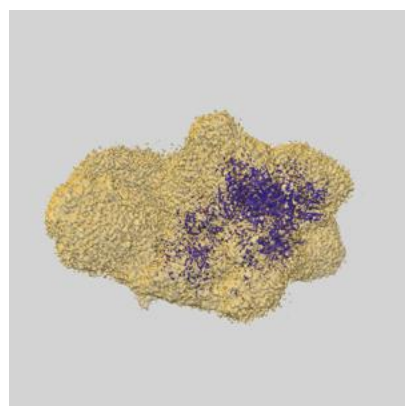
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

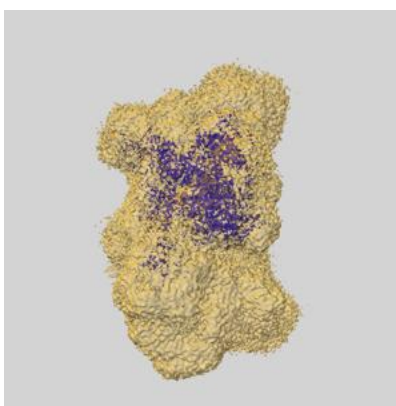
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

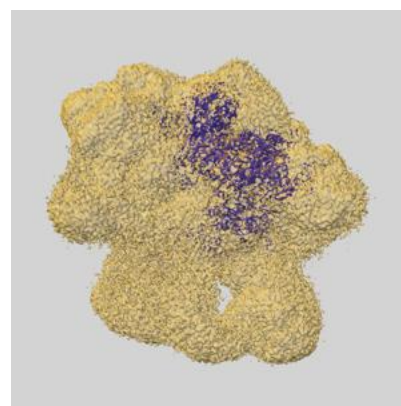
### 6.6.1 emd\_37388\_msk\_1.map [i](#)



X



Y

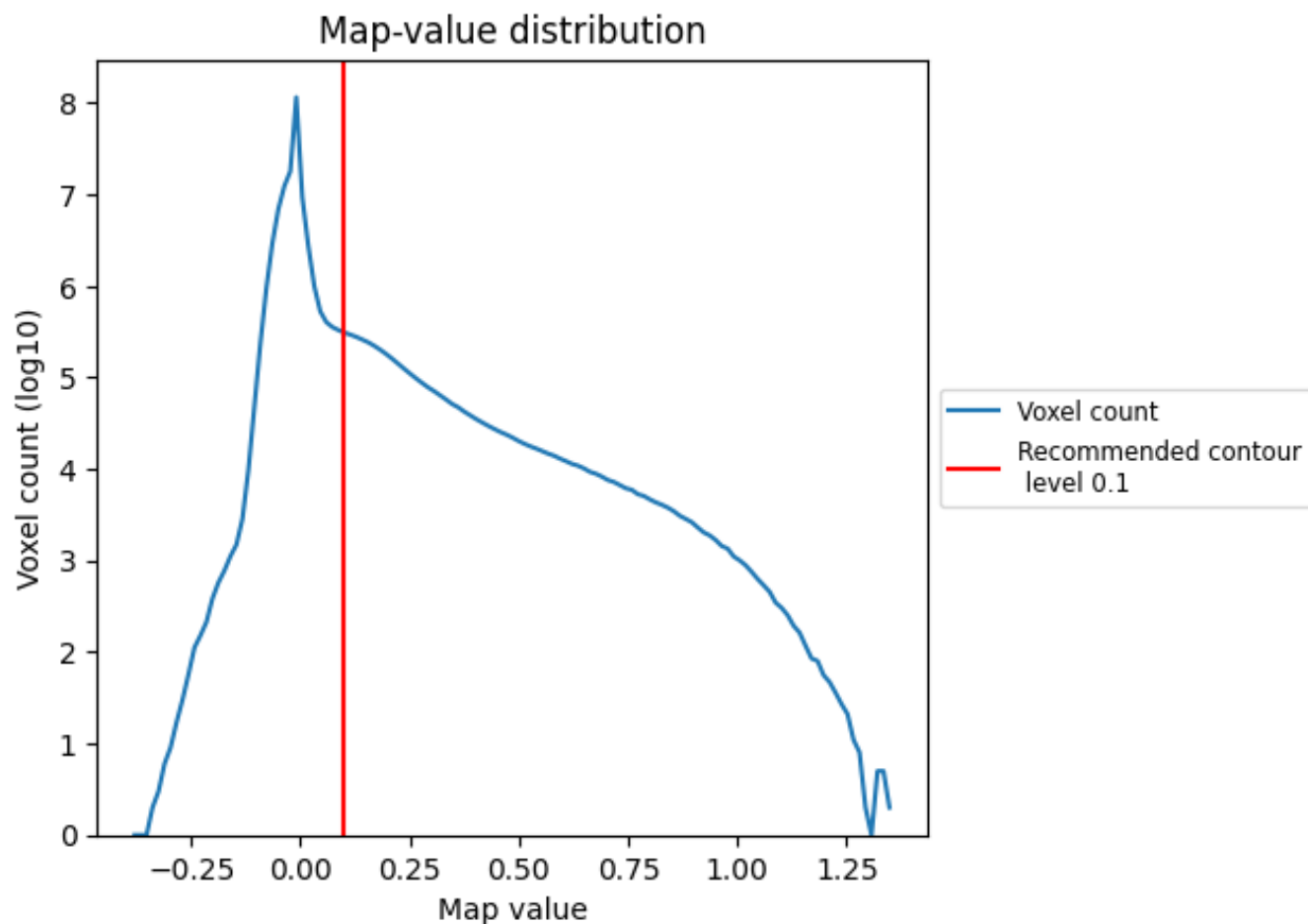


Z

## 7 Map analysis [i](#)

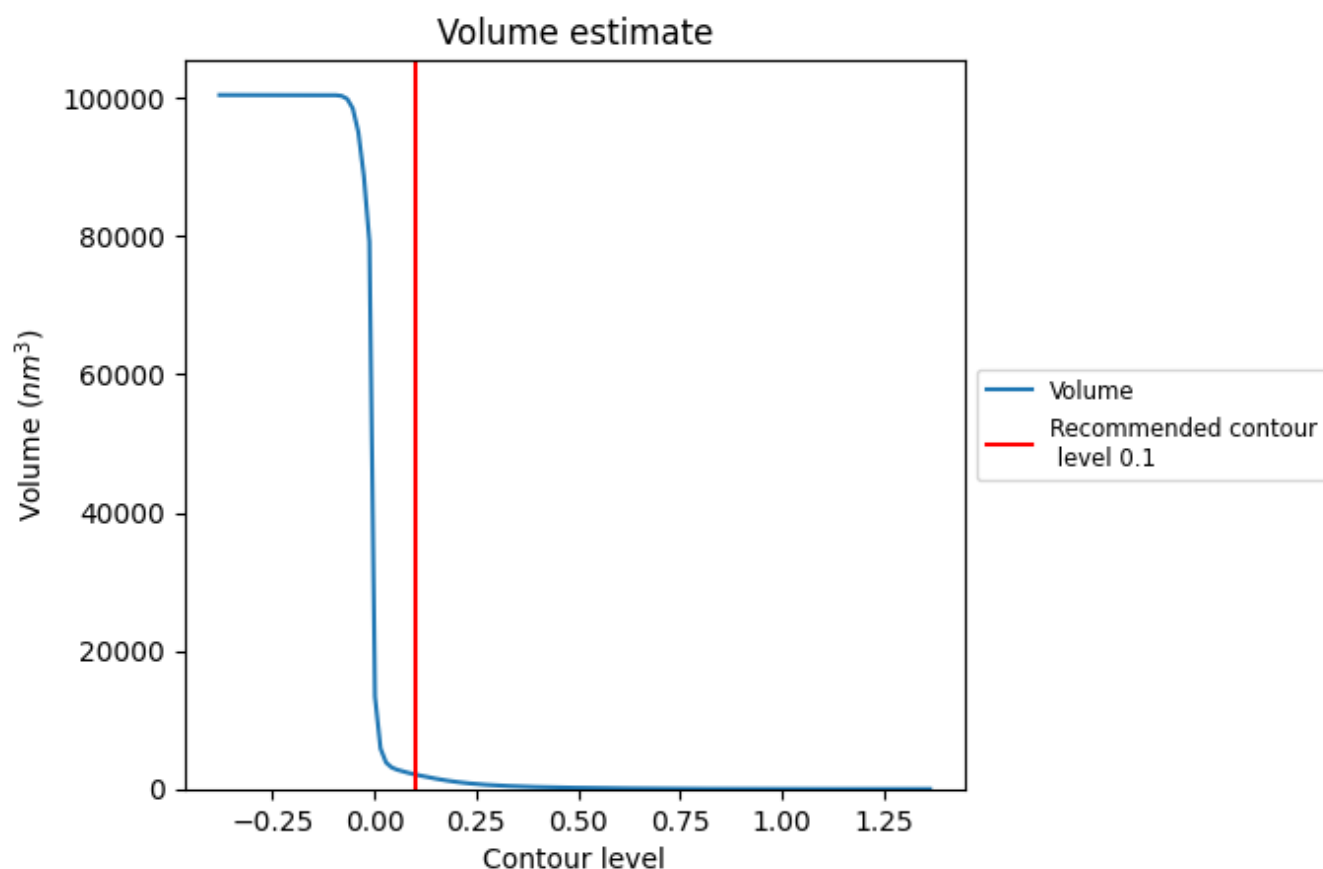
This section contains the results of statistical analysis of the map.

### 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.

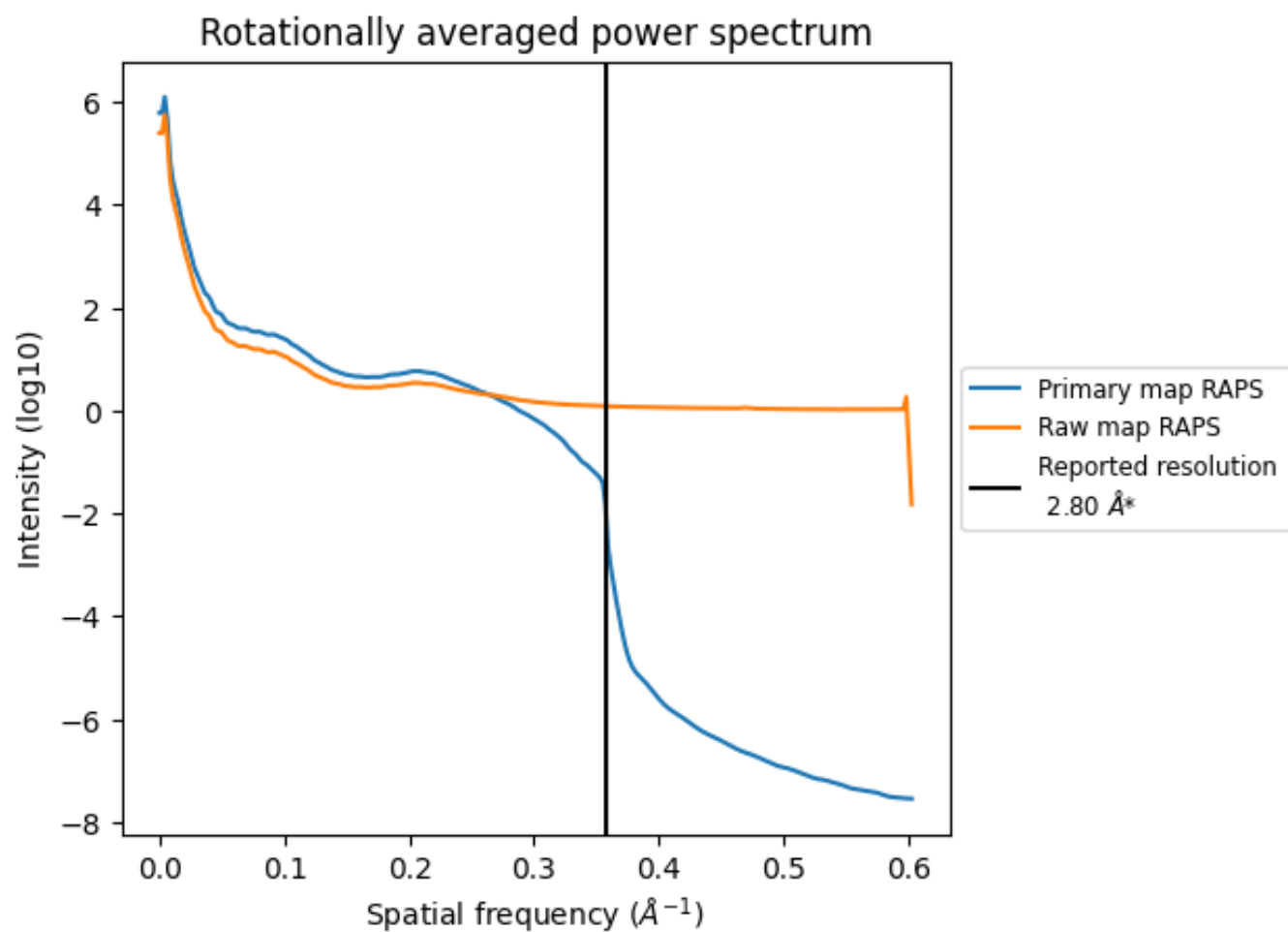
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2097 nm<sup>3</sup>; this corresponds to an approximate mass of 1894 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

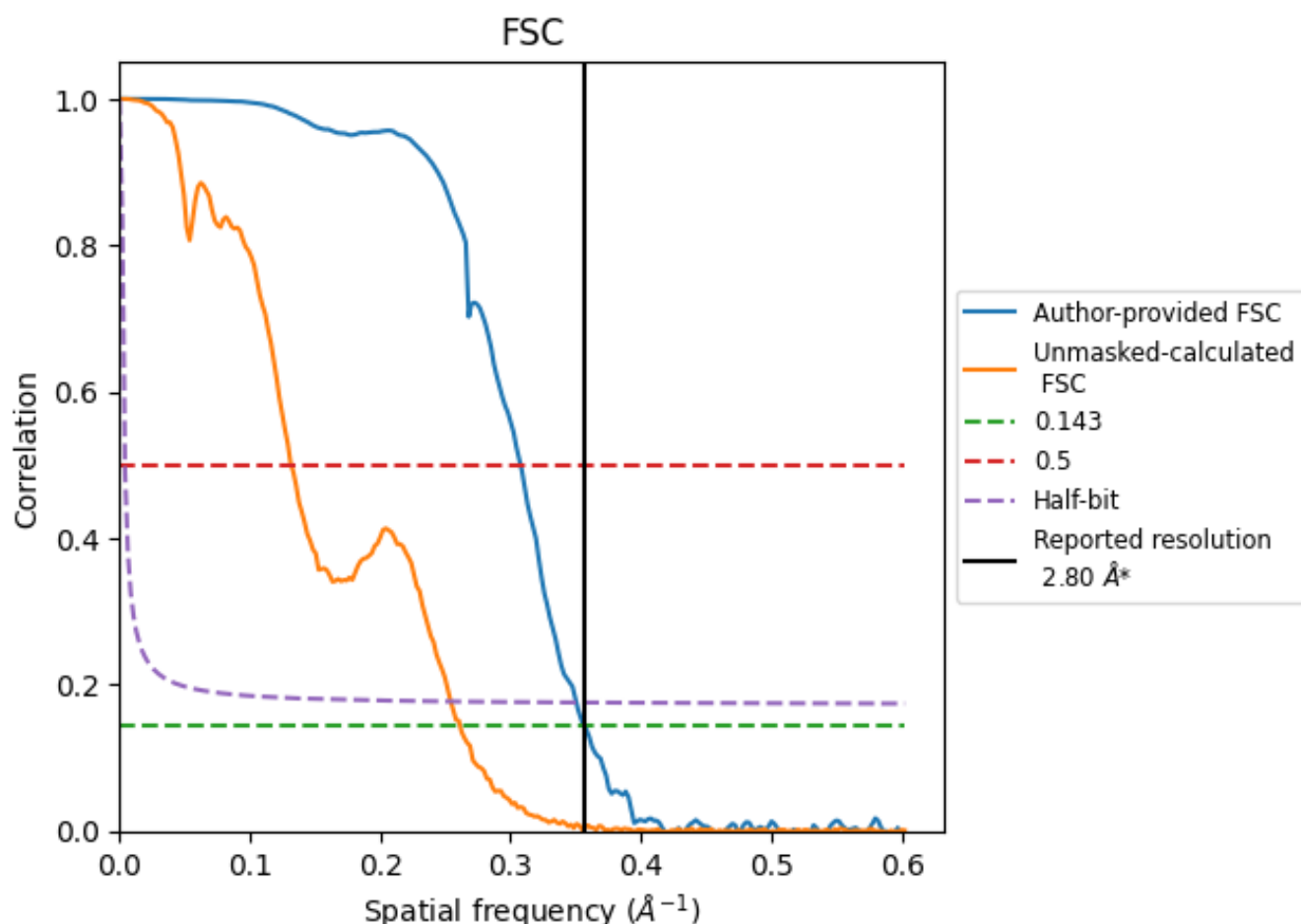


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.81	3.25	2.85
Unmasked-calculated*	3.83	7.59	3.94

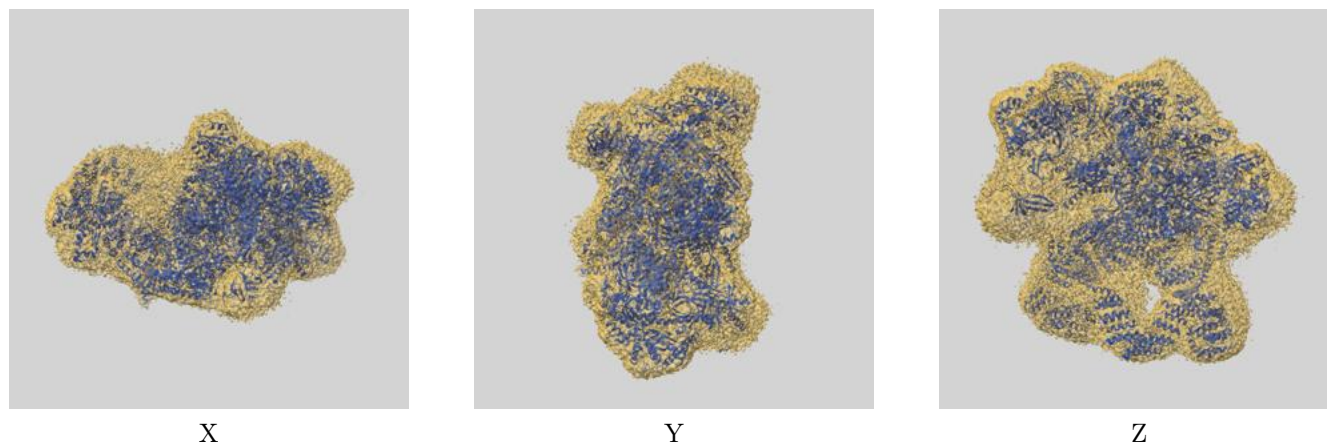
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 2.8 by more than 10 %



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

This section contains information regarding the fit between EMDB map EMD-37388 and PDB model 8WA1. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



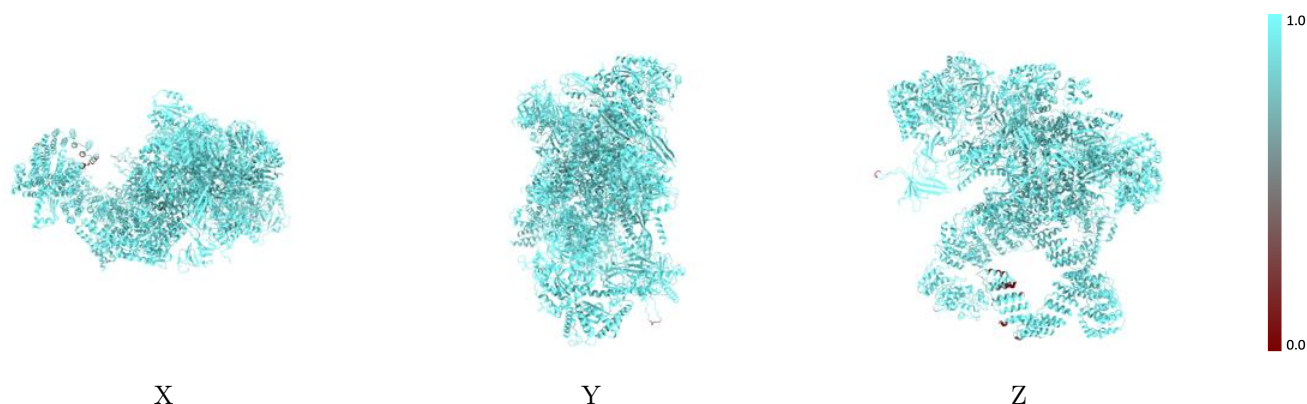
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



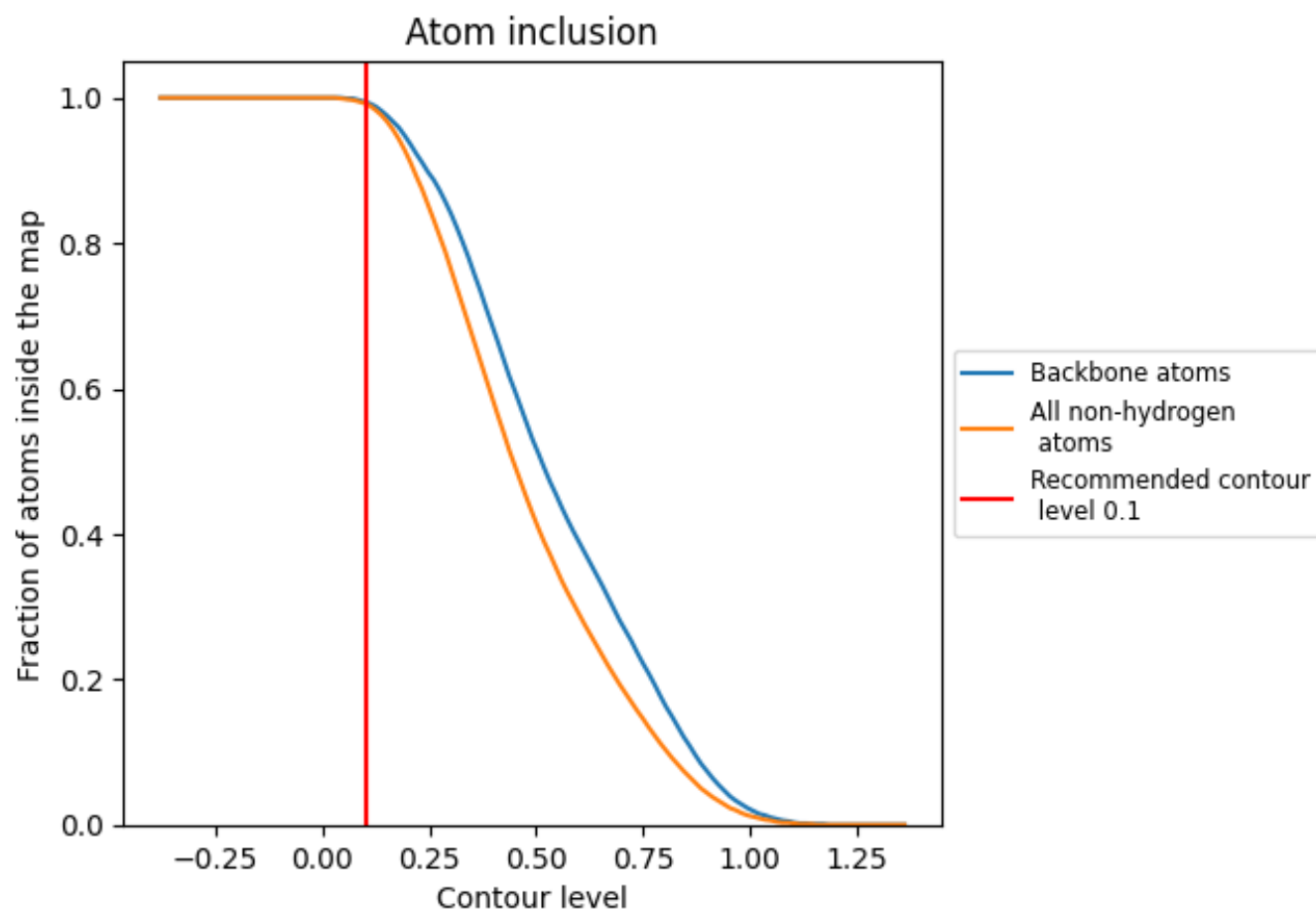
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9920	 0.4140
A	 0.9940	 0.4720
B	 0.9960	 0.4970
C	 0.9920	 0.4530
D	 0.9880	 0.3930
E	 0.9600	 0.1560
F	 0.9970	 0.3910
G	 0.9950	 0.3960
H	 0.9970	 0.5150
I	 0.9980	 0.5290
J	 0.9940	 0.4810
K	 0.9940	 0.4900
L	 0.9990	 0.2920
M	 0.9980	 0.5330
N	 0.9890	 0.1520
O	 0.9960	 0.5040
P	 0.9990	 0.3830
Q	 1.0000	 0.2810
R	 1.0000	 0.3110
S	 1.0000	 0.3220
a	 0.9970	 0.4980
c	 0.9920	 0.4130
i	 0.9970	 0.4850
m	 0.9950	 0.4610

