



Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 09:01 PM JST

PDB ID : 8WA0
EMDB ID : EMD-37387
Title : The cryo-EM structure of the Nicotiana tabacum PEP-PAP-TEC1
Authors : Wu, X.X.; Zhang, Y.
Deposited on : 2023-09-06
Resolution : 2.70 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

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>.

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

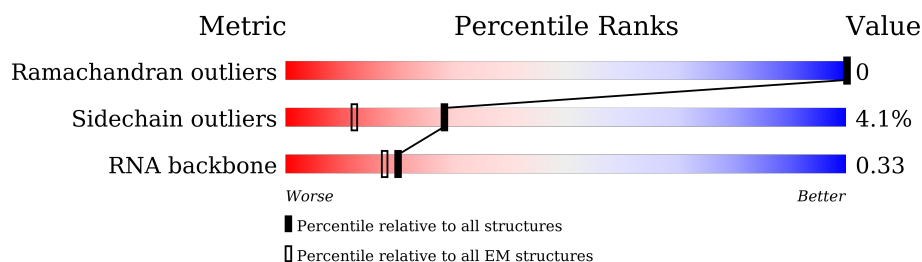
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 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 2.70 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.





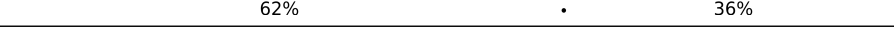
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 ≥ 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	
1	a	337	
2	B	1070	
3	C	688	
4	c	1388	
5	D	892	
6	E	860	
7	F	682	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	G	266	
9	H	531	
10	I	486	
11	i	648	
12	J	507	
13	K	331	
14	L	303	
15	M	178	
15	m	178	
16	N	770	
17	O	151	
18	P	143	
19	R	48	
20	S	20	

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 61128 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
			2164	1368	377	409	10		
1	a	317	Total	C	N	O	S	0	0
			2377	1515	410	442	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	973	Total	C	N	O	S	0	0
			7296	4637	1302	1334	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	661	Total	C	N	O	S	0	0
			4738	3002	860	858	18		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta”.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	c	1176	Total	C	N	O	S	0	0
			8108	5081	1492	1507	28		

- Molecule 5 is a protein called PAP1(pTAC3).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	645	Total	C	N	O	S	0	0
			4772	3012	834	904	22		

- Molecule 6 is a protein called Pentatricopeptide repeat-containing protein At1g74850, chloroplastic-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	700	Total	C	N	O	S	0	0
			4483	2784	816	862	21		

- Molecule 7 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	544	Total	C	N	O	S	0	0
			4185	2645	748	773	19		

- Molecule 8 is a protein called superoxide dismutase.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	218	Total	C	N	O	S	0	0
			1714	1113	289	308	4		

- Molecule 9 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 12-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	260	Total	C	N	O	S	0	0
			2099	1332	370	389	8		

- Molecule 10 is a protein called Fructokinase-like 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	376	Total	C	N	O	S	0	0
			2924	1873	517	522	12		

- Molecule 11 is a protein called Fructokinase-like 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	i	375	Total	C	N	O	S	0	0
			2887	1837	496	540	14		

- Molecule 12 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 14-like isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	421	Total	C	N	O	S	0	0
			3358	2144	575	617	22		

- Molecule 13 is a protein called PAP8(pTAC6).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	204	Total	C	N	O	S	0	0
			1656	1050	289	309	8		

- Molecule 14 is a protein called superoxide dismutase.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	235	Total	C	N	O	S	0	0
			1702	1086	300	312	4		

- Molecule 15 is a protein called Thioredoxin-like protein CITRX1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	116	Total	C	N	O	S	0	0
			931	594	150	180	7		
15	m	109	Total	C	N	O	S	0	0
			822	523	133	159	7		

- Molecule 16 is a protein called UDP-N-acetylmuramoyl-L-alanyl-D-glutamate--2, 6-diaminopimelate ligase-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	537	Total	C	N	O	S	0	0
			2987	1818	579	584	6		

- Molecule 17 is a protein called Protein PLASTID TRANSCRIPTIONALLY ACTIVE 7-like isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	97	Total	C	N	O	S	0	0
			763	482	136	142	3		

- Molecule 18 is a protein called PAP13(pTAC18).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	102	Total	C	N	O	S	0	0
			761	489	133	137	2		

- Molecule 19 is a DNA chain called DNA (48-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	10	Total	C	N	O	P	0	0
			199	96	30	63	10		

- Molecule 20 is a RNA chain called RNA (20-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	9	Total	C	N	O	P	0	0
			198	88	40	61	9		

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

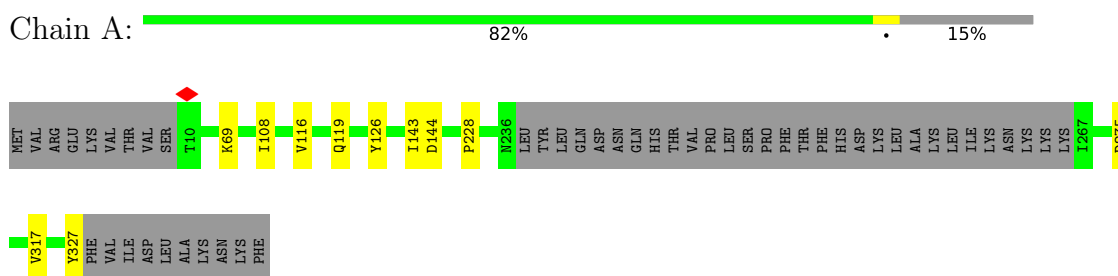
- Molecule 23 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

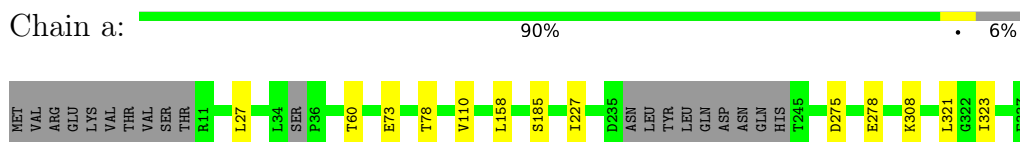
3 Residue-property plots

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.

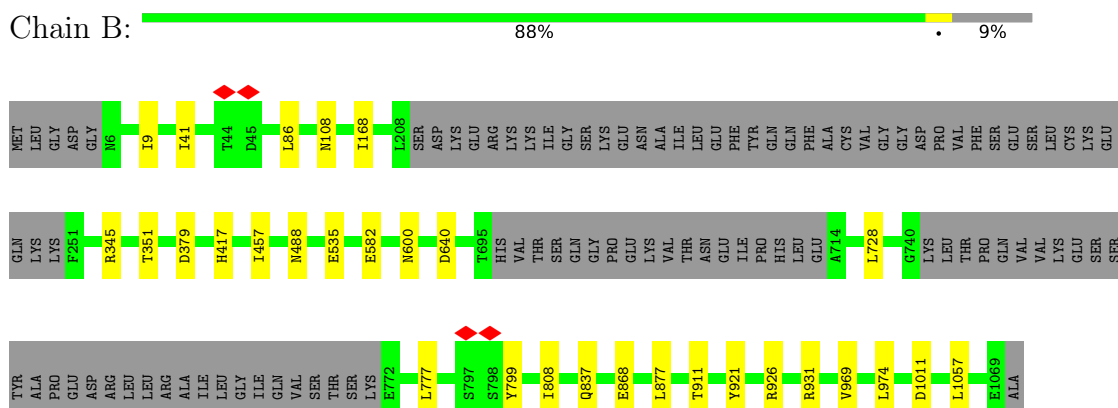
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha

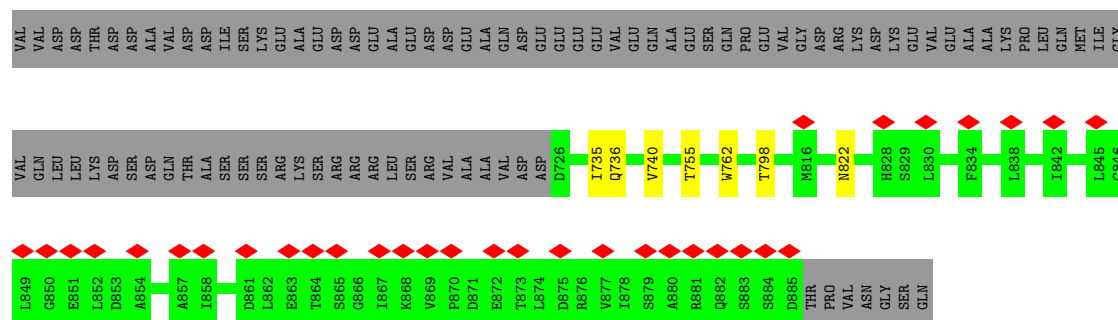


- Molecule 2: DNA-directed RNA polymerase subunit beta

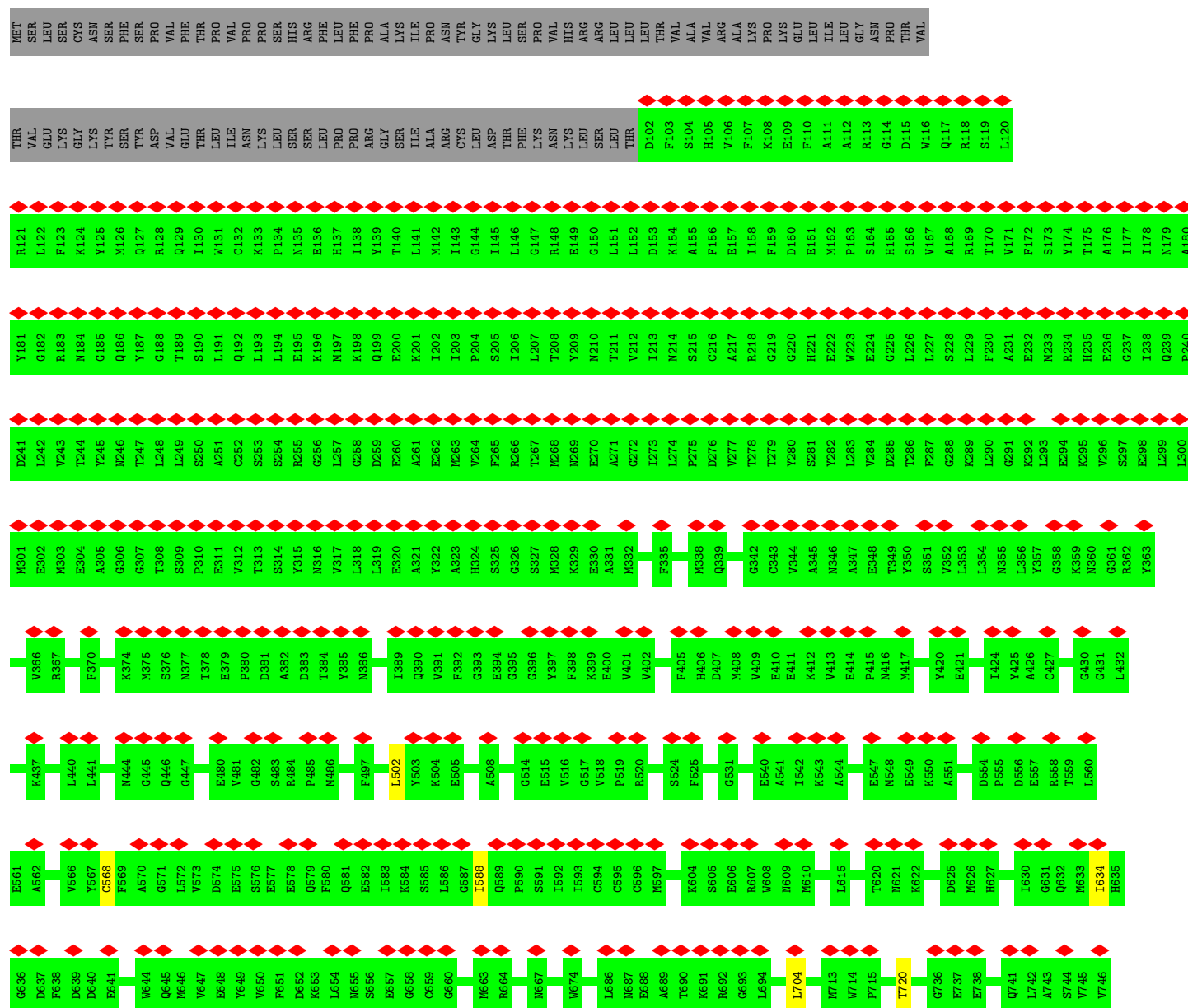
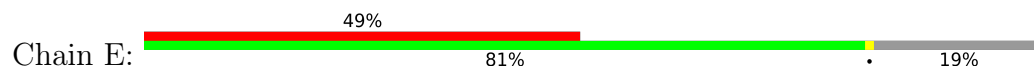


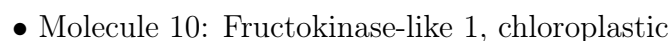
- Molecule 3: DNA-directed RNA polymerase subunit gamma





- Molecule 6: Pentatricopeptide repeat-containing protein At1g74850, chloroplastic-like





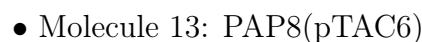
23%



42%

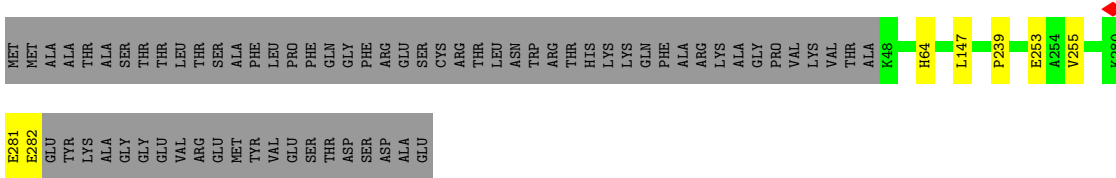
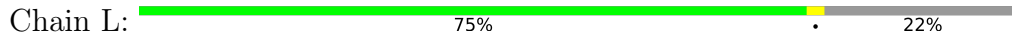


17%

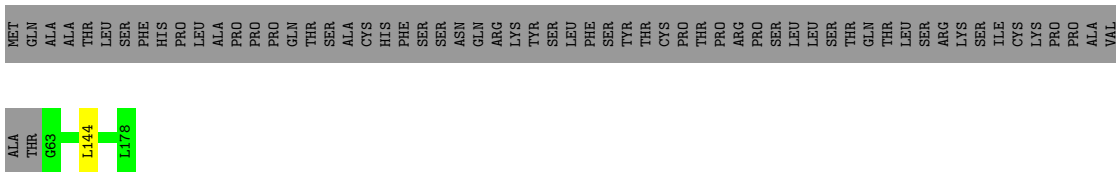


38%

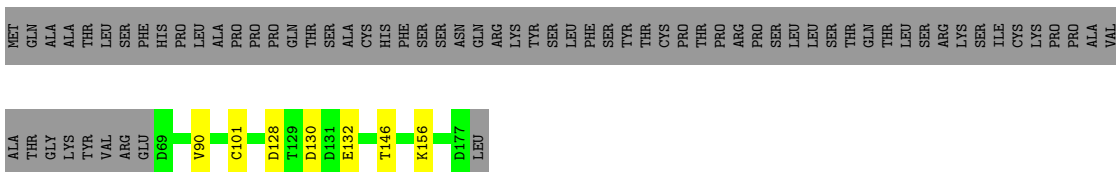
- Molecule 14: superoxide dismutase



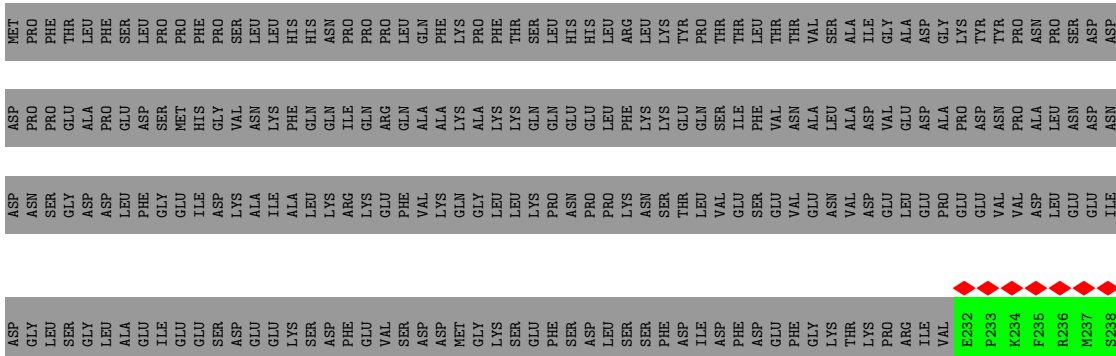
- Molecule 15: Thioredoxin-like protein CITRX1, chloroplastic

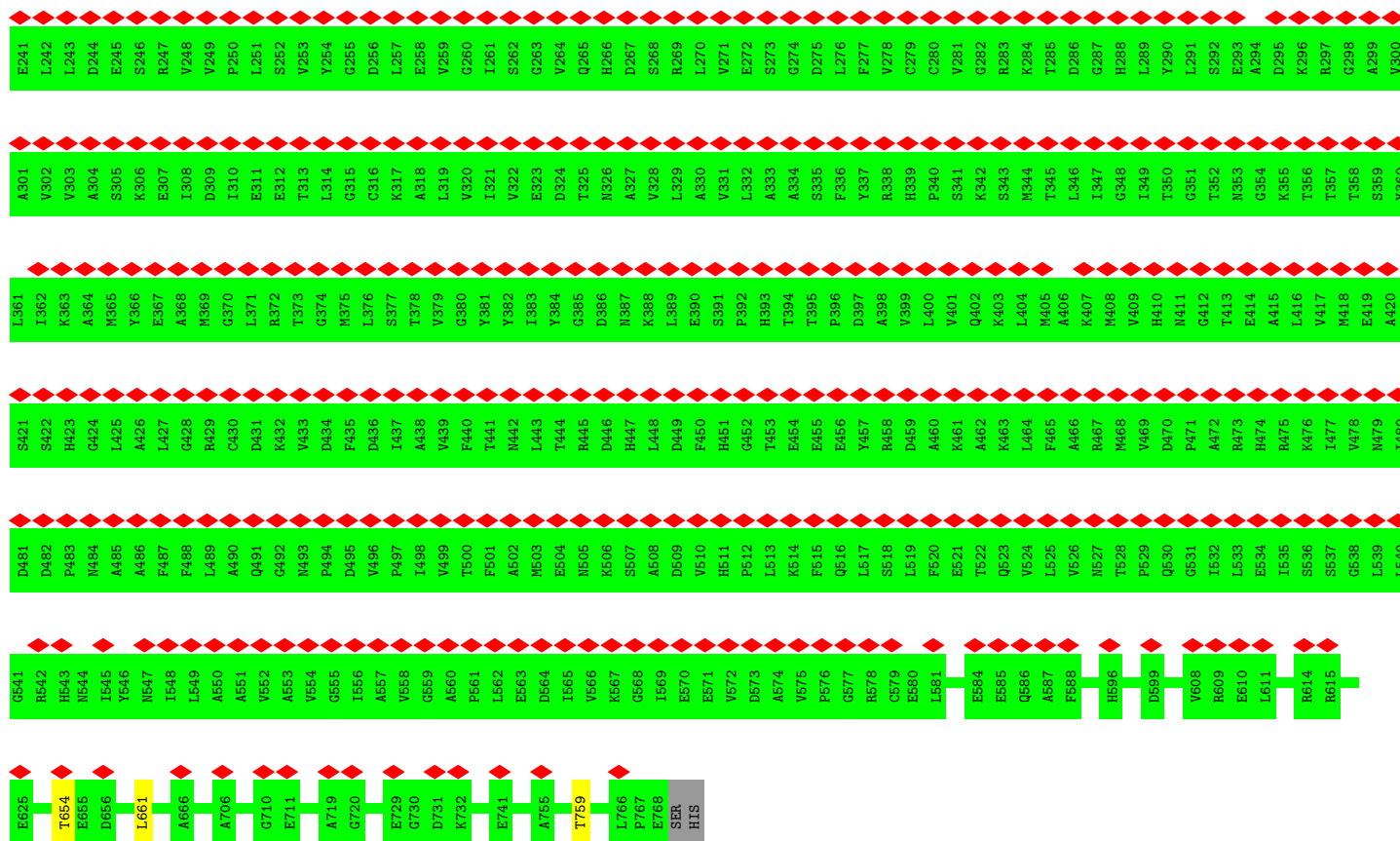


- Molecule 15: Thioredoxin-like protein CITRX1, chloroplastic



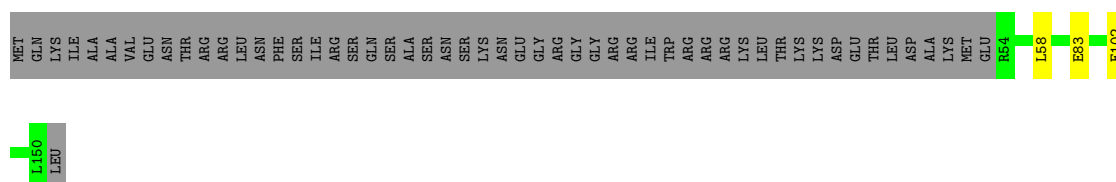
- Molecule 16: UDP-N-acetylmuramoyl-L-alanyl-D-glutamate--2, 6-diaminopimelate ligase-like





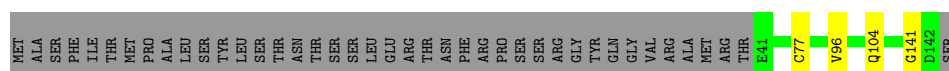
- Molecule 17: Protein PLASTID TRANSCRIPTIONALLY ACTIVE 7-like isoform X2

Chain O: 62% 36%



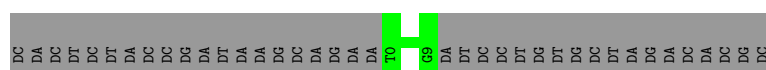
- Molecule 18: PAP13(pTAC18)

Chain P: 69% 29%



- Molecule 19: DNA (48-mer)

Chain R: 21% 79%



- Molecule 20: RNA (20-mer)

Chain S:  45% 55%

A C A A G A U U G U C C U C-9 A-1

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42911	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 ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.229	Depositor
Minimum map value	-0.440	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	444.0, 444.0, 444.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.74, 0.74, 0.74	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	0.65	0/2199	0.76	1/2982 (0.0%)
1	a	0.73	0/2422	0.81	0/3290
2	B	0.75	0/7436	0.79	5/10090 (0.0%)
3	C	0.65	0/4830	0.79	1/6586 (0.0%)
4	c	0.76	0/8235	0.78	1/11232 (0.0%)
5	D	0.73	0/4865	0.74	1/6613 (0.0%)
6	E	0.41	0/4549	0.54	0/6214
7	F	0.74	0/4291	0.73	0/5825
8	G	0.78	0/1765	0.79	0/2405
9	H	0.92	0/2156	0.83	0/2928
10	I	0.85	0/2999	0.84	4/4063 (0.1%)
11	i	0.77	0/2958	0.82	0/4013
12	J	0.80	0/3445	0.82	2/4673 (0.0%)
13	K	0.85	0/1698	0.83	0/2298
14	L	0.50	0/1749	0.71	0/2391
15	M	0.86	0/947	0.88	1/1280 (0.1%)
15	m	0.66	0/834	0.78	0/1134
16	N	0.24	0/3016	0.41	0/4170
17	O	0.91	0/776	0.78	0/1046
18	P	0.59	0/784	0.78	1/1073 (0.1%)
19	R	0.31	0/220	0.67	0/336
20	S	0.30	0/222	0.68	0/345
All	All	0.72	0/62396	0.76	17/84987 (0.0%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	c	233	GLY	N-CA-C	-8.47	91.91	113.10
2	B	911	THR	N-CA-C	-7.05	91.97	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1011	ASP	N-CA-C	7.04	130.00	111.00
18	P	141	GLY	N-CA-C	-6.46	96.95	113.10
15	M	144	LEU	N-CA-C	6.28	127.95	111.00
2	B	9	ILE	N-CA-C	-6.17	94.35	111.00
10	I	115	ASN	N-CA-C	6.03	127.28	111.00
2	B	351	THR	N-CA-C	-5.62	95.83	111.00
3	C	102	VAL	N-CA-C	5.55	126.00	111.00
10	I	467	PHE	N-CA-C	-5.48	96.21	111.00
5	D	296	SER	N-CA-C	5.47	125.78	111.00
10	I	298	LEU	CA-CB-CG	5.47	127.88	115.30
12	J	157	LEU	N-CA-C	5.37	125.51	111.00
2	B	799	TYR	N-CA-C	-5.28	96.75	111.00
12	J	377	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	116	VAL	N-CA-C	-5.24	96.86	111.00
10	I	466	GLY	N-CA-C	5.22	126.15	113.10

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%)	275 (97%)	9 (3%)	0	100	100
1	a	311/337 (92%)	297 (96%)	14 (4%)	0	100	100
2	B	965/1070 (90%)	939 (97%)	26 (3%)	0	100	100
3	C	657/688 (96%)	633 (96%)	24 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	c	1162/1388 (84%)	1136 (98%)	26 (2%)	0	100	100
5	D	639/892 (72%)	625 (98%)	14 (2%)	0	100	100
6	E	698/860 (81%)	679 (97%)	19 (3%)	0	100	100
7	F	542/682 (80%)	532 (98%)	10 (2%)	0	100	100
8	G	216/266 (81%)	213 (99%)	3 (1%)	0	100	100
9	H	258/531 (49%)	253 (98%)	5 (2%)	0	100	100
10	I	374/486 (77%)	365 (98%)	9 (2%)	0	100	100
11	i	373/648 (58%)	361 (97%)	12 (3%)	0	100	100
12	J	419/507 (83%)	413 (99%)	6 (1%)	0	100	100
13	K	202/331 (61%)	198 (98%)	4 (2%)	0	100	100
14	L	233/303 (77%)	222 (95%)	11 (5%)	0	100	100
15	M	114/178 (64%)	108 (95%)	6 (5%)	0	100	100
15	m	107/178 (60%)	103 (96%)	4 (4%)	0	100	100
16	N	535/770 (70%)	521 (97%)	14 (3%)	0	100	100
17	O	95/151 (63%)	92 (97%)	3 (3%)	0	100	100
18	P	100/143 (70%)	92 (92%)	8 (8%)	0	100	100
All	All	8284/10746 (77%)	8057 (97%)	227 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	219/308 (71%)	209 (95%)	10 (5%)	23	49
1	a	240/308 (78%)	227 (95%)	13 (5%)	18	42
2	B	712/924 (77%)	687 (96%)	25 (4%)	31	60
3	C	414/612 (68%)	394 (95%)	20 (5%)	21	48
4	c	680/1238 (55%)	638 (94%)	42 (6%)	15	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	D	435/770 (56%)	422 (97%)	13 (3%)	36	65
6	E	289/741 (39%)	283 (98%)	6 (2%)	48	76
7	F	382/615 (62%)	370 (97%)	12 (3%)	35	64
8	G	167/232 (72%)	159 (95%)	8 (5%)	21	48
9	H	208/472 (44%)	200 (96%)	8 (4%)	28	56
10	I	289/437 (66%)	282 (98%)	7 (2%)	44	73
11	i	299/567 (53%)	285 (95%)	14 (5%)	22	49
12	J	350/449 (78%)	336 (96%)	14 (4%)	27	55
13	K	177/300 (59%)	172 (97%)	5 (3%)	38	68
14	L	142/258 (55%)	135 (95%)	7 (5%)	21	47
15	M	101/160 (63%)	101 (100%)	0	100	100
15	m	85/160 (53%)	78 (92%)	7 (8%)	9	23
16	N	97/659 (15%)	94 (97%)	3 (3%)	35	64
17	O	75/130 (58%)	72 (96%)	3 (4%)	27	55
18	P	61/129 (47%)	58 (95%)	3 (5%)	21	47
All	All	5422/9469 (57%)	5202 (96%)	220 (4%)	28	54

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	108	ILE
1	A	119	GLN
1	A	126	TYR
1	A	143	ILE
1	A	144	ASP
1	A	228	PRO
1	A	275	ASP
1	A	317	VAL
1	A	327	TYR
1	a	27	LEU
1	a	60	THR
1	a	73	GLU
1	a	78	THR
1	a	110	VAL
1	a	158	LEU
1	a	185	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	227	ILE
1	a	275	ASP
1	a	278	GLU
1	a	308	LYS
1	a	321	LEU
1	a	323	ILE
2	B	41	ILE
2	B	86	LEU
2	B	108	ASN
2	B	168	ILE
2	B	345	ARG
2	B	379	ASP
2	B	417	HIS
2	B	457	ILE
2	B	488	ASN
2	B	535	GLU
2	B	582	GLU
2	B	600	ASN
2	B	640	ASP
2	B	728	LEU
2	B	777	LEU
2	B	808	ILE
2	B	837	GLN
2	B	868	GLU
2	B	877	LEU
2	B	921	TYR
2	B	926	ARG
2	B	931	ARG
2	B	969	VAL
2	B	974	LEU
2	B	1057	LEU
3	C	22	VAL
3	C	121	THR
3	C	214	ASP
3	C	218	ILE
3	C	225	GLU
3	C	227	GLU
3	C	254	ARG
3	C	272	VAL
3	C	298	ASP
3	C	340	ASP
3	C	367	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	373	ARG
3	C	496	ASP
3	C	500	ASP
3	C	521	PHE
3	C	524	MET
3	C	531	ILE
3	C	614	TRP
3	C	632	TYR
3	C	680	PHE
4	c	39	LEU
4	c	65	ILE
4	c	71	LEU
4	c	102	GLU
4	c	174	SER
4	c	201	TYR
4	c	262	THR
4	c	290	THR
4	c	291	CYS
4	c	293	SER
4	c	311	LEU
4	c	312	VAL
4	c	320	ILE
4	c	329	PRO
4	c	397	ASN
4	c	436	VAL
4	c	941	ILE
4	c	978	SER
4	c	999	THR
4	c	1006	THR
4	c	1021	ILE
4	c	1041	ARG
4	c	1042	ASN
4	c	1044	ILE
4	c	1045	LEU
4	c	1099	ILE
4	c	1105	LYS
4	c	1121	GLU
4	c	1128	THR
4	c	1129	LEU
4	c	1130	VAL
4	c	1153	LEU
4	c	1158	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	c	1159	ASP
4	c	1161	ILE
4	c	1180	LEU
4	c	1219	ARG
4	c	1232	VAL
4	c	1233	LEU
4	c	1234	VAL
4	c	1266	CYS
4	c	1293	THR
5	D	208	THR
5	D	375	CYS
5	D	442	THR
5	D	496	GLU
5	D	516	LEU
5	D	606	ASN
5	D	735	ILE
5	D	736	GLN
5	D	740	VAL
5	D	755	THR
5	D	762	TRP
5	D	798	THR
5	D	822	ASN
6	E	502	LEU
6	E	568	CYS
6	E	588	ILE
6	E	634	ILE
6	E	704	LEU
6	E	720	THR
7	F	134	ILE
7	F	159	LEU
7	F	174	PRO
7	F	176	ASP
7	F	255	PRO
7	F	257	ARG
7	F	319	ILE
7	F	367	ARG
7	F	371	THR
7	F	517	ILE
7	F	559	GLN
7	F	600	VAL
8	G	60	TYR
8	G	150	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	G	154	GLU
8	G	174	LEU
8	G	184	LEU
8	G	224	TYR
8	G	226	ASN
8	G	228	LYS
9	H	203	LEU
9	H	238	TRP
9	H	242	LYS
9	H	250	ARG
9	H	291	ARG
9	H	322	TRP
9	H	379	GLU
9	H	423	LEU
10	I	152	GLN
10	I	200	ASN
10	I	202	GLU
10	I	407	LEU
10	I	446	GLN
10	I	467	PHE
10	I	486	TRP
11	i	352	PHE
11	i	361	ASN
11	i	402	ASP
11	i	501	ASP
11	i	516	GLU
11	i	518	ILE
11	i	546	ASN
11	i	563	ASP
11	i	577	ARG
11	i	596	LEU
11	i	612	ARG
11	i	629	ASP
11	i	638	GLU
11	i	641	TYR
12	J	90	THR
12	J	134	GLU
12	J	183	THR
12	J	186	ASP
12	J	325	ARG
12	J	355	PHE
12	J	360	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	J	366	VAL
12	J	388	VAL
12	J	412	VAL
12	J	439	ARG
12	J	489	LEU
12	J	503	ASP
12	J	506	LEU
13	K	148	PHE
13	K	199	CYS
13	K	203	THR
13	K	312	ARG
13	K	330	TRP
14	L	64	HIS
14	L	147	LEU
14	L	239	PRO
14	L	253	GLU
14	L	255	VAL
14	L	281	GLU
14	L	282	GLU
15	m	90	VAL
15	m	101	CYS
15	m	128	ASP
15	m	130	ASP
15	m	132	GLU
15	m	146	THR
15	m	156	LYS
16	N	654	THR
16	N	661	LEU
16	N	759	THR
17	O	58	LEU
17	O	83	GLU
17	O	102	GLU
18	P	77	CYS
18	P	96	VAL
18	P	104	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (150) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	196	GLN
1	A	276	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	285	ASN
1	a	41	GLN
1	a	119	GLN
1	a	187	HIS
1	a	196	GLN
1	a	221	ASN
1	a	263	ASN
1	a	276	GLN
1	a	285	ASN
2	B	58	GLN
2	B	108	ASN
2	B	128	GLN
2	B	267	ASN
2	B	278	ASN
2	B	307	ASN
2	B	322	GLN
2	B	334	ASN
2	B	372	HIS
2	B	386	GLN
2	B	488	ASN
2	B	522	GLN
2	B	600	ASN
2	B	615	ASN
2	B	621	HIS
2	B	622	GLN
2	B	636	GLN
2	B	853	ASN
2	B	862	ASN
2	B	865	GLN
2	B	910	GLN
2	B	934	ASN
2	B	938	GLN
2	B	953	GLN
2	B	971	GLN
2	B	1064	GLN
3	C	135	ASN
3	C	300	ASN
3	C	331	GLN
3	C	453	GLN
3	C	471	GLN
3	C	513	GLN
3	C	523	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	525	ASN
3	C	553	ASN
3	C	591	ASN
3	C	605	ASN
3	C	666	HIS
4	c	37	HIS
4	c	41	GLN
4	c	49	GLN
4	c	73	GLN
4	c	77	GLN
4	c	90	ASN
4	c	92	HIS
4	c	145	GLN
4	c	397	ASN
4	c	449	HIS
4	c	497	GLN
4	c	924	GLN
4	c	1007	ASN
4	c	1031	ASN
4	c	1051	ASN
4	c	1095	GLN
4	c	1116	HIS
4	c	1196	GLN
4	c	1207	GLN
4	c	1212	GLN
4	c	1215	GLN
5	D	175	GLN
5	D	188	ASN
5	D	194	ASN
5	D	227	ASN
5	D	394	ASN
5	D	420	GLN
5	D	468	ASN
5	D	606	ASN
5	D	822	ASN
5	D	882	GLN
6	E	476	ASN
6	E	491	ASN
6	E	534	GLN
6	E	579	GLN
6	E	612	HIS
6	E	643	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	E	711	HIS
6	E	792	GLN
7	F	81	ASN
7	F	128	ASN
7	F	148	GLN
7	F	251	GLN
7	F	278	GLN
7	F	288	HIS
7	F	301	HIS
7	F	402	ASN
7	F	417	GLN
7	F	590	HIS
8	G	81	HIS
8	G	92	GLN
8	G	116	ASN
8	G	151	GLN
8	G	226	ASN
8	G	253	GLN
9	H	195	GLN
9	H	216	HIS
9	H	247	GLN
9	H	271	GLN
9	H	320	GLN
9	H	332	GLN
9	H	353	GLN
9	H	399	GLN
10	I	139	GLN
10	I	152	GLN
10	I	193	GLN
10	I	200	ASN
10	I	263	ASN
10	I	317	GLN
10	I	346	GLN
10	I	374	HIS
10	I	440	GLN
11	i	287	GLN
11	i	354	GLN
11	i	361	ASN
11	i	363	ASN
11	i	584	HIS
11	i	607	GLN
12	J	244	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	J	281	GLN
12	J	288	GLN
12	J	313	GLN
12	J	367	ASN
12	J	496	GLN
14	L	84	ASN
14	L	86	ASN
14	L	125	HIS
14	L	169	GLN
14	L	188	ASN
15	M	109	GLN
15	M	121	ASN
15	m	121	ASN
16	N	673	GLN
16	N	691	HIS
17	O	61	GLN
17	O	82	ASN
17	O	99	GLN
17	O	104	ASN
17	O	120	ASN
18	P	104	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	S	8/20 (40%)	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

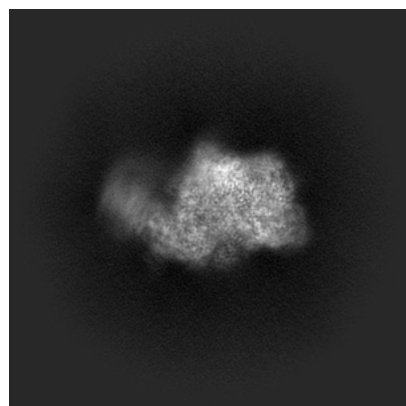
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37387. These allow visual inspection of the internal detail of the map and identification of artifacts.

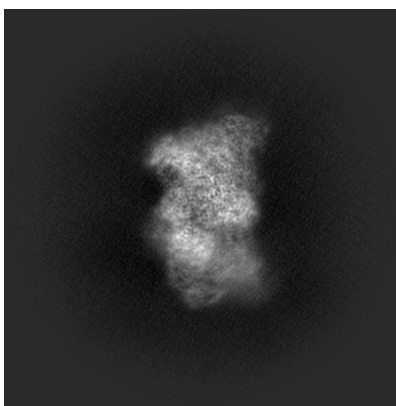
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

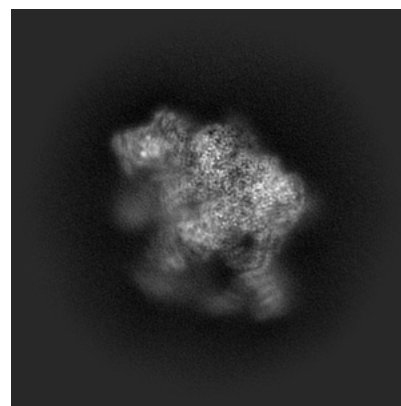
6.1.1 Primary map



X

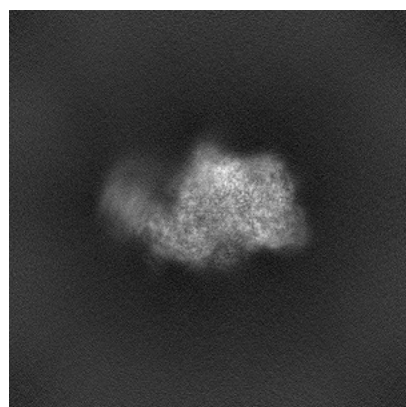


Y

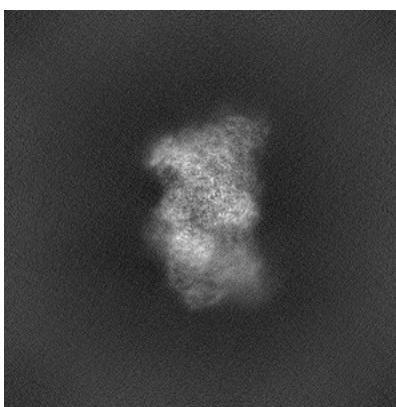


Z

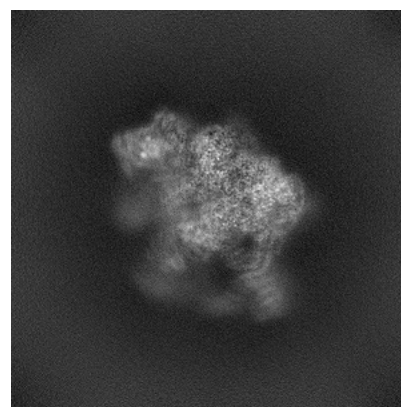
6.1.2 Raw map



X



Y

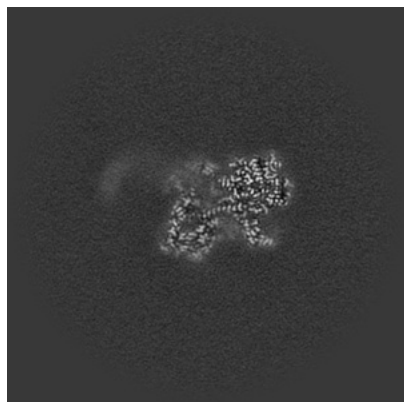


Z

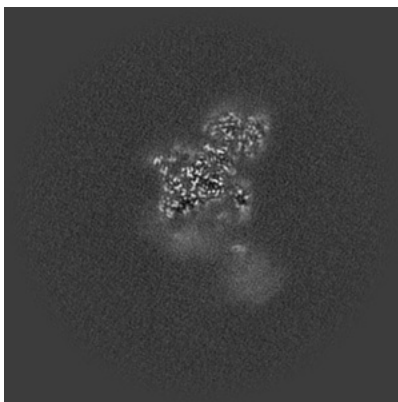
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

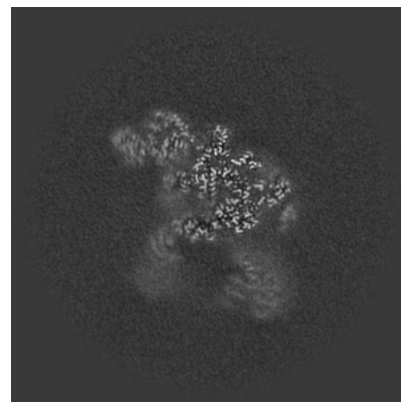
6.2.1 Primary map



X Index: 300

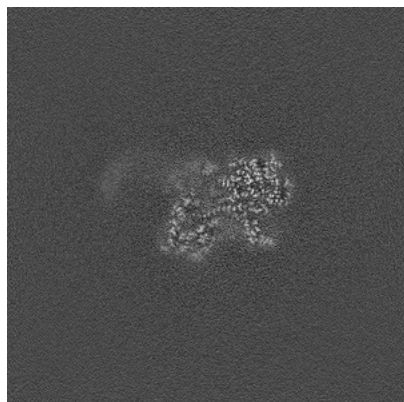


Y Index: 300

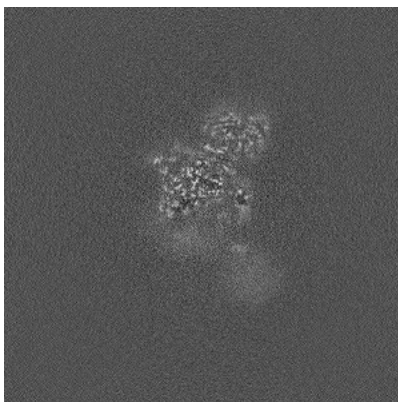


Z Index: 300

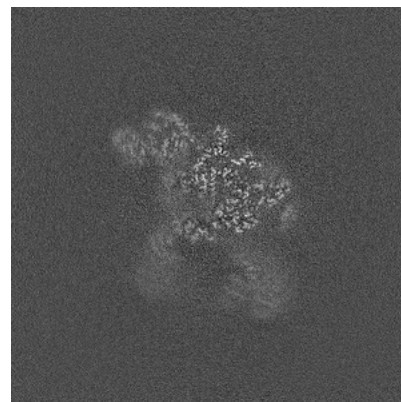
6.2.2 Raw map



X Index: 300



Y Index: 300

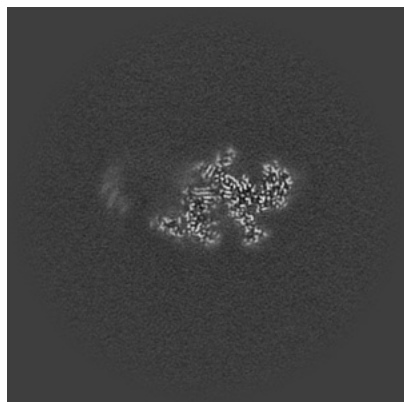


Z Index: 300

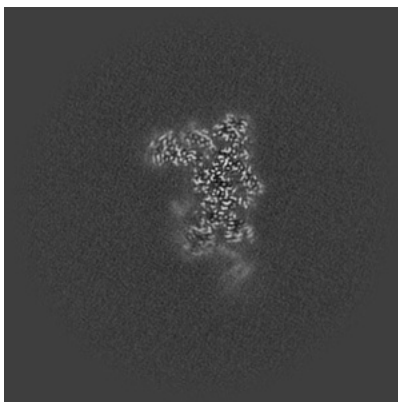
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

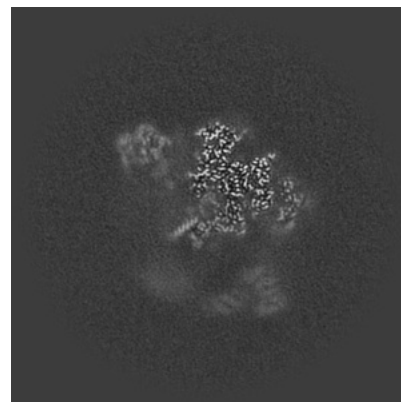
6.3.1 Primary map



X Index: 323

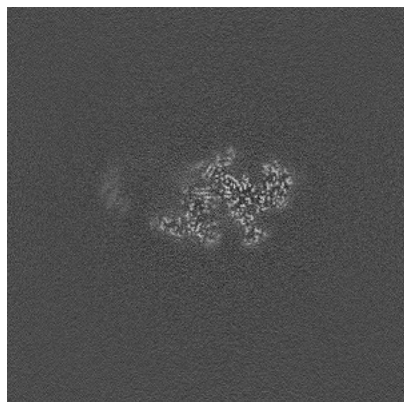


Y Index: 335

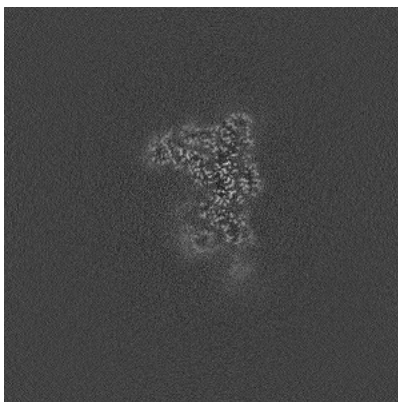


Z Index: 322

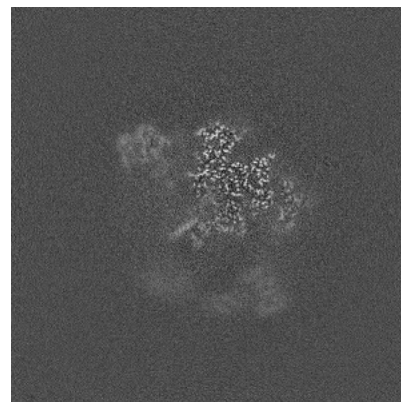
6.3.2 Raw map



X Index: 323



Y Index: 329

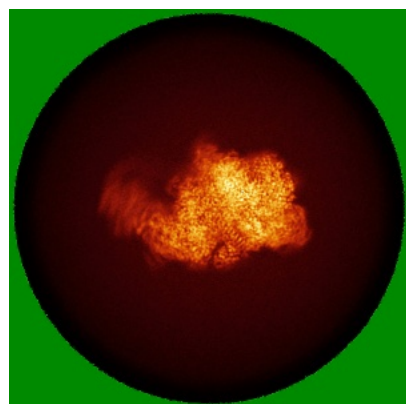


Z Index: 322

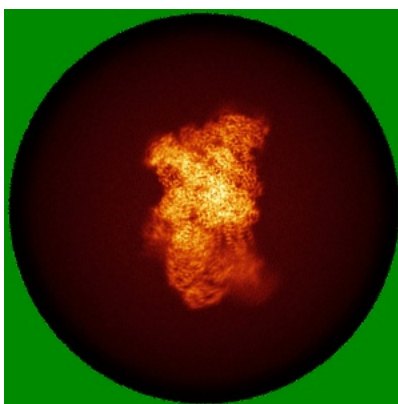
The images above show the largest variance slices of the map in three orthogonal directions.

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

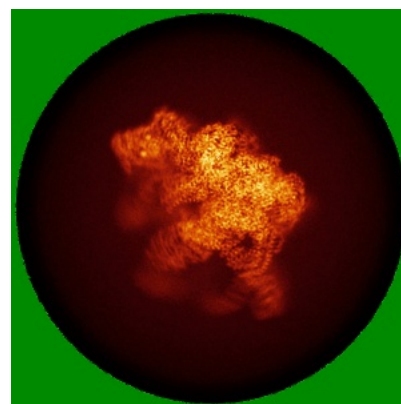
6.4.1 Primary map



X

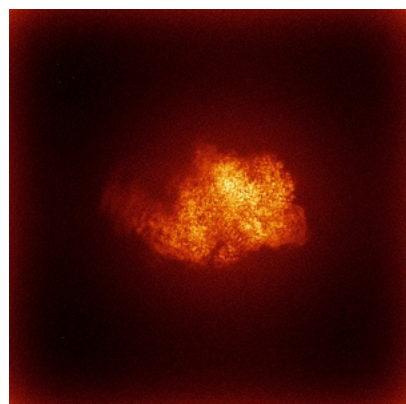


Y

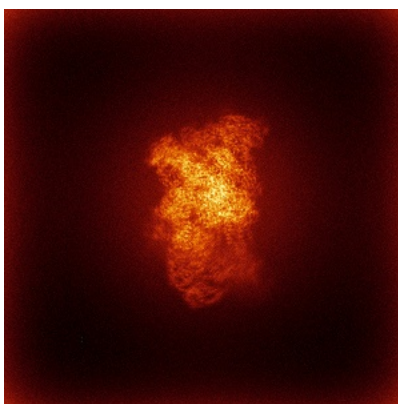


Z

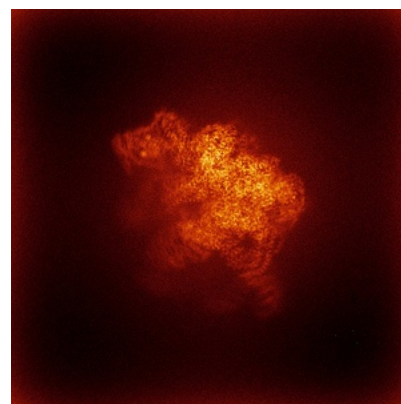
6.4.2 Raw map



X



Y

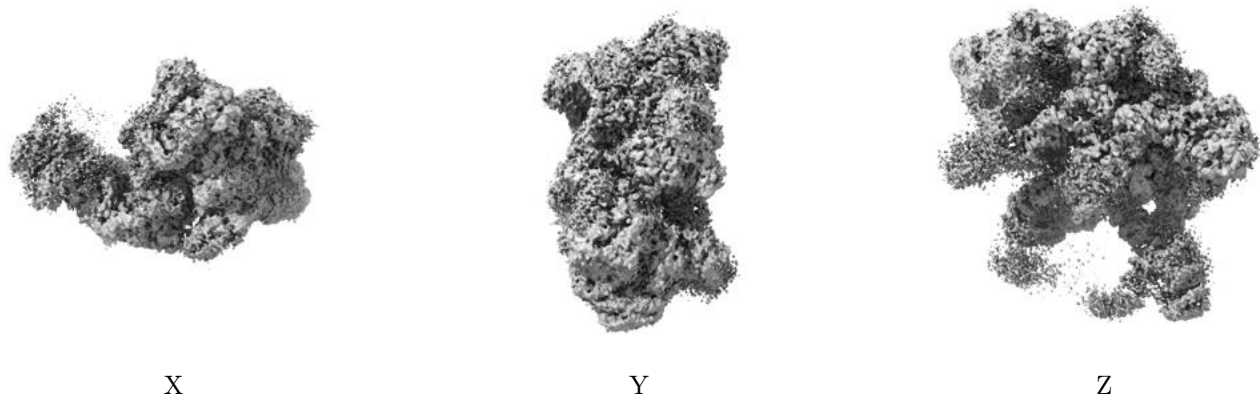


Z

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.

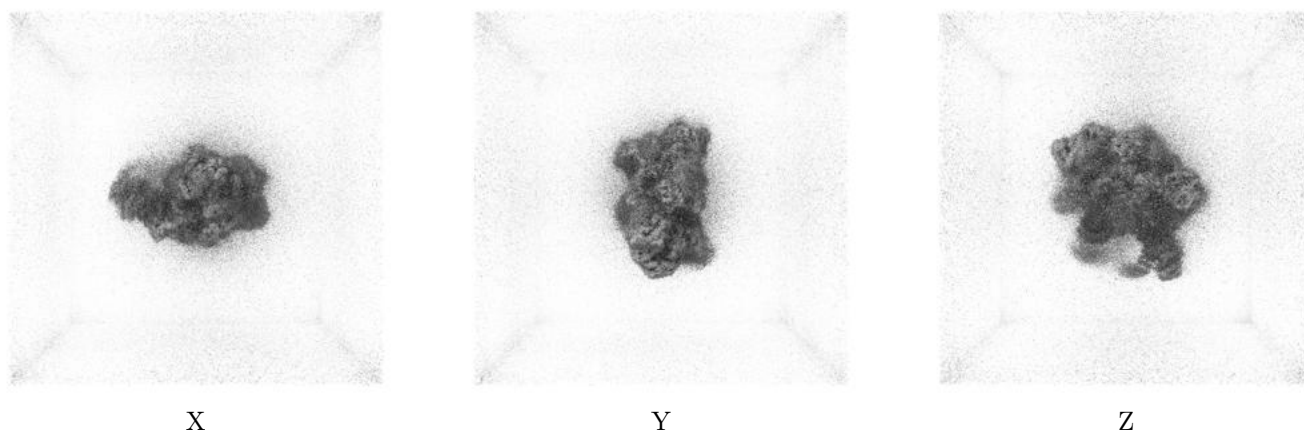
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

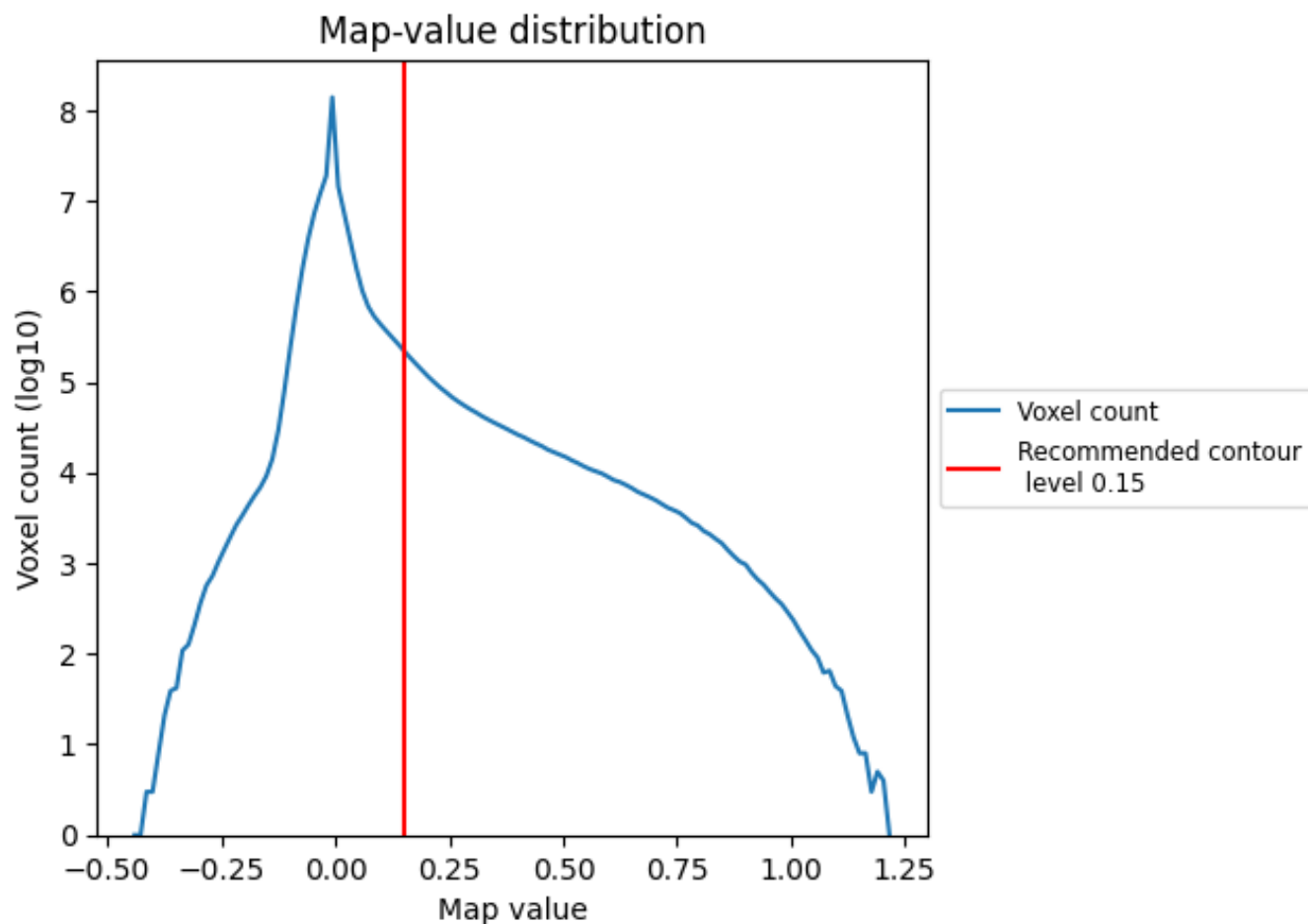
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

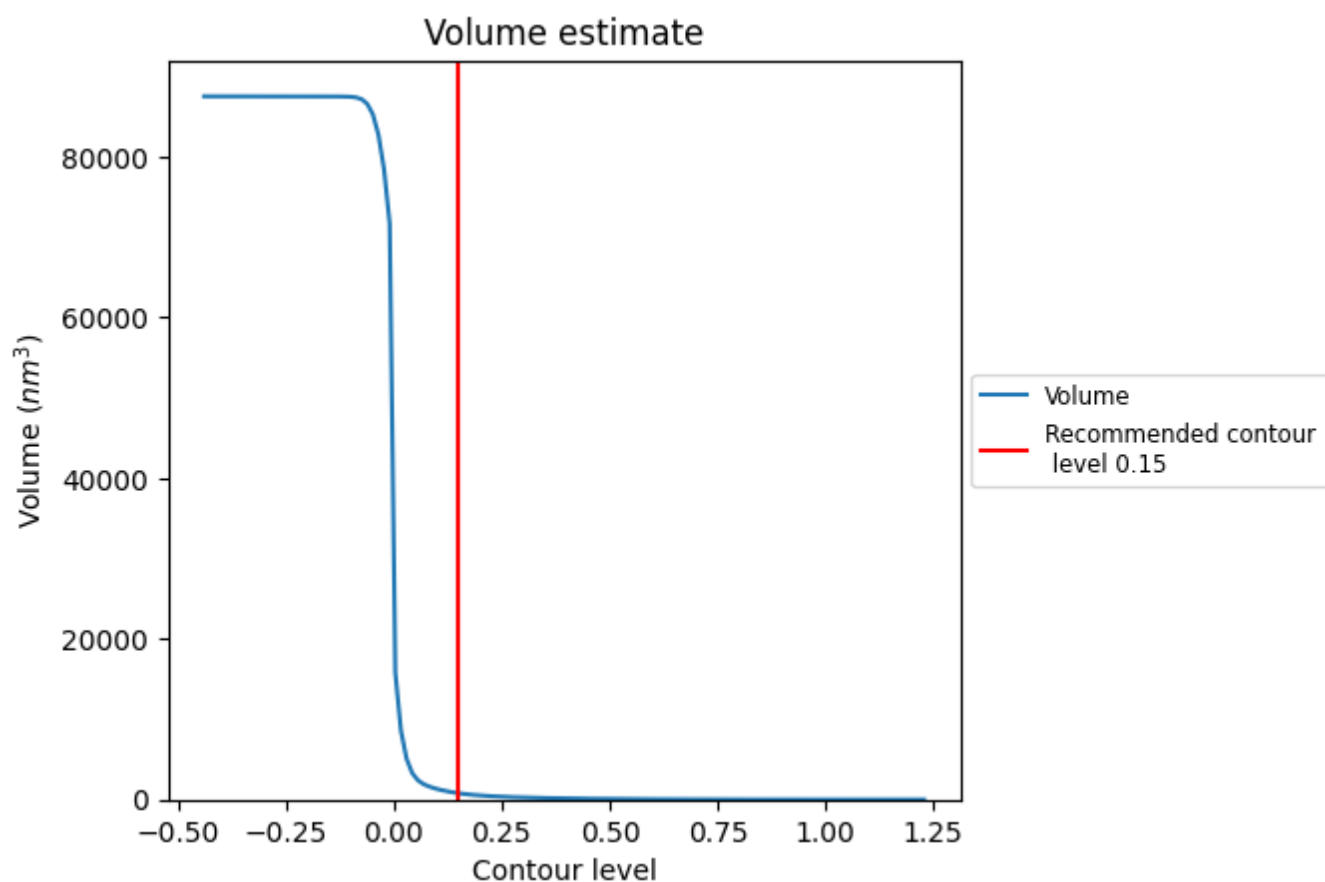
This section contains the results of statistical analysis of the map.

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.

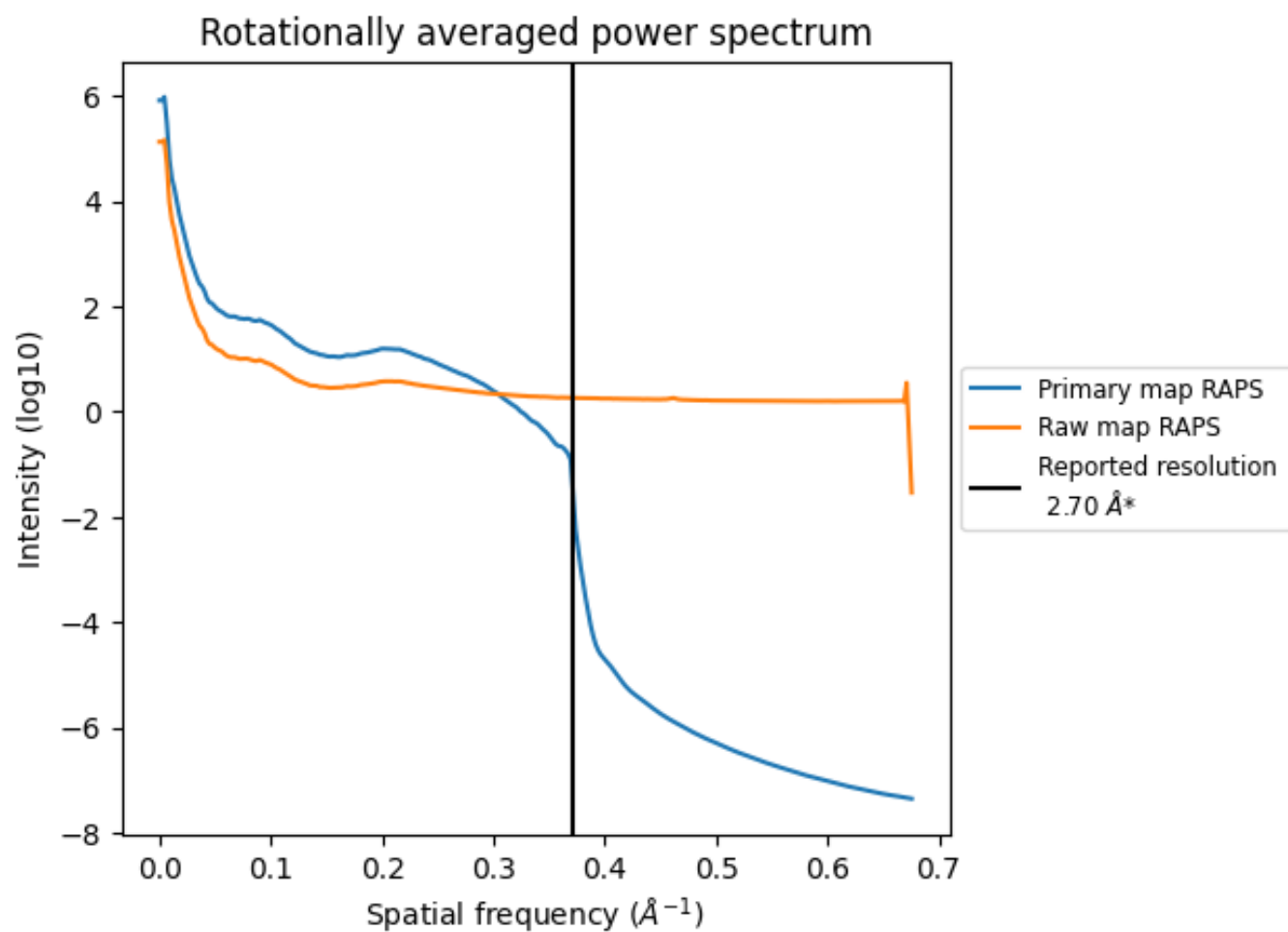
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 787 nm³; this corresponds to an approximate mass of 711 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 ⓘ

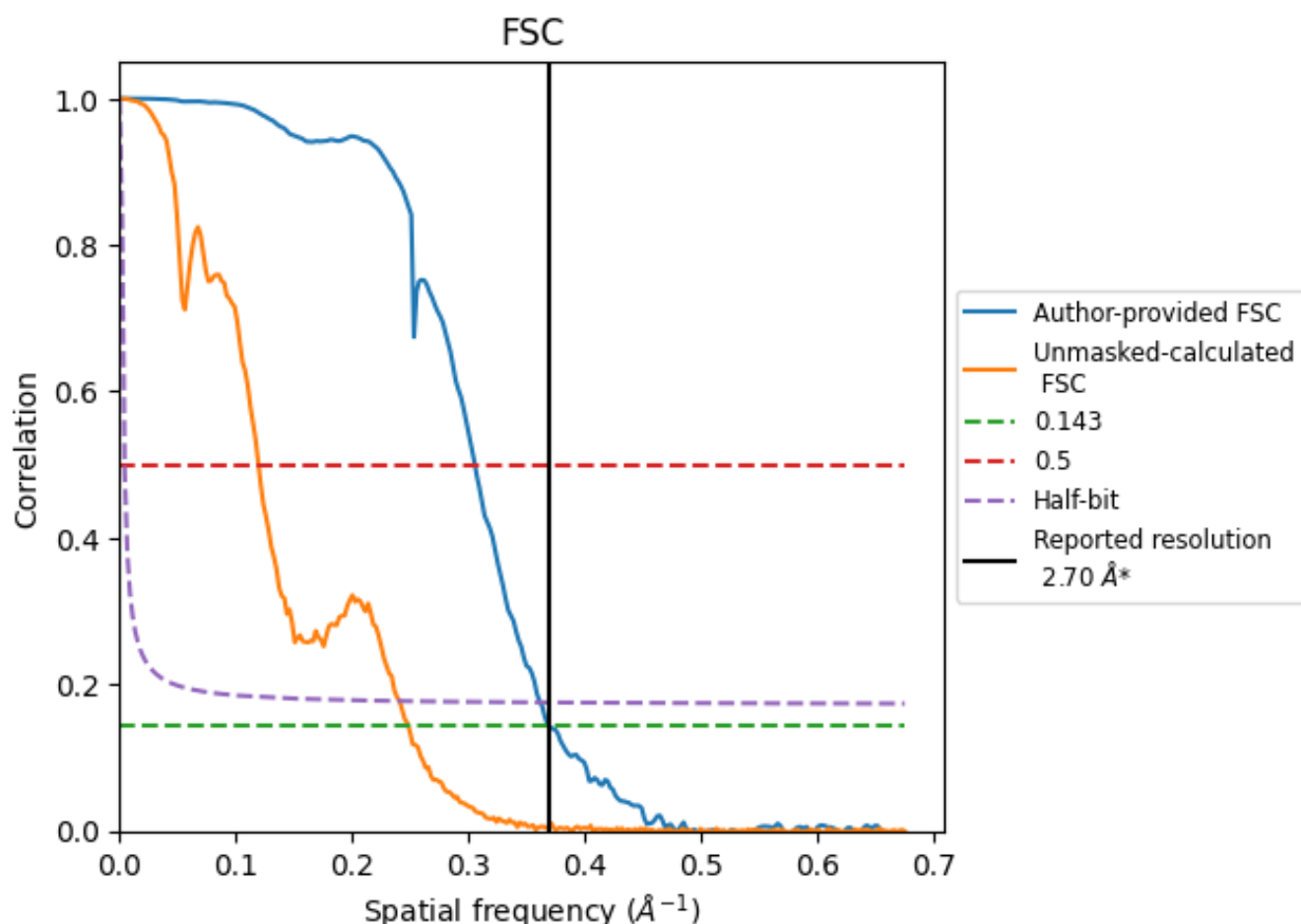


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

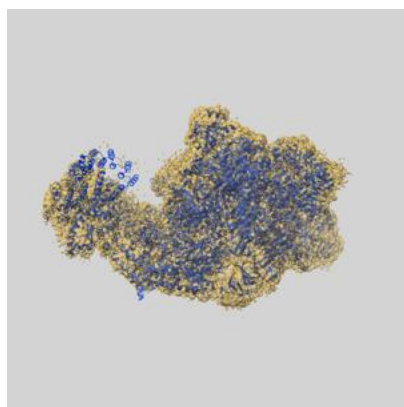
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.27	2.76
Unmasked-calculated*	4.02	8.37	4.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 2.7 by more than 10 %

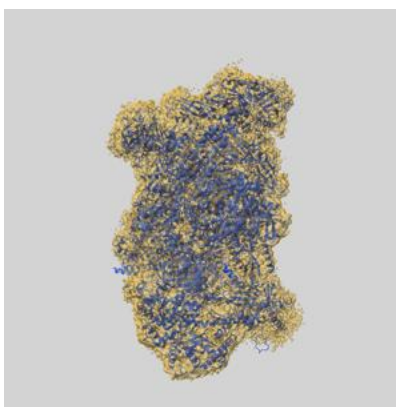
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37387 and PDB model 8WA0. Per-residue inclusion information can be found in section [3](#) on page [8](#).

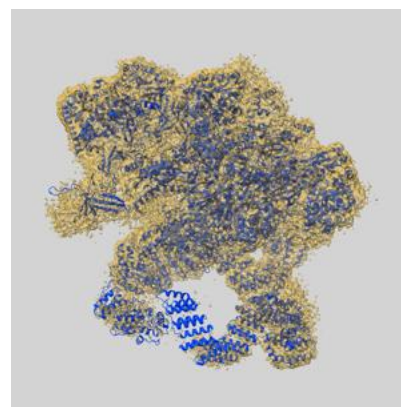
9.1 Map-model overlay [i](#)



X



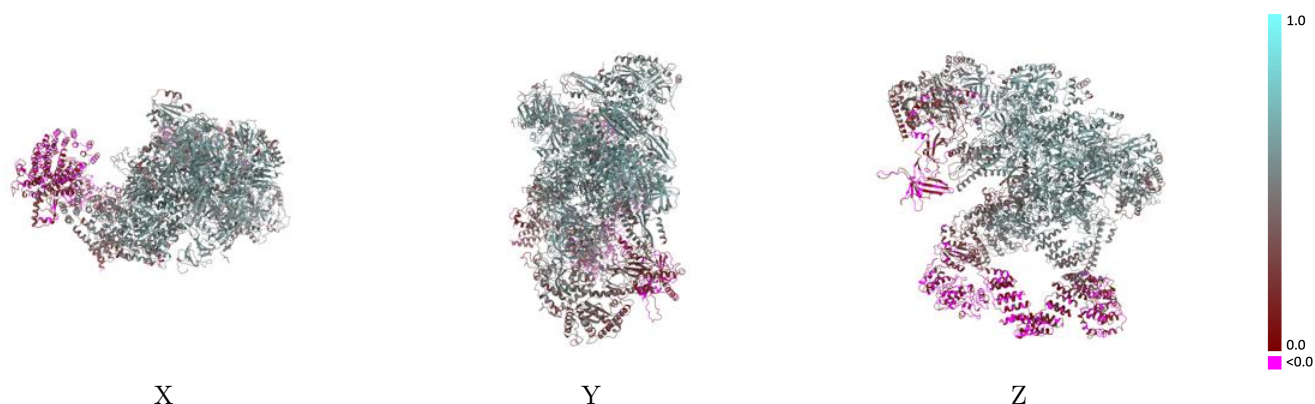
Y



Z

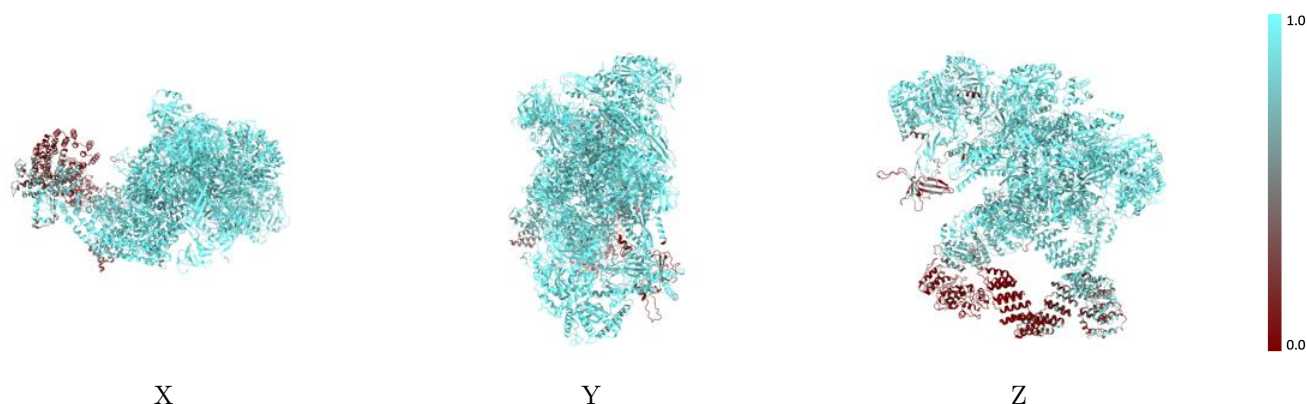
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



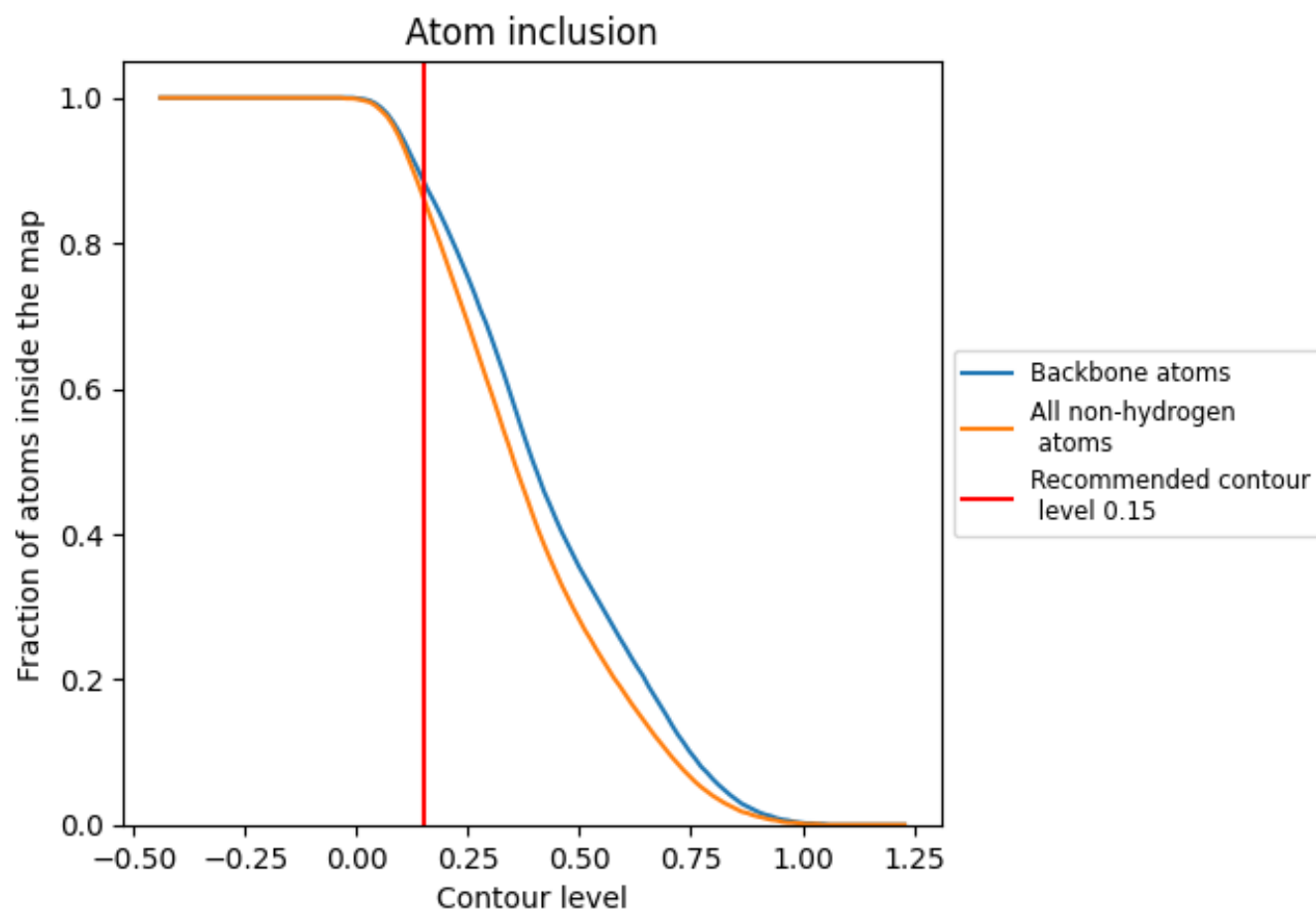
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 86% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8620	 0.4420
A	 0.9500	 0.5240
B	 0.9580	 0.5500
C	 0.9410	 0.4980
D	 0.8630	 0.4180
E	 0.3940	 0.0810
F	 0.9130	 0.4170
G	 0.9450	 0.4510
H	 0.9550	 0.5580
I	 0.9750	 0.5820
J	 0.9610	 0.5210
K	 0.9590	 0.5320
L	 0.9380	 0.3450
M	 0.9610	 0.5700
N	 0.3370	 0.0790
O	 0.9490	 0.5610
P	 0.9610	 0.4330
R	 0.8790	 0.4550
S	 0.8890	 0.4290
a	 0.9680	 0.5450
c	 0.8730	 0.4480
i	 0.9580	 0.5310
m	 0.9260	 0.4910

