wwPDB EM Validation Summary Report (i)

Feb 25, 2024 – 10:42 AM EST

PDB ID	:	5IYC
EMDB ID	:	EMD-8137
Title	:	Human core-PIC in the initial transcribing state
Authors	:	He, Y.; Yan, C.; Fang, J.; Inouye, C.; Tjian, R.; Ivanov, I.; Nogales, E.
Deposited on	:	2016-03-24
Resolution	:	3.90 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 (i) 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 (i)) were used in the production of this report:

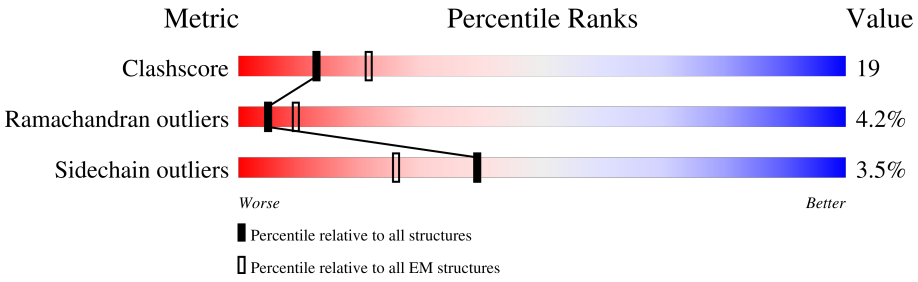
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 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

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	48% 22% 26%
2	B	1174	63% 30% 5%
3	C	275	72% 24%
4	D	142	8% 81% 10% 9%
5	E	210	70% 26%
6	F	127	5% 51% 16% 32%
7	G	172	10% 74% 24%
8	H	150	61% 30% 8%

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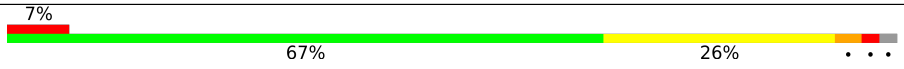
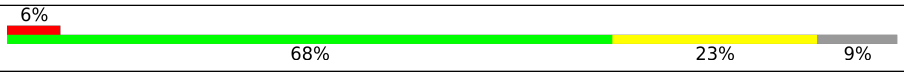
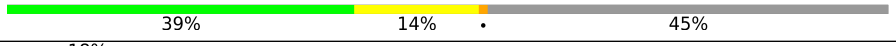
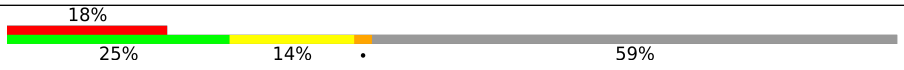
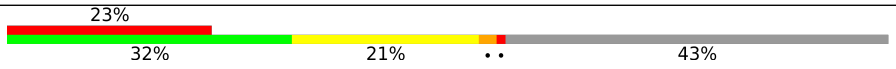
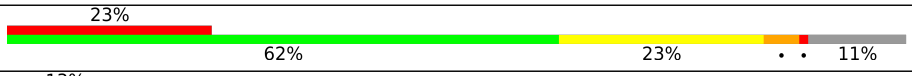
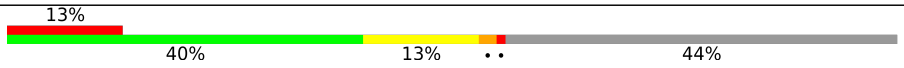
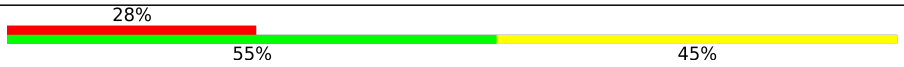
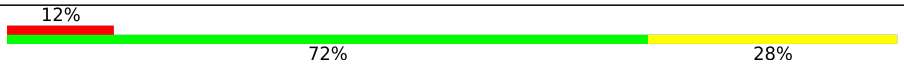
Mol	Chain	Length	Quality of chain
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	316	
14	N	376	
15	O	109	
16	P	339	
17	Q	439	
18	R	291	
19	S	517	
20	T	249	
21	U	301	
22	X	80	
23	Y	80	

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 47927 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	1454	11515	7234	2058	2150	73	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	1165	9317	5878	1637	1738	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	275	2213	1386	380	440	7	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	129	1062	665	179	214	4	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	210	1723	1088	301	325	9	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	86	689	437	120	127	5	0	0

- 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
			1351	875	219	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	150	Total	C	N	O	S	0	0
			1205	764	196	239	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	125	Total	C	N	O	S	0	0
			1013	626	177	198	12		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB10.

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 DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			937	604	154	177	2		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	310	Total	C	N	O	S	0	0
			2391	1490	426	457	18		

- Molecule 14 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 15 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 16 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	185	Total	C	N	O	S	0	0
			1462	946	257	252	7		

- Molecule 17 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	180	Total	C	N	O	S	0	0
			1484	938	262	273	11		

- Molecule 18 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	165	Total	C	N	O	S	0	0
			1357	865	235	253	4		

- Molecule 19 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 20 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 21 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	170	Total	C	N	O	S	0	0
			1343	818	247	263	15		

- Molecule 22 is a DNA chain called SCP-X.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	80	Total	C	N	O	P	0	0
			1645	785	292	489	79		

- Molecule 23 is a DNA chain called SCP-Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	80	Total	C	N	O	P	0	0
			1624	771	291	483	79		

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
24	A	2	Total	Mg	0
			2	2	

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

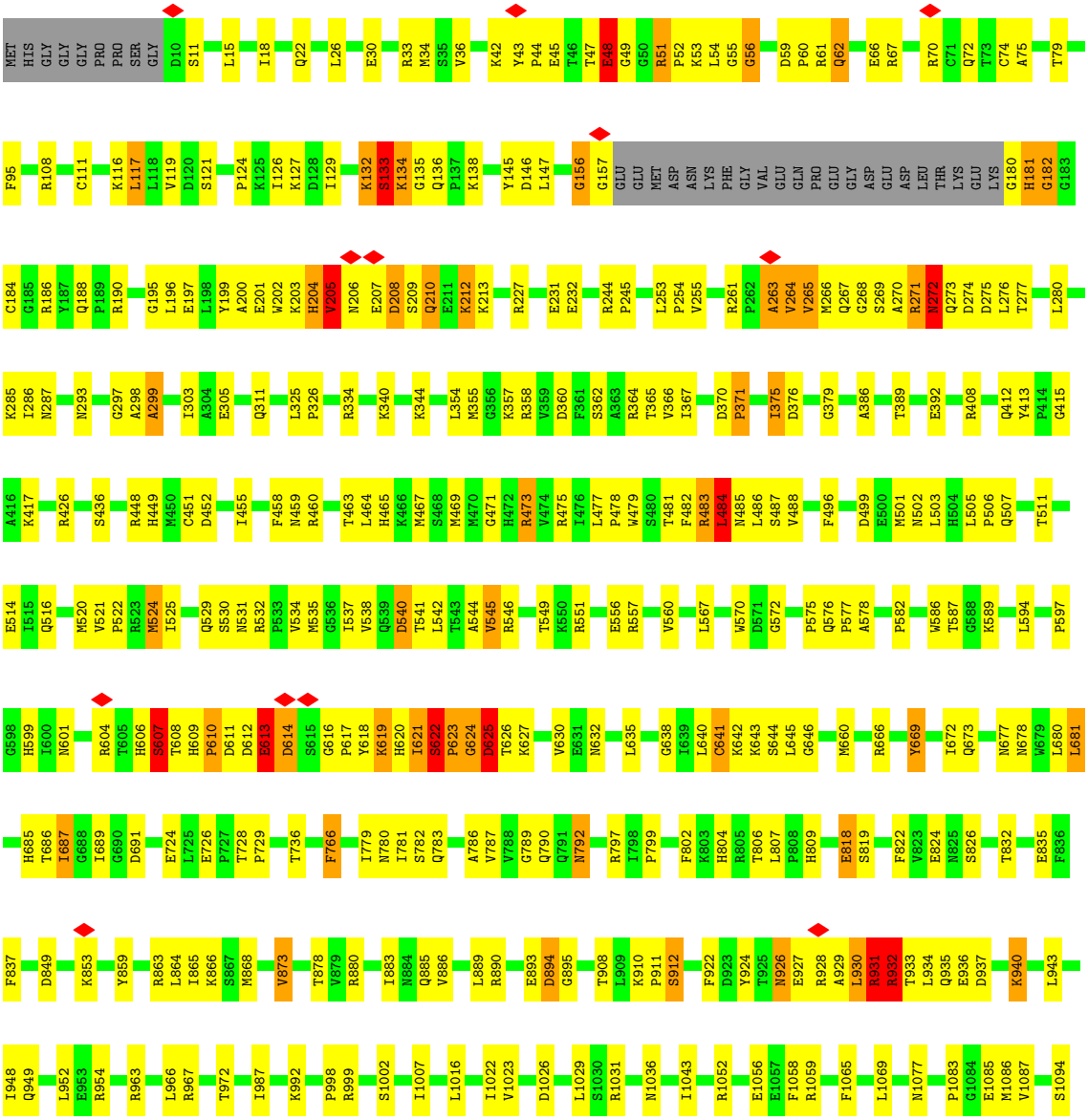
Mol	Chain	Residues	Atoms		AltConf
25	A	2	Total	Zn	0
			2	2	
25	B	1	Total	Zn	0
			1	1	
25	C	1	Total	Zn	0
			1	1	
25	I	2	Total	Zn	0
			2	2	
25	J	1	Total	Zn	0
			1	1	
25	L	1	Total	Zn	0
			1	1	
25	M	1	Total	Zn	0
			1	1	
25	Q	1	Total	Zn	0
			1	1	
25	U	1	Total	Zn	0
			1	1	

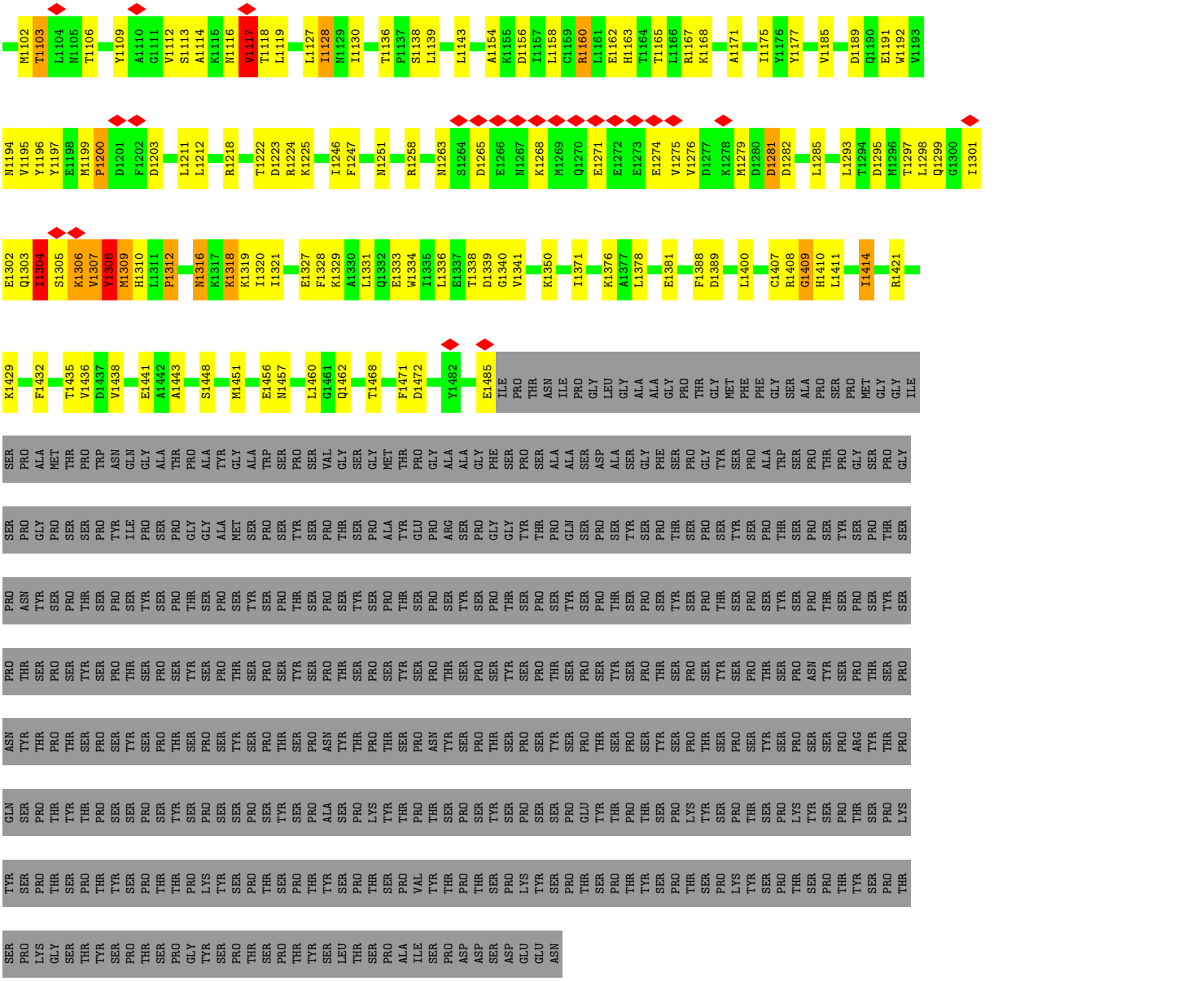
3 Residue-property plots (i)

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

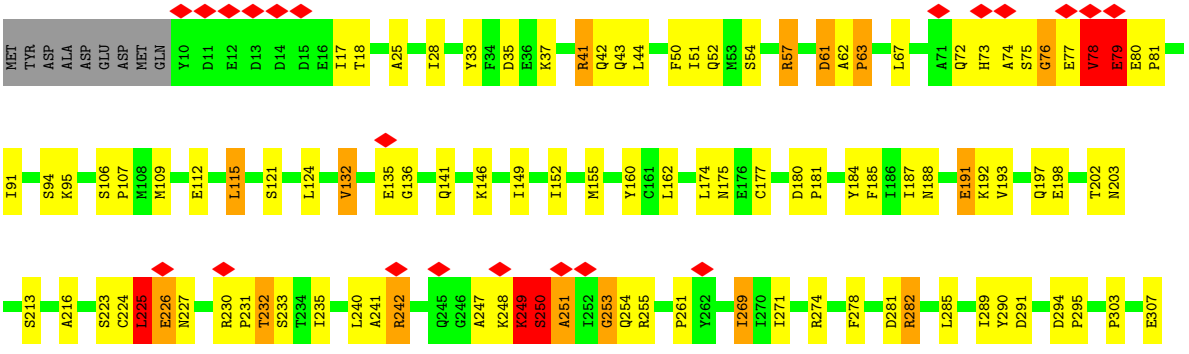
Chain A:

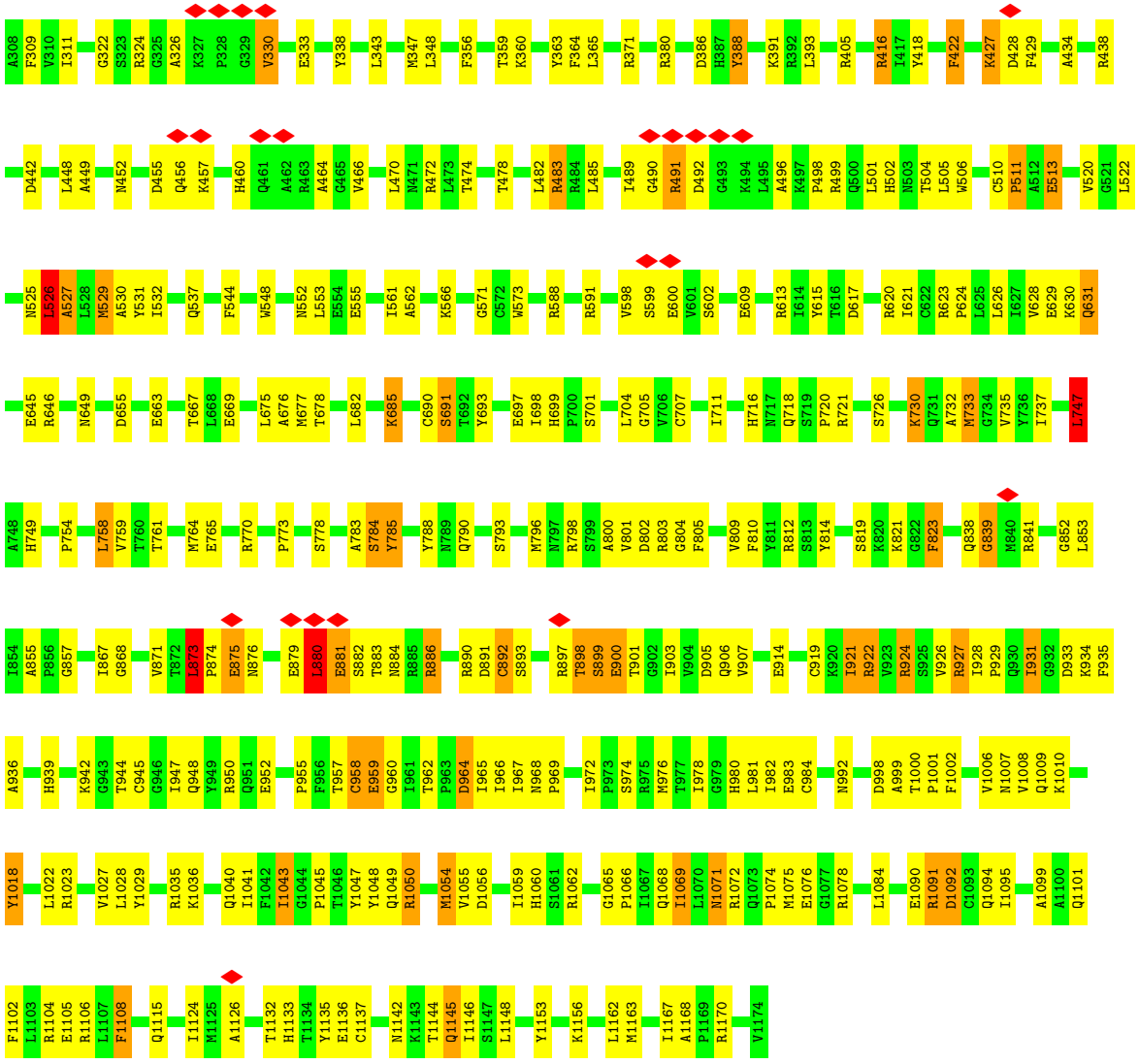




• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

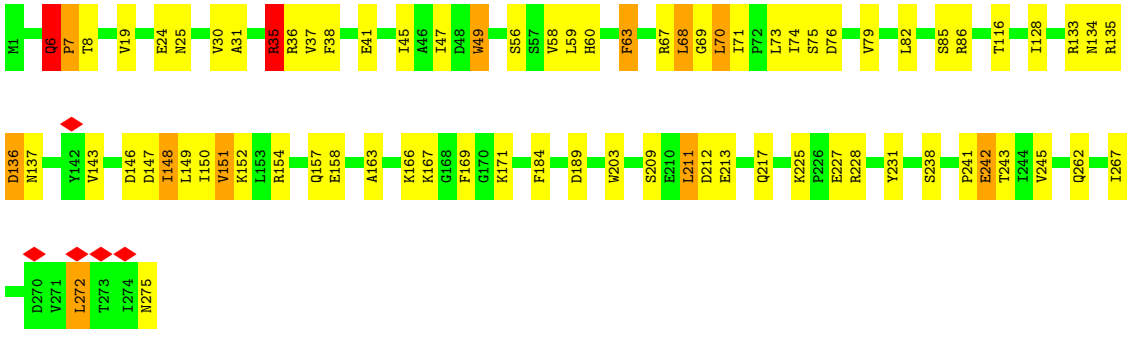
Chain B:





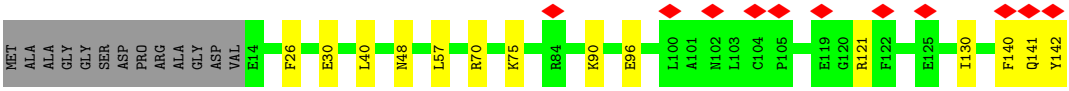
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:

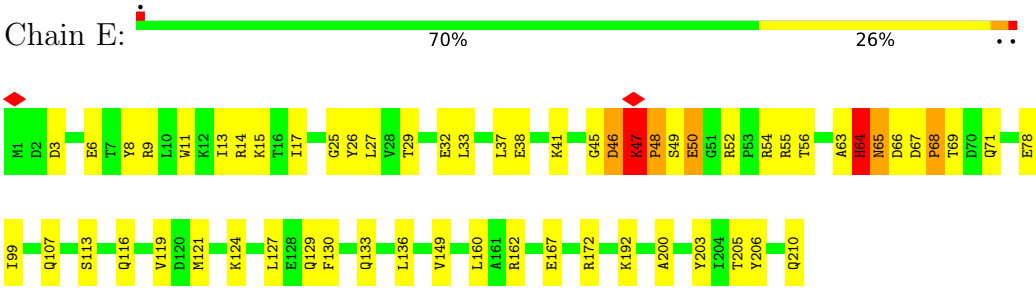


• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

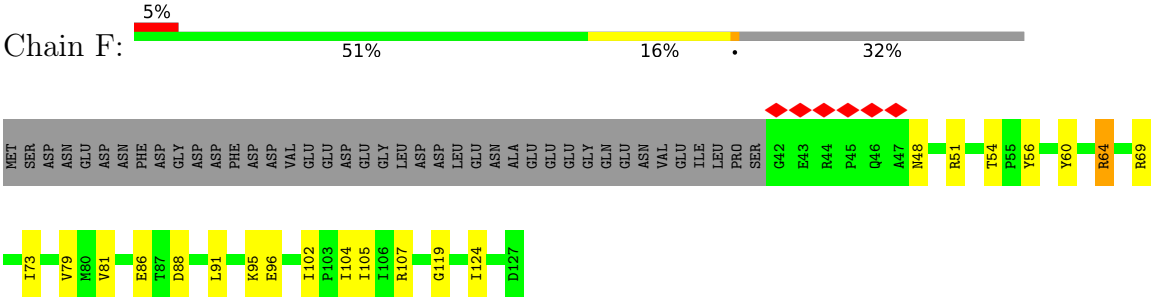
Chain D:



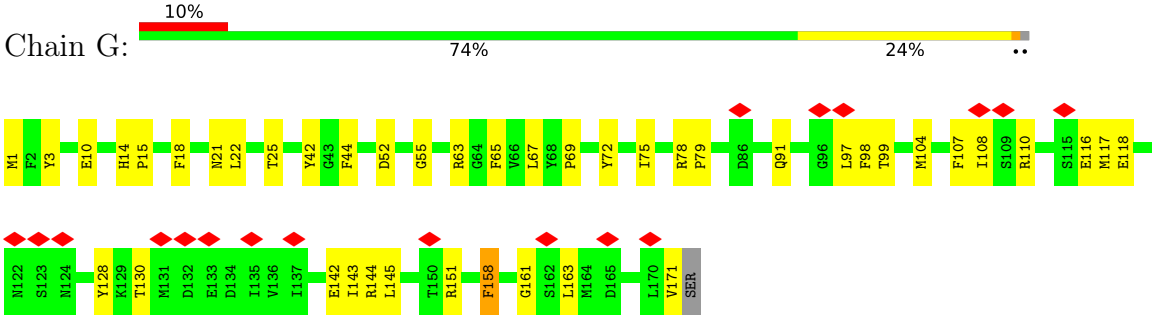
• Molecule 5: DNA-directed RNA polymerase II subunit RPB5



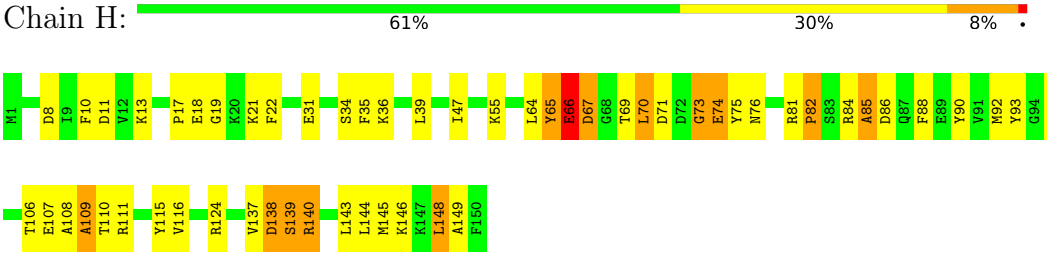
• Molecule 6: DNA-directed RNA polymerase II subunit RPB6



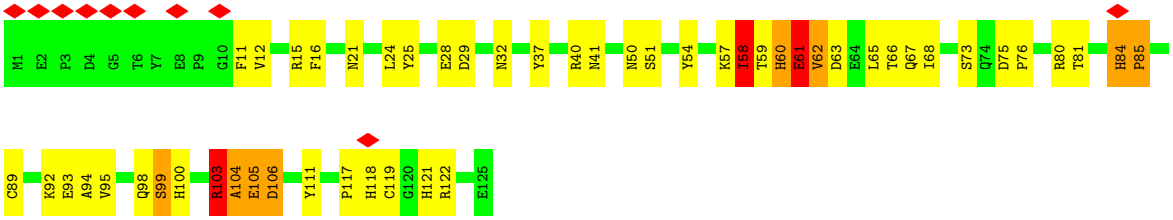
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7



• Molecule 8: DNA-directed RNA polymerase II subunit RPB8

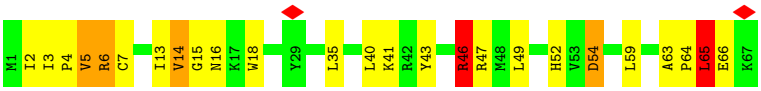


• Molecule 9: DNA-directed RNA polymerase II subunit RPB9



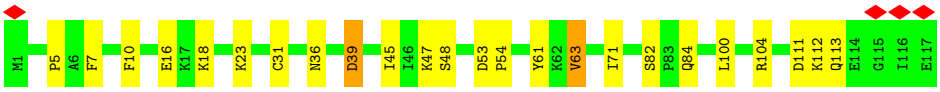
• Molecule 10: DNA-directed RNA polymerase II subunit RPB10

Chain J:



• Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K:

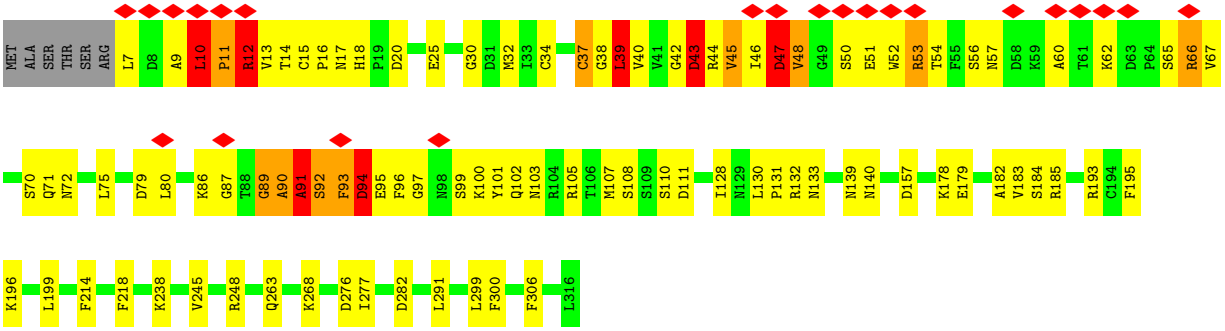


• Molecule 12: DNA-directed RNA polymerase II subunit RPB12

Chain L:

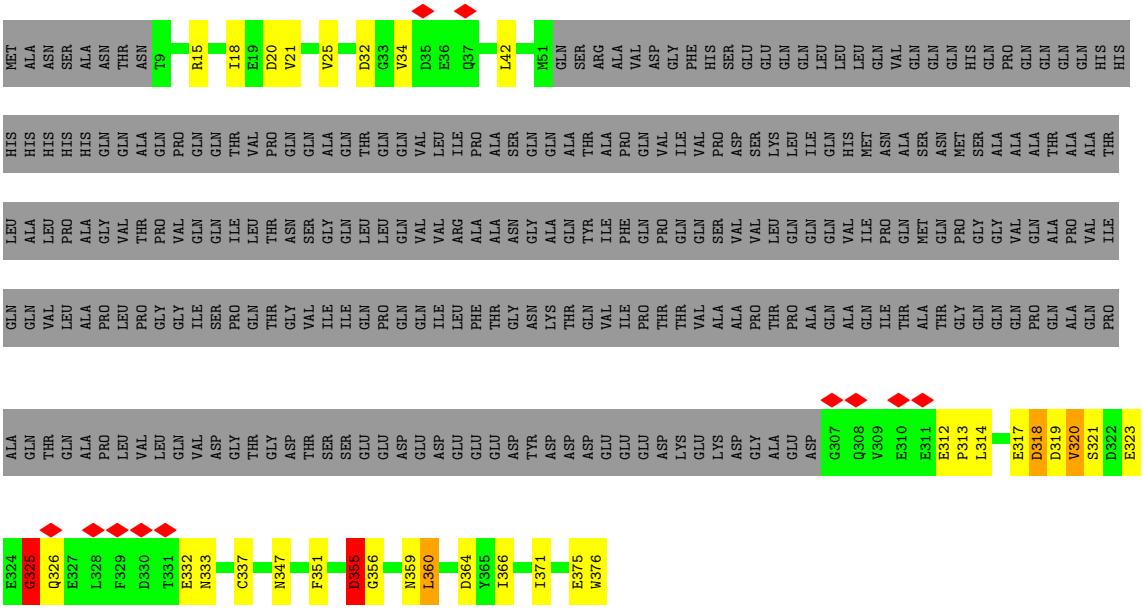
• Molecule 13: Transcription initiation factor IIB

Chain M:

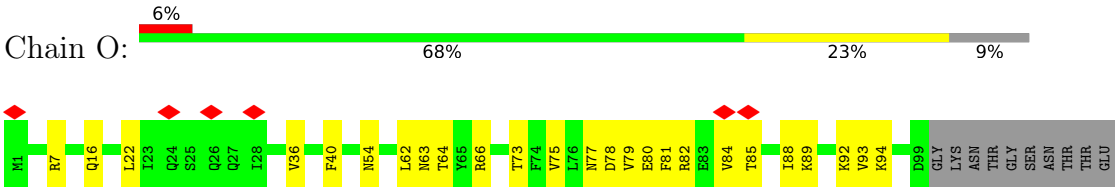


• Molecule 14: Transcription initiation factor IIA subunit 1

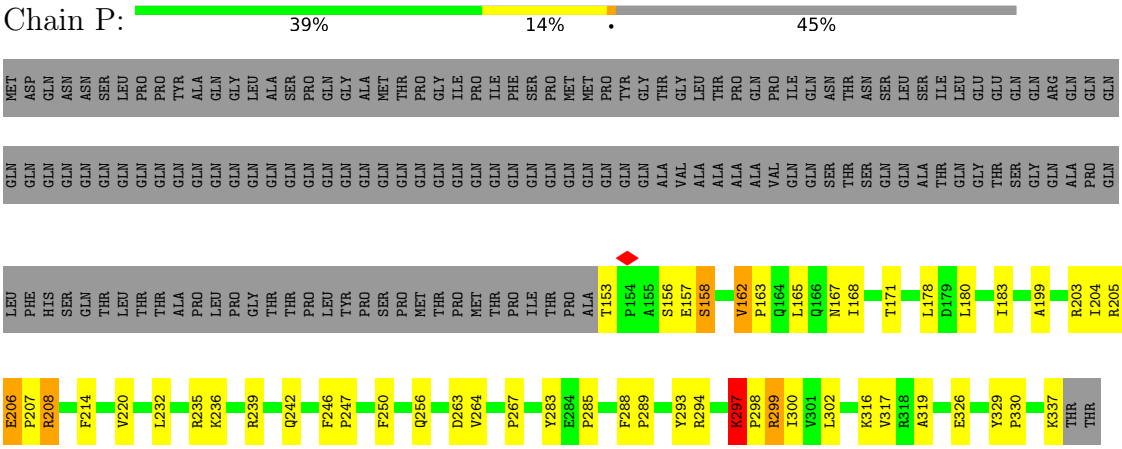
Chain N:



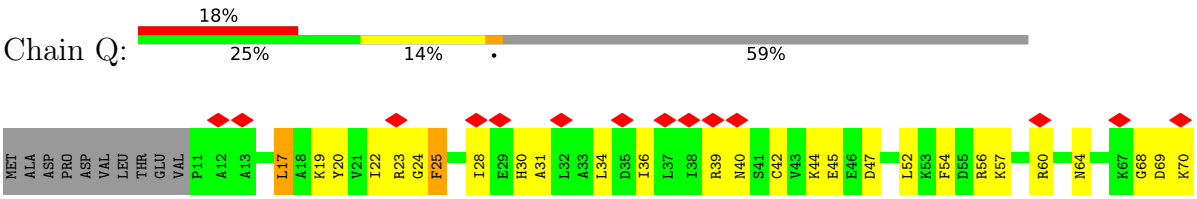
• Molecule 15: Transcription initiation factor IIA subunit 2

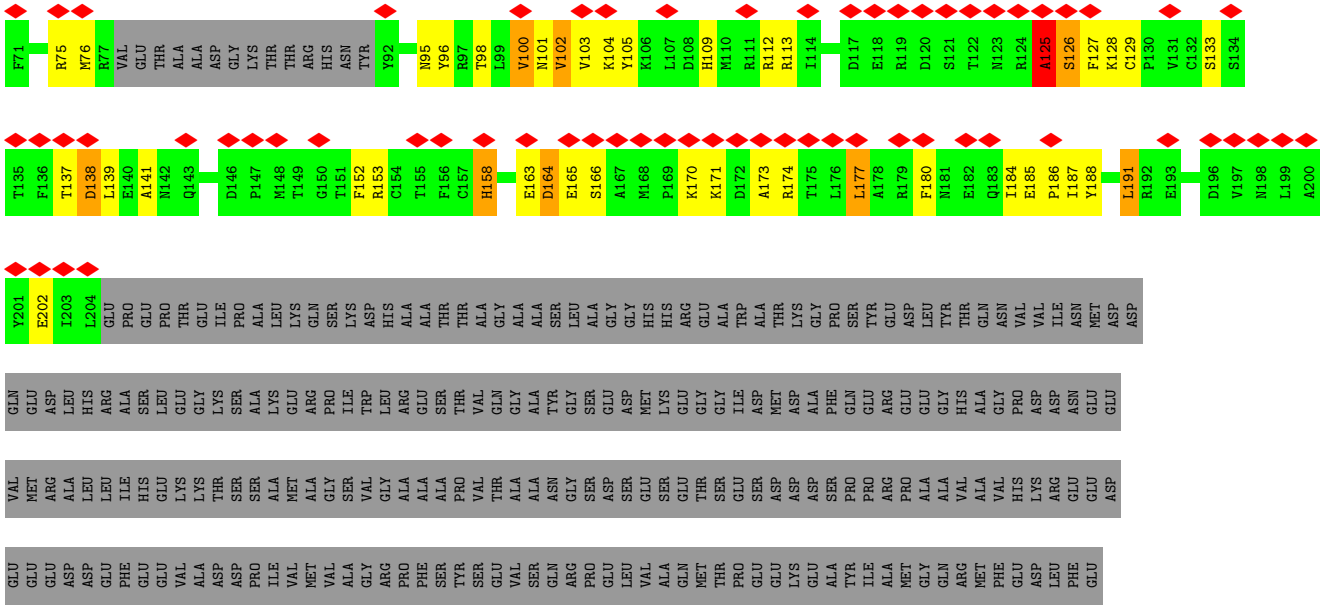


• Molecule 16: TATA-box-binding protein

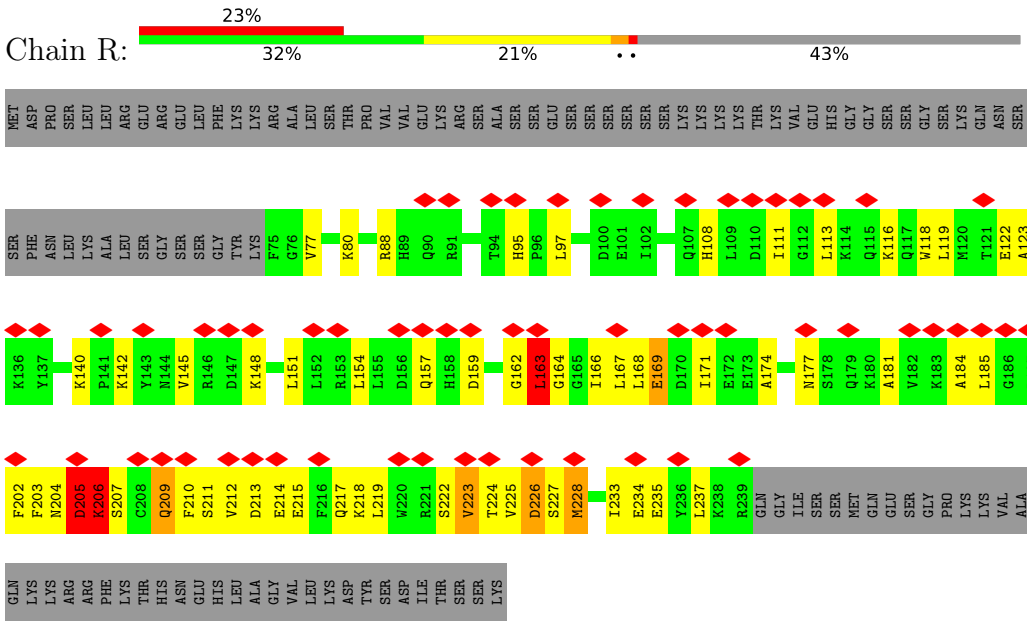


• Molecule 17: General transcription factor IIE subunit 1

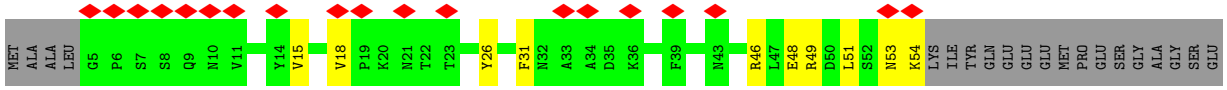


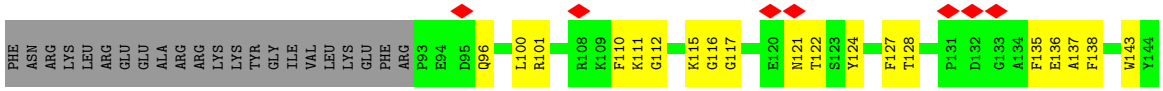


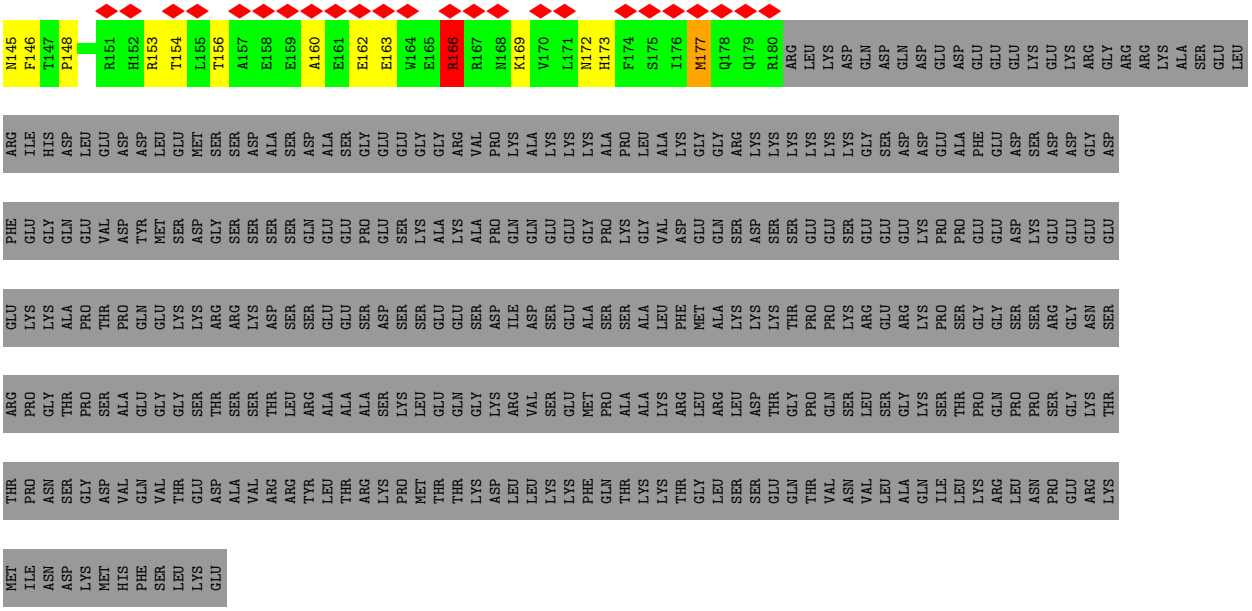
• Molecule 18: Transcription initiation factor IIE subunit beta



• Molecule 19: General transcription factor IIF subunit 1

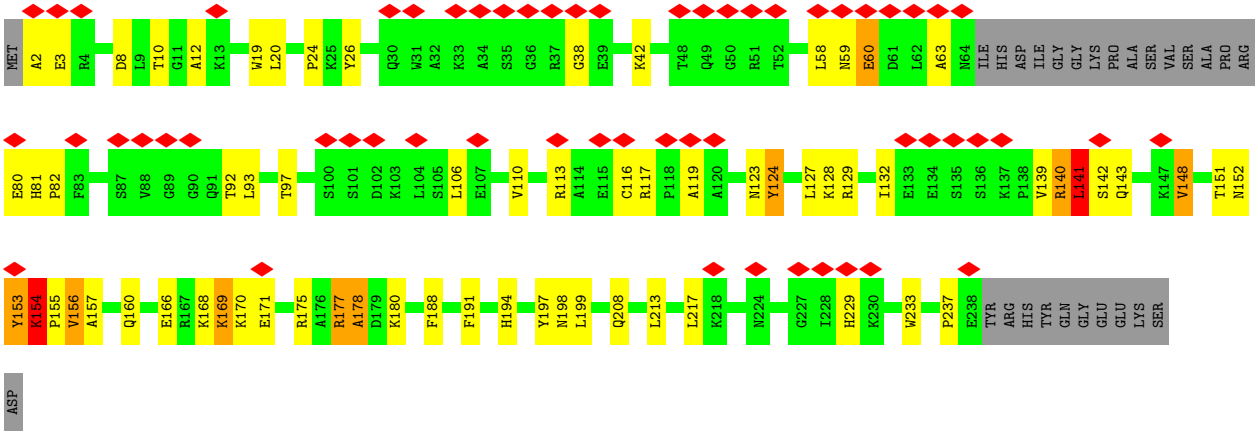






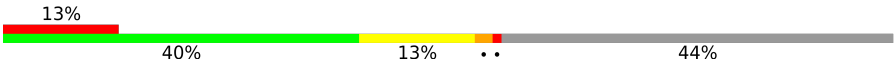
• Molecule 20: General transcription factor IIF subunit 2

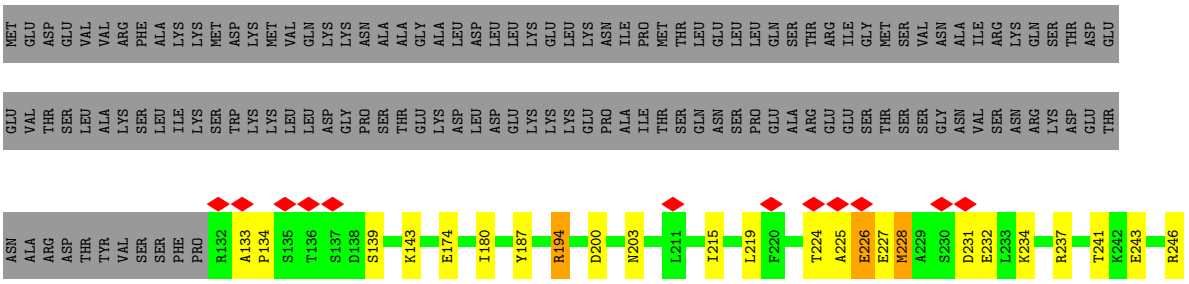
Chain T:

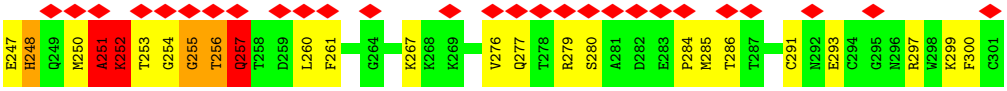


• Molecule 21: Transcription elongation factor A protein 1

Chain U:

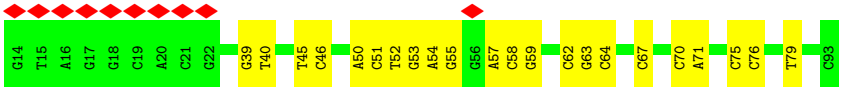






• Molecule 22: SCP-X

• Molecule 23: SCP-Y



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90590	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 ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	27500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.164	Depositor
Minimum map value	-0.103	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	503.03998, 503.03998, 503.03998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	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

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	0.62	4/11727 (0.0%)	0.84	24/15833 (0.2%)
2	B	0.75	9/9503 (0.1%)	0.92	27/12831 (0.2%)
3	C	0.60	0/2259	0.85	6/3073 (0.2%)
4	D	0.24	0/1077	0.44	0/1446
5	E	0.46	0/1753	0.71	0/2368
6	F	0.64	0/700	0.78	0/946
7	G	0.29	0/1382	0.53	0/1874
8	H	0.44	0/1227	0.76	3/1654 (0.2%)
9	I	0.37	0/1038	1.08	5/1407 (0.4%)
10	J	0.75	0/542	0.96	2/730 (0.3%)
11	K	0.49	0/956	0.64	0/1294
12	L	0.53	0/394	0.70	0/524
13	M	0.40	0/2429	0.86	11/3281 (0.3%)
14	N	0.26	0/945	0.68	3/1274 (0.2%)
15	O	0.24	0/816	0.49	0/1105
16	P	0.29	0/1489	0.54	1/2005 (0.0%)
17	Q	0.30	0/1507	0.62	1/2023 (0.0%)
18	R	0.51	0/1380	1.04	5/1854 (0.3%)
19	S	0.25	0/1167	0.54	1/1576 (0.1%)
20	T	0.37	2/1817 (0.1%)	0.70	2/2445 (0.1%)
21	U	0.28	0/1358	0.64	3/1820 (0.2%)
22	X	0.66	0/1843	1.01	0/2847
23	Y	0.60	0/1817	0.95	0/2800
All	All	0.56	15/49126 (0.0%)	0.82	94/67010 (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	3
7	G	0	1
13	M	0	1
14	N	0	2
16	P	0	1
17	Q	0	1
18	R	0	1
19	S	0	1
20	T	0	2
All	All	0	15

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	T	60	GLU	CD-OE1	7.39	1.33	1.25
2	B	191	GLU	CG-CD	6.38	1.61	1.51
20	T	60	GLU	CD-OE2	5.92	1.32	1.25
2	B	1048	TYR	CD2-CE2	-5.68	1.30	1.39
2	B	1047	TYR	CD1-CE1	-5.66	1.30	1.39

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	84	HIS	C-N-CD	-28.89	57.05	120.60
18	R	194	ARG	C-N-CD	-24.66	66.35	120.60
13	M	10	LEU	C-N-CD	-22.77	70.51	120.60
3	C	6	GLN	C-N-CD	-20.32	75.89	120.60
1	A	483	ARG	NE-CZ-NH1	11.54	126.07	120.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1086	MET	Peptide
1	A	1308	TYR	Peptide
2	B	416	ARG	Sidechain
2	B	525	ASN	Peptide
2	B	873	LEU	Mainchain

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	11515	0	11607	525	0
2	B	9317	0	9308	354	0
3	C	2213	0	2153	90	0
4	D	1062	0	1042	11	0
5	E	1723	0	1745	60	0
6	F	689	0	715	18	0
7	G	1351	0	1358	26	0
8	H	1205	0	1168	44	0
9	I	1013	0	932	55	0
10	J	533	0	553	35	0
11	K	937	0	959	32	0
12	L	388	0	393	26	0
13	M	2391	0	2410	126	0
14	N	930	0	888	23	0
15	O	806	0	818	16	0
16	P	1462	0	1549	58	0
17	Q	1484	0	1494	147	0
18	R	1357	0	1379	205	0
19	S	1138	0	1103	35	0
20	T	1788	0	1819	97	0
21	U	1343	0	1338	45	0
22	X	1645	0	908	34	0
23	Y	1624	0	899	27	0
24	A	2	0	0	0	0
25	A	2	0	0	0	0
25	B	1	0	0	0	0
25	C	1	0	0	0	0
25	I	2	0	0	0	0
25	J	1	0	0	0	0
25	L	1	0	0	0	0
25	M	1	0	0	0	0
25	Q	1	0	0	0	0
25	U	1	0	0	0	0
All	All	47927	0	46538	1735	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 19.

The worst 5 of 1735 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)
1:A:932:ARG:CG	1:A:943:LEU:CD1	1.74	1.56
18:R:195:PRO:CG	18:R:199:LYS:CB	1.86	1.52
5:E:64:HIS:CE1	5:E:68:PRO:HG3	1.44	1.52
13:M:37:CYS:SG	13:M:39:LEU:HD22	1.46	1.52
1:A:932:ARG:CD	1:A:943:LEU:HD21	1.38	1.50

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	1450/1970 (74%)	1270 (88%)	118 (8%)	62 (4%)	2 26
2	B	1163/1174 (99%)	1001 (86%)	110 (10%)	52 (4%)	2 25
3	C	273/275 (99%)	242 (89%)	24 (9%)	7 (3%)	5 35
4	D	127/142 (89%)	120 (94%)	7 (6%)	0	100 100
5	E	208/210 (99%)	191 (92%)	8 (4%)	9 (4%)	2 26
6	F	84/127 (66%)	80 (95%)	4 (5%)	0	100 100
7	G	169/172 (98%)	161 (95%)	8 (5%)	0	100 100
8	H	148/150 (99%)	117 (79%)	14 (10%)	17 (12%)	0 7
9	I	123/125 (98%)	90 (73%)	22 (18%)	11 (9%)	1 13
10	J	65/67 (97%)	56 (86%)	5 (8%)	4 (6%)	1 20
11	K	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	17 54
12	L	44/58 (76%)	32 (73%)	9 (20%)	3 (7%)	1 18
13	M	308/316 (98%)	262 (85%)	28 (9%)	18 (6%)	1 21
14	N	109/376 (29%)	95 (87%)	11 (10%)	3 (3%)	5 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	O	97/109 (89%)	96 (99%)	1 (1%)	0	100 100
16	P	183/339 (54%)	170 (93%)	7 (4%)	6 (3%)	4 31
17	Q	176/439 (40%)	160 (91%)	8 (4%)	8 (4%)	2 25
18	R	163/291 (56%)	142 (87%)	15 (9%)	6 (4%)	3 29
19	S	134/517 (26%)	119 (89%)	11 (8%)	4 (3%)	4 33
20	T	218/249 (88%)	190 (87%)	16 (7%)	12 (6%)	2 22
21	U	168/301 (56%)	142 (84%)	18 (11%)	8 (5%)	2 24
All	All	5525/7524 (73%)	4842 (88%)	452 (8%)	231 (4%)	5 26

5 of 231 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	ARG
1	A	70	ARG
1	A	133	SER
1	A	205	VAL
1	A	208	ASP

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	1279/1748 (73%)	1224 (96%)	55 (4%)	29 57
2	B	1020/1028 (99%)	982 (96%)	38 (4%)	34 60
3	C	252/252 (100%)	243 (96%)	9 (4%)	35 61
4	D	119/126 (94%)	119 (100%)	0	100 100
5	E	192/192 (100%)	187 (97%)	5 (3%)	46 68
6	F	74/111 (67%)	72 (97%)	2 (3%)	44 67
7	G	152/153 (99%)	151 (99%)	1 (1%)	84 90
8	H	131/131 (100%)	127 (97%)	4 (3%)	40 64
9	I	112/112 (100%)	109 (97%)	3 (3%)	44 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	J	56/56 (100%)	49 (88%)	7 (12%)	4 23
11	K	106/106 (100%)	103 (97%)	3 (3%)	43 66
12	L	43/55 (78%)	41 (95%)	2 (5%)	26 55
13	M	263/268 (98%)	253 (96%)	10 (4%)	33 59
14	N	105/324 (32%)	101 (96%)	4 (4%)	33 59
15	O	90/98 (92%)	88 (98%)	2 (2%)	52 71
16	P	159/293 (54%)	157 (99%)	2 (1%)	69 82
17	Q	164/373 (44%)	158 (96%)	6 (4%)	34 60
18	R	150/261 (58%)	143 (95%)	7 (5%)	26 55
19	S	121/448 (27%)	117 (97%)	4 (3%)	38 63
20	T	196/218 (90%)	193 (98%)	3 (2%)	65 80
21	U	148/266 (56%)	140 (95%)	8 (5%)	22 52
All	All	4932/6619 (74%)	4757 (96%)	175 (4%)	39 62

5 of 175 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	61	GLU
15	O	63	ASN
10	J	46	ARG
13	M	12	ARG
17	Q	171	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	26	ASN
13	M	71	GLN
18	R	204	ASN
2	B	319	ASN
2	B	175	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

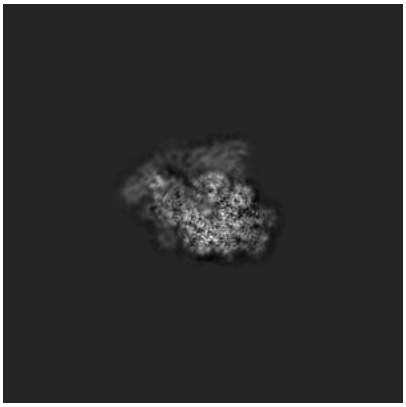
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8137. These allow visual inspection of the internal detail of the map and identification of artifacts.

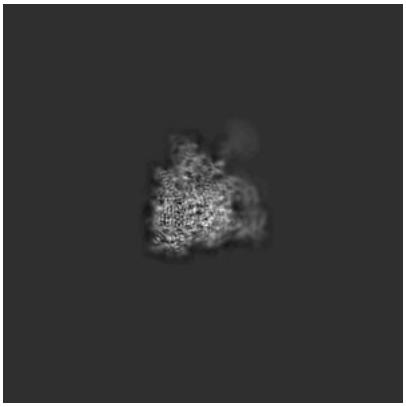
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

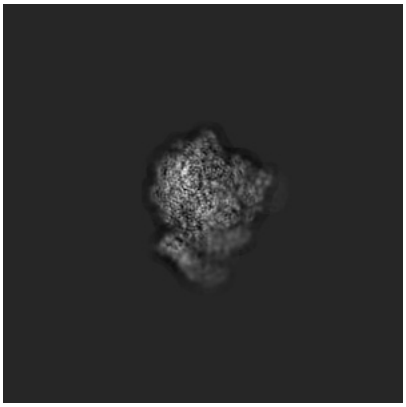
6.1.1 Primary map



X



Y

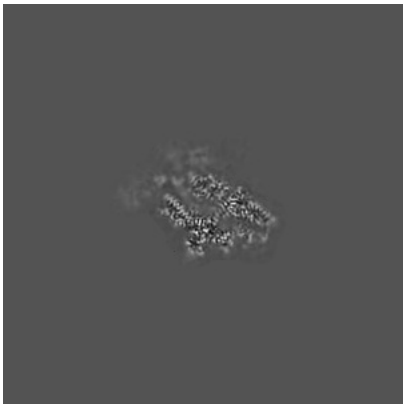


Z

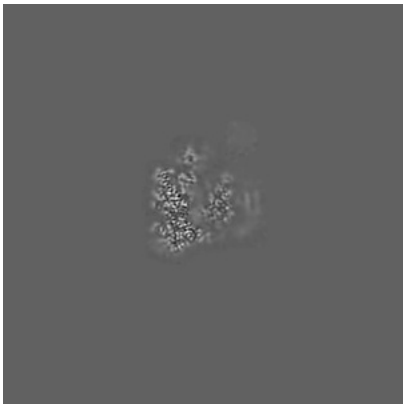
The images above show the map projected in three orthogonal directions.

6.2 Central slices

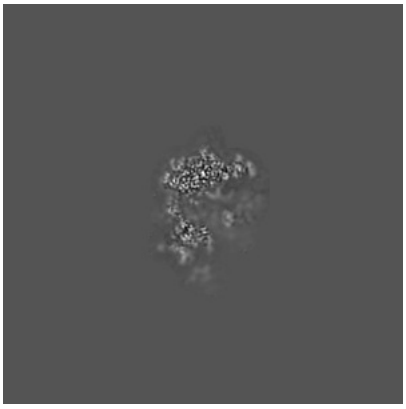
6.2.1 Primary map



X Index: 192



Y Index: 192

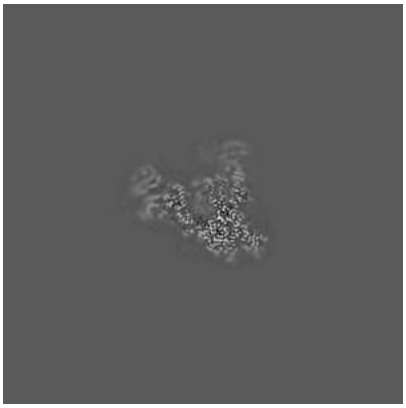


Z Index: 192

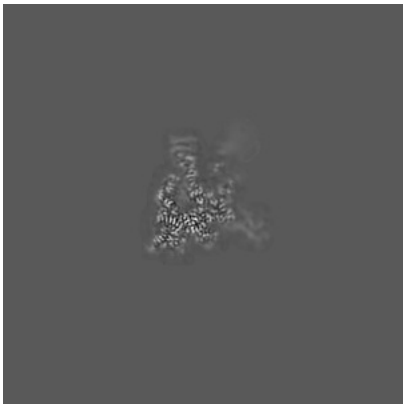
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

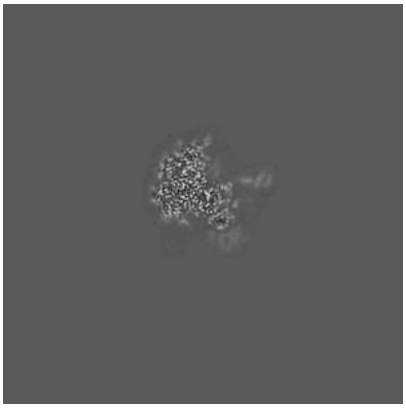
6.3.1 Primary map



X Index: 175



Y Index: 210

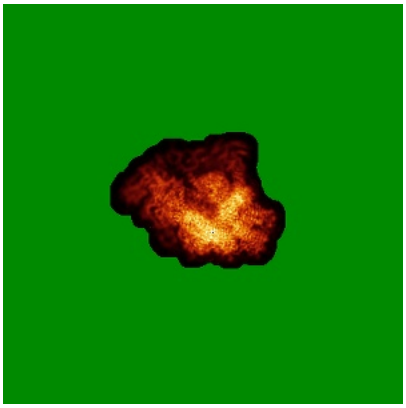


Z Index: 163

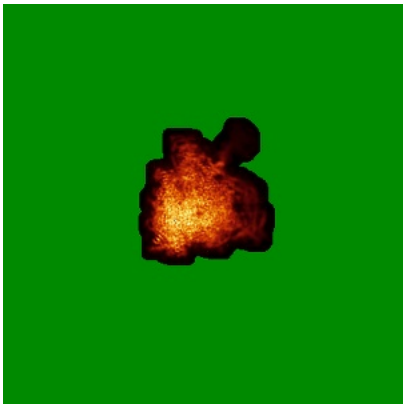
The images above show the largest variance slices of the map in three orthogonal directions.

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

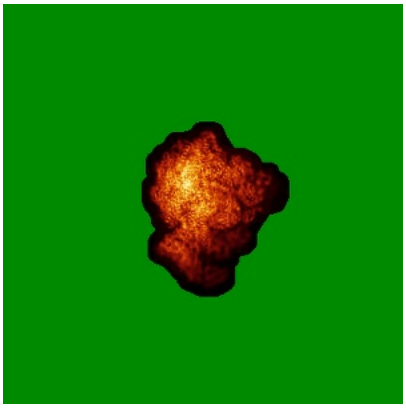
6.4.1 Primary map



X



Y

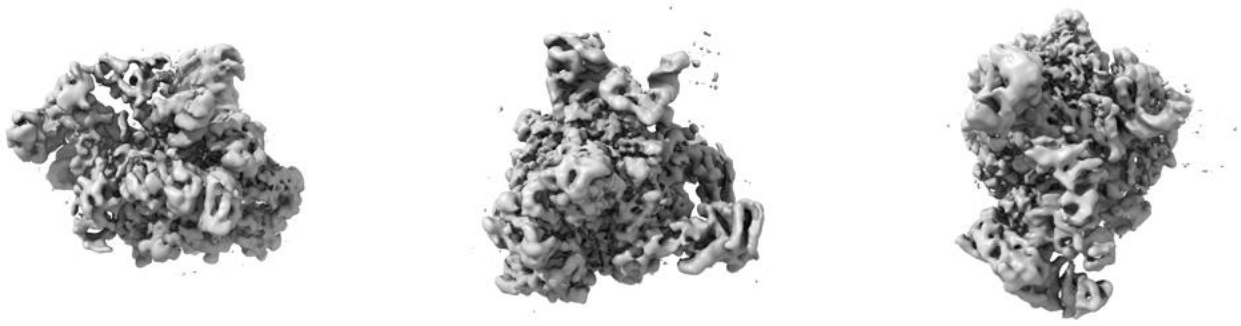


Z

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 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

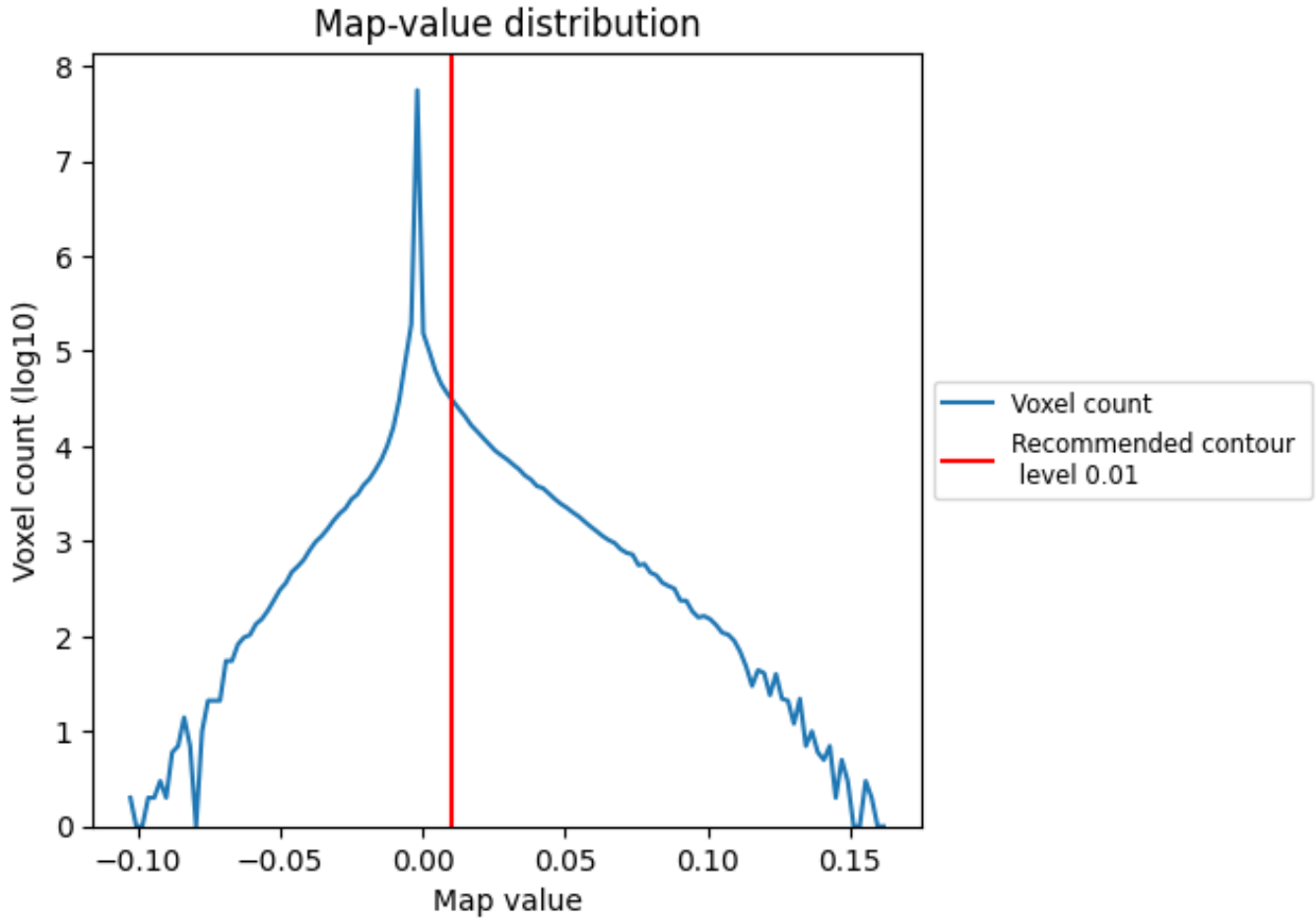
6.6 Mask visualisation (i)

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

7 Map analysis

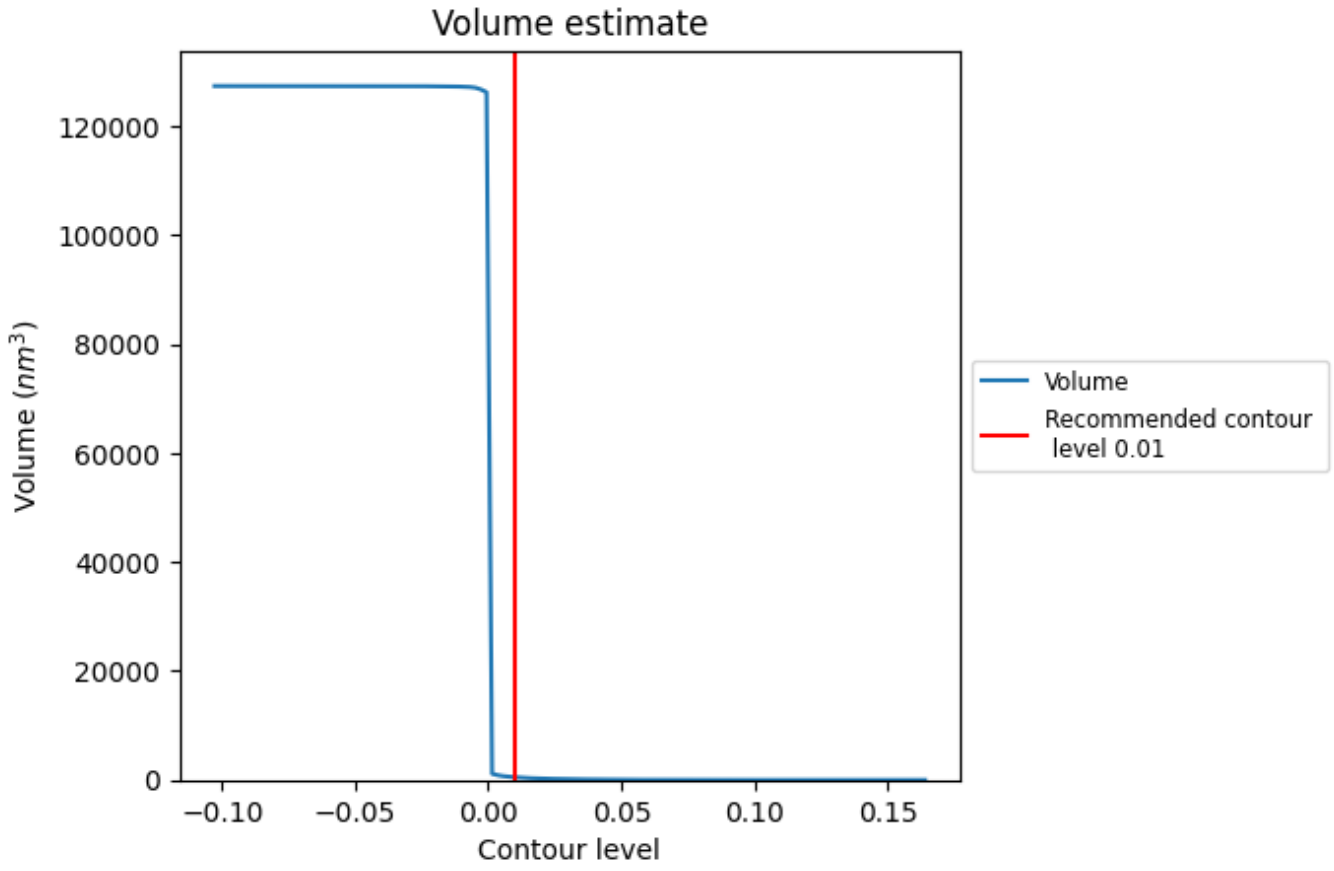
This section contains the results of statistical analysis of the map.

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.

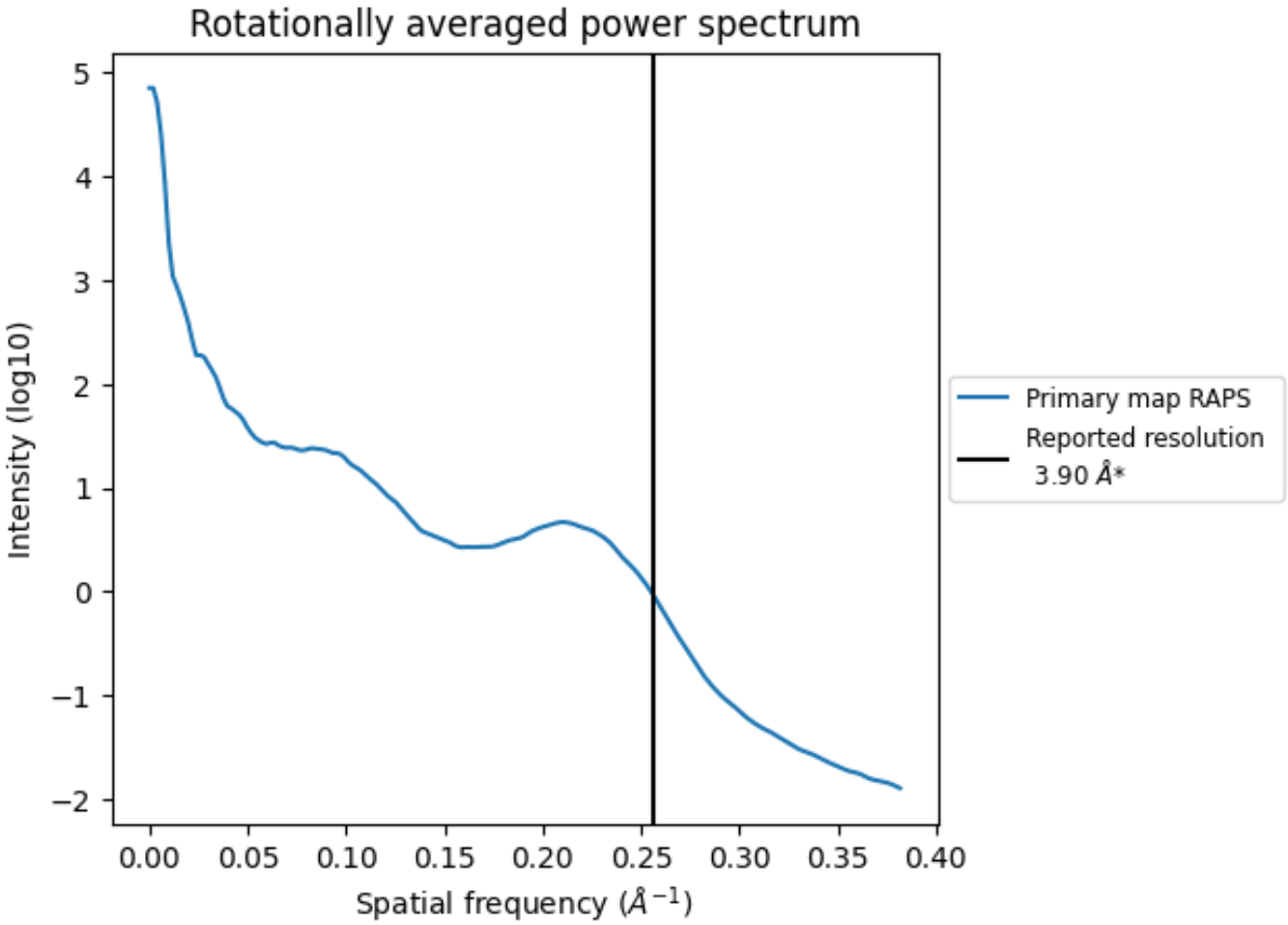
7.2 Volume estimate (i)



The volume at the recommended contour level is 500 nm^3; this corresponds to an approximate mass of 451 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)

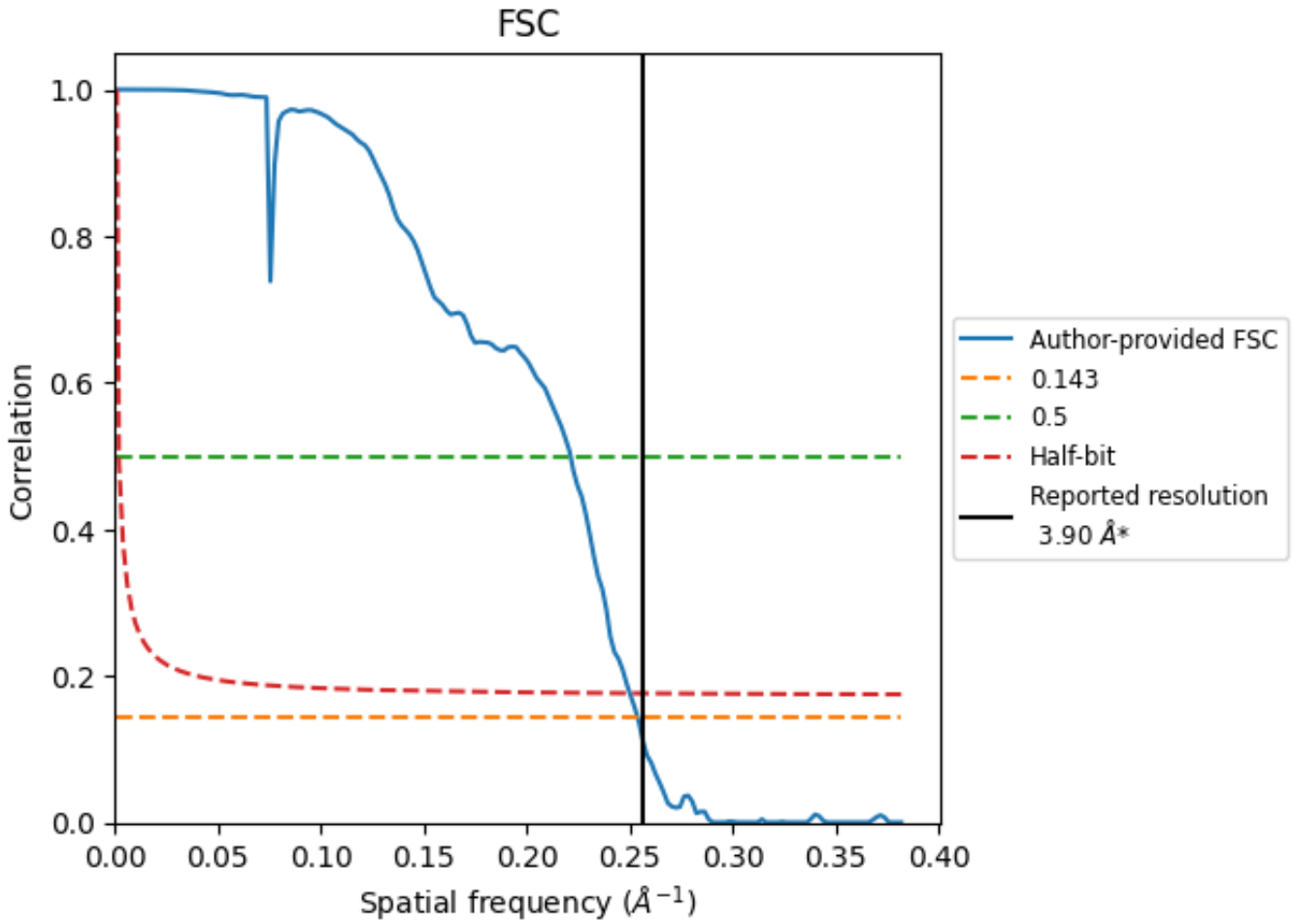


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

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 0.256 Å^{-1}

8.2 Resolution estimates (i)

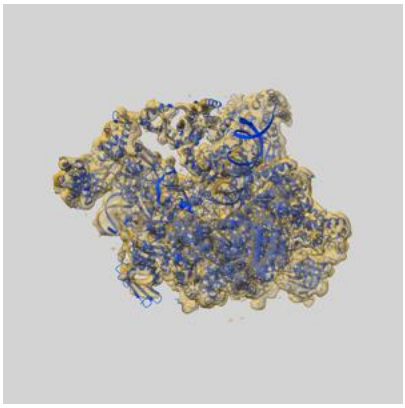
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.94	4.52	4.00
Unmasked-calculated*	-	-	-

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

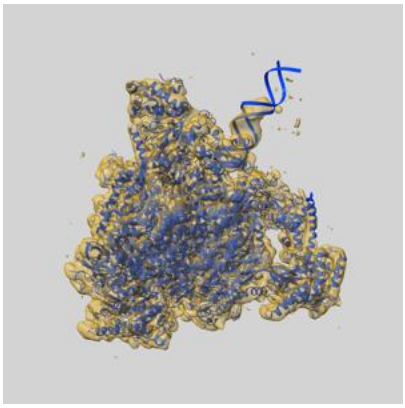
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8137 and PDB model 5IYC. Per-residue inclusion information can be found in section 3 on page 8.

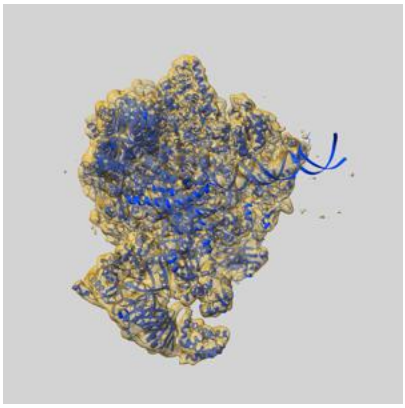
9.1 Map-model overlay



X



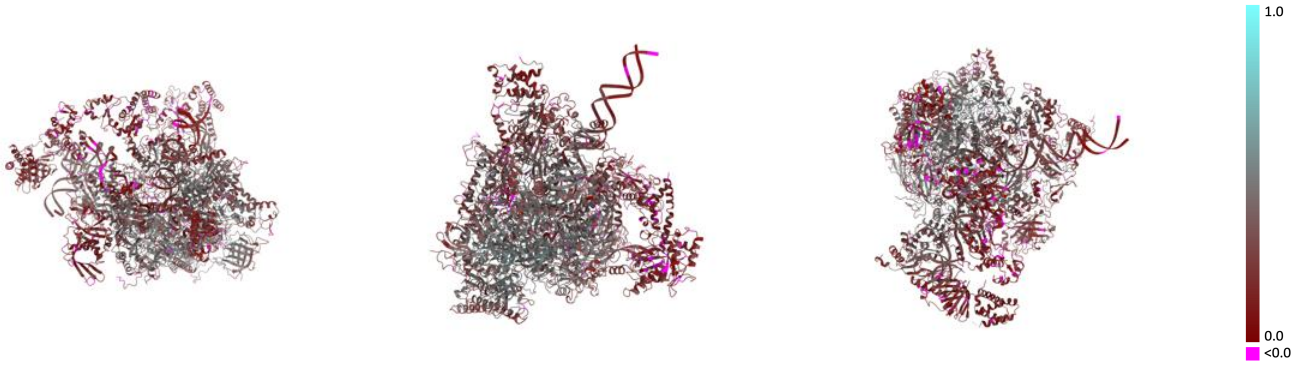
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

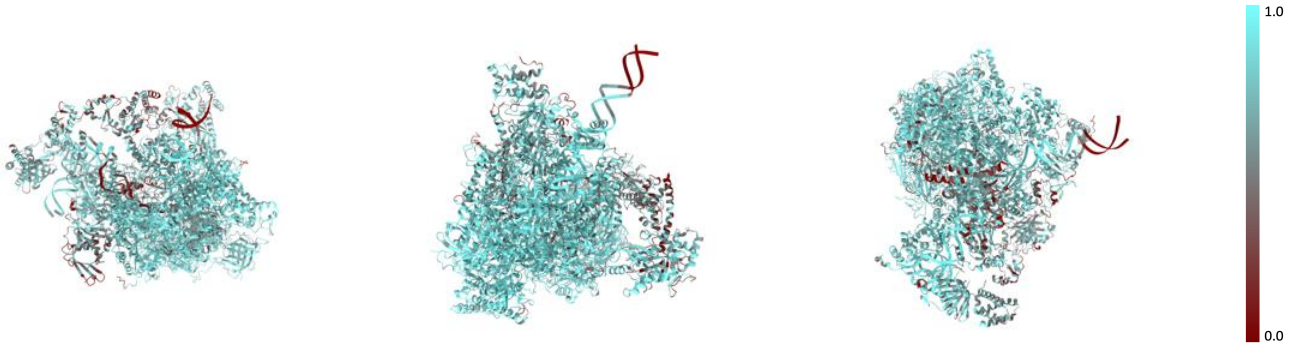
9.2 Q-score mapped to coordinate model



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.

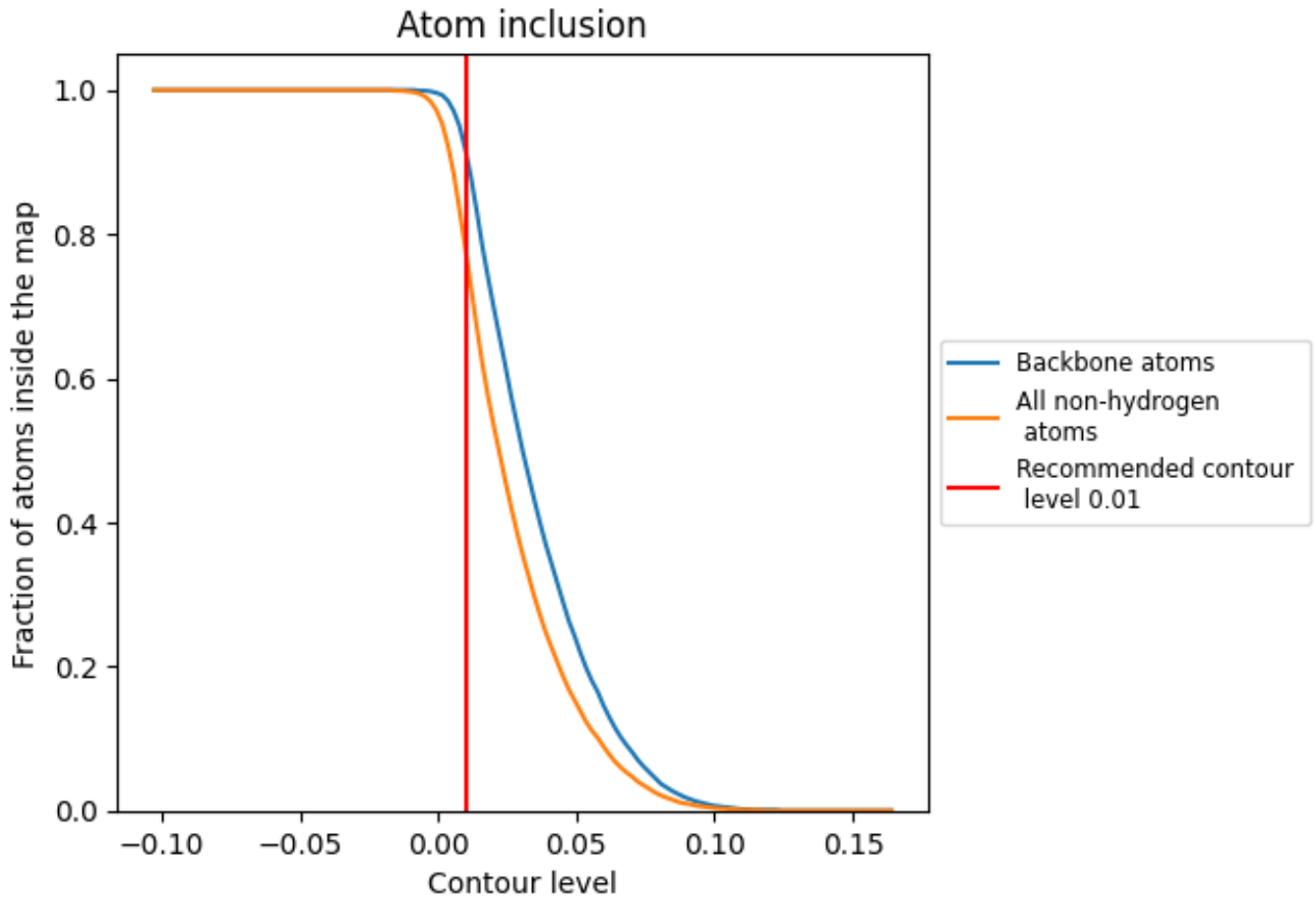
9.3 Atom inclusion mapped to coordinate model



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 78% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7760	0.3060
A	0.8490	0.3730
B	0.8490	0.3980
C	0.8750	0.3840
D	0.7110	0.1630
E	0.8390	0.3450
F	0.8310	0.3900
G	0.7450	0.2050
H	0.8440	0.3320
I	0.7830	0.2840
J	0.8770	0.3930
K	0.8750	0.3840
L	0.8820	0.3710
M	0.7870	0.3020
N	0.6690	0.1670
O	0.6880	0.1690
P	0.8190	0.2500
Q	0.4570	0.1260
R	0.4910	0.1260
S	0.4990	0.1530
T	0.5520	0.1590
U	0.5860	0.1460
X	0.6790	0.2090
Y	0.7800	0.2350