



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 05:26 pm BST

PDB ID : 5G5L
EMDB ID : EMD-3439
Title : RNA polymerase I-Rrn3 complex at 4.8 Å resolution
Authors : Engel, C.; Plitzko, J.; Cramer, P.
Deposited on : 2016-05-26
Resolution : 4.80 Å (reported)
Based on initial model : 4C2M

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) : 2.39

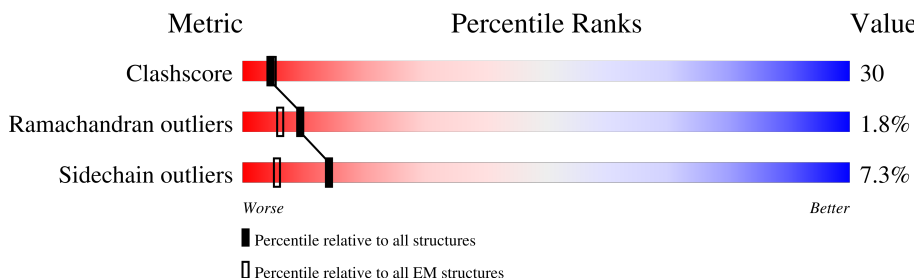
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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	1664	
2	B	1203	
3	C	335	
4	D	137	
5	E	215	
6	F	155	
7	G	326	
8	H	146	

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Mol	Chain	Length	Quality of chain
9	I	125	<div><div></div><div>22%</div><div>54%</div><div>30%</div><div>14%</div></div>
10	J	70	<div><div></div><div>79%</div><div>17%</div><div>...</div></div>
11	K	142	<div><div></div><div>6%</div><div>51%</div><div>19%</div><div>29%</div></div>
12	L	70	<div><div></div><div>6%</div><div>29%</div><div>27%</div><div>6%</div><div>39%</div></div>
13	M	415	<div><div></div><div>8%</div><div>17%</div><div>8%</div><div>75%</div></div>
14	N	233	<div><div></div><div>24%</div><div>47%</div><div>15%</div><div>38%</div></div>
15	O	627	<div><div></div><div>22%</div><div>25%</div><div>40%</div><div>8%</div><div>26%</div></div>

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 37349 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 I SUBUNIT RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1480	Total	C	N	O	S	0	0
			11686	7384	2030	2211	61		

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1174	Total	C	N	O	S	0	0
			9327	5899	1635	1743	50		

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	305	Total	C	N	O	S	0	0
			2423	1539	416	460	8		

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	58	Total	C	N	O	0	0
			459	289	78	92		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	212	Total	C	N	O	S	0	0
			1735	1102	306	316	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	100	Total	C	N	O	S	0	0
			823	522	144	154	3		

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	193	Total	C	N	O	S	0	0
			1520	982	259	274	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	131	Total	C	N	O	S	0	0
			1052	664	176	208	4		

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	107	Total	C	N	O	S	0	0
			820	511	138	162	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			793	496	130	162	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	43	Total	C	N	O	S	0	0
			340	211	66	59	4		

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	105	Total	C	N	O	0	0
			833	528	138	167		

- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	145	Total	C	N	O	S	0	0
			1151	735	188	224	4		

- Molecule 15 is a protein called RNA POLYMERASE I-SPECIFIC TRANSCRIPTION INITIATION FACTOR RRN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	463	Total	C	N	O	S	0	0
			3811	2473	623	694	21		

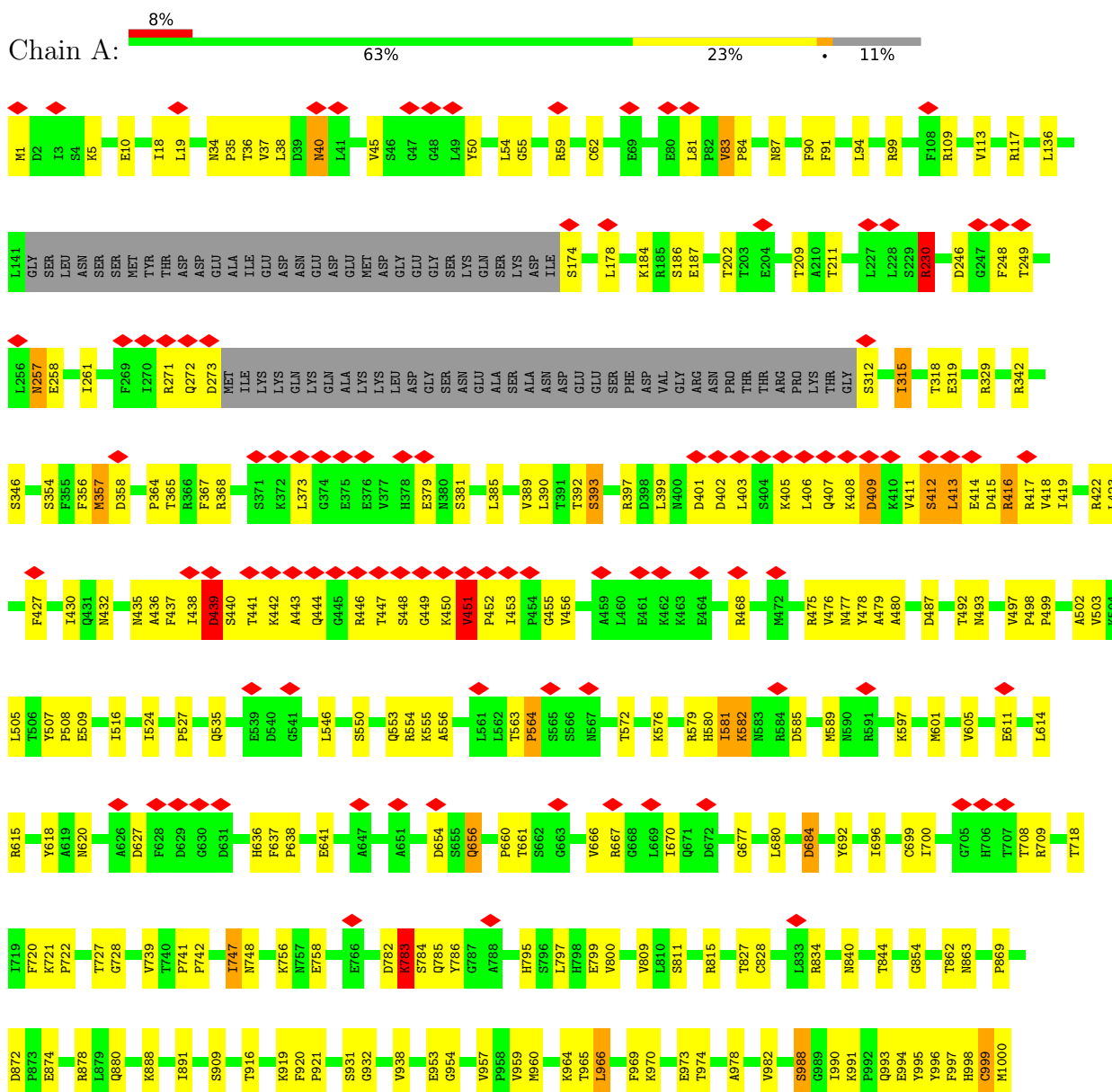
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

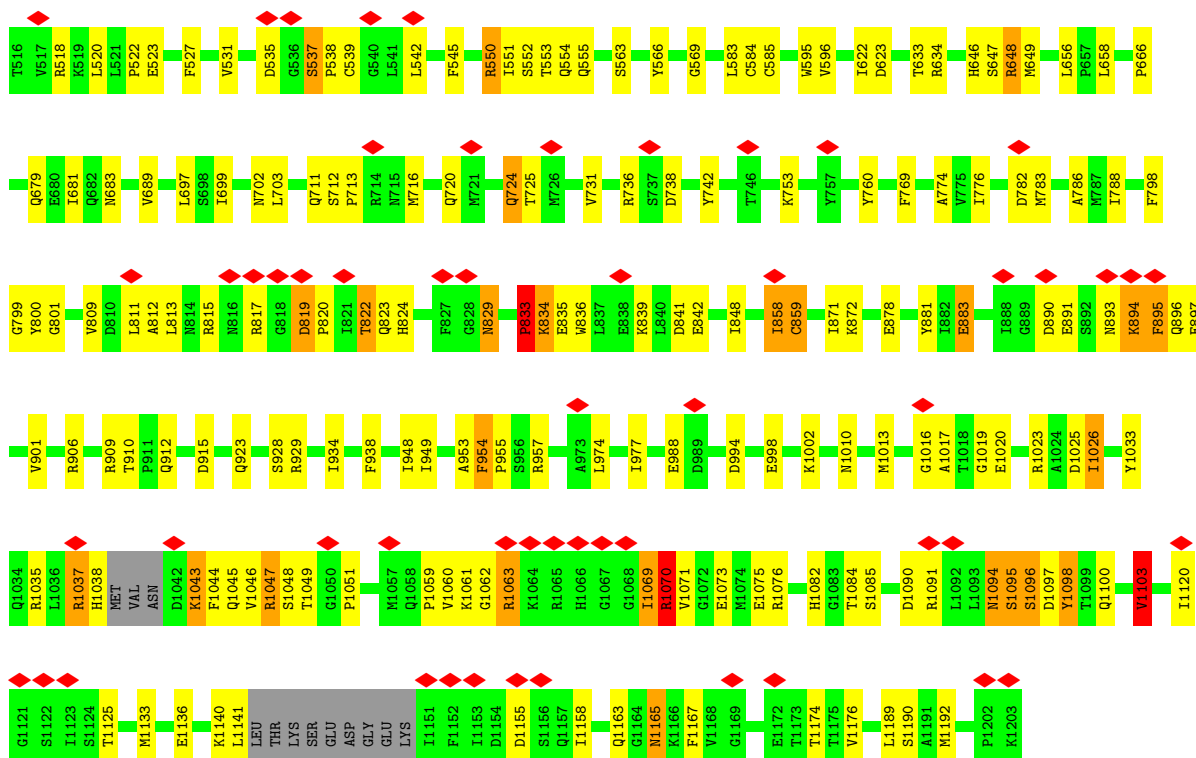
Mol	Chain	Residues	Atoms		AltConf
16	A	2	Total	Zn	0
			2	2	
16	B	1	Total	Zn	0
			1	1	
16	I	2	Total	Zn	0
			2	2	
16	J	1	Total	Zn	0
			1	1	
16	L	1	Total	Zn	0
			1	1	

3 Residue-property plots

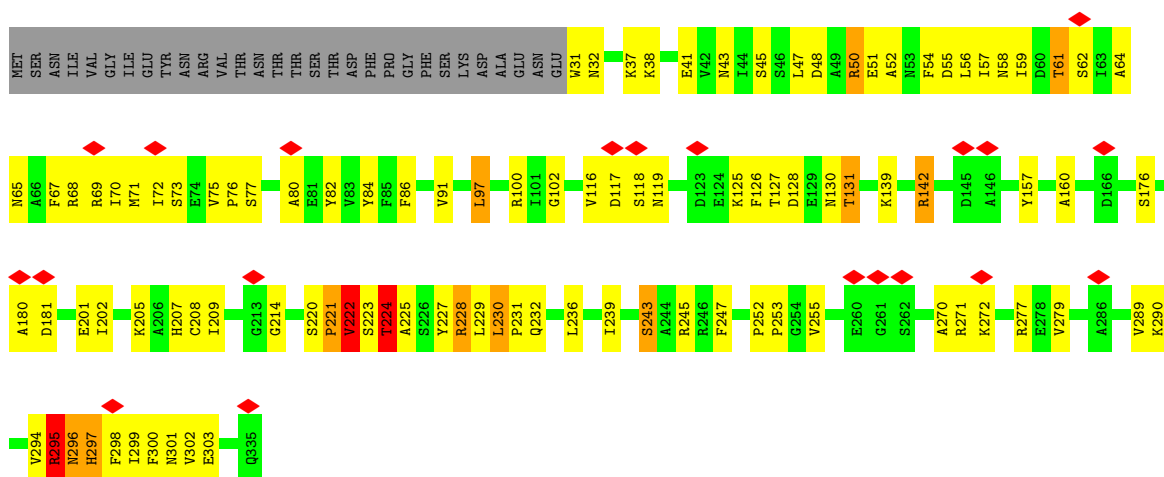
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 I SUBUNIT RPA190

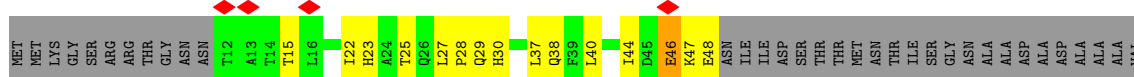


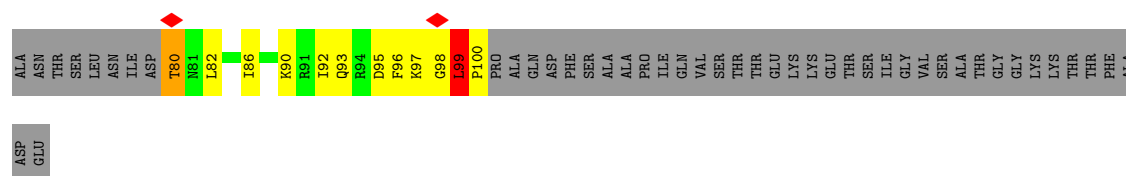


• Molecule 3: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1

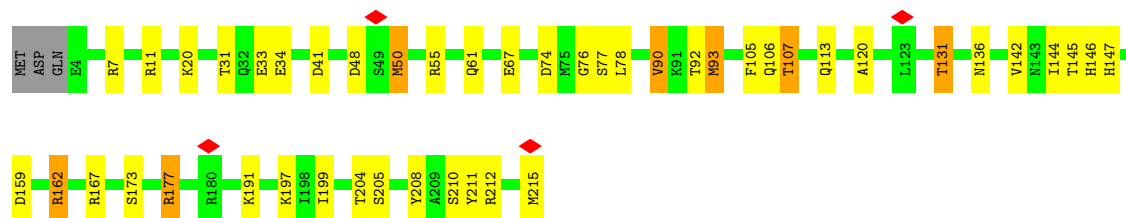
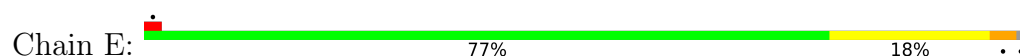


• Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14

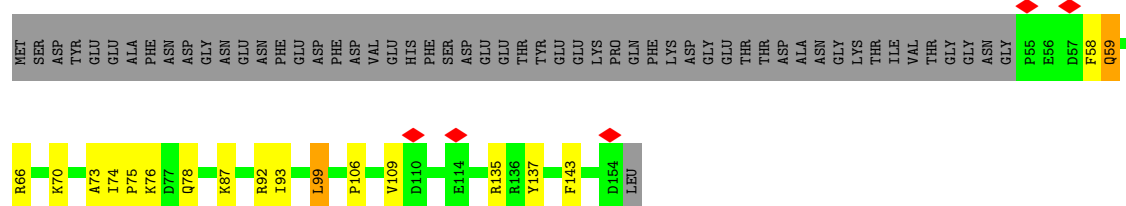




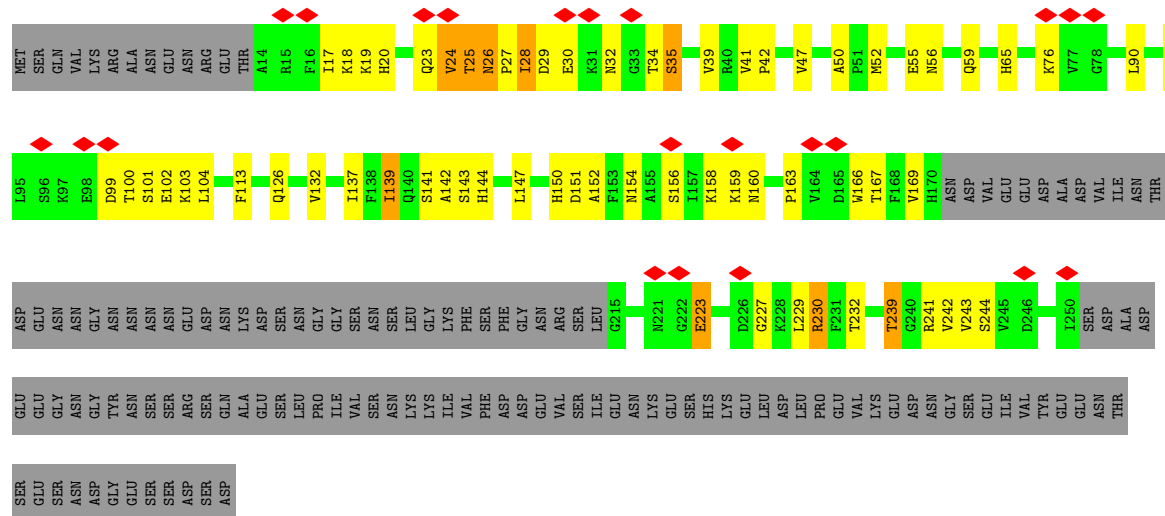
- Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1




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

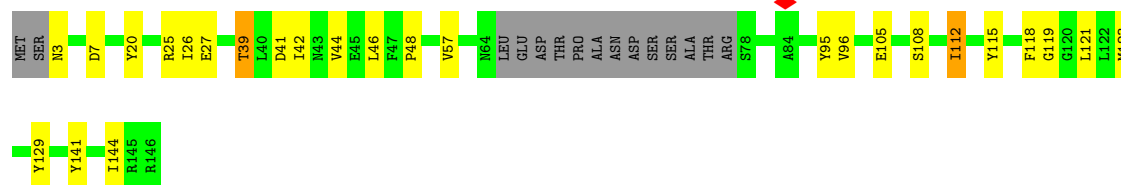


- Molecule 7: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43



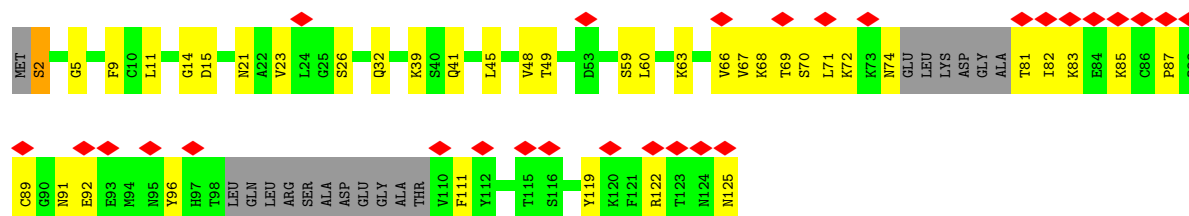
- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H: 




- Molecule 9: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12

Chain I: 



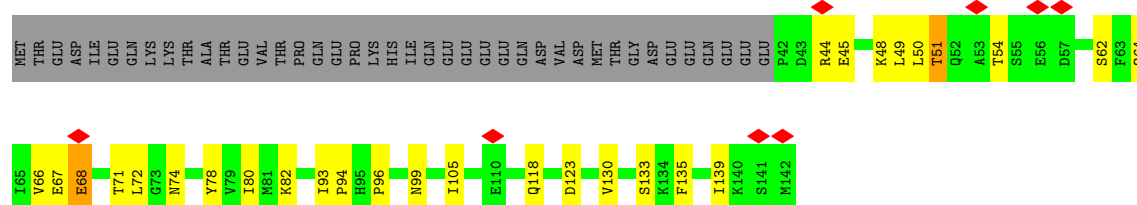
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J: 




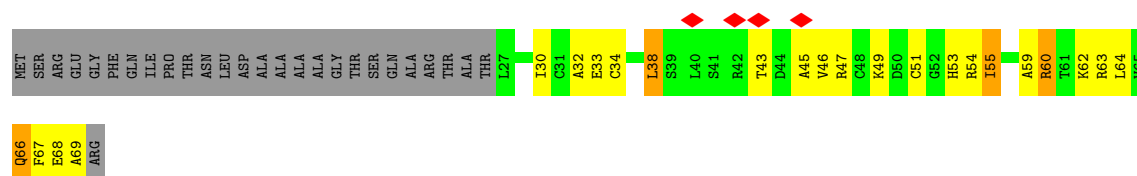
- Molecule 11: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2

Chain K: 

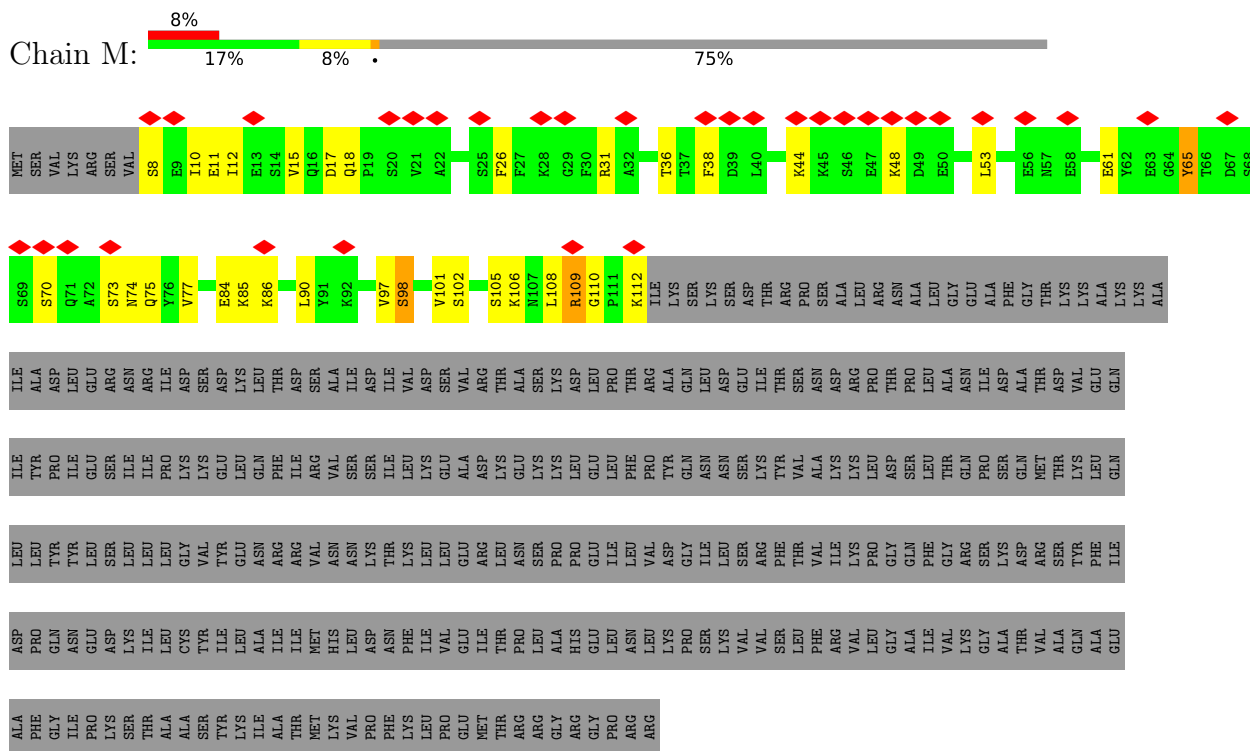


- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

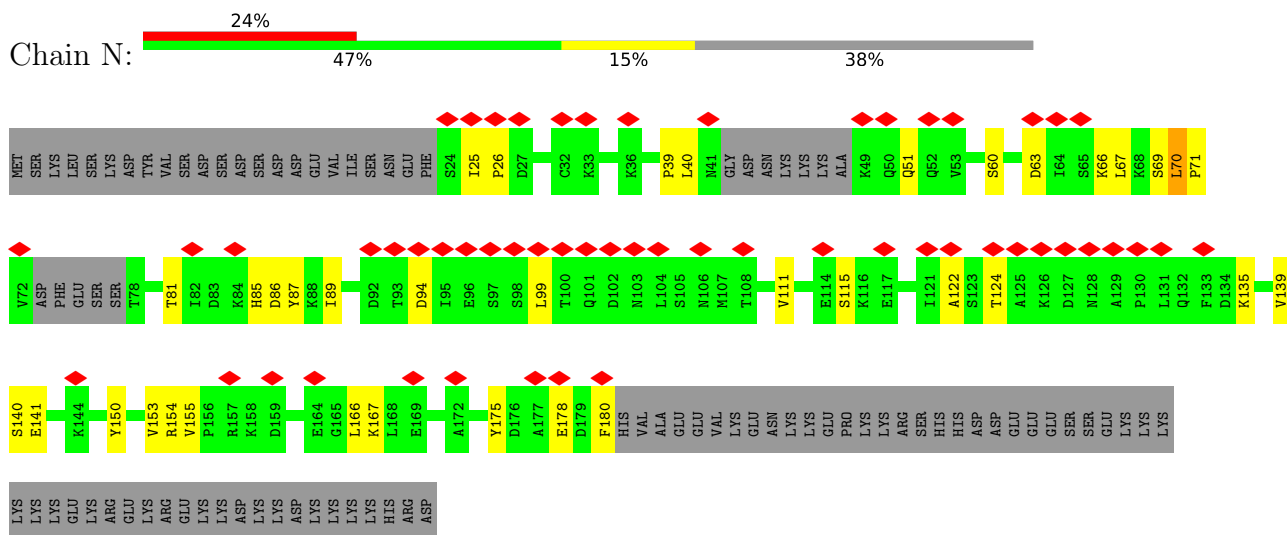
Chain L: 



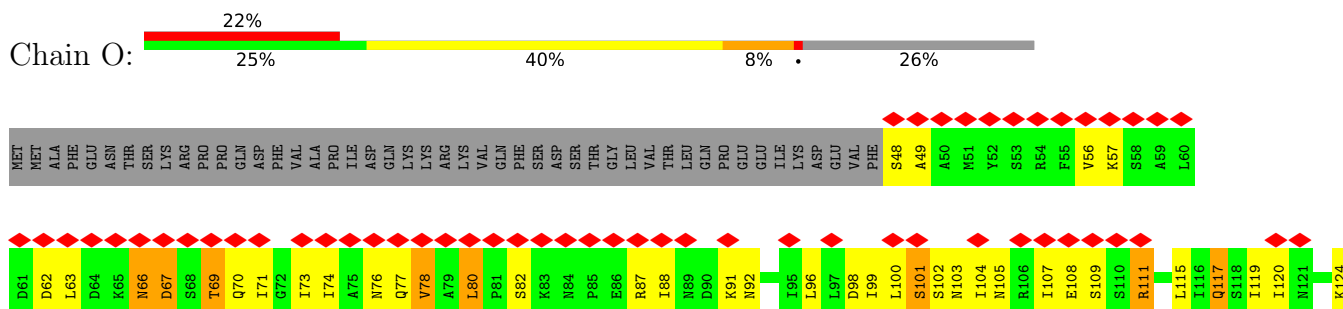
- Molecule 13: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49



- Molecule 14: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34



● Molecule 15: RNA POLYMERASE I-SPECIFIC TRANSCRIPTION INITIATION FACTOR, RRN3



THR	THR	THR	SER	SER	SER	SER	TRP	SER	SER	LEU	ALA	R582	Q583	Q584	F585	I586	D587	L588	Y591	F592	P593	Y594	D595	P596	L597	F598	L599	Y602	M606	K607	E608	Y609	Y610	I611	S614	GLU	ALA	SER	GLY	GLY	TYR	GLU	GLU	SER	ASP	ASP	ASP														
V442	A443	S444	Y445	L446	T447	S448	W449	L450	Y453	V454	I455	E456	R457	E458	E459	E460	V461	D462	Q463	R464	Q465	Q466	M467	E468	R469	F470	K471	H472	F473	Y474	A475	A476	F477	Q478	A479	L480	C481	Y482	I483	F484	C485	F486	R487	H488	R489	T490	F491	R492	D493	T494	D495	G496	N497	W498	E499	L502	D503				
K504	F505	F506	Q507	R508	M509	V510	I511	F514	N515	P516	L517	K518	F519	C520	N521	E522	N523	Y524	M525	L526	M527	F528	I531	V537	A538	Y539	C540	I543	N546	N547	N548	N549	E550	R551	LEU	ARG	GLY	ILE	ILE	GLY	GLY	LYS	ALA	ASP	SER	ASP	LYS	LYS	GLU	ASN	SER	ALA	GLN	ALA	ASN						
S380	I381	Q382	Y383	I384	N385	F386	H387	V388	S389	Q390	Q391	Q392	L395	M396	D397	S398	V401	T402	L403	I404	D405	I406	S407	F408	A409	V410	N411	E412	A413	A414	E415	K416	K417	I418	K419	S420	L421	Q422	Y423	C425	S426	Y427	I428	A429	R430	A431	K432	K433	L434	S435	R436	T437	Q438	I439	F441						
ASP	GLY	THR	THR	GLU	TYR	ASN	VAL	GLU	THR	GLN	G324	I325	K326	L330	L332	L336	T337	T341	H342	V343	E344	E345	Q346	V347	T348	F349	E350	S351	L352	E353	S354	G355	E356	G357	V358	G359	V360	F361	N362	L363	T364	T365	T366	L367	F368	K369	T370	H371	V372	L373	P374	T375	Y376	Y377	R378	R379					
I190	D191	T192	Y193	L194	F197	F198	P199	N200	K201	N202	D203	T204	R205	R206	K207	L208	V209	N210	Y211	T212	ASP	SER	GLY	ASP	ASP	ASP	ASP	L216	K217	ASP	L218	R219	G220	Y221	E224	L225	G226	F227	Q228	I229	W230	S231	L232	L233	E235	K236	I237	I238	S239	I240	D241	V242	E243	L244	Q245	N246	E247	L248	ASP	GLU	LEU
E127	L128	P129	P130	H131	T132	L133	S134	K135	Y136	I137	Y138	F139	I142	L143	C144	S145	I146	I147	P148	K149	W150	W151	Q152	D153	V154	S155	M156	I157	L158	F162	I163	L164	P165	I166	T169	V170	C171	H172	H173	D174	M175	L176	K177	Y178	F179	Y180	L181	M182	I183	P184	S185	M187	G188	F189							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	63445	Depositor
Resolution determination method	Not provided	
CTF correction method	RELION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	37037	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.079	Depositor
Minimum map value	-0.034	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.023	Depositor
Map size (\AA)	324.0, 324.0, 324.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.48	0/11900	0.72	22/16073 (0.1%)
2	B	0.49	1/9533 (0.0%)	0.77	25/12884 (0.2%)
3	C	0.43	0/2475	0.68	5/3354 (0.1%)
4	D	0.40	0/465	0.59	0/630
5	E	0.40	0/1771	0.66	3/2383 (0.1%)
6	F	0.45	0/838	0.58	0/1129
7	G	0.39	0/1558	0.60	3/2120 (0.1%)
8	H	0.42	0/1070	0.61	0/1449
9	I	0.42	0/831	0.57	0/1117
10	J	0.57	1/578 (0.2%)	0.59	0/775
11	K	0.46	0/804	0.79	3/1083 (0.3%)
12	L	0.38	0/342	0.55	0/454
13	M	0.42	0/849	0.56	1/1140 (0.1%)
14	N	0.40	0/1172	0.54	0/1580
15	O	0.38	1/3897 (0.0%)	0.58	3/5268 (0.1%)
All	All	0.45	3/38083 (0.0%)	0.69	65/51439 (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
15	O	0	5
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	10	CYS	CB-SG	7.64	1.95	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	198	PHE	C-N	-7.16	1.20	1.34
2	B	859	CYS	CB-SG	-6.12	1.71	1.82

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1023	ARG	NE-CZ-NH2	-13.90	113.35	120.30
2	B	452	ARG	NE-CZ-NH2	-13.35	113.63	120.30
1	A	397	ARG	NE-CZ-NH1	13.22	126.91	120.30
1	A	329	ARG	NE-CZ-NH2	-13.12	113.74	120.30
2	B	448	ARG	NE-CZ-NH2	-12.97	113.81	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1343	ASP	Peptide
15	O	374	PRO	Peptide
15	O	375	THR	Peptide
15	O	411	ASN	Peptide
15	O	598	PHE	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	11686	0	11770	682	0
2	B	9327	0	9214	482	0
3	C	2423	0	2409	283	0
4	D	459	0	461	103	0
5	E	1735	0	1764	40	0
6	F	823	0	840	64	0
7	G	1520	0	1529	164	0
8	H	1052	0	1021	15	0
9	I	820	0	805	71	0
10	J	569	0	585	6	0
11	K	793	0	790	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	340	0	361	47	0
13	M	833	0	826	32	0
14	N	1151	0	1169	44	0
15	O	3811	0	3800	757	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
All	All	37349	0	37344	2258	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 30.

The worst 5 of 2258 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)
15:O:162:PHE:CB	15:O:214:ASN:CB	1.76	1.62
3:C:75:VAL:HG11	3:C:221:PRO:CG	1.33	1.52
1:A:478:TYR:HA	2:B:1048:SER:CA	1.42	1.50
1:A:436:ALA:CB	1:A:443:ALA:HB2	1.43	1.46
1:A:83:VAL:HG21	1:A:427:PHE:CZ	1.50	1.46

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	1464/1664 (88%)	1370 (94%)	82 (6%)	12 (1%)	16	53
2	B	1166/1203 (97%)	1086 (93%)	56 (5%)	24 (2%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	303/335 (90%)	278 (92%)	18 (6%)	7 (2%)	5	28
4	D	54/137 (39%)	50 (93%)	2 (4%)	2 (4%)	2	20
5	E	210/215 (98%)	197 (94%)	11 (5%)	2 (1%)	13	48
6	F	98/155 (63%)	94 (96%)	4 (4%)	0	100	100
7	G	189/326 (58%)	171 (90%)	13 (7%)	5 (3%)	4	25
8	H	127/146 (87%)	121 (95%)	6 (5%)	0	100	100
9	I	101/125 (81%)	89 (88%)	9 (9%)	3 (3%)	3	22
10	J	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
11	K	99/142 (70%)	92 (93%)	7 (7%)	0	100	100
12	L	41/70 (59%)	32 (78%)	6 (15%)	3 (7%)	1	11
13	M	103/415 (25%)	93 (90%)	8 (8%)	2 (2%)	6	32
14	N	139/233 (60%)	123 (88%)	13 (9%)	3 (2%)	5	29
15	O	457/627 (73%)	400 (88%)	38 (8%)	19 (4%)	2	17
All	All	4618/5863 (79%)	4259 (92%)	277 (6%)	82 (2%)	9	34

5 of 82 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1606	SER
2	B	111	ASP
2	B	117	VAL
2	B	895	PHE
2	B	1069	ILE

5.3.2 Protein sidechains ⓘ

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	1307/1465 (89%)	1221 (93%)	86 (7%)	14	35
2	B	1027/1053 (98%)	956 (93%)	71 (7%)	13	33
3	C	269/296 (91%)	249 (93%)	20 (7%)	11	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	55/116 (47%)	49 (89%)	6 (11%)	5	19
5	E	194/197 (98%)	180 (93%)	14 (7%)	12	32
6	F	90/137 (66%)	86 (96%)	4 (4%)	24	46
7	G	170/291 (58%)	158 (93%)	12 (7%)	12	32
8	H	115/128 (90%)	111 (96%)	4 (4%)	31	52
9	I	97/110 (88%)	91 (94%)	6 (6%)	15	37
10	J	64/65 (98%)	57 (89%)	7 (11%)	5	19
11	K	91/130 (70%)	84 (92%)	7 (8%)	10	30
12	L	38/57 (67%)	34 (90%)	4 (10%)	5	20
13	M	95/371 (26%)	85 (90%)	10 (10%)	5	20
14	N	135/220 (61%)	129 (96%)	6 (4%)	24	46
15	O	427/576 (74%)	378 (88%)	49 (12%)	4	17
All	All	4174/5212 (80%)	3868 (93%)	306 (7%)	14	31

5 of 306 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	51	THR
15	O	350	GLU
12	L	55	ILE
15	O	78	VAL
15	O	526	LEU

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

Mol	Chain	Res	Type
15	O	362	ASN
15	O	547	ASN
15	O	371	HIS
15	O	497	ASN
6	F	59	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 7 ligands modelled in this entry, 7 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.

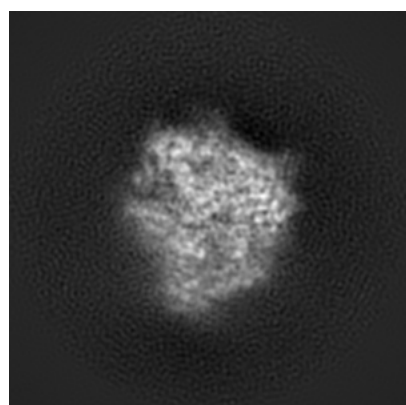
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3439. These allow visual inspection of the internal detail of the map and identification of artifacts.

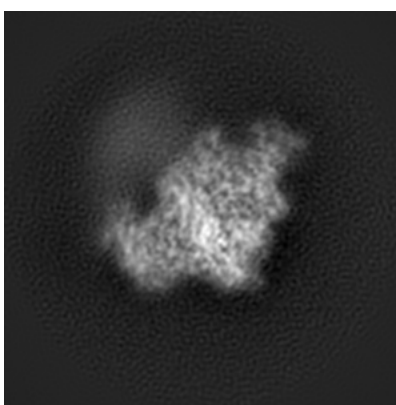
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

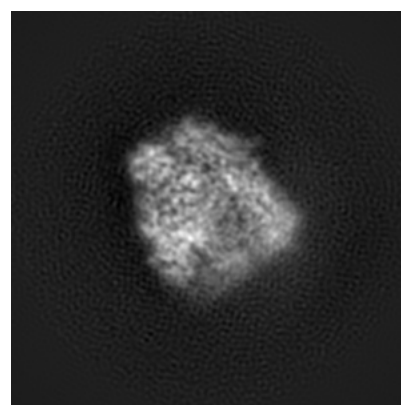
6.1.1 Primary map



X



Y

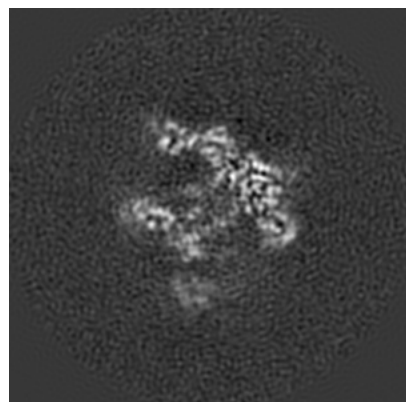


Z

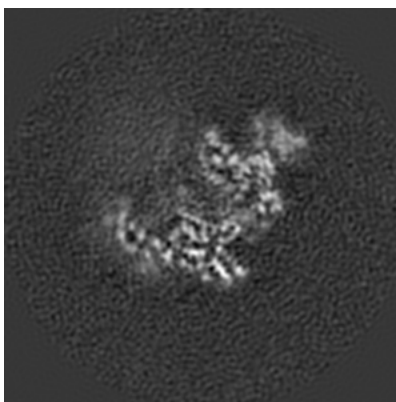
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

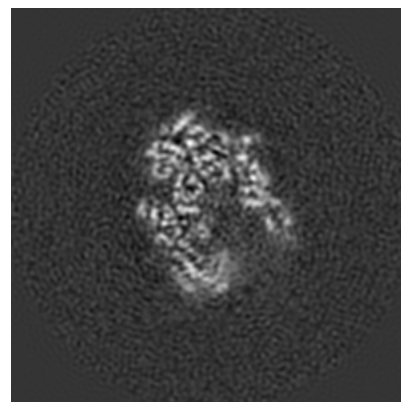
6.2.1 Primary map



X Index: 120



Y Index: 120

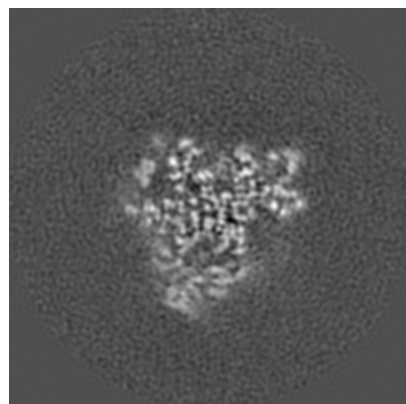


Z Index: 120

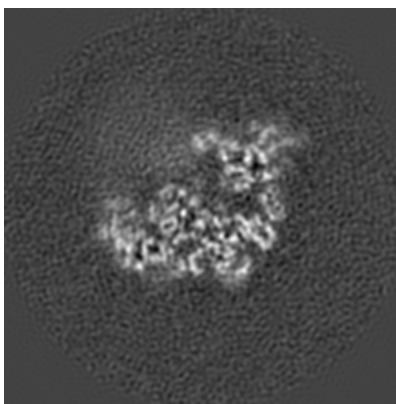
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

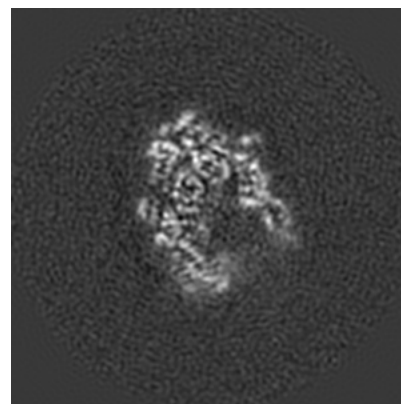
6.3.1 Primary map



X Index: 106



Y Index: 106

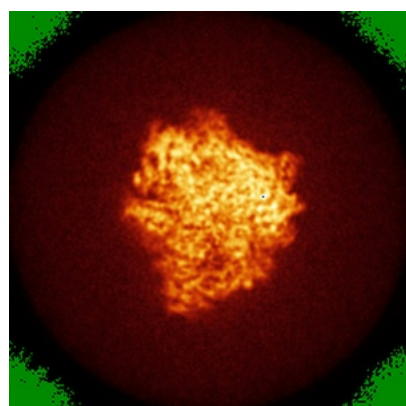


Z Index: 121

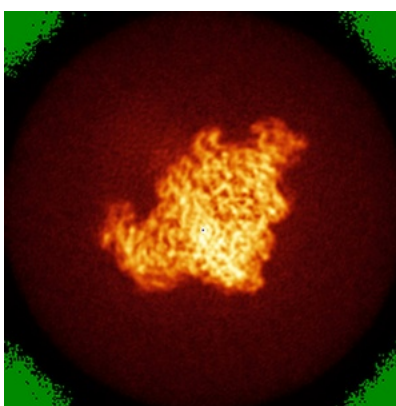
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

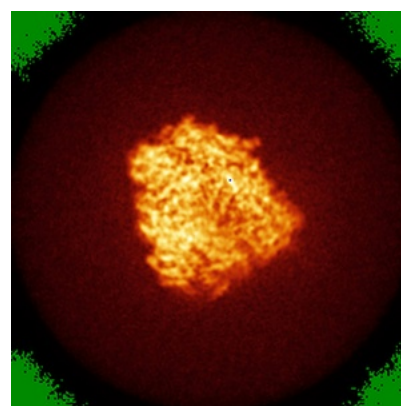
6.4.1 Primary map



X



Y

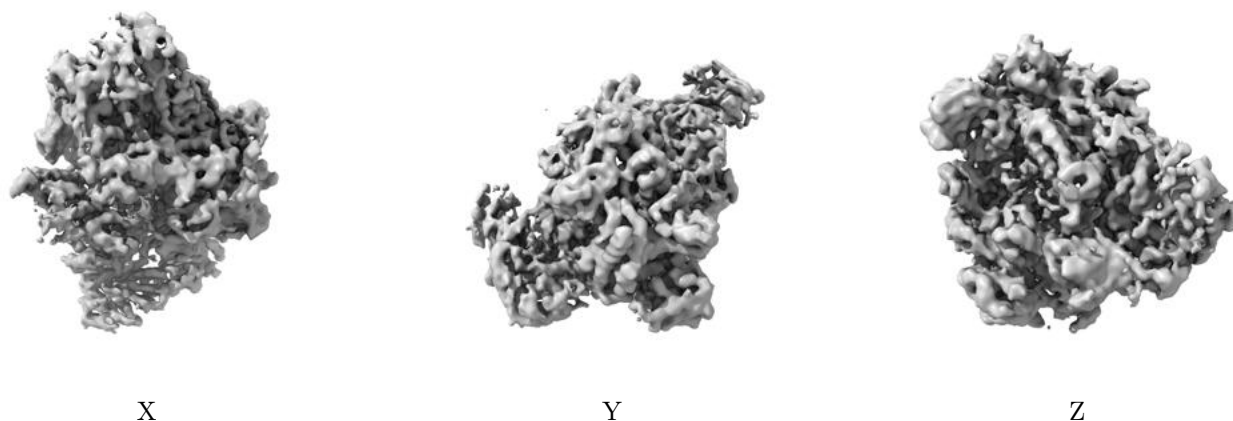


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

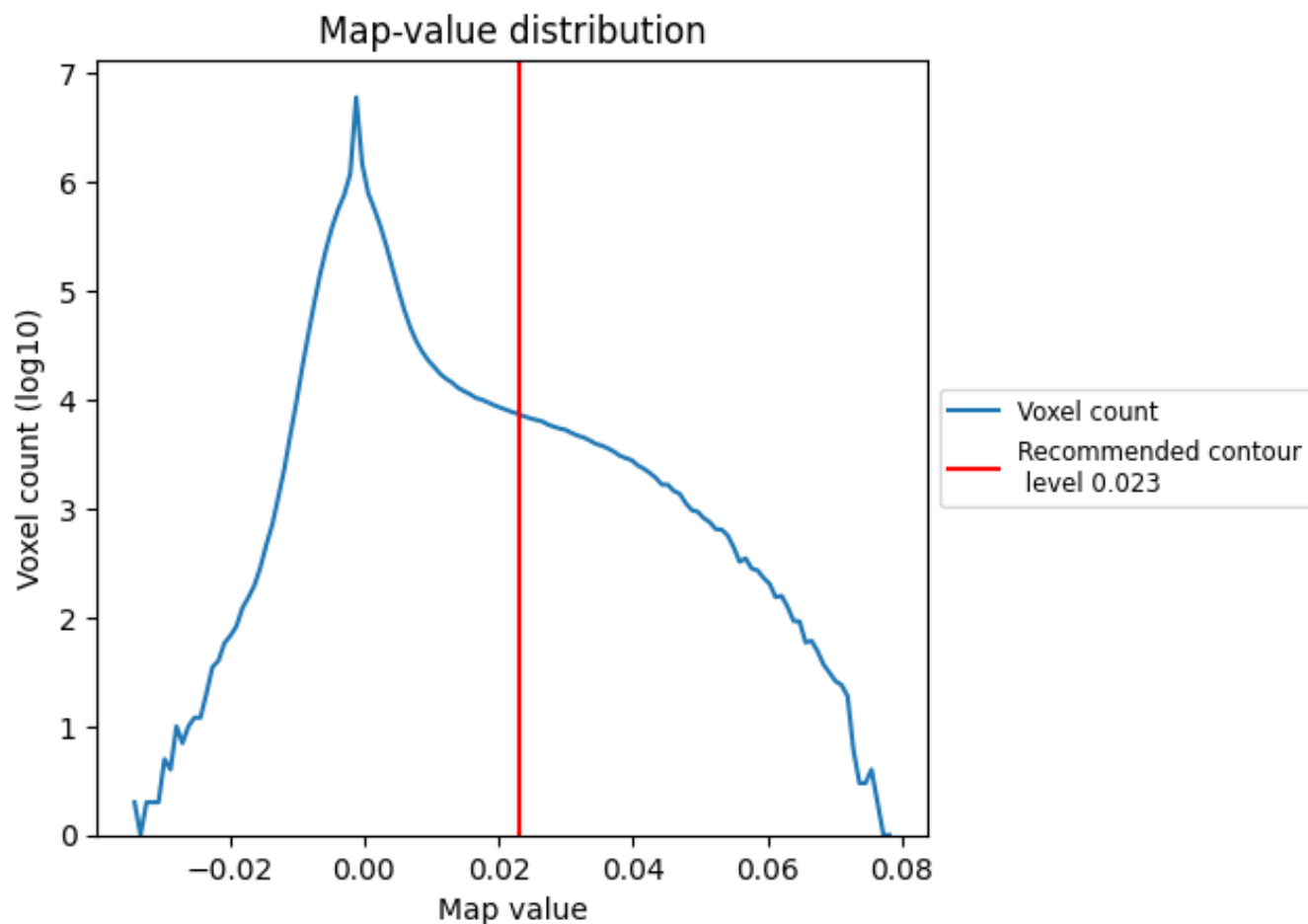
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

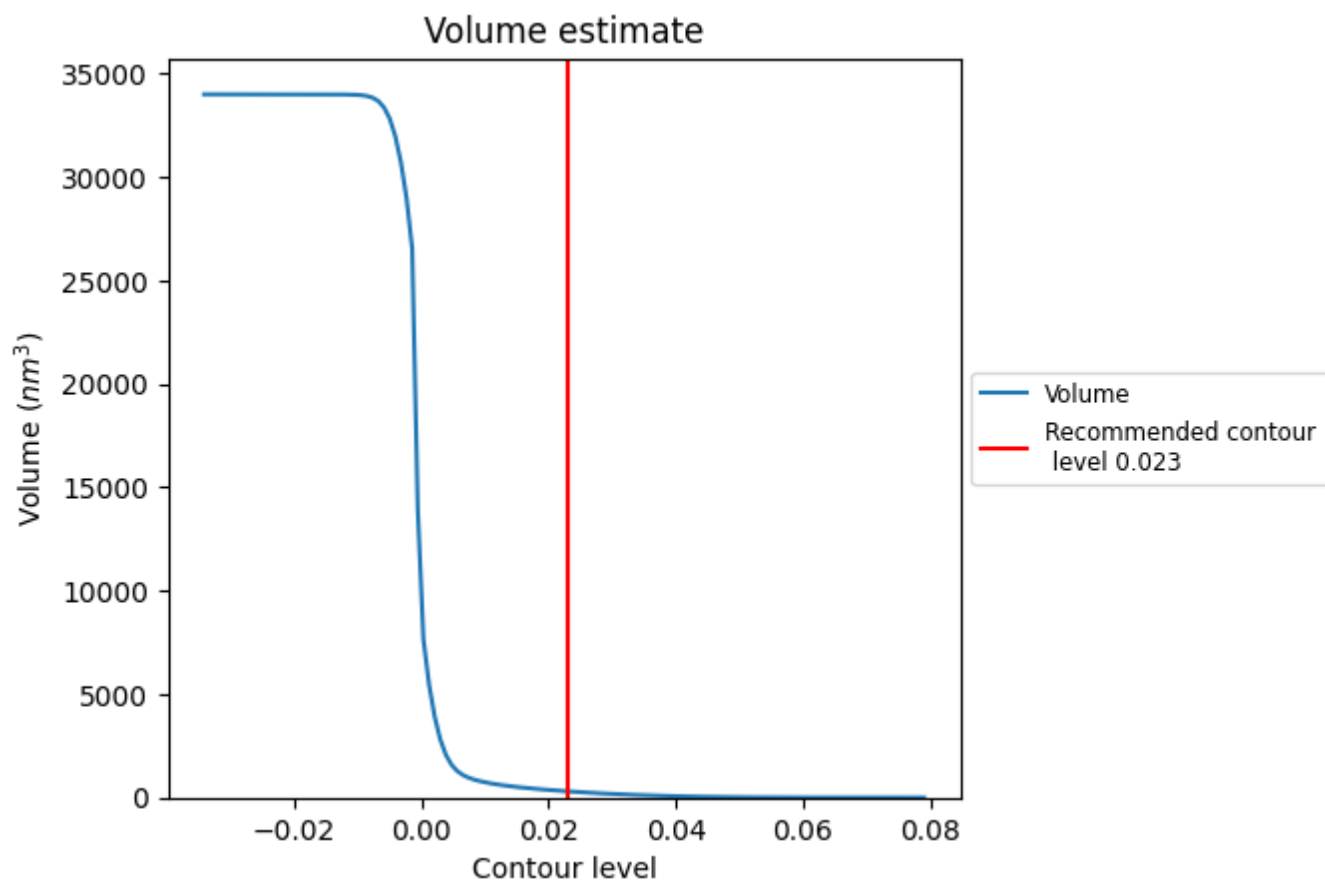
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

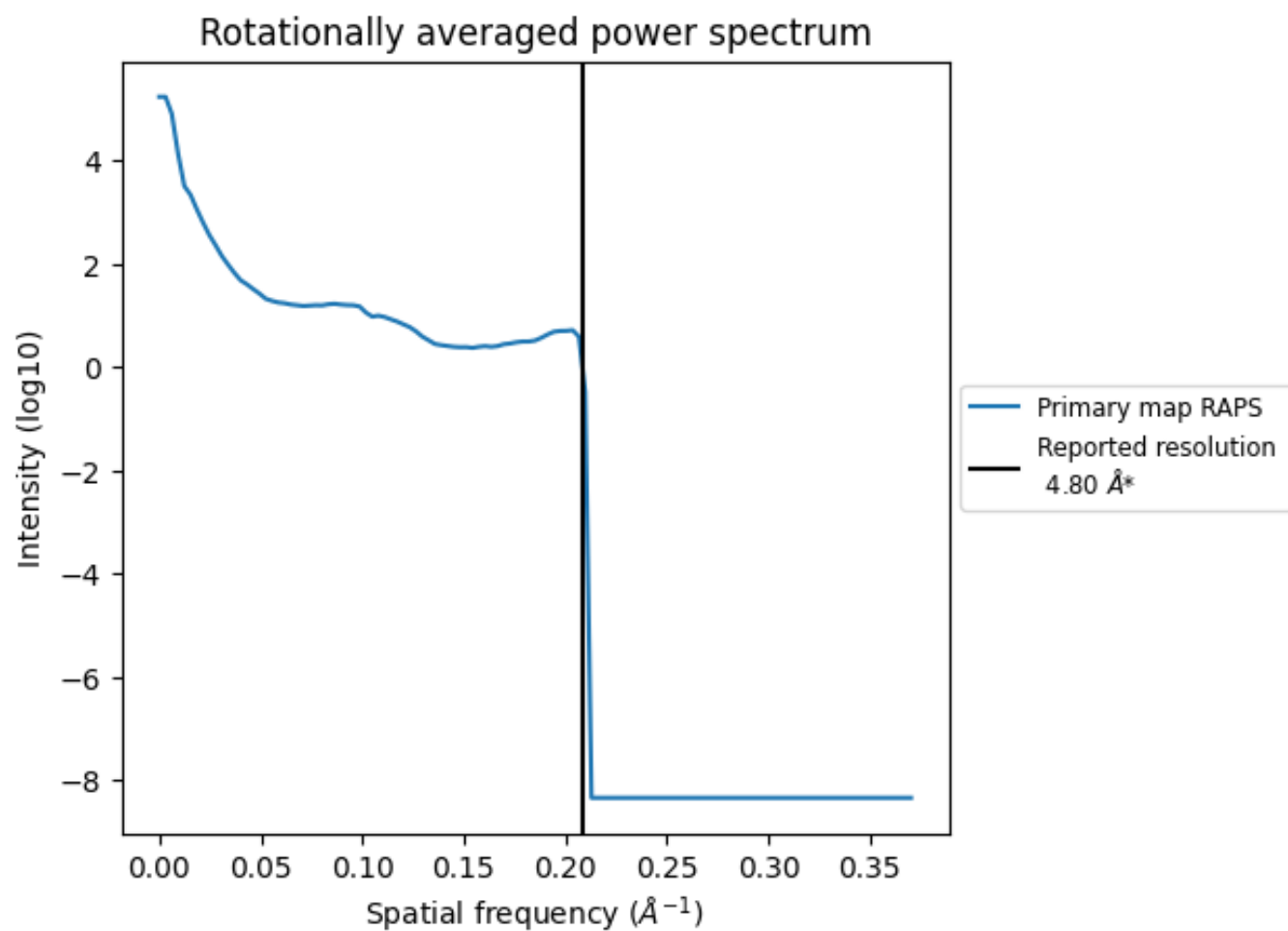
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 300 nm³; this corresponds to an approximate mass of 271 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

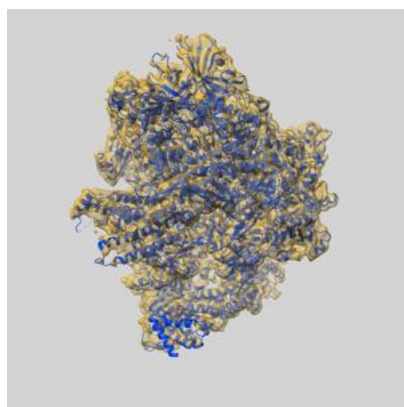
8 Fourier-Shell correlation

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

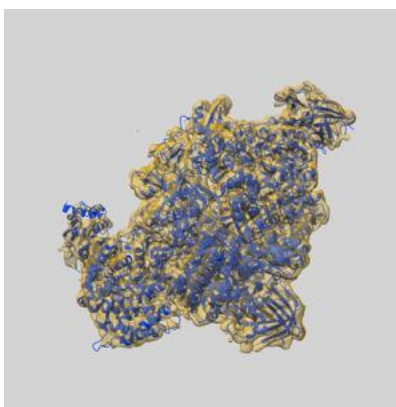
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3439 and PDB model 5G5L. Per-residue inclusion information can be found in section [3](#) on page [7](#).

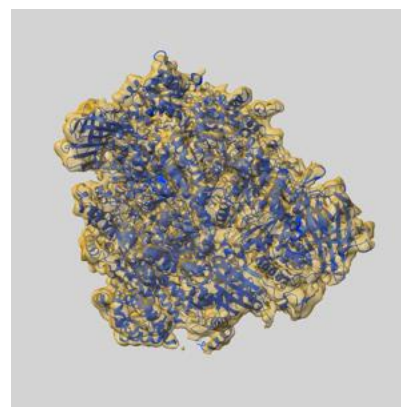
9.1 Map-model overlay [i](#)



X



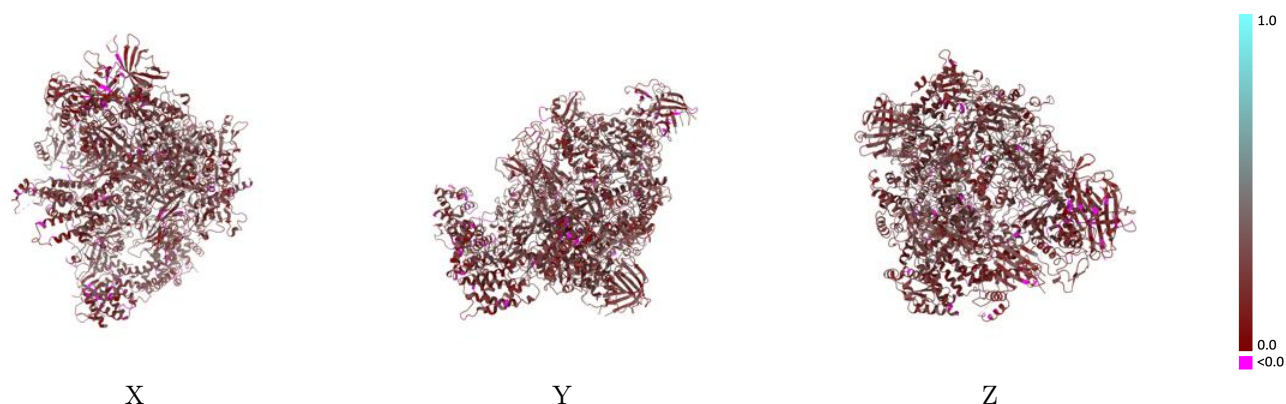
Y



Z

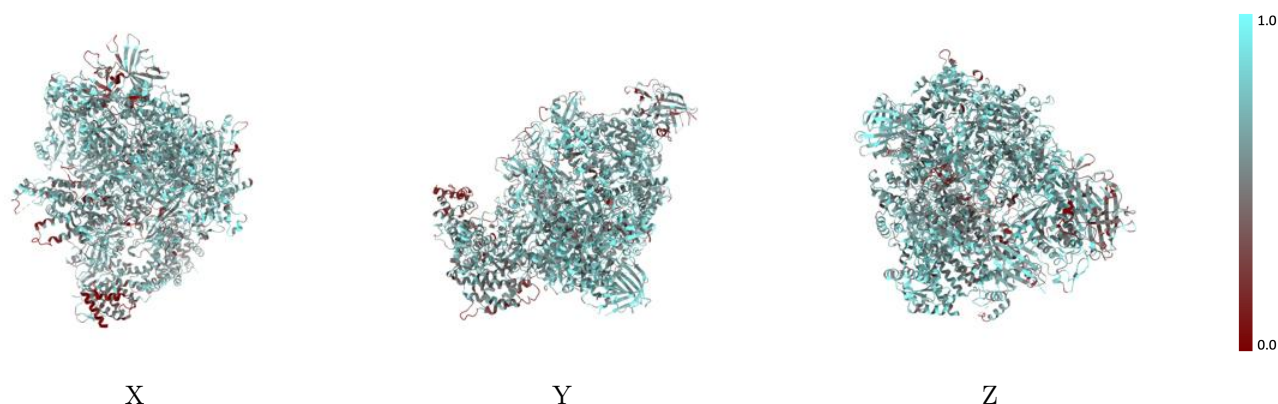
The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



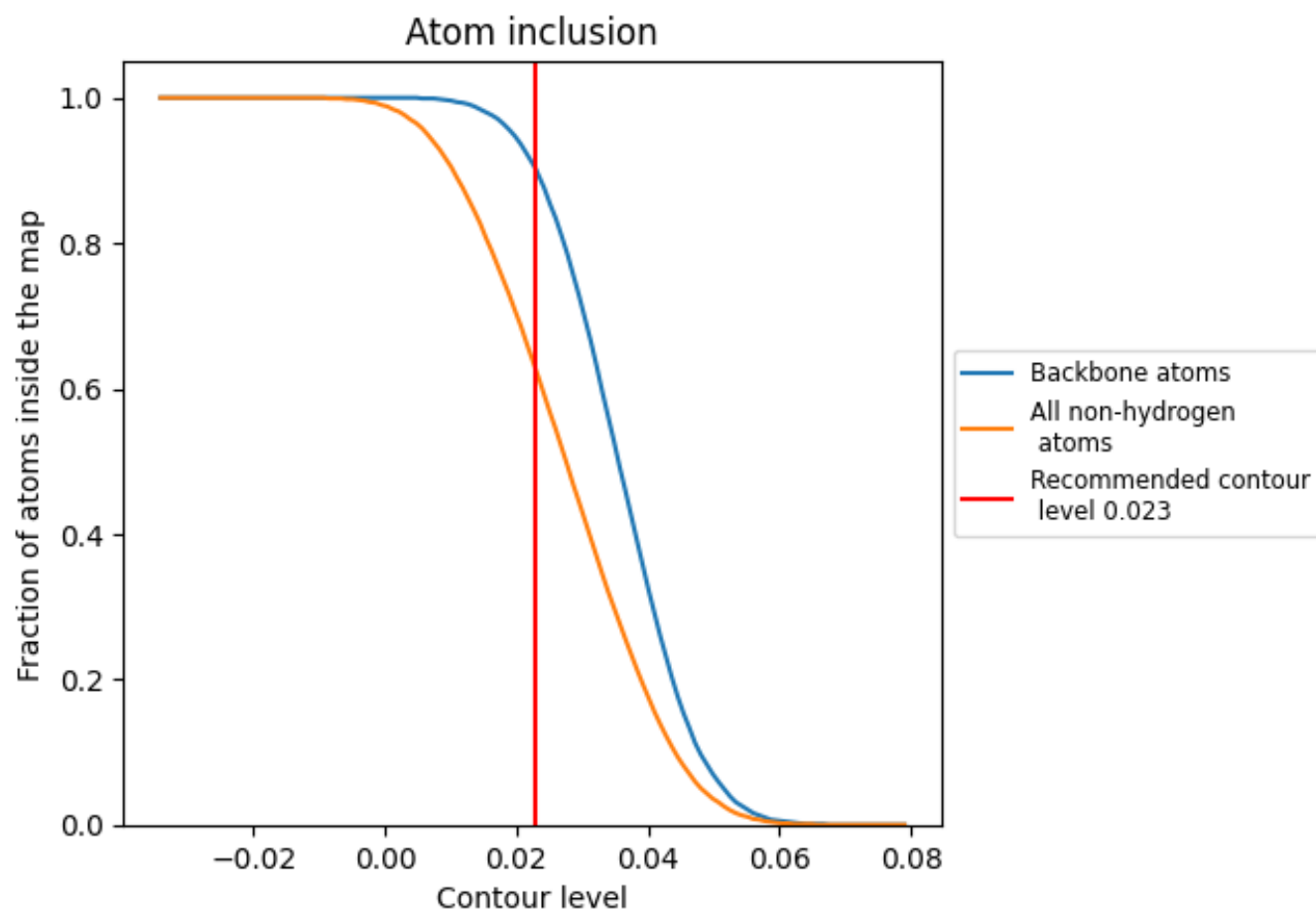
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.023).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 62% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6250	<div></div> 0.2290
A	<div></div> 0.6390	<div></div> 0.2330
B	<div></div> 0.6490	<div></div> 0.2420
C	<div></div> 0.6940	<div></div> 0.2360
D	<div></div> 0.6020	<div></div> 0.2160
E	<div></div> 0.7100	<div></div> 0.2390
F	<div></div> 0.6600	<div></div> 0.2600
G	<div></div> 0.6350	<div></div> 0.2230
H	<div></div> 0.7140	<div></div> 0.2510
I	<div></div> 0.5270	<div></div> 0.2350
J	<div></div> 0.6790	<div></div> 0.2400
K	<div></div> 0.6620	<div></div> 0.2310
L	<div></div> 0.6730	<div></div> 0.2440
M	<div></div> 0.4990	<div></div> 0.1990
N	<div></div> 0.4510	<div></div> 0.1930
O	<div></div> 0.4920	<div></div> 0.1840

