wwPDB EM Validation Summary Report

Apr 30, 2024 – 08:33 pm BST

PDB ID	:	4V1N
EMDB ID	:	EMD-2785
Title	:	Architecture of the RNA polymerase II-Mediator core transcription initiation complex
Authors	:	Plaschka, C.; Lariviere, L.; Wenzeck, L.; Hemann, M.; Tegunov, D.; Petrotchenko, E.V.; Borchers, C.H.; Baumeister, W.; Herzog, F.; Villa, E.; Cramer, P.
Deposited on	:	2014-09-29
Resolution	:	7.80 Å(reported)

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 ⓘ 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:

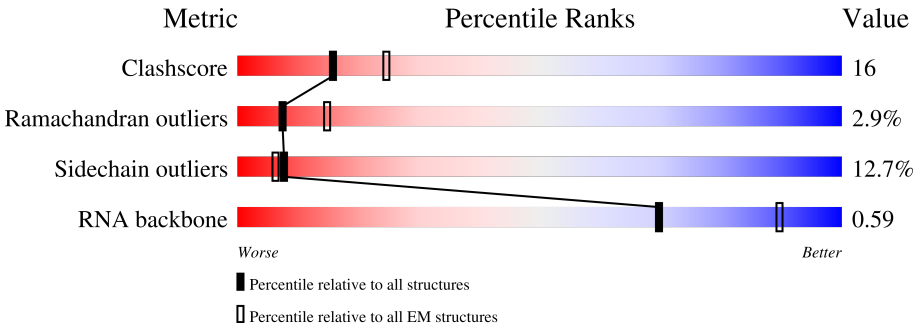
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 7.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
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	1733	7% 55% 23% 18%
2	B	1224	13% 62% 28% 6%
3	C	318	8% 61% 18% 16%
4	D	221	29% 55% 20% 5% 19%
5	E	215	7% 74% 22%
6	F	155	36% 16% 46%
7	G	171	28% 72% 25%

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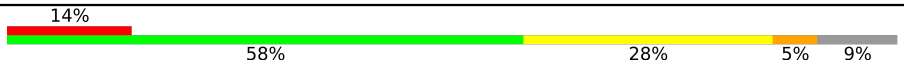
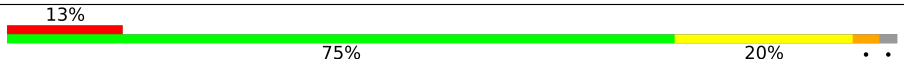
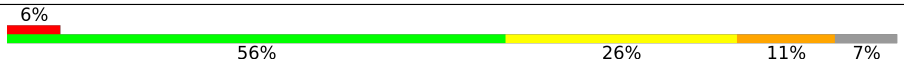
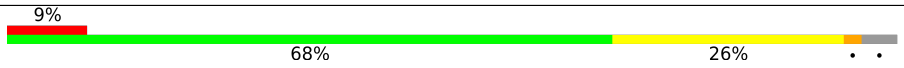
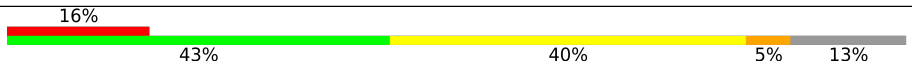
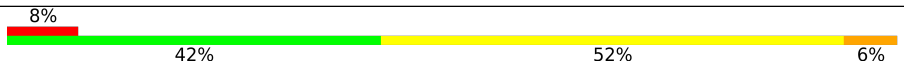
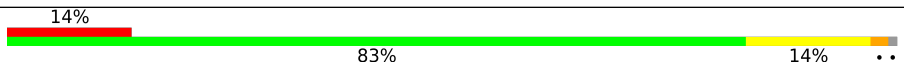
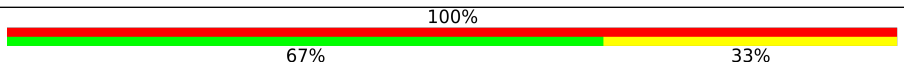
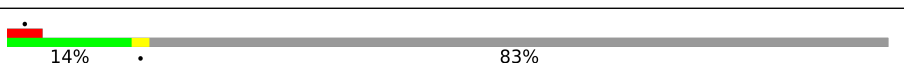
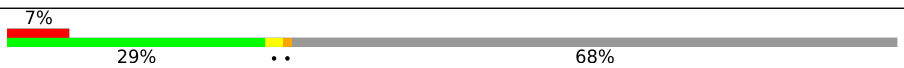
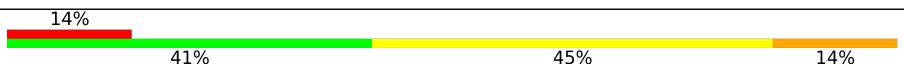
Mol	Chain	Length	Quality of chain
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	345	
14	N	50	
15	O	181	
16	P	6	
17	Q	734	
18	R	331	
19	T	58	

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 38446 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 II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1422	11174	7036	1954	2122	62	0	0

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1156	9140	5781	1606	1697	56	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	266	2095	1317	348	417	13	0	0

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	178	1434	887	257	288	2	0	0

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	214	1752	1111	309	321	11	0	0

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	84	Total	C	N	O	S	0	0
			679	434	115	127	3		

- 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
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1068	673	180	211	4		

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	119	Total	C	N	O	S	0	0
			971	596	179	186	10		

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	1
			920	590	157	171	2		

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			363	224	72	63	4		

- Molecule 13 is a protein called TRANSCRIPTION INITIATION FACTOR IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	300	Total	C	N	O	S	0	1
			2202	1384	380	423	15		

- Molecule 14 is a DNA chain called NONTEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	50	Total	C	N	O	P	0	0
			975	490	191	246	48		

- Molecule 15 is a protein called TATA-BOX-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	60	MET	-	expression tag	UNP P13393

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	6	Total	C	N	O	P	0	0
			123	57	22	39	5		

- Molecule 17 is a protein called TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	122	Total	C	N	O	0	0
			606	362	122	122		

- Molecule 18 is a protein called TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT BETA.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	105	Total	C	N	O	0	0
			521	311	105	105		

- Molecule 19 is a DNA chain called TEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	58	Total	C	N	O	P	0	0
			1125	568	206	294	57		

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
20	A	2	Total	Zn	0
			2	2	
20	B	1	Total	Zn	0
			1	1	
20	C	1	Total	Zn	0
			1	1	
20	I	2	Total	Zn	0
			2	2	
20	J	1	Total	Zn	0
			1	1	
20	L	1	Total	Zn	0
			1	1	
20	M	1	Total	Zn	0
			1	1	

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

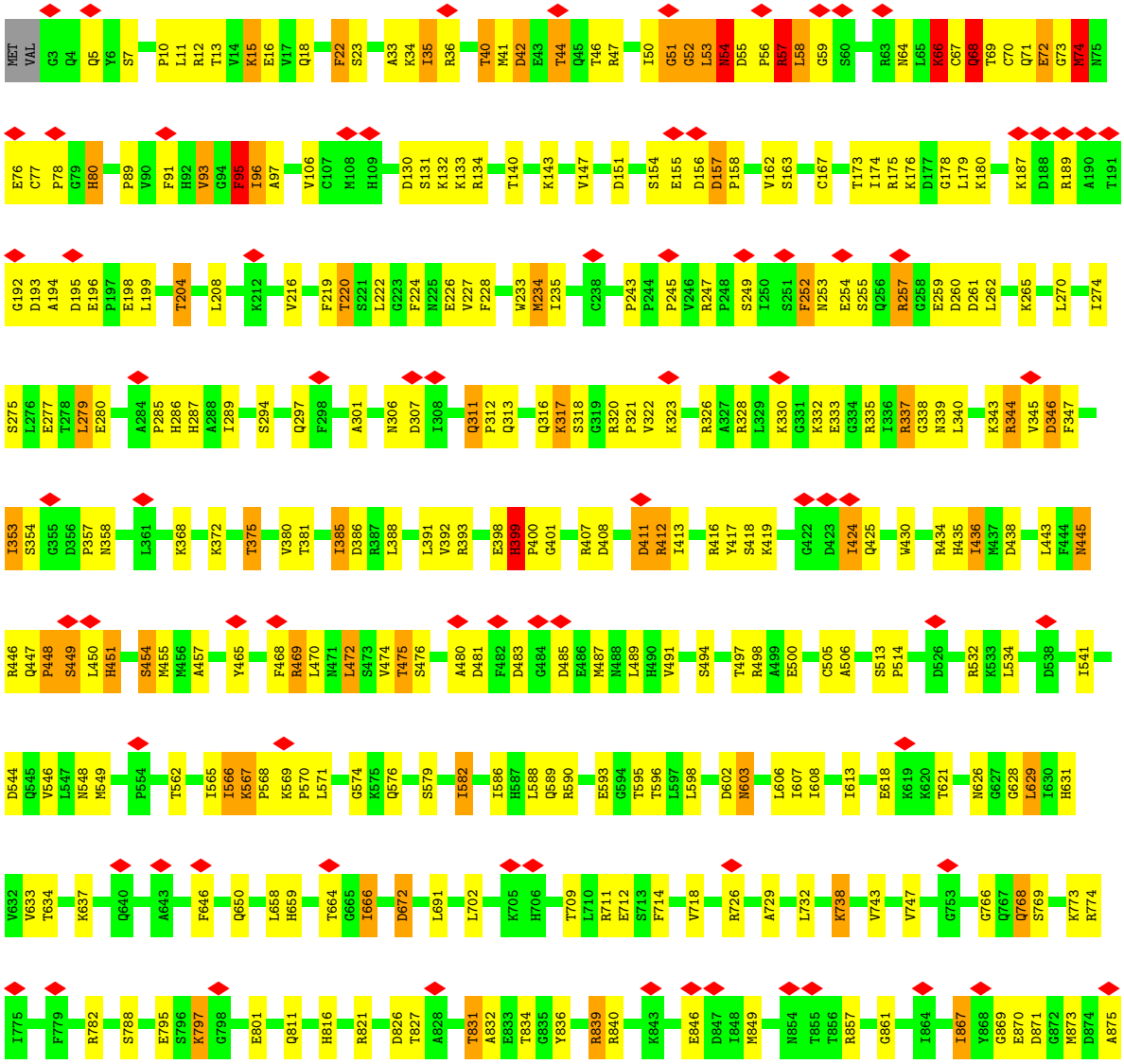
Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	Mg	0
			1	1	

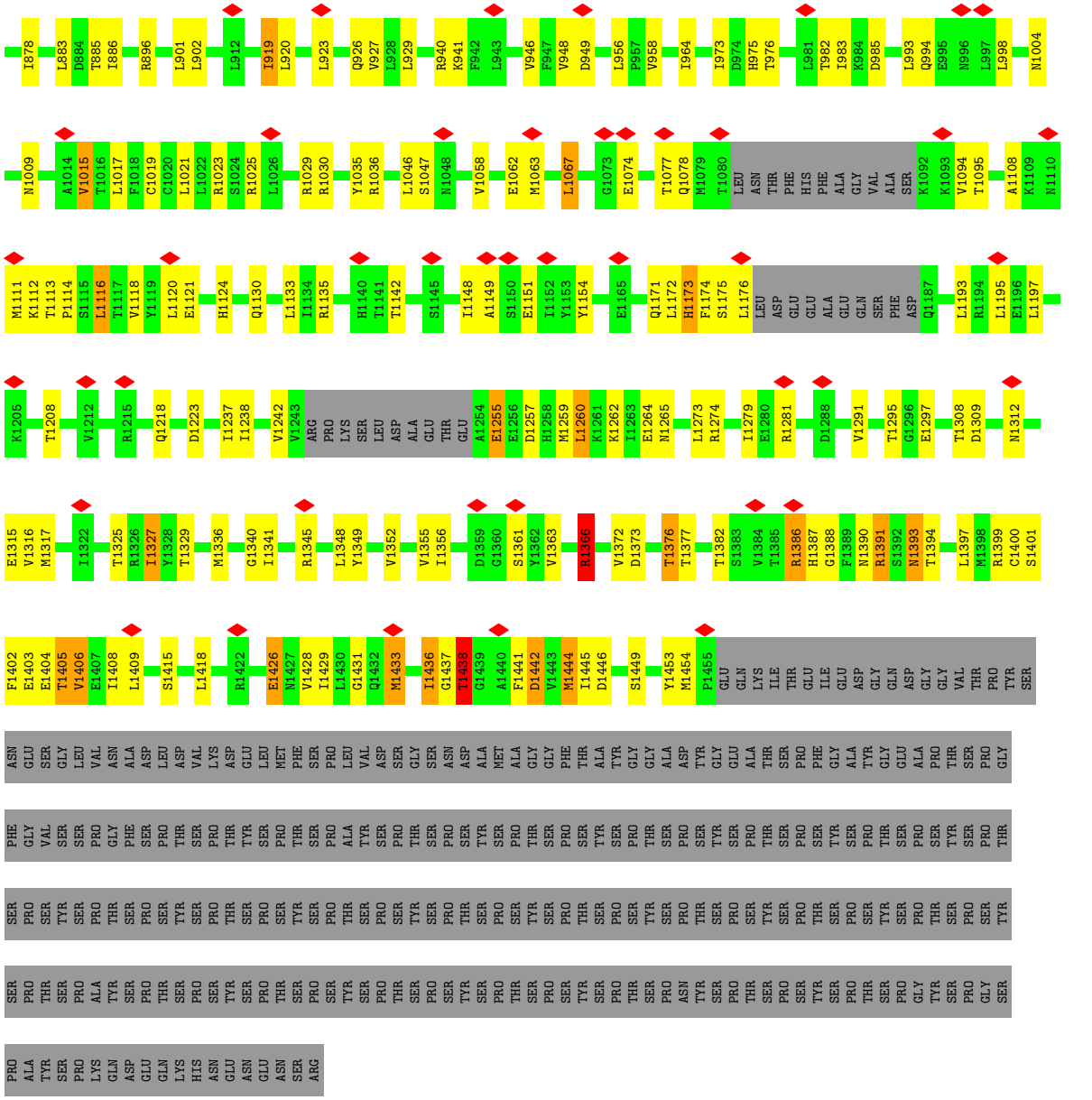
3 Residue-property plots (i)

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

• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1

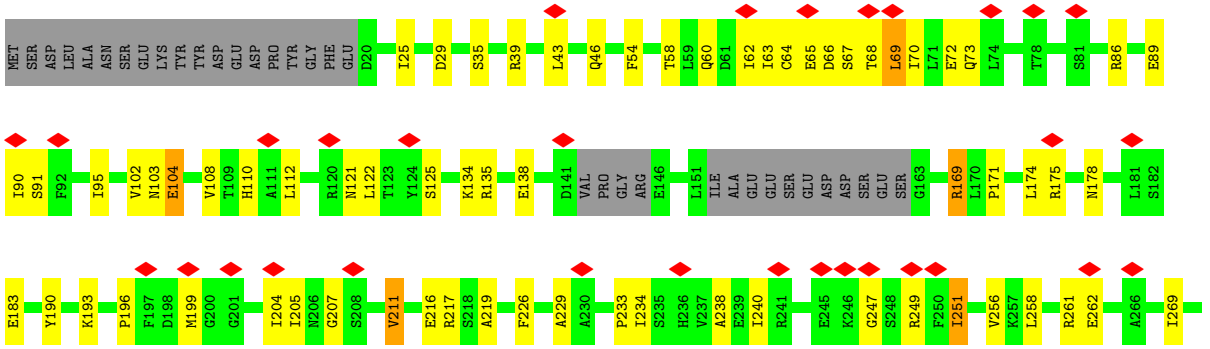
Chain A:

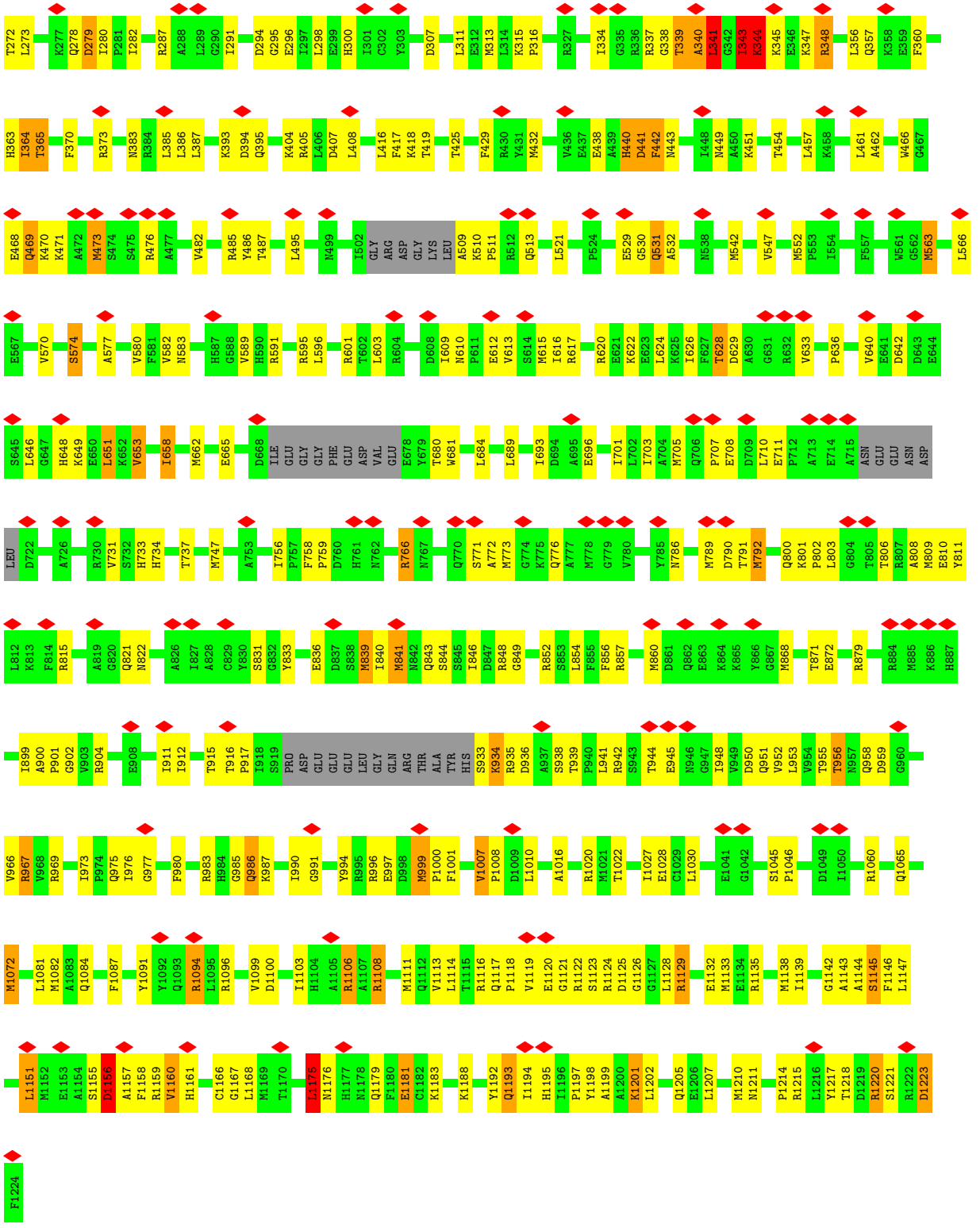




• Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

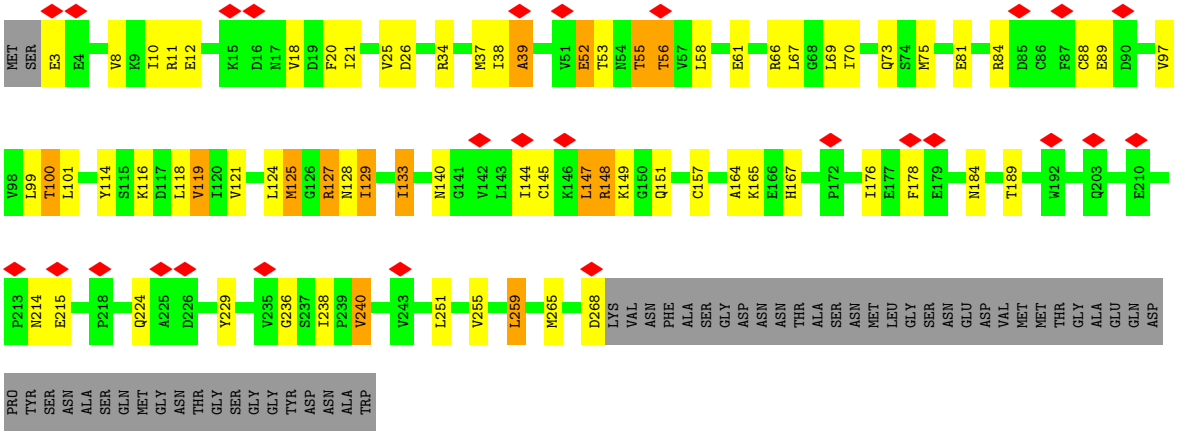
Chain B:





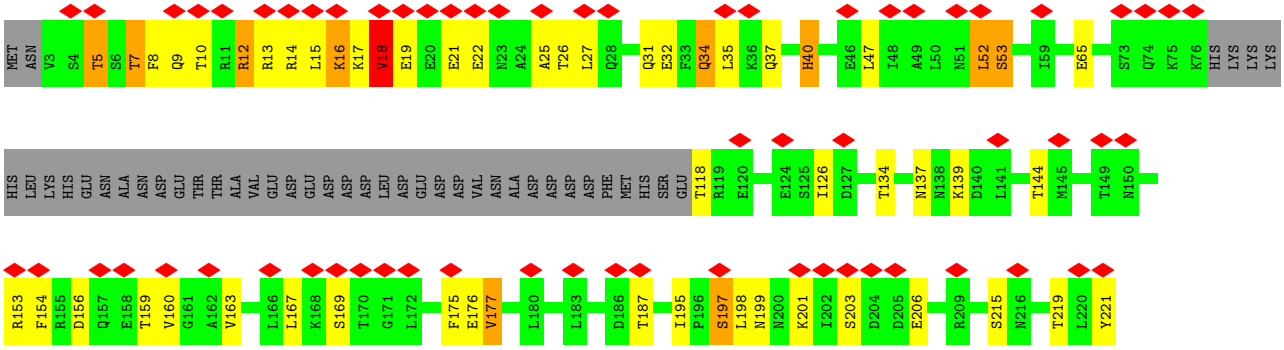
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C:



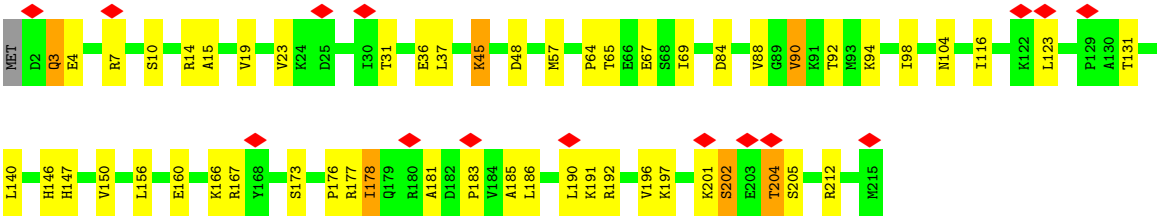
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

Chain D:



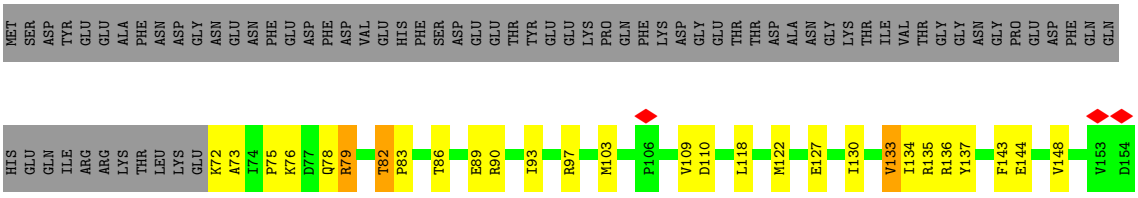
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain E:



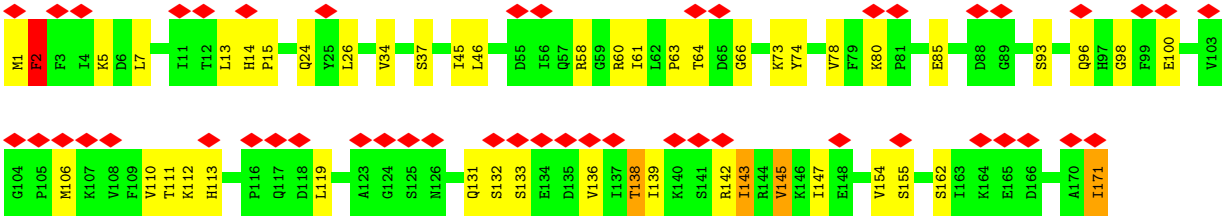
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F:



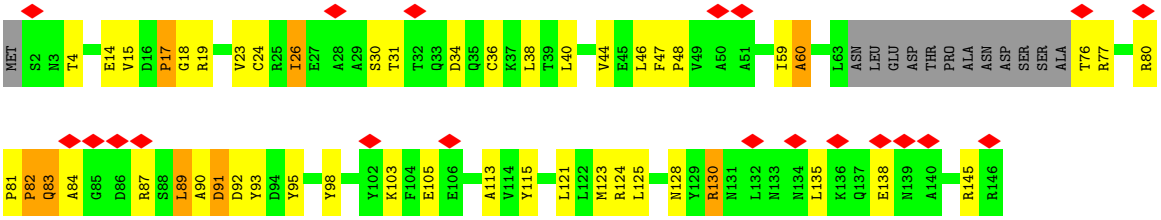
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G:



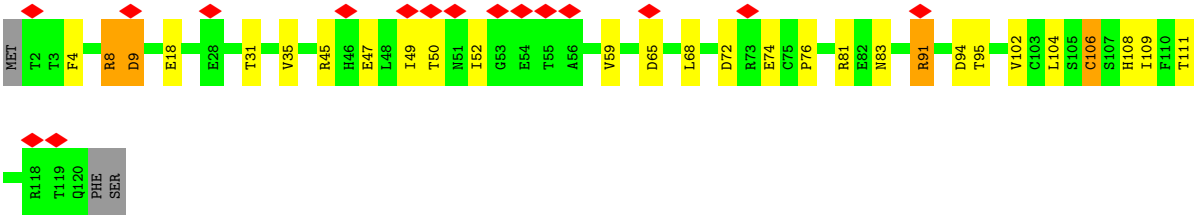
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H:



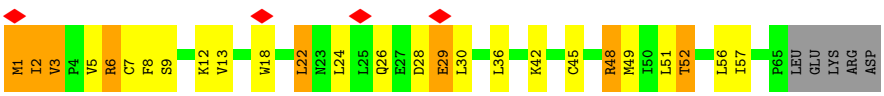
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I:



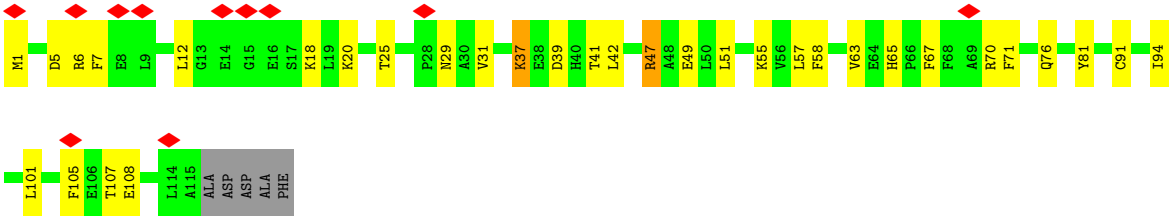
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J:

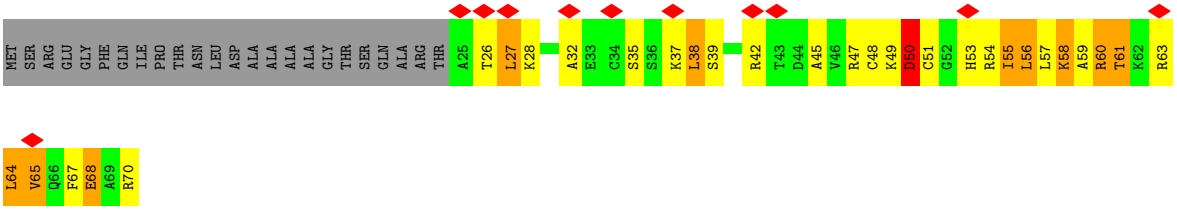


• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

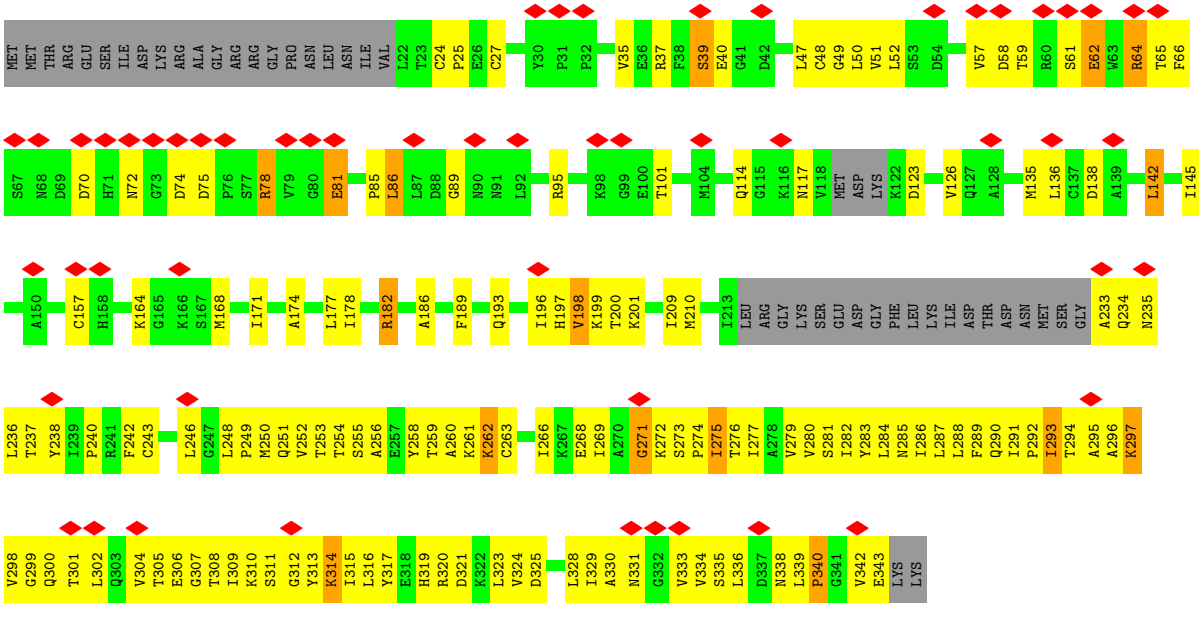
Chain K:



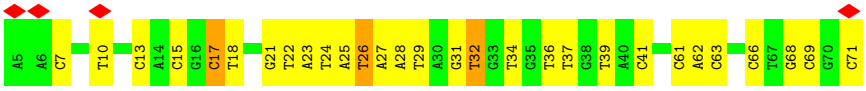
• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4



• Molecule 13: TRANSCRIPTION INITIATION FACTOR IIB

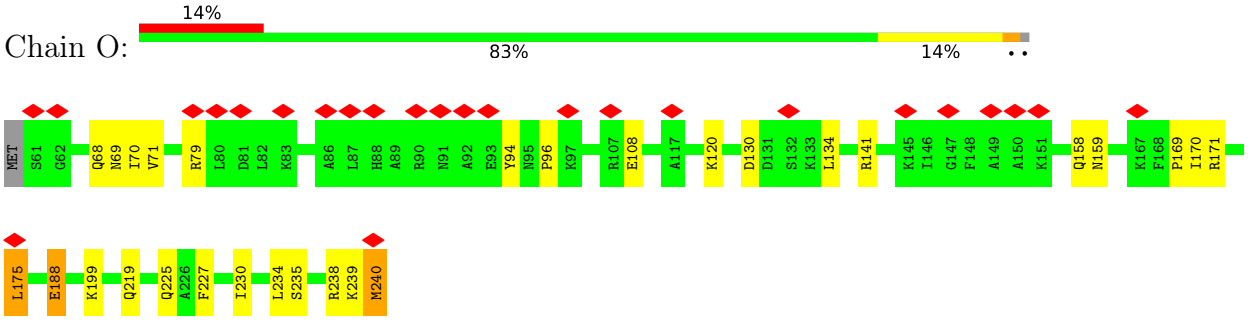


• Molecule 14: NONTEMPLATE DNA



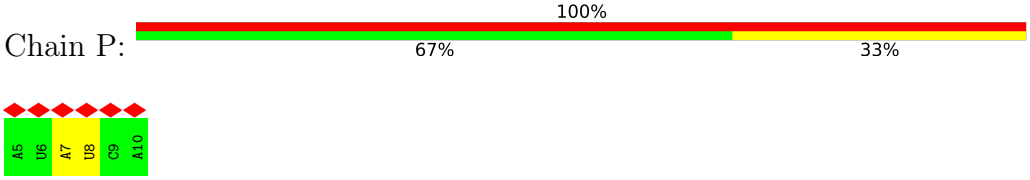
• Molecule 15: TATA-BOX-BINDING PROTEIN

Chain O:



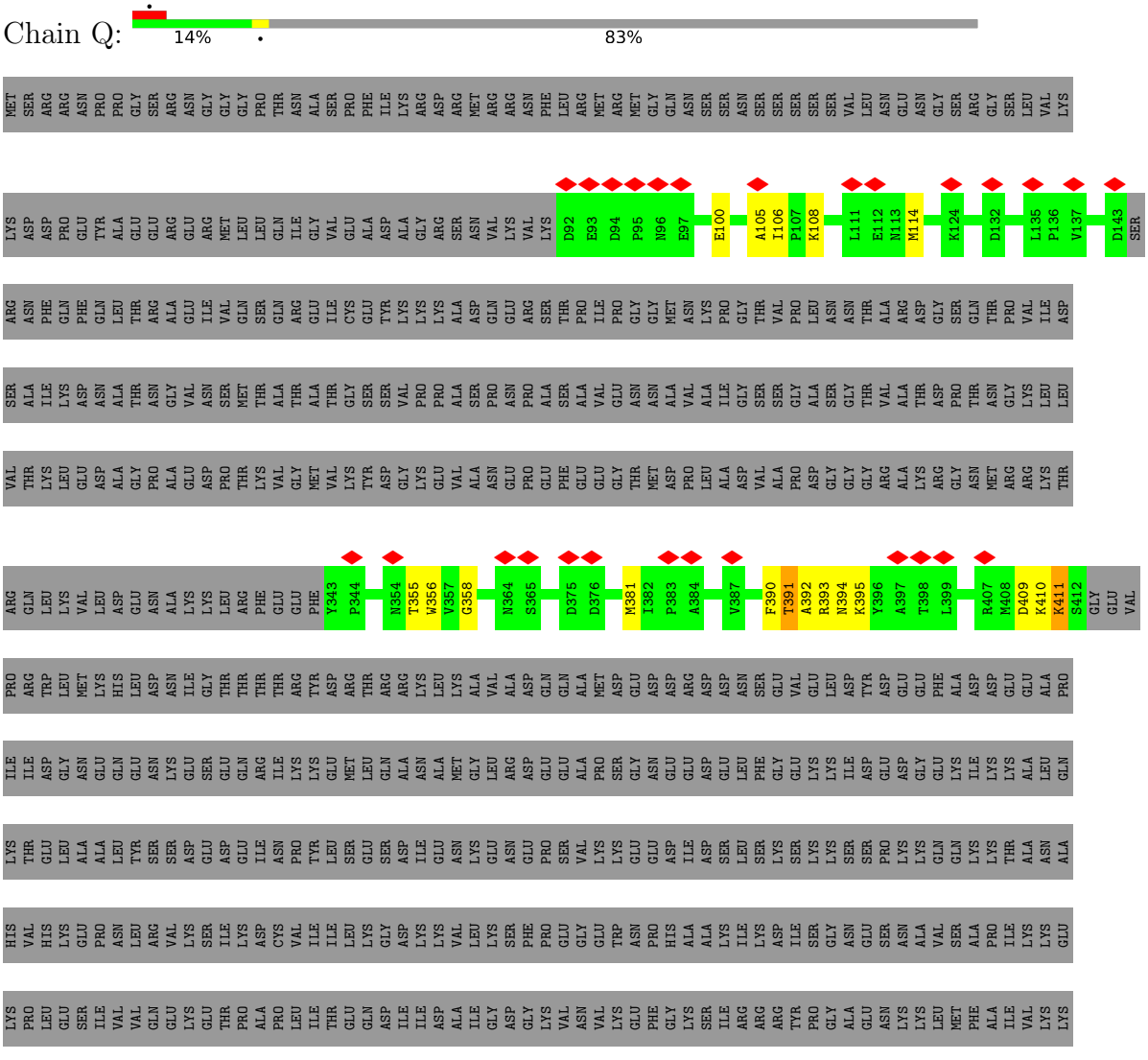
• Molecule 16: RNA

Chain P:



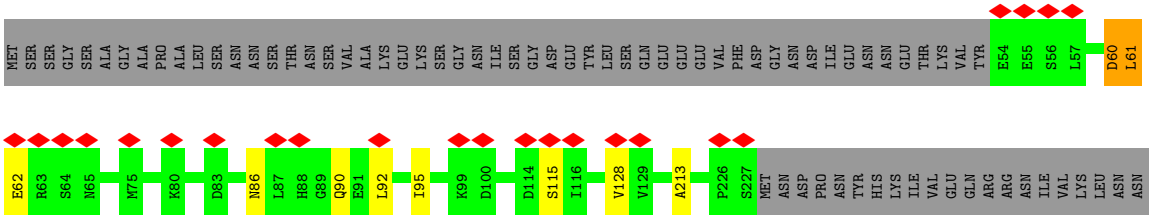
• Molecule 17: TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT ALPHA

Chain Q:



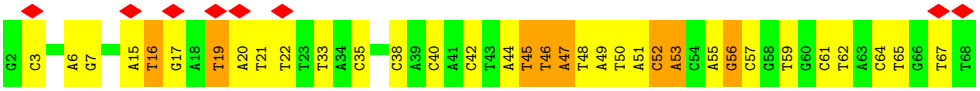
• Molecule 18: TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT BETA

Chain R:



• Molecule 19: TEMPLATE DNA

Chain T:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	4439	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	37169	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.092	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0224	Depositor
Map size (Å)	378.0, 378.0, 378.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.56	4/11374 (0.0%)	0.81	11/15384 (0.1%)
2	B	0.49	1/9316 (0.0%)	0.74	4/12564 (0.0%)
3	C	0.49	0/2133	0.78	2/2891 (0.1%)
4	D	0.51	0/1444	0.83	2/1935 (0.1%)
5	E	0.48	0/1788	0.71	0/2406
6	F	0.62	0/691	0.81	0/933
7	G	0.52	0/1368	0.81	0/1844
8	H	0.50	0/1086	0.80	0/1470
9	I	0.47	0/989	0.78	0/1331
10	J	0.54	0/541	0.88	1/727 (0.1%)
11	K	0.47	0/938	0.71	0/1267
12	L	0.54	0/365	0.95	0/485
13	M	0.61	0/2232	0.77	1/3031 (0.0%)
14	N	1.13	14/1100 (1.3%)	1.31	5/1625 (0.3%)
15	O	0.58	0/1443	0.78	1/1942 (0.1%)
16	P	0.34	0/137	0.80	0/211
17	Q	0.95	0/604	1.19	3/840 (0.4%)
18	R	0.92	0/520	1.21	2/724 (0.3%)
19	T	1.22	18/1265 (1.4%)	1.44	15/1866 (0.8%)
All	All	0.60	37/39334 (0.1%)	0.85	47/53476 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	1
17	Q	0	1
All	All	0	4

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1436	ILE	C-N	14.99	1.60	1.33
1	A	95	PHE	C-N	-14.47	1.00	1.34
19	T	53	DA	P-O5'	-11.71	1.48	1.59
1	A	234	MET	C-N	-11.62	1.07	1.34
19	T	47	DA	C1'-N9	-10.46	1.32	1.47

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	MET	O-C-N	-14.63	99.29	122.70
19	T	46	DT	O4'-C4'-C3'	-11.79	98.93	106.00
19	T	6	DA	O3'-P-O5'	-9.12	86.68	104.00
19	T	42	DC	O5'-P-OP1	-9.08	97.53	105.70
14	N	26	DT	O4'-C4'-C3'	-9.01	100.59	106.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	MET	Mainchain
1	A	95	PHE	Mainchain
2	B	43	LEU	Mainchain
17	Q	410	LYS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11174	0	11223	407	0
2	B	9140	0	9111	313	0
3	C	2095	0	2051	43	0
4	D	1434	0	1460	79	0
5	E	1752	0	1776	28	0
6	F	679	0	701	26	0
7	G	1340	0	1357	33	0
8	H	1068	0	1040	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	971	0	927	15	0
10	J	532	0	542	14	0
11	K	920	0	929	19	0
12	L	363	0	386	26	0
13	M	2202	0	2154	391	0
14	N	975	0	567	22	0
15	O	1416	0	1491	31	0
16	P	123	0	66	1	0
17	Q	606	0	256	30	0
18	R	521	0	216	5	0
19	T	1125	0	661	64	0
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
20	M	1	0	0	0	0
21	A	1	0	0	0	0
All	All	38446	0	36914	1219	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 1219 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:868:MET:CE	13:M:182:ARG:HG2	1.34	1.54
1:A:867:ILE:CG1	1:A:867:ILE:CD1	1.83	1.53
17:Q:356:TRP:CA	17:Q:392:ALA:HA	1.06	1.52
2:B:1215:ARG:NH1	4:D:15:LEU:HD13	1.27	1.49
17:Q:356:TRP:HA	17:Q:392:ALA:CA	0.93	1.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1414/1733 (82%)	1248 (88%)	115 (8%)	51 (4%)	3 25
2	B	1140/1224 (93%)	1019 (89%)	85 (8%)	36 (3%)	4 26
3	C	264/318 (83%)	242 (92%)	20 (8%)	2 (1%)	19 60
4	D	174/221 (79%)	148 (85%)	18 (10%)	8 (5%)	2 21
5	E	212/215 (99%)	195 (92%)	13 (6%)	4 (2%)	8 38
6	F	82/155 (53%)	75 (92%)	7 (8%)	0	100 100
7	G	169/171 (99%)	158 (94%)	8 (5%)	3 (2%)	8 40
8	H	129/146 (88%)	106 (82%)	14 (11%)	9 (7%)	1 14
9	I	117/122 (96%)	98 (84%)	16 (14%)	3 (3%)	5 31
10	J	63/70 (90%)	51 (81%)	9 (14%)	3 (5%)	2 21
11	K	113/120 (94%)	109 (96%)	4 (4%)	0	100 100
12	L	44/70 (63%)	27 (61%)	9 (20%)	8 (18%)	0 3
13	M	294/345 (85%)	267 (91%)	24 (8%)	3 (1%)	15 55
15	O	178/181 (98%)	174 (98%)	4 (2%)	0	100 100
17	Q	118/734 (16%)	106 (90%)	11 (9%)	1 (1%)	19 60
18	R	103/331 (31%)	96 (93%)	3 (3%)	4 (4%)	3 23
All	All	4614/6156 (75%)	4119 (89%)	360 (8%)	135 (3%)	7 29

5 of 135 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	MET
1	A	96	ILE
1	A	189	ARG
1	A	195	ASP
1	A	286	HIS

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	1240/1520 (82%)	1065 (86%)	175 (14%)	3 16
2	B	985/1061 (93%)	868 (88%)	117 (12%)	5 20
3	C	234/274 (85%)	206 (88%)	28 (12%)	5 20
4	D	160/200 (80%)	129 (81%)	31 (19%)	1 8
5	E	196/197 (100%)	175 (89%)	21 (11%)	6 23
6	F	74/137 (54%)	67 (90%)	7 (10%)	8 27
7	G	152/152 (100%)	135 (89%)	17 (11%)	6 22
8	H	117/128 (91%)	103 (88%)	14 (12%)	5 20
9	I	113/116 (97%)	106 (94%)	7 (6%)	18 43
10	J	60/65 (92%)	49 (82%)	11 (18%)	1 10
11	K	99/102 (97%)	87 (88%)	12 (12%)	5 20
12	L	40/57 (70%)	27 (68%)	13 (32%)	0 2
13	M	231/299 (77%)	208 (90%)	23 (10%)	7 26
15	O	152/153 (99%)	140 (92%)	12 (8%)	12 35
All	All	3853/4461 (86%)	3365 (87%)	488 (13%)	8 18

5 of 488 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	646	LEU
12	L	42	ARG
2	B	1193	GLN
11	K	101	LEU
13	M	293	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
8	H	83	GLN

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Mol	Chain	Res	Type
15	O	158	GLN
9	I	83	ASN
13	M	235	ASN
2	B	300	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	5/6 (83%)	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 (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 10 ligands modelled in this entry, 10 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
19	T	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	23:DT	O3'	33:DT	P	36.30
1	B	351:TYR	C	352:ALA	N	3.29
1	A	234:MET	C	235:ILE	N	1.07
1	A	95:PHE	C	96:ILE	N	1.00

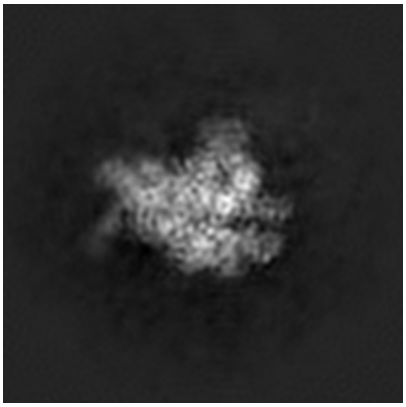
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2785. These allow visual inspection of the internal detail of the map and identification of artifacts.

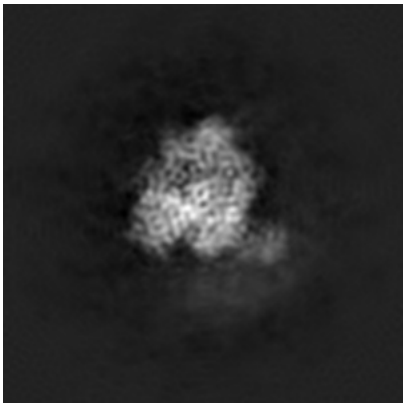
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

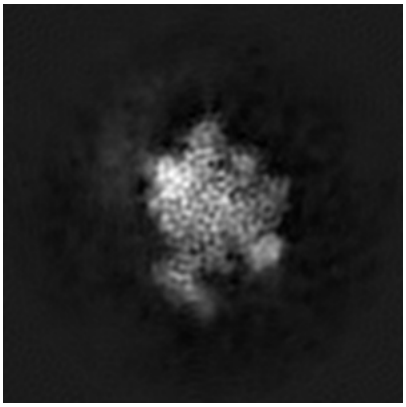
6.1.1 Primary map



X



Y

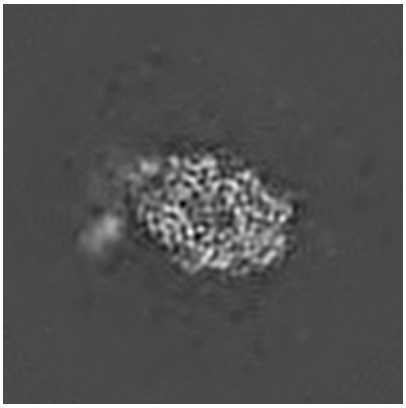


Z

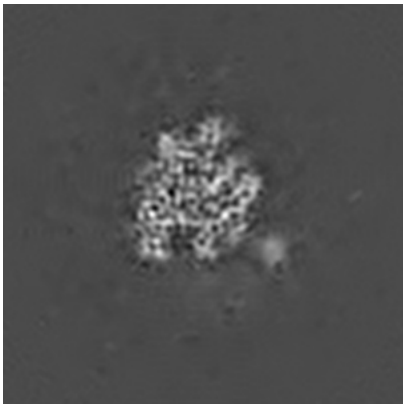
The images above show the map projected in three orthogonal directions.

6.2 Central slices

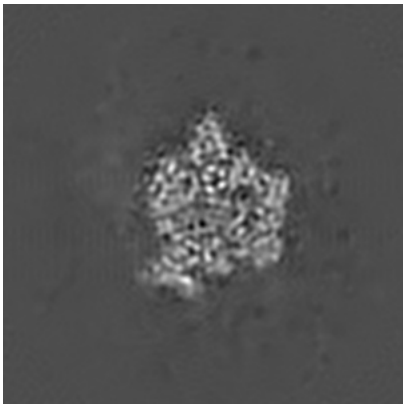
6.2.1 Primary map



X Index: 140



Y Index: 140

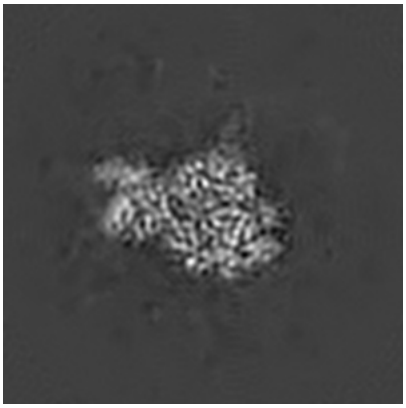


Z Index: 140

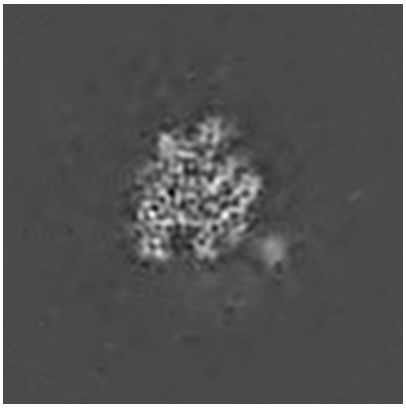
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

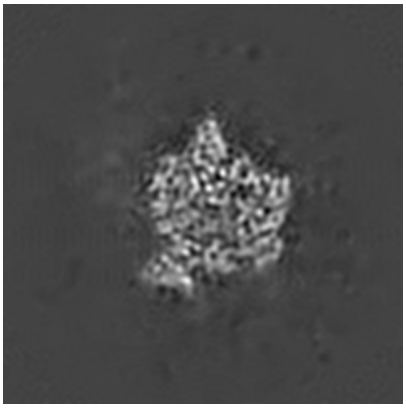
6.3.1 Primary map



X Index: 130



Y Index: 140

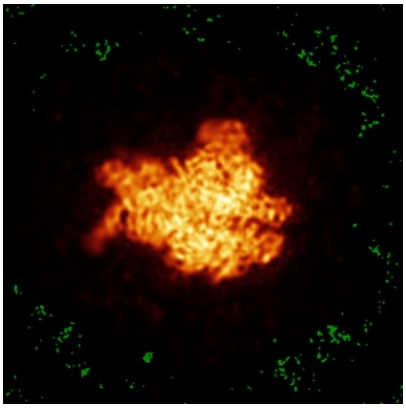


Z Index: 142

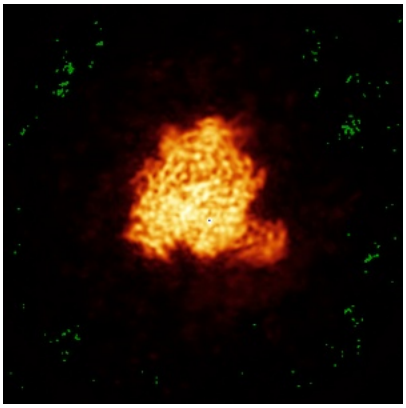
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

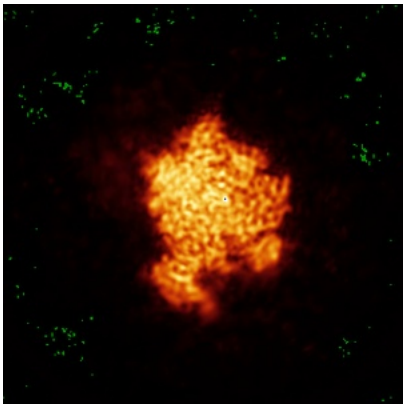
6.4.1 Primary map



X



Y

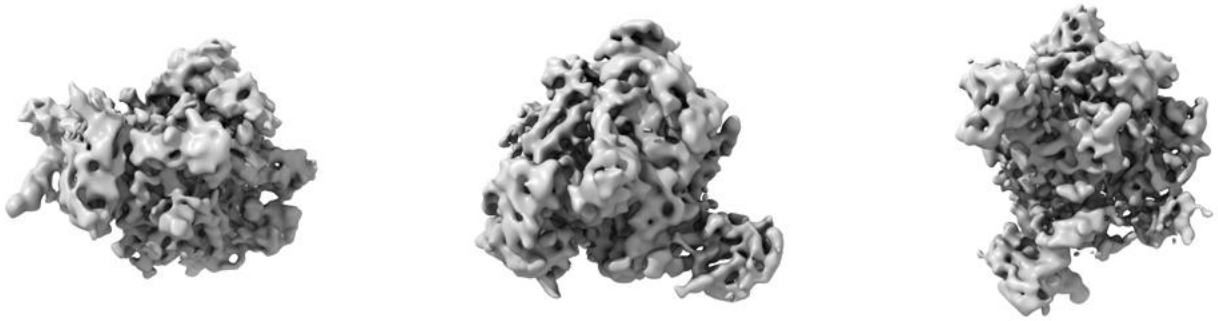


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0224. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

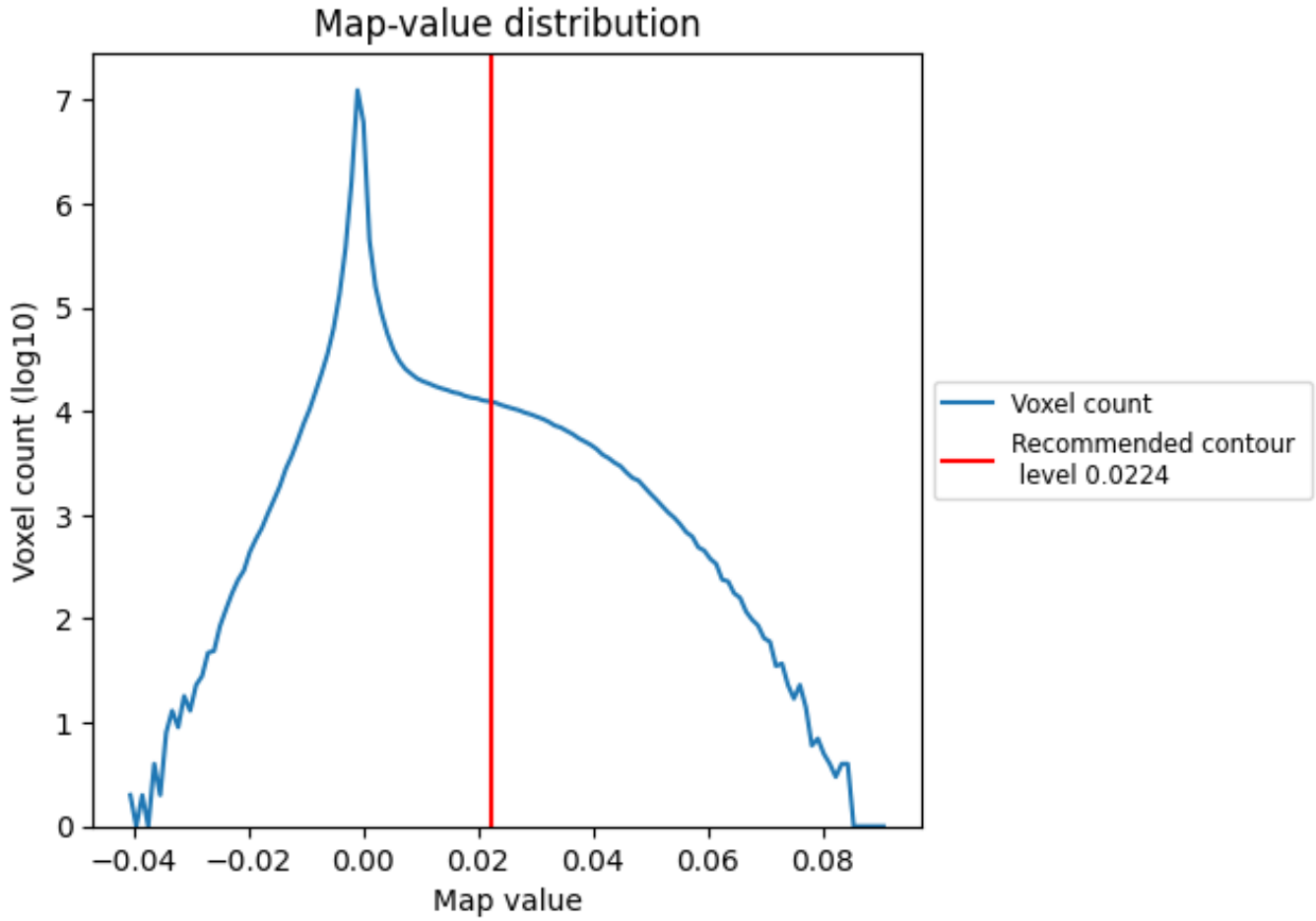
6.6 Mask visualisation (i)

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

7 Map analysis

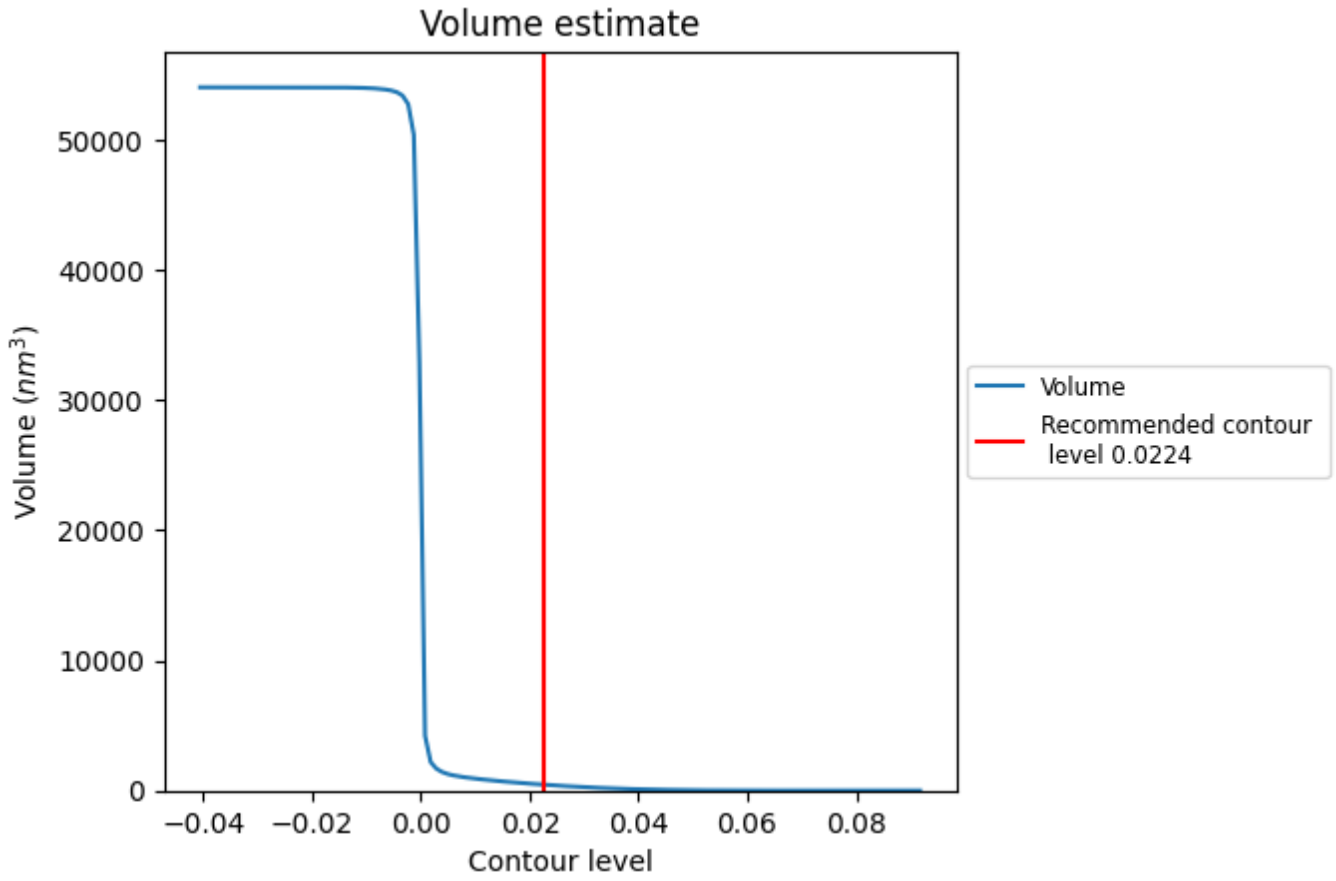
This section contains the results of statistical analysis of the map.

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.

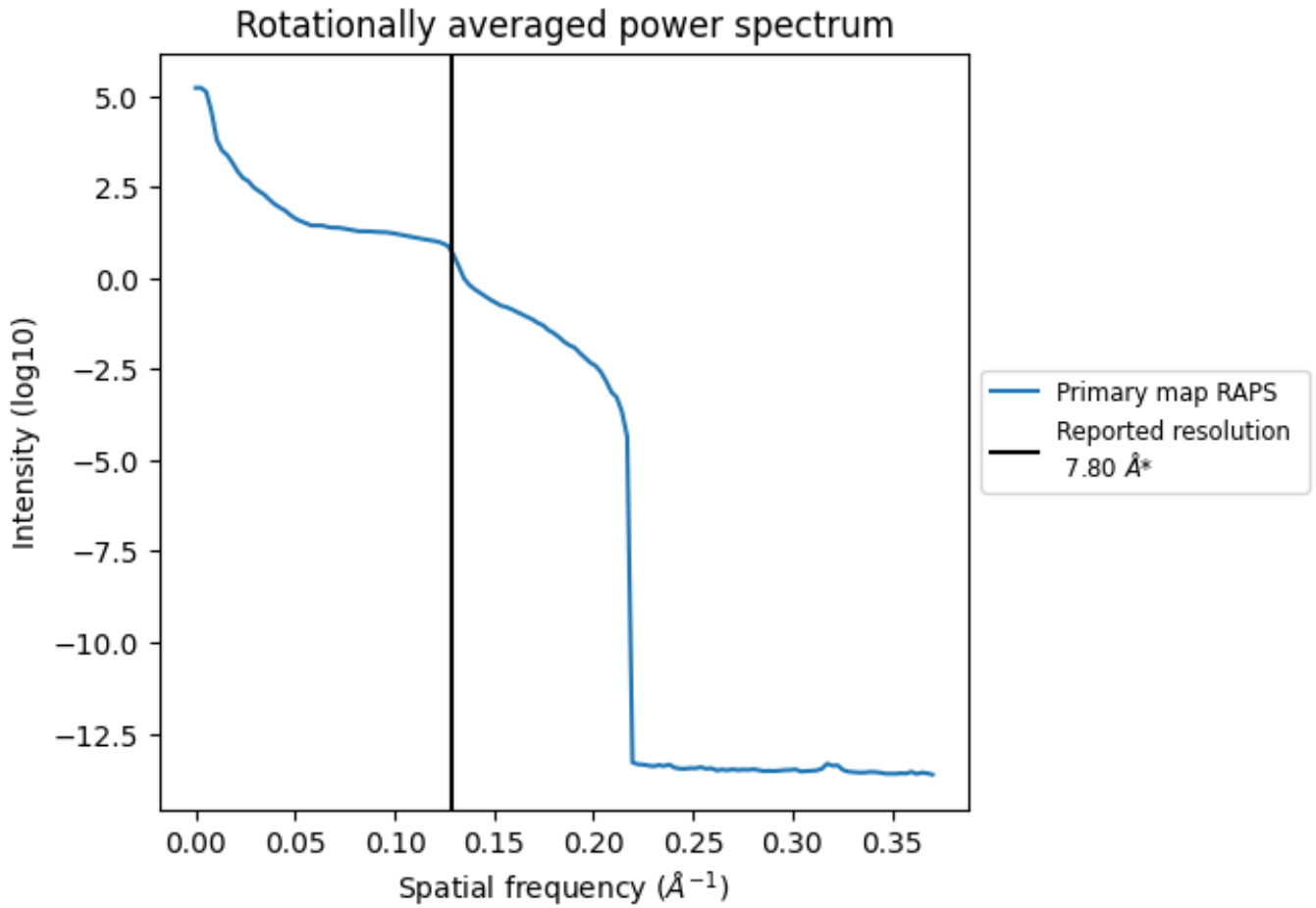
7.2 Volume estimate (i)



The volume at the recommended contour level is 458 nm^3; this corresponds to an approximate mass of 414 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 0.128 Å^{-1}

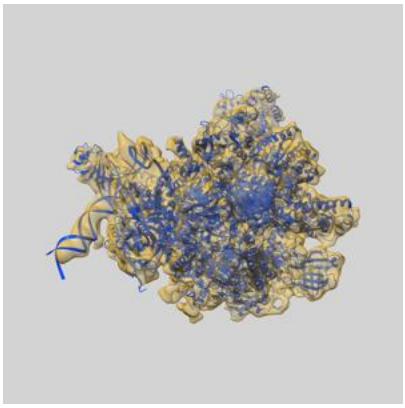
8 Fourier-Shell correlation (i)

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

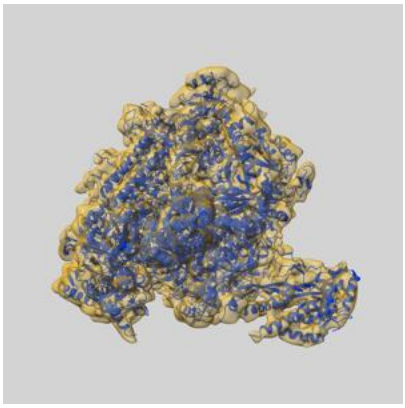
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2785 and PDB model 4V1N. Per-residue inclusion information can be found in section 3 on page 8.

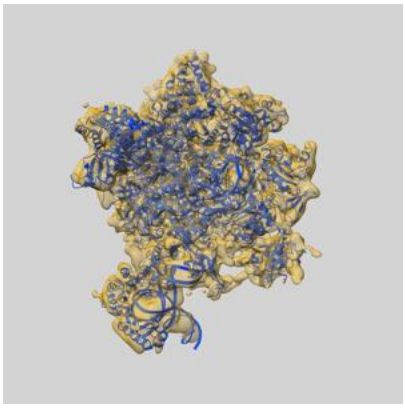
9.1 Map-model overlay



X



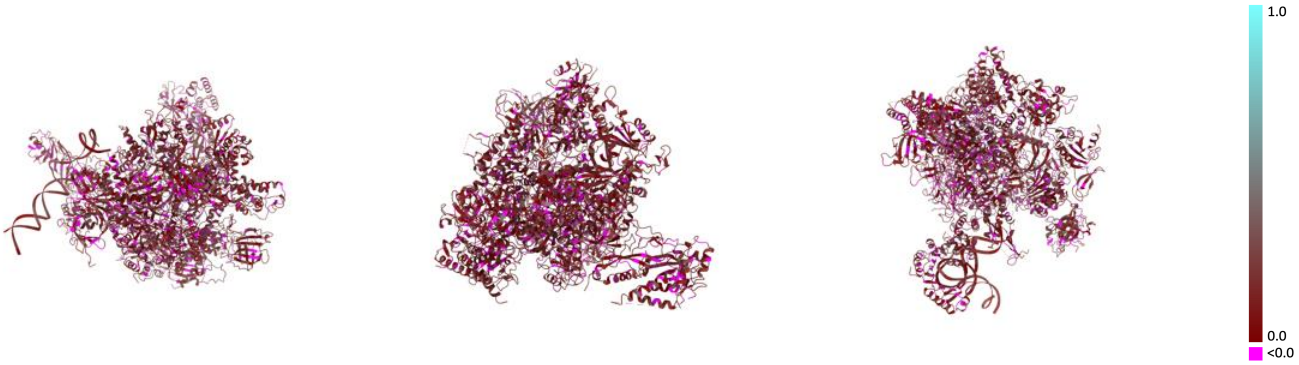
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0224 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.

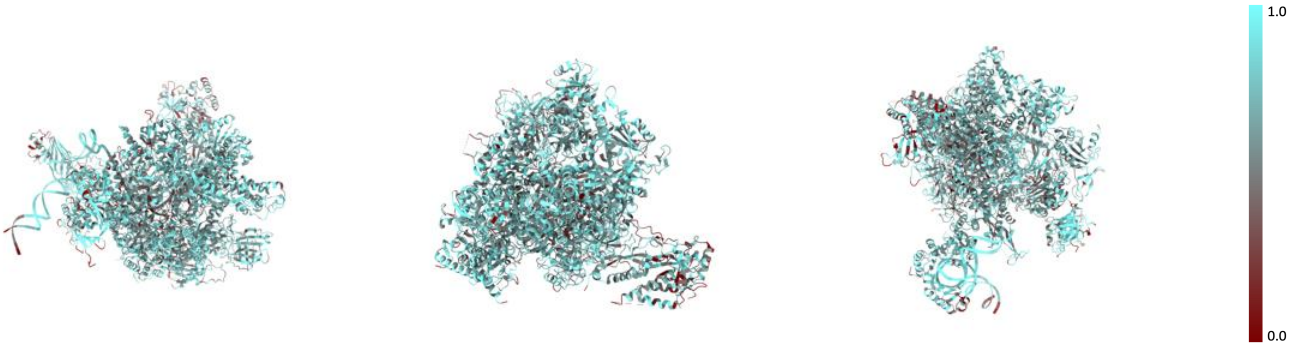
9.2 Q-score mapped to coordinate model (i)



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.

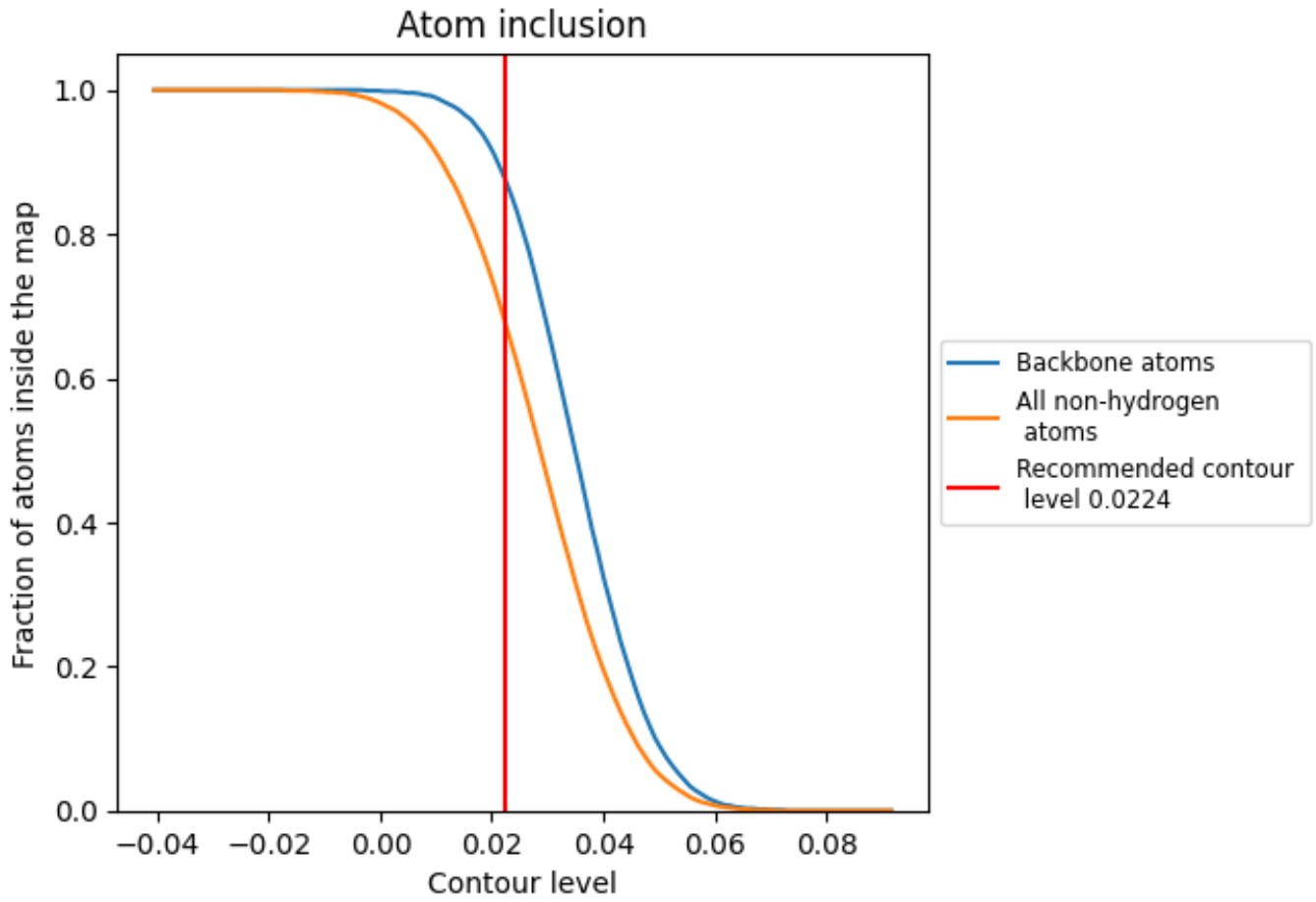
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0224).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 68% 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 (0.0224) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6770	0.1290
A	0.6900	0.1330
B	0.6550	0.1210
C	0.7220	0.1380
D	0.5330	0.1120
E	0.7230	0.1400
F	0.7190	0.1400
G	0.5680	0.1040
H	0.7070	0.1390
I	0.6840	0.1280
J	0.7220	0.1230
K	0.7120	0.1500
L	0.6130	0.1020
M	0.6210	0.1250
N	0.8060	0.1680
O	0.7010	0.1040
P	0.1540	0.0140
Q	0.7410	0.1820
R	0.7430	0.1360
T	0.7550	0.1400