



Full wwPDB EM Validation Report ⓘ

May 25, 2024 – 10:42 AM EDT

PDB ID : 7NAC
EMDB ID : EMD-24269
Title : State E2 nucleolar 60S ribosomal biogenesis intermediate - Composite model
Authors : Cruz, V.E.; Sekulski, K.; Peddada, N.; Erzberger, J.P.
Deposited on : 2021-06-21
Resolution : 3.04 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

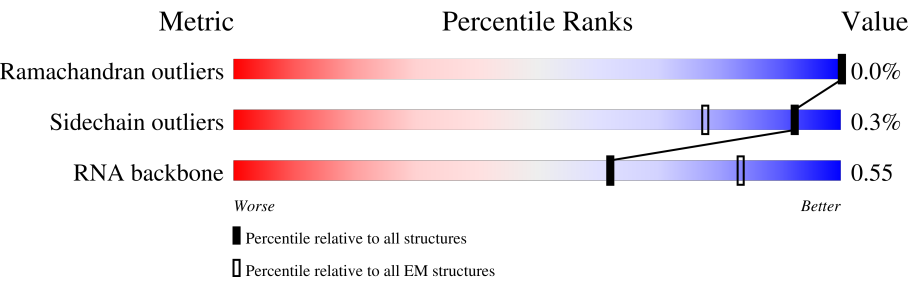
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.04 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	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 $\leq 5\%$. 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	1	3396	
2	2	158	
3	7	204	
4	A	291	
5	B	387	
6	C	362	
7	E	176	
8	F	244	



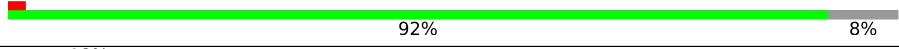
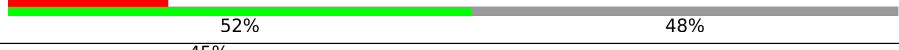


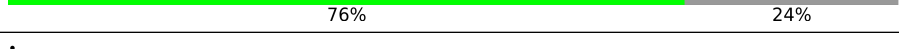
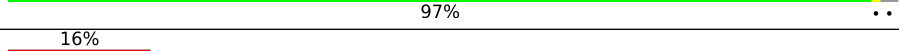
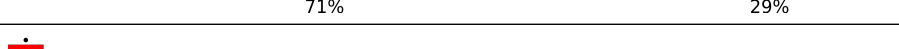
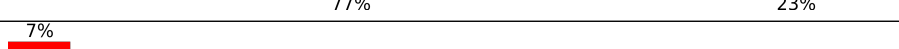
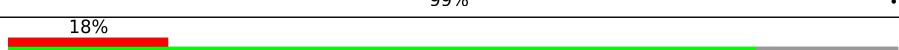

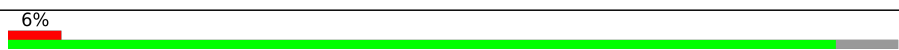
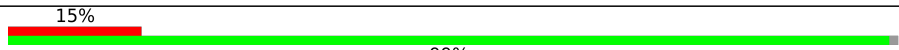
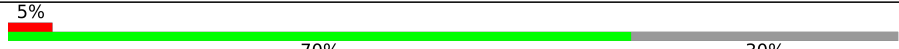






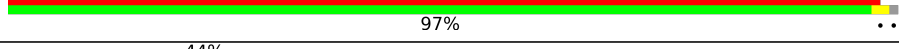



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Mol	Chain	Length	Quality of chain
9	H	191	
10	J	427	
11	L	199	
12	M	138	
13	N	204	
14	O	199	
15	P	184	
16	Q	186	
17	S	172	
18	T	160	
19	W	236	
20	X	142	
21	Y	127	
22	b	647	
23	d	113	
24	e	130	
25	f	107	
26	h	120	
27	i	100	
28	j	88	
29	l	181	
30	m	807	
31	q	618	
32	r	261	
33	s	520	

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Mol	Chain	Length	Quality of chain
34	u	199	
35	v	231	
36	y	245	
37	z	106	
38	8	710	
39	I	663	
40	K	376	
41	V	137	
42	R	189	
43	G	256	
44	Z	136	
45	U	121	
46	c	105	
47	g	121	
48	k	78	
49	n	605	
50	p	460	
51	t	322	
52	6	87	
53	D	505	
54	o	220	
55	w	841	
56	a	217	
57	5	235	
58	x	606	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 158246 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 RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2661	Total	C	N	O	P	0	0
			56944	25427	10267	18590	2660		

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 3 is a protein called 60S ribosomal subunit assembly/export protein LOC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	7	129	Total	C	N	O	0	0
			1048	650	204	194		

- Molecule 4 is a protein called Ribosome biogenesis protein BRX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	266	Total	C	N	O	S	0	0
			2174	1382	386	400	6		

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	335	Total	C	N	O	S	0	0
			2661	1691	492	472	6		

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	359	Total	C	N	O	S	0	0
			2731	1720	518	490	3		

- Molecule 7 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	164	Total	C	N	O	S	0	0
			1309	845	234	229	1		

- Molecule 8 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 9 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	190	Total	C	N	O	S	0	0
			1510	957	273	276	4		

- Molecule 10 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	145	Total	C	N	O	S	0	0
			1215	759	225	228	3		

- Molecule 11 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	121	Total	C	N	O		0	0
			991	623	208	160			

- Molecule 12 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 13 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	189	Total	C	N	O	S	0	0
			1621	1015	343	262	1		

- Molecule 14 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 15 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	183	Total	C	N	O	S	0	0
			1442	896	287	259			

- Molecule 16 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	134	Total	C	N	O	S	0	0
			1035	659	196	179	1		

- Molecule 17 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	170	Total	C	N	O	S	0	0
			1432	922	265	242	3		

- Molecule 18 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	52	Total	C	N	O	S	0	0
			401	244	82	74	1		

- Molecule 19 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	232	Total	C	N	O	S	0	0
			1870	1184	321	360	5		

- Molecule 20 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	137	Total	C	N	O	S	0	0
			1068	682	192	192	2		

- Molecule 21 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Y	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 22 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	b	502	Total	C	N	O	S	0	0
			4066	2581	710	754	21		

- Molecule 23 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	107	Total	C	N	O	S	0	0
			873	553	165	154	1		

- Molecule 24 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	125	Total	C	N	O	S	0	0
			1009	641	203	164	1		

- Molecule 25 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 26 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 27 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	i	79	Total	C	N	O	S	0	0
			628	388	130	108	2		

- Molecule 28 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	j	73	Total	C	N	O	S	0	0
			580	353	126	96	5		

- Molecule 29 is a protein called 60S ribosome subunit biogenesis protein NIP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	l	176	Total	C	N	O	S	0	0
			1394	896	244	247	7		

- Molecule 30 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	m	666	Total	C	N	O	S	0	0
			5377	3421	936	1005	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	551	ALA	GLU	conflict	UNP Q04660

- Molecule 31 is a protein called 25S rRNA (cytosine(2870)-C(5))-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	q	358	Total	C	N	O	S	0	0
			2799	1779	490	518	12		

- Molecule 32 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	r	176	Total	C	N	O	S	0	0
			1438	906	279	248	5		

- Molecule 33 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	s	36	Total	C	N	O	S	0	0
			301	184	69	46	2		

- Molecule 34 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	u	140	Total	C	N	O	S	0	0
			1183	742	237	195	9		

- Molecule 35 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	v	130	Total	C	N	O	S	0	0
			1087	678	211	195	3		

- Molecule 36 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	y	225	Total	C	N	O	S	0	0
			1701	1056	295	343	7		

- Molecule 37 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	z	55	Total	C	N	O	0	0
			444	273	88	83		

- Molecule 38 is a protein called NOC2 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	8	470	Total	C	N	O	S	0	0
			3567	2269	632	655	11		

- Molecule 39 is a protein called Nucleolar complex-associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	I	533	Total	C	N	O	S	0	0
			4247	2693	726	808	20		

- Molecule 40 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	K	284	Total	C	N	O	S	0	0
			2274	1462	375	433	4		

- Molecule 41 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	V	134	Total	C	N	O	S	0	0
			993	623	187	176	7		

- Molecule 42 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	R	134	Total	C	N	O		0	0
			1082	679	220	183			

- Molecule 43 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	G	198	Total	C	N	O	S	0	0
			1549	998	271	277	3		

- Molecule 44 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Z	135	Total	C	N	O		0	0
			1092	710	202	180			

- Molecule 45 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	U	102	Total	C	N	O		0	0
			808	524	132	152			

- Molecule 46 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	c	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 47 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	g	112	Total	C	N	O	S	0	0
			881	546	179	152	4		

- Molecule 48 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	k	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 49 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	n	425	Total	C	N	O	S	0	0
			3470	2241	600	615	14		

- Molecule 50 is a protein called YTM1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	p	337	Total	C	N	O	S	0	0
			2628	1633	470	518	7		

- Molecule 51 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	285	Total	C	N	O	S	0	0
			2293	1453	425	412	3		

- Molecule 52 is a RNA chain called 5.8S ribosomal RNA gene and internal transcribed spacer 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	6	87	Total	C	N	O	P	0	0
			1838	823	309	619	87		

- Molecule 53 is a protein called ATP-dependent RNA helicase HAS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	D	432	Total	C	N	O	S	0	0
			3451	2227	591	621	12		

- Molecule 54 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	o	133	Total	C	N	O	S	0	0
			1107	716	198	189	4		

- Molecule 55 is a protein called 27S pre-rRNA (guanosine(2922)-2'-O)-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	w	672	Total	C	N	O	S	0	0
			5451	3430	980	1013	28		

- Molecule 56 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	a	214	Total	C	N	O	S	0	0
			1695	1083	295	308	9		

- Molecule 57 is a protein called RRP17 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	5	141	Total	C	N	O	S	0	0
			1208	749	226	232	1		

- Molecule 58 is a protein called ATP-dependent rRNA helicase SPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	x	539	Total	C	N	O	S	0	0
			4340	2781	744	795	20		

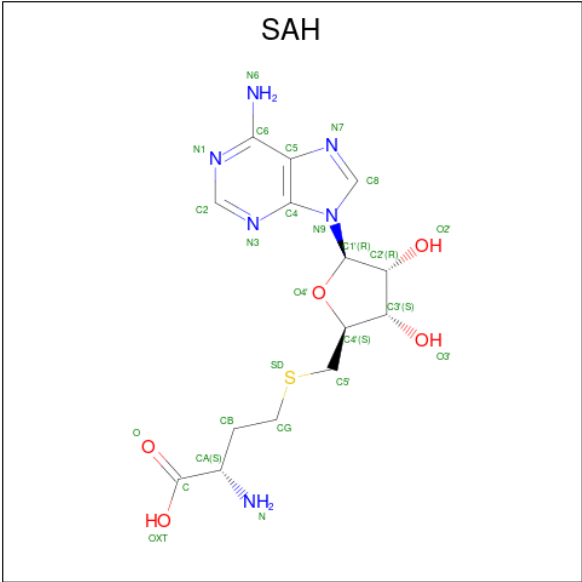
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	405	ALA	THR	conflict	UNP A7A237

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	j	1	Total	Zn	0
			1	1	
59	g	1	Total	Zn	0
			1	1	

- Molecule 60 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S) (labeled as "Ligand of Interest" by depositor).

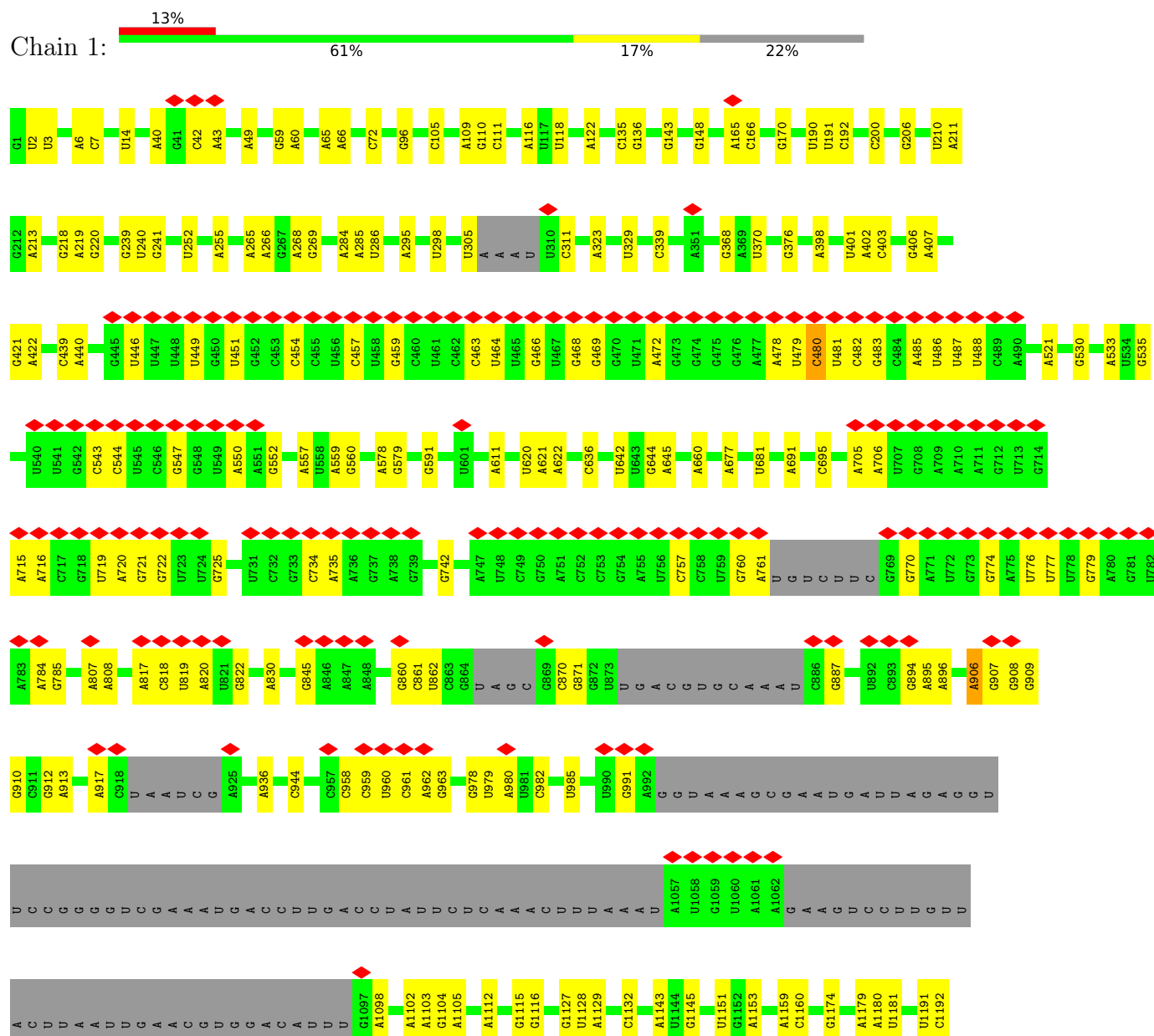


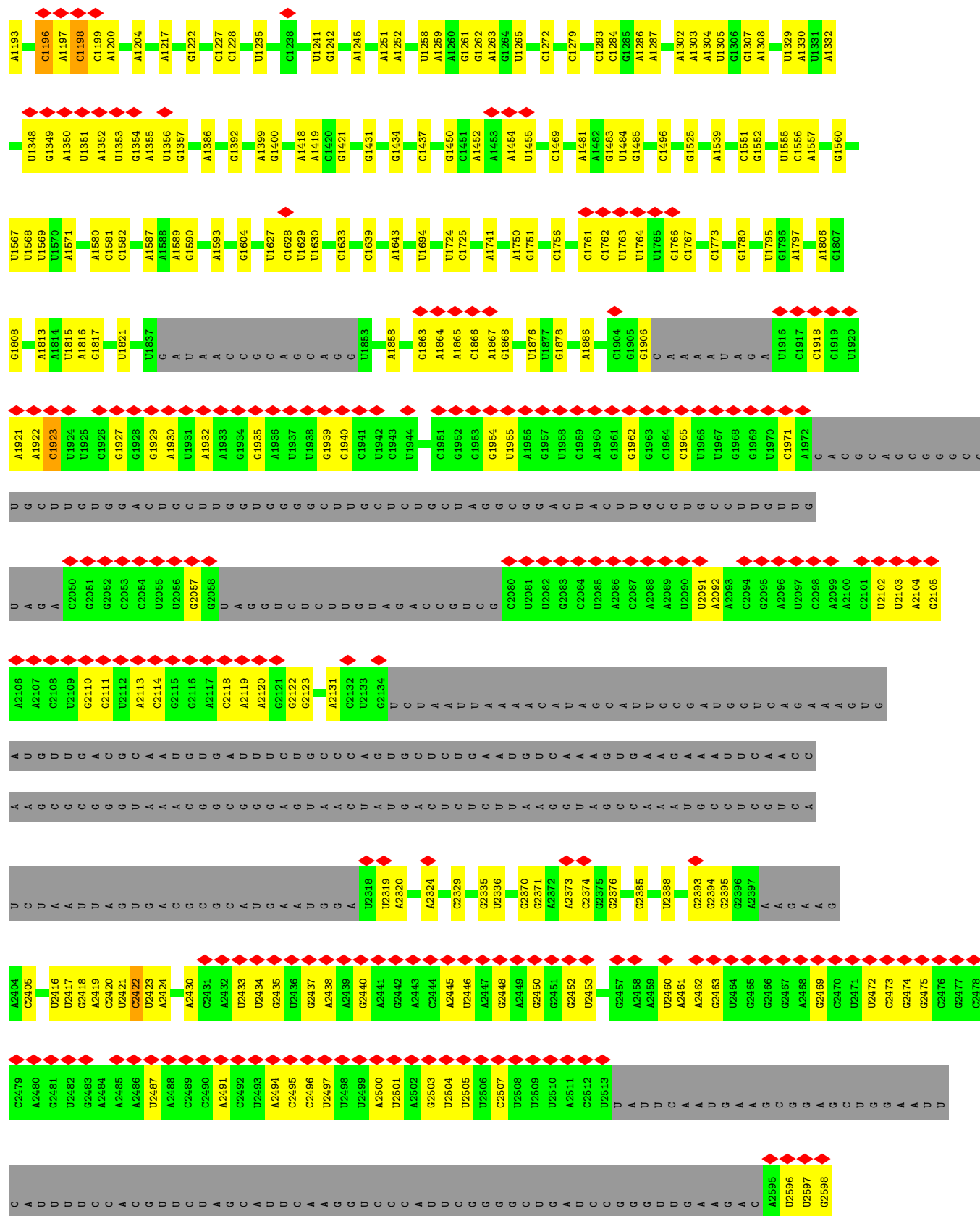
Mol	Chain	Residues	Atoms					AltConf
60	w	1	Total	C	N	O	S	0
			26	14	6	5	1	

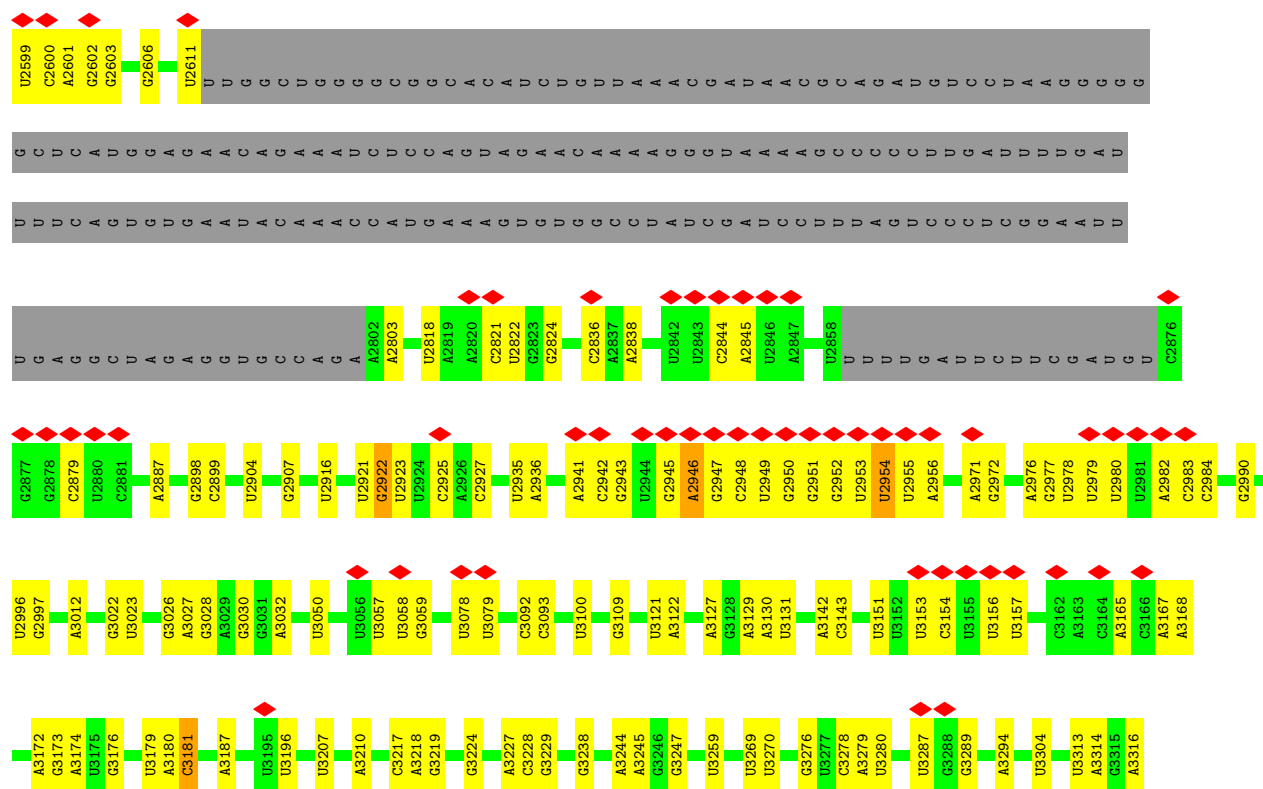
3 Residue-property plots

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.

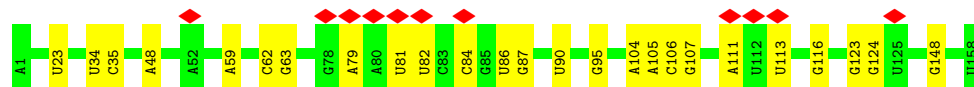
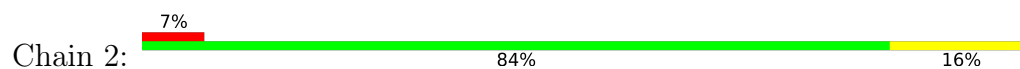
• Molecule 1: 25S rRNA



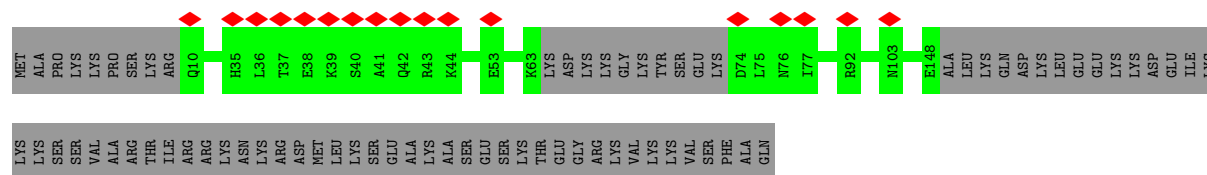




• Molecule 2: 5.8S rRNA

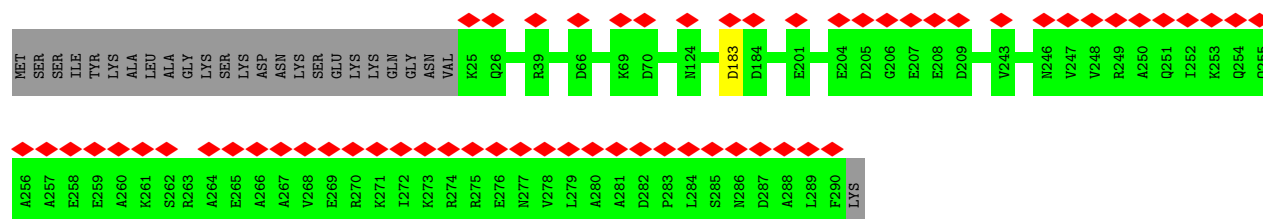


• Molecule 3: 60S ribosomal subunit assembly/export protein LOC1

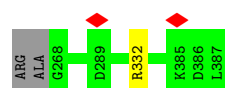
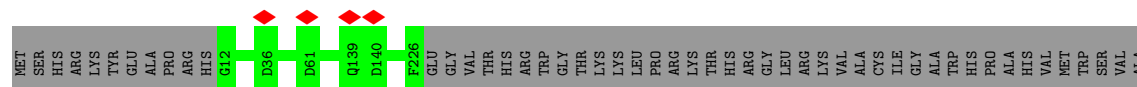
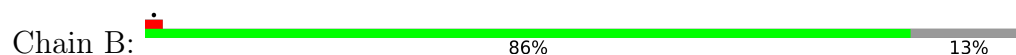


• Molecule 4: Ribosome biogenesis protein BRX1

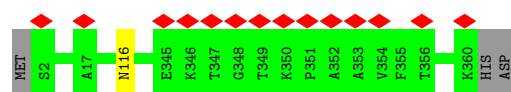




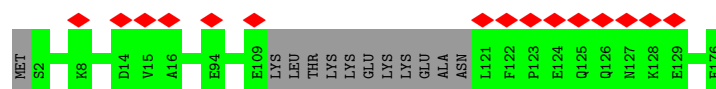
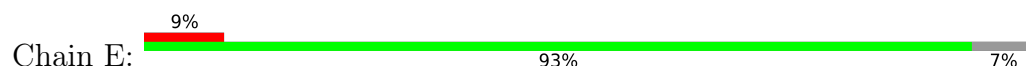
• Molecule 5: 60S ribosomal protein L3



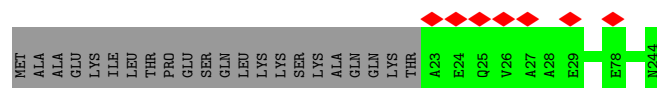
• Molecule 6: 60S ribosomal protein L4-A



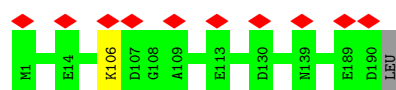
• Molecule 7: 60S ribosomal protein L6-A



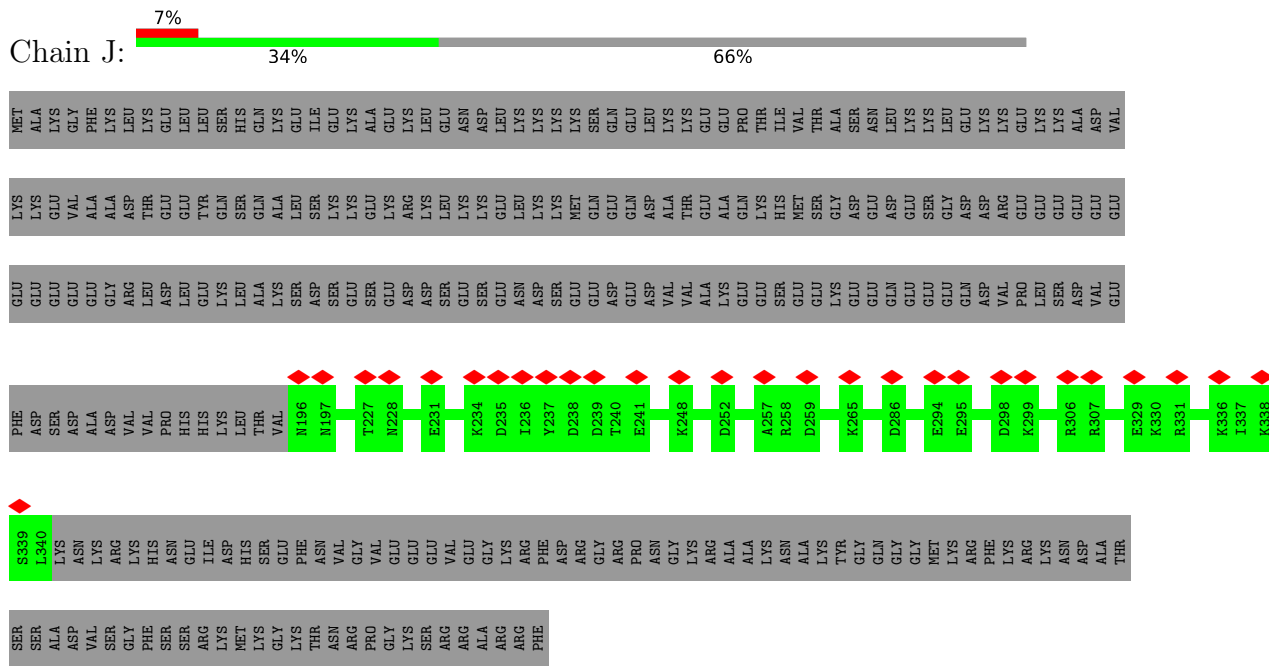
• Molecule 8: 60S ribosomal protein L7-A



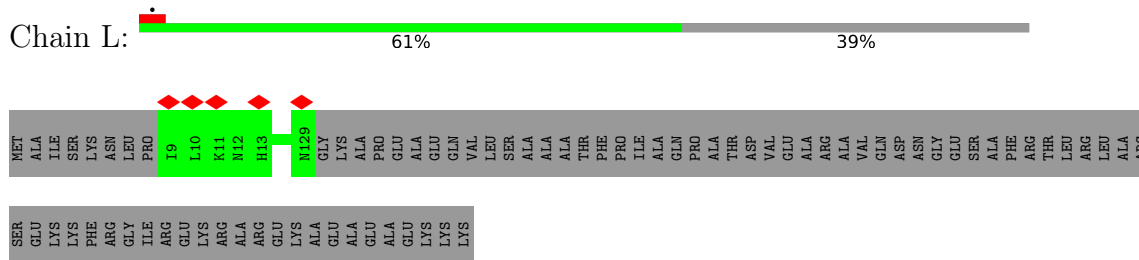
• Molecule 9: 60S ribosomal protein L9-A



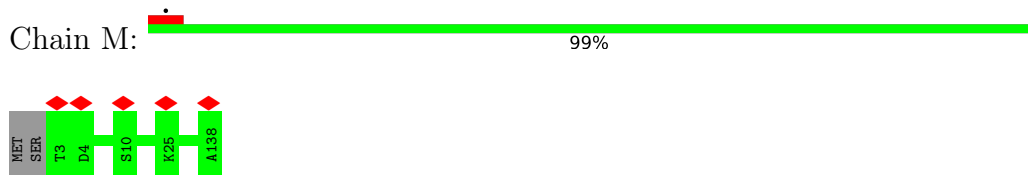
• Molecule 10: rRNA-processing protein EBP2



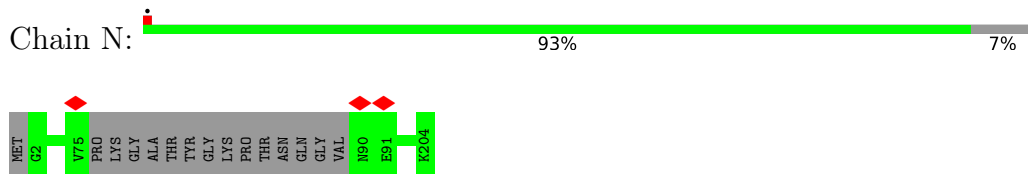
- Molecule 11: 60S ribosomal protein L13-A



- Molecule 12: 60S ribosomal protein L14-A

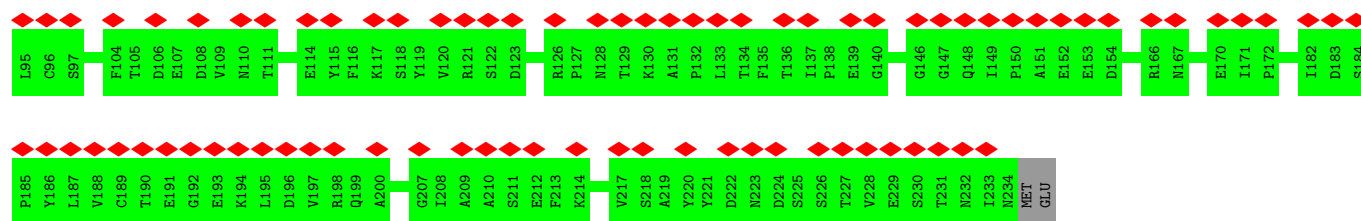


- Molecule 13: 60S ribosomal protein L15-A



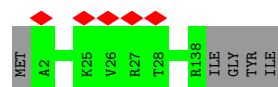
- Molecule 14: 60S ribosomal protein L16-A





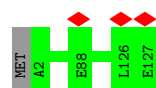
- Molecule 20: 60S ribosomal protein L25

Chain X: 96%



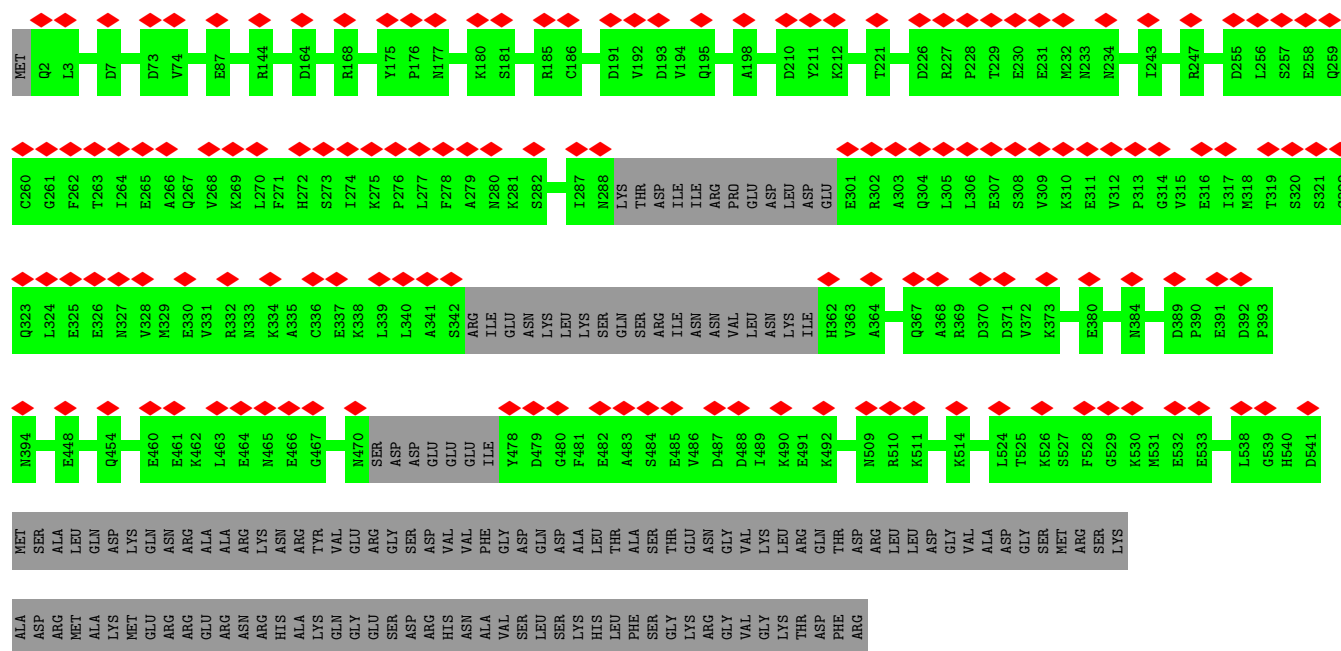
- Molecule 21: 60S ribosomal protein L26-A

Chain Y: 99%



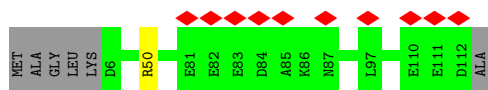
- Molecule 22: Nucleolar GTP-binding protein 1

Chain b: 78%

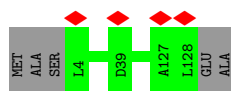


- Molecule 23: 60S ribosomal protein L31-A

Chain d: 94%



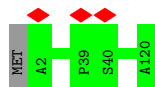
- Molecule 24: 60S ribosomal protein L32



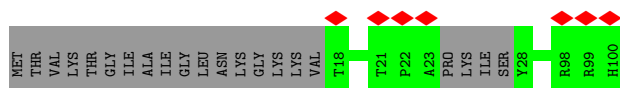
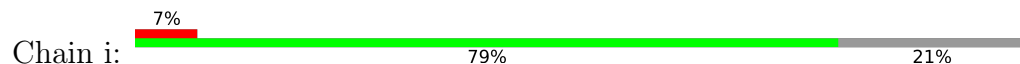
- Molecule 25: 60S ribosomal protein L33-A



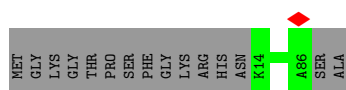
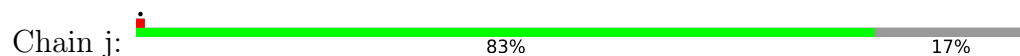
- Molecule 26: 60S ribosomal protein L35-A



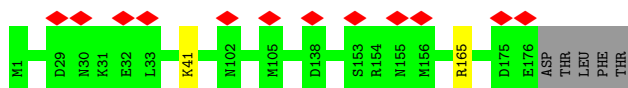
- Molecule 27: 60S ribosomal protein L36-A



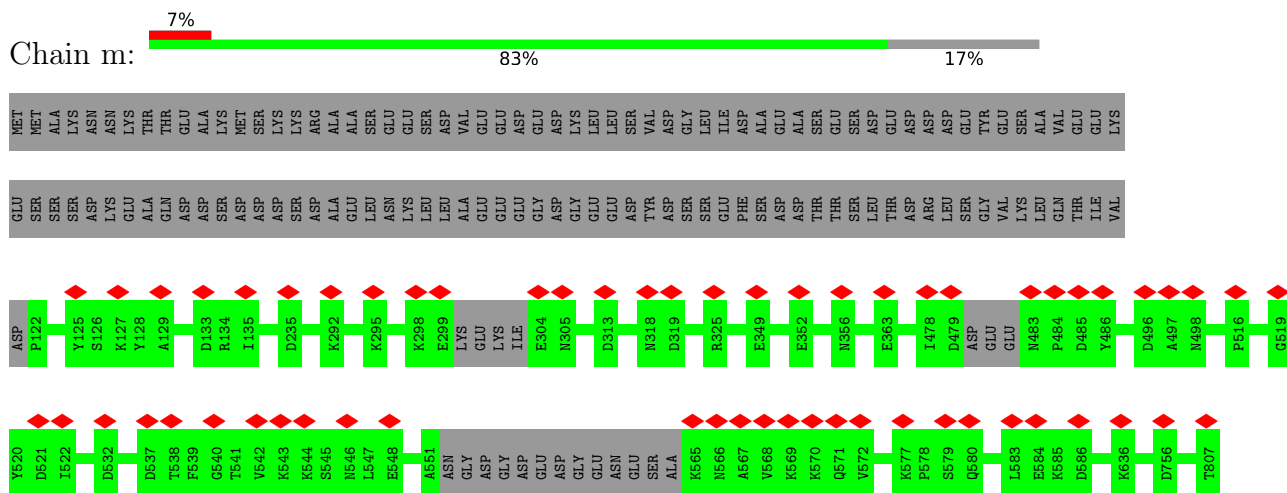
- Molecule 28: 60S ribosomal protein L37-A



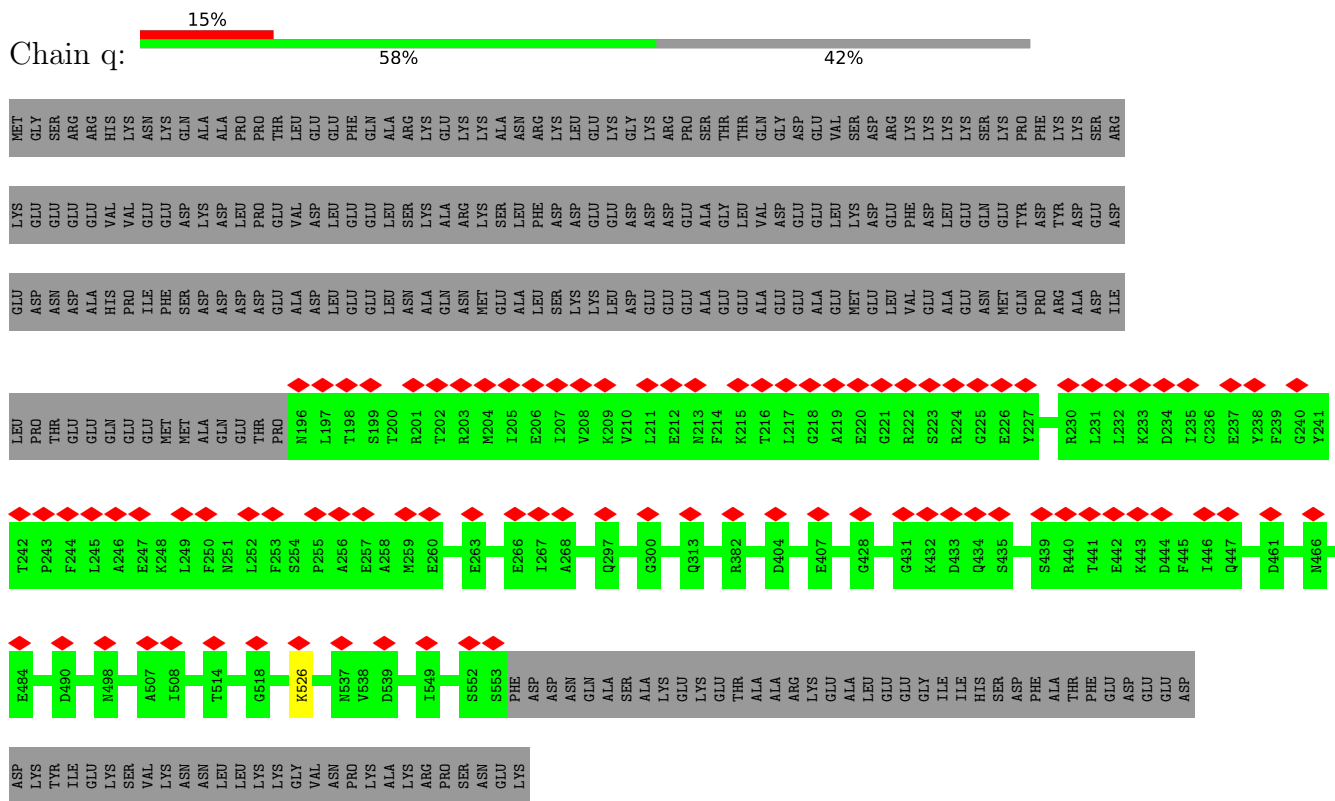
- Molecule 29: 60S ribosome subunit biogenesis protein NIP7



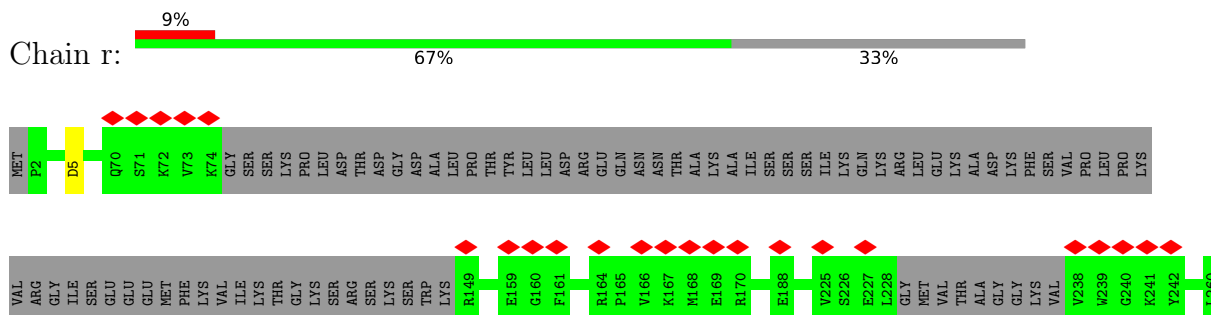
- Molecule 30: Ribosome biogenesis protein ERB1



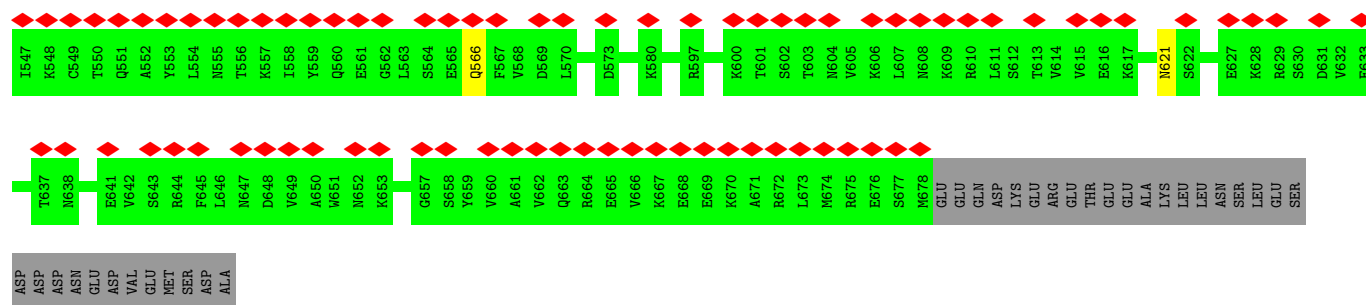
- Molecule 31: 25S rRNA (cytosine(2870)-C(5))-methyltransferase



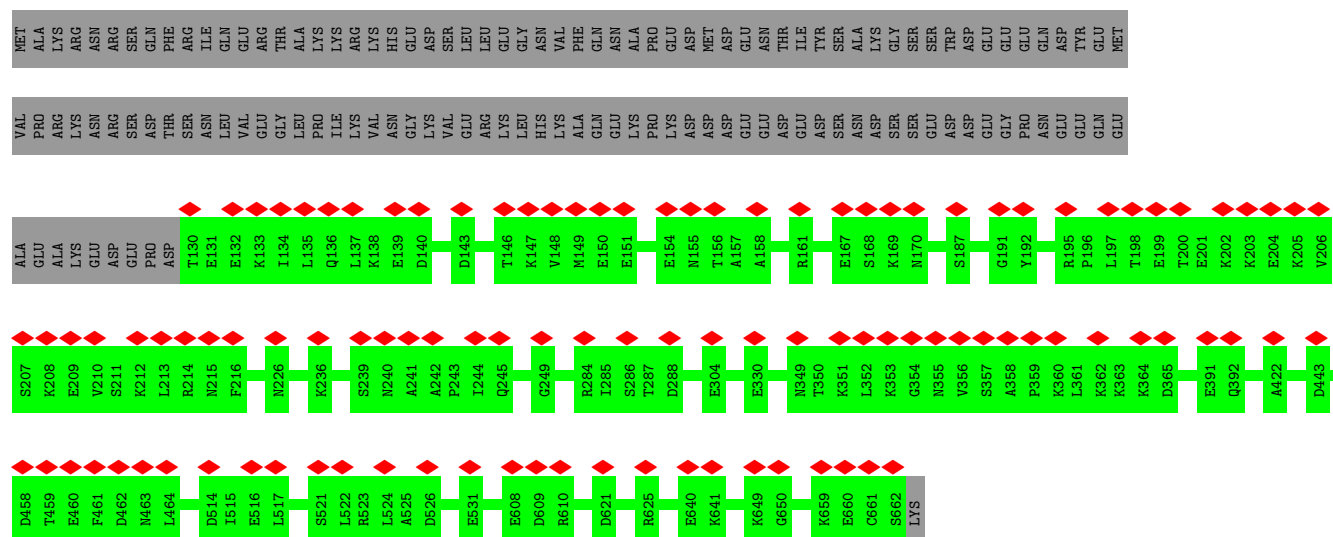
- Molecule 32: Ribosome biogenesis protein NSA2



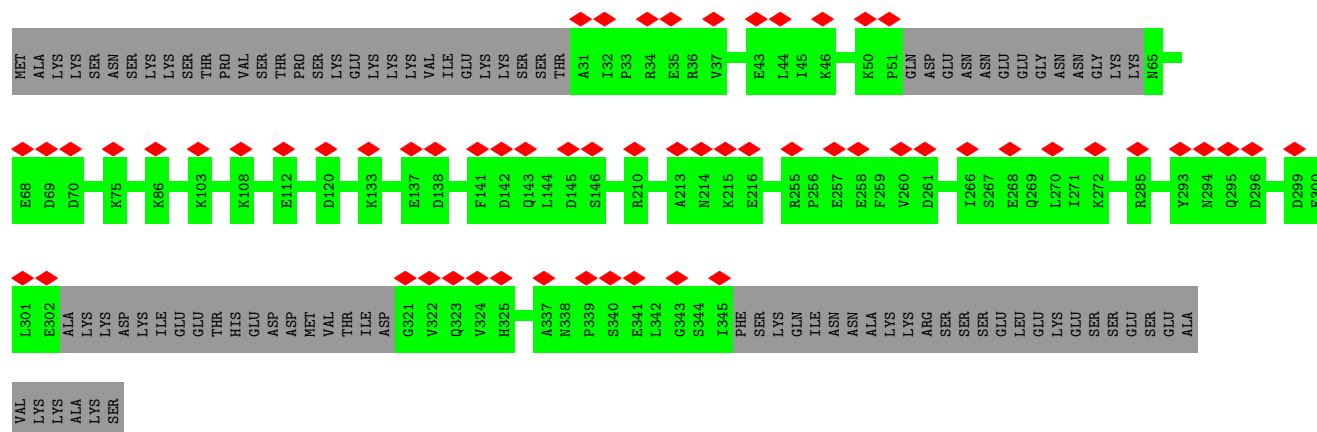
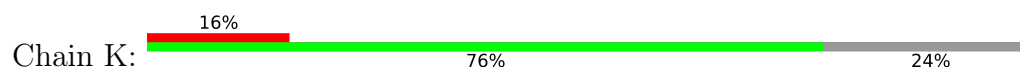
- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|
| R469 | Q470 | L471 | I472 | V476 | I483 | R484 | L485 | I486 | P487 | Q490 | F491 | F492 | R495 | F496 | Y497 | L498 | I499 | K500 | S501 | L502 | L503 | R504 | L505 | S506 | Q507 | N508 | I515 | E521 | I522 | L523 | T524 | S525 | T526 | A527 | F528 | T529 | K530 | A531 | P532 | K533 | LYS | SER | PRO | ASN | LEU | ALA | A540 | F541 | D542 | F543 | E544 | H545 | N546 | H546 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|



• Molecule 39: Nucleolar complex-associated protein 3

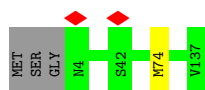


• Molecule 40: Proteasome-interacting protein CIC1

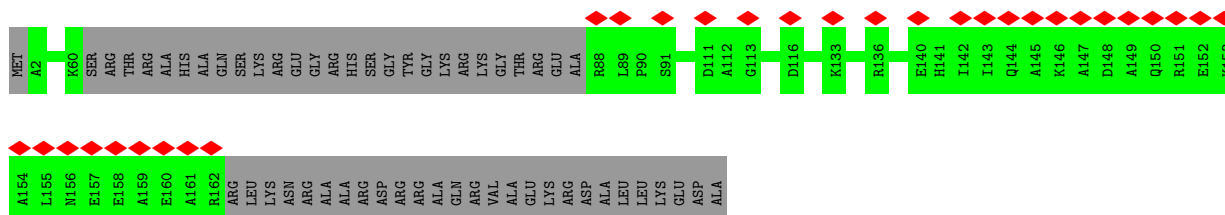


• Molecule 41: 60S ribosomal protein L23-A

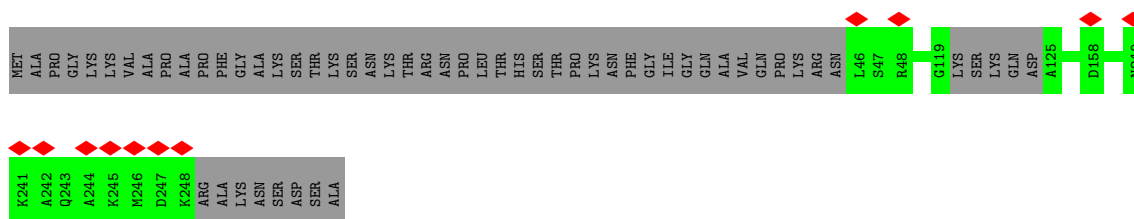
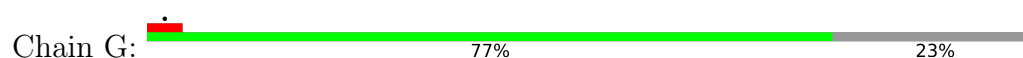




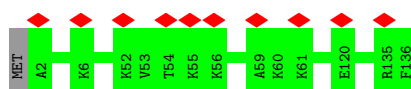
- Molecule 42: 60S ribosomal protein L19-A



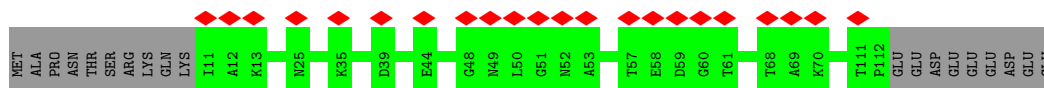
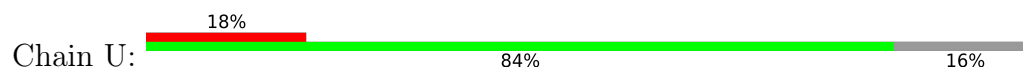
- Molecule 43: 60S ribosomal protein L8-A



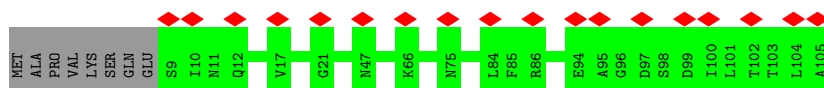
- Molecule 44: 60S ribosomal protein L27-A



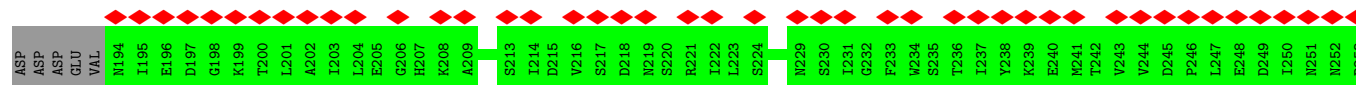
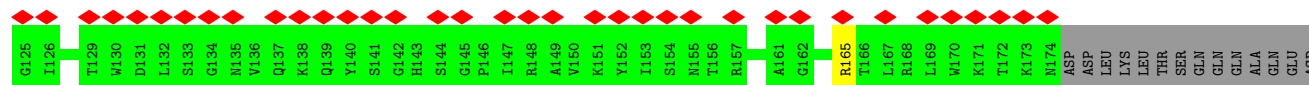
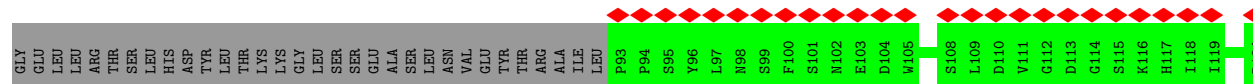
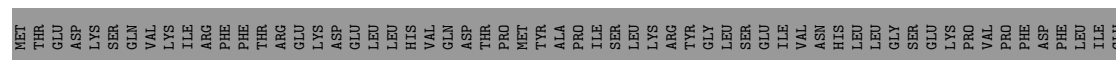
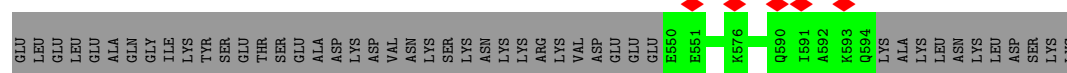
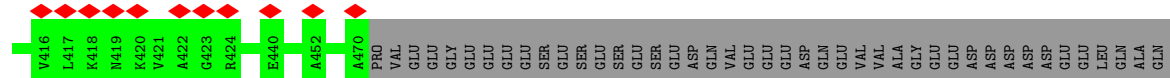
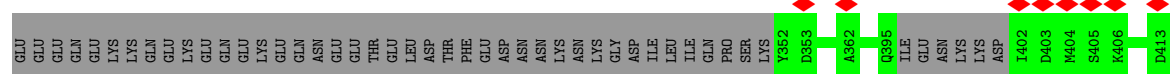
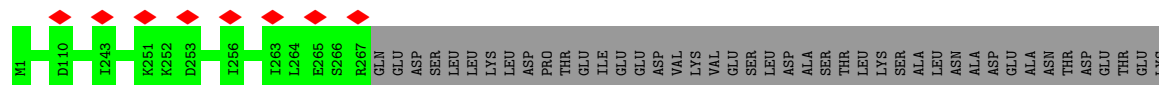
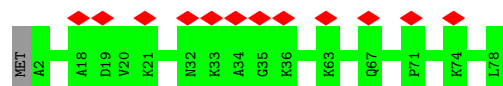
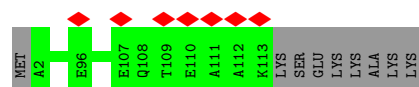
- Molecule 45: 60S ribosomal protein L22-A

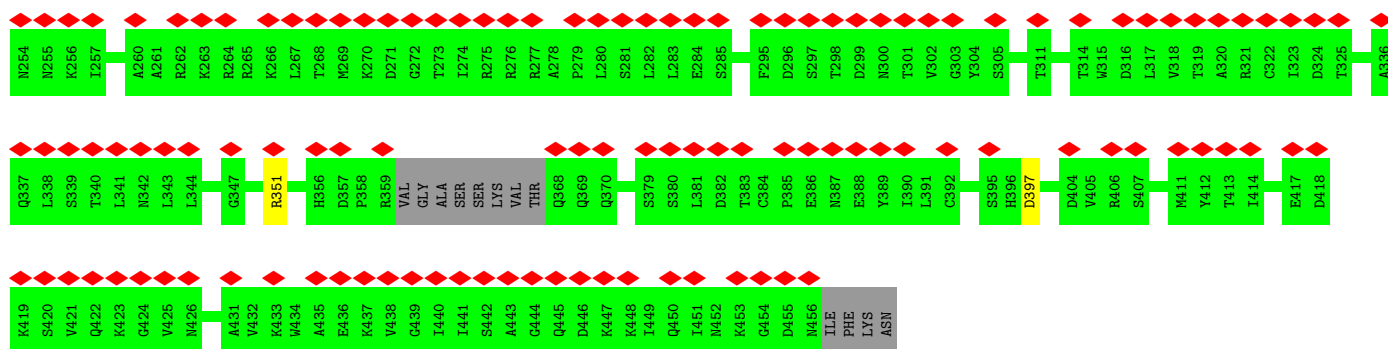


- Molecule 46: 60S ribosomal protein L30

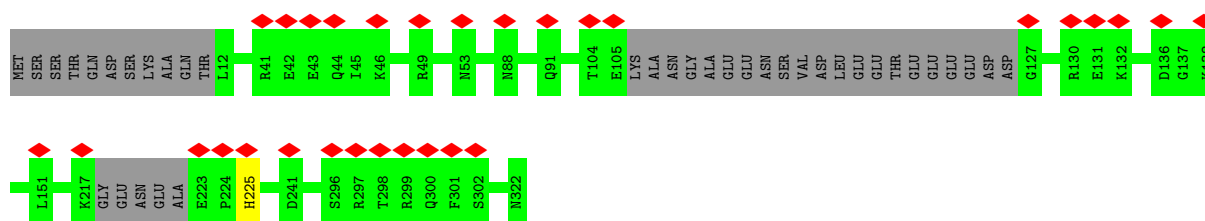
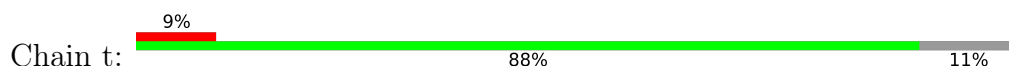


- Molecule 47: 60S ribosomal protein L34-A

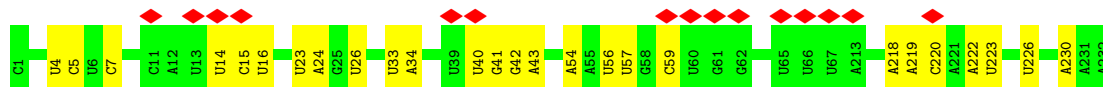




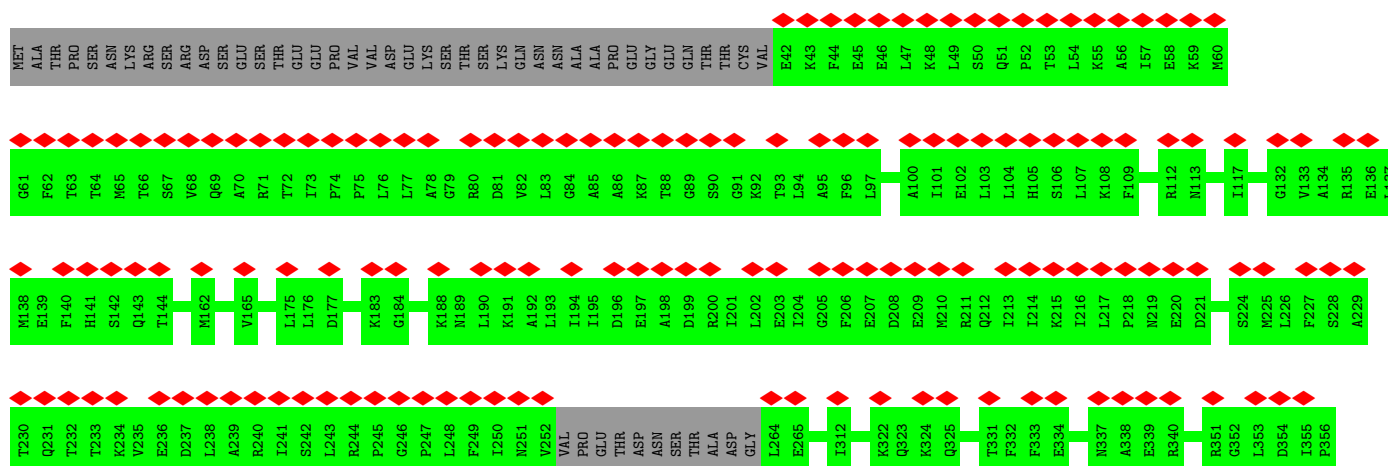
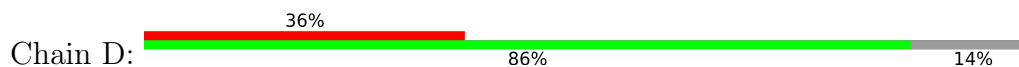
• Molecule 51: Ribosome biogenesis protein RLP7



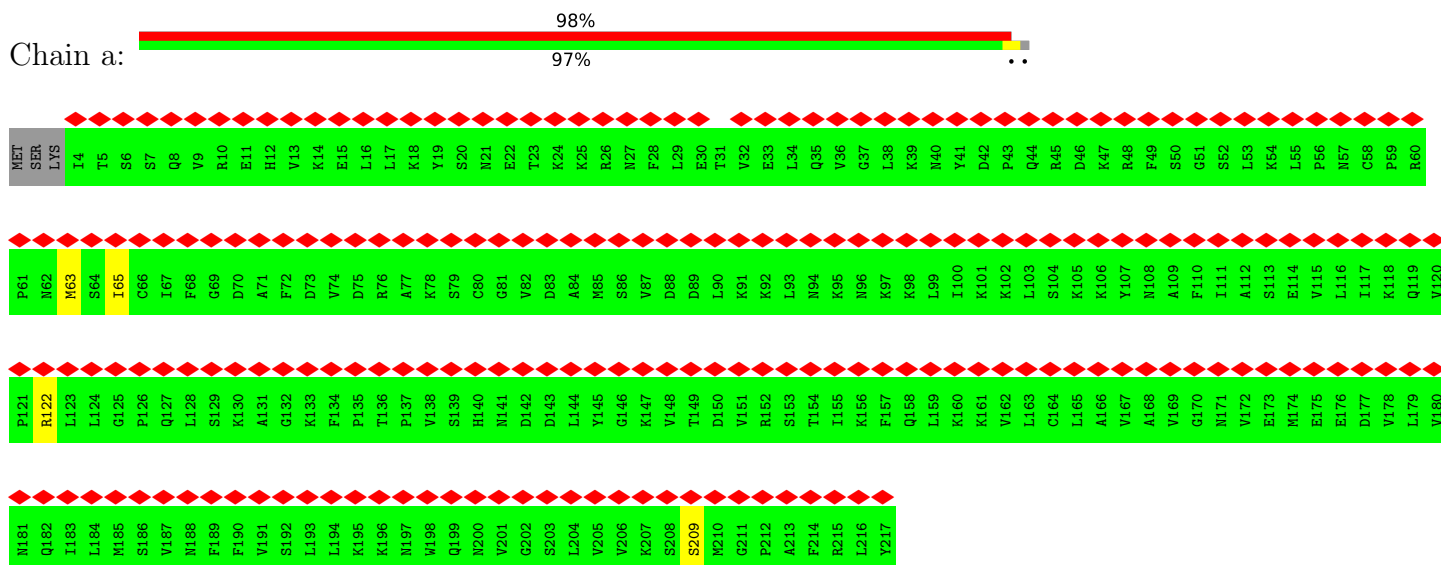
• Molecule 52: 5.8S ribosomal RNA gene and internal transcribed spacer 2



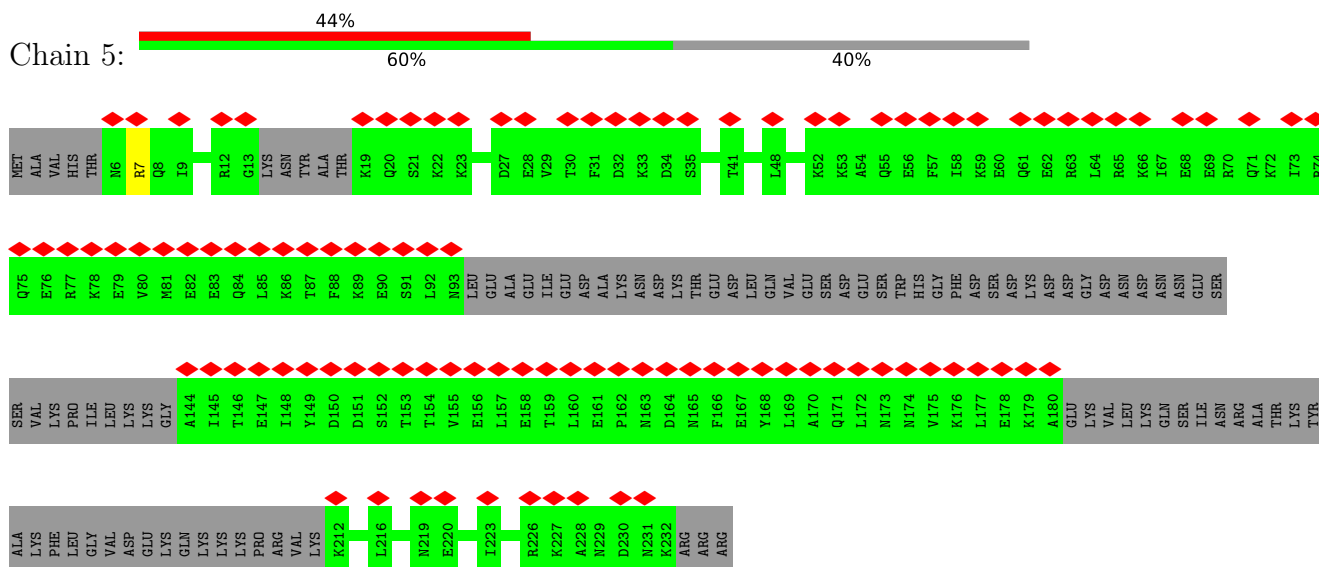
• Molecule 53: ATP-dependent RNA helicase HAS1



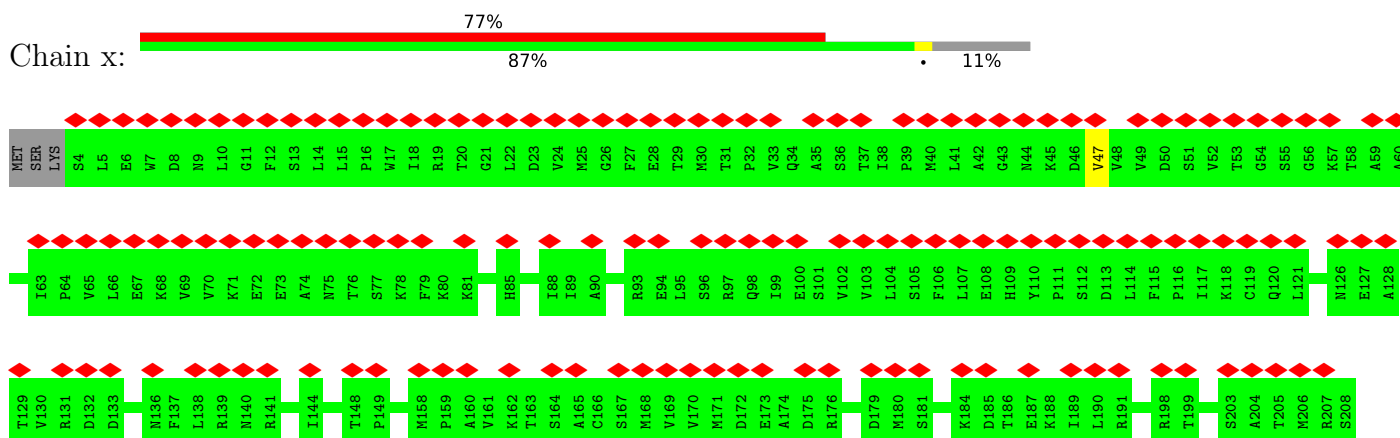
- Molecule 56: Ribosomal protein



- Molecule 57: RRP17 isoform 1



- Molecule 58: ATP-dependent rRNA helicase SPB4



GLU	ASN	ALA	GLU	GLU	GLU	ARG	ILE	LYS	GLU	ASP	TRP	LYS	GLU	ILE	VAL	GLN	ASN	LYS	ARG	LYS	LYS	VAL	SER	SER	LYS	ALA	GLN	ALA	PRO	S234	S235	L236	K237	L238	N239	Y240	C241	V242	V243	N244	P245	A246	E247	K248	L249	Q250	L251	L252	V253	S254	I255	L256	N257	N258	Y259	K260	F261	K262	K263	C264	I265	V266	Y267	F268	F269	T270
A209	G210	S211	D212	I213	E214	L218	R219	N220	P221	V222	R223	I224	T225	V226	N227	S228	LYS	ASN	GLN	ALA	PRO	S234	S235	L236	K237	L238	N239	Y240	C241	V242	V243	N244	P245	A246	E247	K248	L249	Q250	L251	L252	V253	S254	I255	L256	N257	N258	Y259	K260	F261	K262	K263	C264	I265	V266	Y267	F268	F269	T270								
C271	V272	S273	V274	S275	Y276	F277	Y278	S279	F280	I281	Q282	Y283	L284	G285	K286	R287	N288	I289	L290	V291	N292	E293	V294	E295	I296	F297	S298	L299	H300	G301	K302	L303	Q304	T305	S306	A307	R308	T309	K310	T311	L312	T313	A314	F315	T316	D317	SER	LEU	S320	N321	S322	V323	L324	F325	T326	T327	D328	V329	A330							
A331	R332	G333	I334	D335	I336	P337	D338	V339	D340	L341	V342	I343	Q344	L345	D346	P347	P348	T349	N350	T351	D352	M353	F354	M355	H356	R357	C358	G359	R360	T361	G362	R363	A364	N365	R366	V367	G368	K369	A370	I371	T372	F373	L374	N375	E376	G377	R378	E379	E380	D381	F382	I383	P384	F385	M386	Q387	V388	K389	N390							
V391	E392	L393	E394	E395	L396	D397	L398	E399	V400	K401	G402	I403	T404	A405	N406	F407	Y408	E409	D410	F411	R412	N413	W414	I415	L416	E417	D418	R419	D420	R421	F422	D423	K424	G425	V426	K427	A428	Y429	V430	A431	F432	I433	K434	Y435	Y436	S437	N438	H439	S440	A441	T442	S443	I444	F445	R446	L447	Q448	S449	L450							
D451	Y452	V453	G454	I455	A456	K457	L458	Y459	G460	L461	F462	R463	L464	P465	R466	P467	P468	E469	I470	T471	K472	Y473	L474	ALA	THR	GLU	LYS	GLN	GLU	GLY	ILE	PHE	PRO	GLY	M486	W487	L488	V489	D490	P491	P492	V493	W494	M495	D496	E497	Y498	K499	Y500	K501	D502	K503	K504	R505	E506	K507	E508	R509	Q510							
E511	T512	L513	K514	N515	I516	S517	L518	I519	N520	D521	K522	K523	K524	L525	K526	S527	E528	L529	K530	K531	K532	N533	L534	A535	W536	S537	D538	K539	T540	L541	T542	K543	E544	R545	K546	L547	E548	R549	K550	E551	K552	M553	S554	L555	K556	R557	K558	A559	I560	GLU	GLU	GLU	LYS	ALA	GLU	GLU	LEU	ASP								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	198000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.2	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.216	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0275	Depositor
Map size (\AA)	453.6, 453.6, 453.6	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A2M, OMG, OMU, ZN, SAH, PSU

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	1	0.36	0/63625	0.79	11/99173 (0.0%)
2	2	0.39	0/3746	0.76	0/5832
3	7	0.26	0/1056	0.52	0/1408
4	A	0.27	0/2222	0.51	1/2998 (0.0%)
5	B	0.31	0/2715	0.55	0/3647
6	C	0.29	0/2782	0.52	0/3766
7	E	0.28	0/1332	0.50	0/1791
8	F	0.28	0/1821	0.50	0/2451
9	H	0.28	0/1531	0.50	0/2062
10	J	0.24	0/1232	0.47	0/1642
11	L	0.30	0/1009	0.58	0/1355
12	M	0.28	0/1068	0.50	0/1438
13	N	0.30	0/1654	0.58	0/2212
14	O	0.29	0/1585	0.50	0/2128
15	P	0.27	0/1465	0.54	0/1968
16	Q	0.26	0/1050	0.52	0/1419
17	S	0.29	0/1468	0.53	0/1973
18	T	0.24	0/404	0.52	0/542
19	W	0.26	0/1902	0.52	0/2564
20	X	0.28	0/1083	0.50	0/1458
21	Y	0.31	0/1004	0.58	0/1341
22	b	0.26	0/4141	0.49	0/5575
23	d	0.27	0/887	0.54	0/1191
24	e	0.27	0/1030	0.52	0/1379
25	f	0.31	0/868	0.54	0/1168
26	h	0.28	0/978	0.50	0/1301
27	i	0.27	0/633	0.56	0/839
28	j	0.30	0/592	0.58	0/785
29	l	0.27	0/1425	0.52	0/1922
30	m	0.27	0/5511	0.50	0/7471
31	q	0.27	0/2854	0.52	0/3860
32	r	0.26	0/1462	0.53	1/1952 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	s	0.26	0/301	0.56	0/386
34	u	0.27	0/1205	0.53	0/1603
35	v	0.27	0/1100	0.51	0/1456
36	y	0.27	0/1722	0.54	0/2343
37	z	0.25	0/445	0.46	0/585
38	8	0.25	0/3624	0.46	1/4891 (0.0%)
39	I	0.25	0/4310	0.47	0/5807
40	K	0.26	0/2310	0.46	0/3118
41	V	0.28	0/1008	0.53	0/1356
42	R	0.25	0/1095	0.51	0/1465
43	G	0.29	0/1575	0.47	0/2125
44	Z	0.28	0/1118	0.46	0/1497
45	U	0.27	0/825	0.47	0/1120
46	c	0.26	0/751	0.46	0/1008
47	g	0.27	0/891	0.55	0/1191
48	k	0.28	0/618	0.52	0/826
49	n	0.28	0/3544	0.47	0/4766
50	p	0.25	0/2674	0.53	0/3623
51	t	0.25	0/2319	0.51	0/3108
52	6	0.28	0/2050	0.78	1/3186 (0.0%)
53	D	0.26	0/3516	0.48	0/4741
54	o	0.27	0/1129	0.49	0/1502
55	w	0.26	0/5531	0.49	0/7389
56	a	0.25	0/1722	0.51	0/2313
57	5	0.24	0/1217	0.48	0/1613
58	x	0.26	0/4419	0.49	0/5958
All	All	0.31	0/167154	0.65	15/239587 (0.0%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	906	A	C2'-C3'-O3'	6.74	124.49	113.70
38	8	306	PRO	N-CA-CB	5.69	110.13	103.30
1	1	1196	C	N1-C2-O2	5.65	122.29	118.90
52	6	226	U	C2-N1-C1'	5.58	124.39	117.70
1	1	1198	C	C2-N1-C1'	5.45	124.79	118.80
1	1	1196	C	C2-N1-C1'	5.29	124.62	118.80
1	1	3181	C	N1-C2-O2	5.27	122.06	118.90
4	A	183	ASP	CB-CG-OD1	5.17	122.95	118.30
1	1	2422	C	C2-N1-C1'	5.13	124.44	118.80
1	1	1923	C	C2-N1-C1'	5.12	124.43	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	r	5	ASP	CB-CG-OD1	5.09	122.89	118.30
1	1	480	C	P-O3'-C3'	5.09	125.81	119.70
1	1	3317	U	C2-N1-C1'	5.08	123.79	117.70
1	1	2954	U	P-O3'-C3'	5.04	125.74	119.70
1	1	3181	C	C2-N1-C1'	5.03	124.34	118.80

There are no chirality outliers.

There are no planarity outliers.

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	
3	7	125/204 (61%)	117 (94%)	8 (6%)	0	100	100
4	A	264/291 (91%)	245 (93%)	19 (7%)	0	100	100
5	B	331/387 (86%)	315 (95%)	16 (5%)	0	100	100
6	C	357/362 (99%)	347 (97%)	10 (3%)	0	100	100
7	E	160/176 (91%)	150 (94%)	10 (6%)	0	100	100
8	F	220/244 (90%)	213 (97%)	7 (3%)	0	100	100
9	H	188/191 (98%)	179 (95%)	9 (5%)	0	100	100
10	J	143/427 (34%)	136 (95%)	7 (5%)	0	100	100
11	L	119/199 (60%)	113 (95%)	6 (5%)	0	100	100
12	M	134/138 (97%)	128 (96%)	6 (4%)	0	100	100
13	N	185/204 (91%)	181 (98%)	4 (2%)	0	100	100
14	O	195/199 (98%)	193 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	P	181/184 (98%)	173 (96%)	8 (4%)	0	100	100
16	Q	132/186 (71%)	130 (98%)	2 (2%)	0	100	100
17	S	168/172 (98%)	162 (96%)	6 (4%)	0	100	100
18	T	50/160 (31%)	45 (90%)	5 (10%)	0	100	100
19	W	230/236 (98%)	217 (94%)	13 (6%)	0	100	100
20	X	135/142 (95%)	127 (94%)	8 (6%)	0	100	100
21	Y	124/127 (98%)	122 (98%)	2 (2%)	0	100	100
22	b	494/647 (76%)	473 (96%)	21 (4%)	0	100	100
23	d	105/113 (93%)	102 (97%)	3 (3%)	0	100	100
24	e	123/130 (95%)	119 (97%)	4 (3%)	0	100	100
25	f	104/107 (97%)	103 (99%)	1 (1%)	0	100	100
26	h	117/120 (98%)	114 (97%)	3 (3%)	0	100	100
27	i	75/100 (75%)	69 (92%)	6 (8%)	0	100	100
28	j	71/88 (81%)	69 (97%)	2 (3%)	0	100	100
29	l	174/181 (96%)	164 (94%)	9 (5%)	1 (1%)	25	60
30	m	658/807 (82%)	629 (96%)	29 (4%)	0	100	100
31	q	356/618 (58%)	330 (93%)	26 (7%)	0	100	100
32	r	170/261 (65%)	165 (97%)	5 (3%)	0	100	100
33	s	34/520 (6%)	34 (100%)	0	0	100	100
34	u	138/199 (69%)	137 (99%)	1 (1%)	0	100	100
35	v	124/231 (54%)	119 (96%)	5 (4%)	0	100	100
36	y	223/245 (91%)	213 (96%)	10 (4%)	0	100	100
37	z	53/106 (50%)	53 (100%)	0	0	100	100
38	8	456/710 (64%)	435 (95%)	21 (5%)	0	100	100
39	I	531/663 (80%)	511 (96%)	20 (4%)	0	100	100
40	K	278/376 (74%)	267 (96%)	11 (4%)	0	100	100
41	V	132/137 (96%)	128 (97%)	4 (3%)	0	100	100
42	R	130/189 (69%)	128 (98%)	2 (2%)	0	100	100
43	G	194/256 (76%)	190 (98%)	4 (2%)	0	100	100
44	Z	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
45	U	100/121 (83%)	94 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	c	95/105 (90%)	95 (100%)	0	0	100	100
47	g	110/121 (91%)	109 (99%)	1 (1%)	0	100	100
48	k	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
49	n	417/605 (69%)	401 (96%)	16 (4%)	0	100	100
50	p	331/460 (72%)	303 (92%)	28 (8%)	0	100	100
51	t	279/322 (87%)	271 (97%)	8 (3%)	0	100	100
53	D	426/505 (84%)	413 (97%)	13 (3%)	0	100	100
54	o	131/220 (60%)	128 (98%)	3 (2%)	0	100	100
55	w	656/841 (78%)	614 (94%)	42 (6%)	0	100	100
56	a	212/217 (98%)	192 (91%)	17 (8%)	3 (1%)	11	40
57	5	133/235 (57%)	126 (95%)	7 (5%)	0	100	100
58	x	531/606 (88%)	508 (96%)	22 (4%)	1 (0%)	47	80
All	All	11810/15605 (76%)	11302 (96%)	503 (4%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
56	a	63	MET
58	x	406	ASN
56	a	209	SER
56	a	65	ILE
29	l	41	LYS

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	
3	7	114/181 (63%)	114 (100%)	0	100	100
4	A	242/263 (92%)	242 (100%)	0	100	100
5	B	281/323 (87%)	280 (100%)	1 (0%)	91	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	C	286/289 (99%)	285 (100%)	1 (0%)	92	97
7	E	142/153 (93%)	142 (100%)	0	100	100
8	F	186/205 (91%)	186 (100%)	0	100	100
9	H	170/171 (99%)	169 (99%)	1 (1%)	86	94
10	J	133/383 (35%)	133 (100%)	0	100	100
11	L	100/159 (63%)	100 (100%)	0	100	100
12	M	107/109 (98%)	107 (100%)	0	100	100
13	N	165/176 (94%)	165 (100%)	0	100	100
14	O	160/162 (99%)	159 (99%)	1 (1%)	86	94
15	P	145/146 (99%)	144 (99%)	1 (1%)	84	93
16	Q	110/151 (73%)	110 (100%)	0	100	100
17	S	155/156 (99%)	151 (97%)	4 (3%)	46	76
18	T	41/137 (30%)	41 (100%)	0	100	100
19	W	209/213 (98%)	209 (100%)	0	100	100
20	X	114/118 (97%)	114 (100%)	0	100	100
21	Y	109/110 (99%)	109 (100%)	0	100	100
22	b	447/573 (78%)	447 (100%)	0	100	100
23	d	94/97 (97%)	93 (99%)	1 (1%)	73	90
24	e	108/111 (97%)	108 (100%)	0	100	100
25	f	90/91 (99%)	90 (100%)	0	100	100
26	h	104/105 (99%)	104 (100%)	0	100	100
27	i	65/82 (79%)	65 (100%)	0	100	100
28	j	60/71 (84%)	60 (100%)	0	100	100
29	l	151/156 (97%)	150 (99%)	1 (1%)	84	93
30	m	599/722 (83%)	599 (100%)	0	100	100
31	q	304/535 (57%)	303 (100%)	1 (0%)	92	97
32	r	156/229 (68%)	156 (100%)	0	100	100
33	s	32/445 (7%)	32 (100%)	0	100	100
34	u	125/180 (69%)	125 (100%)	0	100	100
35	v	116/205 (57%)	116 (100%)	0	100	100
36	y	193/211 (92%)	193 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	z	48/95 (50%)	48 (100%)	0	100	100
38	8	351/647 (54%)	348 (99%)	3 (1%)	78	91
39	I	484/602 (80%)	484 (100%)	0	100	100
40	K	261/346 (75%)	261 (100%)	0	100	100
41	V	103/105 (98%)	102 (99%)	1 (1%)	76	91
42	R	112/154 (73%)	112 (100%)	0	100	100
43	G	161/208 (77%)	161 (100%)	0	100	100
44	Z	115/116 (99%)	115 (100%)	0	100	100
45	U	89/107 (83%)	89 (100%)	0	100	100
46	c	81/88 (92%)	81 (100%)	0	100	100
47	g	95/103 (92%)	95 (100%)	0	100	100
48	k	68/69 (99%)	68 (100%)	0	100	100
49	n	381/548 (70%)	381 (100%)	0	100	100
50	p	300/413 (73%)	297 (99%)	3 (1%)	76	91
51	t	256/287 (89%)	255 (100%)	1 (0%)	91	96
53	D	378/440 (86%)	378 (100%)	0	100	100
54	o	118/199 (59%)	118 (100%)	0	100	100
55	w	592/745 (80%)	591 (100%)	1 (0%)	93	98
56	a	195/198 (98%)	194 (100%)	1 (0%)	88	95
57	5	133/217 (61%)	132 (99%)	1 (1%)	81	92
58	x	489/548 (89%)	480 (98%)	9 (2%)	59	83
All	All	10423/13653 (76%)	10391 (100%)	32 (0%)	92	97

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	332	ARG
6	C	116	ASN
9	H	106	LYS
14	O	101	ARG
15	P	30	ARG
17	S	8	GLN
17	S	26	ARG
17	S	119	ARG
17	S	122	HIS

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Mol	Chain	Res	Type
23	d	50	ARG
29	l	165	ARG
31	q	526	LYS
38	8	450	ARG
38	8	566	GLN
38	8	621	ASN
41	V	74	MET
50	p	165	ARG
50	p	351	ARG
50	p	397	ASP
51	t	225	HIS
55	w	7	LYS
56	a	122	ARG
57	5	7	ARG
58	x	47	VAL
58	x	292	ASN
58	x	349	THR
58	x	403	ILE
58	x	411	PHE
58	x	435	TYR
58	x	498	TYR
58	x	500	TYR
58	x	538	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	255	GLN
5	B	198	HIS
17	S	142	GLN
18	T	146	ASN
31	q	402	ASN
40	K	295	GLN
42	R	134	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2643/3396 (77%)	554 (20%)	38 (1%)
2	2	157/158 (99%)	24 (15%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	6	85/87 (97%)	24 (28%)	4 (4%)
All	All	2885/3641 (79%)	602 (20%)	43 (1%)

All (602) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	U
1	1	3	U
1	1	6	A
1	1	7	C
1	1	14	U
1	1	40	A
1	1	42	C
1	1	43	A
1	1	49	A
1	1	59	G
1	1	60	A
1	1	65	A
1	1	66	A
1	1	72	C
1	1	96	G
1	1	105	C
1	1	109	A
1	1	110	G
1	1	111	C
1	1	116	A
1	1	118	U
1	1	122	A
1	1	135	C
1	1	136	G
1	1	143	G
1	1	148	G
1	1	165	A
1	1	166	C
1	1	170	G
1	1	190	U
1	1	191	U
1	1	192	C
1	1	200	C
1	1	206	G
1	1	210	U
1	1	211	A

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Mol	Chain	Res	Type
1	1	213	A
1	1	218	G
1	1	219	A
1	1	220	G
1	1	240	U
1	1	241	G
1	1	252	U
1	1	255	A
1	1	265	A
1	1	266	A
1	1	268	A
1	1	269	G
1	1	284	A
1	1	285	A
1	1	286	U
1	1	295	A
1	1	298	U
1	1	305	U
1	1	311	C
1	1	323	A
1	1	329	U
1	1	339	C
1	1	368	G
1	1	370	U
1	1	376	G
1	1	398	A
1	1	401	U
1	1	402	A
1	1	403	C
1	1	407	A
1	1	421	G
1	1	422	A
1	1	439	C
1	1	440	A
1	1	446	U
1	1	449	U
1	1	451	U
1	1	454	C
1	1	457	C
1	1	459	G
1	1	463	C
1	1	464	U

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Mol	Chain	Res	Type
1	1	466	G
1	1	468	G
1	1	469	G
1	1	472	A
1	1	478	A
1	1	479	U
1	1	480	C
1	1	481	U
1	1	482	C
1	1	483	G
1	1	485	A
1	1	486	U
1	1	487	U
1	1	488	U
1	1	521	A
1	1	530	G
1	1	533	A
1	1	535	G
1	1	543	C
1	1	544	C
1	1	547	G
1	1	550	A
1	1	552	G
1	1	557	A
1	1	559	A
1	1	560	G
1	1	578	A
1	1	579	G
1	1	591	G
1	1	611	A
1	1	620	U
1	1	621	A
1	1	622	A
1	1	636	C
1	1	642	U
1	1	645	A
1	1	660	A
1	1	677	A
1	1	681	U
1	1	691	A
1	1	695	C
1	1	705	A

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Mol	Chain	Res	Type
1	1	706	A
1	1	715	A
1	1	716	A
1	1	719	U
1	1	721	G
1	1	722	G
1	1	725	G
1	1	734	C
1	1	735	A
1	1	742	G
1	1	757	C
1	1	760	G
1	1	761	A
1	1	770	G
1	1	774	G
1	1	776	U
1	1	777	U
1	1	779	G
1	1	784	A
1	1	785	G
1	1	807	A
1	1	808	A
1	1	817	A
1	1	818	C
1	1	819	U
1	1	820	A
1	1	822	G
1	1	830	A
1	1	845	G
1	1	860	G
1	1	861	C
1	1	862	U
1	1	871	G
1	1	887	G
1	1	894	G
1	1	895	A
1	1	896	A
1	1	906	A
1	1	907	G
1	1	908	G
1	1	909	G
1	1	910	G

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Mol	Chain	Res	Type
1	1	912	G
1	1	913	A
1	1	917	A
1	1	936	A
1	1	944	C
1	1	958	C
1	1	959	C
1	1	960	U
1	1	961	C
1	1	962	A
1	1	963	G
1	1	978	G
1	1	979	U
1	1	980	A
1	1	982	C
1	1	985	U
1	1	991	G
1	1	1098	A
1	1	1103	A
1	1	1104	G
1	1	1105	A
1	1	1112	A
1	1	1115	G
1	1	1116	G
1	1	1127	G
1	1	1129	A
1	1	1132	C
1	1	1143	A
1	1	1145	G
1	1	1151	U
1	1	1153	A
1	1	1160	C
1	1	1174	G
1	1	1179	A
1	1	1180	A
1	1	1181	U
1	1	1191	U
1	1	1192	C
1	1	1193	A
1	1	1196	C
1	1	1197	A
1	1	1198	C

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Mol	Chain	Res	Type
1	1	1199	C
1	1	1200	A
1	1	1204	A
1	1	1217	A
1	1	1222	G
1	1	1228	C
1	1	1235	U
1	1	1241	U
1	1	1242	G
1	1	1245	A
1	1	1251	A
1	1	1252	A
1	1	1258	U
1	1	1259	A
1	1	1261	G
1	1	1262	G
1	1	1263	A
1	1	1265	U
1	1	1272	C
1	1	1279	C
1	1	1284	C
1	1	1286	A
1	1	1287	A
1	1	1303	A
1	1	1304	A
1	1	1305	U
1	1	1307	G
1	1	1308	A
1	1	1330	A
1	1	1332	A
1	1	1348	U
1	1	1349	G
1	1	1350	A
1	1	1351	U
1	1	1352	A
1	1	1353	U
1	1	1354	G
1	1	1355	A
1	1	1356	U
1	1	1357	G
1	1	1386	A
1	1	1392	G

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Mol	Chain	Res	Type
1	1	1399	A
1	1	1400	G
1	1	1418	A
1	1	1419	A
1	1	1421	G
1	1	1431	G
1	1	1434	G
1	1	1437	C
1	1	1450	G
1	1	1452	A
1	1	1454	A
1	1	1455	U
1	1	1469	C
1	1	1481	A
1	1	1483	G
1	1	1484	U
1	1	1485	G
1	1	1496	C
1	1	1525	G
1	1	1539	A
1	1	1552	G
1	1	1555	U
1	1	1556	C
1	1	1557	A
1	1	1560	G
1	1	1567	U
1	1	1568	U
1	1	1569	U
1	1	1571	A
1	1	1580	A
1	1	1581	C
1	1	1582	C
1	1	1587	A
1	1	1589	A
1	1	1590	G
1	1	1593	A
1	1	1604	G
1	1	1627	U
1	1	1628	C
1	1	1629	U
1	1	1630	U
1	1	1633	C

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Mol	Chain	Res	Type
1	1	1639	C
1	1	1643	A
1	1	1694	U
1	1	1724	U
1	1	1725	C
1	1	1741	A
1	1	1750	A
1	1	1751	G
1	1	1756	C
1	1	1761	C
1	1	1762	C
1	1	1763	U
1	1	1764	U
1	1	1766	G
1	1	1767	C
1	1	1773	C
1	1	1780	G
1	1	1795	U
1	1	1797	A
1	1	1806	A
1	1	1808	G
1	1	1813	A
1	1	1815	U
1	1	1816	A
1	1	1817	G
1	1	1821	U
1	1	1858	A
1	1	1863	G
1	1	1864	A
1	1	1865	A
1	1	1866	C
1	1	1867	A
1	1	1868	G
1	1	1876	U
1	1	1878	G
1	1	1886	A
1	1	1906	G
1	1	1918	C
1	1	1921	A
1	1	1922	A
1	1	1923	C
1	1	1927	G

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Mol	Chain	Res	Type
1	1	1929	G
1	1	1930	A
1	1	1932	A
1	1	1935	G
1	1	1939	G
1	1	1940	G
1	1	1955	U
1	1	1962	G
1	1	1965	C
1	1	1971	C
1	1	2057	G
1	1	2091	U
1	1	2092	A
1	1	2102	U
1	1	2103	U
1	1	2104	A
1	1	2105	G
1	1	2110	G
1	1	2111	G
1	1	2113	A
1	1	2114	C
1	1	2118	C
1	1	2119	A
1	1	2120	A
1	1	2122	G
1	1	2123	G
1	1	2131	A
1	1	2319	U
1	1	2320	A
1	1	2324	A
1	1	2329	C
1	1	2335	G
1	1	2336	U
1	1	2370	G
1	1	2371	G
1	1	2373	A
1	1	2374	C
1	1	2376	G
1	1	2385	G
1	1	2388	U
1	1	2393	G
1	1	2394	G

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Mol	Chain	Res	Type
1	1	2395	G
1	1	2405	C
1	1	2416	U
1	1	2418	G
1	1	2419	A
1	1	2420	C
1	1	2421	U
1	1	2422	C
1	1	2423	U
1	1	2424	A
1	1	2430	A
1	1	2433	U
1	1	2434	U
1	1	2435	G
1	1	2437	G
1	1	2438	A
1	1	2440	G
1	1	2445	A
1	1	2446	U
1	1	2448	G
1	1	2450	G
1	1	2452	G
1	1	2453	U
1	1	2460	U
1	1	2461	A
1	1	2462	A
1	1	2463	G
1	1	2469	G
1	1	2472	U
1	1	2473	C
1	1	2474	G
1	1	2475	G
1	1	2487	U
1	1	2491	A
1	1	2494	A
1	1	2495	C
1	1	2497	U
1	1	2501	U
1	1	2503	G
1	1	2504	U
1	1	2505	U
1	1	2507	C

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Mol	Chain	Res	Type
1	1	2596	U
1	1	2598	G
1	1	2599	U
1	1	2600	C
1	1	2601	A
1	1	2602	G
1	1	2603	G
1	1	2606	G
1	1	2611	U
1	1	2803	A
1	1	2818	U
1	1	2821	C
1	1	2822	U
1	1	2824	G
1	1	2836	C
1	1	2838	A
1	1	2844	C
1	1	2845	A
1	1	2879	C
1	1	2887	A
1	1	2898	G
1	1	2899	C
1	1	2904	U
1	1	2907	G
1	1	2916	U
1	1	2922	OMG
1	1	2925	C
1	1	2927	C
1	1	2935	U
1	1	2936	A
1	1	2941	A
1	1	2942	C
1	1	2943	G
1	1	2945	G
1	1	2946	A2M
1	1	2947	G
1	1	2948	C
1	1	2949	U
1	1	2950	G
1	1	2951	G
1	1	2952	G
1	1	2953	U

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Mol	Chain	Res	Type
1	1	2955	U
1	1	2956	A
1	1	2971	A
1	1	2972	G
1	1	2976	A
1	1	2977	G
1	1	2978	U
1	1	2979	U
1	1	2980	U
1	1	2982	A
1	1	2983	C
1	1	2984	C
1	1	2990	G
1	1	2996	U
1	1	2997	G
1	1	3012	A
1	1	3022	G
1	1	3023	U
1	1	3026	G
1	1	3027	A
1	1	3028	G
1	1	3030	G
1	1	3032	A
1	1	3050	U
1	1	3057	U
1	1	3058	U
1	1	3059	G
1	1	3078	U
1	1	3079	U
1	1	3092	C
1	1	3093	C
1	1	3100	U
1	1	3109	G
1	1	3122	A
1	1	3127	A
1	1	3129	A
1	1	3130	A
1	1	3131	U
1	1	3142	A
1	1	3143	C
1	1	3151	U
1	1	3153	U

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Mol	Chain	Res	Type
1	1	3154	C
1	1	3156	U
1	1	3157	U
1	1	3165	A
1	1	3167	A
1	1	3168	A
1	1	3172	A
1	1	3173	G
1	1	3174	A
1	1	3176	G
1	1	3179	U
1	1	3180	A
1	1	3181	C
1	1	3187	A
1	1	3196	U
1	1	3207	U
1	1	3210	A
1	1	3217	C
1	1	3218	A
1	1	3219	G
1	1	3224	G
1	1	3227	A
1	1	3228	C
1	1	3229	G
1	1	3238	G
1	1	3244	A
1	1	3245	A
1	1	3247	G
1	1	3259	U
1	1	3270	U
1	1	3276	G
1	1	3278	C
1	1	3279	A
1	1	3280	U
1	1	3287	U
1	1	3289	G
1	1	3294	A
1	1	3304	U
1	1	3313	U
1	1	3314	A
1	1	3316	A
1	1	3317	U

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Mol	Chain	Res	Type
1	1	3319	U
1	1	3334	U
1	1	3335	A
1	1	3341	U
1	1	3349	C
1	1	3358	U
1	1	3362	A
1	1	3369	G
1	1	3378	C
1	1	3382	U
1	1	3383	G
1	1	3386	G
1	1	3389	U
1	1	3396	U
2	2	23	U
2	2	34	U
2	2	35	C
2	2	48	A
2	2	59	A
2	2	62	C
2	2	63	G
2	2	79	A
2	2	81	U
2	2	82	U
2	2	84	C
2	2	86	U
2	2	87	G
2	2	90	U
2	2	95	G
2	2	104	A
2	2	105	A
2	2	106	C
2	2	107	G
2	2	111	A
2	2	113	U
2	2	116	G
2	2	124	G
2	2	148	G
52	6	4	U
52	6	5	C
52	6	7	C
52	6	14	U

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Mol	Chain	Res	Type
52	6	15	C
52	6	16	U
52	6	23	U
52	6	24	A
52	6	26	U
52	6	33	U
52	6	34	A
52	6	40	U
52	6	41	G
52	6	42	G
52	6	43	A
52	6	54	A
52	6	56	U
52	6	57	U
52	6	59	C
52	6	218	A
52	6	219	A
52	6	220	C
52	6	223	U
52	6	230	A

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	165	A
1	1	239	G
1	1	406	G
1	1	480	C
1	1	487	U
1	1	644	G
1	1	720	A
1	1	734	C
1	1	817	A
1	1	870	C
1	1	906	A
1	1	908	G
1	1	1102	A
1	1	1104	G
1	1	1128	U
1	1	1159	A
1	1	1227	C
1	1	1241	U

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Mol	Chain	Res	Type
1	1	1283	C
1	1	1302	A
1	1	1307	G
1	1	1329	U
1	1	1355	A
1	1	1551	C
1	1	1954	G
1	1	2417	U
1	1	2419	A
1	1	2445	A
1	1	2496	C
1	1	2500	A
1	1	2597	U
1	1	2600	C
1	1	2602	G
1	1	2954	U
1	1	3121	U
1	1	3218	A
1	1	3228	C
1	1	3269	U
2	2	123	G
52	6	42	G
52	6	56	U
52	6	218	A
52	6	222	A

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	A2M	1	2946	1	18,25,26	1.50	1 (5%)	18,36,39	0.99	1 (5%)
1	OMG	1	2922	1	18,26,27	1.38	3 (16%)	19,38,41	1.45	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	1	2921	1	19,22,23	0.74	0	26,31,34	0.96	2 (7%)
1	PSU	1	2923	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	1	2946	1	-	1/5/27/28	0/3/3/3
1	OMG	1	2922	1	-	2/5/27/28	0/3/3/3
1	OMU	1	2921	1	-	0/9/27/28	0/2/2/2
1	PSU	1	2923	1	-	1/7/25/26	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2946	A2M	O5'-C5'	-4.32	1.34	1.44
1	1	2922	OMG	C6-N1	4.17	1.44	1.37
1	1	2923	PSU	C6-C5	3.09	1.38	1.35
1	1	2923	PSU	C4-N3	-2.63	1.33	1.38
1	1	2922	OMG	C2-N2	2.56	1.40	1.34
1	1	2922	OMG	C5-C6	-2.13	1.43	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2923	PSU	N1-C2-N3	5.91	121.83	115.13
1	1	2923	PSU	C4-N3-C2	-3.88	120.75	126.34
1	1	2922	OMG	O6-C6-N1	-3.71	116.27	120.65
1	1	2923	PSU	O2-C2-N1	-3.32	119.14	122.79
1	1	2922	OMG	O6-C6-C5	3.23	130.67	124.37
1	1	2921	OMU	CM2-O2'-C2'	-2.53	107.89	114.52
1	1	2921	OMU	C4-N3-C2	-2.26	123.60	126.58
1	1	2946	A2M	C2-N1-C6	-2.06	115.23	118.75

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	2922	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	1	2923	PSU	O4'-C1'-C5-C4
1	1	2946	A2M	C4'-C5'-O5'-P
1	1	2922	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	SAH	w	901	-	24,28,28	1.20	3 (12%)	25,40,40	1.70	5 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SAH	w	901	-	-	4/11/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	w	901	SAH	C2-N3	3.92	1.38	1.32
60	w	901	SAH	C2-N1	2.42	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	w	901	SAH	OXT-C	-2.15	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	w	901	SAH	N3-C2-N1	-5.39	120.26	128.68
60	w	901	SAH	C5'-SD-CG	-3.85	90.71	102.27
60	w	901	SAH	C3'-C2'-C1'	2.80	105.20	100.98
60	w	901	SAH	OXT-C-O	-2.55	118.30	124.09
60	w	901	SAH	OXT-C-CA	2.30	121.22	113.38

There are no chirality outliers.

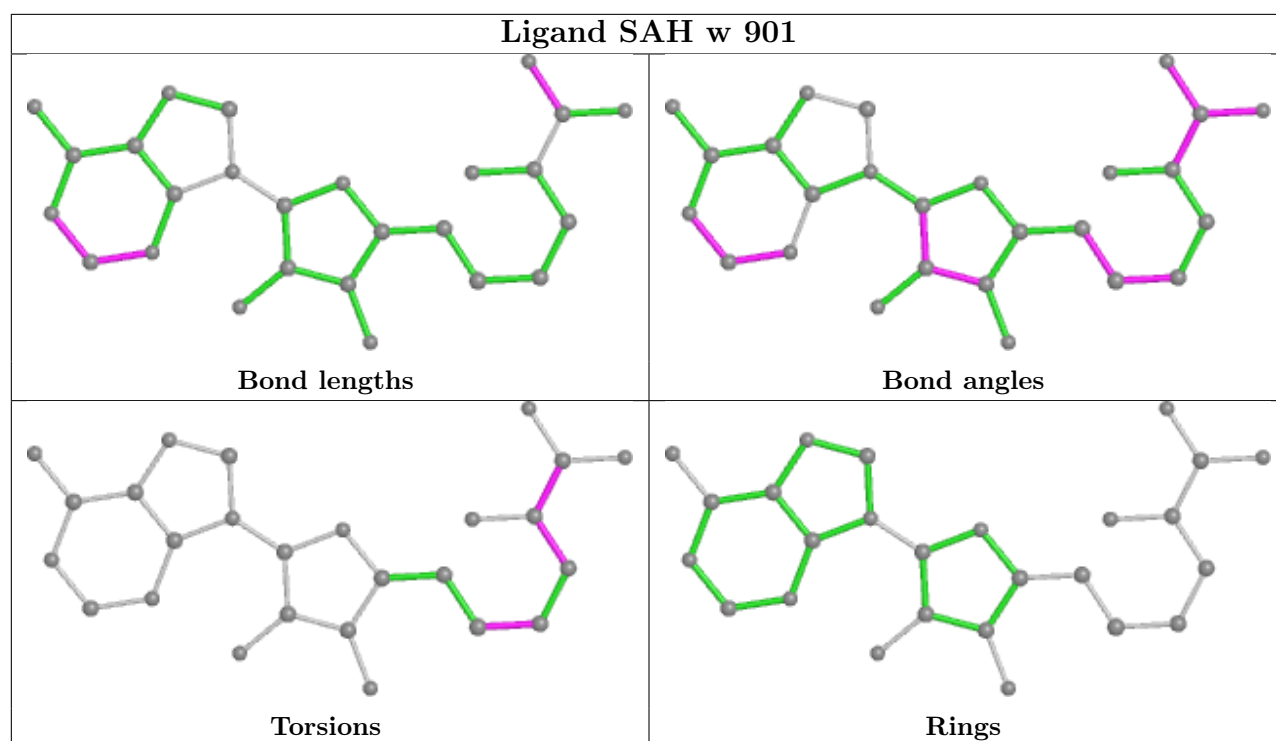
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	w	901	SAH	C-CA-CB-CG
60	w	901	SAH	N-CA-CB-CG
60	w	901	SAH	CB-CG-SD-C5'
60	w	901	SAH	OXT-C-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
52	6	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	6	67:U	O3'	213:A	P	14.86

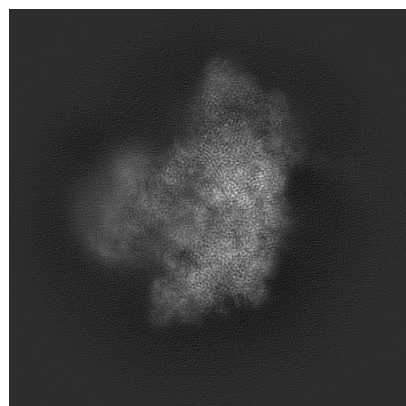
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24269. These allow visual inspection of the internal detail of the map and identification of artifacts.

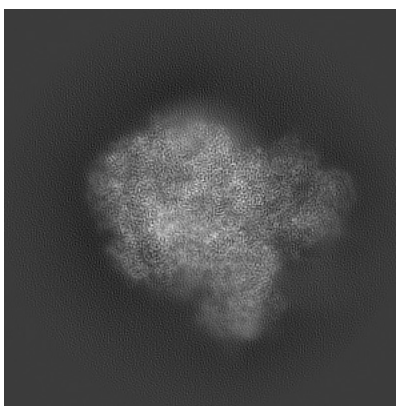
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

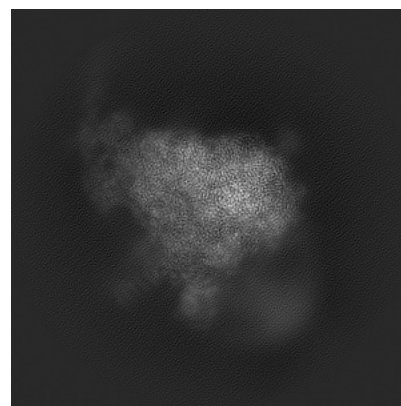
6.1.1 Primary map



X

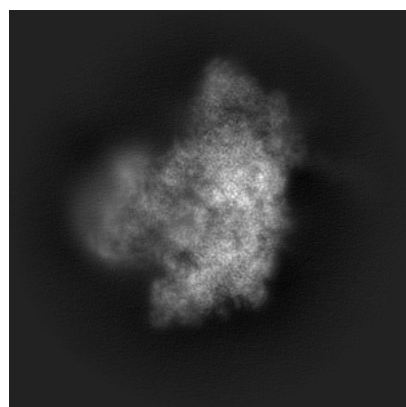


Y

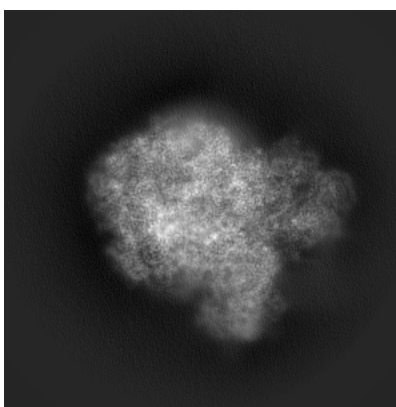


Z

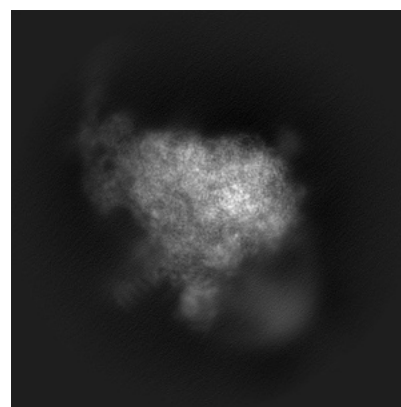
6.1.2 Raw map



X



Y

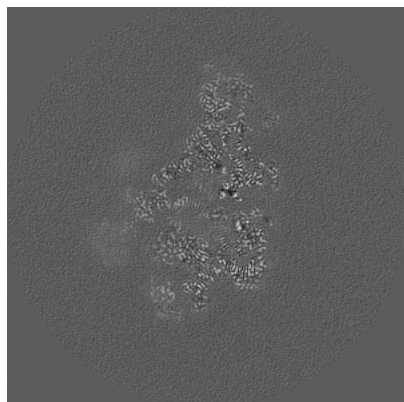


Z

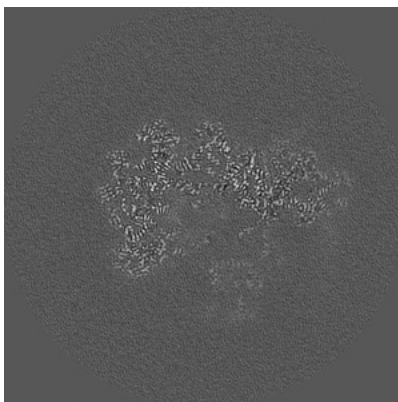
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

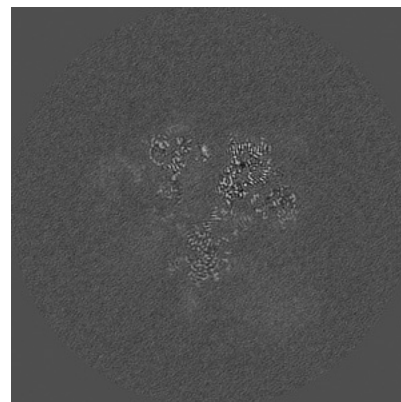
6.2.1 Primary map



X Index: 210

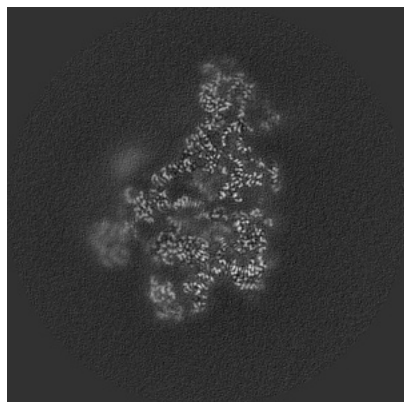


Y Index: 210

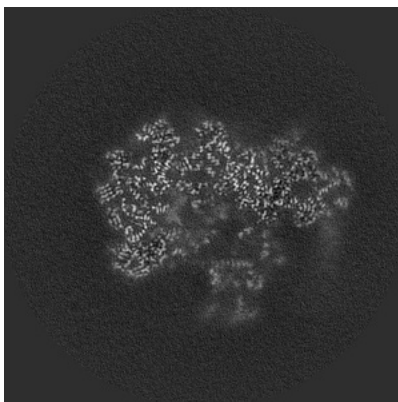


Z Index: 210

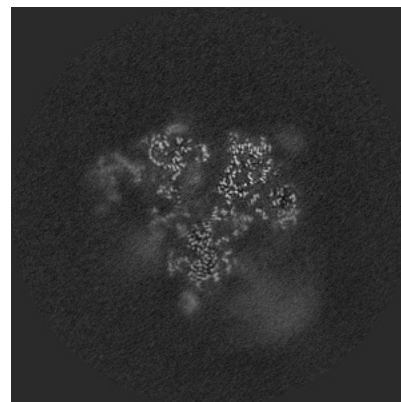
6.2.2 Raw map



X Index: 210



Y Index: 210

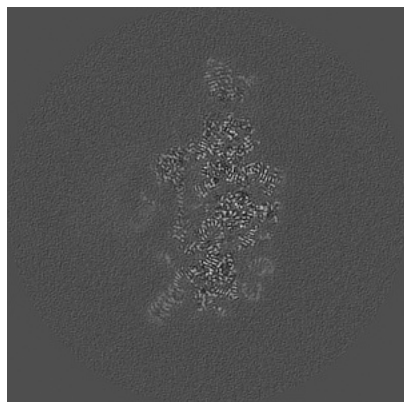


Z Index: 210

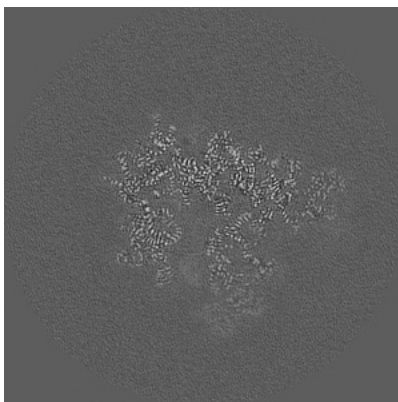
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

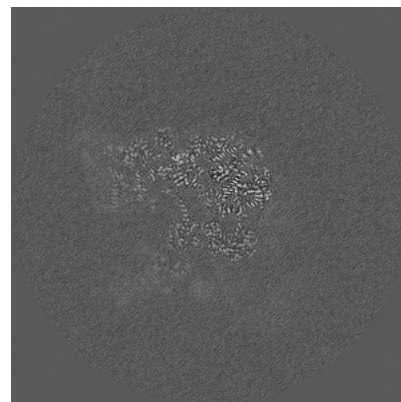
6.3.1 Primary map



X Index: 234

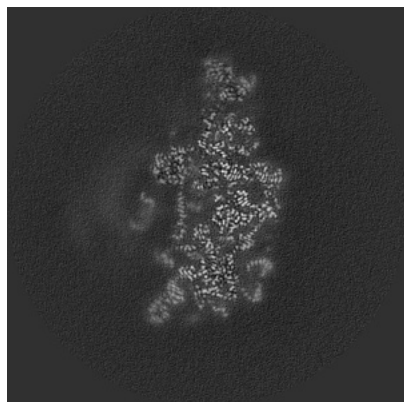


Y Index: 233

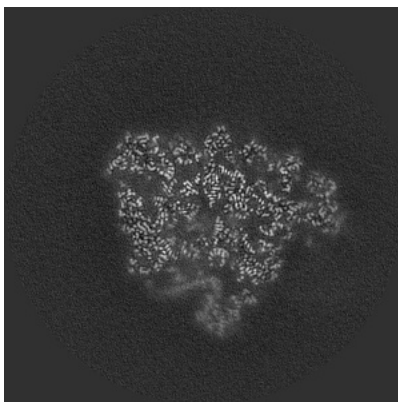


Z Index: 247

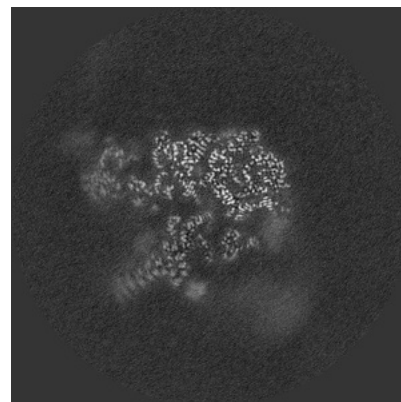
6.3.2 Raw map



X Index: 236



Y Index: 246

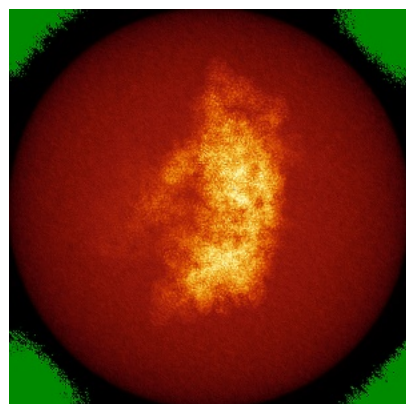


Z Index: 235

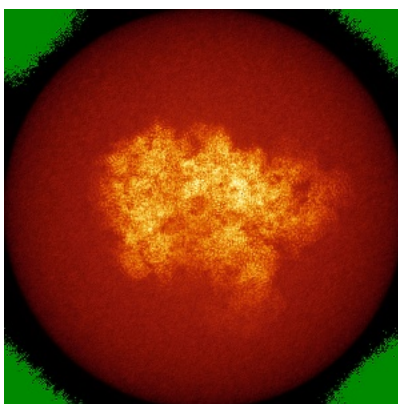
The images above show the largest variance slices of the map in three orthogonal directions.

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

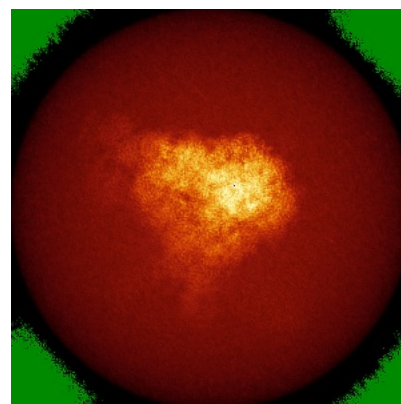
6.4.1 Primary map



X

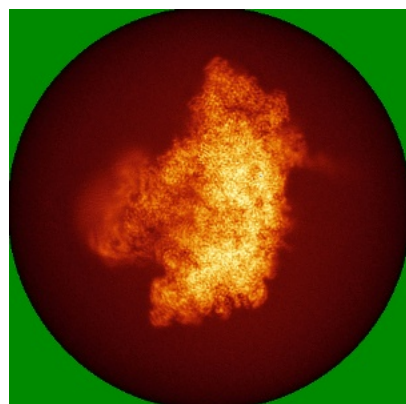


Y

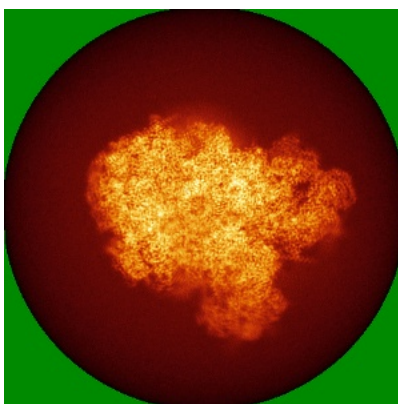


Z

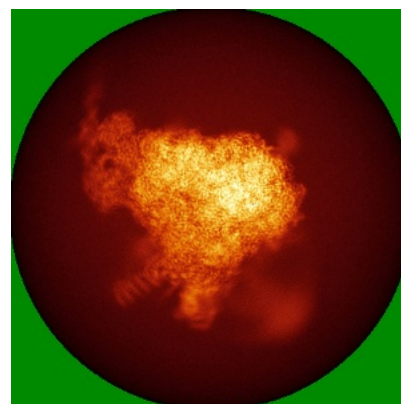
6.4.2 Raw map



X



Y

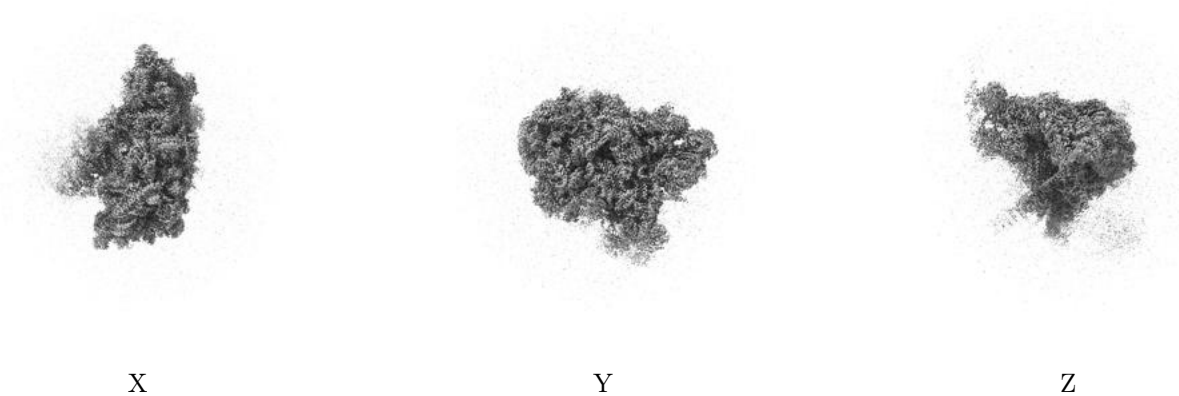


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.0275. 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



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.

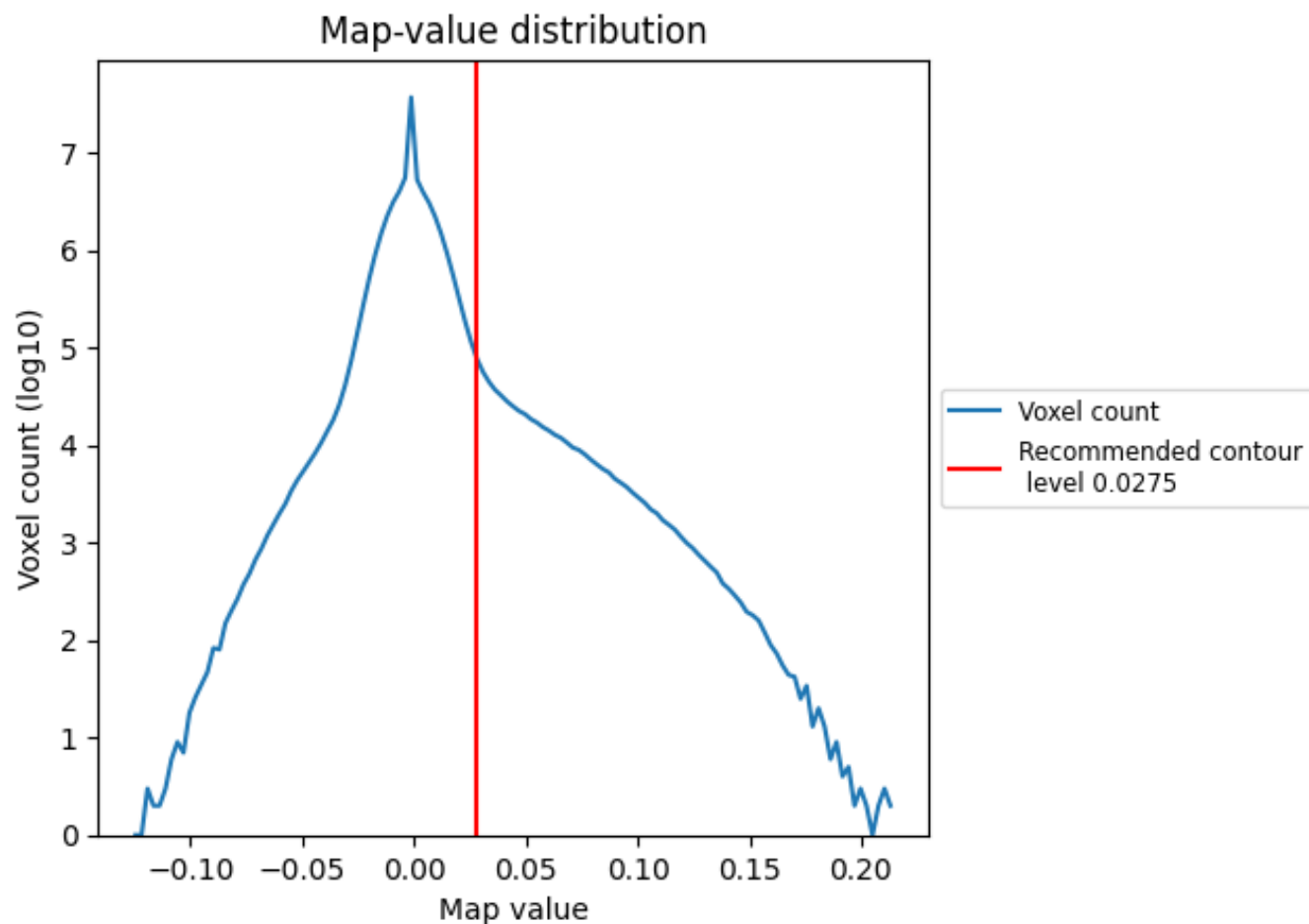
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

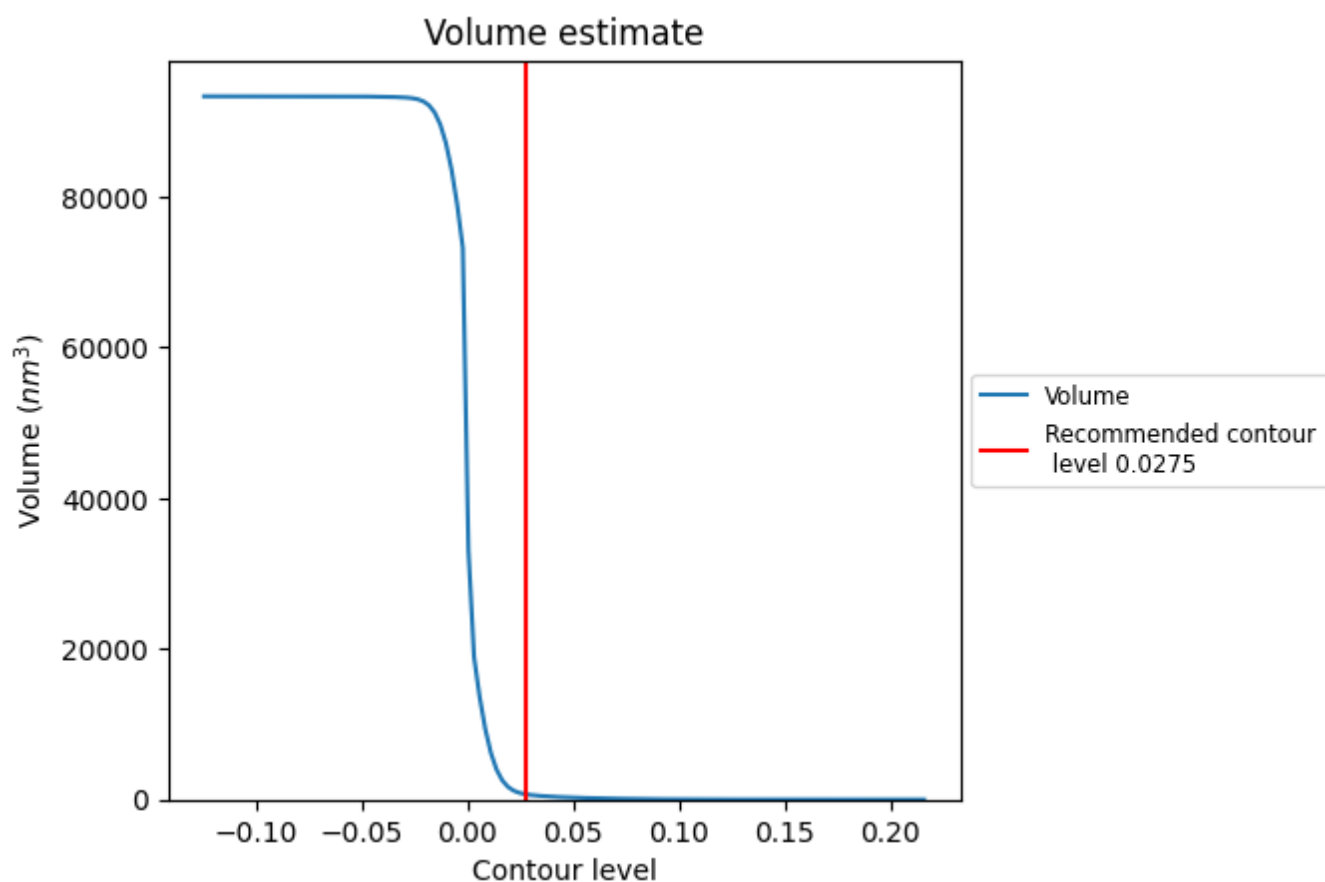
This section contains the results of statistical analysis of the map.

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.

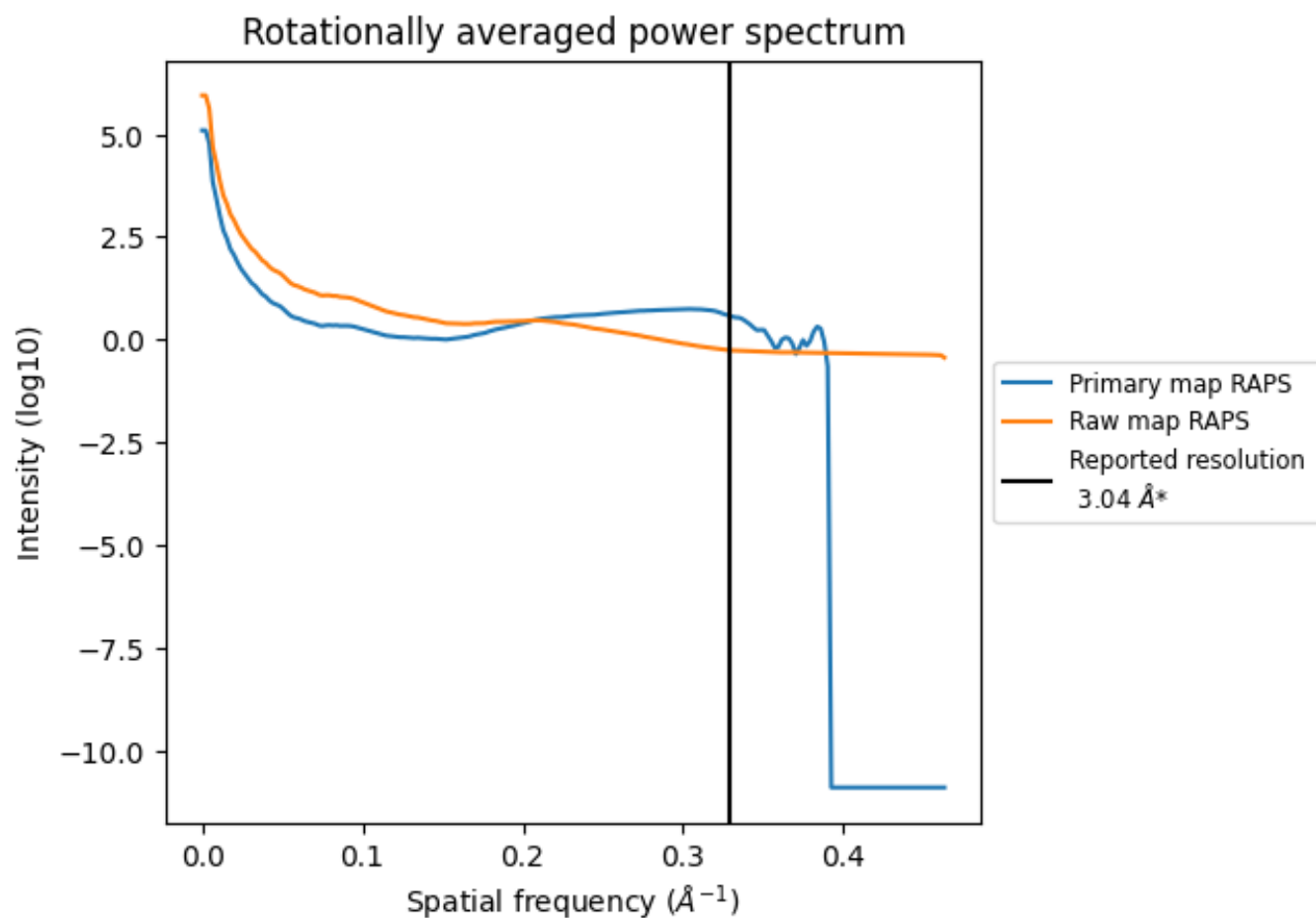
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 704 nm^3 ; this corresponds to an approximate mass of 636 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 ⓘ

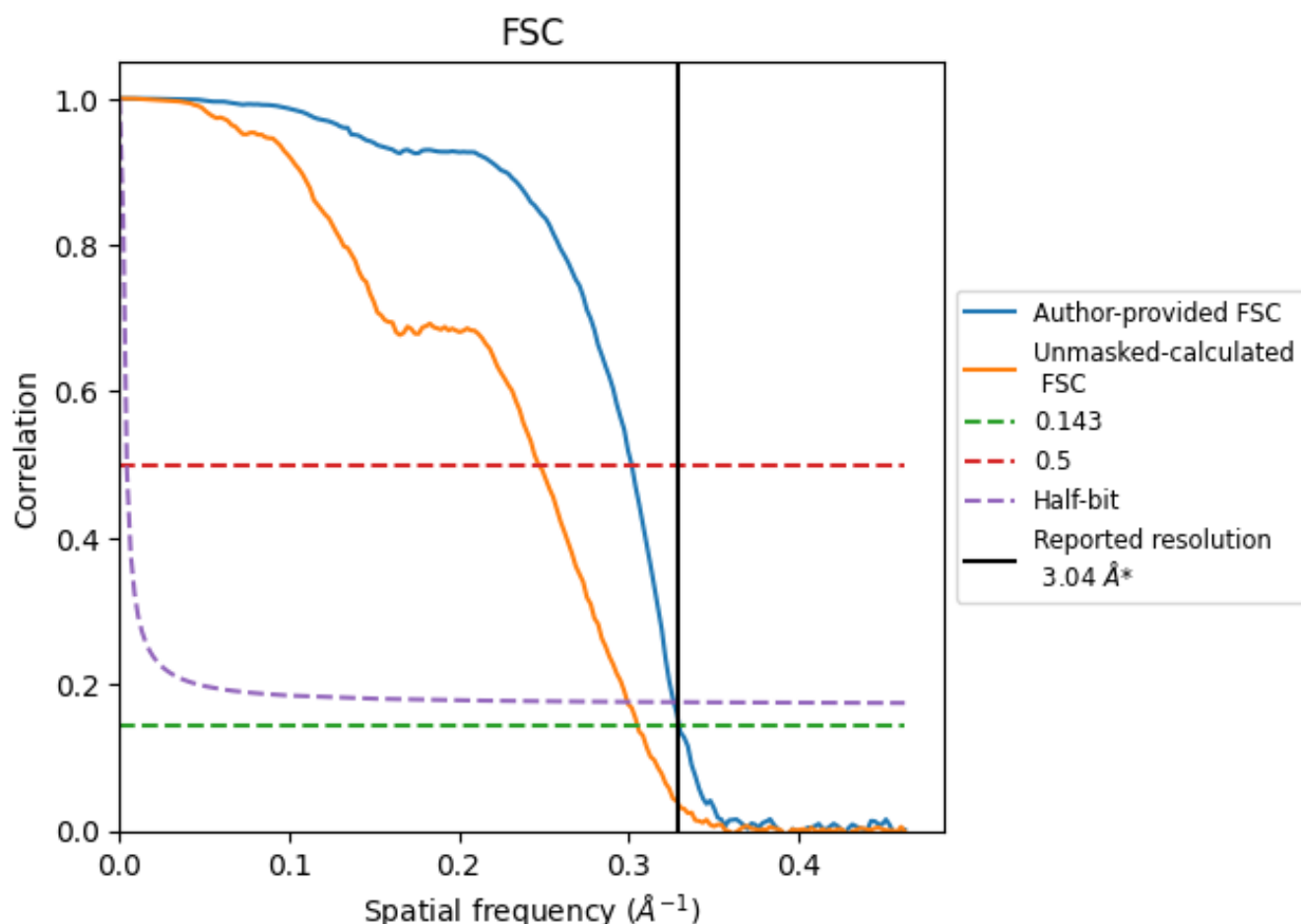


*Reported resolution corresponds to spatial frequency of 0.329 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.329 Å⁻¹

8.2 Resolution estimates [i](#)

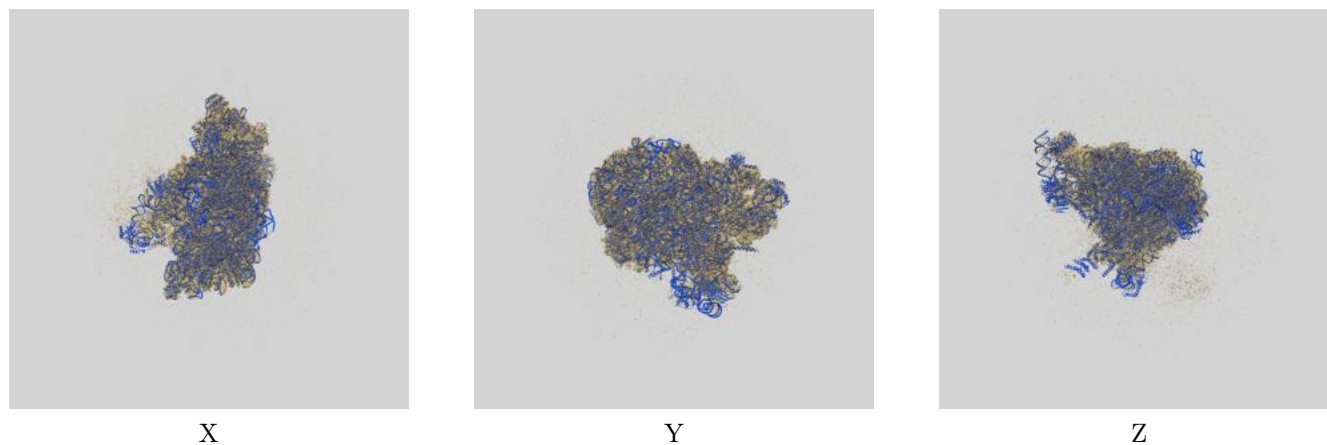
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.03	3.31	3.06
Unmasked-calculated*	3.27	4.05	3.34

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

9 Map-model fit [i](#)

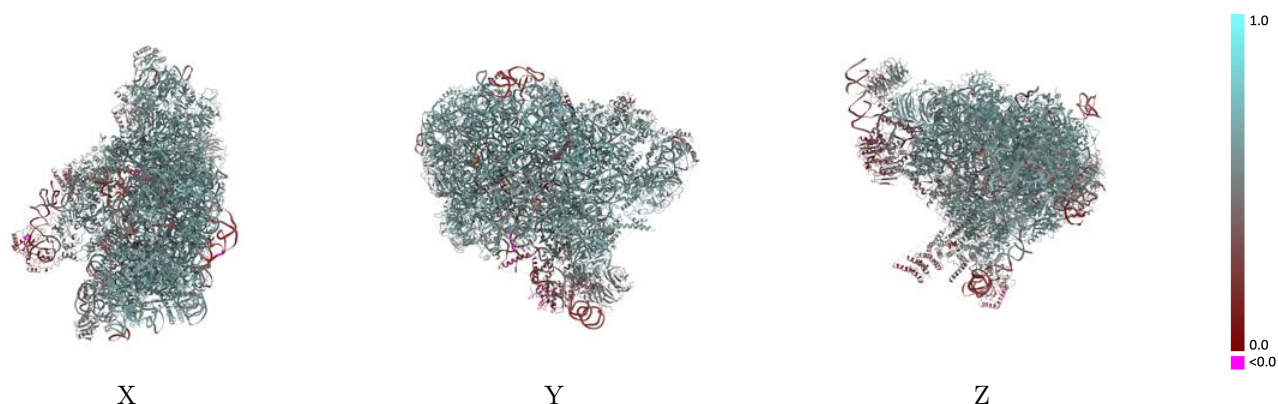
This section contains information regarding the fit between EMDB map EMD-24269 and PDB model 7NAC. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



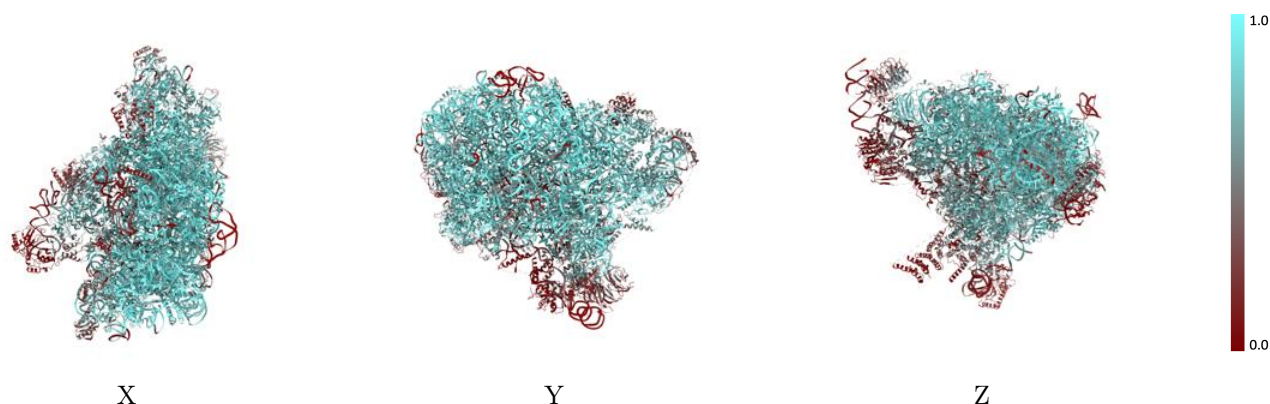
The images above show the 3D surface view of the map at the recommended contour level 0.0275 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



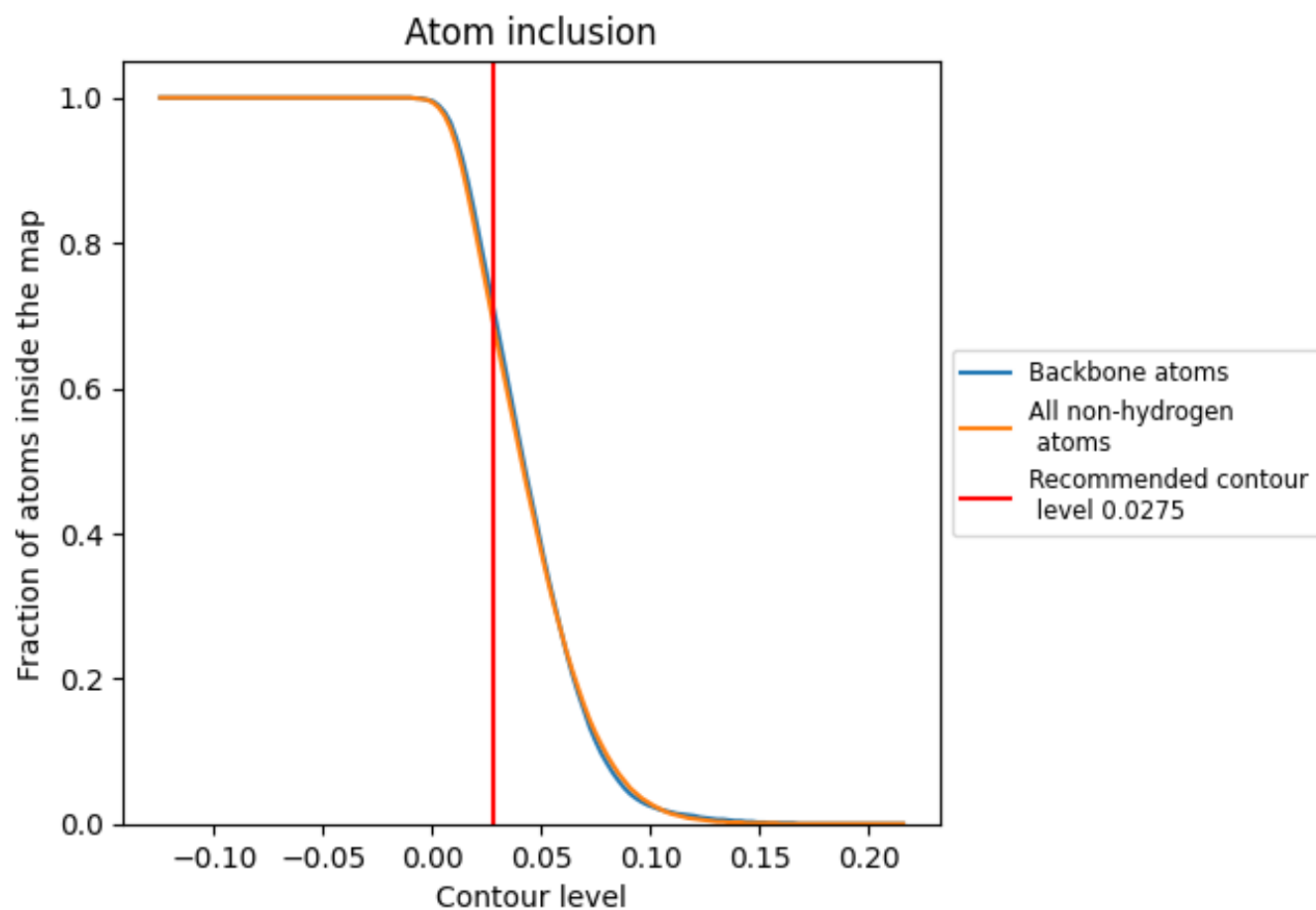
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0275).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 70% 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 (0.0275) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6970	 0.5490
1	 0.7670	 0.5470
2	 0.9030	 0.6080
5	 0.2830	 0.4650
6	 0.7140	 0.5480
7	 0.6390	 0.5610
8	 0.3090	 0.4270
A	 0.6680	 0.5390
B	 0.8900	 0.6200
C	 0.8700	 0.6250
D	 0.4970	 0.5230
E	 0.7690	 0.5870
F	 0.8230	 0.6100
G	 0.8380	 0.6120
H	 0.8040	 0.6050
I	 0.6150	 0.5450
J	 0.6210	 0.5550
K	 0.6280	 0.5510
L	 0.8710	 0.6240
M	 0.8310	 0.6110
N	 0.9340	 0.6420
O	 0.9030	 0.6290
P	 0.7790	 0.5880
Q	 0.8090	 0.6090
R	 0.6550	 0.5550
S	 0.7390	 0.5850
T	 0.0330	 0.3610
U	 0.6250	 0.5490
V	 0.8300	 0.6170
W	 0.4160	 0.4790
X	 0.8200	 0.6170
Y	 0.8850	 0.6230
Z	 0.7620	 0.5990
a	 0.0230	 0.2310
b	 0.5820	 0.5370



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Chain	Atom inclusion	Q-score
c	 0.6210	 0.5600
d	 0.7530	 0.5810
e	 0.8820	 0.6320
f	 0.9460	 0.6500
g	 0.8280	 0.6130
h	 0.8660	 0.6260
i	 0.7870	 0.5850
j	 0.9080	 0.6390
k	 0.6930	 0.5830
l	 0.7590	 0.5940
m	 0.7530	 0.5940
n	 0.7830	 0.6010
o	 0.6510	 0.5500
p	 0.3150	 0.4580
q	 0.5830	 0.5280
r	 0.6930	 0.5770
s	 0.7750	 0.6040
t	 0.7190	 0.5860
u	 0.7490	 0.5890
v	 0.8220	 0.6080
w	 0.5630	 0.5320
x	 0.1590	 0.3020
y	 0.8050	 0.5930
z	 0.4950	 0.5320