wwPDB EM Validation Summary Report ⓘ

Mar 5, 2024 – 01:05 AM 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)

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

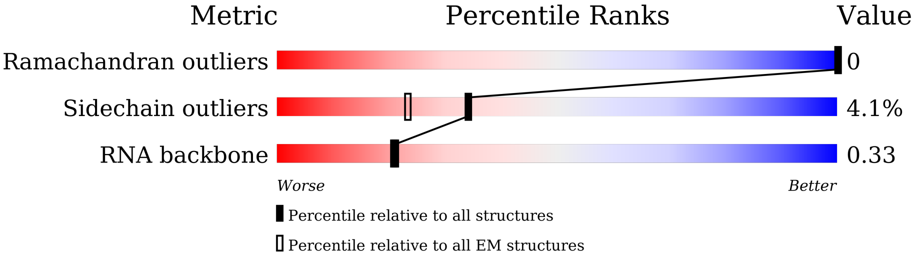
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

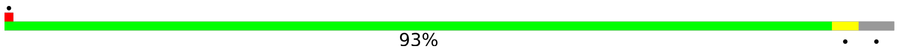
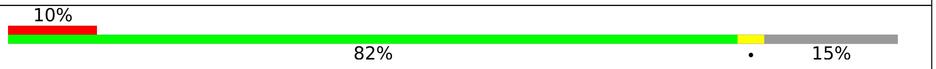
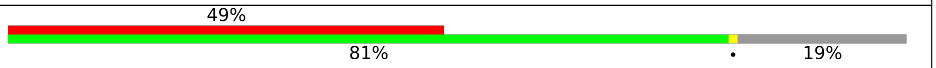
The reported resolution of this entry is 2.70 Å.

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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	

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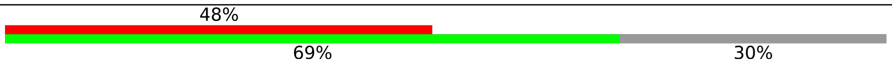
Mol	Chain	Length	Quality of chain
8	G	266	
9	H	531	
10	I	486	
11	i	648	
12	J	507	
13	K	331	
14	L	303	
15	M	178	
15	m	178	
16	N	770	
17	O	151	
18	P	143	
19	R	48	
20	S	20	

2 Entry composition ⓘ

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
			Total	C	N	O	S		
1	A	288	2164	1368	377	409	10	0	0
1	a	317	2377	1515	410	442	10	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 8 is a protein called superoxide dismutase.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 14 is a protein called superoxide dismutase.

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

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

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

- 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 2987	C 1818	N 579	O 584	S 6	0	0

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

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

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

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

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

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

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

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

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

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

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

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

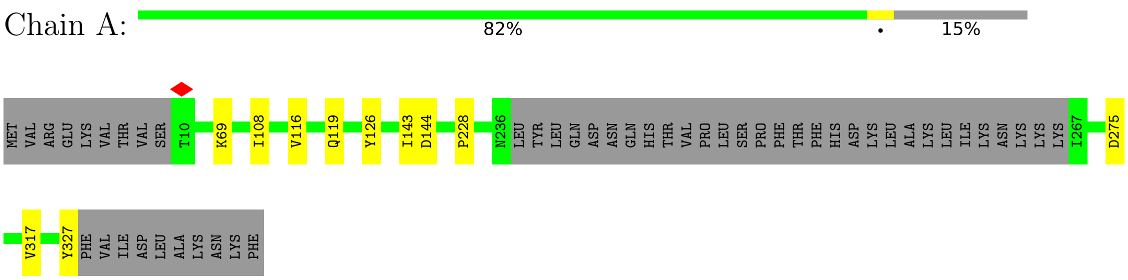
- Molecule 23 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

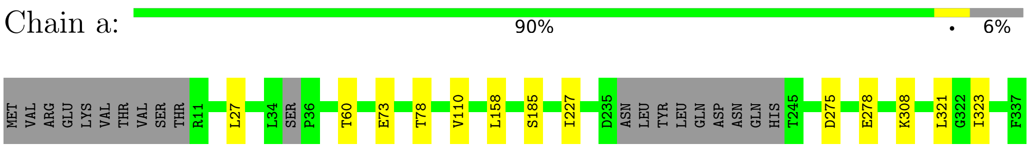
3 Residue-property plots ⓘ

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.

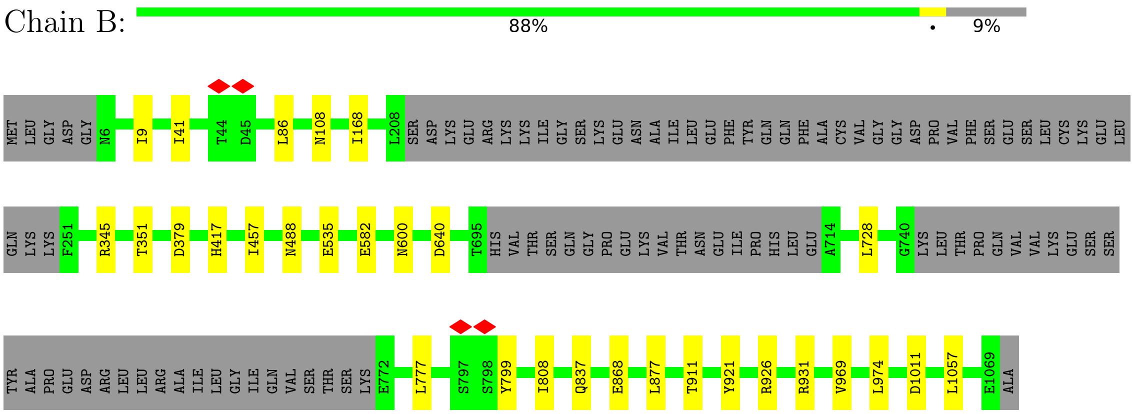
- Molecule 1: DNA-directed RNA polymerase subunit alpha



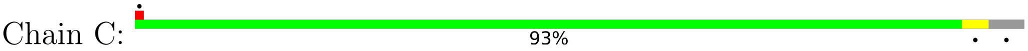
- Molecule 1: DNA-directed RNA polymerase subunit alpha

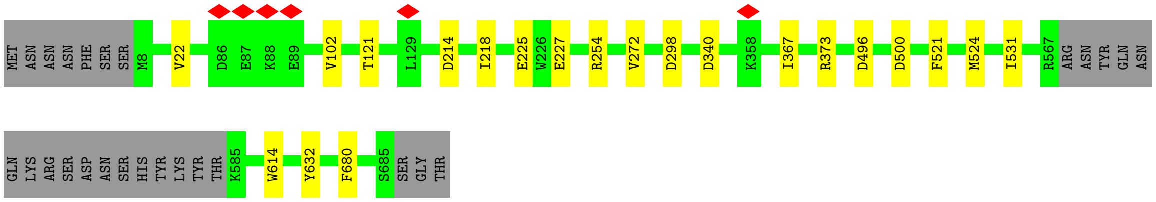


- Molecule 2: DNA-directed RNA polymerase subunit beta



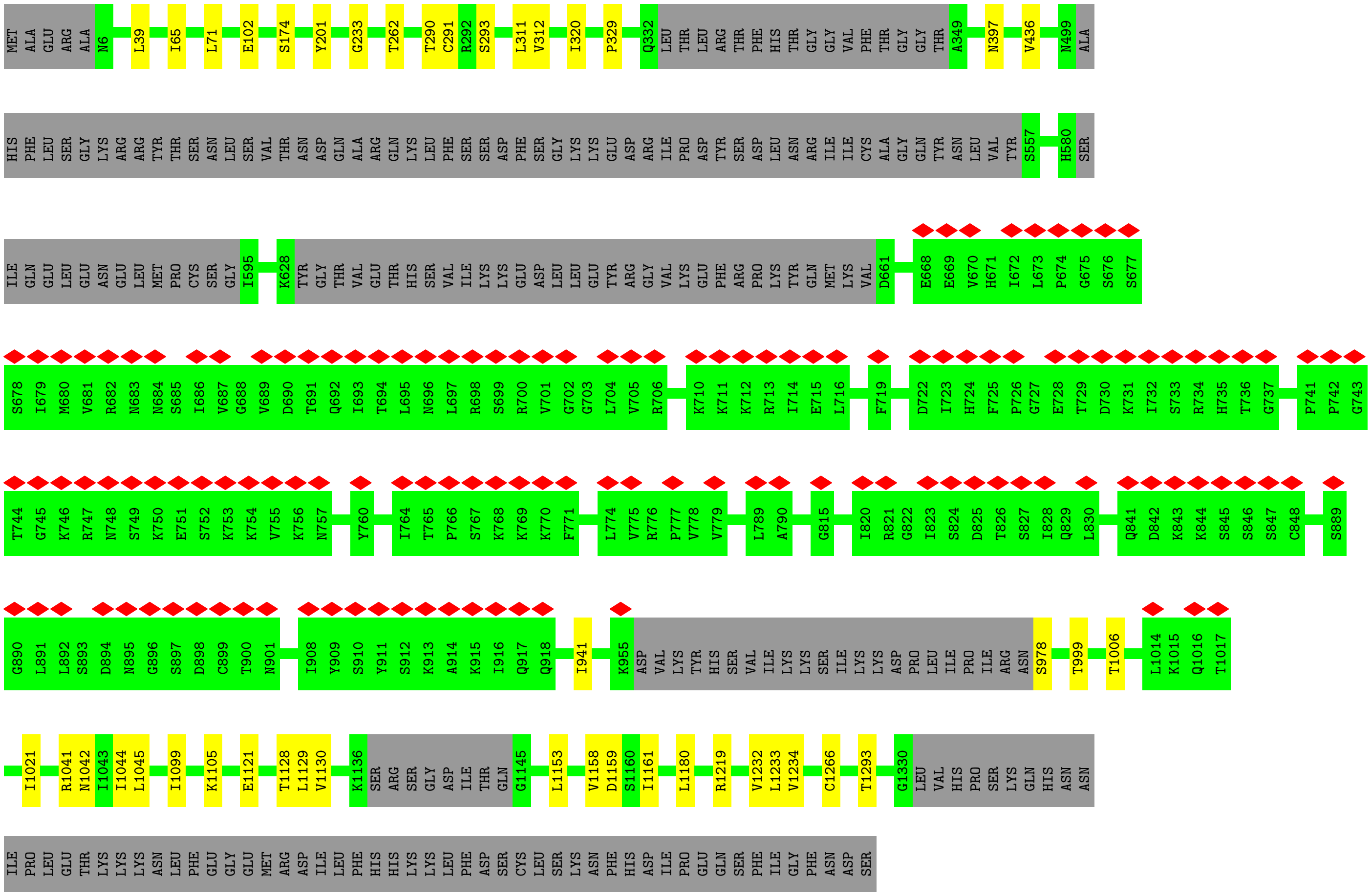
- Molecule 3: DNA-directed RNA polymerase subunit gamma





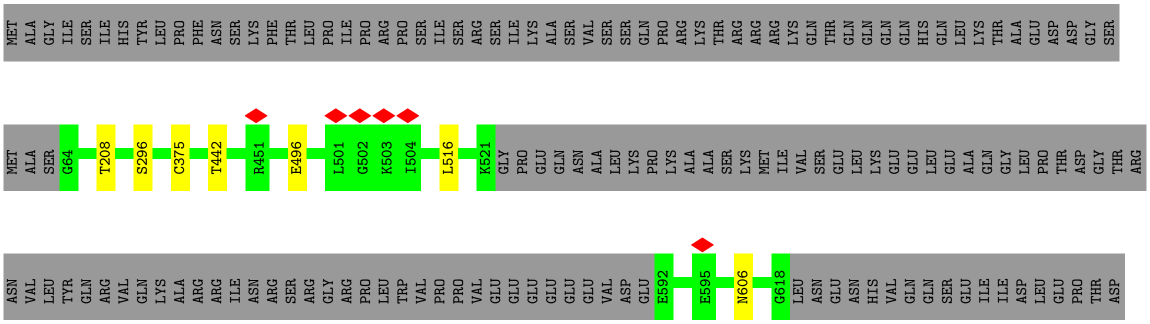
- Molecule 4: DNA-directed RNA polymerase subunit beta”

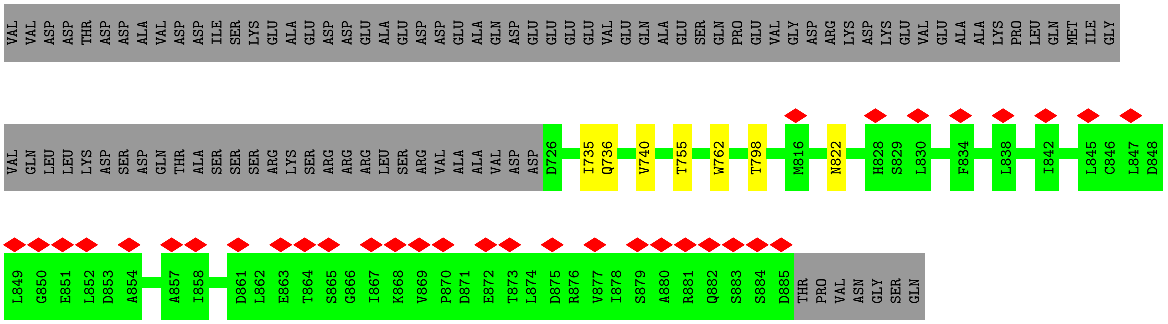
Chain c:



- Molecule 5: PAP1(pTAC3)

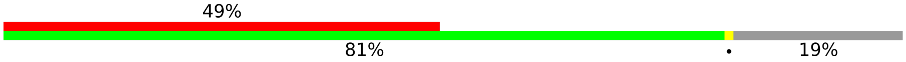
Chain D:

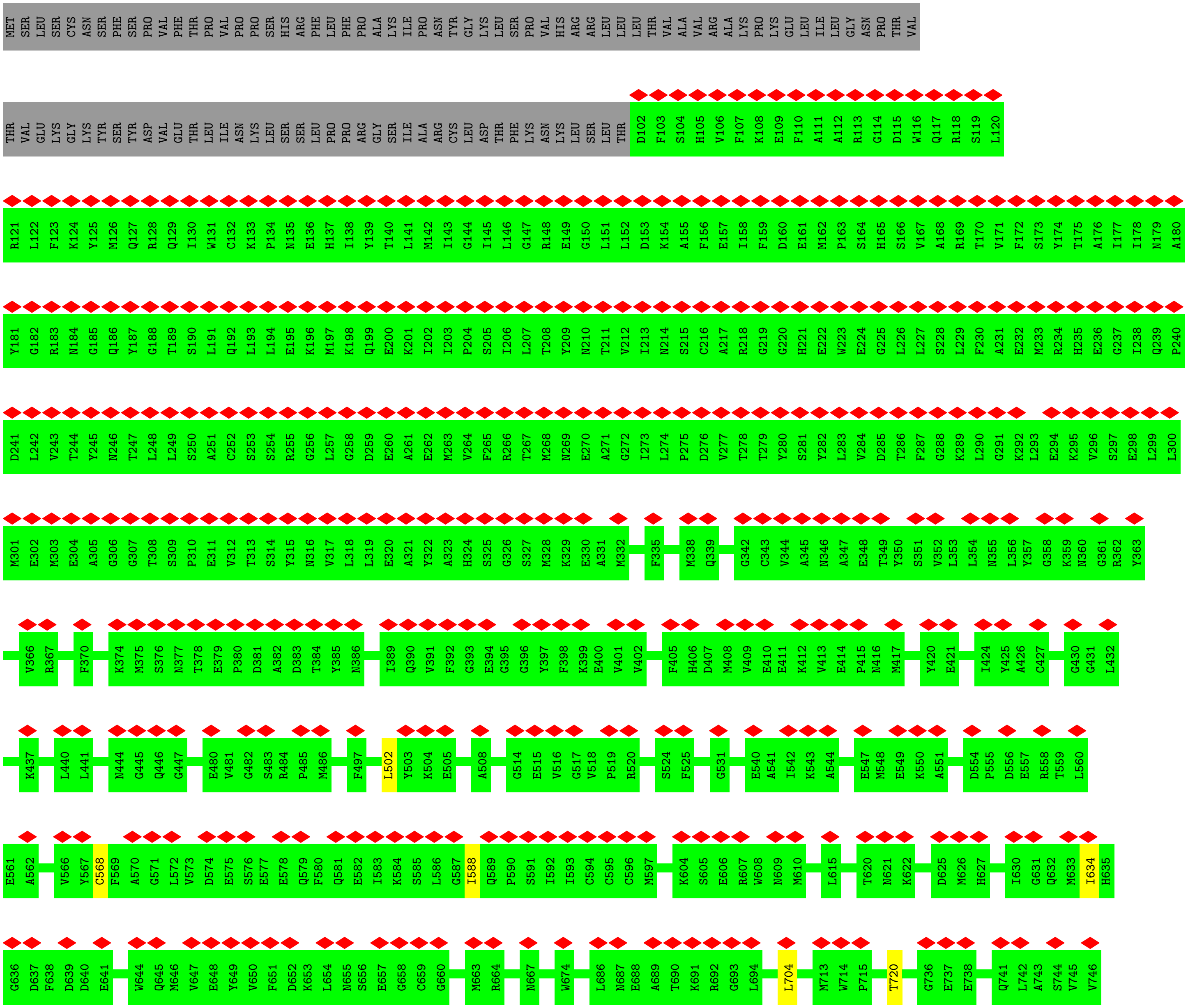




- Molecule 6: Pentatricopeptide repeat-containing protein At1g74850, chloroplastic-like

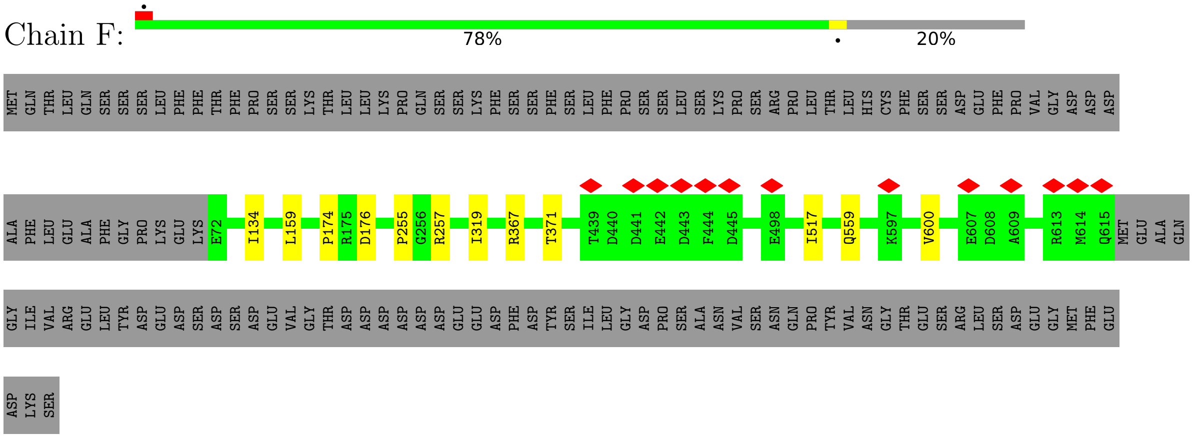
Chain E:





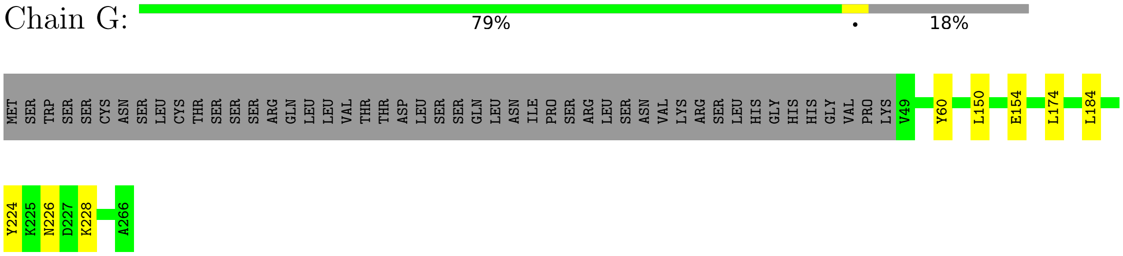
- Molecule 7: Protein PLASTID TRANSCRIPTIONALLY ACTIVE 10-like

Chain F:



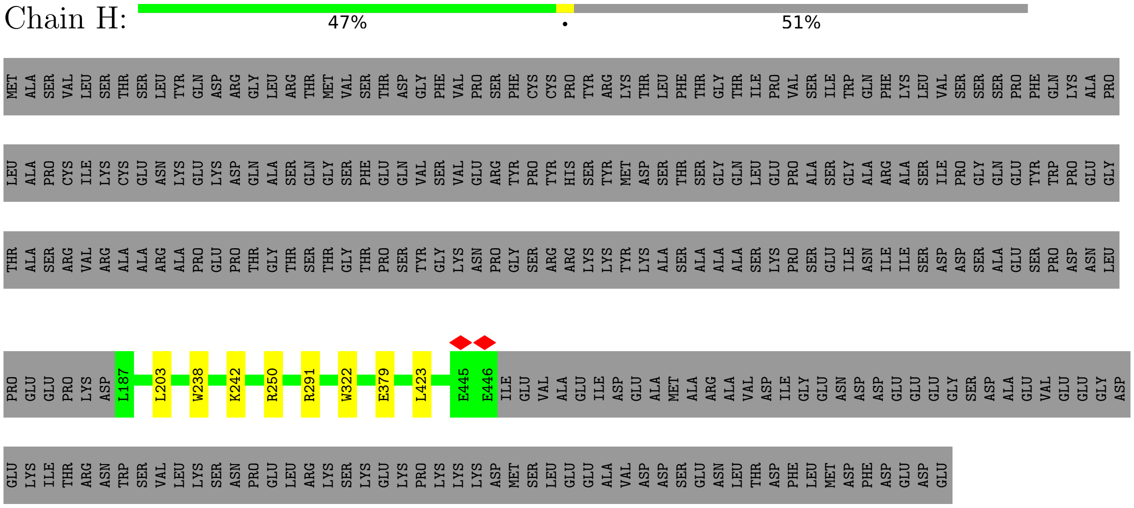
- Molecule 8: superoxide dismutase

Chain G:

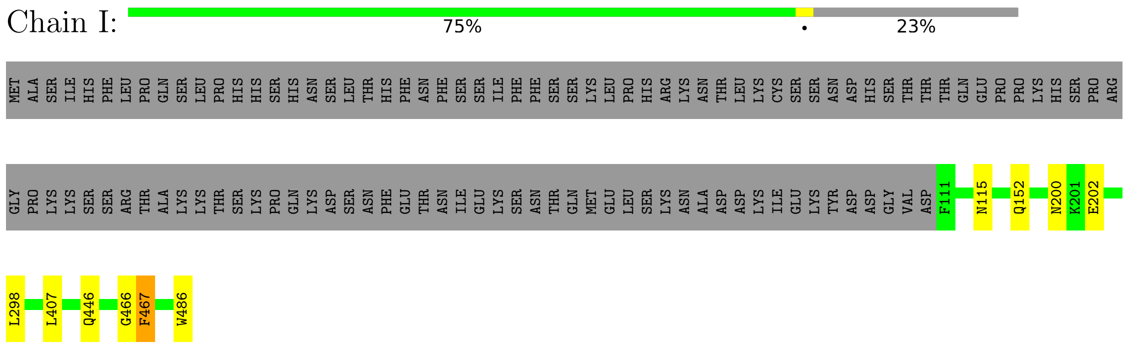


- Molecule 9: Protein PLASTID TRANSCRIPTIONALLY ACTIVE 12-like

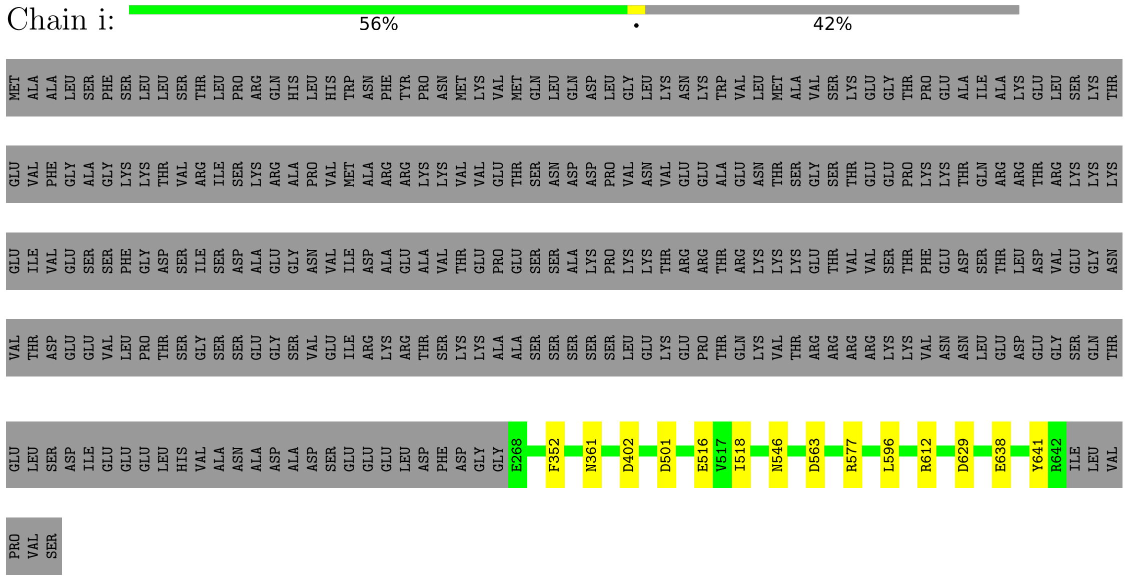
Chain H:



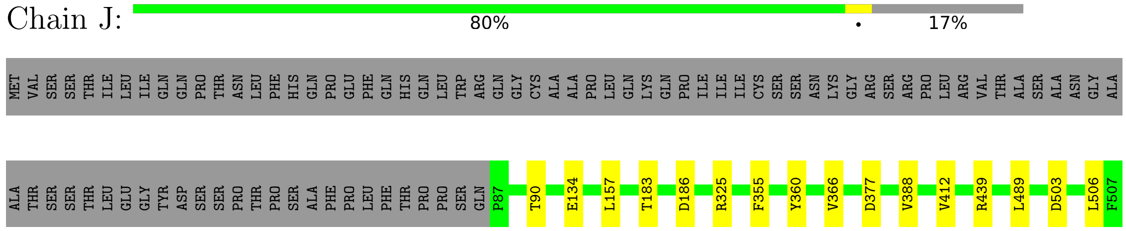
- Molecule 10: Fructokinase-like 1, chloroplastic



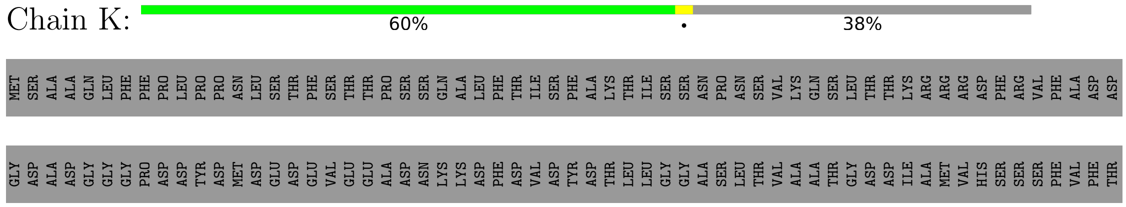
- Molecule 11: Fructokinase-like 2, chloroplastic

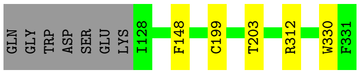


- Molecule 12: Protein PLASTID TRANSCRIPTIONALLY ACTIVE 14-like isoform X2

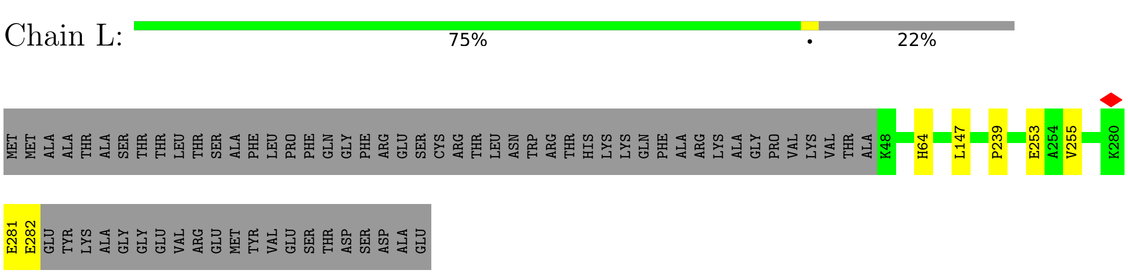


- Molecule 13: PAP8(pTAC6)

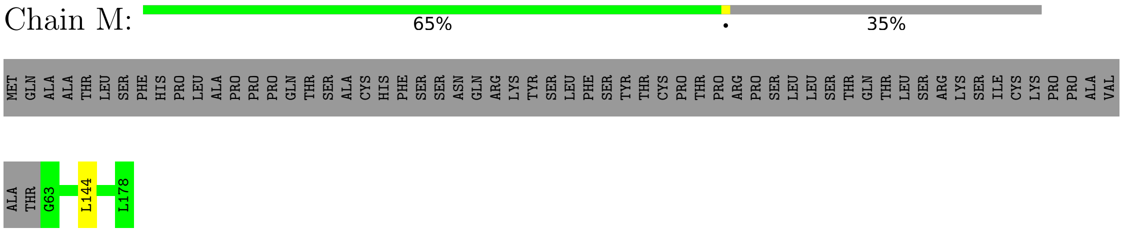




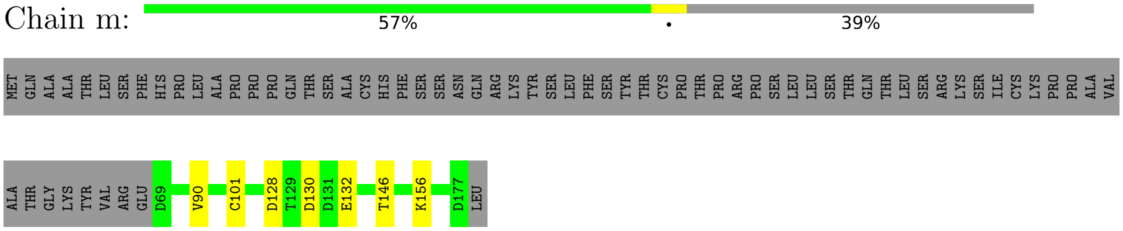
- Molecule 14: superoxide dismutase



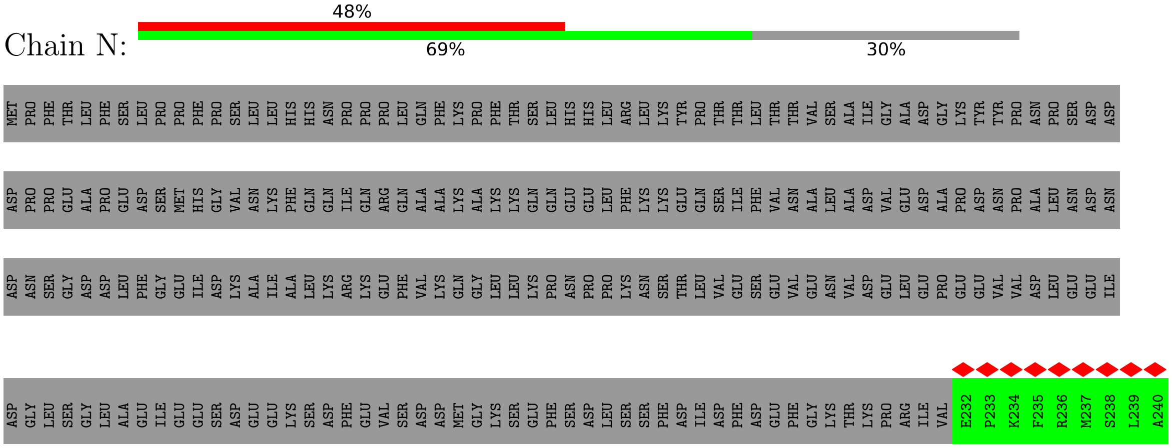
- Molecule 15: Thioredoxin-like protein CITRX1, chloroplastic

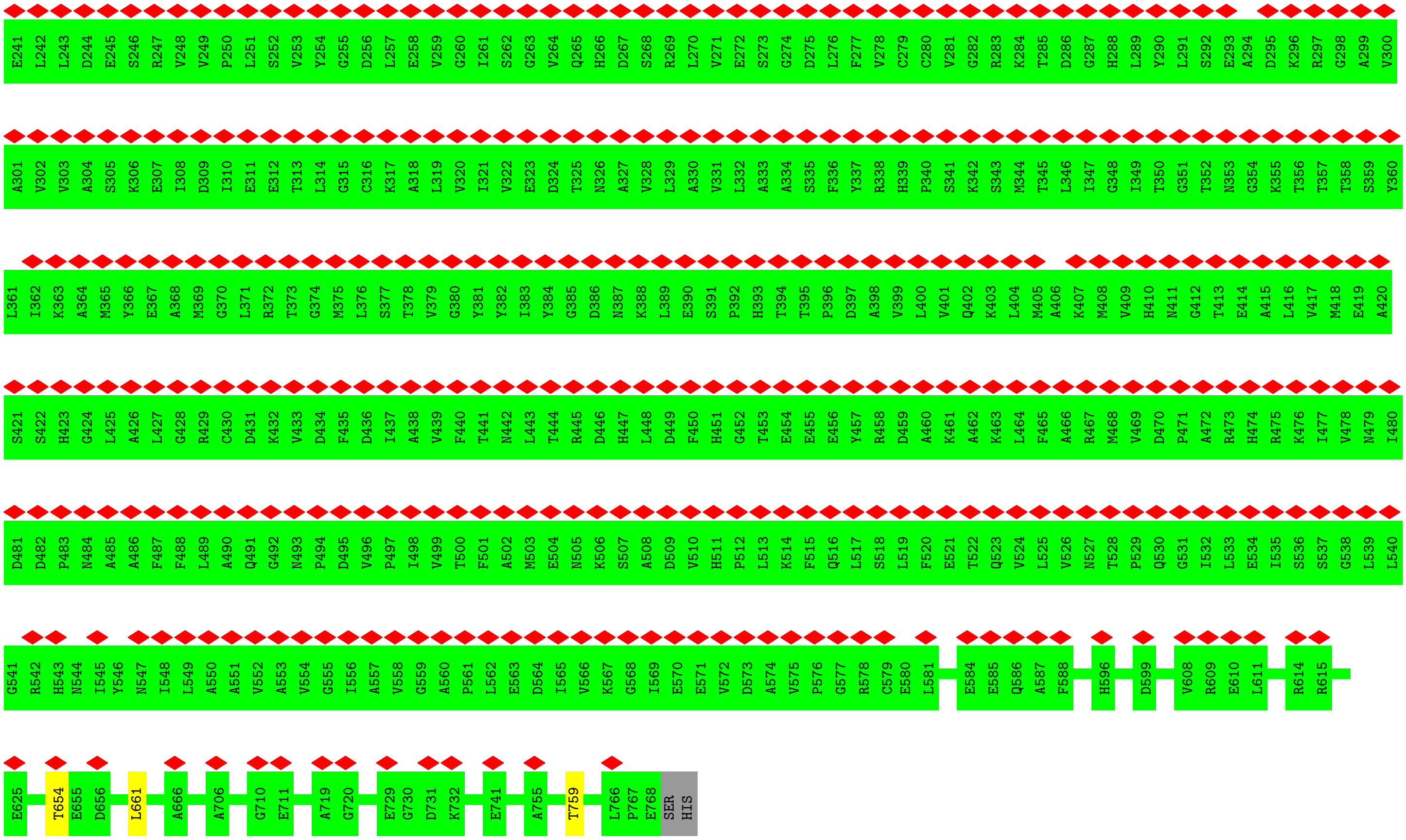


- Molecule 15: Thioredoxin-like protein CITRX1, chloroplastic

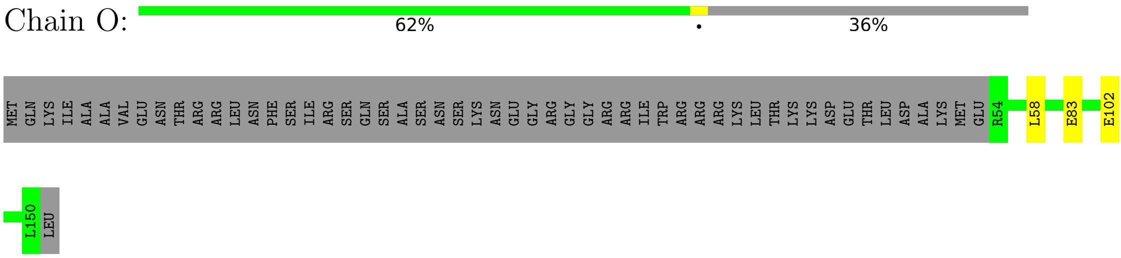


- Molecule 16: UDP-N-acetylmuramoyl-L-alanyl-D-glutamate--2, 6-diaminopimelate ligase-like

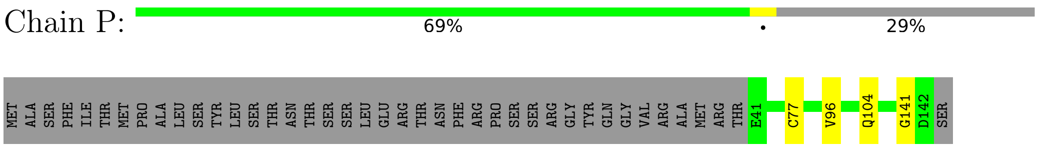




- Molecule 17: Protein PLASTID TRANSCRIPTIONALLY ACTIVE 7-like isoform X2



- Molecule 18: PAP13(pTAC18)



- Molecule 19: DNA (48-mer)

- Molecule 20: RNA (20-mer)

Chain S:

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 ($e^{-}/\text{Å}^{2}$)	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, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.65	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.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	27	54
1	a	240/308 (78%)	227 (95%)	13 (5%)	22	47
2	B	712/924 (77%)	687 (96%)	25 (4%)	36	65
3	C	414/612 (68%)	394 (95%)	20 (5%)	25	53
4	c	680/1238 (55%)	638 (94%)	42 (6%)	18	40
5	D	435/770 (56%)	422 (97%)	13 (3%)	41	70
6	E	289/741 (39%)	283 (98%)	6 (2%)	53	80
7	F	382/615 (62%)	370 (97%)	12 (3%)	40	69
8	G	167/232 (72%)	159 (95%)	8 (5%)	25	53
9	H	208/472 (44%)	200 (96%)	8 (4%)	33	62
10	I	289/437 (66%)	282 (98%)	7 (2%)	49	77
11	i	299/567 (53%)	285 (95%)	14 (5%)	26	54
12	J	350/449 (78%)	336 (96%)	14 (4%)	31	60
13	K	177/300 (59%)	172 (97%)	5 (3%)	43	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	L	142/258 (55%)	135 (95%)	7 (5%)	25	52
15	M	101/160 (63%)	101 (100%)	0	100	100
15	m	85/160 (53%)	78 (92%)	7 (8%)	11	26
16	N	97/659 (15%)	94 (97%)	3 (3%)	40	69
17	O	75/130 (58%)	72 (96%)	3 (4%)	31	60
18	P	61/129 (47%)	58 (95%)	3 (5%)	25	52
All	All	5422/9469 (57%)	5202 (96%)	220 (4%)	34	59

5 of 220 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	606	ASN
8	G	154	GLU
18	P	104	GLN
14	L	239	PRO
5	D	755	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 150 such sidechains are listed below:

Mol	Chain	Res	Type
10	I	193	GLN
16	N	691	HIS
10	I	346	GLN
12	J	288	GLN
3	C	605	ASN

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 monosaccharides 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.

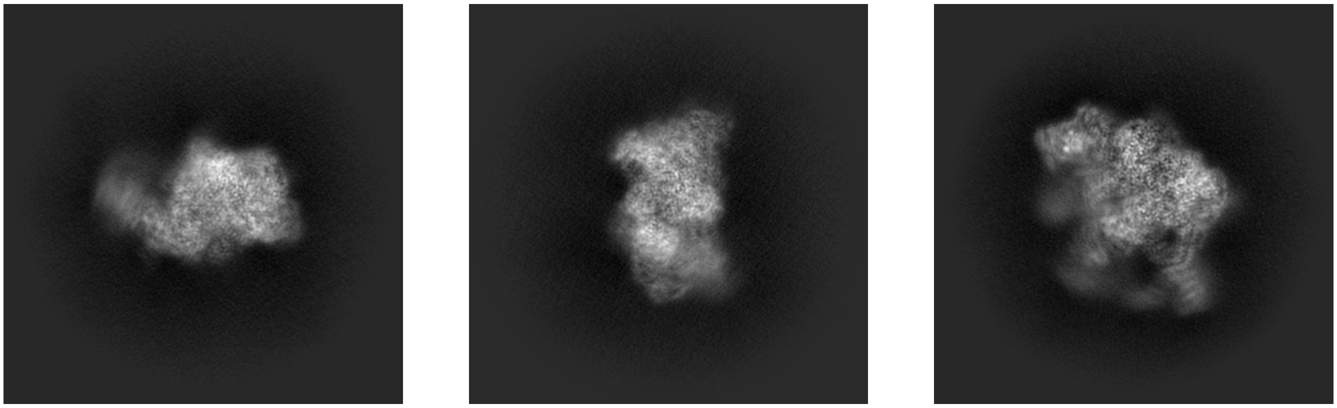
6 Map visualisation ⓘ

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.

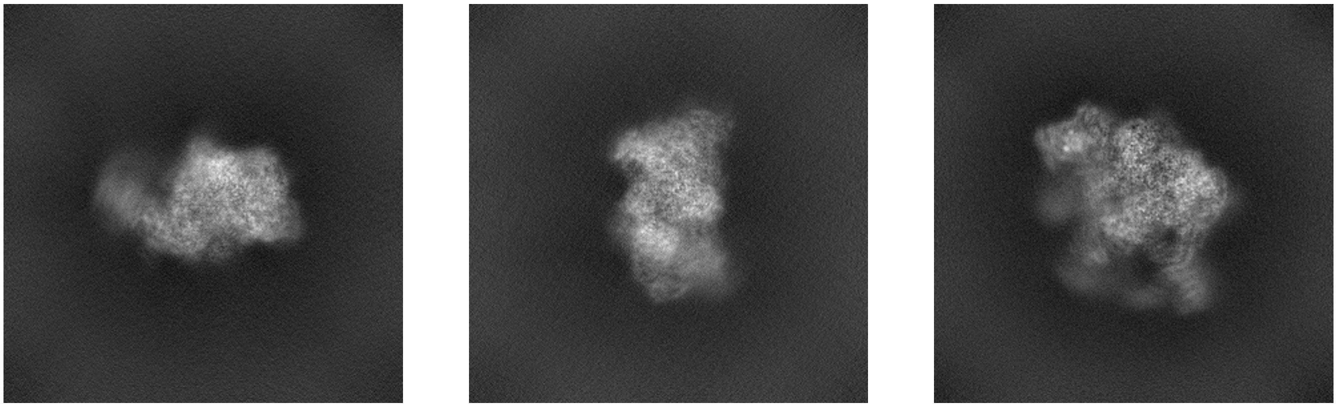
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

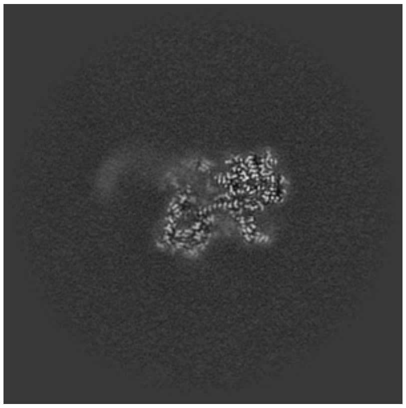


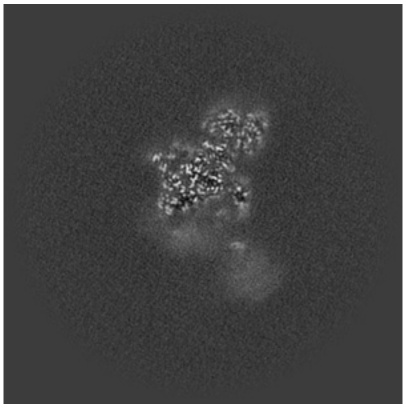
X Y Z

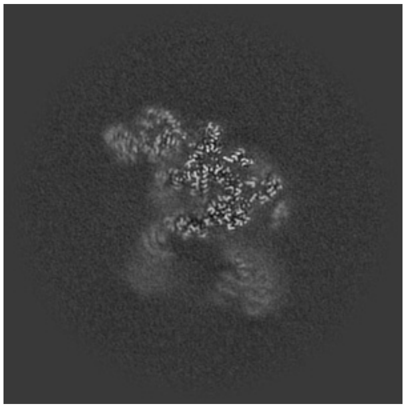
The images above show the map projected in three orthogonal directions.

6.2 Central slices

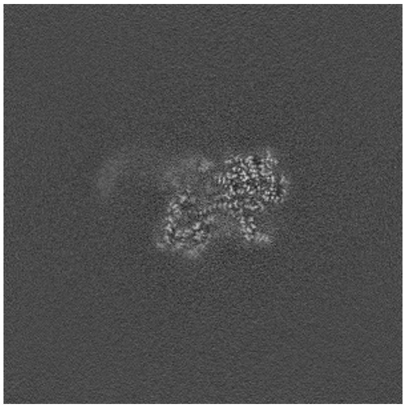
6.2.1 Primary map

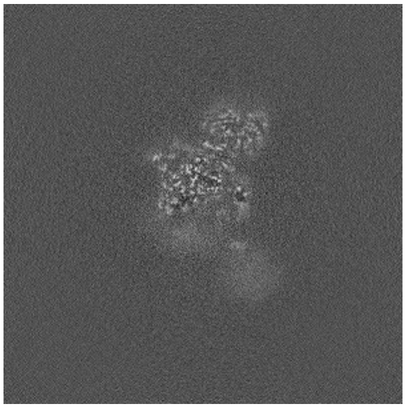

X Index: 300

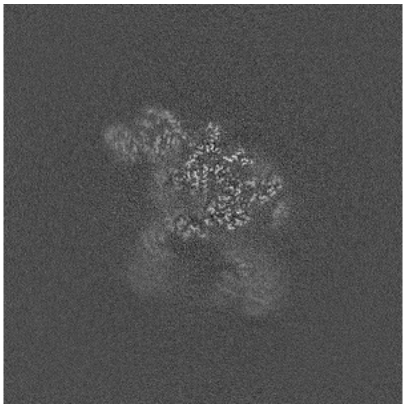

Y Index: 300


Z Index: 300

6.2.2 Raw map


X Index: 300

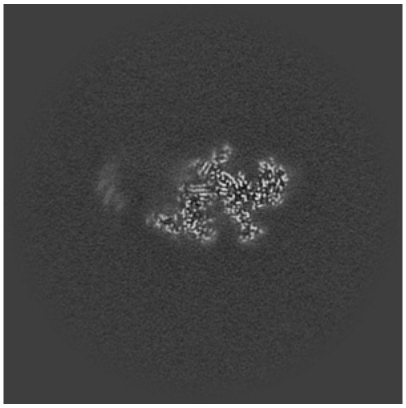

Y Index: 300

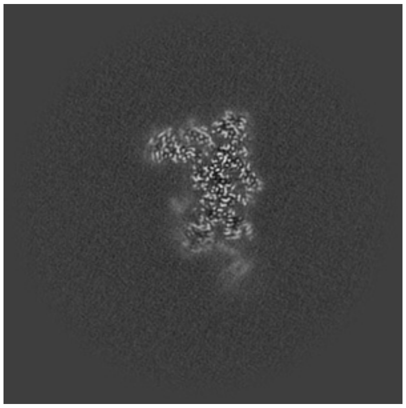

Z Index: 300

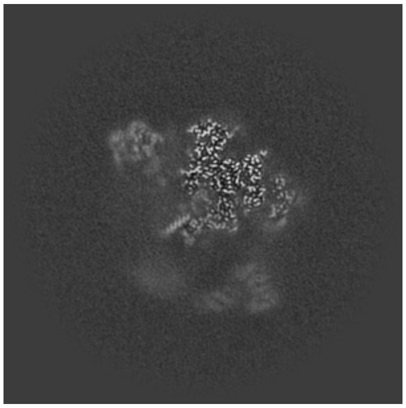
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

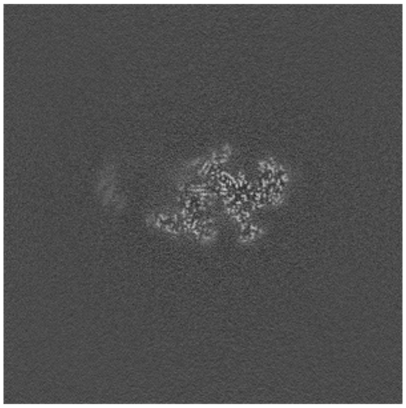
6.3.1 Primary map

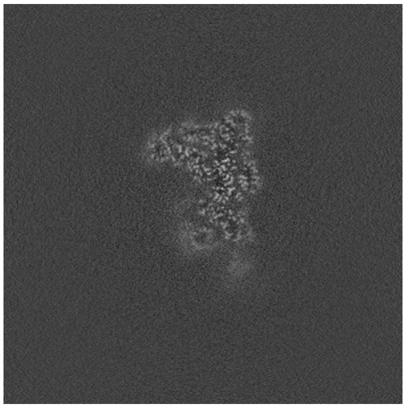

X Index: 323

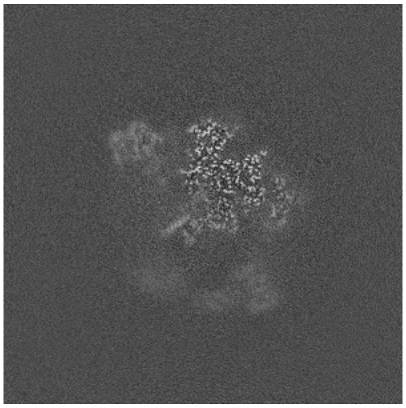

Y Index: 335


Z Index: 322

6.3.2 Raw map


X Index: 323

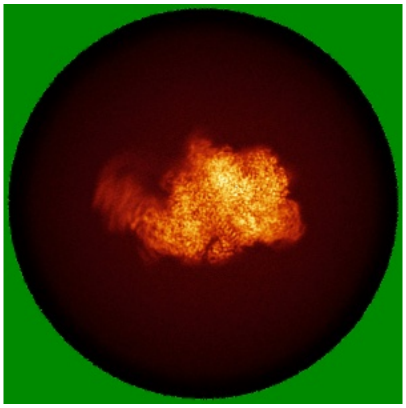

Y Index: 329


Z Index: 322

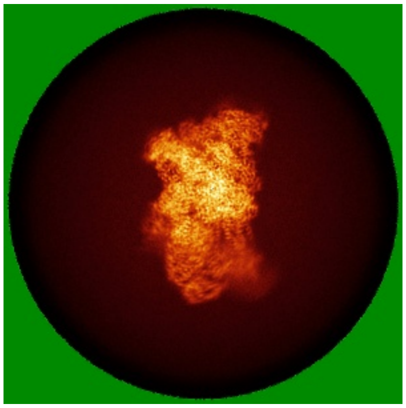
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

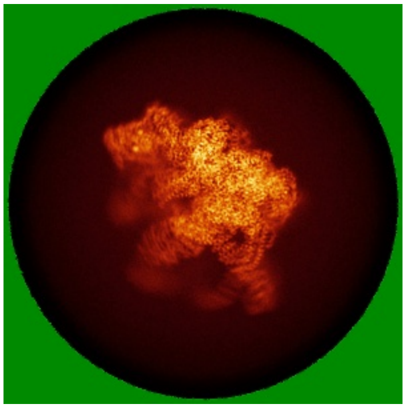
6.4.1 Primary map



X

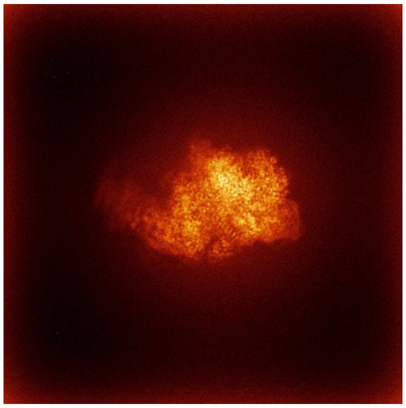


Y

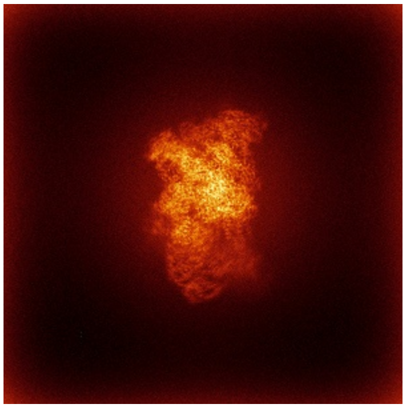


Z

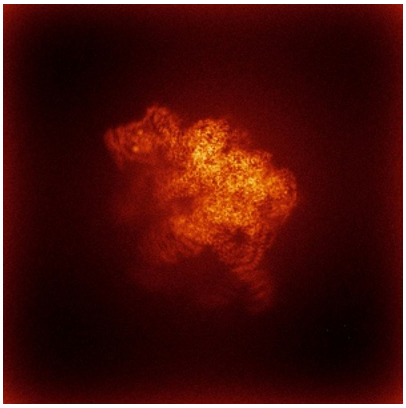
6.4.2 Raw map



X



Y



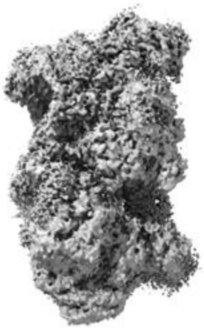
Z

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.

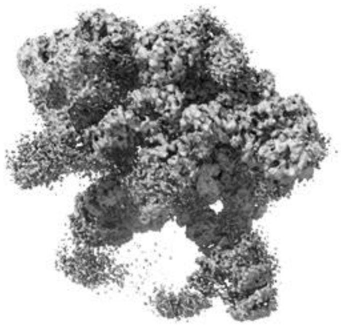
6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X



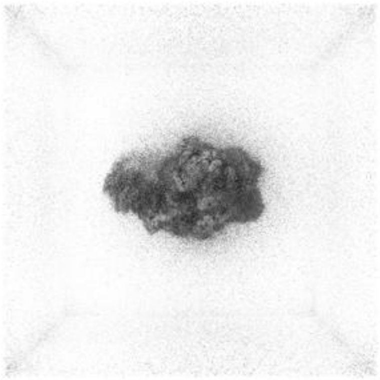
Y



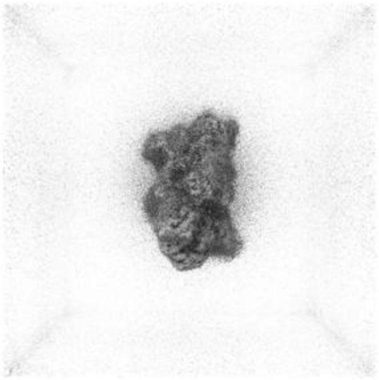
Z

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.

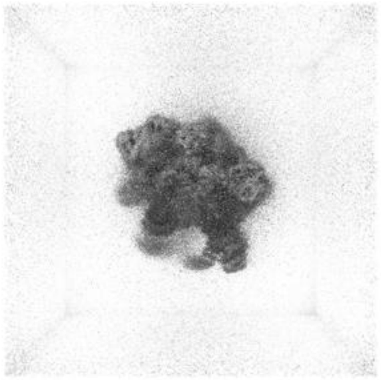
6.5.2 Raw map



X



Y



Z

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.

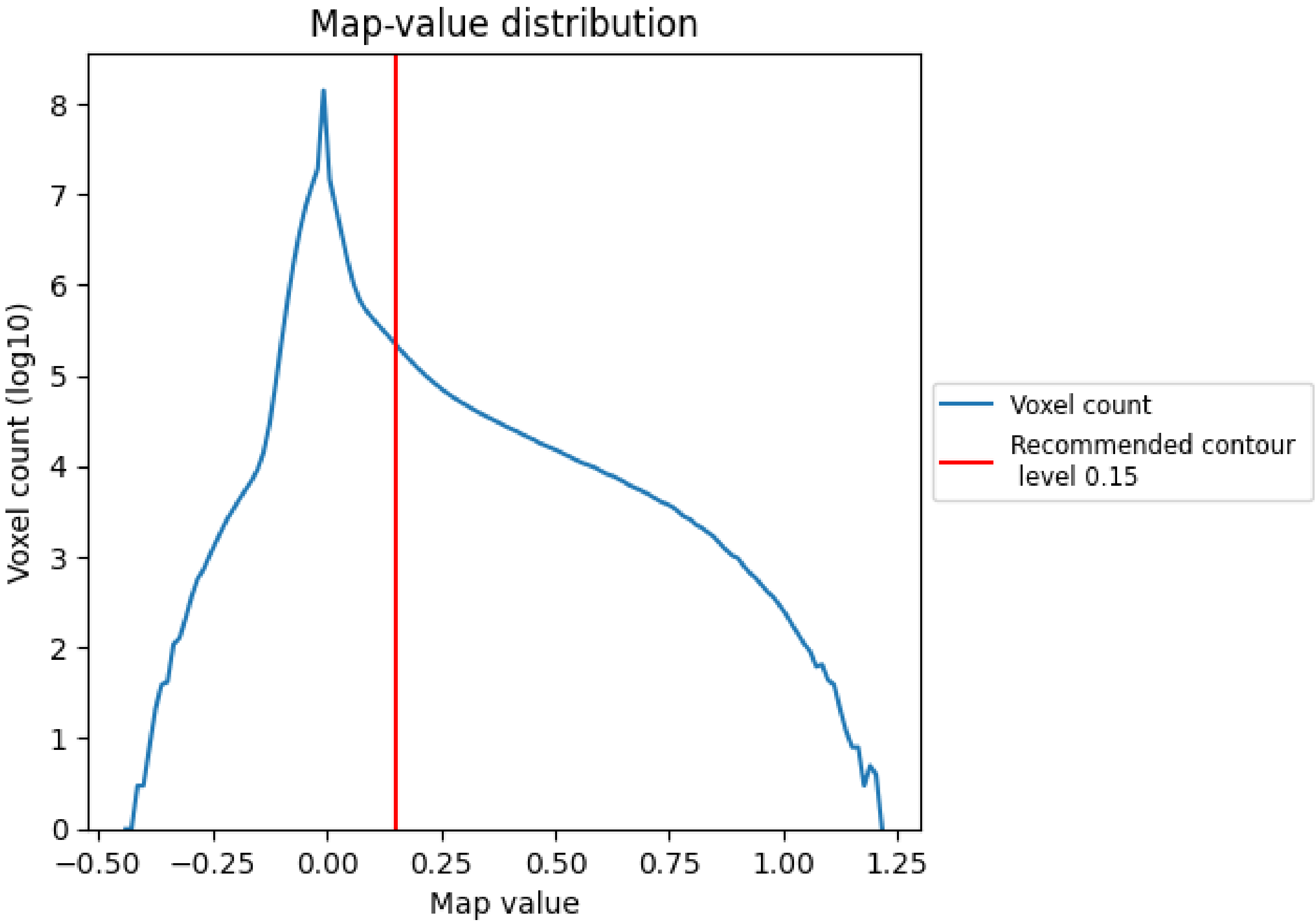
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

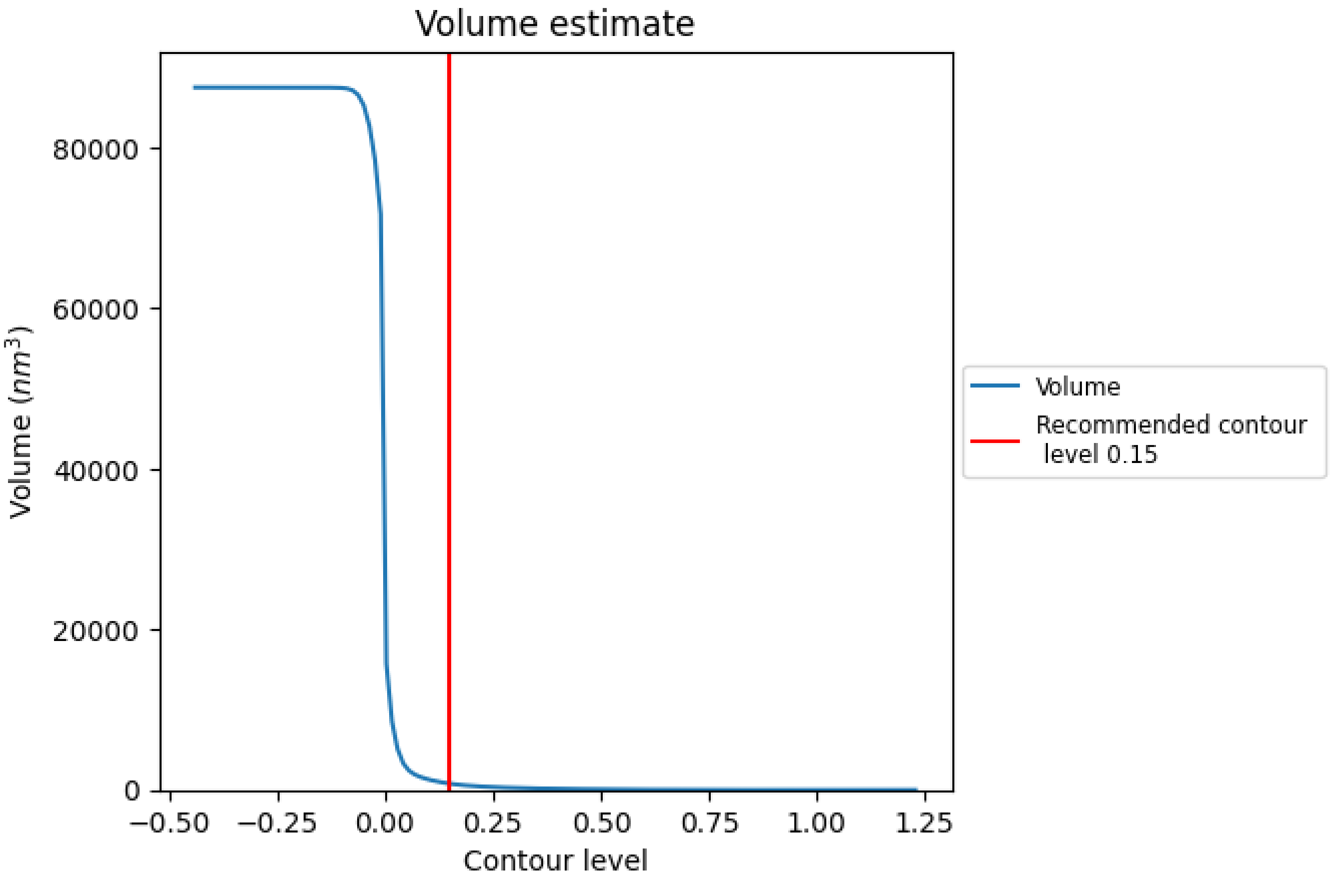
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

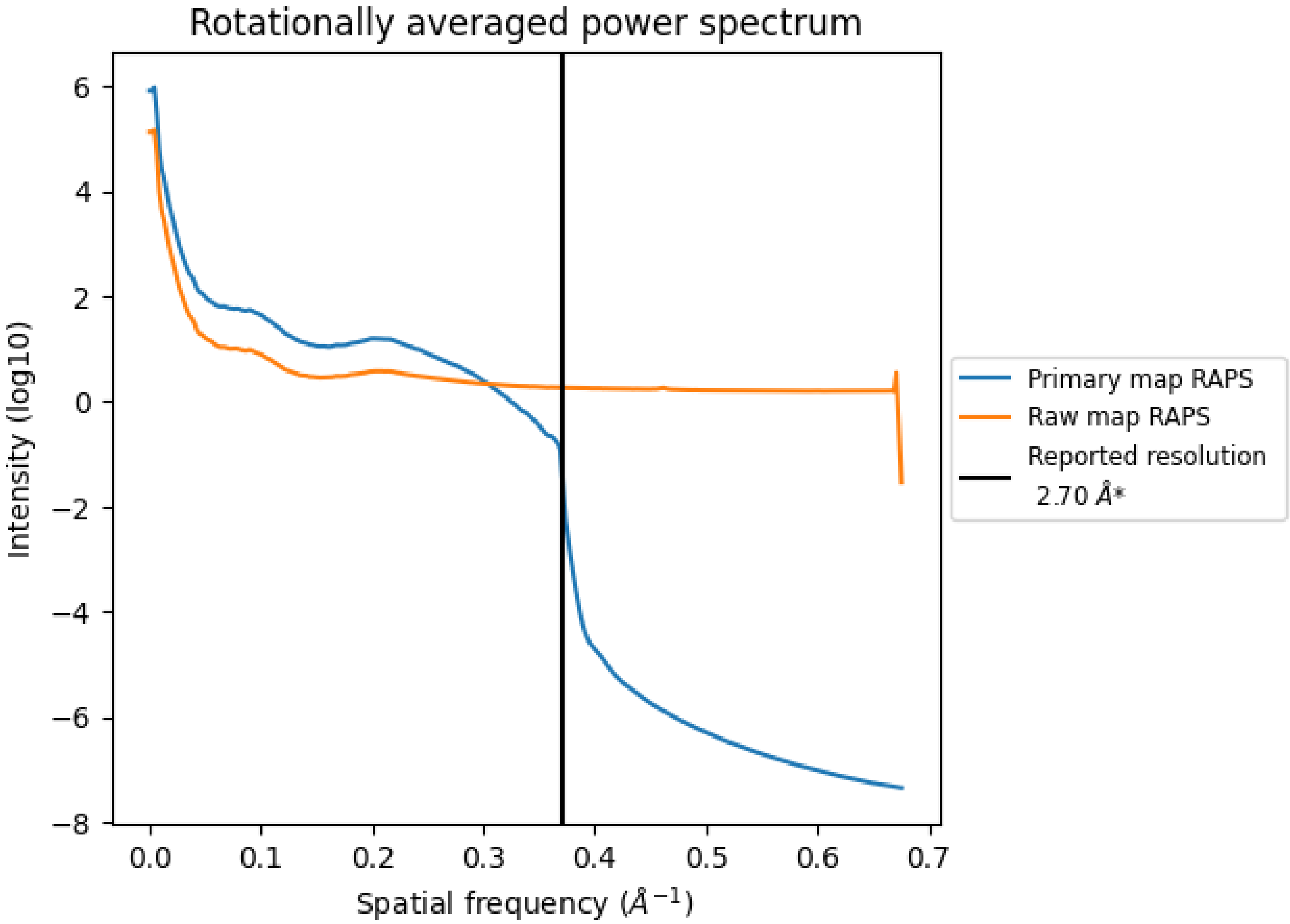
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 787 nm^3; 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 ⓘ

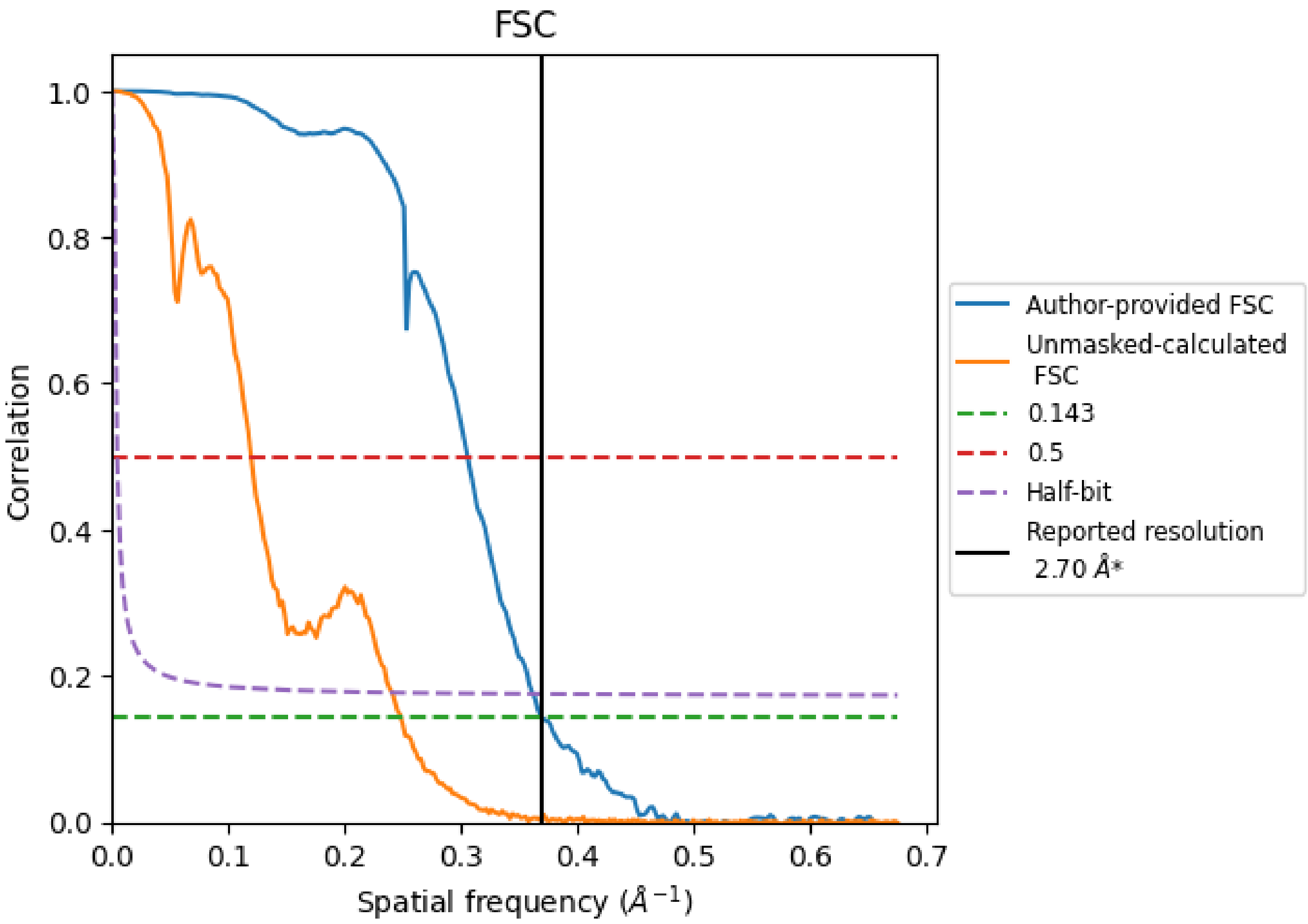


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates ⓘ

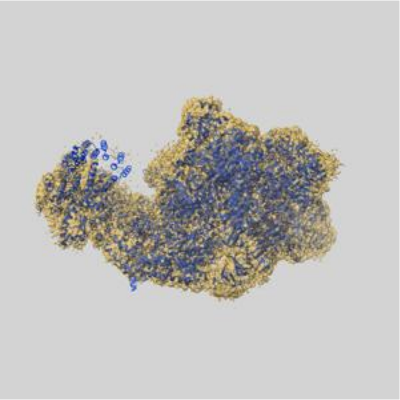
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.27	2.76
Unmasked-calculated*	4.02	8.37	4.15

*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 %

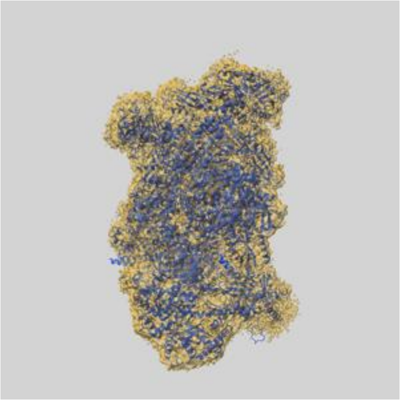
9 Map-model fit

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.

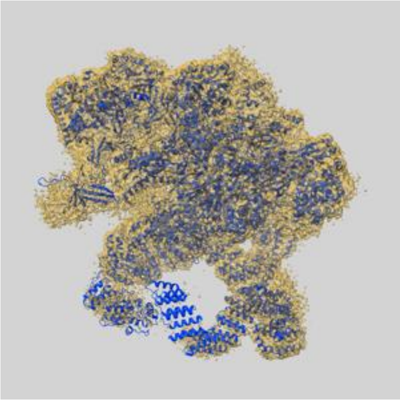
9.1 Map-model overlay



X



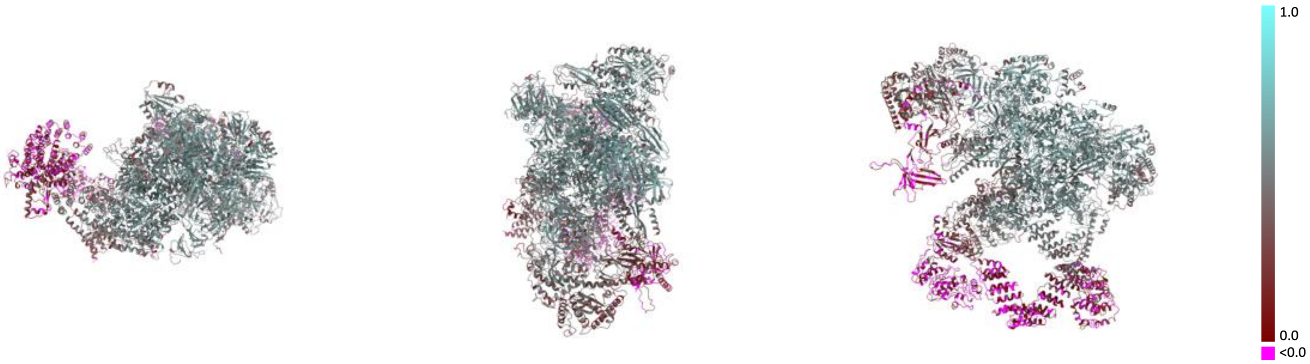
Y



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.

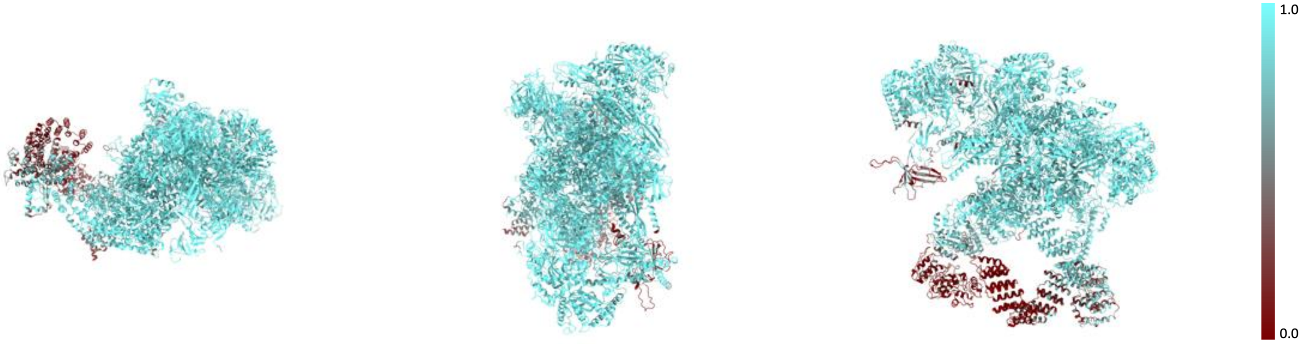
9.2 Q-score mapped to coordinate model



X Y Z

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.

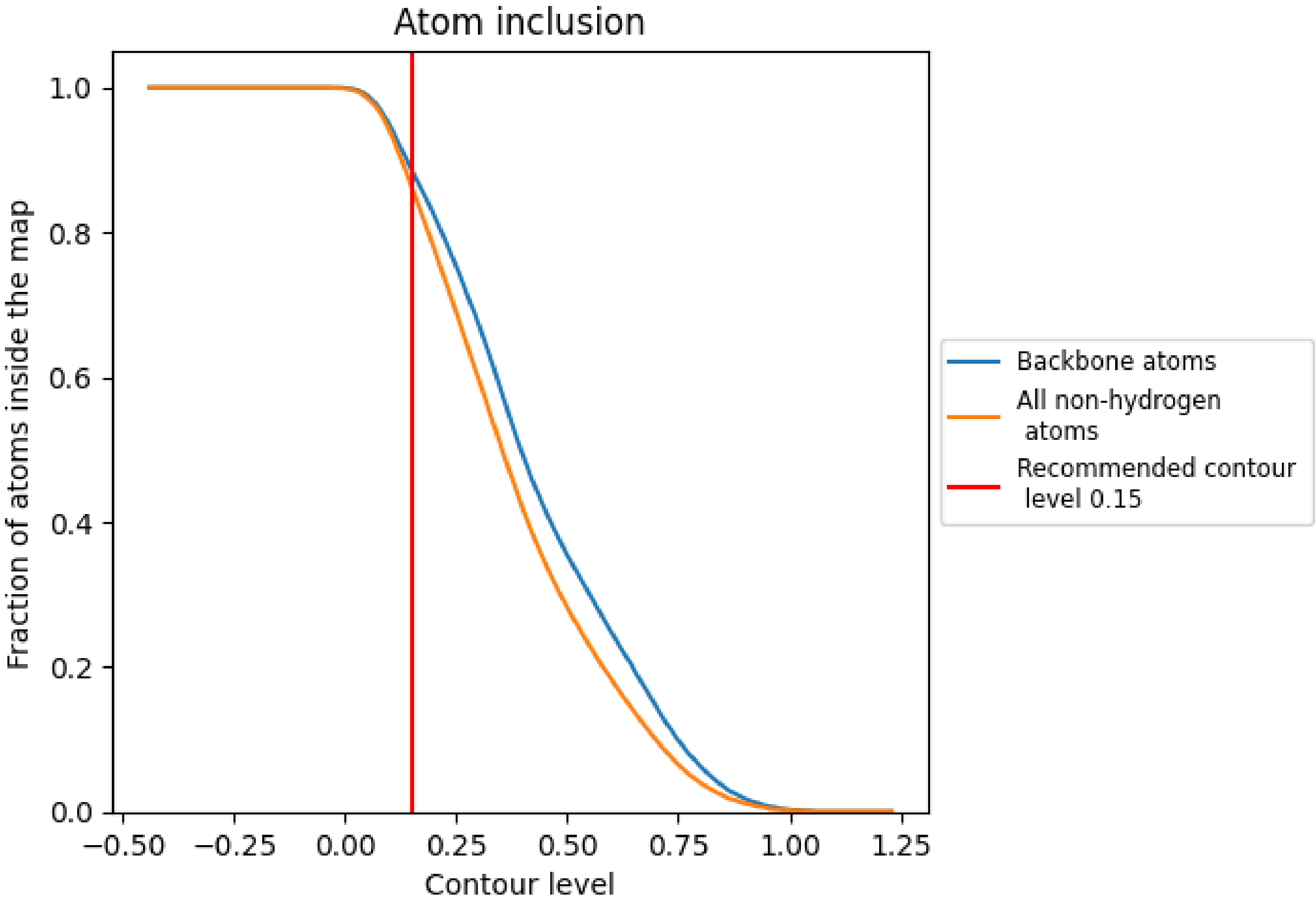
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 ⓘ



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