wwPDB EM Validation Summary Report ⓘ

Jan 6, 2025 – 08:55 PM EST

PDB ID	:	9BZ0
EMDB ID	:	EMD-45050
Title	:	Structure of an STK19-containing TC-NER complex
Authors	:	Mevissen, T.E.T.; Kuemmecke, M.; Farnung, L.; Walter, J.C.
Deposited on	:	2024-05-24
Resolution	:	1.90 Å(reported)
Based on initial models	:	8B3F, .

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

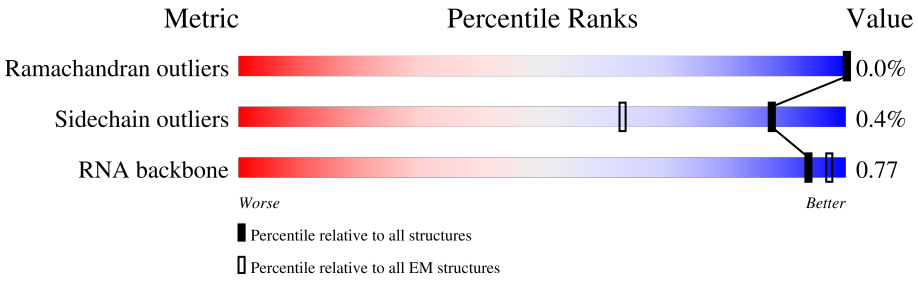
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 1.90 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.



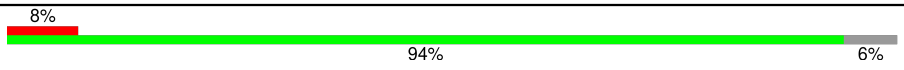
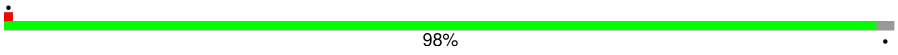
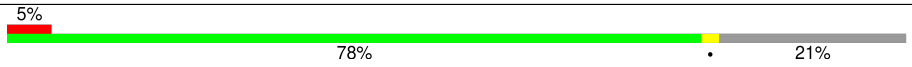
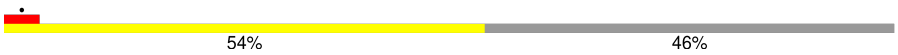
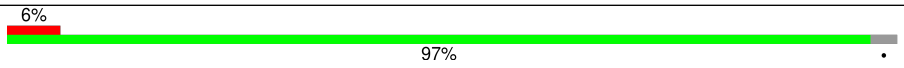
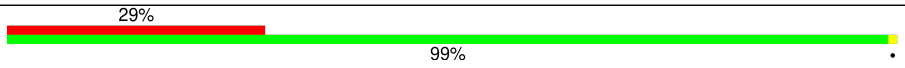
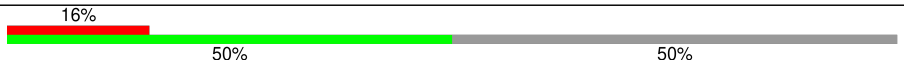
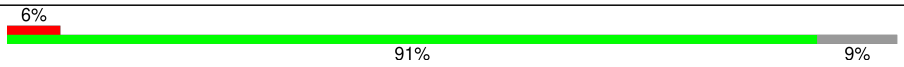
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1984	71% · 28%
2	B	1251	90% 10%
3	C	275	94% 5%
4	D	142	11% 89% · 10%
5	E	210	100%
6	F	127	6% 65% 35%
7	G	172	17% 99% ·
8	H	150	99% ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	85	
14	N	90	
15	P	10	
16	T	90	
17	a	396	
18	b	1496	
19	c	712	
20	d	1143	
21	e	105	
22	f	254	

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 54687 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1425	11289	7096	2018	2103	72	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	1129	9038	5719	1587	1668	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 RNA polymerase Rpb4/RPC9 core 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	1721	1089	300	324	8	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	82	658	418	113	122	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
			950	587	169	183	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			534	345	90	93	6		

- Molecule 11 is a protein called RNA polymerase II subunit J.

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
			389	241	75	67	6		

- Molecule 13 is a protein called Transcription elongation factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	64	Total	C	N	O	S	0	0
			505	312	81	105	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-1	SER	-	expression tag	UNP A0A2K5RSX0
M	0	ASN	-	expression tag	UNP A0A2K5RSX0
M	1	ALA	-	expression tag	UNP A0A2K5RSX0

- Molecule 14 is a DNA chain called DNA (35-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	35	Total	C	N	O	P	0	0
			732	346	146	205	35		

- Molecule 15 is a RNA chain called RNA (5'-R(P*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	10	Total	C	N	O	P	0	0
			220	98	45	67	10		

- Molecule 16 is a DNA chain called DNA (49-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	49	Total	C	N	O	P	0	0
			984	472	161	302	49		

- Molecule 17 is a protein called DNA excision repair protein ERCC-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	386	Total	C	N	O	S	0	0
			3017	1880	529	589	19		

- Molecule 18 is a protein called DNA excision repair protein ERCC-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	621	Total	C	N	O	S	0	0
			5065	3238	895	909	23		

There are 5 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	1213	GLY	ARG	variant	UNP Q03468

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
b	1413	ARG	GLN	variant	UNP Q03468

- Molecule 19 is a protein called UV-stimulated scaffold protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	c	243	Total	C	N	O	S	0	0
			1865	1162	364	331	8		

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 20 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	d	1140	Total	C	N	O	S	0	0
			8918	5642	1503	1724	49		

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 21 is a protein called DET1- and DDB1-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	e	53	Total	C	N	O	S	0	0
			429	271	76	80	2		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	-2	SER	-	expression tag	UNP Q9BW61
e	-1	ASN	-	expression tag	UNP Q9BW61
e	0	ALA	-	expression tag	UNP Q9BW61

- Molecule 22 is a protein called Inactive serine/threonine-protein kinase 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	f	232	Total	C	N	O	S	0	0
			1817	1161	324	326	6		

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	Mg	0
			1	1	
24	b	1	Total	Mg	0
			1	1	

- Molecule 25 is water.

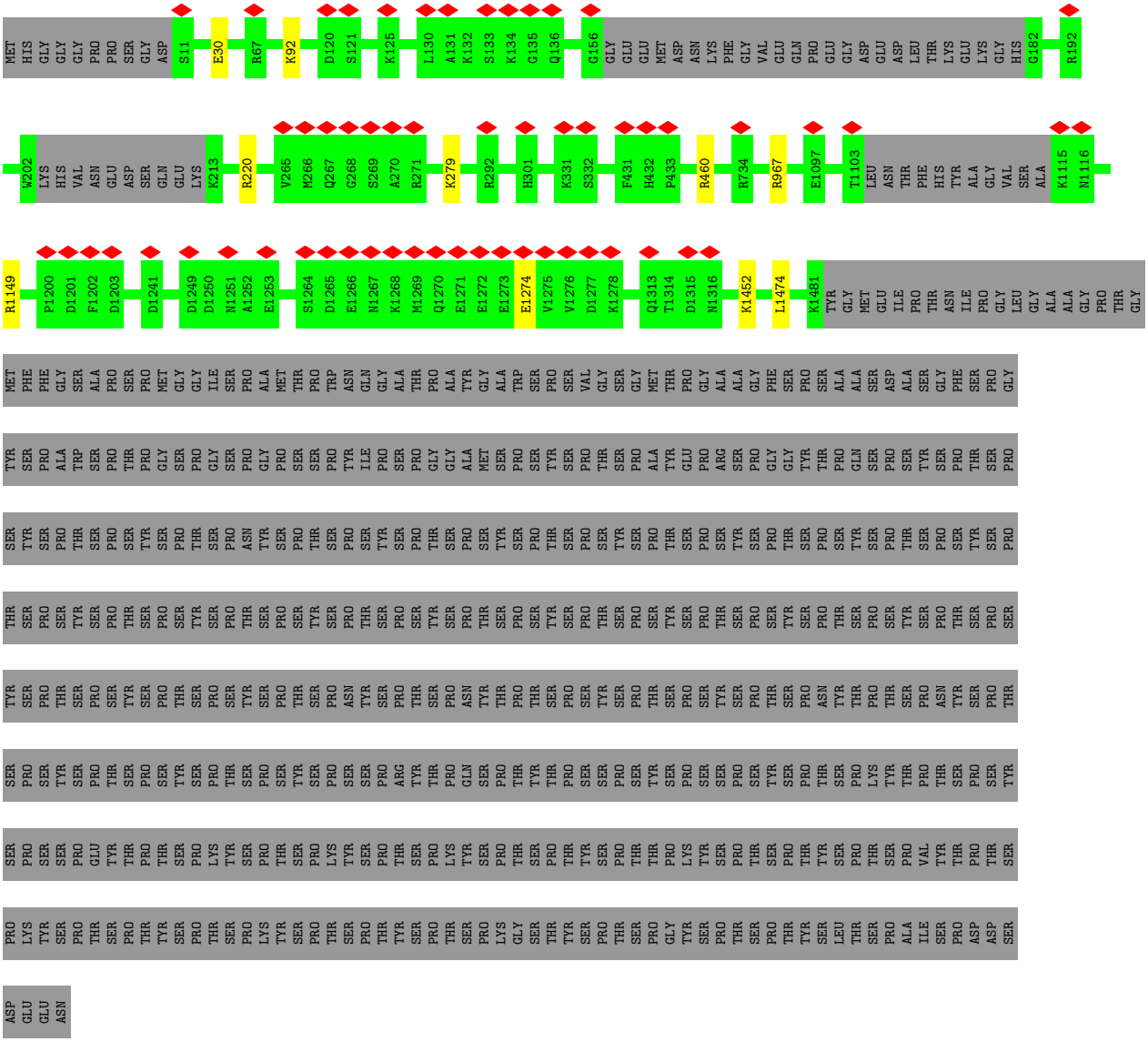
Mol	Chain	Residues	Atoms		AltConf
25	A	2	Total	O	0
			2	2	

3 Residue-property plots (i)

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

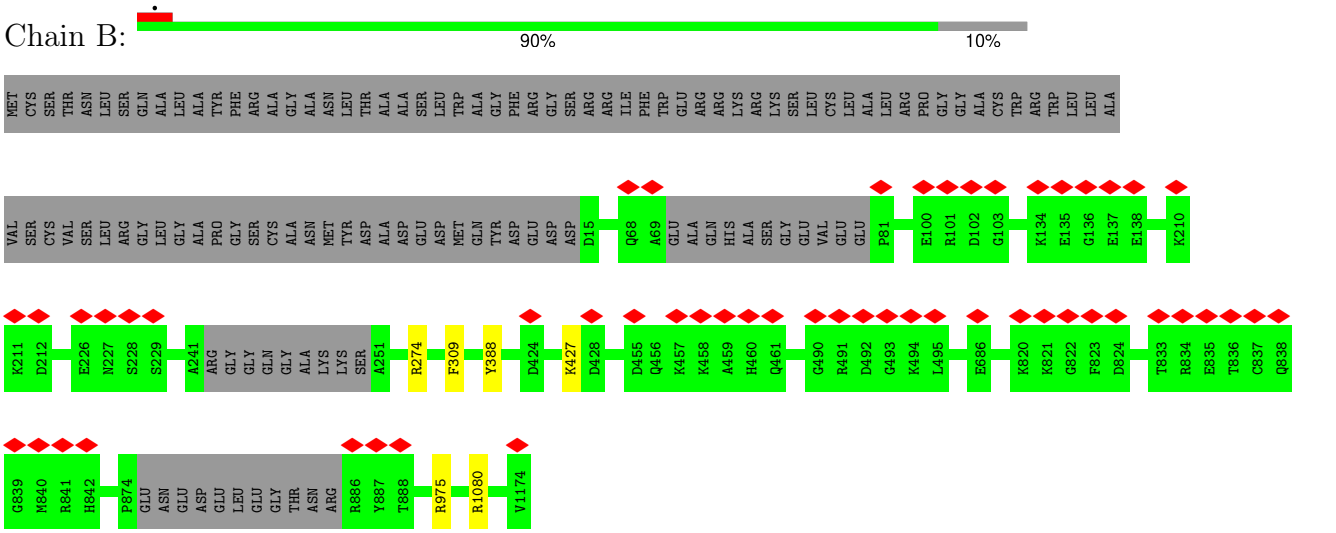
- Molecule 1: DNA-directed RNA polymerase subunit

Chain A:



• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:

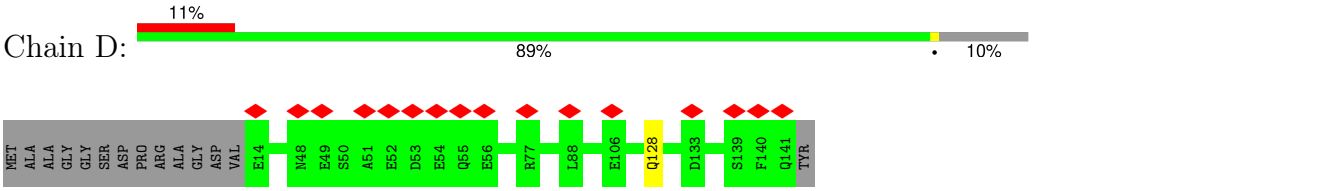


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:

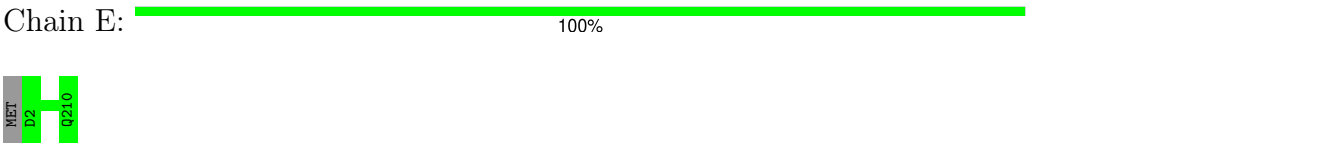
• Molecule 4: RNA polymerase Rpb4/RPC9 core domain-containing protein

Chain D:



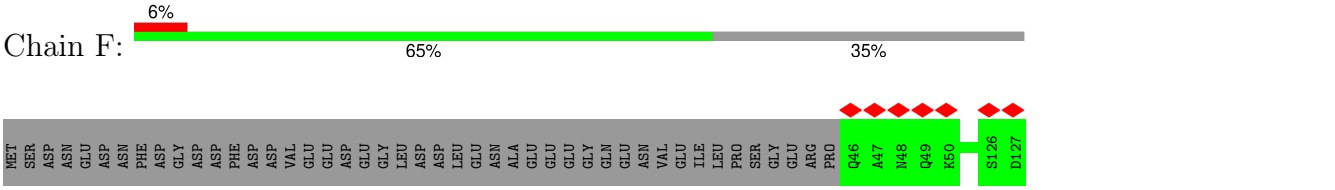
• Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E:



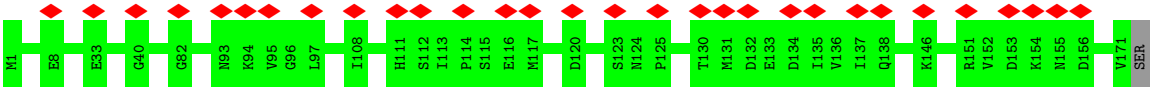
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:

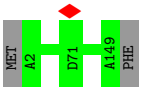


• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

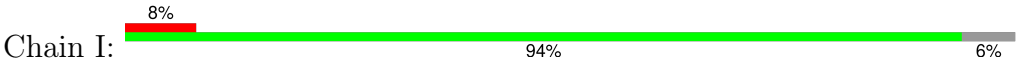
Chain G:

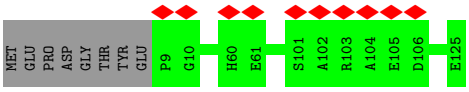


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



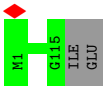
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9



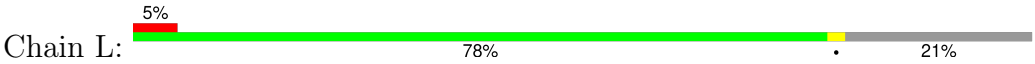


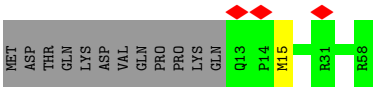
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

• Molecule 11: RNA polymerase II subunit J

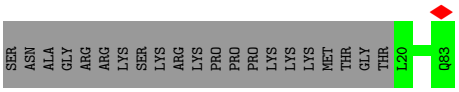


• Molecule 12: RNA polymerase II subunit K



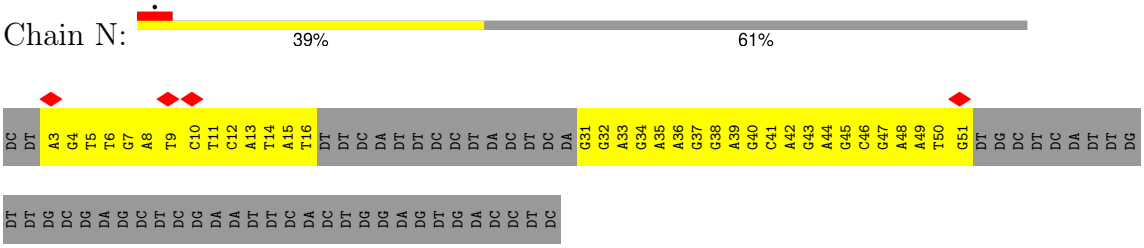


• Molecule 13: Transcription elongation factor 1 homolog



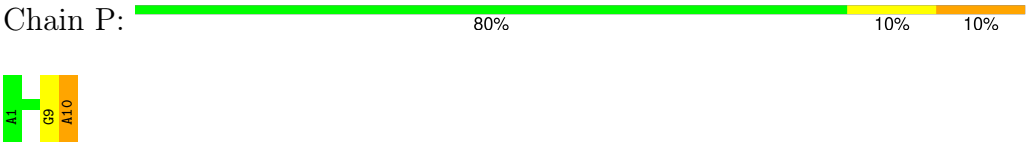
• Molecule 14: DNA (35-MER)

Chain N:



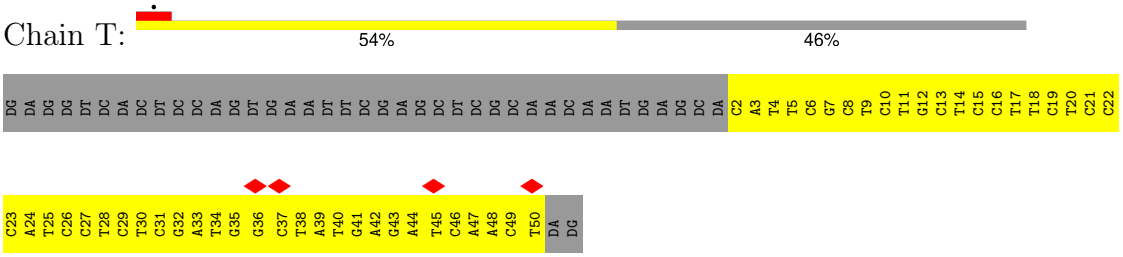
• Molecule 15: RNA (5'-R(P*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3')

Chain P:



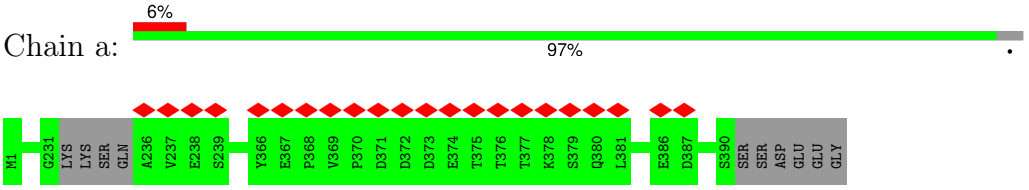
• Molecule 16: DNA (49-MER)

Chain T:



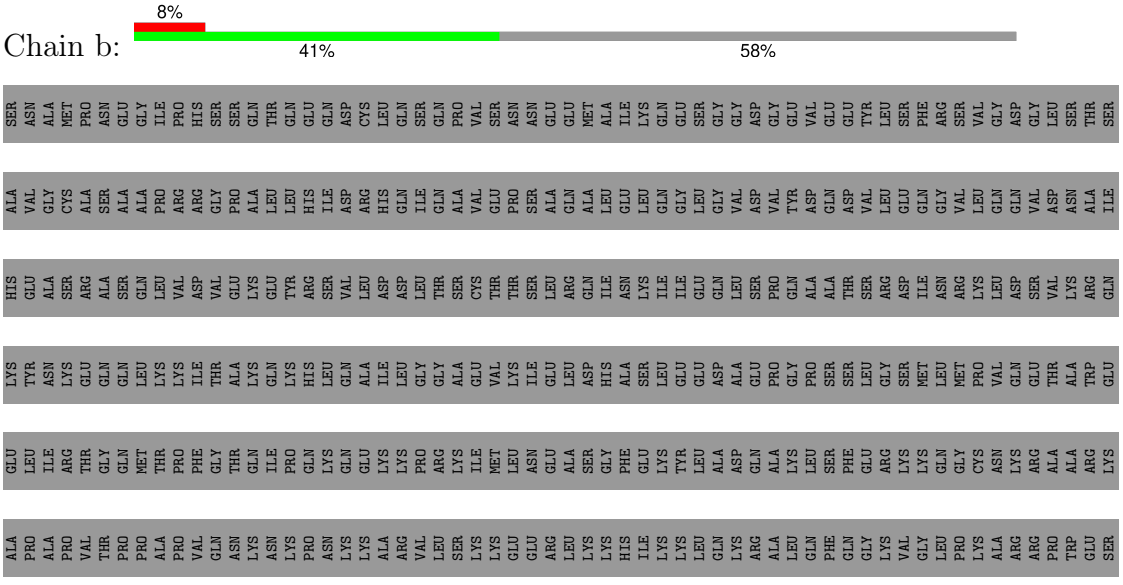
• Molecule 17: DNA excision repair protein ERCC-8

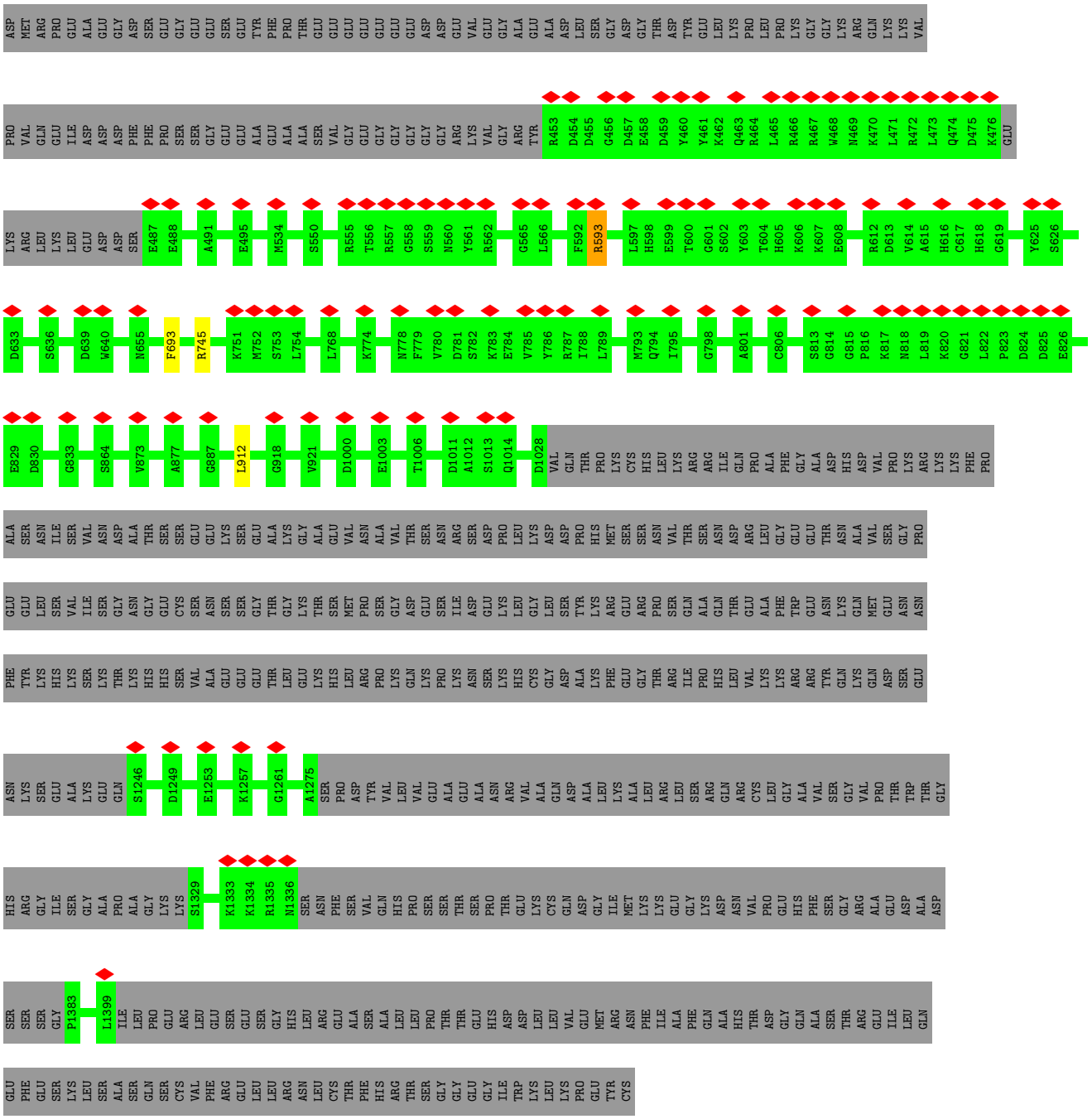
Chain a:



• Molecule 18: DNA excision repair protein ERCC-6

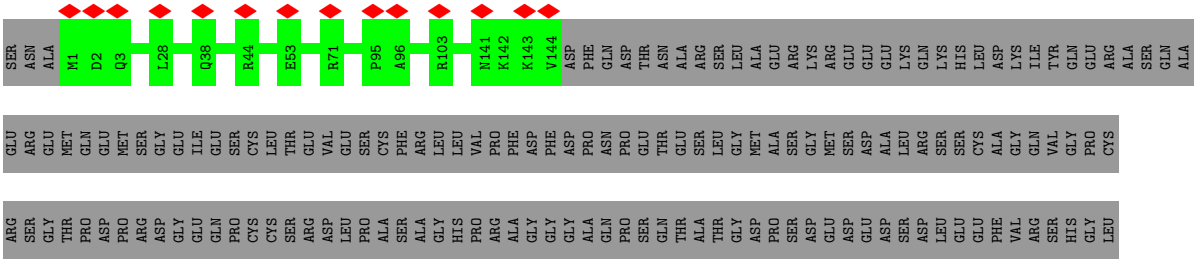
Chain b:

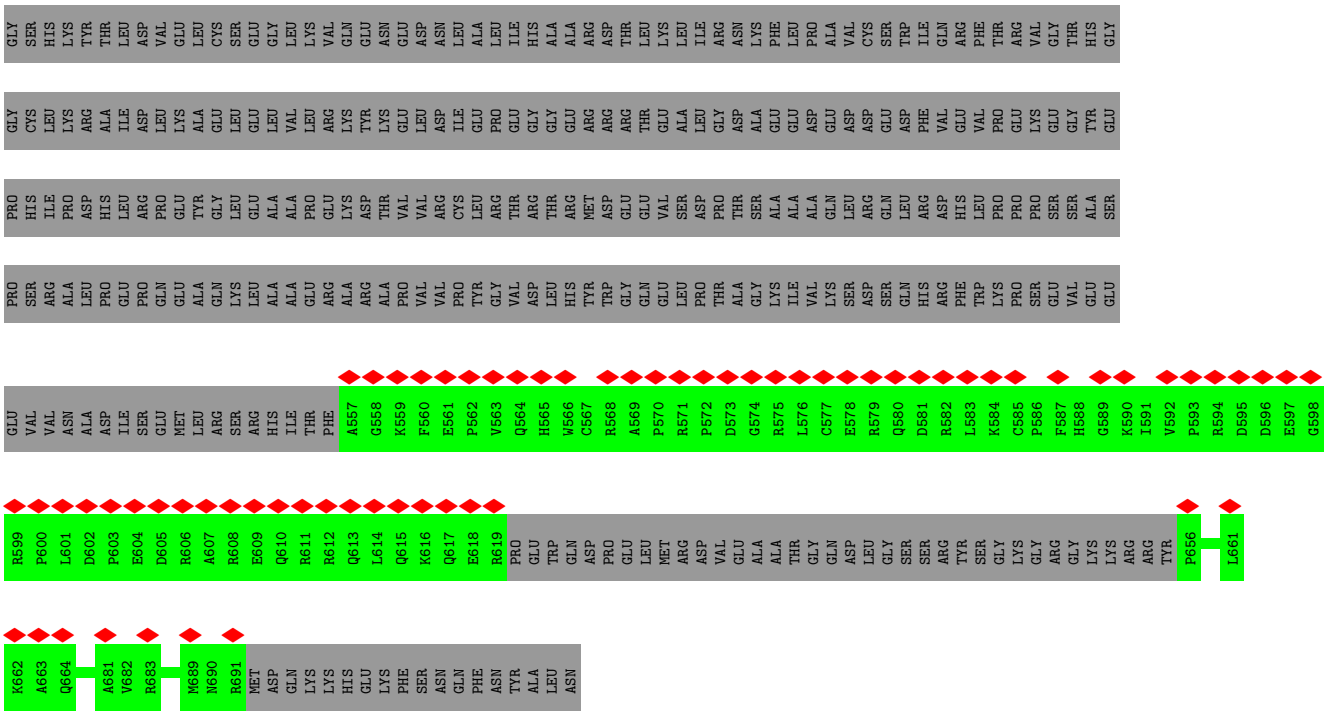




• Molecule 19: UV-stimulated scaffold protein A

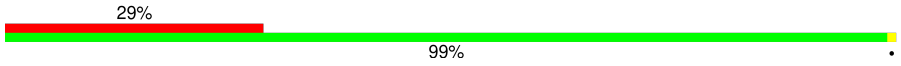
Chain c:

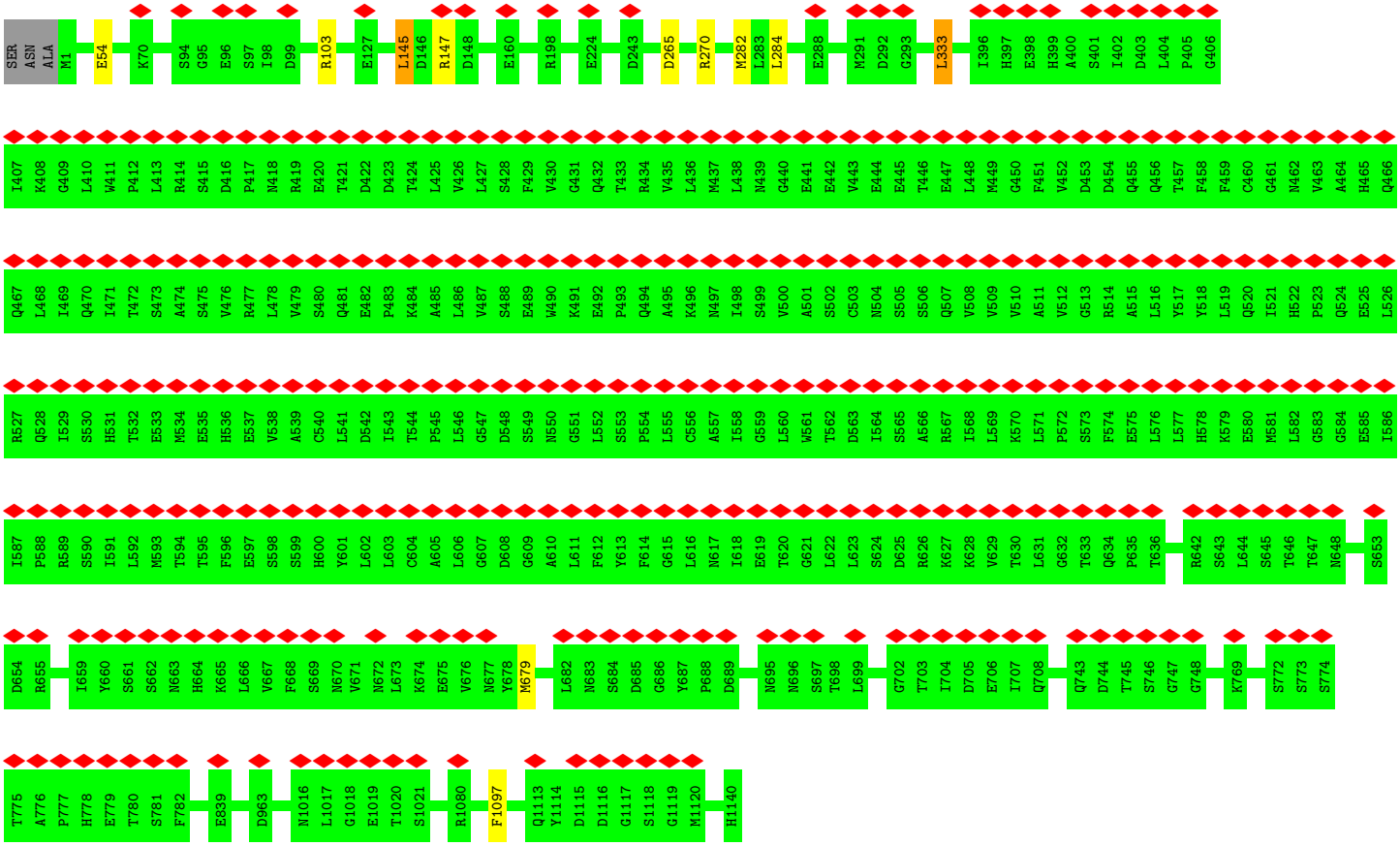




• Molecule 20: DNA damage-binding protein 1

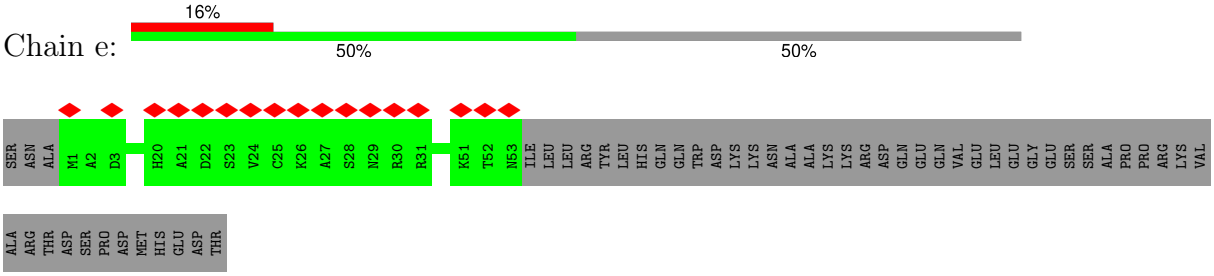
Chain d:





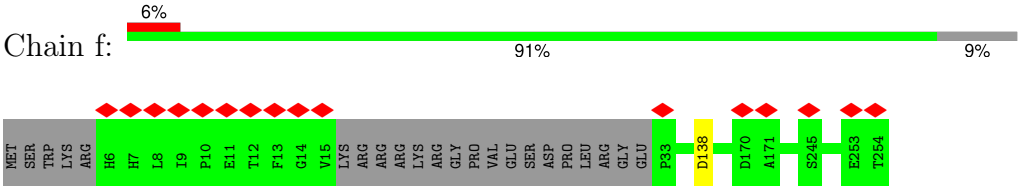
• Molecule 21: DET1- and DDB1-associated protein 1

Chain e:



• Molecule 22: Inactive serine/threonine-protein kinase 19

Chain f:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	484012	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52.4	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	142.479	Depositor
Minimum map value	-0.208	Depositor
Average map value	0.017	Depositor
Map value standard deviation	1.349	Depositor
Recommended contour level	3.06	Depositor
Map size (Å)	439.92, 439.92, 439.92	wwPDB
Map dimensions	468, 468, 468	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.94000006, 0.94000006, 0.94000006	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.38	0/11493	0.59	2/15515 (0.0%)
2	B	0.43	0/9219	0.58	1/12444 (0.0%)
3	C	0.41	0/2132	0.57	0/2896
4	D	0.25	0/1027	0.49	0/1384
5	E	0.45	0/1752	0.59	0/2366
6	F	0.41	0/668	0.57	0/901
7	G	0.30	0/1365	0.54	0/1853
8	H	0.40	0/1207	0.57	0/1628
9	I	0.45	0/973	0.57	0/1316
10	J	0.41	0/543	0.63	0/730
11	K	0.36	0/939	0.53	0/1271
12	L	0.43	0/395	0.66	0/524
13	M	0.46	0/515	0.49	0/700
14	N	1.10	1/824 (0.1%)	1.79	58/1270 (4.6%)
15	P	0.94	0/247	1.30	4/384 (1.0%)
16	T	1.11	1/1096 (0.1%)	1.88	85/1685 (5.0%)
17	a	0.54	0/3082	0.59	0/4182
18	b	0.64	0/5180	0.61	1/6982 (0.0%)
19	c	0.28	0/1899	0.55	0/2540
20	d	0.50	0/9083	0.61	3/12306 (0.0%)
21	e	0.26	0/439	0.56	0/593
22	f	0.58	0/1853	0.61	0/2509
All	All	0.49	2/55931 (0.0%)	0.69	154/75979 (0.2%)

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

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
15	P	0	1
18	b	0	1
20	d	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	T	43	DG	C3'-O3'	-7.23	1.34	1.44
14	N	13	DA	N3-C4	-5.06	1.31	1.34

The worst 5 of 154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	T	34	DT	OP1-P-OP2	-8.30	107.15	119.60
16	T	33	DA	OP1-P-O3'	8.16	123.16	105.20
15	P	10	A	N1-C6-N6	-8.05	113.77	118.60
14	N	45	DG	OP1-P-OP2	-8.05	107.53	119.60
14	N	11	DT	OP1-P-O3'	7.74	122.23	105.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	967	ARG	Sidechain
2	B	274	ARG	Sidechain
15	P	10	A	Sidechain
18	b	593	ARG	Sidechain
20	d	103	ARG	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1417/1984 (71%)	1370 (97%)	46 (3%)	1 (0%)	48	41
2	B	1121/1251 (90%)	1086 (97%)	35 (3%)	0	100	100
3	C	256/275 (93%)	247 (96%)	9 (4%)	0	100	100
4	D	126/142 (89%)	120 (95%)	6 (5%)	0	100	100
5	E	207/210 (99%)	206 (100%)	1 (0%)	0	100	100
6	F	80/127 (63%)	77 (96%)	3 (4%)	0	100	100
7	G	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
8	H	146/150 (97%)	141 (97%)	5 (3%)	0	100	100
9	I	115/125 (92%)	109 (95%)	6 (5%)	0	100	100
10	J	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	109 (96%)	4 (4%)	0	100	100
12	L	44/58 (76%)	41 (93%)	3 (7%)	0	100	100
13	M	62/85 (73%)	61 (98%)	1 (2%)	0	100	100
17	a	382/396 (96%)	367 (96%)	15 (4%)	0	100	100
18	b	611/1496 (41%)	587 (96%)	24 (4%)	0	100	100
19	c	237/712 (33%)	230 (97%)	7 (3%)	0	100	100
20	d	1138/1143 (100%)	1083 (95%)	55 (5%)	0	100	100
21	e	51/105 (49%)	45 (88%)	6 (12%)	0	100	100
22	f	228/254 (90%)	221 (97%)	7 (3%)	0	100	100
All	All	6568/8869 (74%)	6329 (96%)	238 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1274	GLU

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	1256/1763 (71%)	1250 (100%)	6 (0%)	86 88
2	B	991/1084 (91%)	987 (100%)	4 (0%)	89 90
3	C	237/252 (94%)	236 (100%)	1 (0%)	89 90
4	D	108/126 (86%)	107 (99%)	1 (1%)	75 77
5	E	191/192 (100%)	191 (100%)	0	100 100
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%)	42 (98%)	1 (2%)	45 41
13	M	59/77 (77%)	59 (100%)	0	100 100
17	a	339/348 (97%)	339 (100%)	0	100 100
18	b	553/1298 (43%)	550 (100%)	3 (0%)	86 88
19	c	186/610 (30%)	186 (100%)	0	100 100
20	d	999/1001 (100%)	990 (99%)	9 (1%)	75 77
21	e	49/95 (52%)	49 (100%)	0	100 100
22	f	194/214 (91%)	193 (100%)	1 (0%)	86 88
All	All	5817/7784 (75%)	5791 (100%)	26 (0%)	88 90

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	b	693	PHE
20	d	145	LEU
20	d	1097	PHE
20	d	54	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	d	147	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
17	a	98	HIS
18	b	525	GLN
18	b	522	HIS
18	b	669	HIS
2	B	749	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/10 (90%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 12 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.

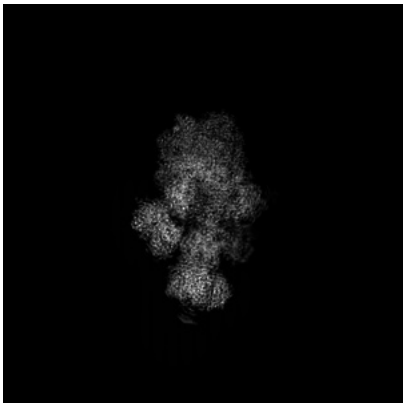
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45050. These allow visual inspection of the internal detail of the map and identification of artifacts.

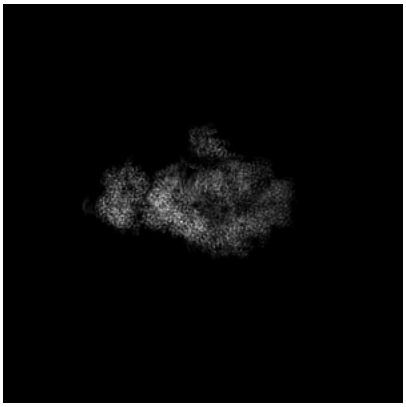
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

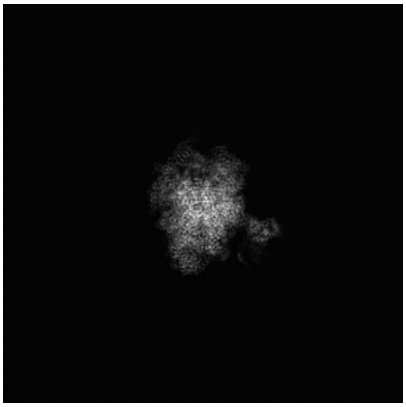
6.1.1 Primary map



X



Y



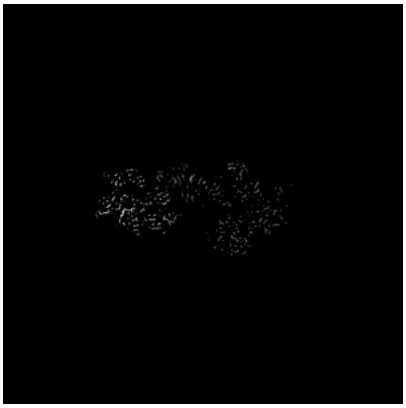
Z

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

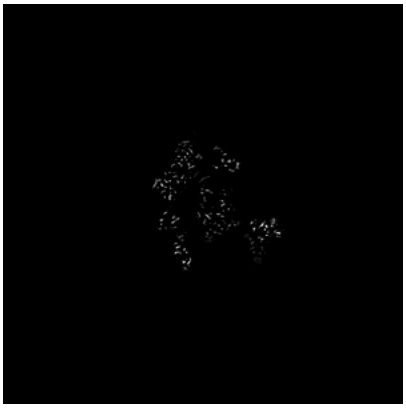
6.2 Central slices

6.2.1 Primary map

X Index: 234



Y Index: 234

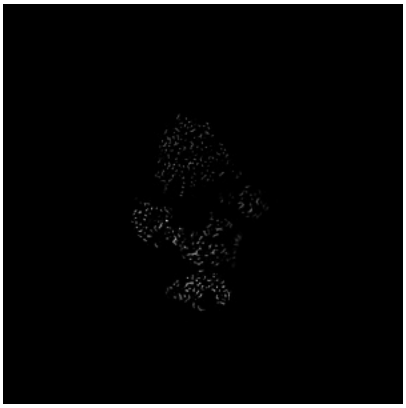


Z Index: 234

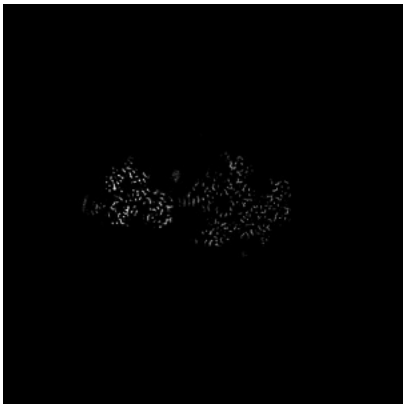
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

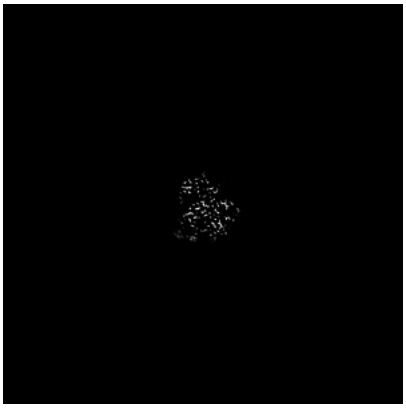
6.3.1 Primary map



X Index: 218



Y Index: 219

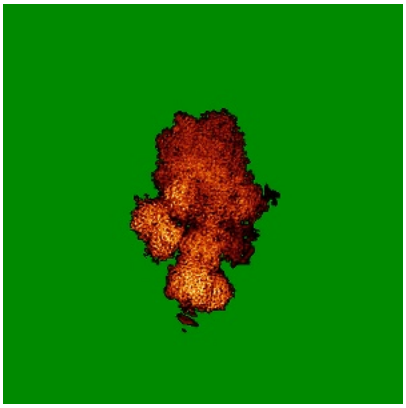


Z Index: 132

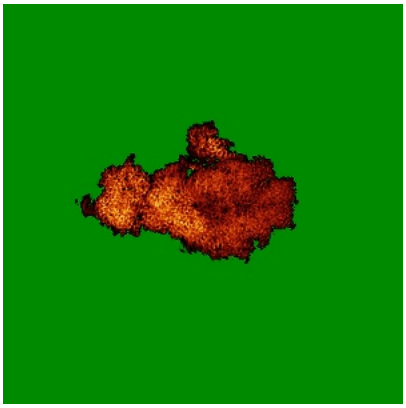
The images above show the largest variance slices of the map in three orthogonal directions.

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

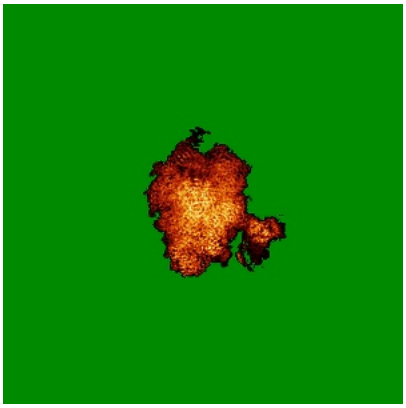
6.4.1 Primary map



X



Y

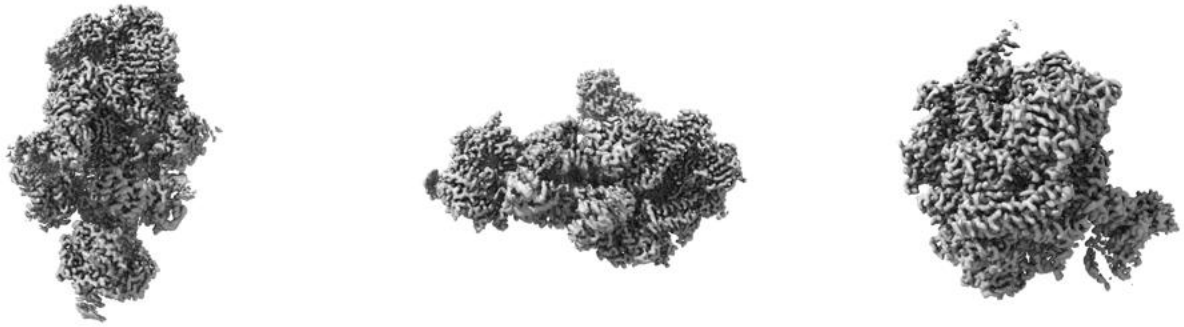


Z

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

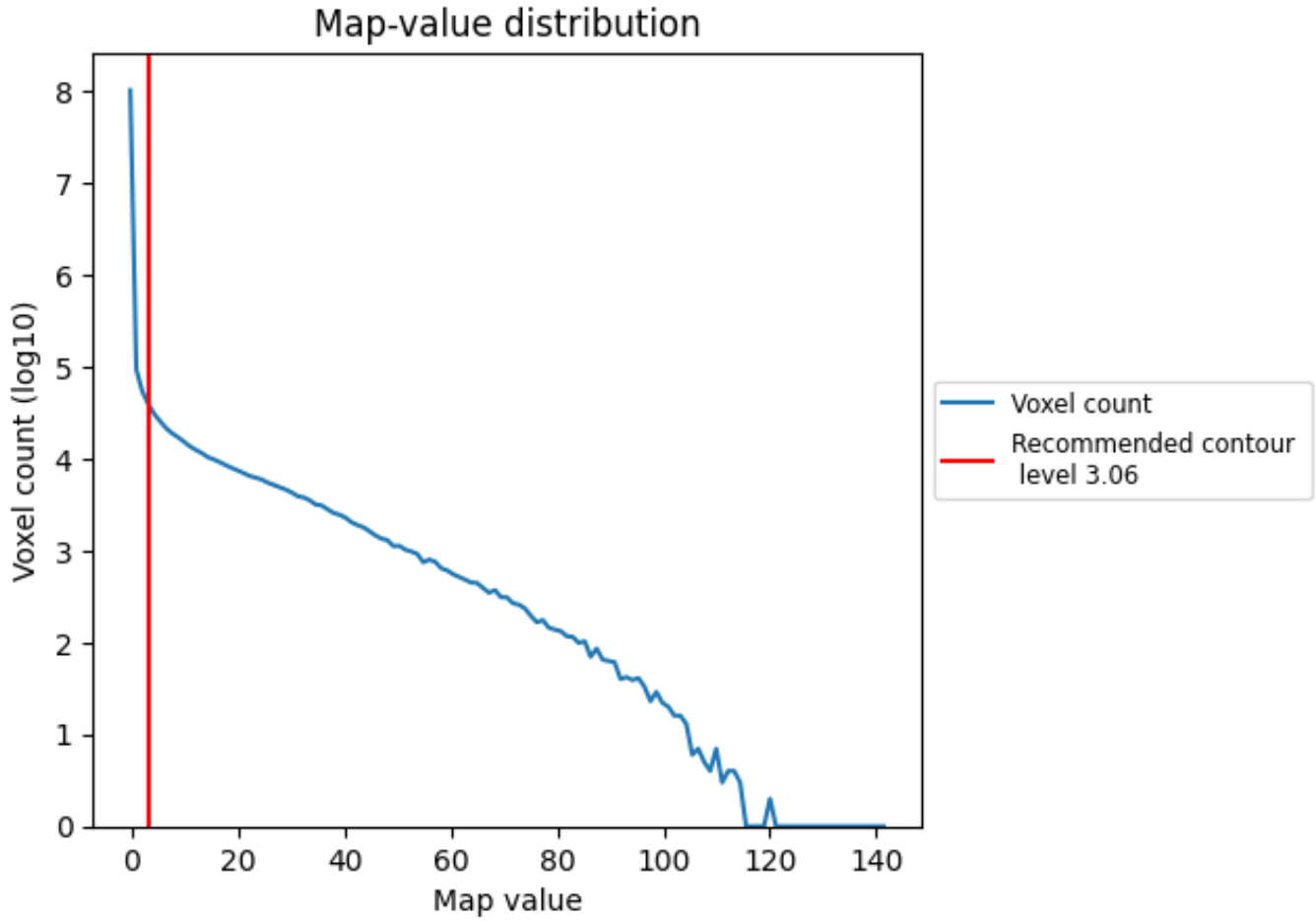
6.6 Mask visualisation (i)

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

7 Map analysis

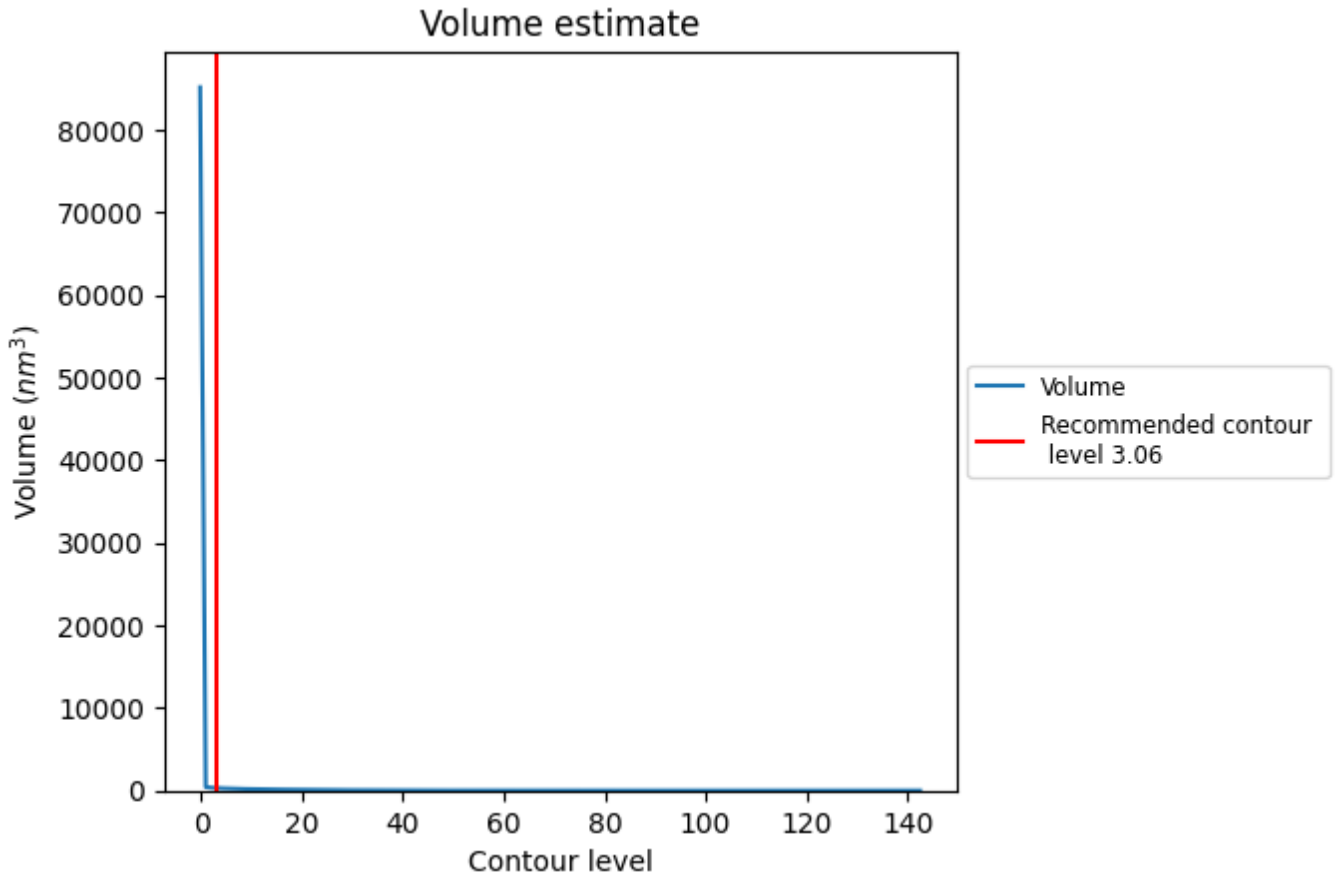
This section contains the results of statistical analysis of the map.

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.

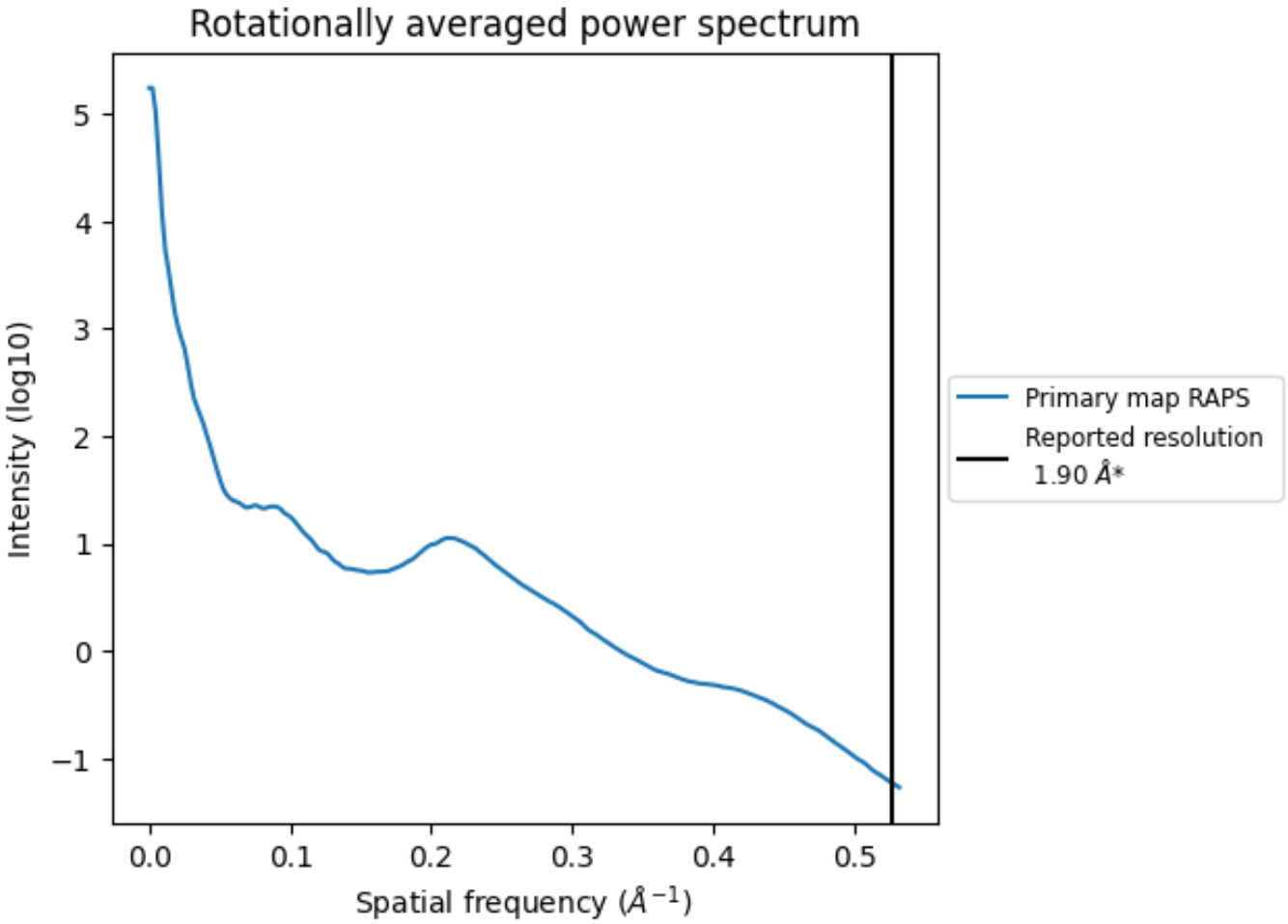
7.2 Volume estimate (i)



The volume at the recommended contour level is 306 nm^3; this corresponds to an approximate mass of 276 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)

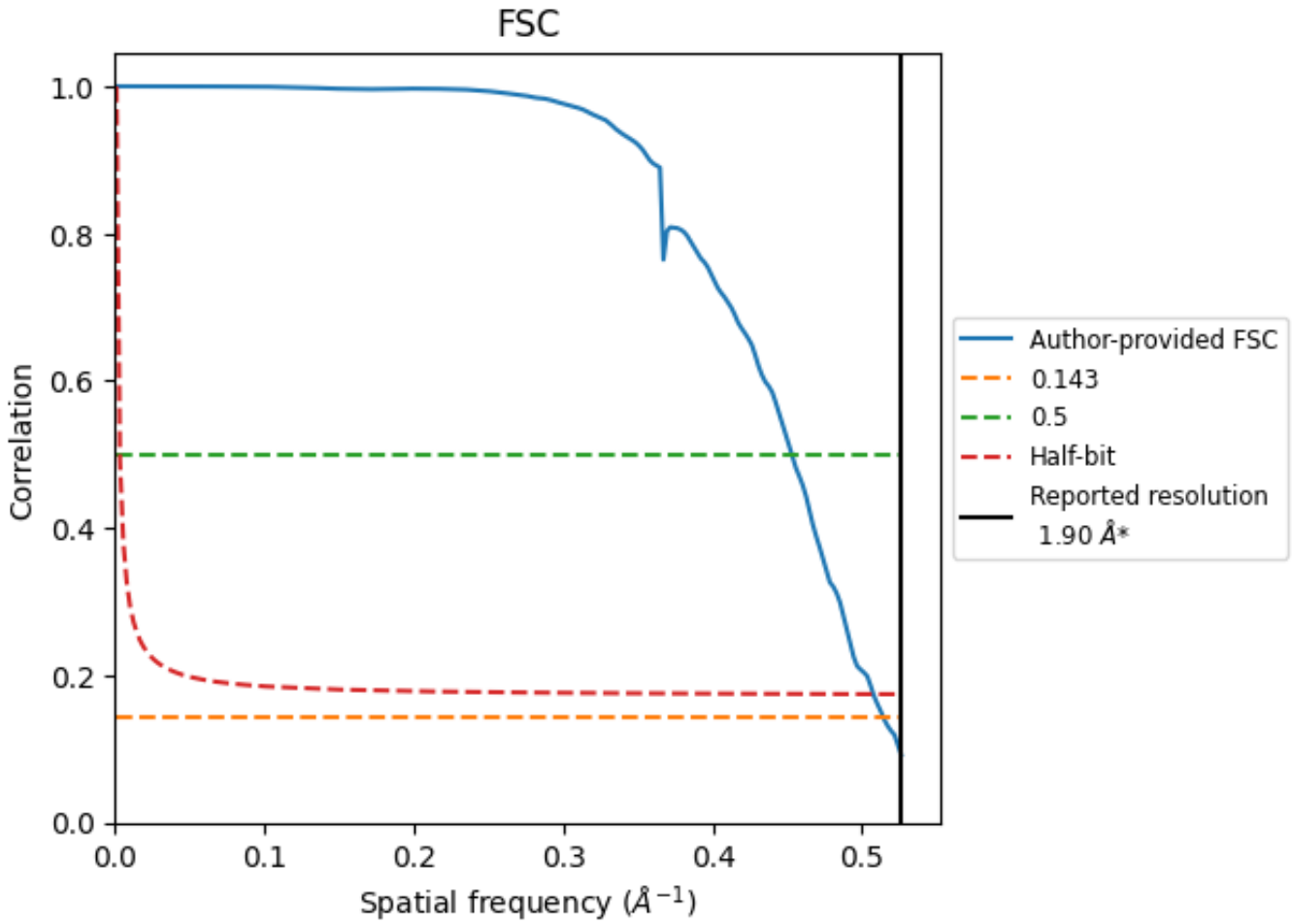


*Reported resolution corresponds to spatial frequency of 0.526 Å^{-1}

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 0.526 Å^{-1}

8.2 Resolution estimates (i)

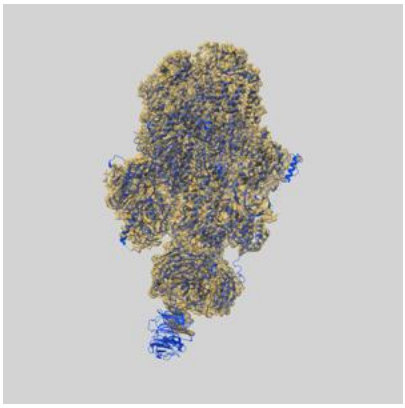
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.90	-	-
Author-provided FSC curve	1.95	2.21	1.97
Unmasked-calculated*	-	-	-

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

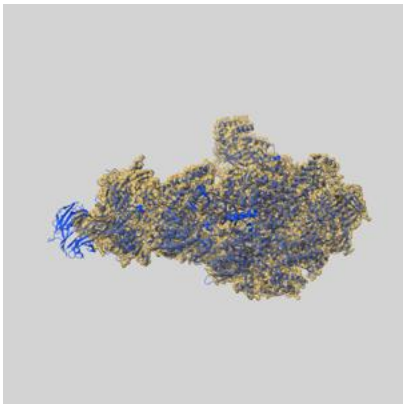
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45050 and PDB model 9BZ0. Per-residue inclusion information can be found in section 3 on page 9.

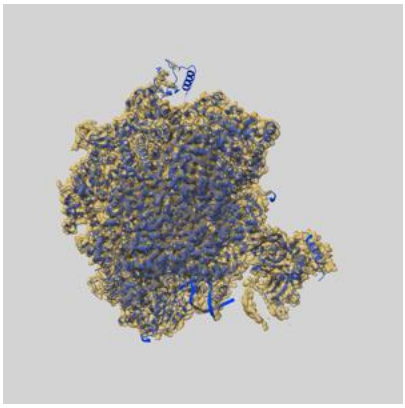
9.1 Map-model overlay



X



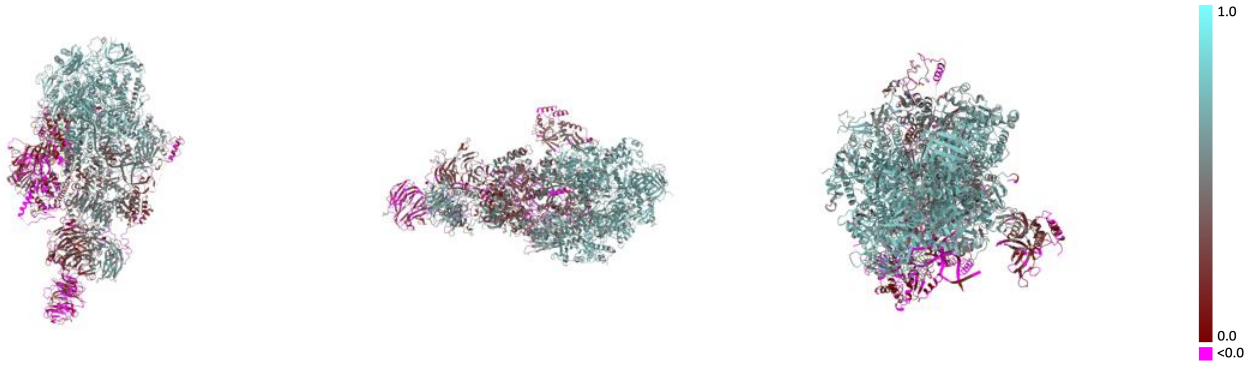
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

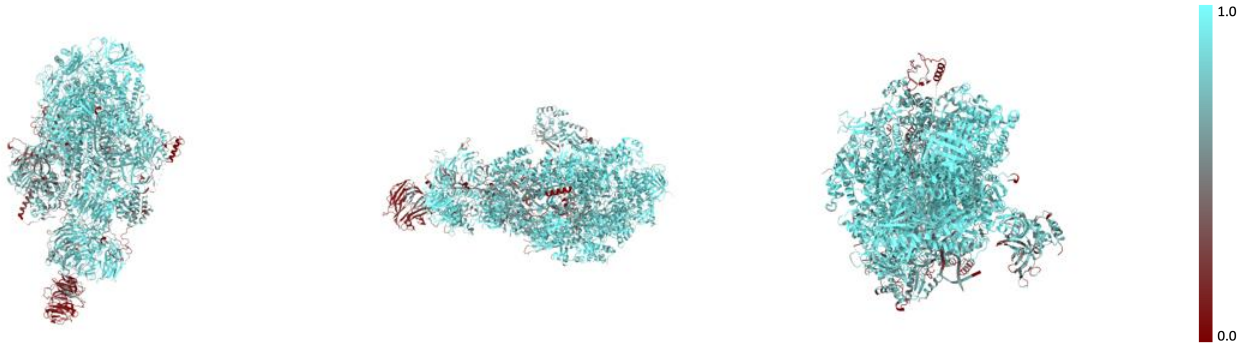
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

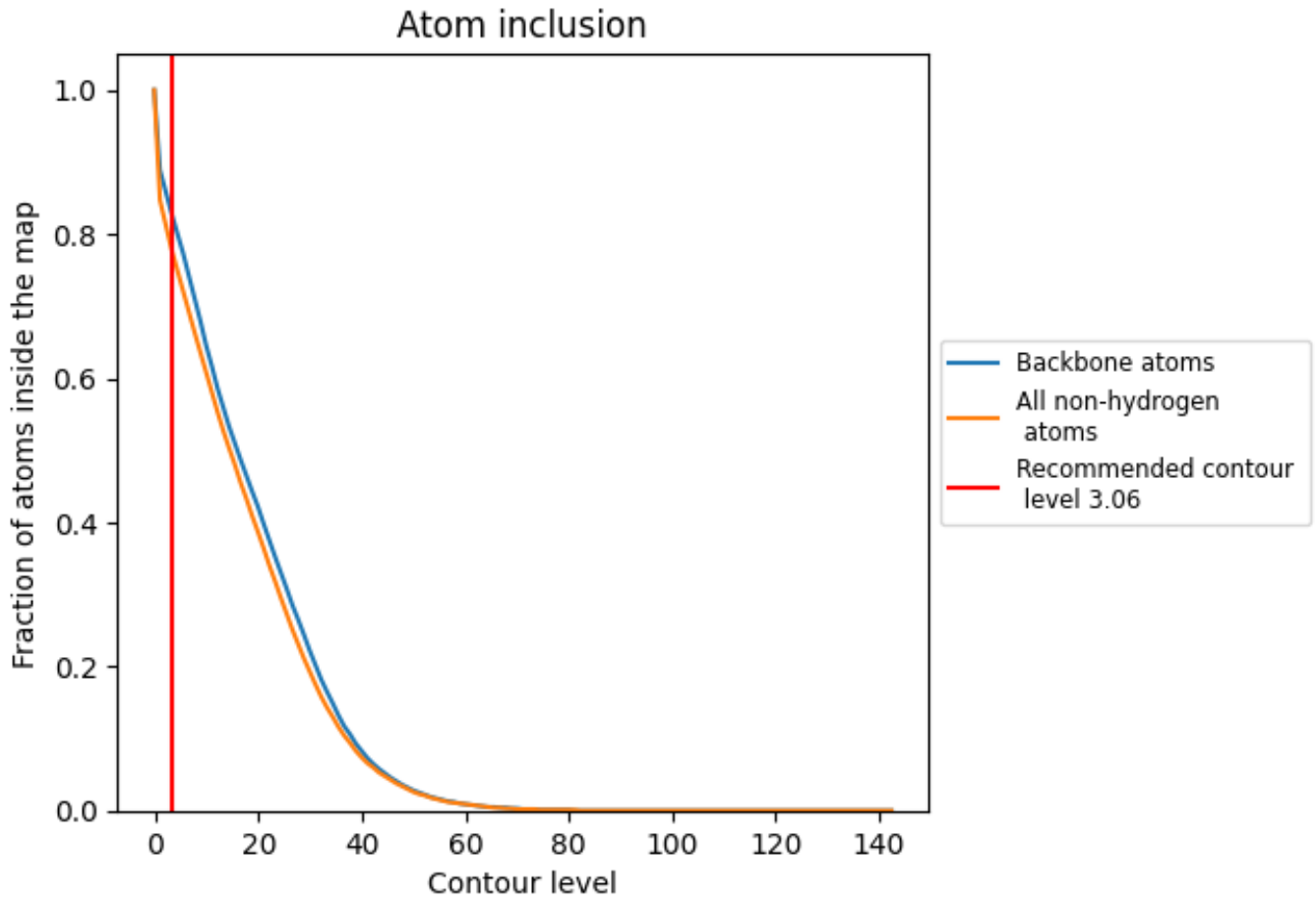
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.06).

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 (3.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7810	0.4480
A	0.8680	0.5810
B	0.8880	0.6130
C	0.8980	0.6430
D	0.6710	0.1430
E	0.9040	0.5940
F	0.8700	0.5870
G	0.6780	0.2670
H	0.9030	0.6370
I	0.8270	0.5440
J	0.9120	0.6590
K	0.9180	0.6540
L	0.7830	0.5240
M	0.8640	0.5220
N	0.7250	0.2710
P	0.9550	0.6300
T	0.7730	0.3400
a	0.8810	0.4870
b	0.6620	0.1040
c	0.5420	0.2750
d	0.6180	0.2740
e	0.5360	0.2360
f	0.7940	0.3990