wwPDB EM Validation Summary Report

Nov 30, 2021 – 02:19 pm GMT

PDB ID	:	7PKS
EMDB ID	:	EMD-13479
Title	:	Structural basis of Integrator-mediated transcription regulation
Authors	:	Fianu, I.; Chen, Y.; Dienemann, C.; Cramer, P.
Deposited on	:	2021-08-26
Resolution	:	3.60 Å(reported)
Based on initial models	:	7CUN, 7BFP, 3DW8, 6GML

This is a wwPDB EM Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

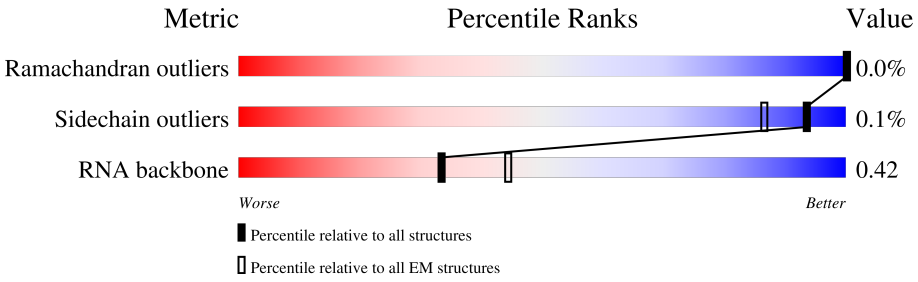
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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	1970	71% 29%
2	B	1174	95% 5%
3	C	275	95% 5%
4	D	142	12% 89% 11%
5	E	210	99%
6	F	127	61% 39%
7	G	172	5% 99%
8	H	150	5% 99%

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Mol	Chain	Length	Quality of chain
9	I	125	94% 6%
10	J	67	99%
11	K	117	5% 98%
12	L	58	79% 21%
13	M	13	100%
14	N	48	50% 50%
15	P	17	59% 41%
16	T	48	69% 31%
17	U	528	5% 34% 65%
18	V	614	73% 27%
19	W	616	5% 82% 18%
20	X	22	100%
21	Z	1087	25% 75%
22	a	2190	11% 56% 44%
23	b	1204	87% 13%
24	d	963	85% 15%
25	e	1019	64% 36%
26	f	887	60% 40%
27	g	962	92% 8%
28	h	995	89% 11%
29	i	658	83% 16%
30	k	600	76% 24%
31	p	589	97%
32	q	309	94% 6%
33	u	27	100%

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 101147 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1392	11012	6933	1973	2037	69	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2

- 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	1112	8901	5634	1560	1643	64	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	261	2096	1314	360	416	6	0	0

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	126	Total	C	N	O	S	0	0
			975	613	166	192	4		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	78	Total	C	N	O	S	0	0
			627	401	106	115	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1316	858	208	242	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	117	Total	C	N	O	S	0	0
			944	584	166	183	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			383	238	72	67	6		

- Molecule 13 is a protein called RPBI C-terminal domain peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	13	Total	C	N	O	0	0
			95	60	13	22		

- Molecule 14 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	24	Total	C	N	O	P	0	0
			489	234	90	141	24		

- Molecule 15 is a RNA chain called TAR RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	17	Total	C	N	O	P	0	0
			361	162	66	116	17		

- Molecule 16 is a DNA chain called DNA Template.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	33	Total	C	N	O	P	0	0
			682	325	122	202	33		

- Molecule 17 is a protein called Negative elongation factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	183	Total	C	N	O	S	0	0
			1398	889	238	264	7		

- Molecule 18 is a protein called Negative elongation factor B.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	V	451	Total 2040	C 1102	N 466	O 472	0	0

- Molecule 19 is a protein called Negative elongation factor C/D.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	508	Total 3854	C 2468	N 654	O 713	S 19	0	0

- Molecule 20 is a protein called Negative elongation factor E.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	X	22	Total 110	C 66	N 22	O 22	0	0

- Molecule 21 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	273	Total 2174	C 1369	N 392	O 402	S 11	0	0

- Molecule 22 is a protein called Integrator complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	1227	Total 8337	C 5233	N 1513	O 1550	S 41	0	0

- Molecule 23 is a protein called Integrator complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	1047	Total 7926	C 5085	N 1332	O 1447	S 62	0	0

- Molecule 24 is a protein called Integrator complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	d	820	Total 6410	C 4090	N 1093	O 1193	S 34	0	0

- Molecule 25 is a protein called Integrator complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	e	649	Total	C	N	O	S	0	0
			4671	2973	857	824	17		

- Molecule 26 is a protein called Integrator complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	f	536	Total	C	N	O	S	0	0
			4075	2617	692	743	23		

- Molecule 27 is a protein called Integrator complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	g	886	Total	C	N	O	S	0	0
			6710	4250	1163	1257	40		

- Molecule 28 is a protein called Integrator complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	h	887	Total	C	N	O	S	0	0
			6749	4332	1156	1223	38		

- Molecule 29 is a protein called Integrator complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	i	550	Total	C	N	O	S	0	0
			4249	2741	689	788	31		

- Molecule 30 is a protein called Integrator complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	k	458	Total	C	N	O	S	0	0
			3336	2143	575	593	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	487	GLU	ASP	conflict	UNP Q5TA45

- Molecule 31 is a protein called Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	p	575	Total	C	N	O	S	0	0
			4388	2795	748	818	27		

- Molecule 32 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	q	290	Total	C	N	O	S	0	0
			2322	1467	403	437	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	88	ASN	ASP	conflict	UNP P67775

- Molecule 33 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	u	27	Total	C	N	O	0	0
			144	89	28	27		

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
34	A	1	Total	Mg	0
			1	1	

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
35	A	2	Total	Zn	0
			2	2	
35	B	1	Total	Zn	0
			1	1	
35	C	1	Total	Zn	0
			1	1	
35	I	2	Total	Zn	0
			2	2	
35	J	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
35	L	1	Total Zn 1 1	0
35	k	2	Total Zn 2 2	0

- Molecule 36 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

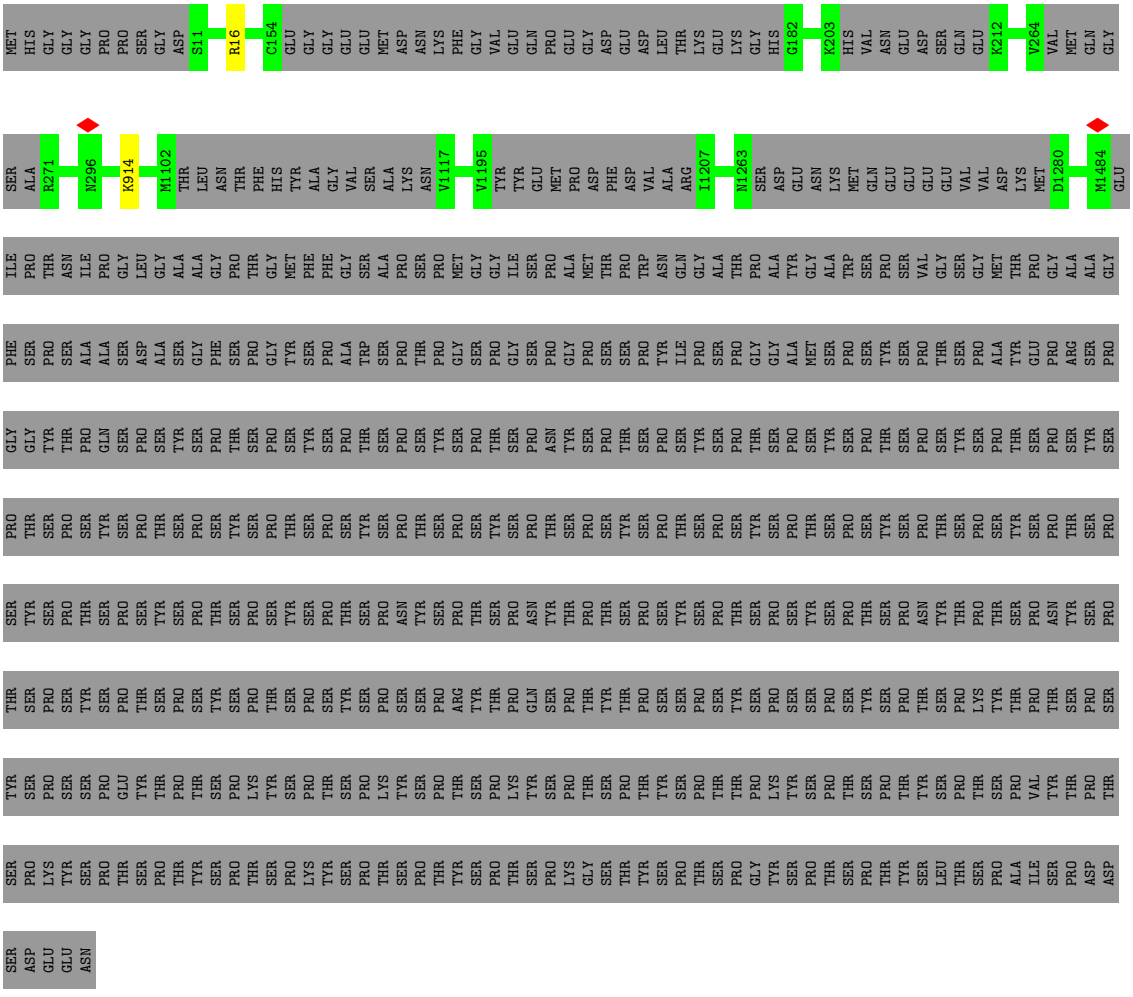
Mol	Chain	Residues	Atoms	AltConf
36	q	2	Total Mn 2 2	0

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.

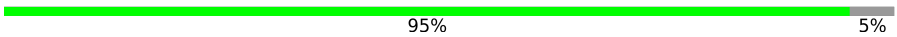
• Molecule 1: DNA-directed RNA polymerase subunit

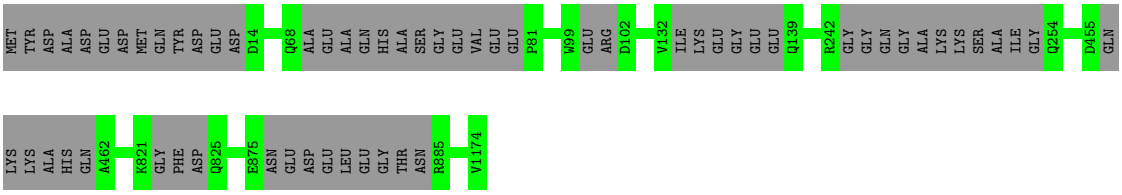
Chain A:



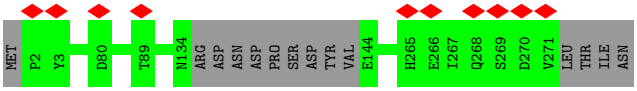
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:

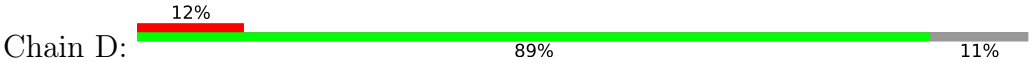


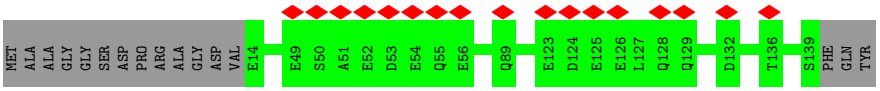


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



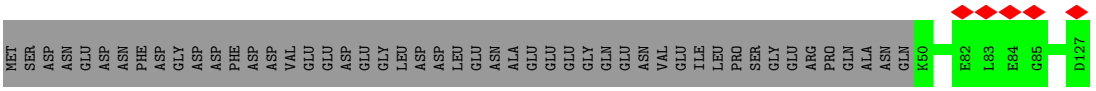
• Molecule 4: RNA polymerase II subunit D



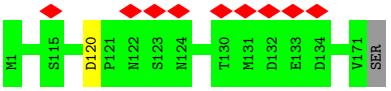


• Molecule 5: DNA-directed RNA polymerase II subunit E

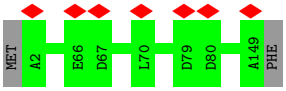
• Molecule 6: DNA-directed RNA polymerase II subunit F



• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

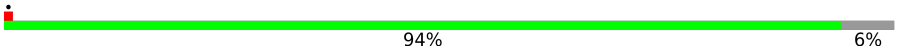


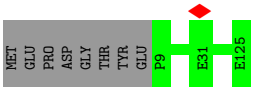
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

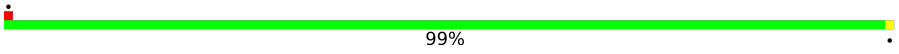
Chain I:

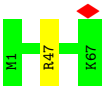




• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

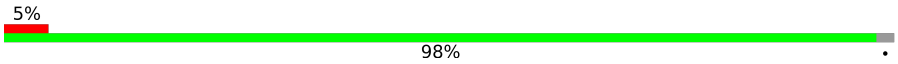
Chain J:

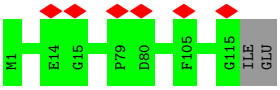




• Molecule 11: RNA_pol_L_2 domain-containing protein

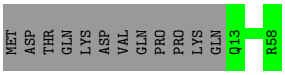
Chain K:





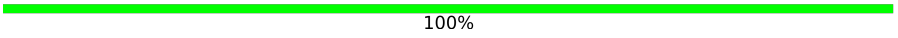
• Molecule 12: RNA polymerase II subunit K

Chain L:



• Molecule 13: RPBI C-terminal domain peptide

Chain M:



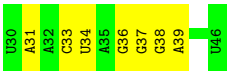
There are no outlier residues recorded for this chain.

• Molecule 14: Non-template DNA

Chain N:

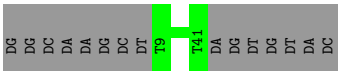
• Molecule 15: TAR RNA

Chain P:



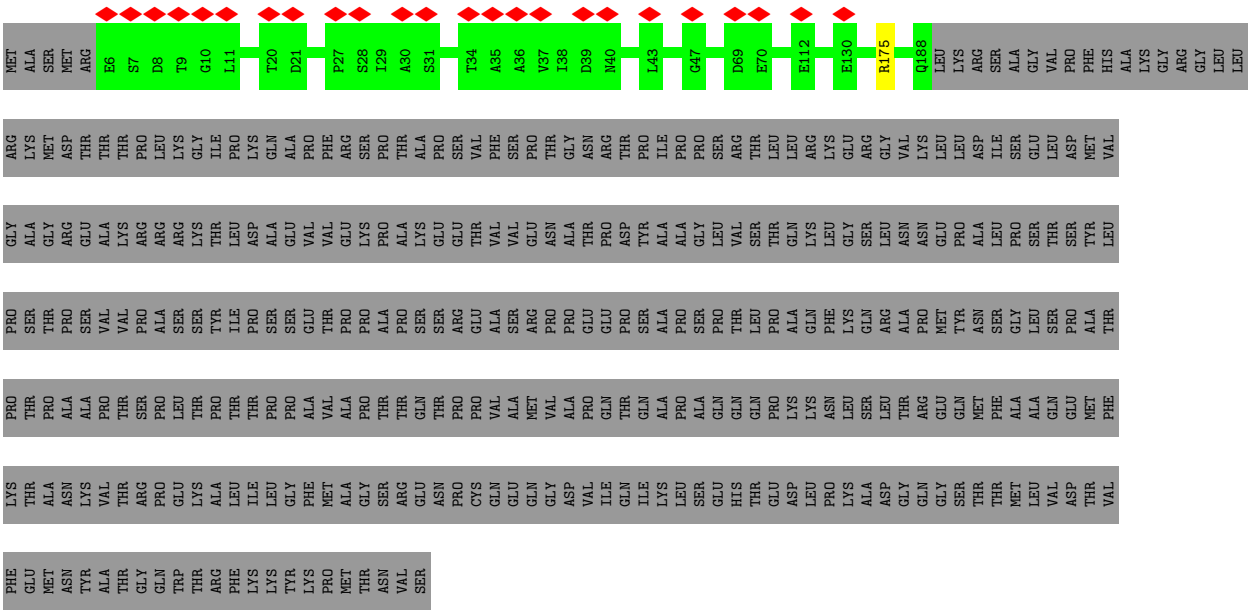
• Molecule 16: DNA Template

Chain T:



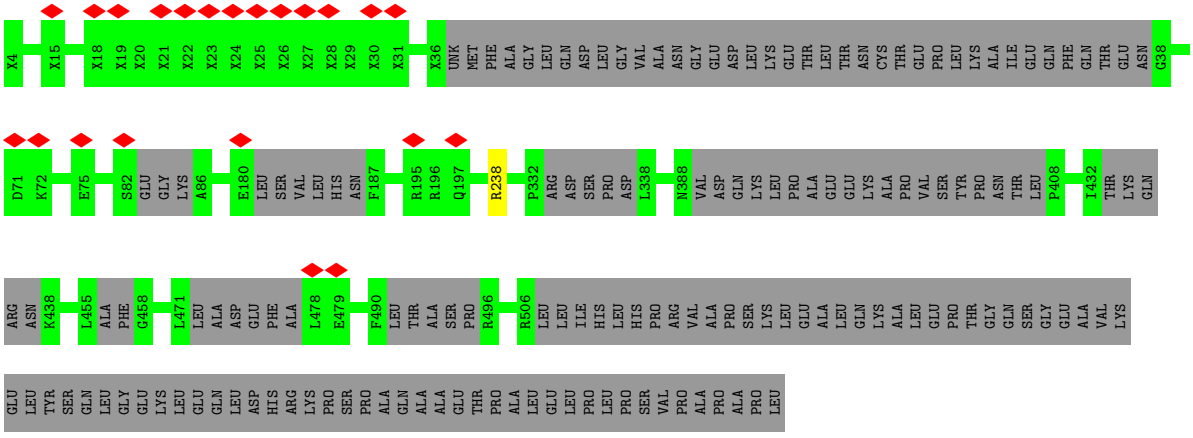
• Molecule 17: Negative elongation factor A

Chain U:



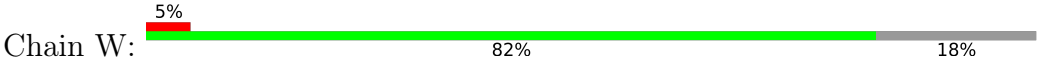
• Molecule 18: Negative elongation factor B

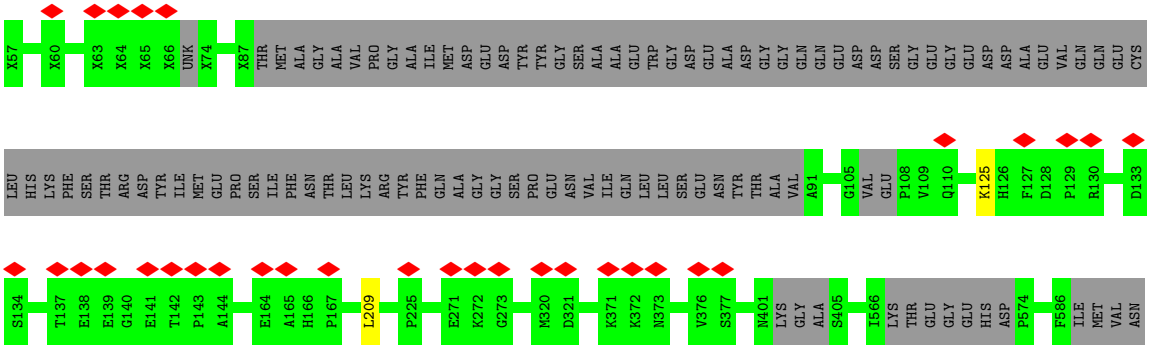
Chain V:



• Molecule 19: Negative elongation factor C/D

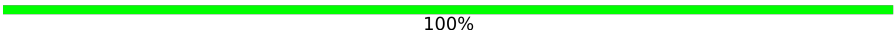
Chain W:





• Molecule 20: Negative elongation factor E

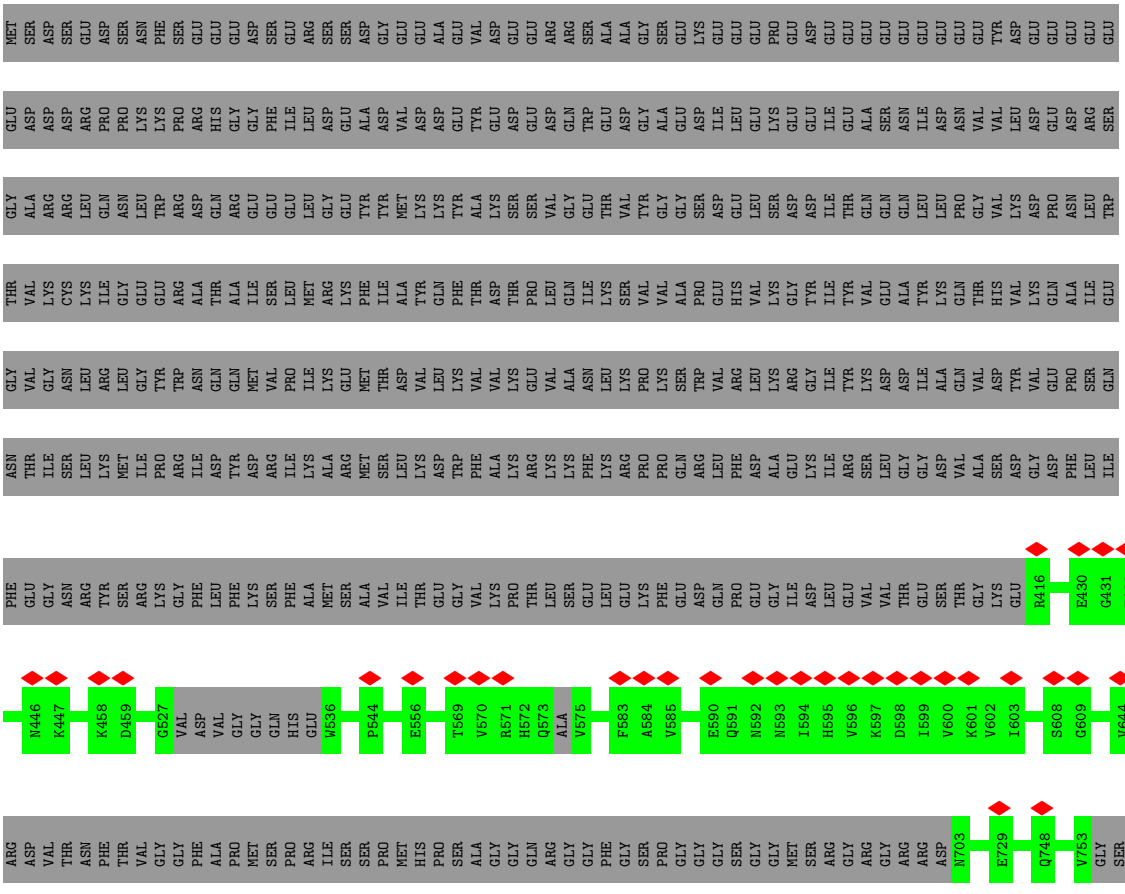
Chain X:

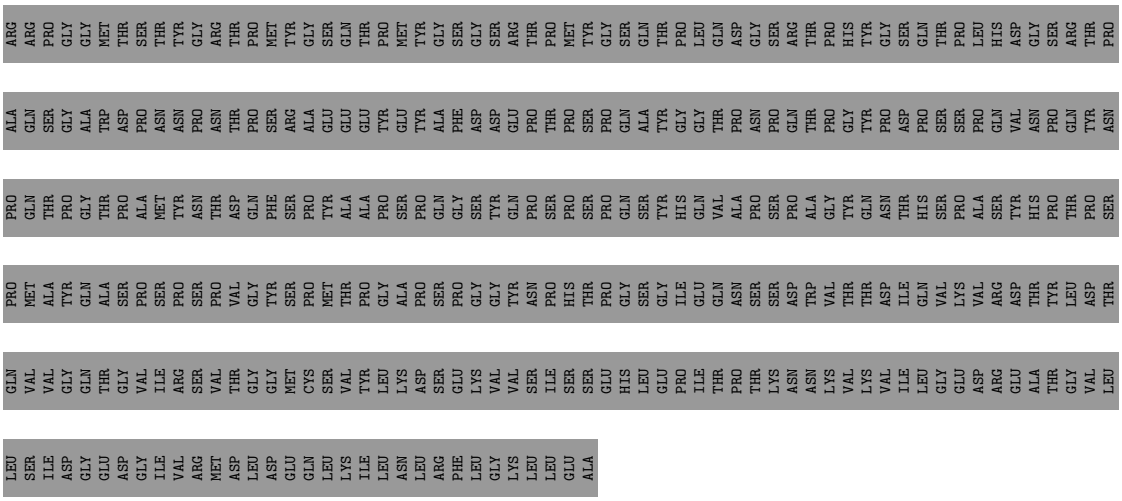


There are no outlier residues recorded for this chain.

• Molecule 21: Transcription elongation factor SPT5

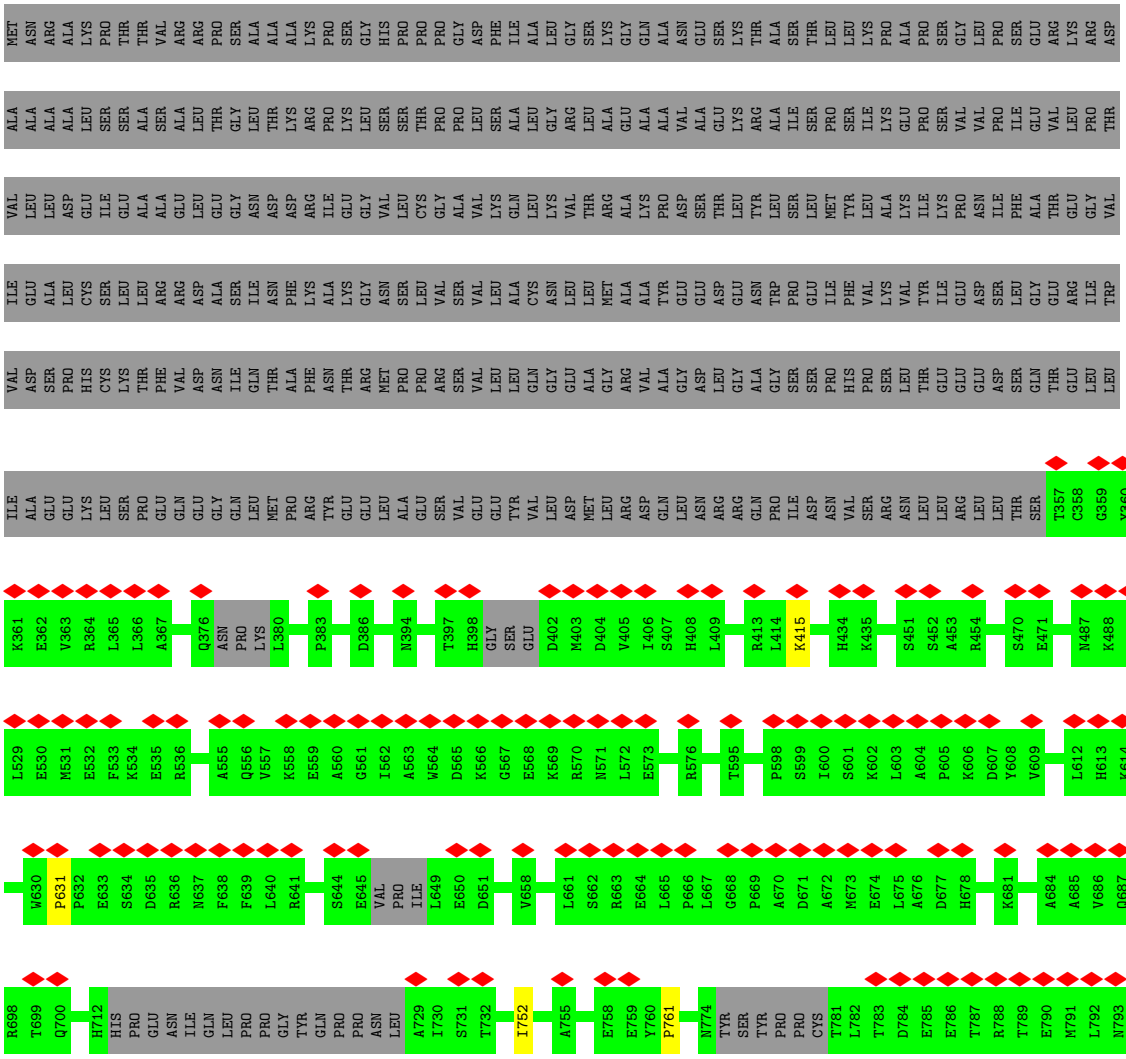
Chain Z:

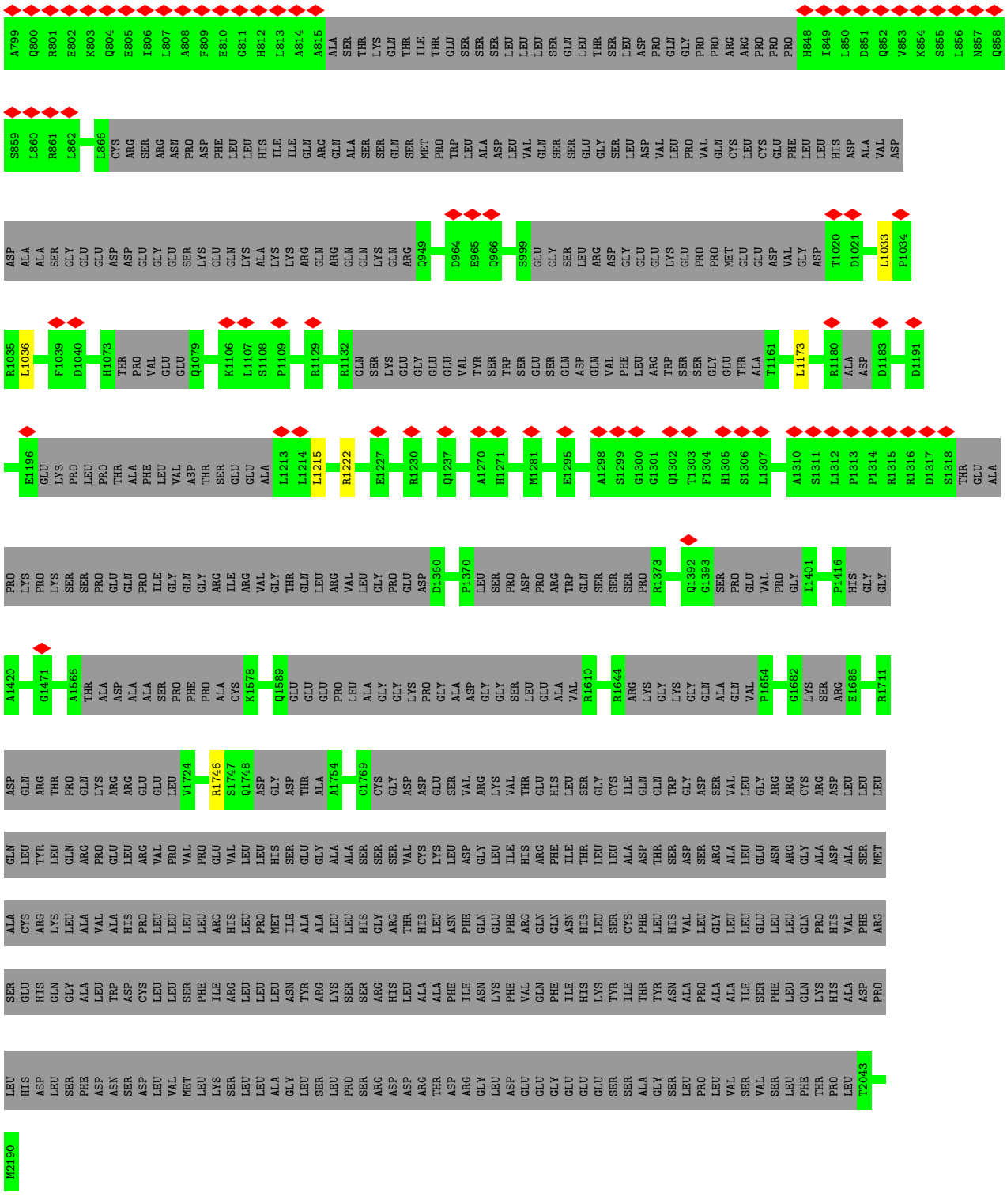




• Molecule 22: Integrator complex subunit 1

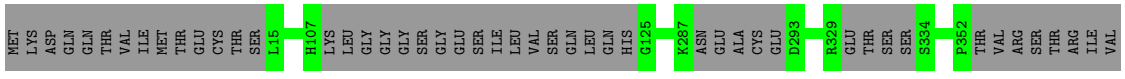
Chain a:

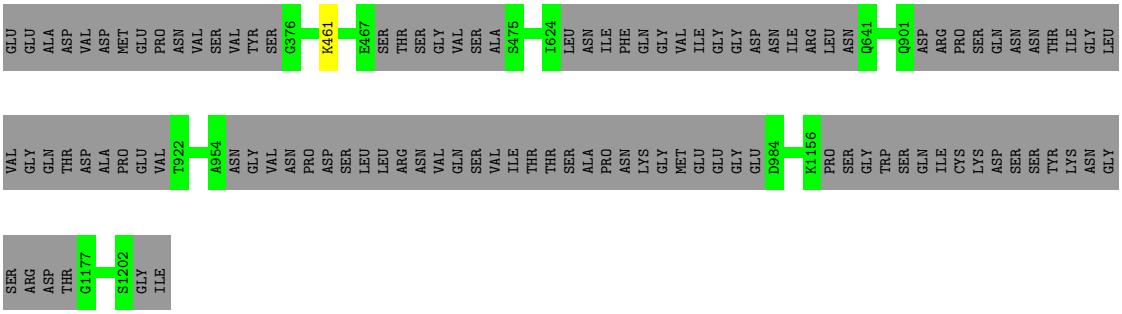




• Molecule 23: Integrator complex subunit 2

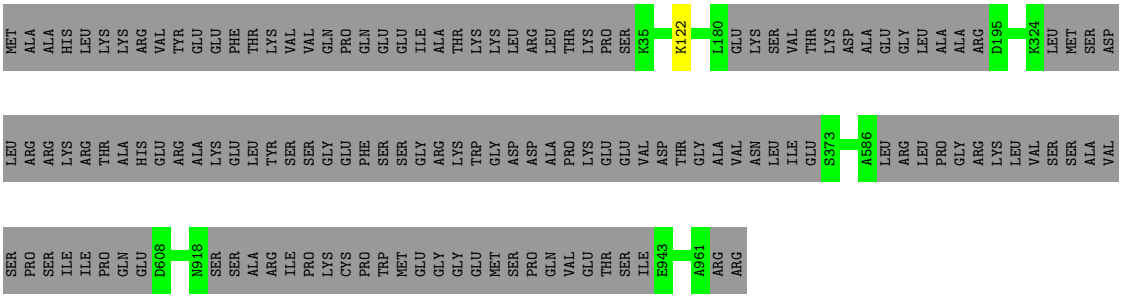
Chain b:





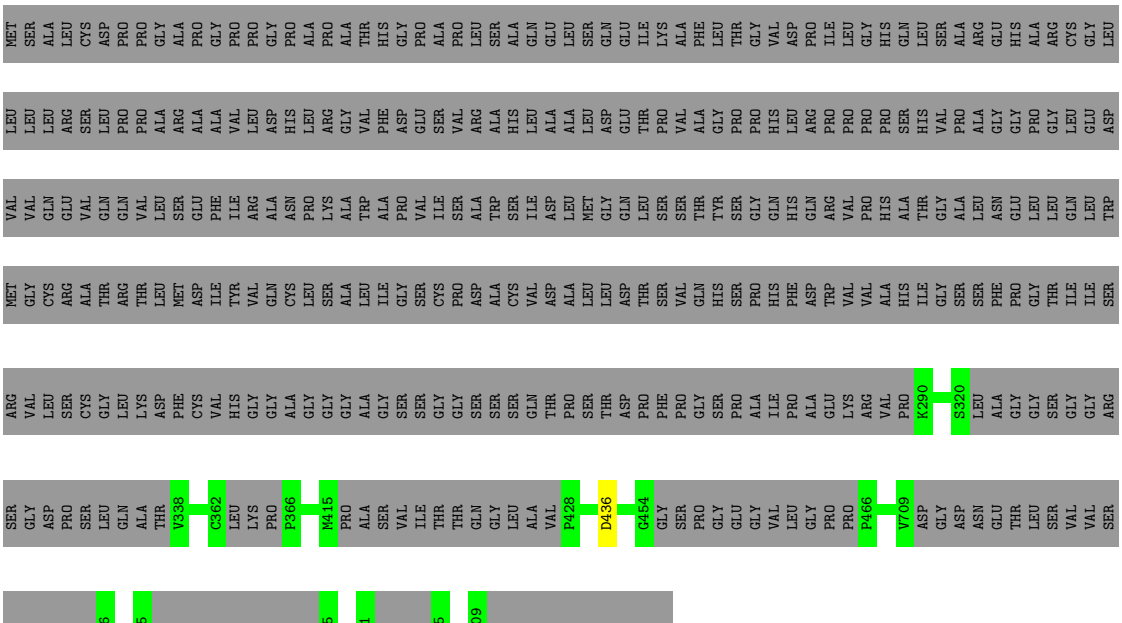
• Molecule 24: Integrator complex subunit 4

Chain d:



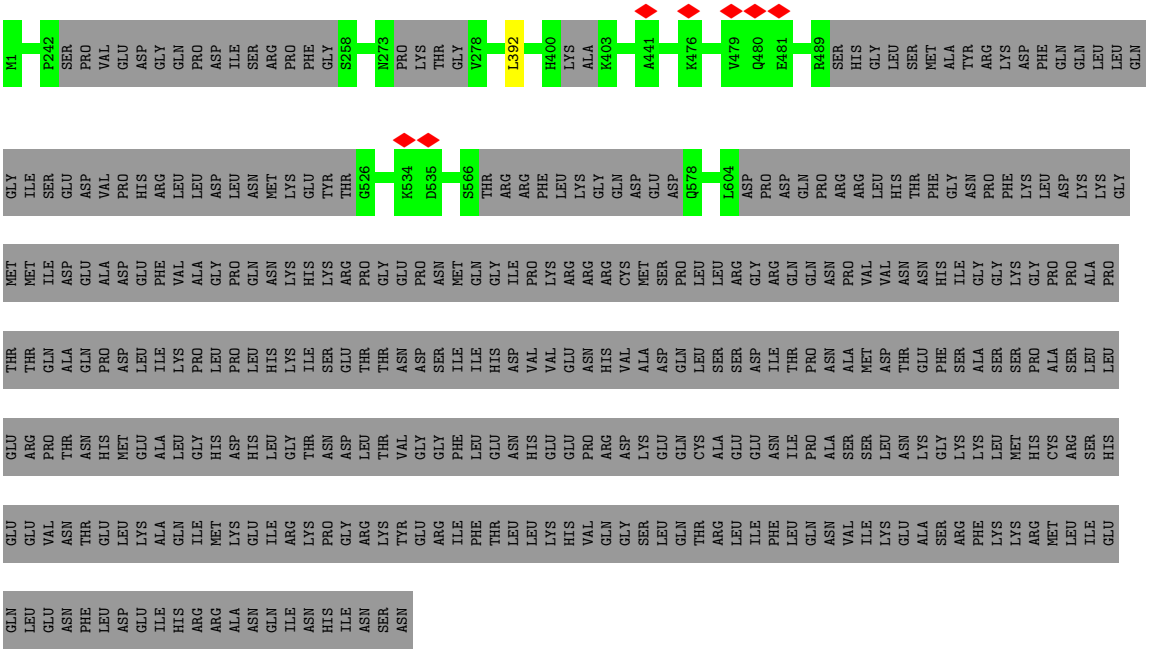
• Molecule 25: Integrator complex subunit 5

Chain e:



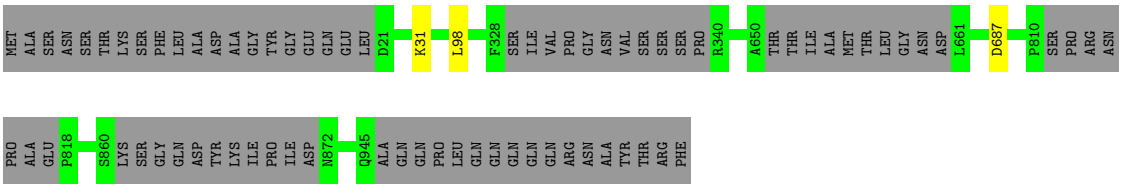
• Molecule 26: Integrator complex subunit 6

Chain f:



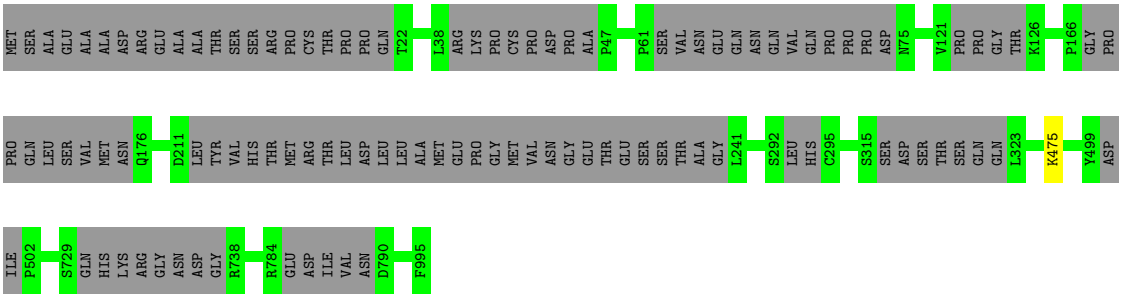
• Molecule 27: Integrator complex subunit 7

Chain g:



• Molecule 28: Integrator complex subunit 8

Chain h:

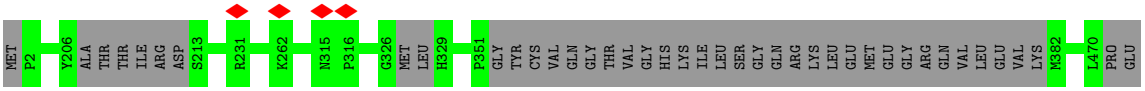


• Molecule 29: Integrator complex subunit 9

Chain i:

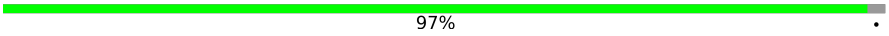
• Molecule 30: Integrator complex subunit 11

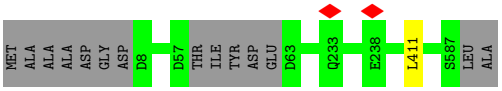
Chain k:



• Molecule 31: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform

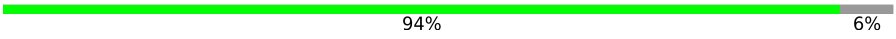
Chain p:





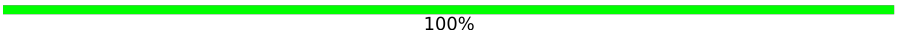
• Molecule 32: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain q:



• Molecule 33: Unknown

Chain u:



There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	614283	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	46.18	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.203	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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	0/11210	0.54	0/15130
2	B	0.31	0/9076	0.55	0/12250
3	C	0.33	0/2139	0.53	0/2906
4	D	0.27	0/988	0.62	0/1333
5	E	0.28	0/1752	0.54	0/2366
6	F	0.30	0/637	0.56	0/859
7	G	0.28	0/1347	0.55	1/1833 (0.1%)
8	H	0.31	0/1207	0.56	0/1628
9	I	0.30	0/967	0.58	0/1309
10	J	0.33	0/542	0.57	0/730
11	K	0.31	0/939	0.53	0/1271
12	L	0.35	0/389	0.67	0/517
13	M	0.29	0/100	0.42	0/139
14	N	0.52	0/547	0.93	0/838
15	P	0.28	0/403	0.94	0/625
16	T	0.52	0/764	0.98	0/1179
17	U	0.26	0/1422	0.56	0/1933
18	V	0.23	0/1912	0.45	0/2453
19	W	0.26	0/3812	0.52	1/5186 (0.0%)
21	Z	0.26	0/2206	0.54	0/2968
22	a	0.27	0/8430	0.58	2/11494 (0.0%)
23	b	0.28	0/8065	0.53	0/10992
24	d	0.28	0/6535	0.53	0/8877
25	e	0.28	0/4775	0.53	1/6511 (0.0%)
26	f	0.29	0/4179	0.55	1/5705 (0.0%)
27	g	0.29	0/6817	0.54	2/9246 (0.0%)
28	h	0.29	0/6867	0.51	0/9329
29	i	0.31	0/4360	0.54	1/5957 (0.0%)
30	k	0.29	0/3408	0.53	0/4632
31	p	0.27	0/4460	0.57	1/6064 (0.0%)
32	q	0.30	0/2378	0.54	0/3228
33	u	0.24	0/15	0.26	0/20

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	0.29	0/102648	0.55	10/139508 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
22	a	0	1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	g	687	ASP	CB-CG-OD2	7.46	125.01	118.30
22	a	1036	LEU	CA-CB-CG	7.46	132.45	115.30
22	a	1173	LEU	CA-CB-CG	7.37	132.25	115.30
19	W	209	LEU	CA-CB-CG	7.21	131.87	115.30
31	p	411	LEU	CA-CB-CG	7.01	131.43	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	a	1033	LEU	Peptide

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	1378/1970 (70%)	1351 (98%)	27 (2%)	0	100	100
2	B	1096/1174 (93%)	1066 (97%)	30 (3%)	0	100	100
3	C	257/275 (94%)	252 (98%)	5 (2%)	0	100	100
4	D	124/142 (87%)	119 (96%)	5 (4%)	0	100	100
5	E	207/210 (99%)	202 (98%)	5 (2%)	0	100	100
6	F	76/127 (60%)	76 (100%)	0	0	100	100
7	G	169/172 (98%)	155 (92%)	14 (8%)	0	100	100
8	H	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
9	I	115/125 (92%)	109 (95%)	6 (5%)	0	100	100
10	J	65/67 (97%)	65 (100%)	0	0	100	100
11	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
12	L	44/58 (76%)	39 (89%)	5 (11%)	0	100	100
13	M	11/13 (85%)	11 (100%)	0	0	100	100
17	U	181/528 (34%)	174 (96%)	7 (4%)	0	100	100
18	V	400/614 (65%)	366 (92%)	34 (8%)	0	100	100
19	W	476/616 (77%)	455 (96%)	21 (4%)	0	100	100
21	Z	265/1087 (24%)	250 (94%)	15 (6%)	0	100	100
22	a	1177/2190 (54%)	1103 (94%)	69 (6%)	5 (0%)	34	71
23	b	1027/1204 (85%)	977 (95%)	50 (5%)	0	100	100
24	d	810/963 (84%)	784 (97%)	26 (3%)	0	100	100
25	e	633/1019 (62%)	609 (96%)	24 (4%)	0	100	100
26	f	524/887 (59%)	506 (97%)	18 (3%)	0	100	100
27	g	876/962 (91%)	842 (96%)	34 (4%)	0	100	100
28	h	865/995 (87%)	825 (95%)	40 (5%)	0	100	100
29	i	544/658 (83%)	516 (95%)	28 (5%)	0	100	100
30	k	448/600 (75%)	423 (94%)	25 (6%)	0	100	100
31	p	571/589 (97%)	556 (97%)	15 (3%)	0	100	100
32	q	288/309 (93%)	276 (96%)	12 (4%)	0	100	100
33	u	1/27 (4%)	1 (100%)	0	0	100	100
All	All	12887/17848 (72%)	12361 (96%)	521 (4%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	a	631	PRO
22	a	761	PRO
22	a	415	LYS
22	a	1215	LEU
22	a	752	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1223/1749 (70%)	1221 (100%)	2 (0%)	93 98
2	B	978/1027 (95%)	978 (100%)	0	100 100
3	C	238/252 (94%)	238 (100%)	0	100 100
4	D	101/126 (80%)	101 (100%)	0	100 100
5	E	191/192 (100%)	189 (99%)	2 (1%)	76 88
6	F	68/111 (61%)	68 (100%)	0	100 100
7	G	141/153 (92%)	141 (100%)	0	100 100
8	H	129/131 (98%)	129 (100%)	0	100 100
9	I	104/112 (93%)	104 (100%)	0	100 100
10	J	56/56 (100%)	55 (98%)	1 (2%)	59 81
11	K	104/106 (98%)	104 (100%)	0	100 100
12	L	42/55 (76%)	42 (100%)	0	100 100
13	M	13/13 (100%)	13 (100%)	0	100 100
17	U	155/451 (34%)	154 (99%)	1 (1%)	86 94
18	V	49/515 (10%)	48 (98%)	1 (2%)	55 79
19	W	398/514 (77%)	397 (100%)	1 (0%)	92 97
21	Z	243/940 (26%)	243 (100%)	0	100 100
22	a	684/1907 (36%)	682 (100%)	2 (0%)	92 97
23	b	859/1072 (80%)	858 (100%)	1 (0%)	93 98
24	d	704/845 (83%)	703 (100%)	1 (0%)	93 98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
25	e	444/812 (55%)	444 (100%)	0	100 100
26	f	431/796 (54%)	431 (100%)	0	100 100
27	g	719/840 (86%)	718 (100%)	1 (0%)	93 98
28	h	700/896 (78%)	699 (100%)	1 (0%)	93 98
29	i	482/600 (80%)	482 (100%)	0	100 100
30	k	317/520 (61%)	317 (100%)	0	100 100
31	p	480/512 (94%)	480 (100%)	0	100 100
32	q	251/274 (92%)	250 (100%)	1 (0%)	91 97
33	u	1/1 (100%)	1 (100%)	0	100 100
All	All	10305/15578 (66%)	10290 (100%)	15 (0%)	93 98

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	W	125	LYS
28	h	475	LYS
22	a	1222	ARG
32	q	144	LYS
24	d	122	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	260	GLN
19	W	95	ASN
23	b	622	GLN
28	h	988	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	16/17 (94%)	6 (37%)	1 (6%)

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	31	A

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Mol	Chain	Res	Type
15	P	33	C
15	P	34	U
15	P	36	G
15	P	37	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	38	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 13 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.

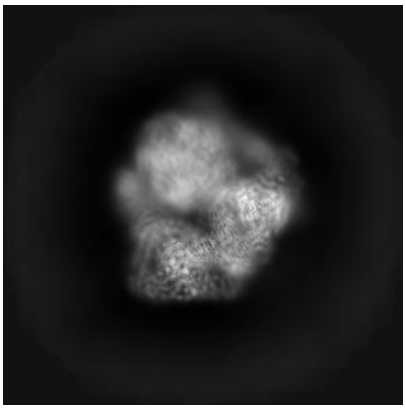
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13479. These allow visual inspection of the internal detail of the map and identification of artifacts.

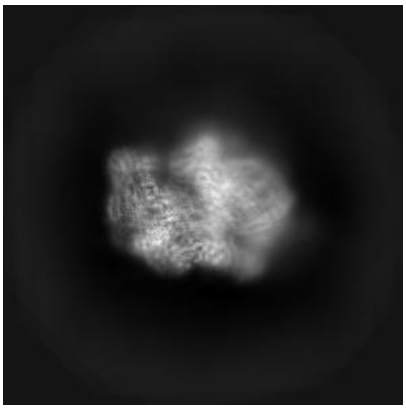
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

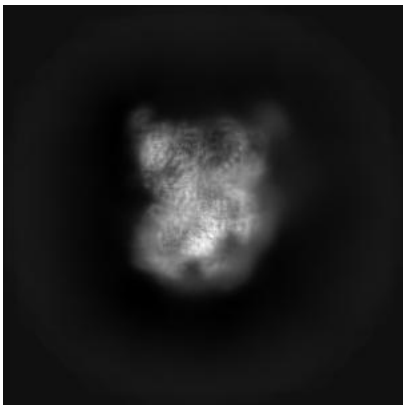
6.1.1 Primary map



X

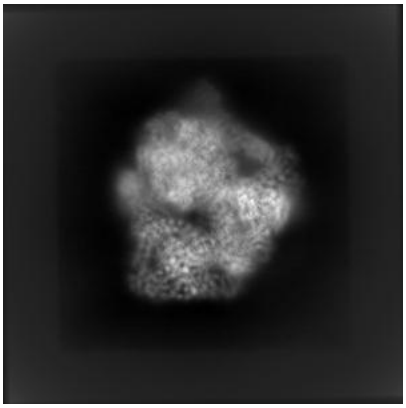


Y

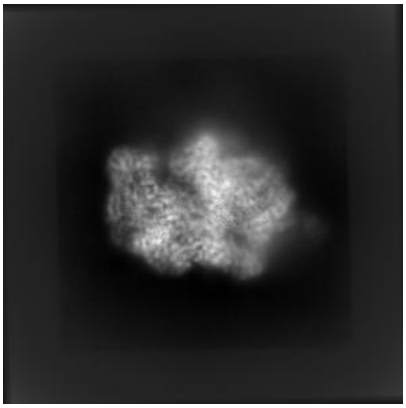


Z

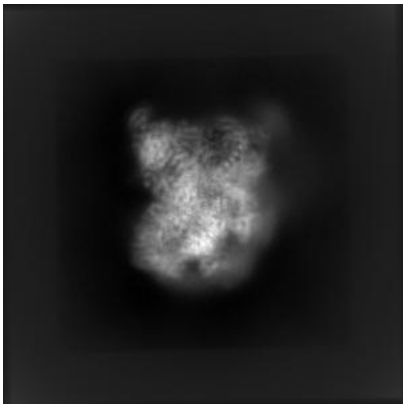
6.1.2 Raw map



X



Y

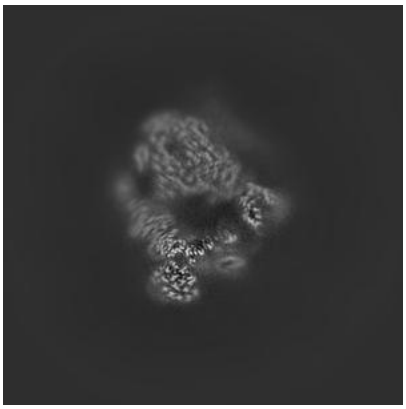


Z

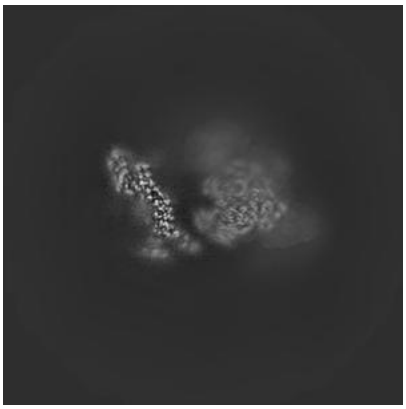
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

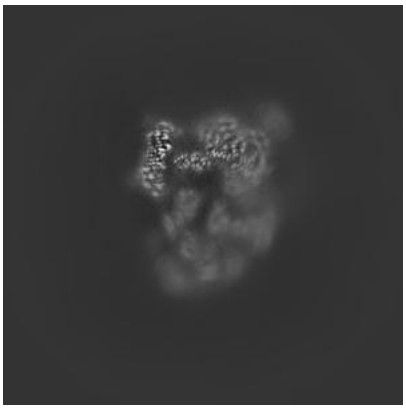
6.2.1 Primary map



X Index: 240

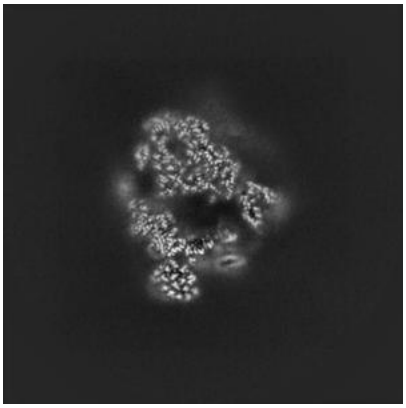


Y Index: 240

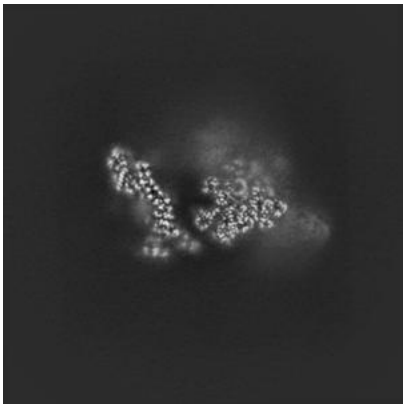


Z Index: 240

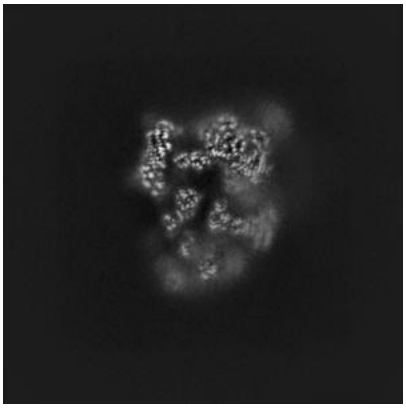
6.2.2 Raw map



X Index: 240



Y Index: 240

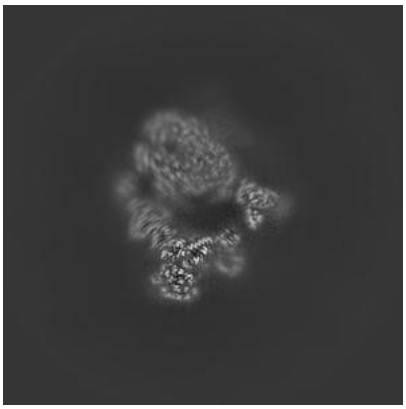


Z Index: 240

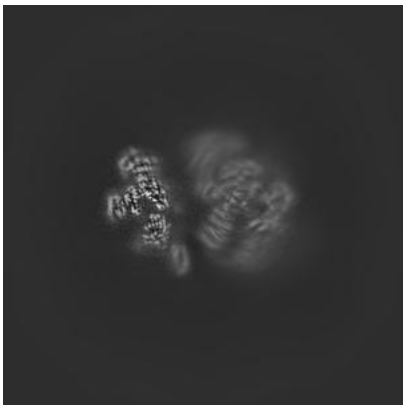
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

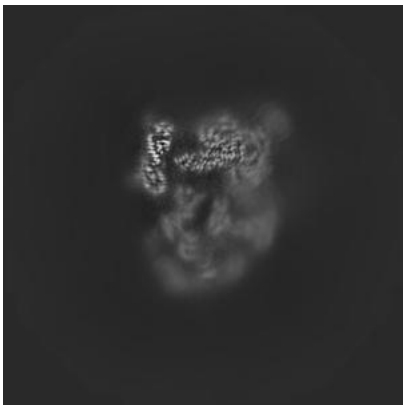
6.3.1 Primary map



X Index: 244

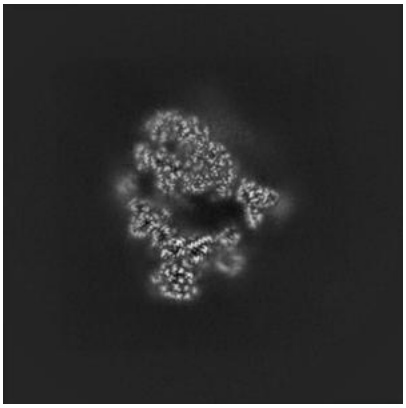


Y Index: 211

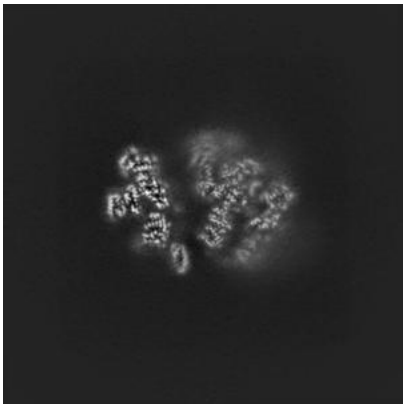


Z Index: 243

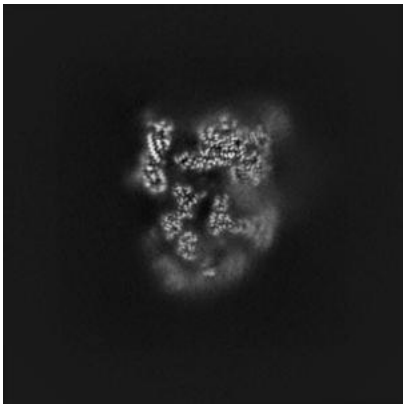
6.3.2 Raw map



X Index: 244



Y Index: 211

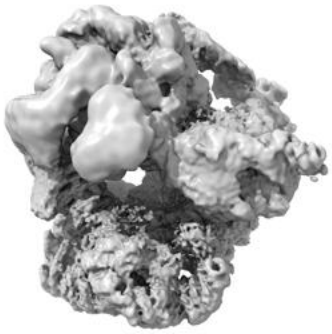


Z Index: 244

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

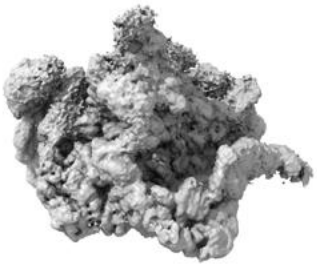
Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

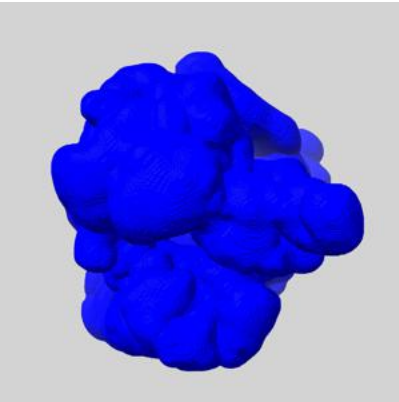
6.5 Mask visualisation (i)

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

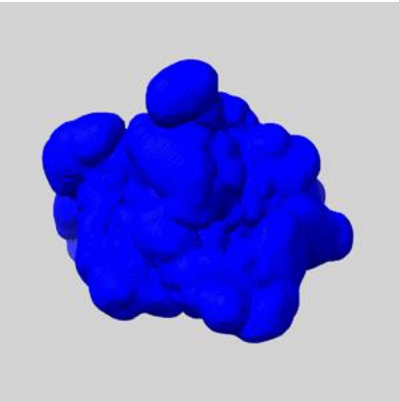
A mask typically either:

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

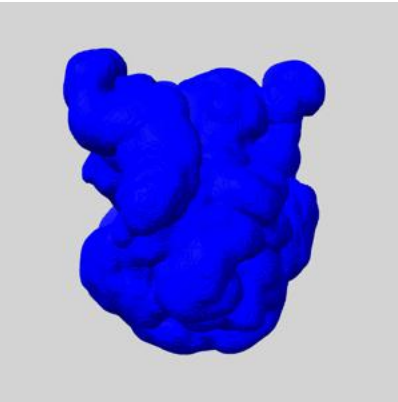
6.5.1 emd_13479_msk_1.map (i)



X



Y

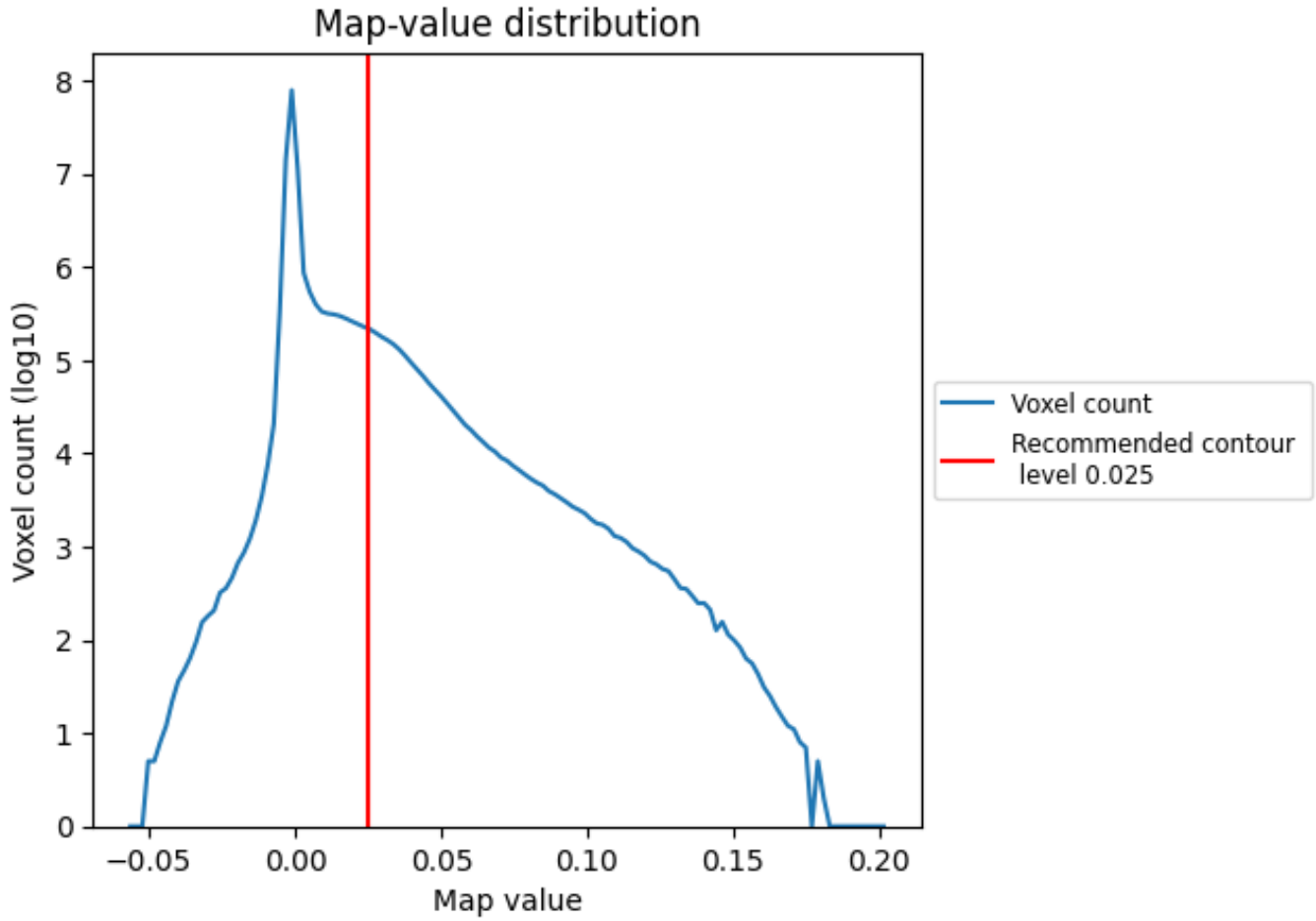


Z

7 Map analysis

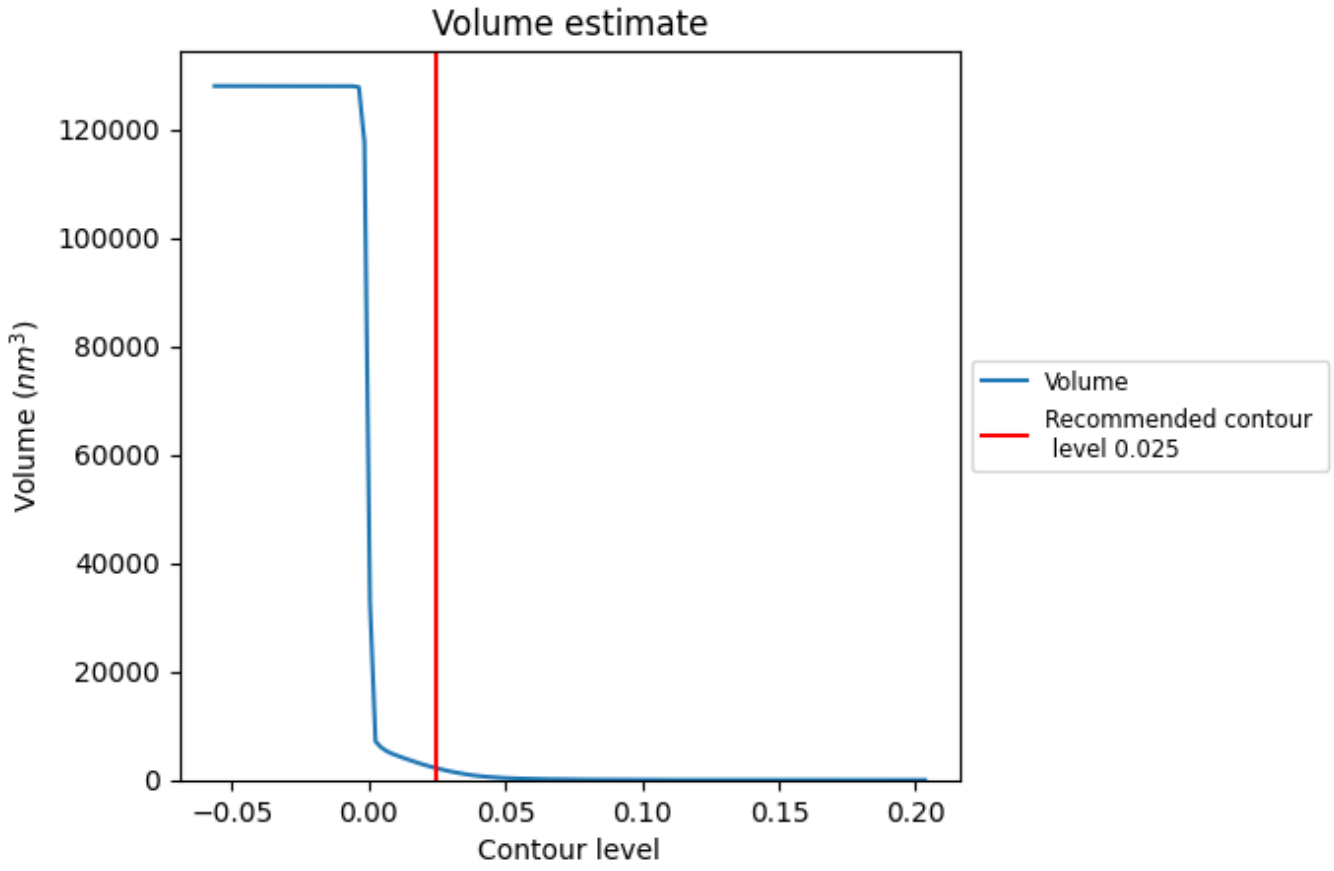
This section contains the results of statistical analysis of the map.

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.

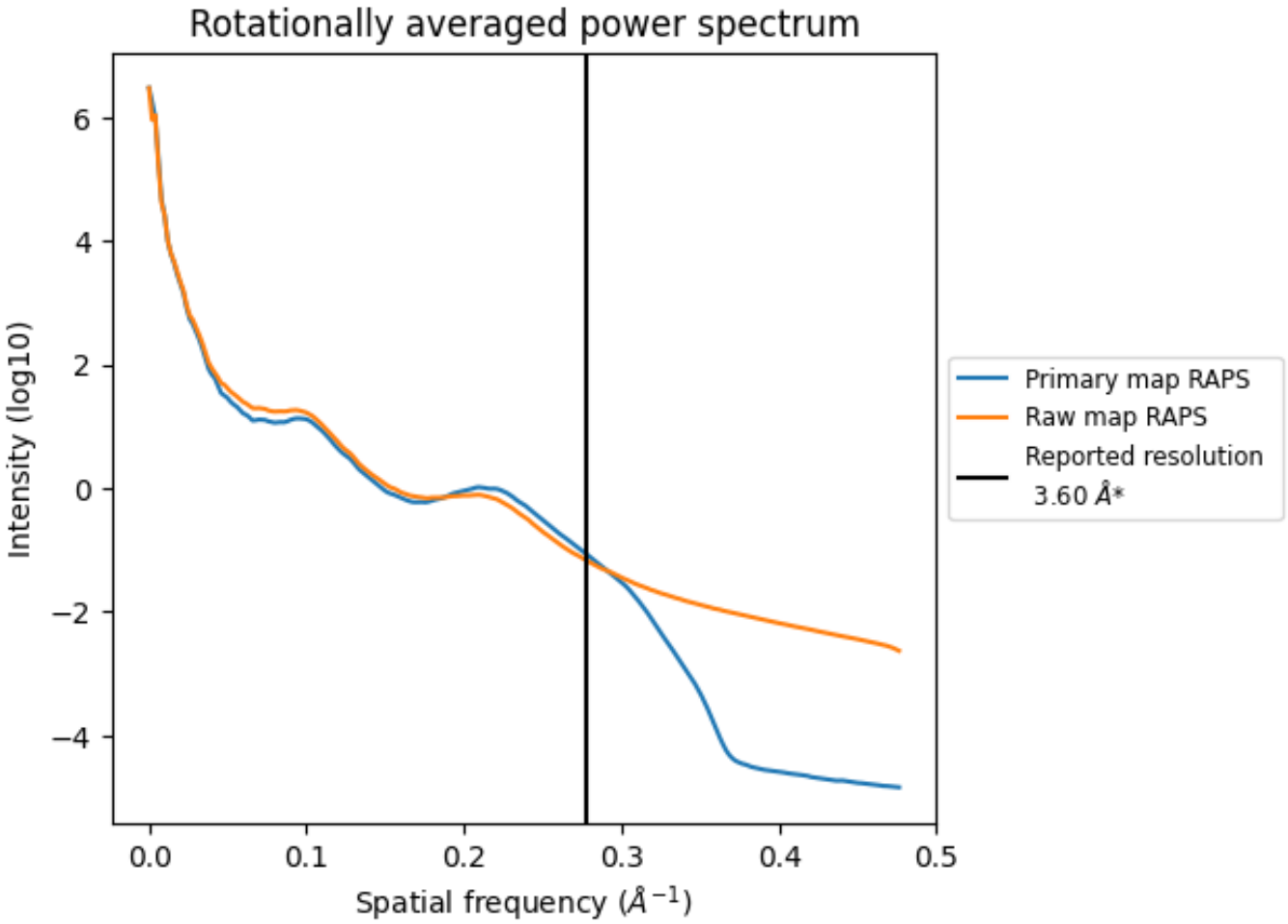
7.2 Volume estimate (i)



The volume at the recommended contour level is 2154 nm^3; this corresponds to an approximate mass of 1946 kDa.

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

7.3 Rotationally averaged power spectrum (i)

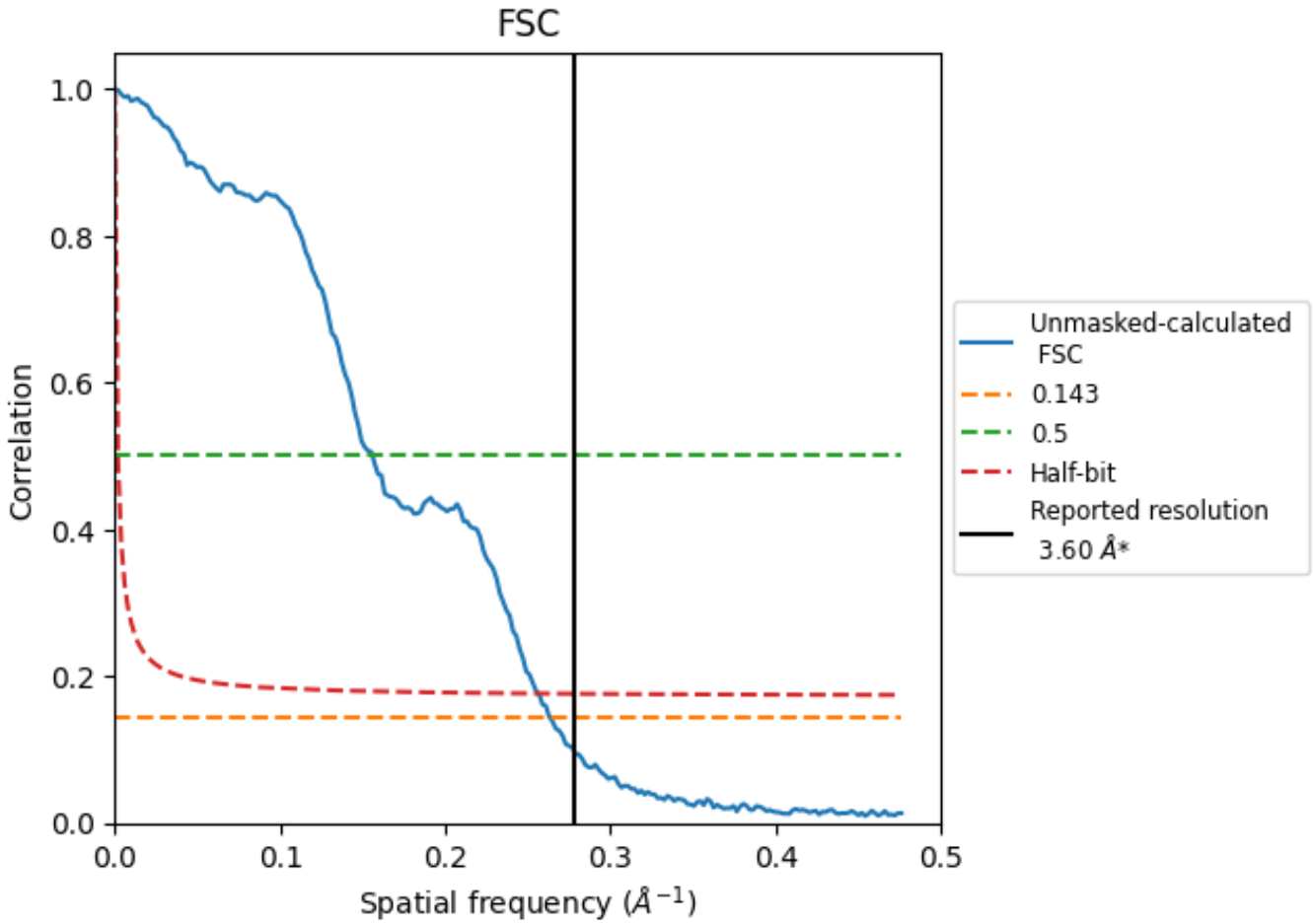


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

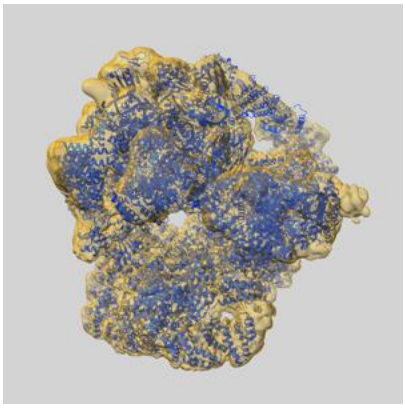
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	6.41	3.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

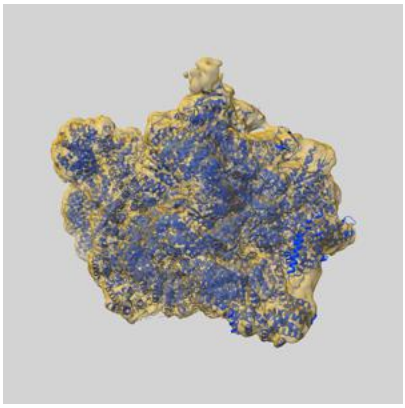
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13479 and PDB model 7PKS. Per-residue inclusion information can be found in section 3 on page 11.

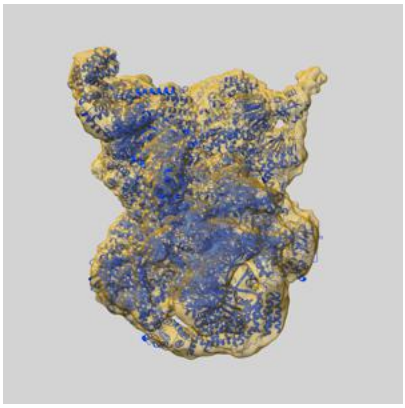
9.1 Map-model overlay



X



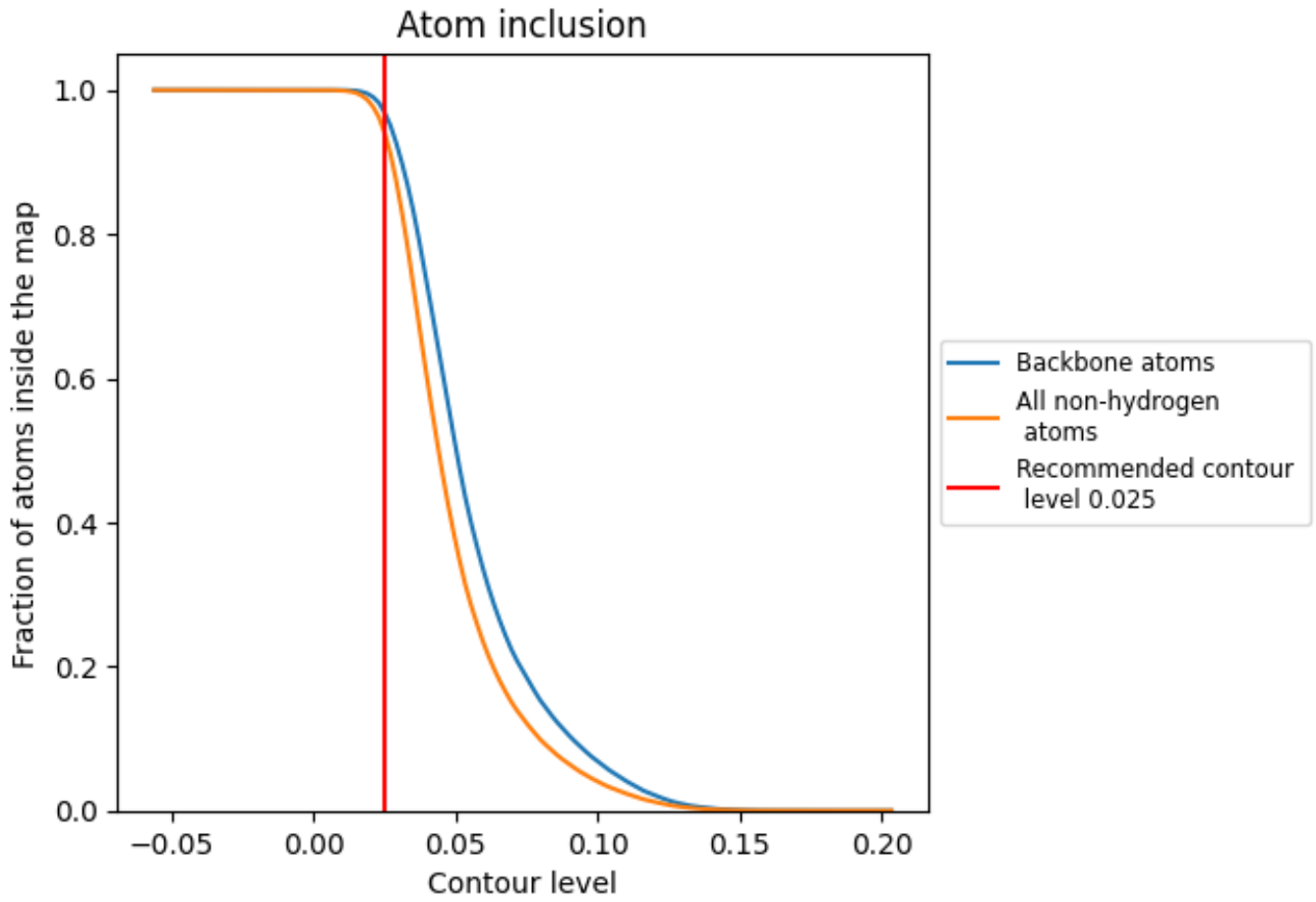
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.