wwPDB EM Validation Summary Report (i)

Jul 8, 2024 – 05:45 pm BST

PDB ID	:	7OPD
EMDB ID	:	EMD-13016
Title	:	Pol II-CSB-CRL4CSA-UVSSA-SPT6-PAF (Structure 5)
Authors	:	Kokic, G.; Cramer, P.
Deposited on	:	2021-05-31
Resolution	:	3.00 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:

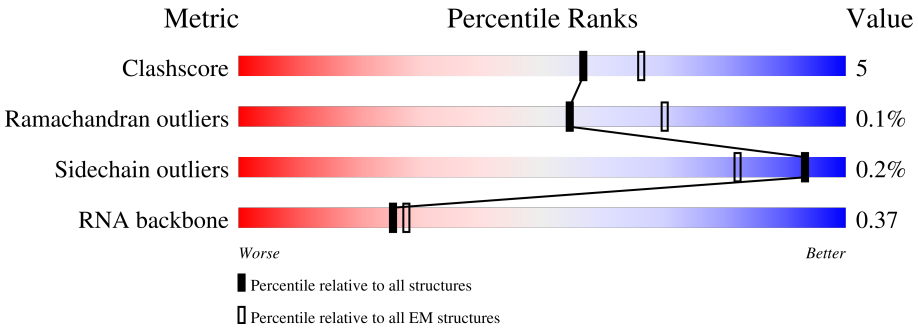
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.00 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	1970	65% 7% 28%
2	B	1174	5% 89% 7%
3	C	275	87% 7% 5%
4	D	142	16% 73% 15% 10%
5	E	210	91% 9%
6	F	127	61% 35%
7	G	172	13% 73% 24%

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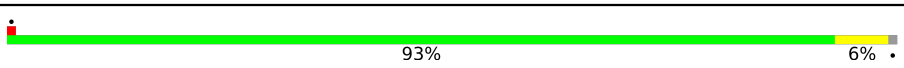
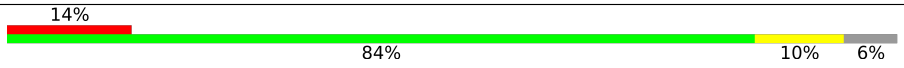
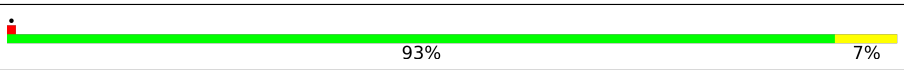
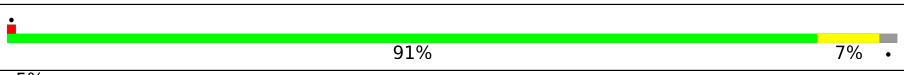
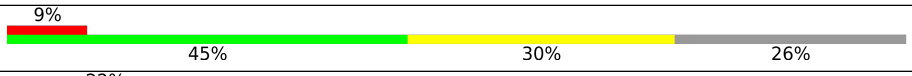
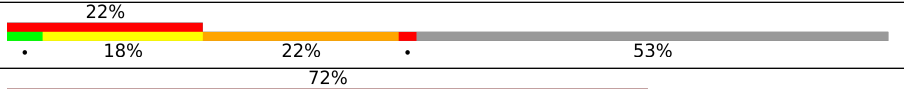
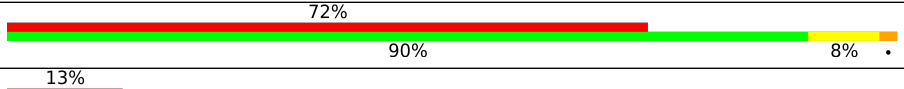
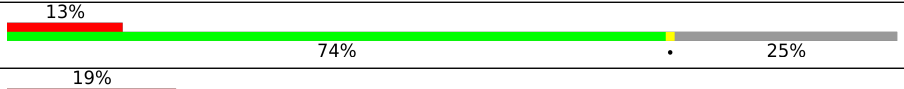
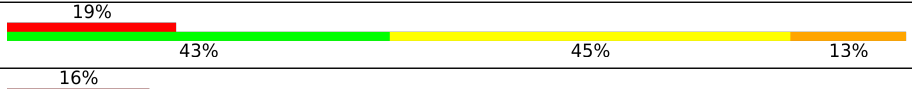
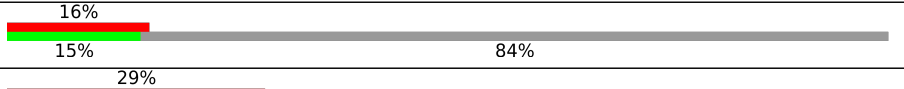
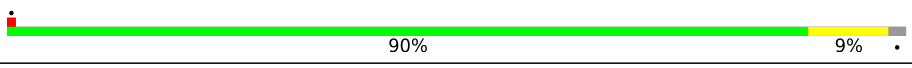
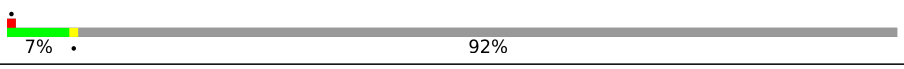
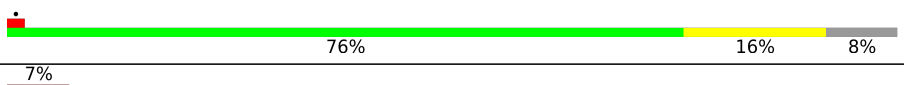
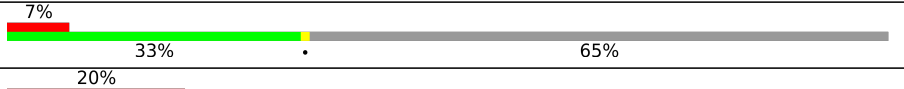
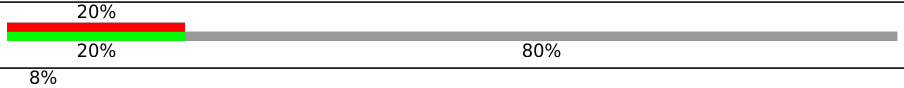
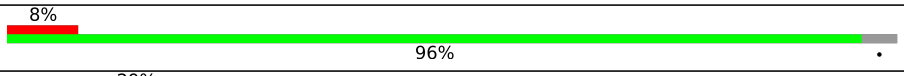
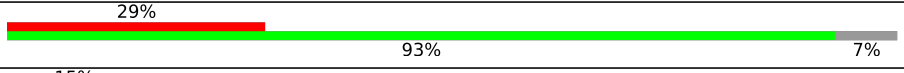
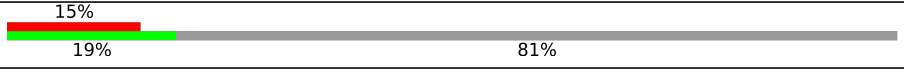
Mol	Chain	Length	Quality of chain
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	1729	
14	N	47	
15	P	45	
16	R	40	
17	S	1179	
18	T	47	
19	U	666	
20	V	531	
21	Y	305	
22	Z	531	
23	a	396	
24	b	1496	
25	c	712	
26	d	1143	
27	e	762	
28	f	108	

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 64227 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	1412	11179	7033	2002	2074	70	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1131	9052	5727	1592	1669	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	260	2089	1309	359	415	6	0	0

- Molecule 4 is a protein called RPOL4c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	128	1013	636	172	201	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	209	1720	1089	300	323	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	82	657	418	113	121	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
			1334	867	216	243	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
			949	587	169	182	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
			388	241	75	66	6		

- Molecule 13 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	810	Total	C	N	O	S	0	0
			6648	4226	1155	1234	33		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP Q7KZ85
M	-1	ASN	-	expression tag	UNP Q7KZ85
M	0	ALA	-	expression tag	UNP Q7KZ85

- Molecule 14 is a DNA chain called NTS.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	35	Total	C	N	O	P	0	0
			727	344	142	206	35		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	21	Total	C	N	O	P	0	0
			454	204	89	140	21		

- Molecule 16 is a protein called LEO1 helix.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	R	40	Total	C	N	O	0	0
			160	80	40	40		

- Molecule 17 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	S	890	Total	C	N	O	0	0
			3560	1780	890	890		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	1174	GLU	-	expression tag	UNP Q6PD62
S	1175	ASN	-	expression tag	UNP Q6PD62
S	1176	LEU	-	expression tag	UNP Q6PD62
S	1177	TYR	-	expression tag	UNP Q6PD62
S	1178	PHE	-	expression tag	UNP Q6PD62
S	1179	GLN	-	expression tag	UNP Q6PD62

- Molecule 18 is a DNA chain called TS.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	47	Total	C	N	O	P	0	0
			947	453	159	288	47		

- Molecule 19 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	U	104	Total	C	N	O	0	0
			416	208	104	104		

- Molecule 20 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	V	217	Total	C	N	O	0	0
			868	434	217	217		

- Molecule 21 is a protein called WD repeat-containing protein 61.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Y	300	Total	C	N	O	0	0
			1200	600	300	300		

- Molecule 22 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	Z	43	Total	C	N	O	0	0
			172	86	43	43		

- Molecule 23 is a protein called DNA excision repair protein ERCC-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	365	Total	C	N	O	S	0	0
			2849	1775	507	548	19		

- Molecule 24 is a protein called DNA excision repair protein ERCC-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	520	Total	C	N	O	S	0	0
			4261	2746	748	746	21		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	-2	SER	-	expression tag	UNP Q03468
b	-1	ASN	-	expression tag	UNP Q03468
b	0	ALA	-	expression tag	UNP Q03468
b	538	ARG	LYS	conflict	UNP Q03468

- Molecule 25 is a protein called UV-stimulated scaffold protein A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	c	141	Total	C	N	O	0	0
			564	282	141	141		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	-2	SER	-	expression tag	UNP Q2YD98
c	-1	ASN	-	expression tag	UNP Q2YD98
c	0	ALA	-	expression tag	UNP Q2YD98

- Molecule 26 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	1096	Total	C	N	O	S	0	0
			7443	4562	1354	1493	34		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-2	SER	-	expression tag	UNP Q16531
d	-1	ASN	-	expression tag	UNP Q16531
d	0	ALA	-	expression tag	UNP Q16531

- Molecule 27 is a protein called Cullin-4A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	e	711	Total	C	N	O	0	0
			2845	1422	711	712		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	-2	SER	-	expression tag	UNP Q13619
e	-1	ASN	-	expression tag	UNP Q13619
e	0	ALA	-	expression tag	UNP Q13619

- Molecule 28 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	f	21	Total 84	C 42	N 21	O 21	0	0

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

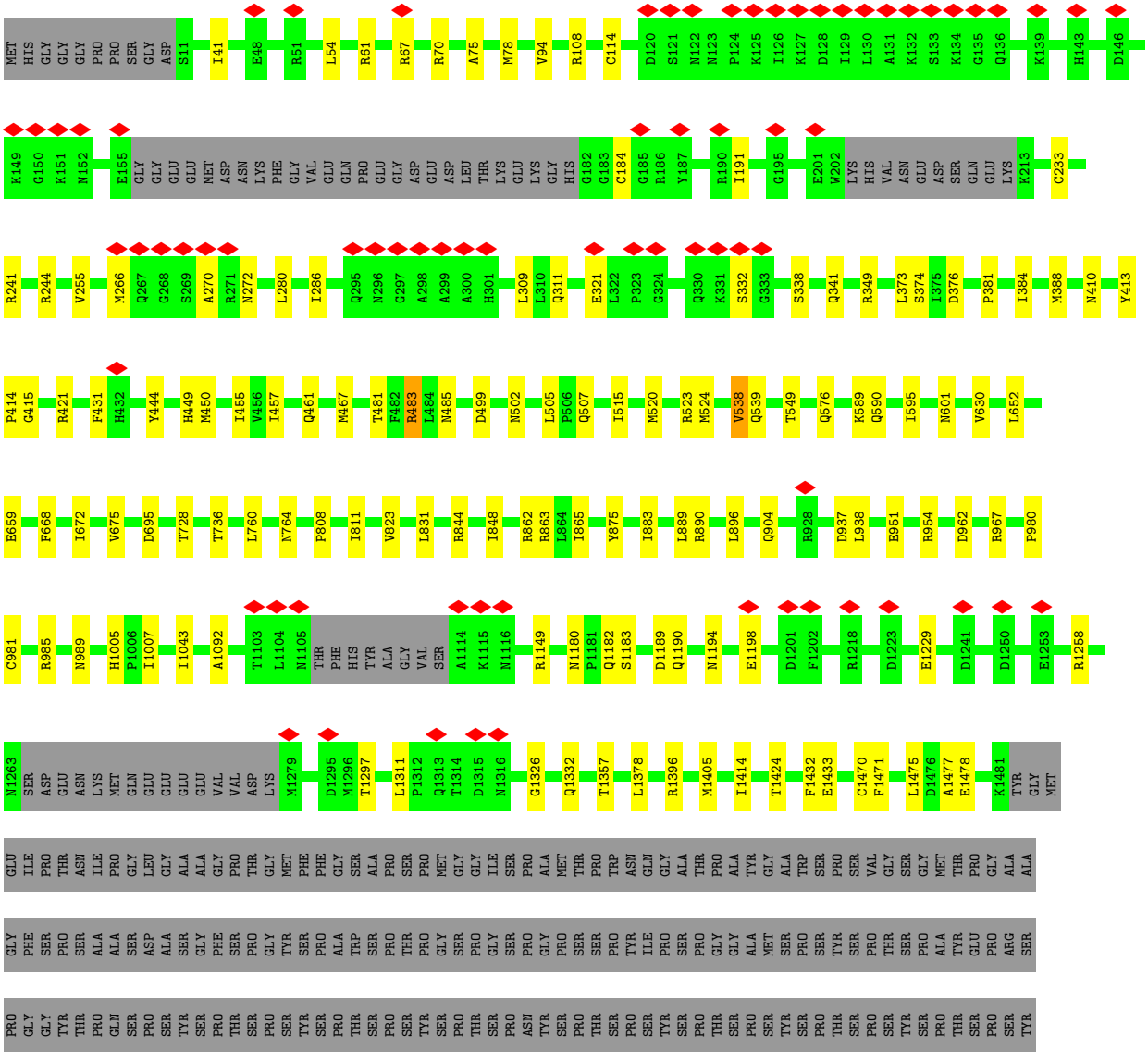
Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total 1	Mg 1	0

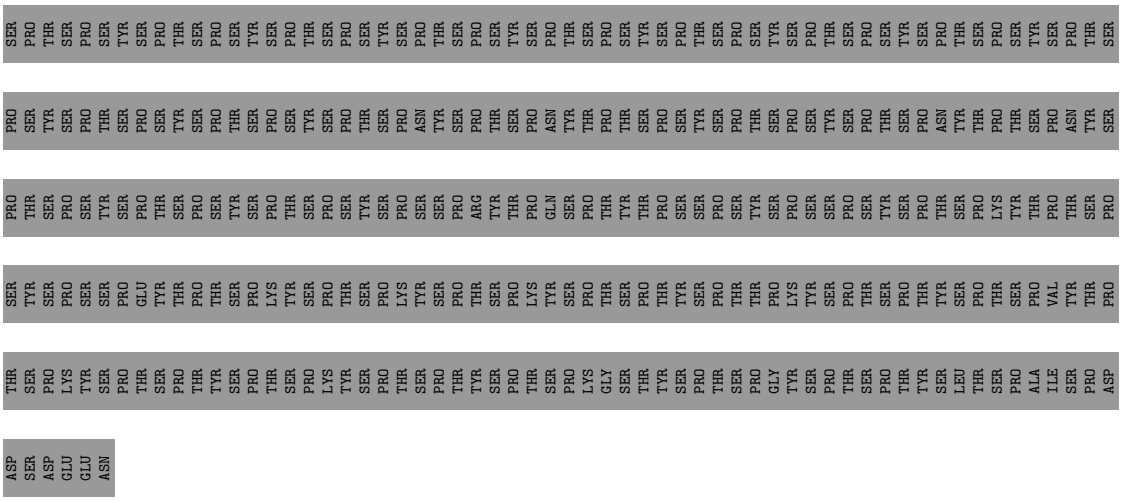
3 Residue-property plots (i)

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 II subunit RPB1

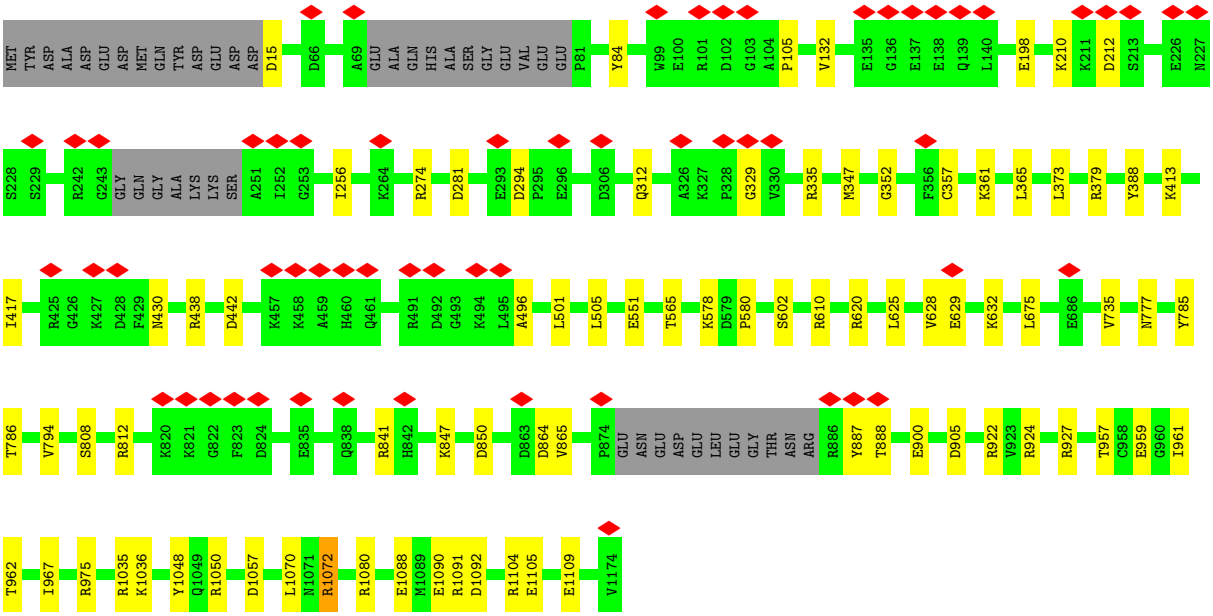
Chain A:





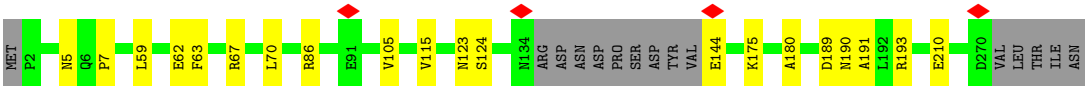
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:



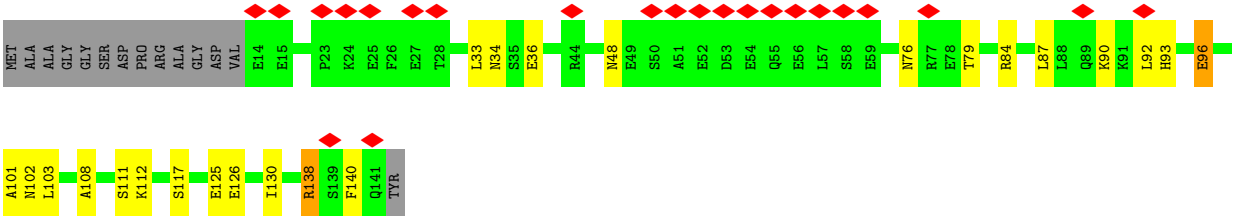
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:

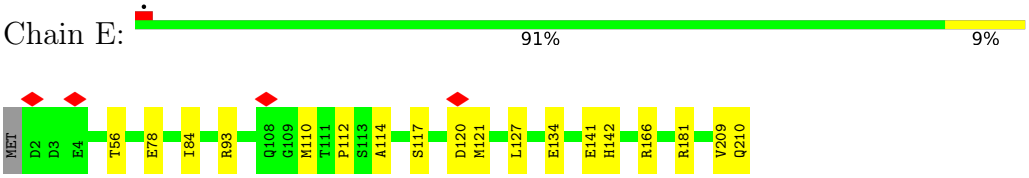


• Molecule 4: RPOL4c domain-containing protein

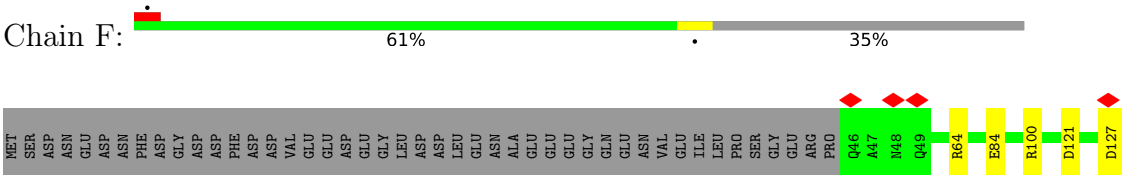
Chain D:



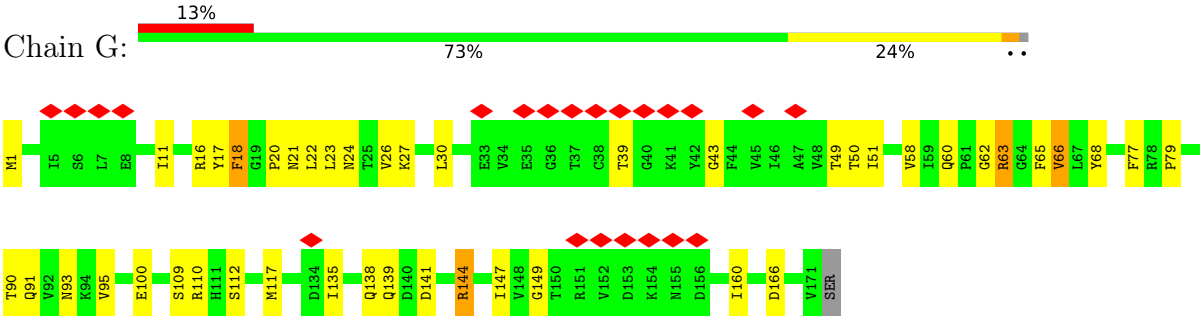
• Molecule 5: DNA-directed RNA polymerase II subunit E



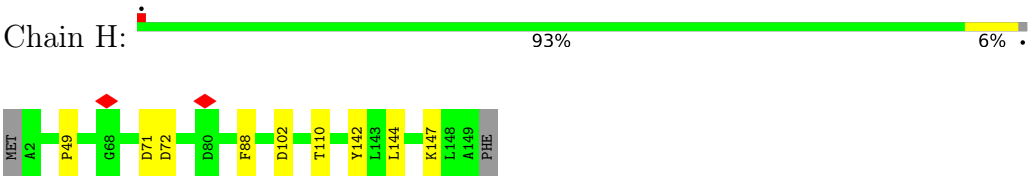
• Molecule 6: DNA-directed RNA polymerase II subunit F



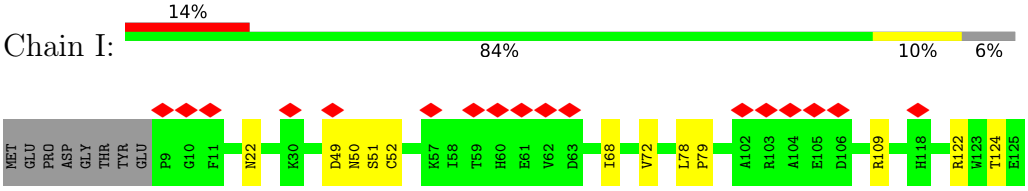
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7



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

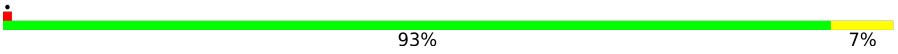


• Molecule 9: DNA-directed RNA polymerase II subunit RPB9



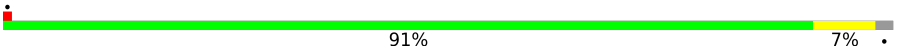
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



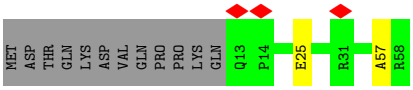
• Molecule 11: RNA_pol_L_2 domain-containing protein

Chain K:



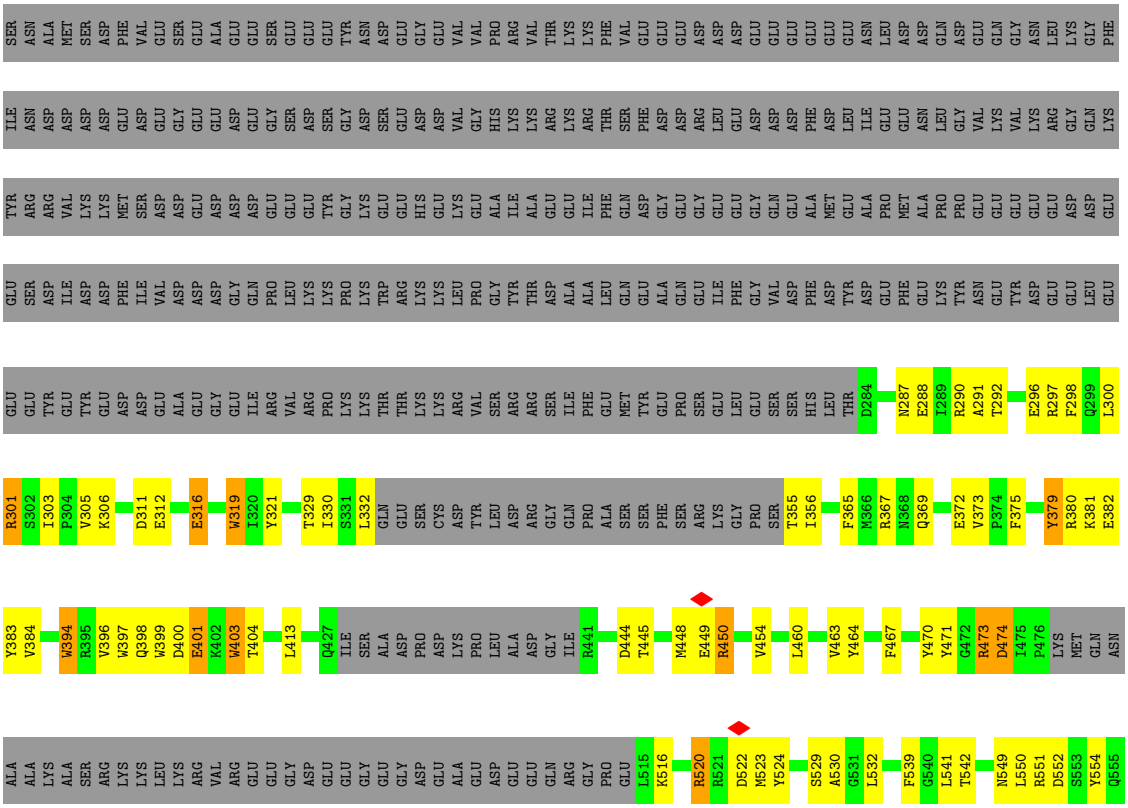
• Molecule 12: RNA polymerase II subunit K

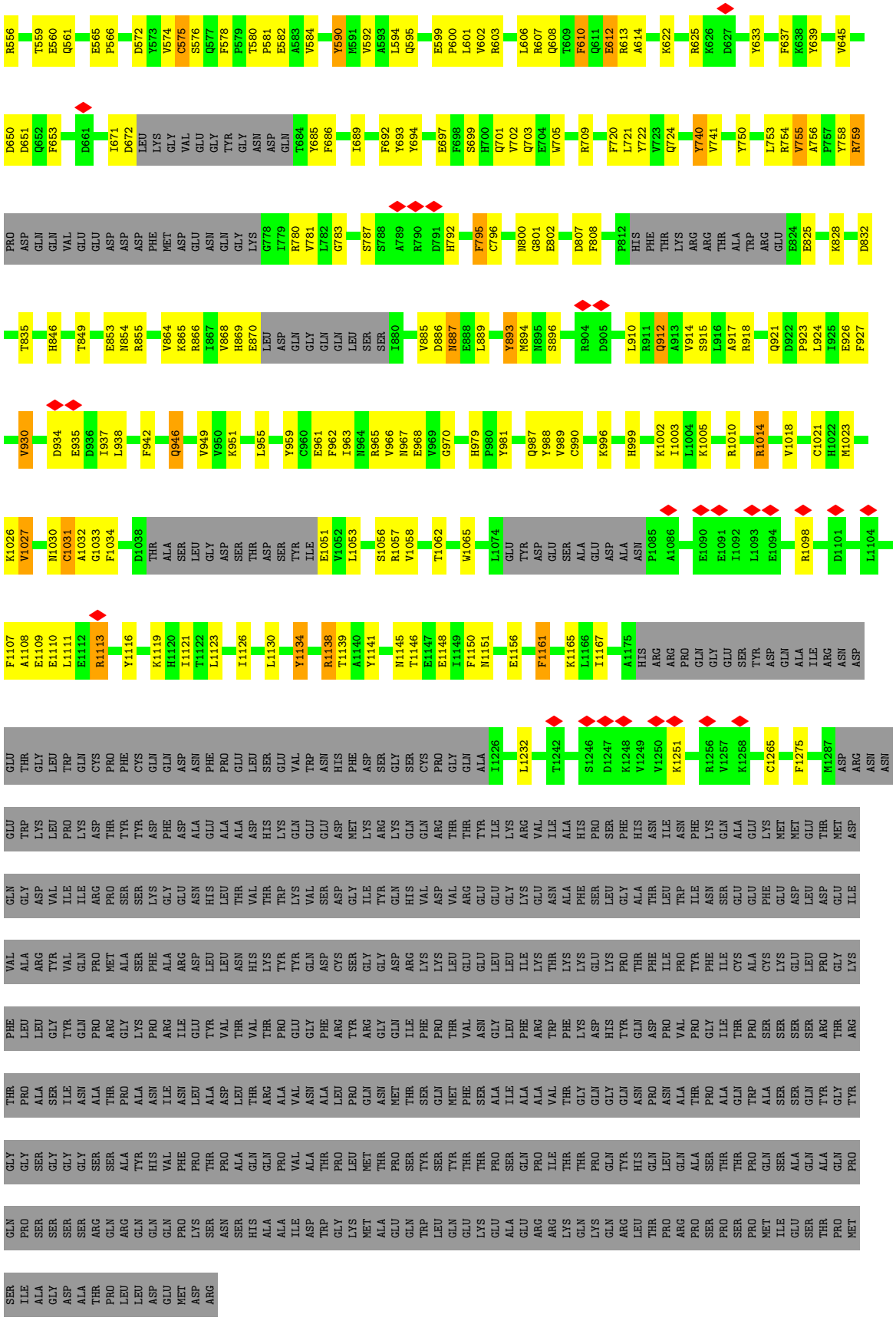
Chain L:



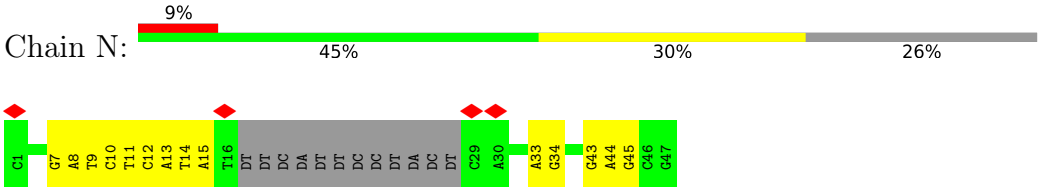
• Molecule 13: Transcription elongation factor SPT6

Chain M:

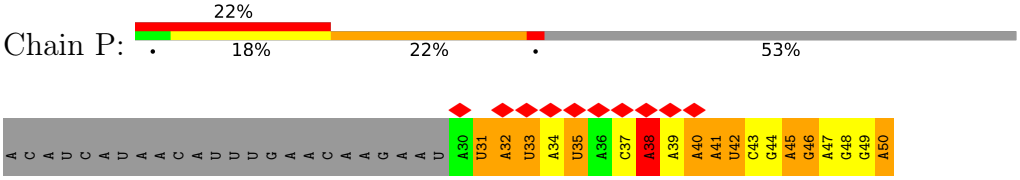




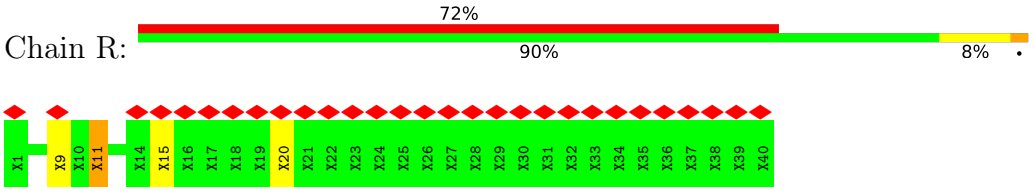
- Molecule 14: NTS



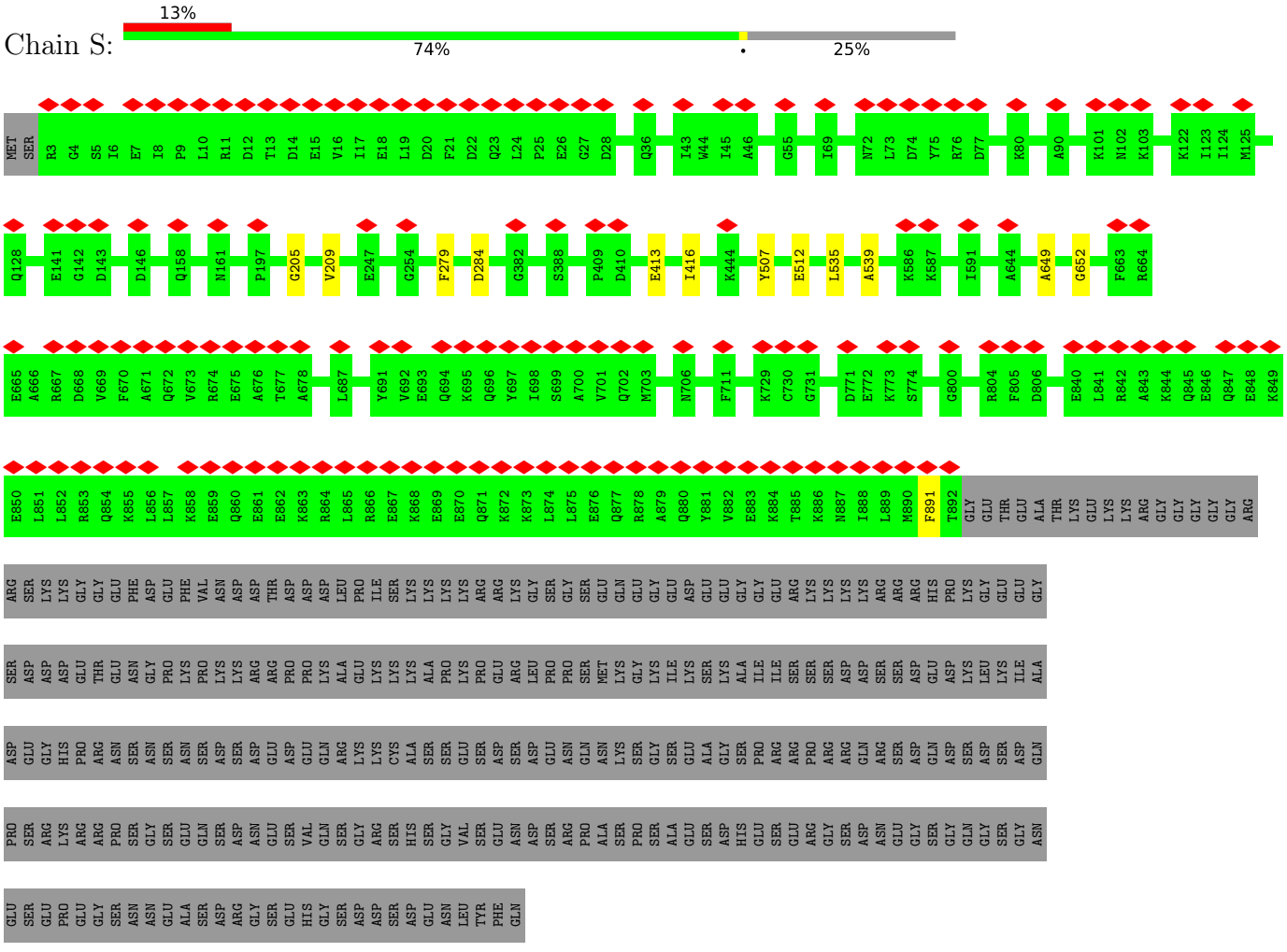
• Molecule 15: RNA



• Molecule 16: LEO1 helix

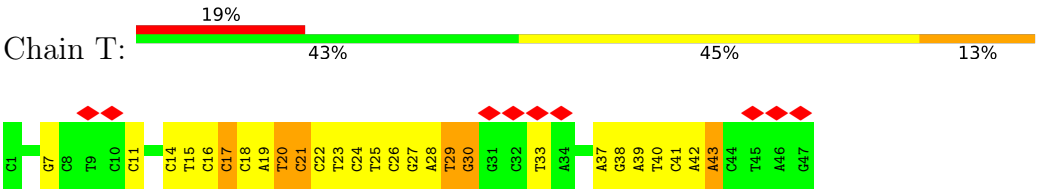


• Molecule 17: RNA polymerase-associated protein CTR9 homolog



• Molecule 18: TS

Chain T:

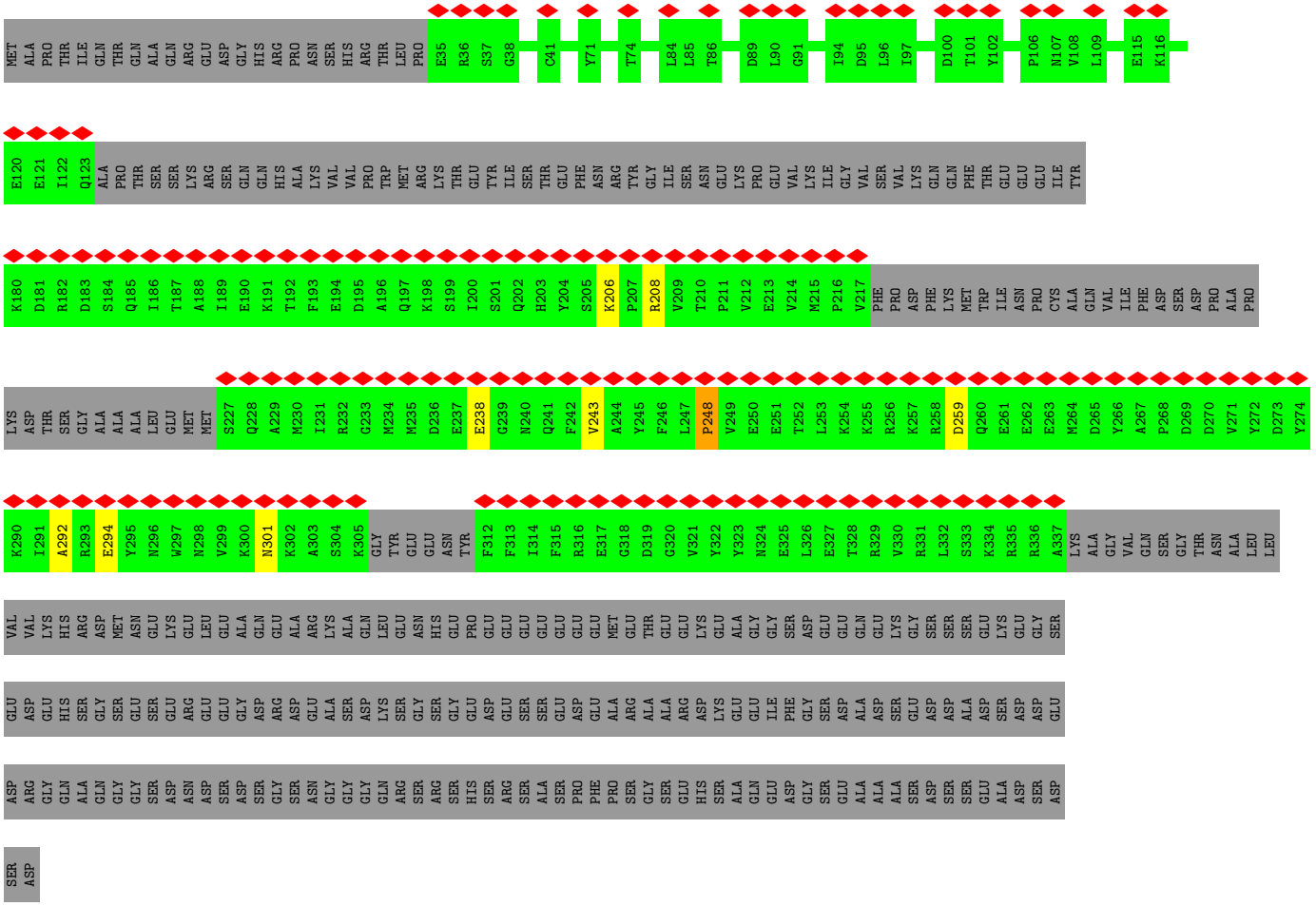


• Molecule 19: RNA polymerase-associated protein LEO1

Chain U:

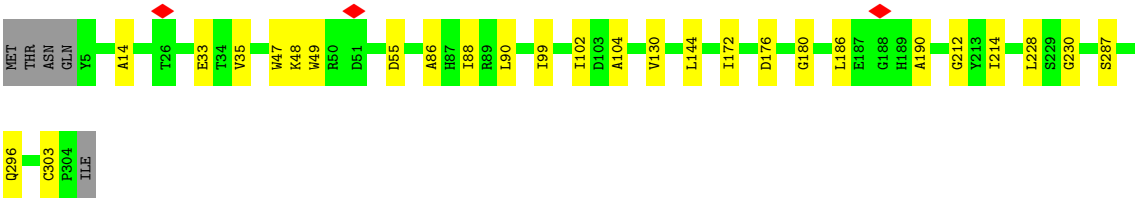
• Molecule 20: RNA polymerase II-associated factor 1 homolog

Chain V:



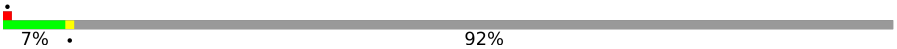
• Molecule 21: WD repeat-containing protein 61

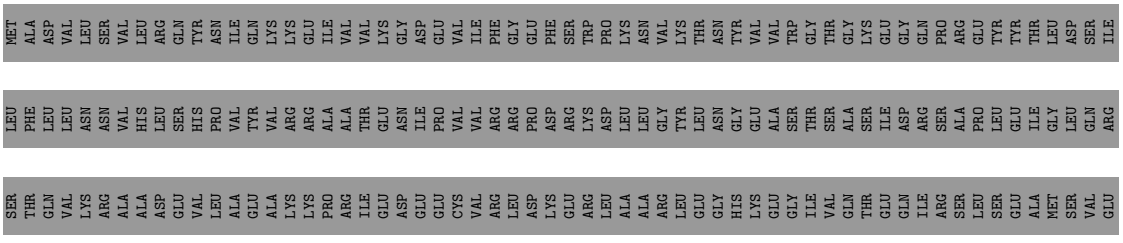
Chain Y:

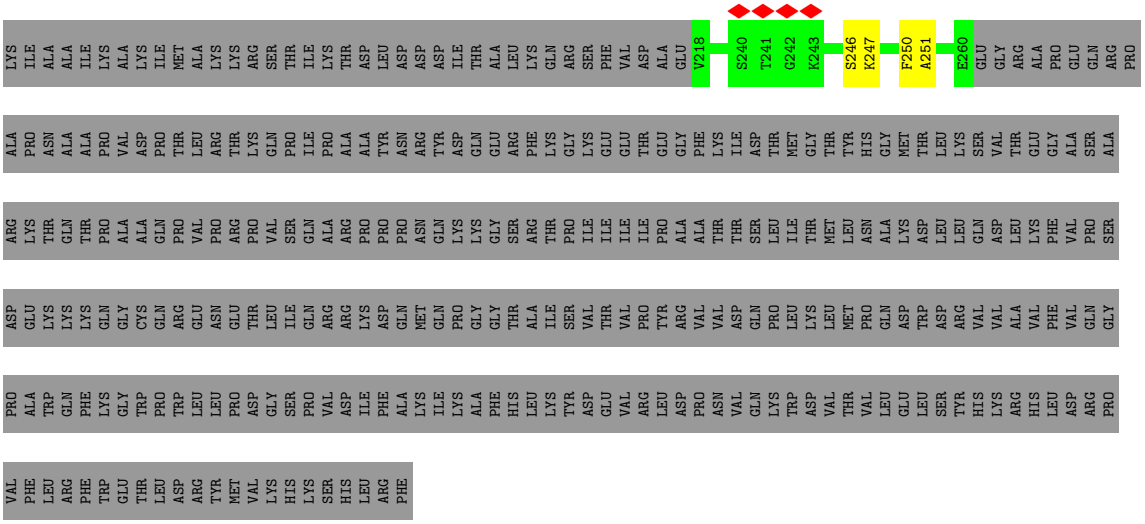


• Molecule 22: Parafibromin

Chain Z:

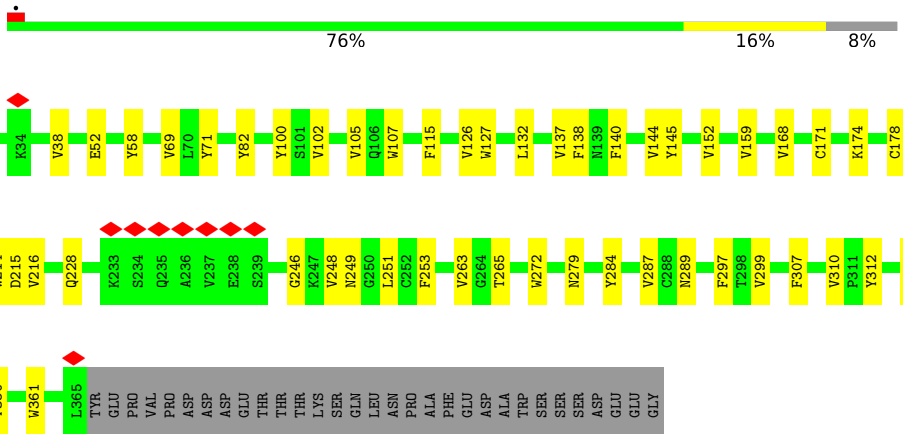






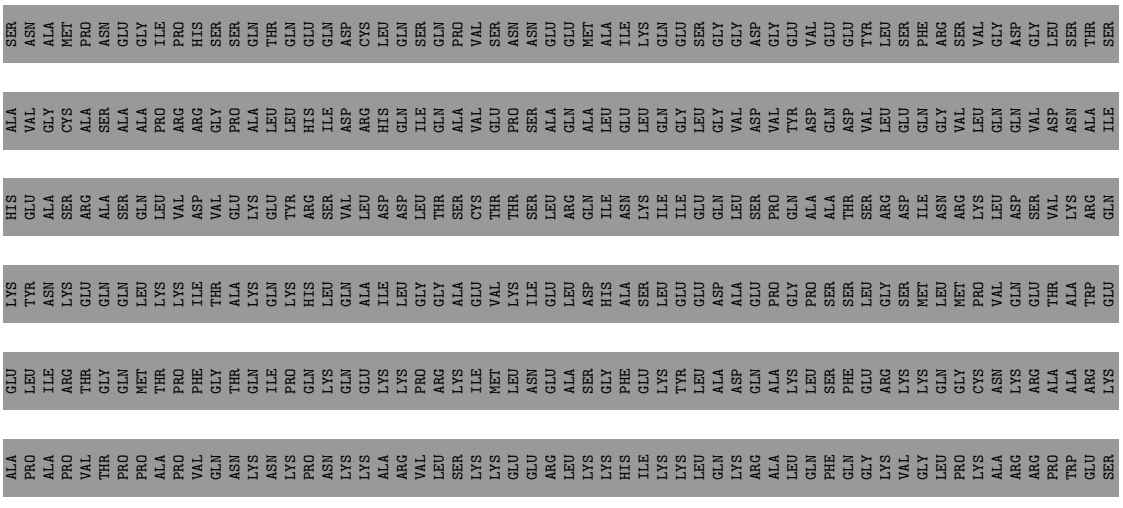
• Molecule 23: DNA excision repair protein ERCC-8

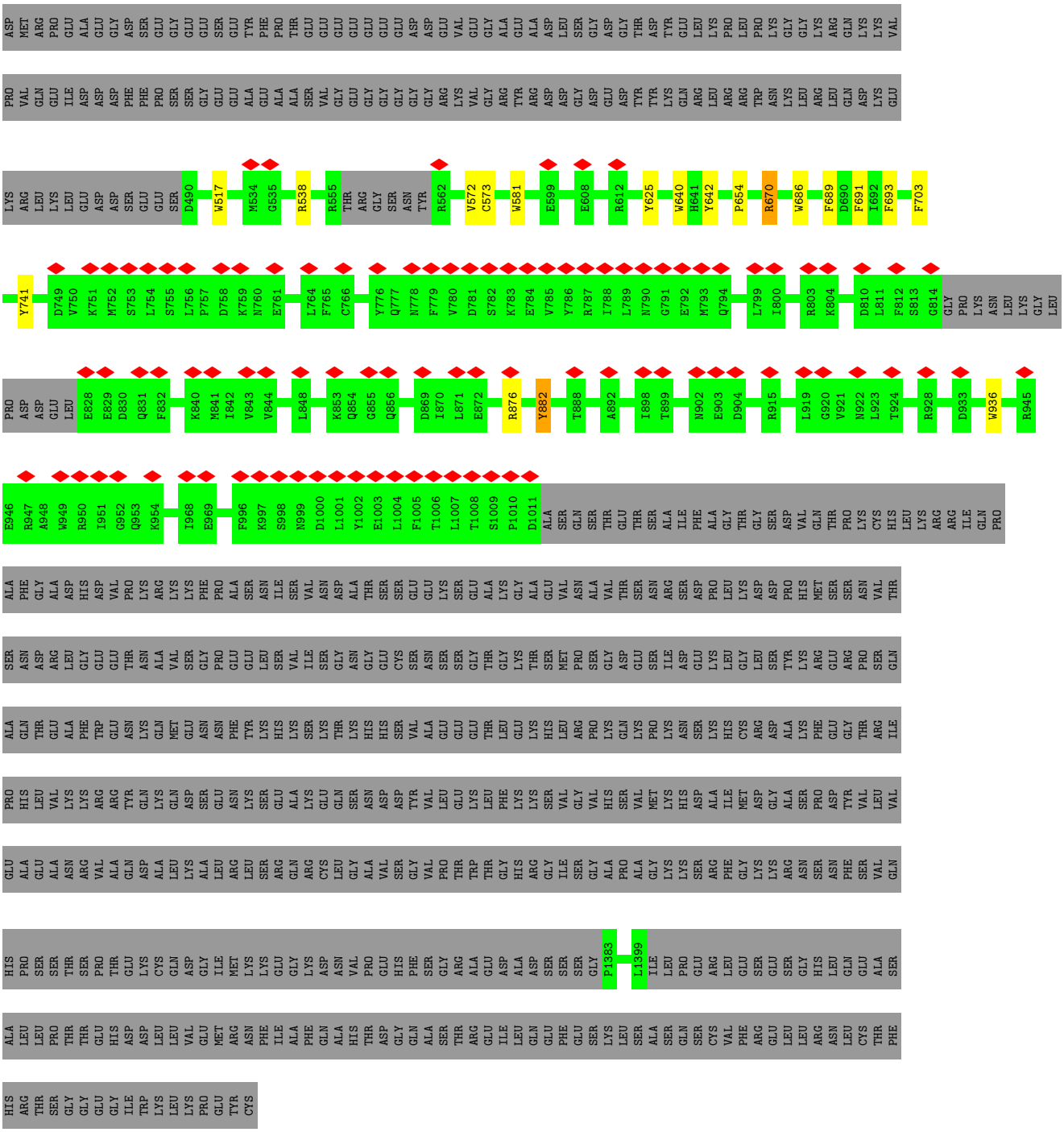
Chain a:



• Molecule 24: DNA excision repair protein ERCC-6

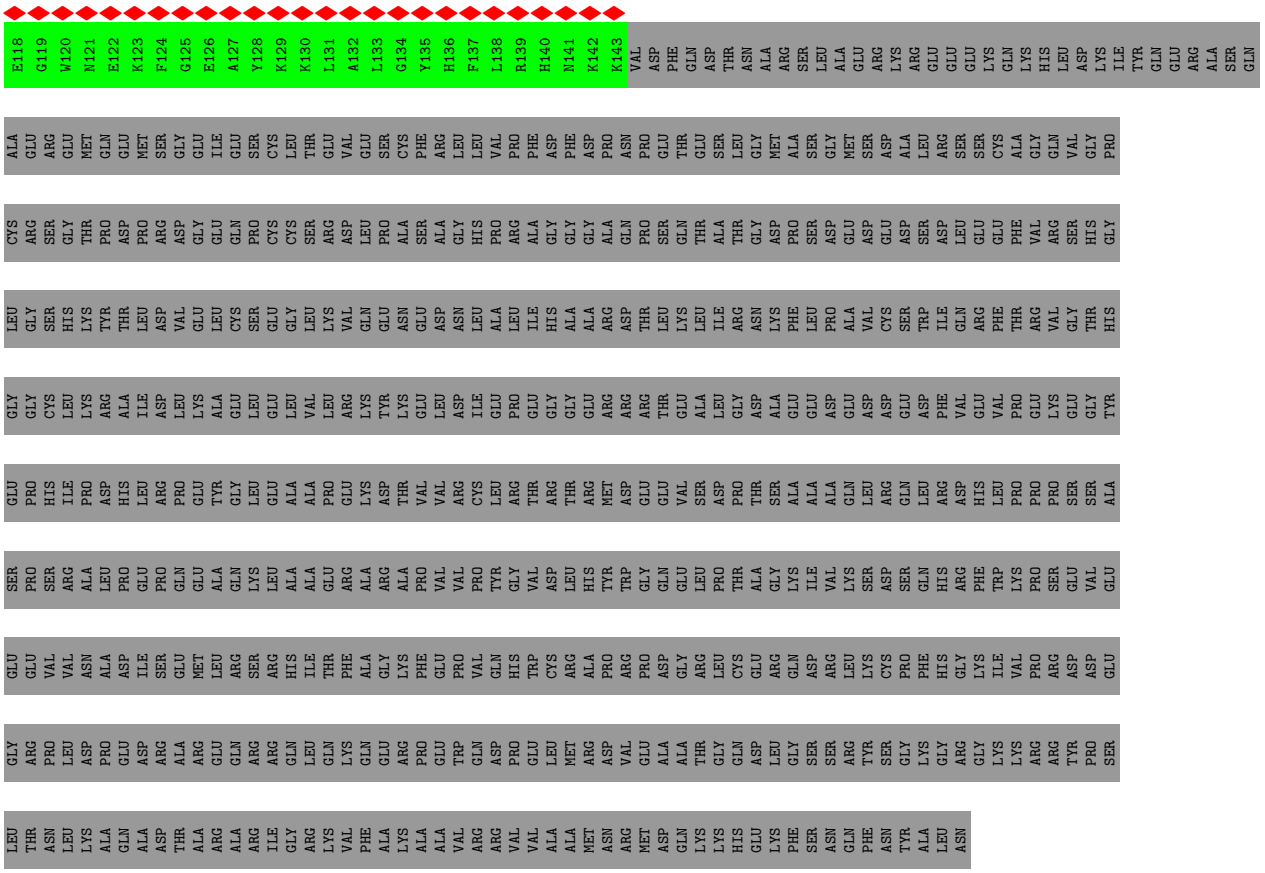
Chain b:



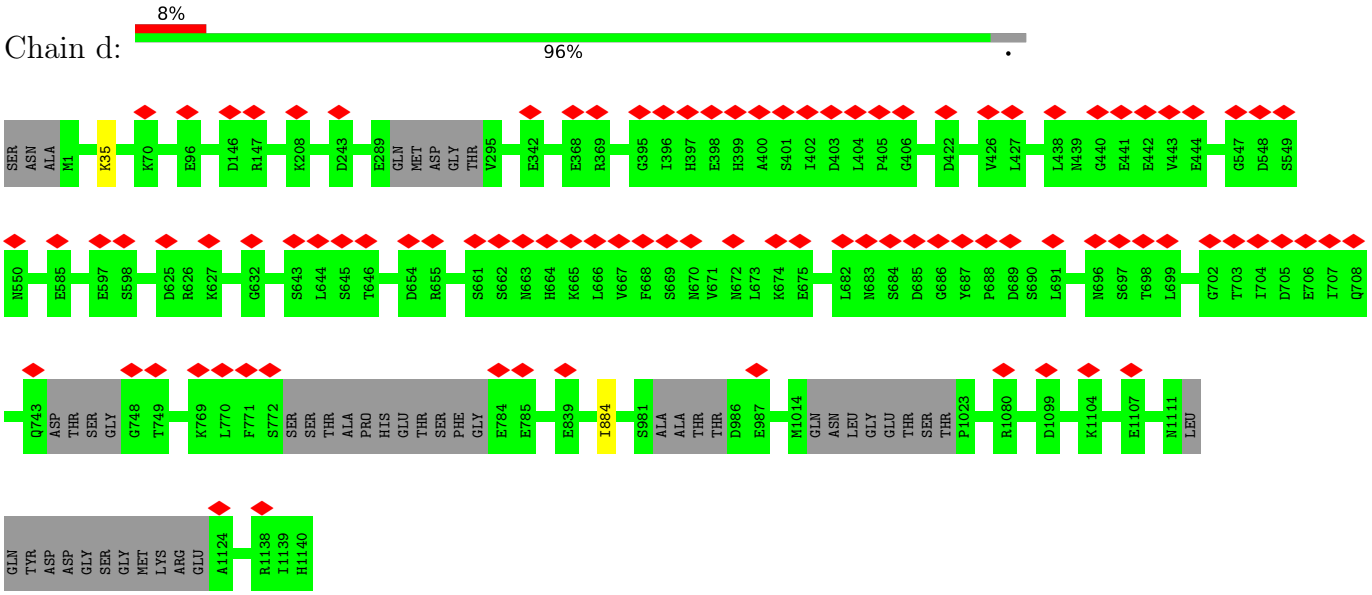


• Molecule 25: UV-stimulated scaffold protein A

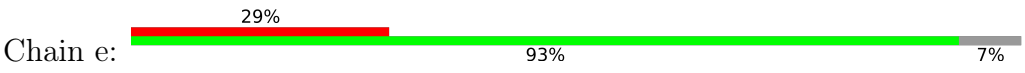
Chain c:

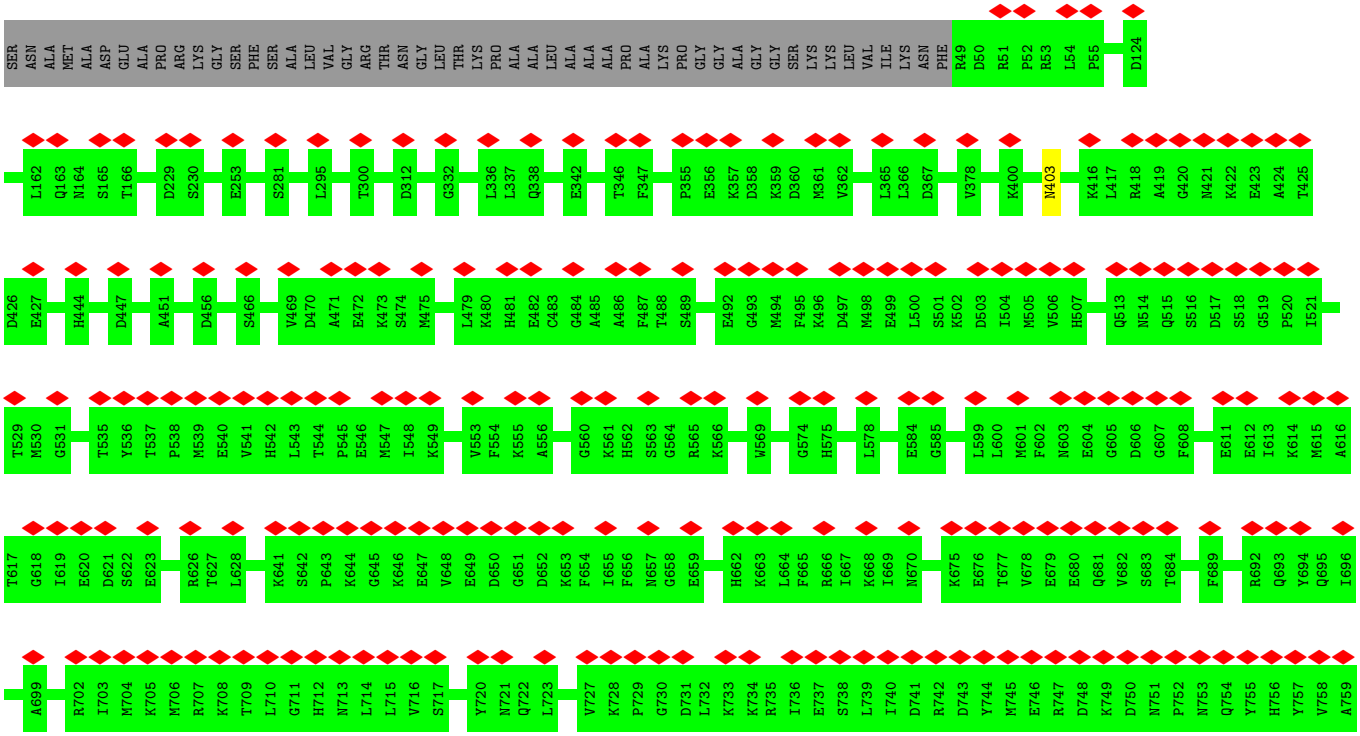


• Molecule 26: DNA damage-binding protein 1

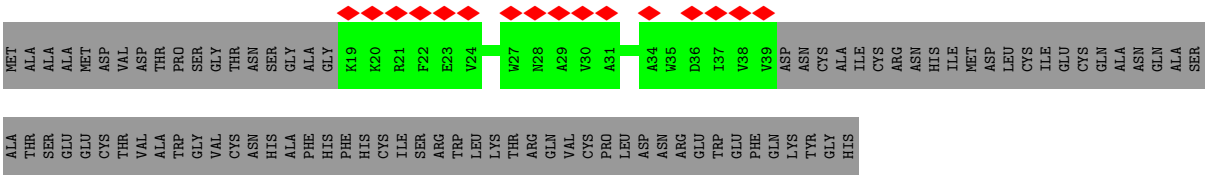


• Molecule 27: Cullin-4A





• Molecule 28: E3 ubiquitin-protein ligase RBX1



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100000	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 ($e^-/Å^2$)	40.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.167	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	440.99997, 440.99997, 440.99997	wwPDB
Map dimensions	420, 420, 420	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: 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	0.30	0/11382	0.54	1/15368 (0.0%)
2	B	0.32	0/9233	0.54	0/12463
3	C	0.34	0/2132	0.56	1/2896 (0.0%)
4	D	0.85	1/1027 (0.1%)	0.78	1/1384 (0.1%)
5	E	0.29	0/1751	0.53	0/2366
6	F	0.32	0/667	0.50	0/901
7	G	1.28	12/1365 (0.9%)	0.86	5/1853 (0.3%)
8	H	0.34	0/1207	0.53	0/1628
9	I	0.30	0/972	0.54	0/1316
10	J	0.32	0/542	0.51	0/730
11	K	0.31	0/939	0.49	0/1271
12	L	0.34	0/394	0.59	0/524
13	M	1.76	177/6770 (2.6%)	0.98	14/9119 (0.2%)
14	N	2.38	41/817 (5.0%)	1.00	0/1258
15	P	4.52	108/510 (21.2%)	2.04	32/793 (4.0%)
17	S	0.28	0/3559	0.52	0/4447
18	T	4.09	207/1056 (19.6%)	1.40	18/1624 (1.1%)
19	U	0.29	0/413	0.47	0/511
20	V	0.28	0/864	0.54	0/1073
21	Y	0.32	0/1199	0.62	1/1497 (0.1%)
22	Z	0.29	0/171	0.53	0/212
23	a	2.01	99/2908 (3.4%)	0.95	5/3939 (0.1%)
24	b	1.16	29/4364 (0.7%)	0.74	2/5893 (0.0%)
25	c	0.22	0/563	0.42	0/702
26	d	0.35	0/7551	0.54	0/10076
27	e	0.29	0/2844	0.57	0/3552
28	f	0.23	0/83	0.62	0/102
All	All	1.10	674/65283 (1.0%)	0.70	80/87498 (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	1
13	M	0	1
16	R	0	1
23	a	0	1
26	d	0	2
27	e	0	1
All	All	0	7

The worst 5 of 674 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	P	48	G	C5-C4	-17.85	1.25	1.38
18	T	25	DT	C5-C6	-16.39	1.22	1.34
18	T	22	DC	N3-C4	-16.37	1.22	1.33
18	T	27	DG	N7-C5	-15.77	1.29	1.39
15	P	46	G	N9-C8	-15.30	1.27	1.37

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	P	50	A	O5'-P-OP1	-15.91	91.38	105.70
13	M	1014	ARG	NE-CZ-NH1	-13.18	113.71	120.30
18	T	19	DA	O5'-P-OP2	-11.54	95.32	105.70
13	M	1014	ARG	NE-CZ-NH2	10.53	125.57	120.30
15	P	45	A	N1-C6-N6	-10.48	112.31	118.60

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	538	VAL	Peptide
13	M	575	CYS	Peptide
16	R	11	UNK	Peptide
23	a	174	LYS	Peptide
26	d	35	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	11179	0	11313	102	0
2	B	9052	0	9087	56	0
3	C	2089	0	2031	14	0
4	D	1013	0	972	18	0
5	E	1720	0	1737	14	0
6	F	657	0	684	4	0
7	G	1334	0	1333	26	0
8	H	1186	0	1147	5	0
9	I	949	0	879	9	0
10	J	533	0	553	5	0
11	K	920	0	942	6	0
12	L	388	0	393	2	0
13	M	6648	0	6644	138	0
14	N	727	0	393	1	0
15	P	454	0	210	12	0
16	R	160	0	2	3	0
17	S	3560	0	940	8	0
18	T	947	0	519	13	0
19	U	416	0	111	0	0
20	V	868	0	212	3	0
21	Y	1200	0	341	15	0
22	Z	172	0	44	2	0
23	a	2849	0	2778	0	0
24	b	4261	0	4302	0	0
25	c	564	0	143	0	0
26	d	7443	0	6536	0	0
27	e	2845	0	753	0	0
28	f	84	0	20	0	0
29	A	2	0	0	0	0
29	B	1	0	0	0	0
29	C	1	0	0	0	0
29	I	2	0	0	0	0
29	J	1	0	0	0	0
29	L	1	0	0	0	0
30	A	1	0	0	0	0
All	All	64227	0	55019	405	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 5.

The worst 5 of 405 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:114:CYS:SG	1:A:184:CYS:HB3	1.83	1.18
13:M:926:GLU:OE1	13:M:981:TYR:OH	1.90	0.88
1:A:338:SER:OG	1:A:341:GLN:OE1	1.92	0.88
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.57	0.87
13:M:1014:ARG:NH1	13:M:1032:ALA:O	2.08	0.87

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	1402/1970 (71%)	1366 (97%)	36 (3%)	0	100	100
2	B	1123/1174 (96%)	1076 (96%)	47 (4%)	0	100	100
3	C	256/275 (93%)	249 (97%)	7 (3%)	0	100	100
4	D	126/142 (89%)	118 (94%)	8 (6%)	0	100	100
5	E	207/210 (99%)	204 (99%)	3 (1%)	0	100	100
6	F	80/127 (63%)	75 (94%)	5 (6%)	0	100	100
7	G	169/172 (98%)	158 (94%)	11 (6%)	0	100	100
8	H	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
9	I	115/125 (92%)	111 (96%)	4 (4%)	0	100	100
10	J	65/67 (97%)	65 (100%)	0	0	100	100
11	K	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
12	L	44/58 (76%)	40 (91%)	4 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	M	788/1729 (46%)	710 (90%)	76 (10%)	2 (0%)	41 76
17	S	888/1179 (75%)	842 (95%)	46 (5%)	0	100 100
19	U	98/666 (15%)	82 (84%)	14 (14%)	2 (2%)	7 34
20	V	209/531 (39%)	174 (83%)	31 (15%)	4 (2%)	8 36
21	Y	298/305 (98%)	278 (93%)	20 (7%)	0	100 100
22	Z	41/531 (8%)	40 (98%)	1 (2%)	0	100 100
23	a	363/396 (92%)	336 (93%)	27 (7%)	0	100 100
24	b	512/1496 (34%)	470 (92%)	42 (8%)	0	100 100
25	c	139/712 (20%)	136 (98%)	3 (2%)	0	100 100
26	d	1082/1143 (95%)	1004 (93%)	78 (7%)	0	100 100
27	e	709/762 (93%)	652 (92%)	57 (8%)	0	100 100
28	f	19/108 (18%)	18 (95%)	1 (5%)	0	100 100
All	All	8992/14145 (64%)	8457 (94%)	527 (6%)	8 (0%)	54 85

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	V	248	PRO
19	U	481	GLY
19	U	463	PRO
20	V	238	GLU
20	V	259	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	1242/1749 (71%)	1240 (100%)	2 (0%)	93 98
2	B	992/1027 (97%)	990 (100%)	2 (0%)	93 98
3	C	237/252 (94%)	237 (100%)	0	100 100
4	D	108/126 (86%)	107 (99%)	1 (1%)	78 92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	E	191/192 (100%)	190 (100%)	1 (0%)	88 96
6	F	71/111 (64%)	71 (100%)	0	100 100
7	G	147/153 (96%)	147 (100%)	0	100 100
8	H	129/131 (98%)	129 (100%)	0	100 100
9	I	105/112 (94%)	105 (100%)	0	100 100
10	J	56/56 (100%)	56 (100%)	0	100 100
11	K	104/106 (98%)	104 (100%)	0	100 100
12	L	43/55 (78%)	43 (100%)	0	100 100
13	M	722/1524 (47%)	717 (99%)	5 (1%)	84 94
23	a	320/348 (92%)	320 (100%)	0	100 100
24	b	466/1299 (36%)	463 (99%)	3 (1%)	86 95
26	d	690/1001 (69%)	690 (100%)	0	100 100
All	All	5623/8242 (68%)	5609 (100%)	14 (0%)	93 98

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	1098	ARG
13	M	1113	ARG
24	b	882	TYR
24	b	538	ARG
24	b	670	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	93	HIS
13	M	561	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	20/45 (44%)	9 (45%)	1 (5%)

5 of 9 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	31	U
15	P	32	A
15	P	33	U
15	P	34	A
15	P	35	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	32	A

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 9 ligands modelled in this entry, 9 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.

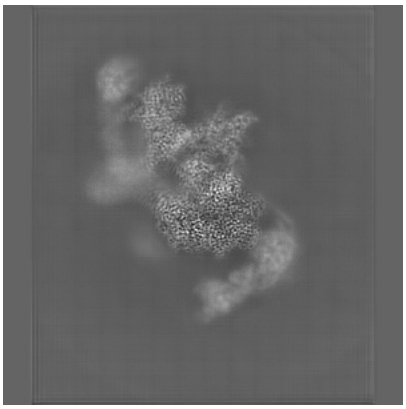
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13016. These allow visual inspection of the internal detail of the map and identification of artifacts.

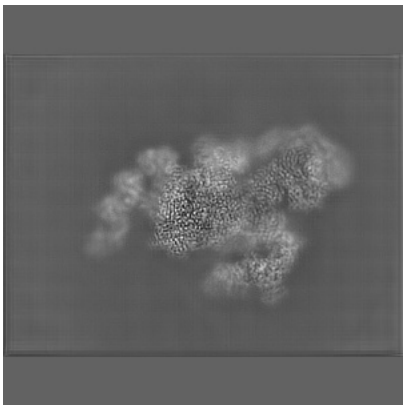
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

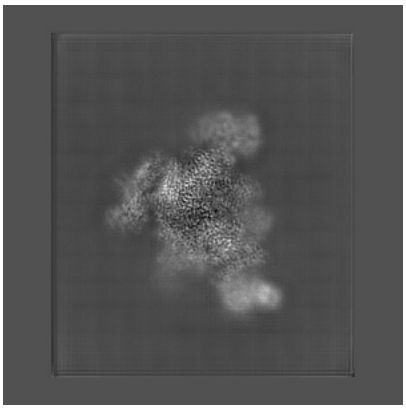
6.1.1 Primary map



X

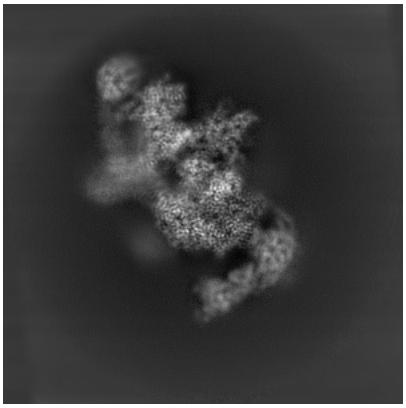


Y

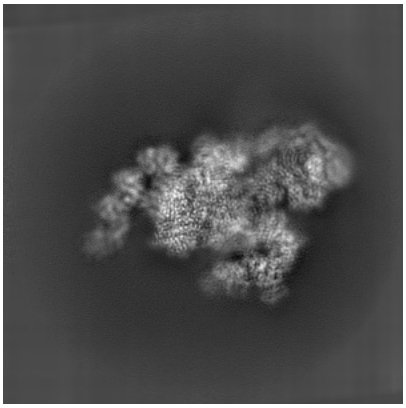


Z

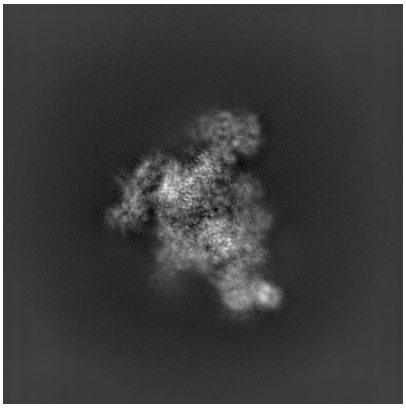
6.1.2 Raw map



X



Y

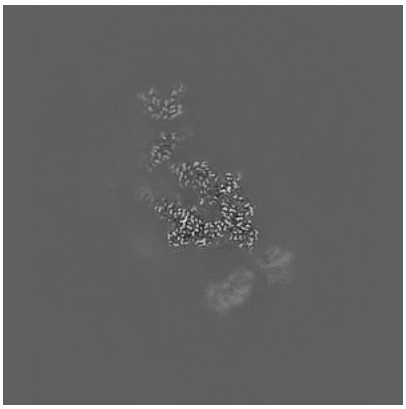


Z

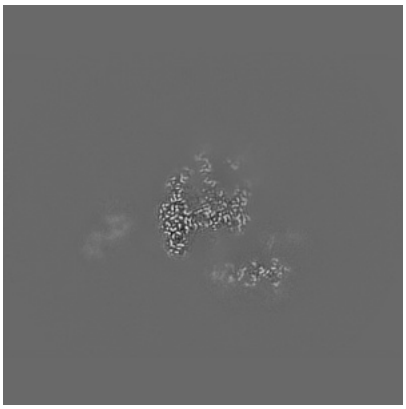
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

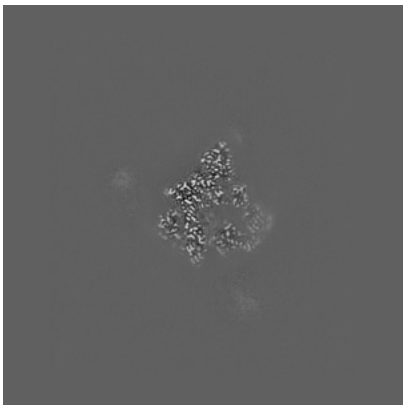
6.2.1 Primary map



X Index: 210

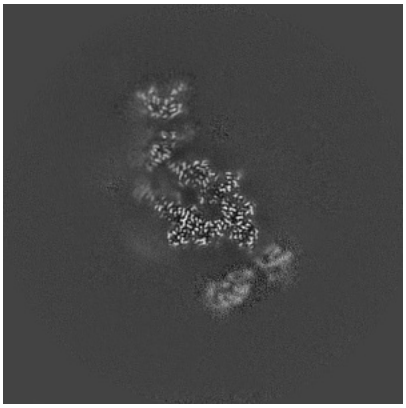


Y Index: 210

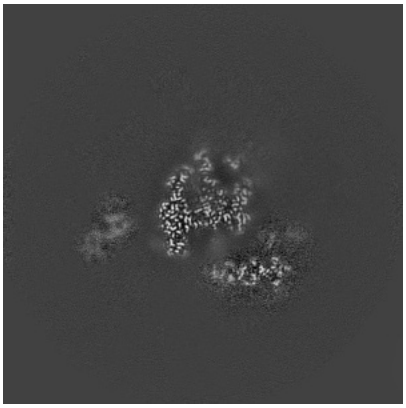


Z Index: 210

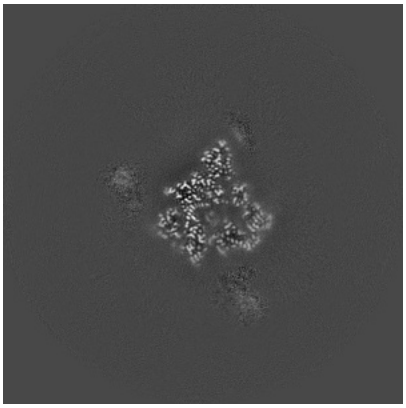
6.2.2 Raw map



X Index: 210



Y Index: 210

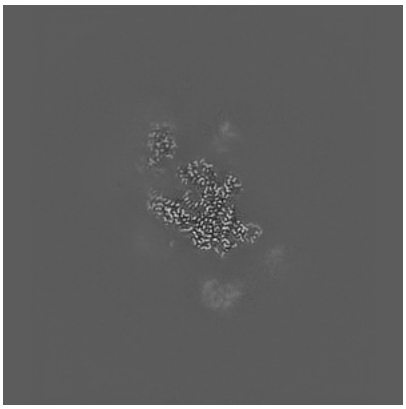


Z Index: 210

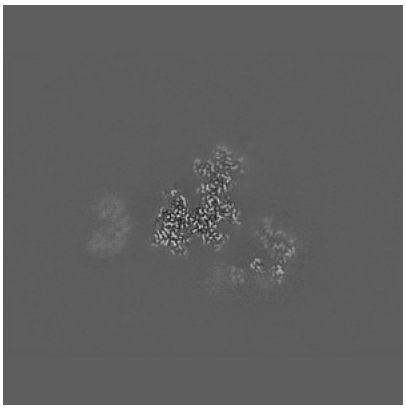
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

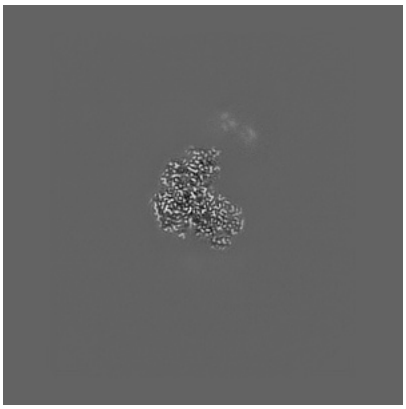
6.3.1 Primary map



X Index: 197

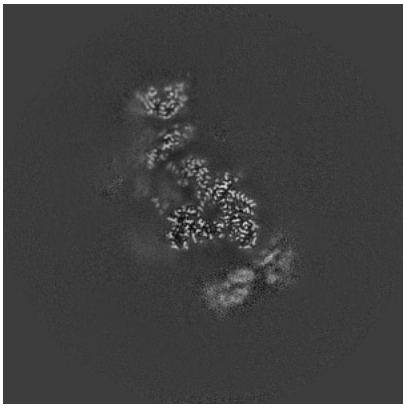


Y Index: 222

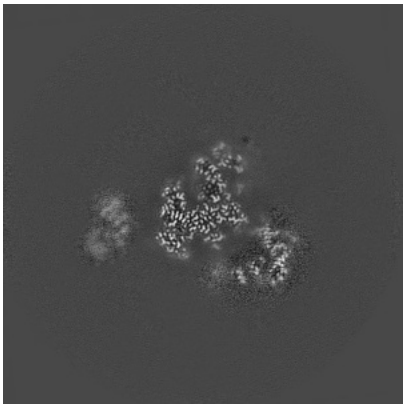


Z Index: 183

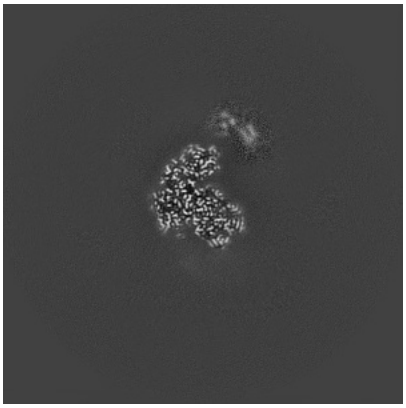
6.3.2 Raw map



X Index: 213



Y Index: 218

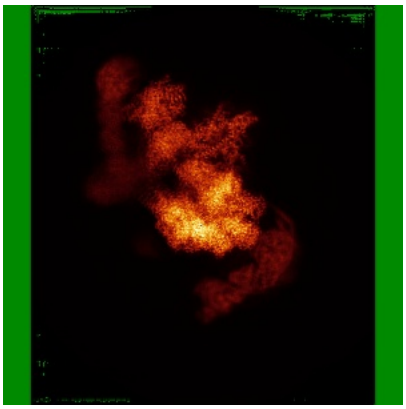


Z Index: 181

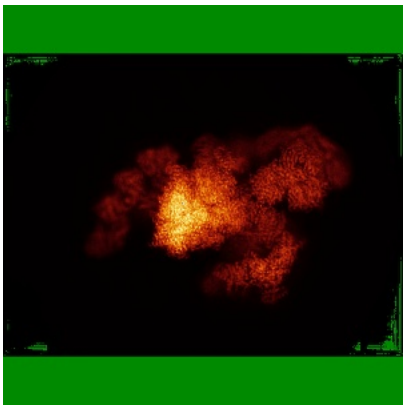
The images above show the largest variance slices of the map in three orthogonal directions.

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

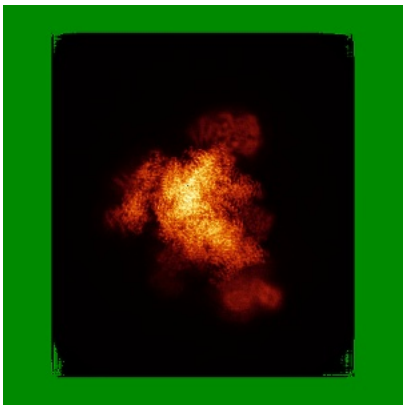
6.4.1 Primary map



X

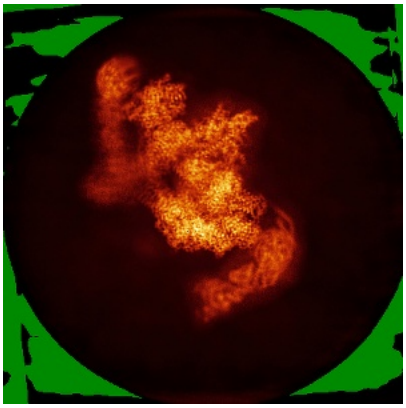


Y

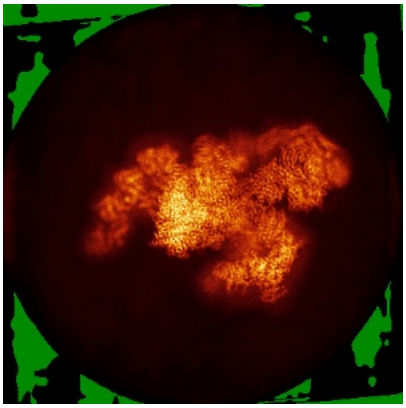


Z

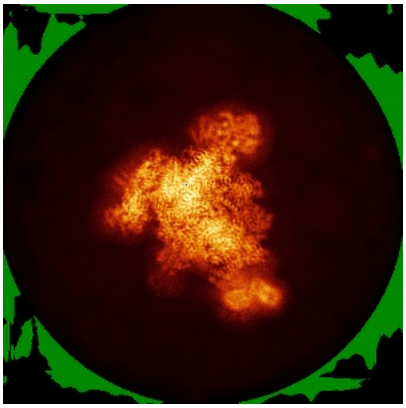
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

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.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

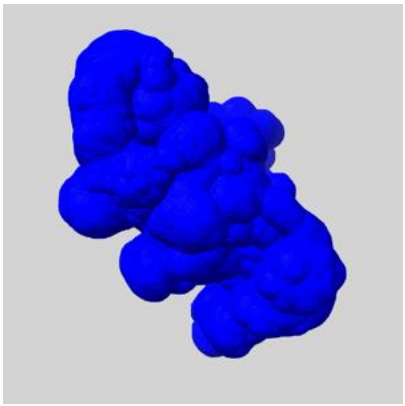
6.6 Mask visualisation

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

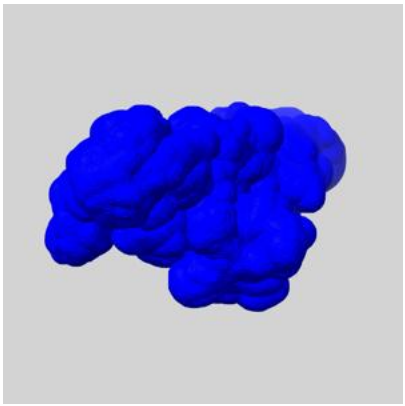
A mask typically either:

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

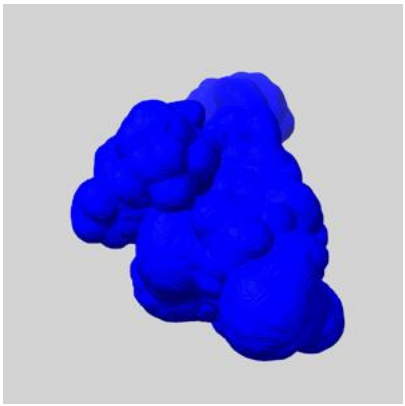
6.6.1 emd_13016_msk_1.map



X

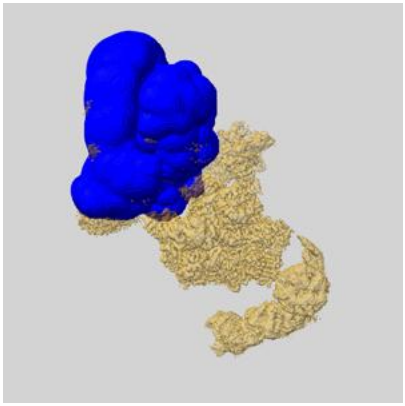


Y

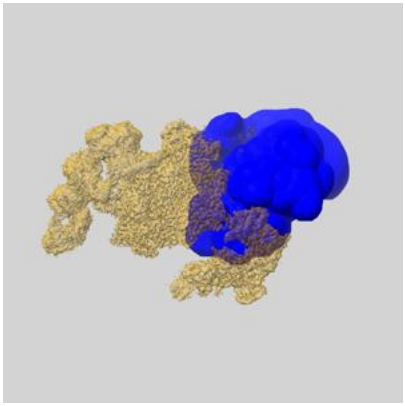


Z

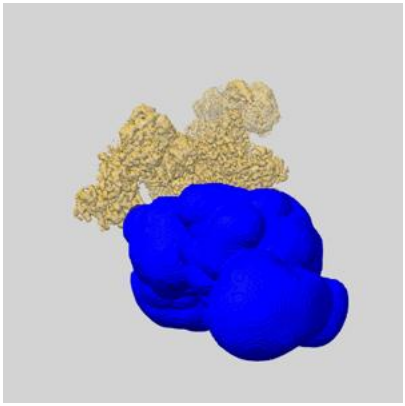
6.6.2 emd_13016_msk_2.map



X

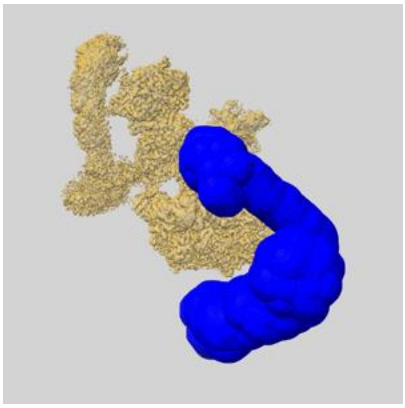


Y

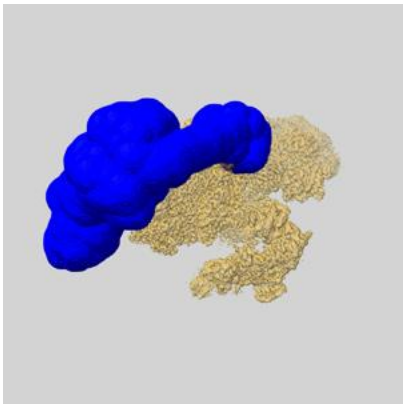


Z

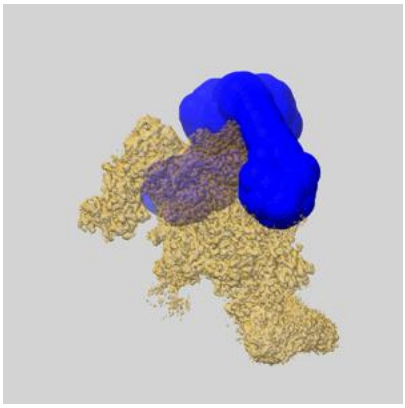
6.6.3 emd_13016_msk_3.map



X

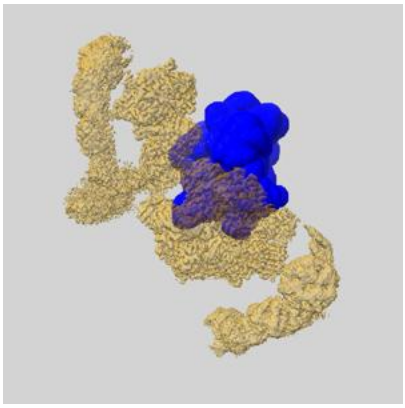


Y

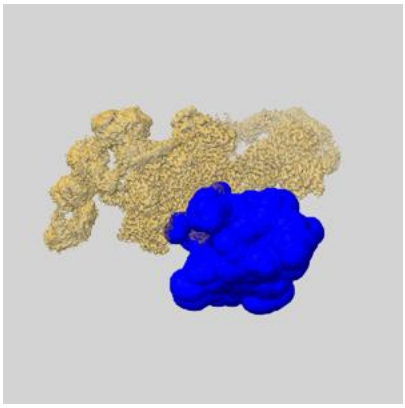


Z

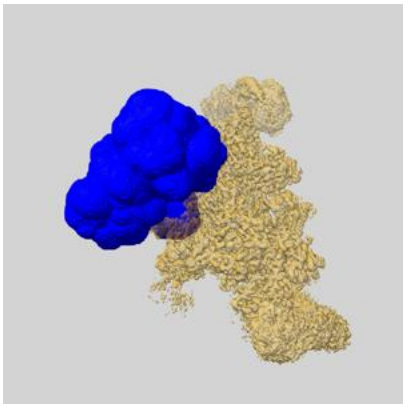
6.6.4 emd_13016_msk_4.map



X

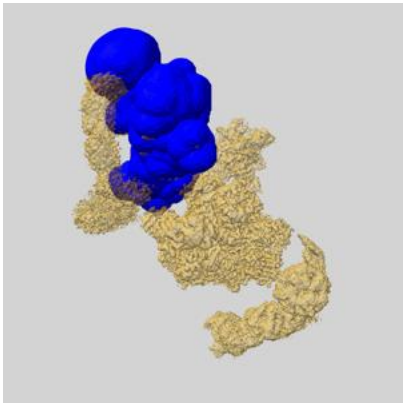


Y

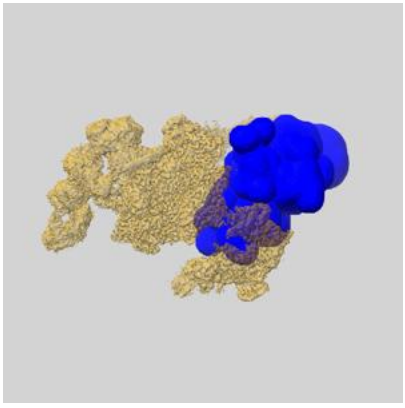


Z

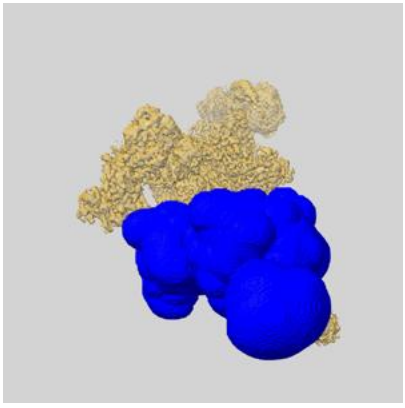
6.6.5 emd_13016_msk_5.map



X

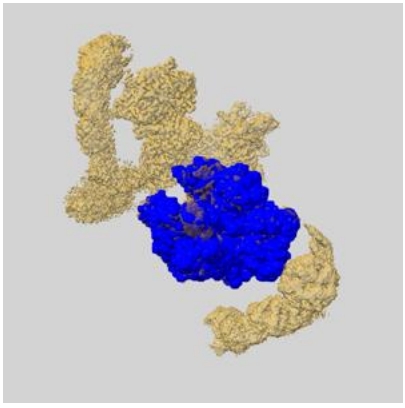


Y

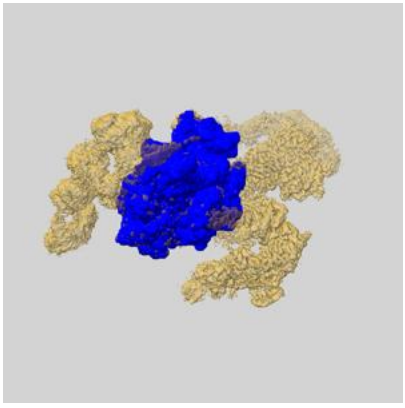


Z

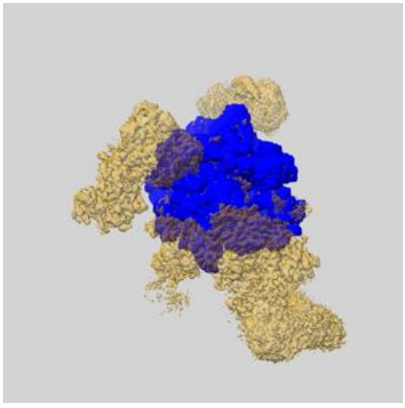
6.6.6 emd_13016_msk_6.map ⓘ



X



Y

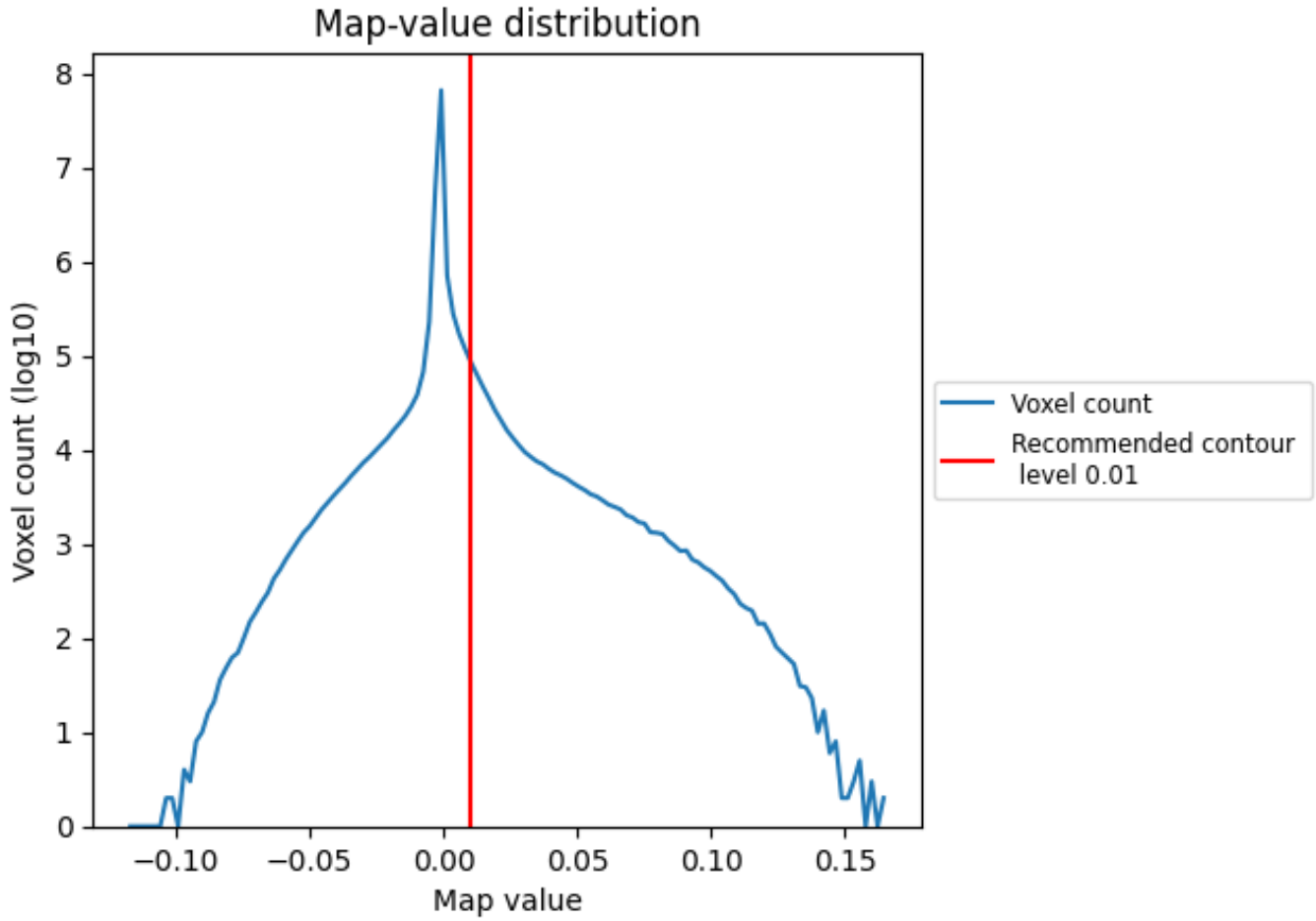


Z

7 Map analysis

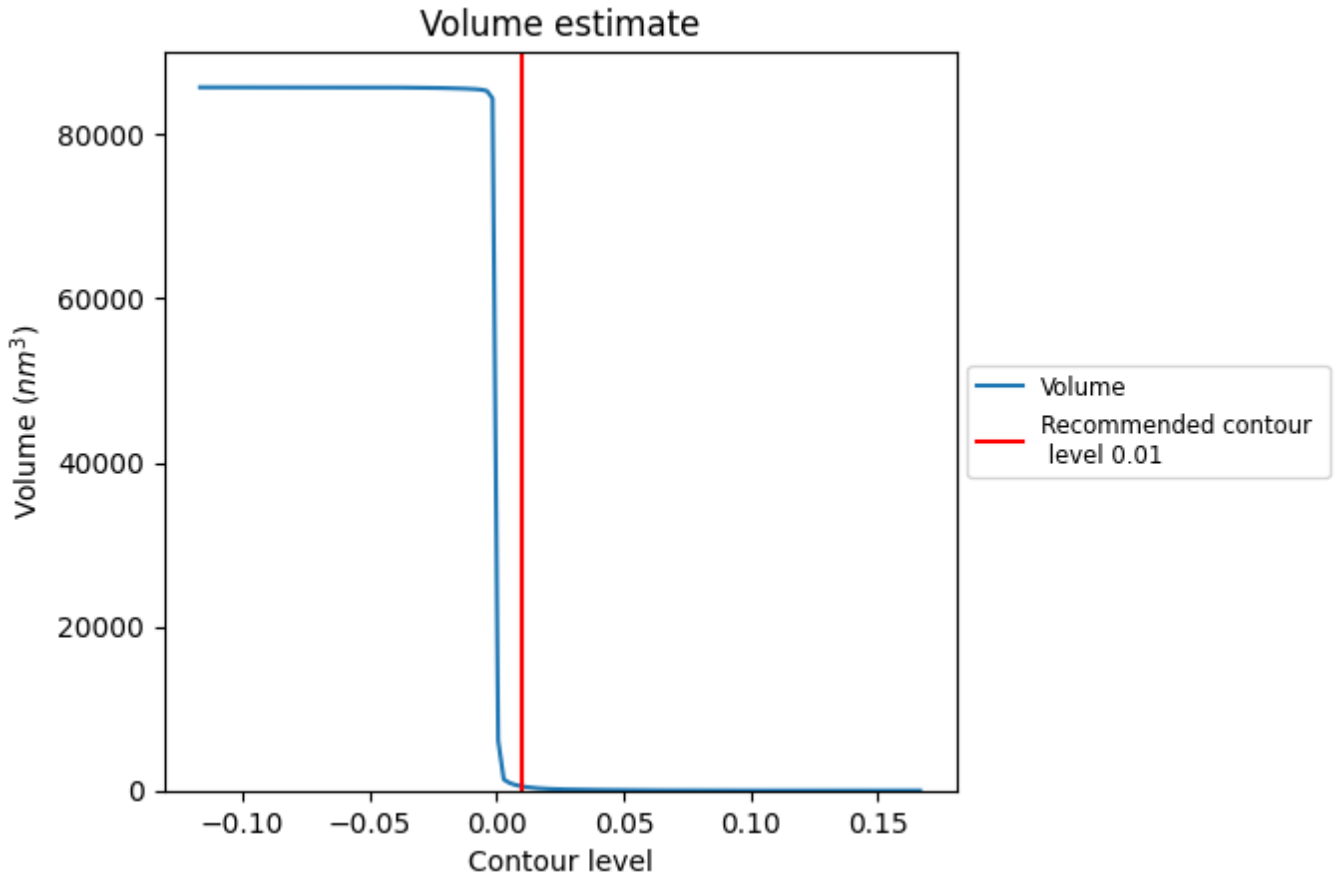
This section contains the results of statistical analysis of the map.

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.

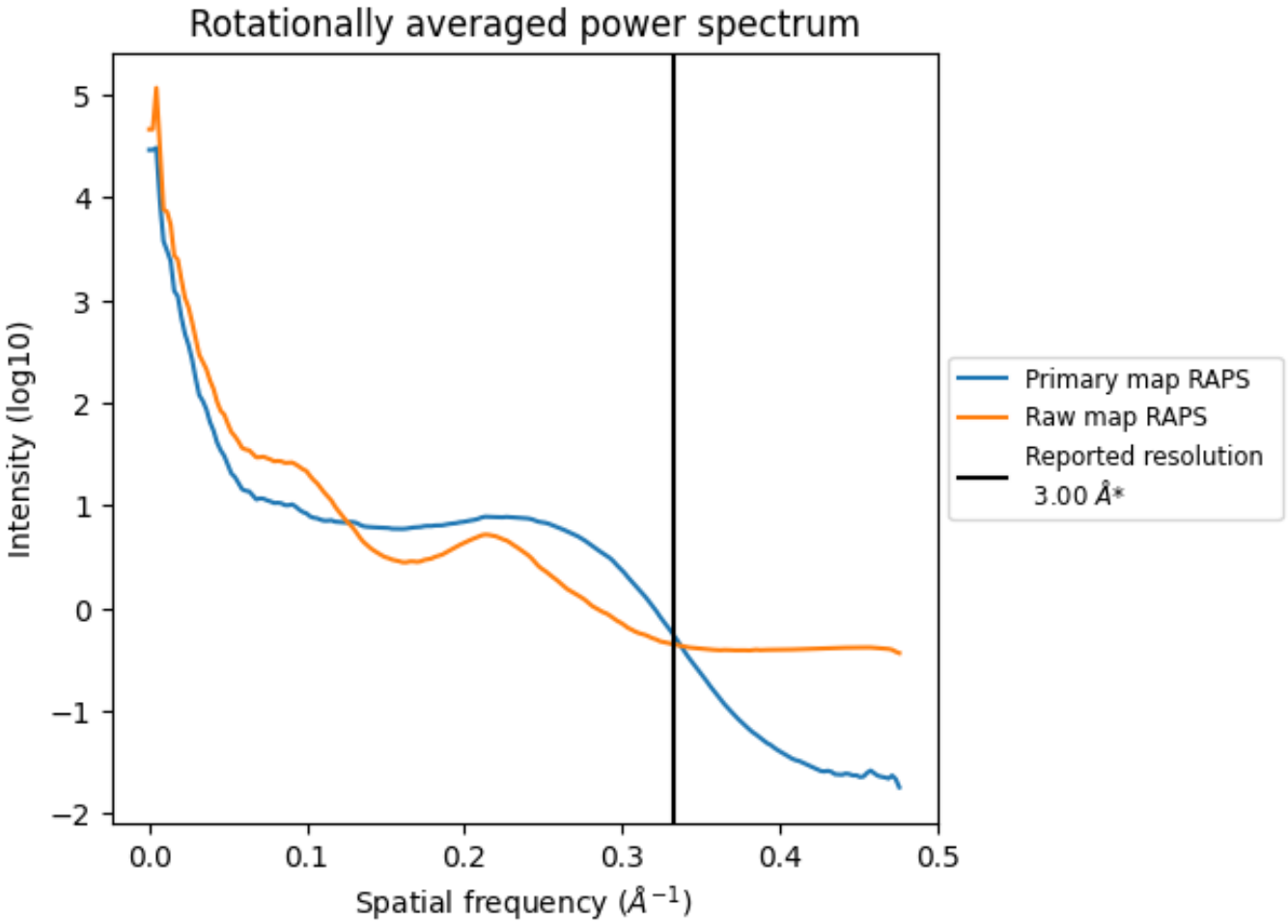
7.2 Volume estimate (i)



The volume at the recommended contour level is 512 nm^3; this corresponds to an approximate mass of 463 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)

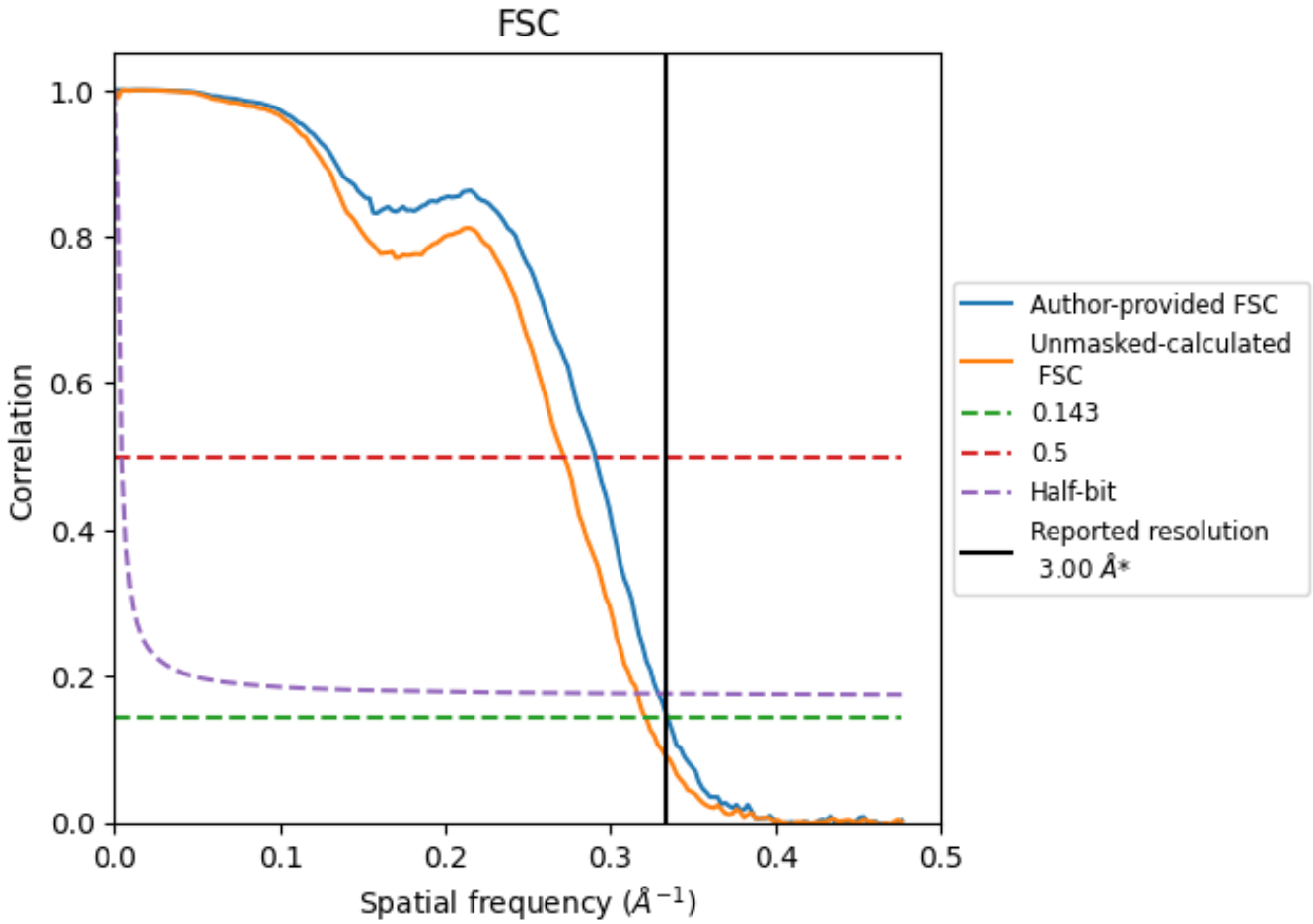


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

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 0.333 $Å^{-1}$

8.2 Resolution estimates (i)

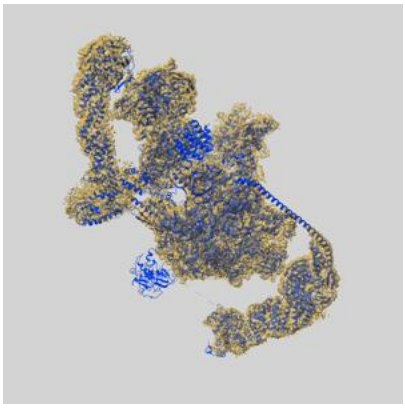
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.99	3.44	3.04
Unmasked-calculated*	3.11	3.68	3.16

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

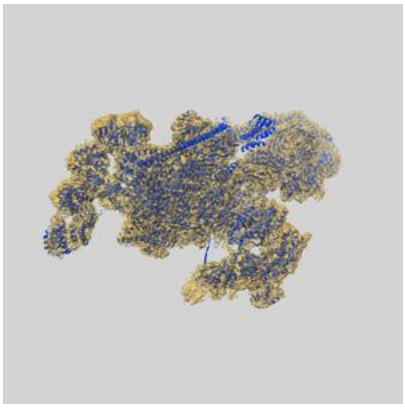
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13016 and PDB model 7OPD. Per-residue inclusion information can be found in section 3 on page 10.

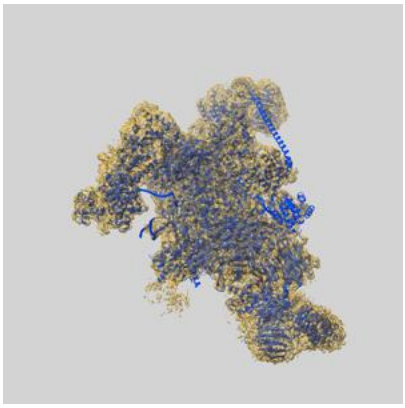
9.1 Map-model overlay



X



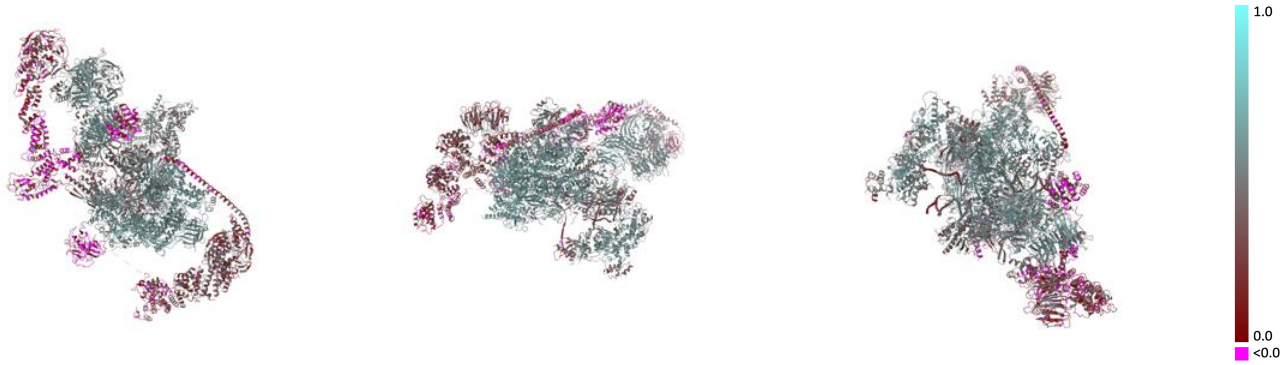
Y



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.

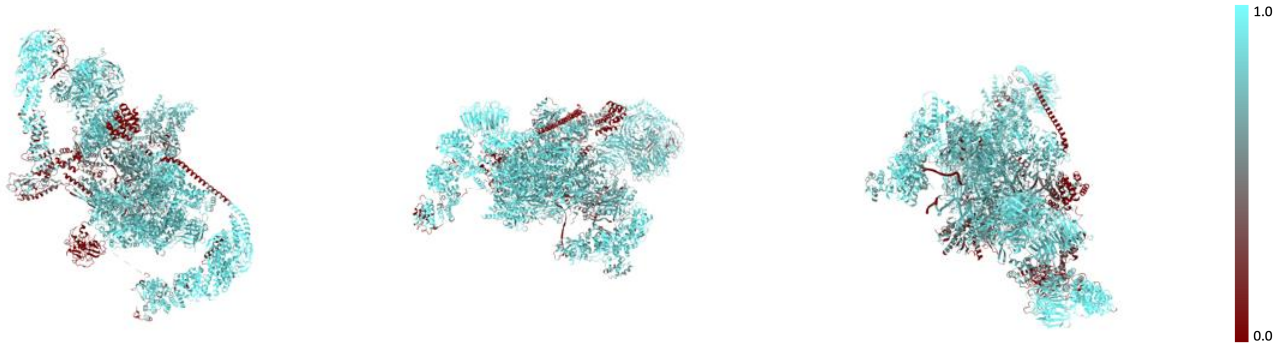
9.2 Q-score mapped to coordinate model



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.

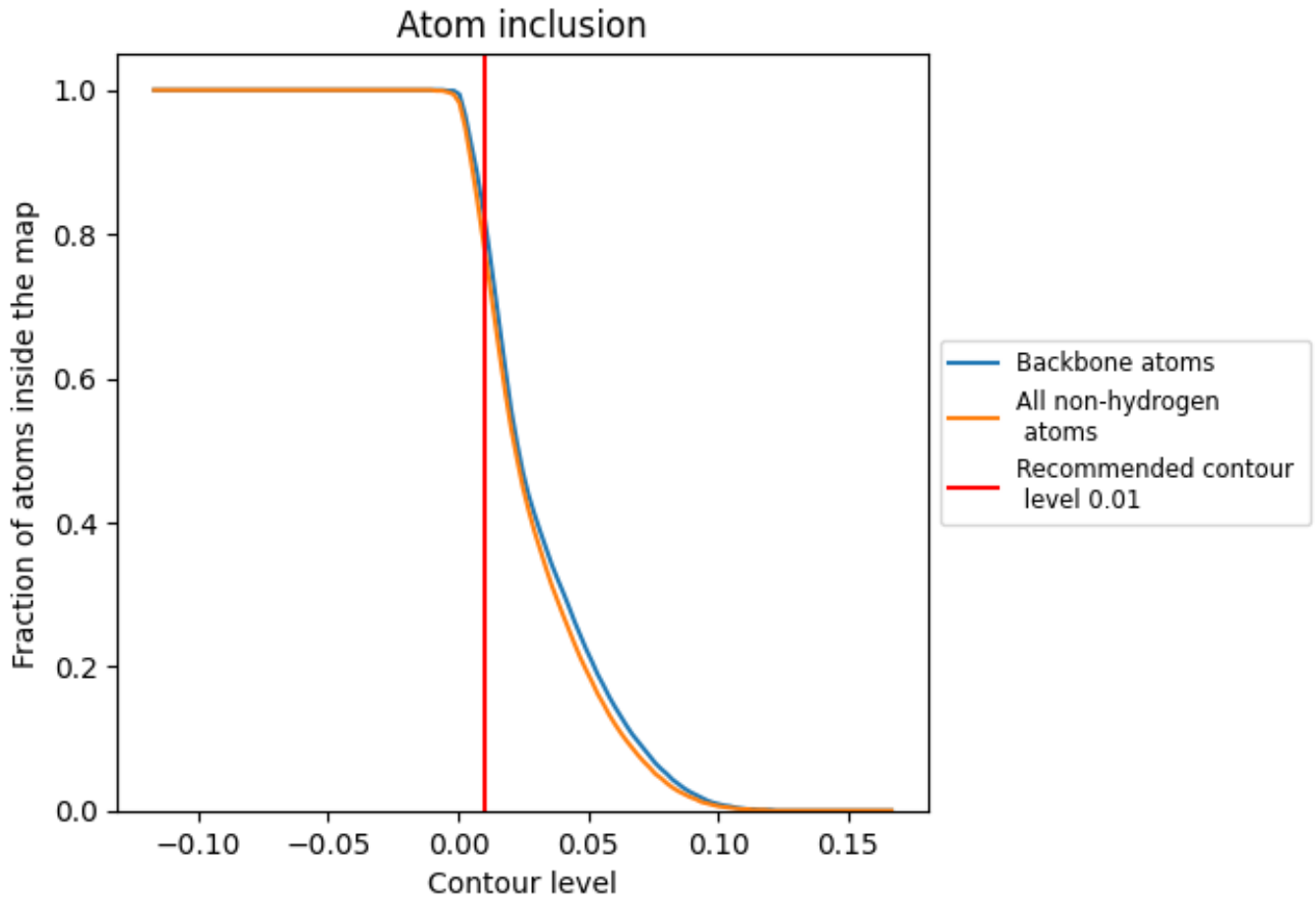
9.3 Atom inclusion mapped to coordinate model



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, 83% 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	0.7850	0.4720
A	0.8420	0.5530
B	0.8510	0.5600
C	0.9120	0.5890
D	0.6760	0.4030
E	0.8620	0.5410
F	0.8720	0.5720
G	0.7160	0.4960
H	0.8900	0.5830
I	0.7500	0.4910
J	0.9330	0.6180
K	0.9200	0.5950
L	0.8090	0.5080
M	0.8370	0.5000
N	0.6600	0.4260
P	0.5020	0.3840
R	0.2000	0.3300
S	0.7810	0.2280
T	0.6830	0.4590
U	0.0000	0.0120
V	0.2500	0.0820
Y	0.9600	0.3240
Z	0.8550	0.3060
a	0.9070	0.5870
b	0.6660	0.4790
c	0.0050	0.0250
d	0.8000	0.4670
e	0.5960	0.1270
f	0.2380	0.1570