



wwPDB EM Validation Summary Report ⓘ

Jun 23, 2026 – 03:35 PM JST

PDB ID : 8INK / pdb_00008ink
EMDB ID : EMD-35599
Title : human nuclear pre-60S ribosomal particle - State D
Authors : Zhang, Y.; Gao, N.
Deposited on : 2023-03-10
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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:

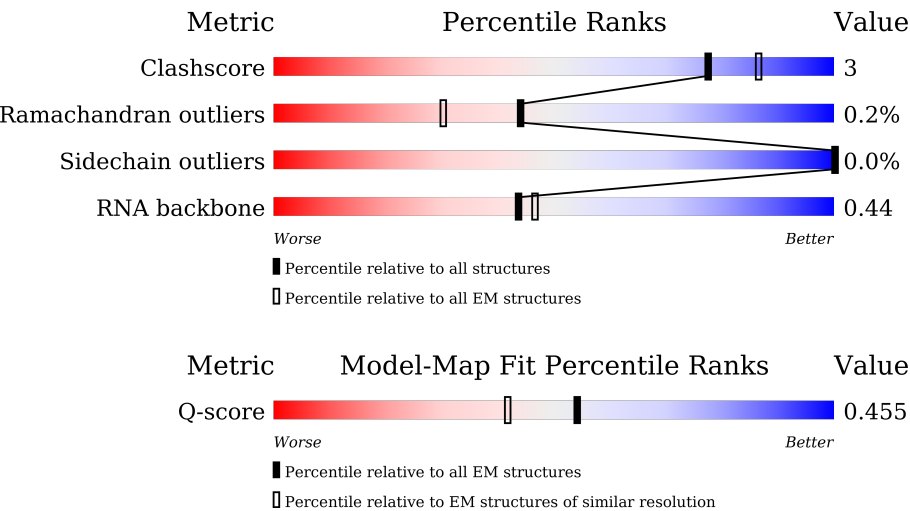
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	N	687	46% 43%5%52%
2	6	245	5% 87%13%
3	7	163	75%8%17%

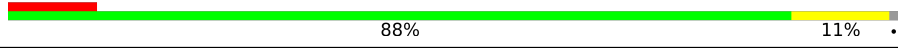
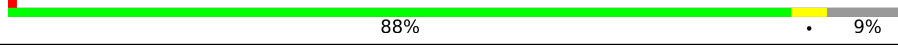
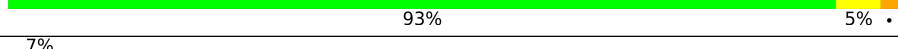
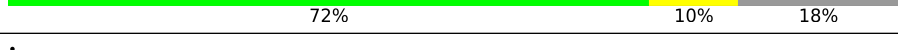
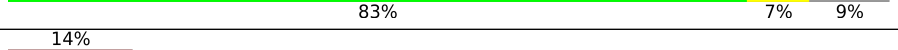
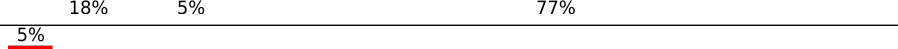
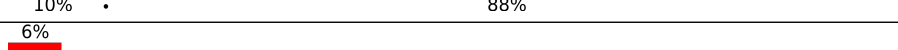
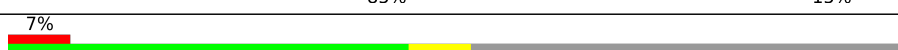
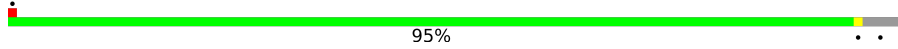
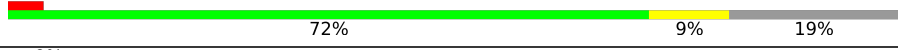
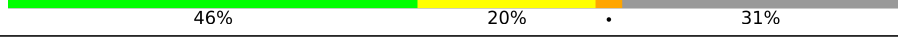
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Mol	Chain	Length	Quality of chain
4	8	156	
5	9	134	
6	A	159	
7	B	403	
8	D	427	
9	E	115	
10	F	117	
11	G	266	
12	H	123	
13	I	192	
14	J	260	
15	K	105	
16	L	148	
17	M	97	
18	O	70	
19	P	51	
20	Q	211	
21	S	215	
22	U	204	
23	V	203	
24	X	92	
25	Z	188	
26	a	196	
27	b	176	
28	e	140	

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Mol	Chain	Length	Quality of chain
29	g	156	
30	h	145	
31	i	136	
32	l	137	
33	m	257	
34	n	110	
35	o	288	
36	p	248	
37	r	360	
38	u	549	
39	w	731	
40	y	165	
41	z	129	
42	C	178	
43	R	297	
44	W	485	
45	T	160	
46	4	634	
47	Y	184	
48	k	135	
49	j	125	
50	d	128	
51	3	120	
52	v	239	
53	2	5054	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 152807 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 Protein SDA1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	332	Total	C	N	O	S	0	0
			2719	1762	461	475	21		

- Molecule 2 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	6	244	Total	C	N	O	S	0	0
			1852	1149	318	372	13		

- Molecule 3 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	7	135	Total	C	N	O	S	0	0
			1159	737	225	187	10		

- Molecule 4 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	8	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 5 is a protein called Zinc finger protein 593.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	9	86	Total	C	N	O	S	0	0
			711	433	154	121	3		

- Molecule 6 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	45	Total	C	N	O	S	0	0
			352	221	76	52	3		

- Molecule 7 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	402	Total	C	N	O	S	1	0
			3244	2065	609	556	14		

- Molecule 8 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	358	Total	C	N	O	S	0	0
			2853	1797	570	473	13		

- Molecule 9 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 10 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	109	Total	C	N	O	S	0	0
			868	544	179	139	6		

- Molecule 11 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

- Molecule 12 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 13 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 14 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	217	Total	C	N	O	S	0	0
			1772	1134	334	296	8		

- Molecule 15 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 16 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	112	Total	C	N	O	S	0	0
			877	557	172	145	3		

- Molecule 17 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 18 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 19 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 20 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 21 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	135	Total	C	N	O	S	0	0
			1111	713	213	178	7		

- Molecule 22 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 23 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 24 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 25 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	151	Total	C	N	O	S	0	0
			1223	768	247	203	5		

- Molecule 26 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	148	Total	C	N	O	S	0	0
			1239	772	266	192	9		

- Molecule 27 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

- Molecule 28 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 29 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	g	117	Total	C	N	O	S	0	0
			958	612	179	166	1		

- Molecule 30 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 31 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 32 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	l	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 33 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	m	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 34 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	n	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 35 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	o	235	Total	C	N	O	S	0	0
			1897	1217	360	316	4		

- Molecule 36 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	p	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 37 is a protein called Coiled-coil domain-containing protein 86.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	r	82	Total	C	N	O	S	0	0
			723	442	158	121	2		

- Molecule 38 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	u	68	Total	C	N	O	S	0	0
			578	362	121	92	3		

- Molecule 39 is a protein called G Protein Nucleolar 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	w	433	Total	C	N	O	S	0	0
			3472	2201	615	643	13		

- Molecule 40 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	y	165	Total	C	N	O	S	0	0
			1250	779	232	234	5		

- Molecule 41 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	z	67	Total	C	N	O	S	0	0
			581	363	128	88	2		

- Molecule 42 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	C	165	Total	C	N	O	S	0	0
			1319	836	245	233	5		

- Molecule 43 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	R	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 44 is a protein called Notchless protein homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	W	388	Total	C	N	O	S	0	0
			3018	1889	556	562	11		

- Molecule 45 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	T	124	Total	C	N	O	S	0	0
			1001	632	194	171	4		

- Molecule 46 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	4	611	Total	C	N	O	S	0	0
			5016	3151	918	920	27		

- Molecule 47 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Y	167	Total	C	N	O	S	0	0
			1355	848	260	238	9		

- Molecule 48 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	k	129	Total	C	N	O	S	0	0
			1064	673	220	166	5		

- Molecule 49 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	j	111	Total	C	N	O	S	0	0
			918	578	178	160	2		

- Molecule 50 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	d	104	Total	C	N	O	S	0	0
			850	542	149	157	2		

- Molecule 51 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	115	Total	C	N	O	P	0	0
			2453	1093	437	808	115		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	92	C	G	conflict	GB NR_023363
3	93	G	C	conflict	GB NR_023363
3	95	C	U	conflict	GB NR_023363
3	96	U	G	conflict	GB NR_023363

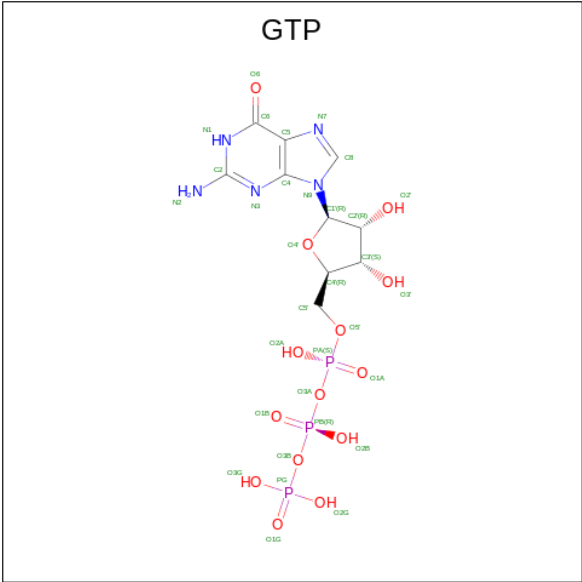
- Molecule 52 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	v	217	Total	C	N	O	S	0	0
			1771	1129	311	320	11		

- Molecule 53 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2	3495	Total	C	N	O	P	0	0
			75023	33449	13712	24368	3494		

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



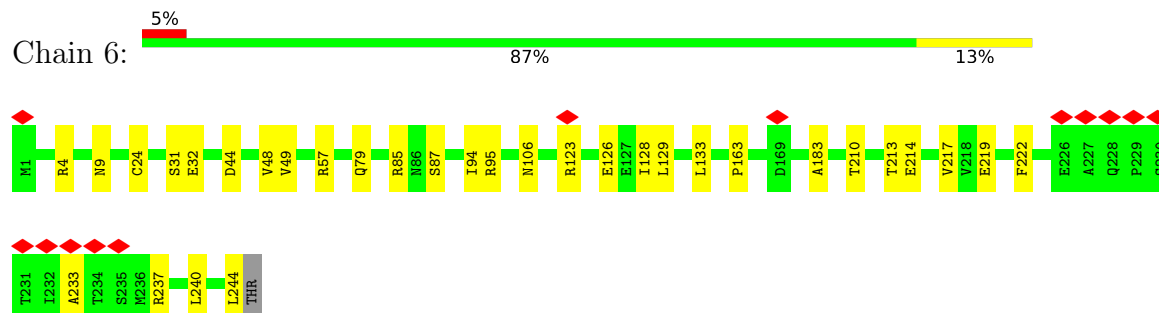
Mol	Chain	Residues	Atoms					AltConf
54	w	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

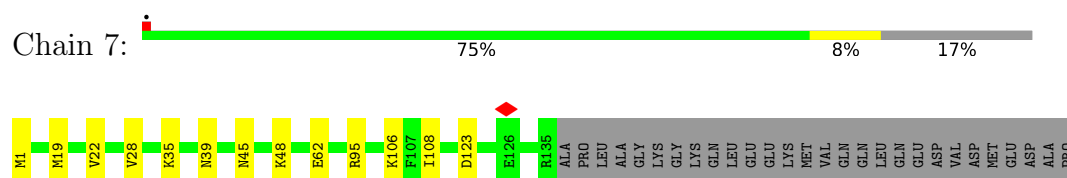
Mol	Chain	Residues	Atoms		AltConf
55	w	1	Total	Mg	0
			1	1	

LEU	HIS	LYS	LYS	PRO	LYS	SER	ASP	GLU	THR	ARG	LEU	ALA	THR	ALA	MET	GLY	LYS	THR	LYS	THR	LYS	ASN	PRO	PHE	SER	SER	SER	ASN	LYS	GLU	LYS	LYS	LYS	GLN	LYS	ASN	PHE	MET	MET	ARG	TYR	SER	GLN	ASN	VAL	ARG
SER	LYS	ASN	LYS	ARG	SER	PHE	ARG	GLU	LYS	GLN	LEU	LEU	ALA	ARG	ASP	ALA	LEU	LEU	LYS	LYS	ARG	ARG	LYS	ARG	LYS	GLU	PHE	MET	LYS																	

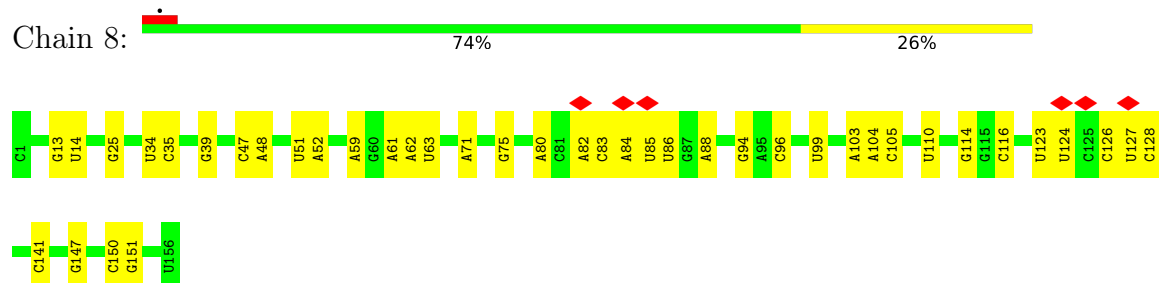
- Molecule 2: Eukaryotic translation initiation factor 6



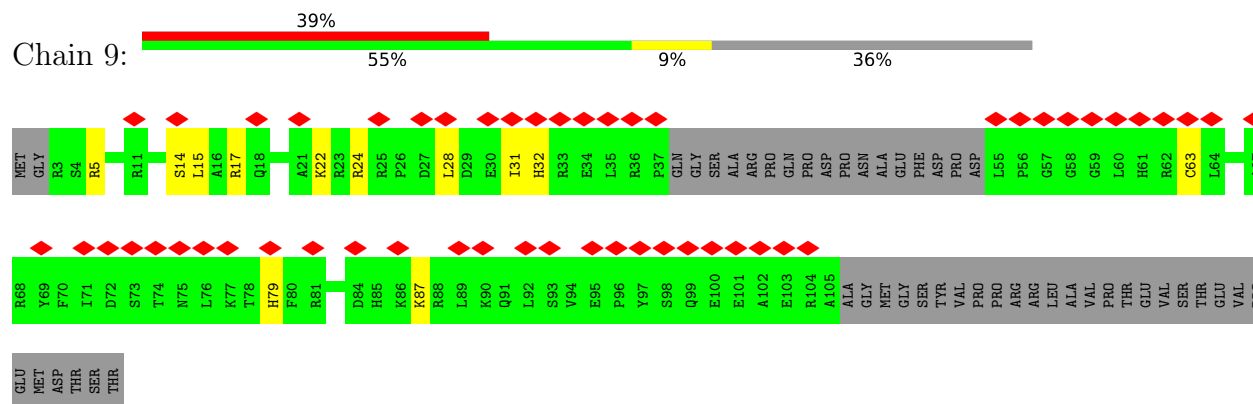
- Molecule 3: Probable ribosome biogenesis protein RLP24



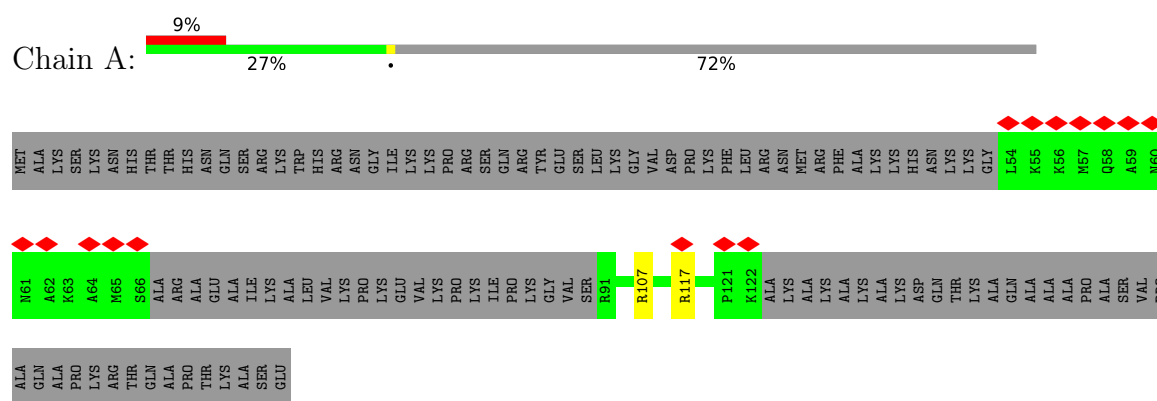
- Molecule 4: 5.8S rRNA



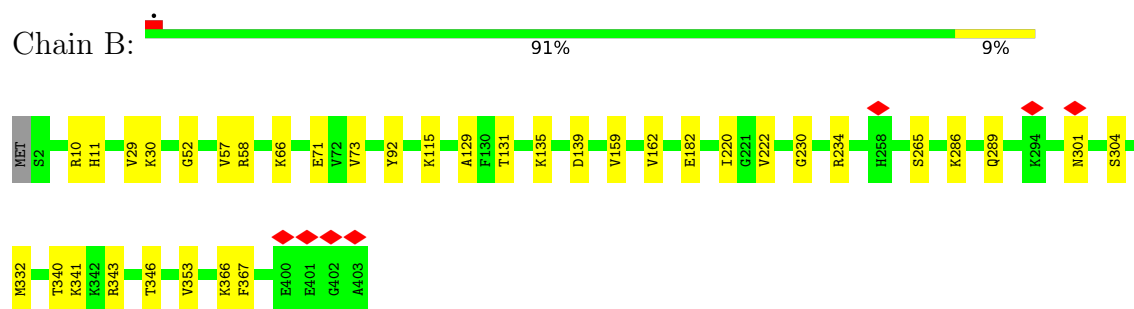
- Molecule 5: Zinc finger protein 593



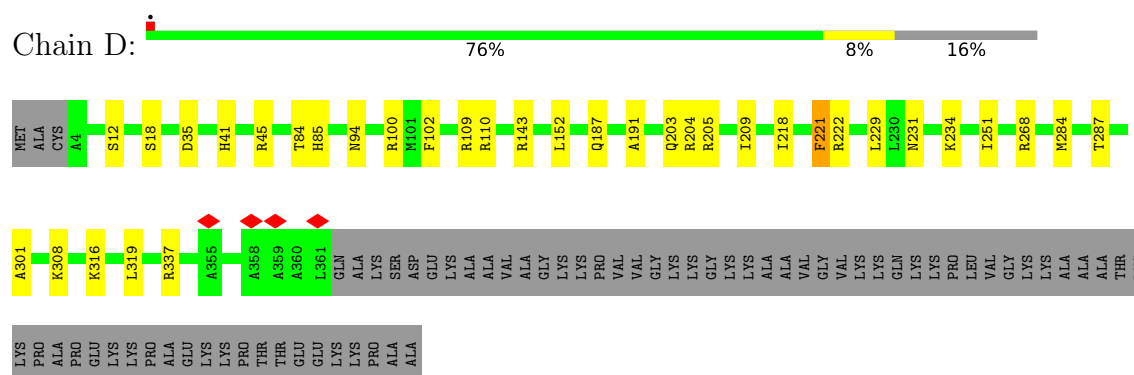
- Molecule 6: 60S ribosomal protein L29



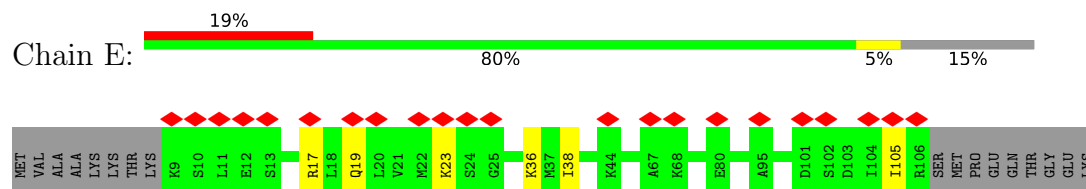
- Molecule 7: 60S ribosomal protein L3



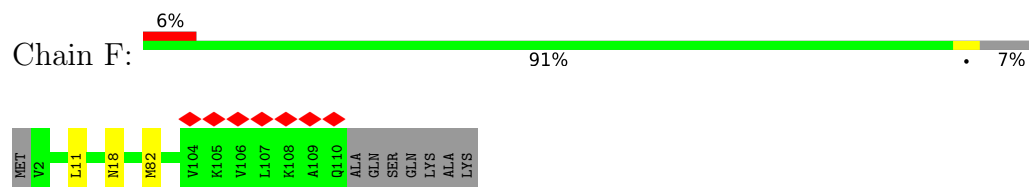
- Molecule 8: 60S ribosomal protein L4



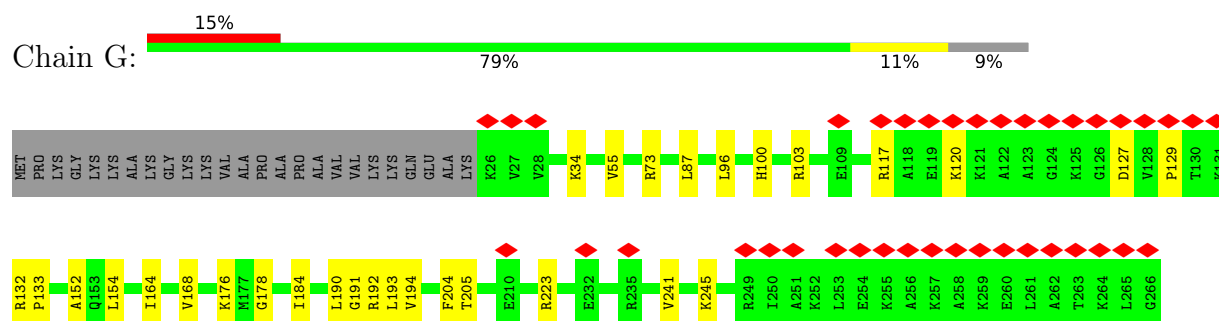
- Molecule 9: 60S ribosomal protein L30



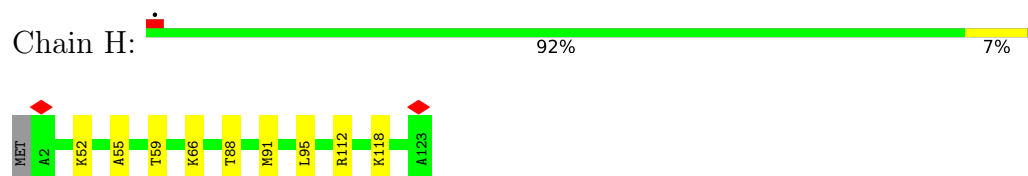
- Molecule 10: 60S ribosomal protein L34



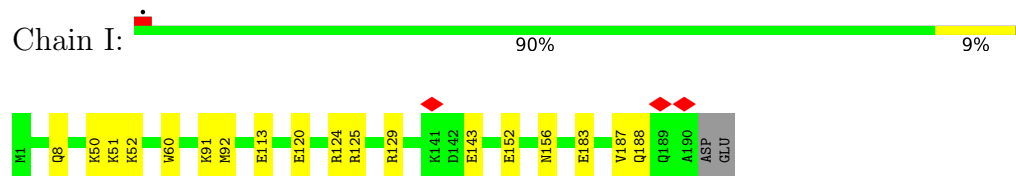
- Molecule 11: 60S ribosomal protein L7a



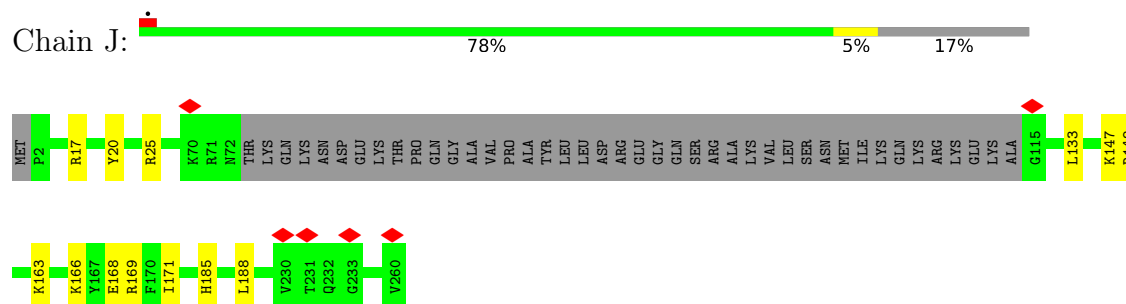
- Molecule 12: 60S ribosomal protein L35



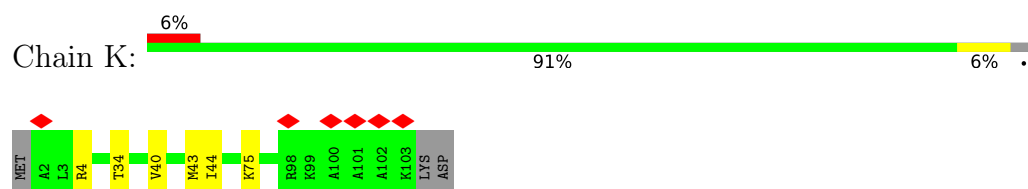
- Molecule 13: 60S ribosomal protein L9



- Molecule 14: Ribosome biogenesis protein NSA2 homolog

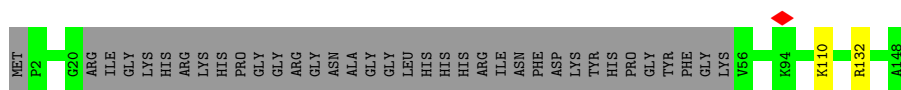


- Molecule 15: 60S ribosomal protein L36



- Molecule 16: 60S ribosomal protein L27a





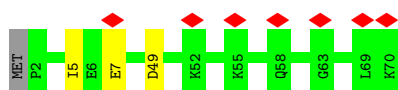
- Molecule 17: 60S ribosomal protein L37

Chain M:



- Molecule 18: 60S ribosomal protein L38

Chain O:



- Molecule 19: 60S ribosomal protein L39

Chain P:



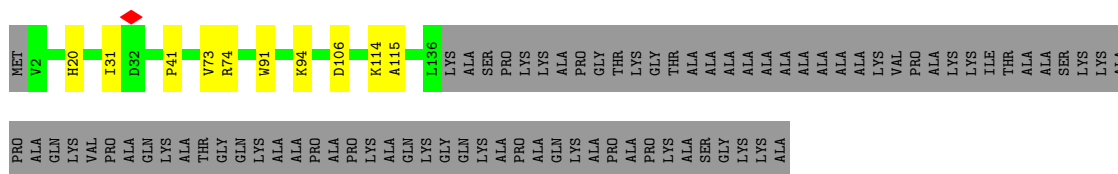
- Molecule 20: 60S ribosomal protein L13

Chain Q:



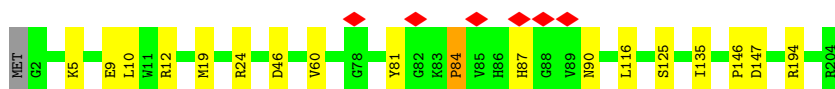
- Molecule 21: 60S ribosomal protein L14

Chain S:



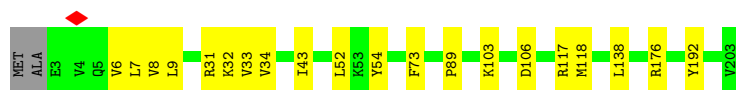
- Molecule 22: 60S ribosomal protein L15

Chain U:



- Molecule 23: 60S ribosomal protein L13a

Chain V:  89% 10%



- Molecule 24: 60S ribosomal protein L37a

Chain X:  7% 86% 13%



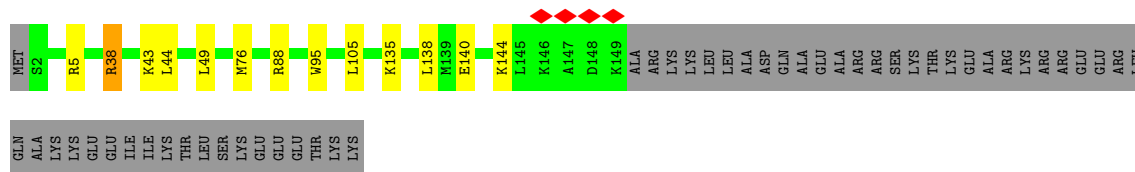
- Molecule 25: 60S ribosomal protein L18

Chain Z:  68% 12% 20%



- Molecule 26: 60S ribosomal protein L19

Chain a:  69% 6% 24%



- Molecule 27: 60S ribosomal protein L18a

Chain b:  88% 12%



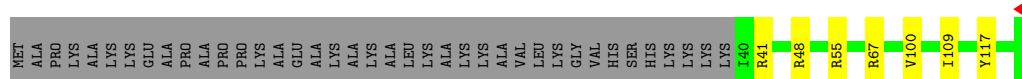
- Molecule 28: 60S ribosomal protein L23

Chain e:  80% 14% 6%



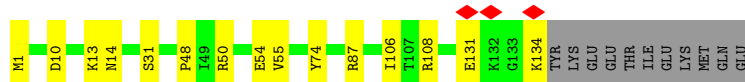
- Molecule 29: 60S ribosomal protein L23a

Chain g:  71% 25%



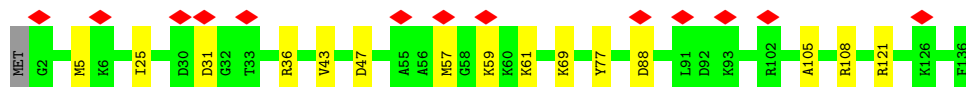
- Molecule 30: 60S ribosomal protein L26

Chain h:  82% 10% 8%



- Molecule 31: 60S ribosomal protein L27

Chain i:  10% 88% 11%



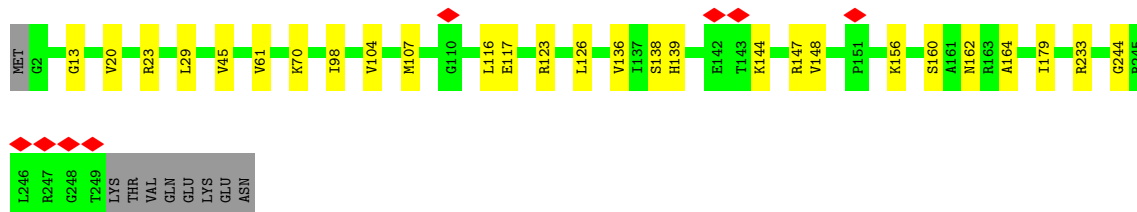
- Molecule 32: 60S ribosomal protein L28

Chain l:  88% 9%



- Molecule 33: 60S ribosomal protein L8

Chain m:  86% 11%



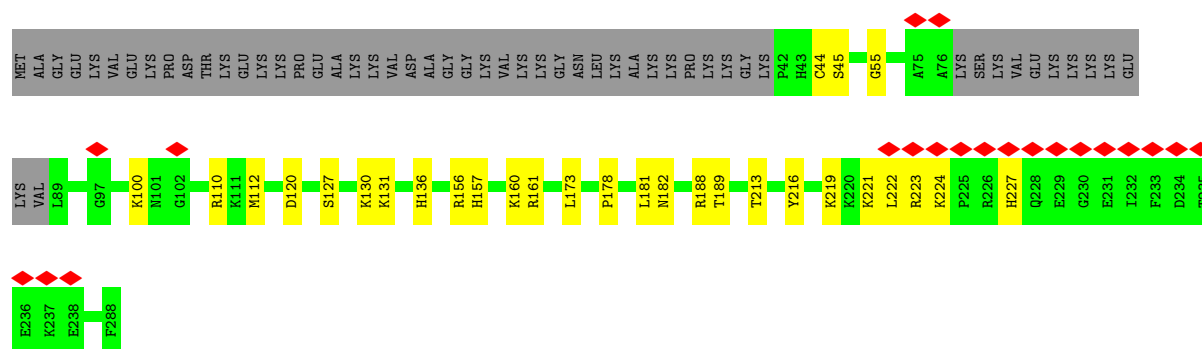
- Molecule 34: 60S ribosomal protein L35a

Chain n:  93% 5%

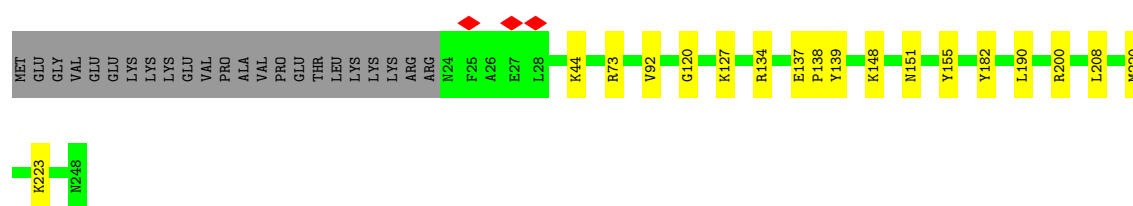
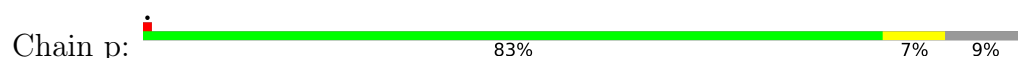


- Molecule 35: 60S ribosomal protein L6

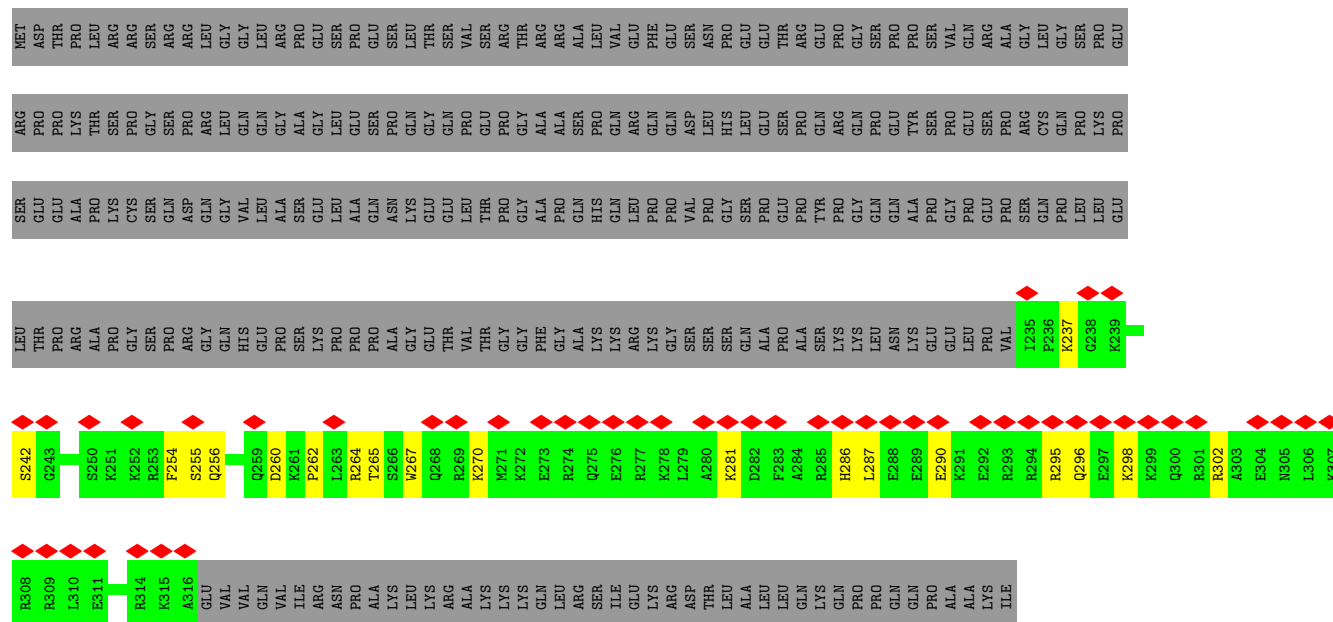
Chain o:  7% 72% 10% 18%



- Molecule 36: 60S ribosomal protein L7

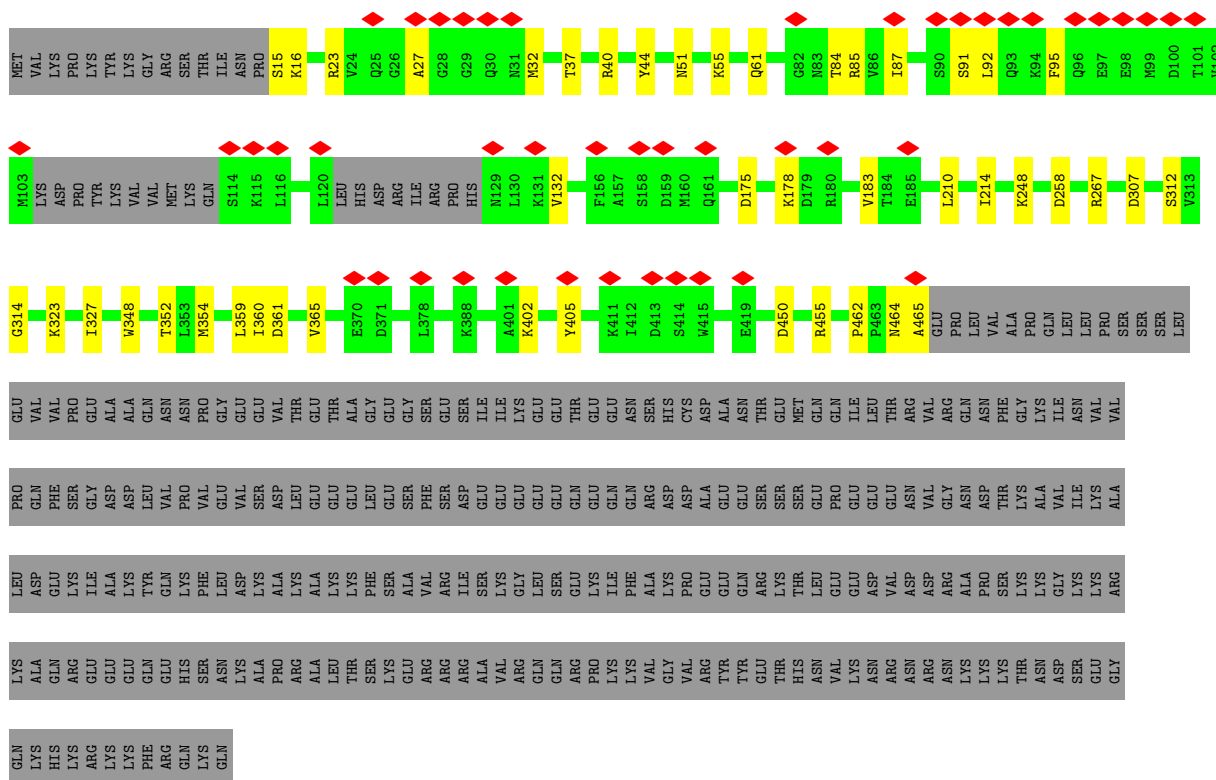


- Molecule 37: Coiled-coil domain-containing protein 86

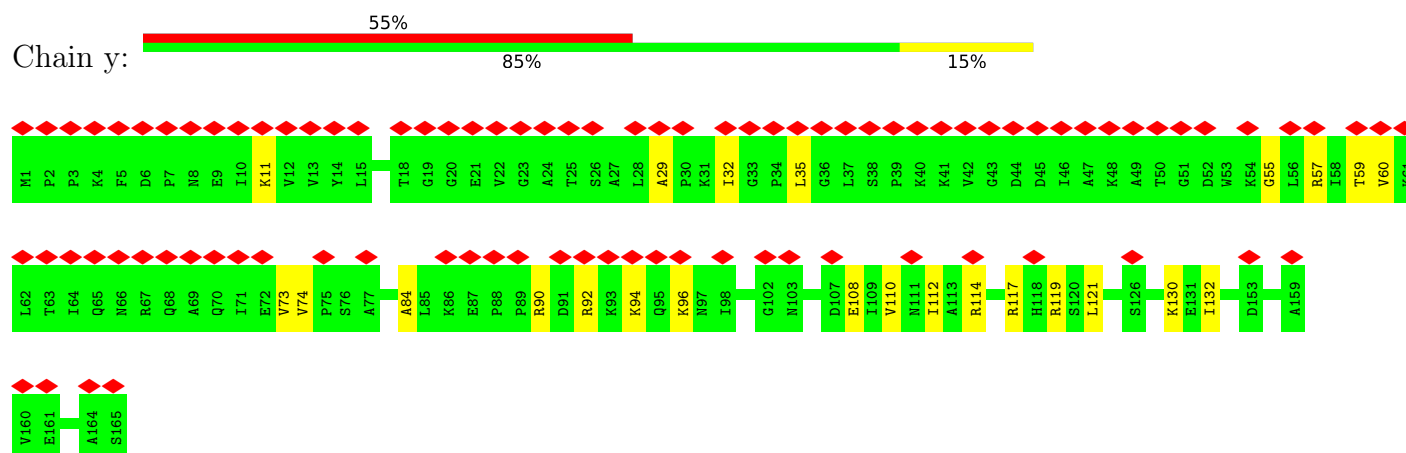


- Molecule 38: Guanine nucleotide-binding protein-like 3

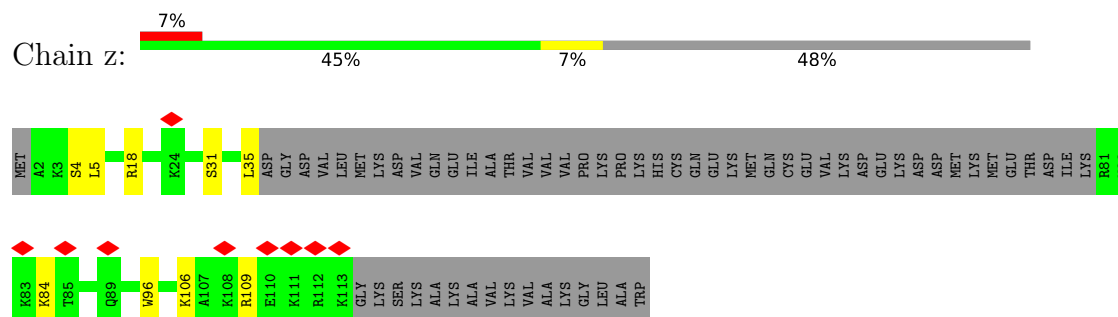




- Molecule 40: 60S ribosomal protein L12



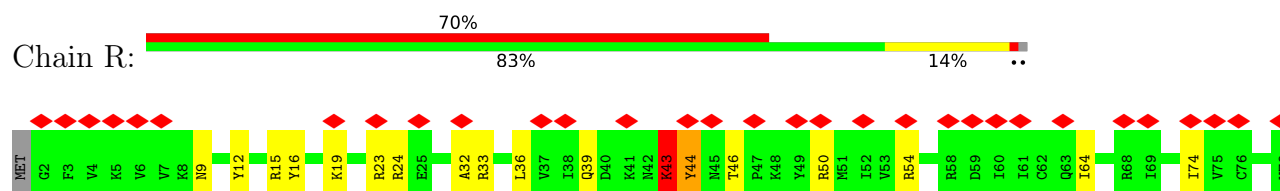
- Molecule 41: Protein LLP homolog

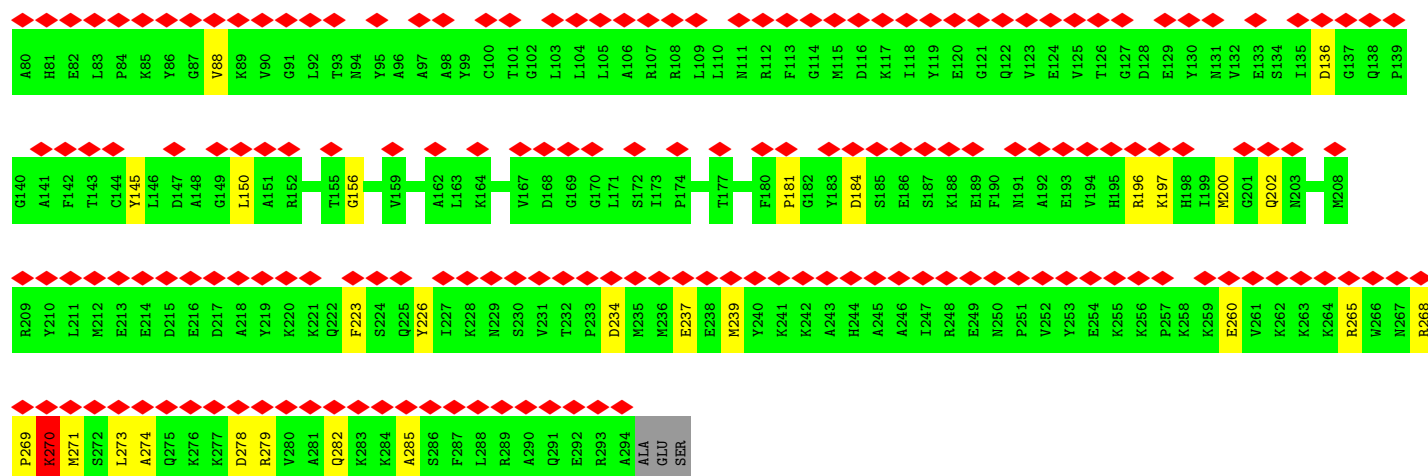


- Molecule 42: 60S ribosomal protein L11

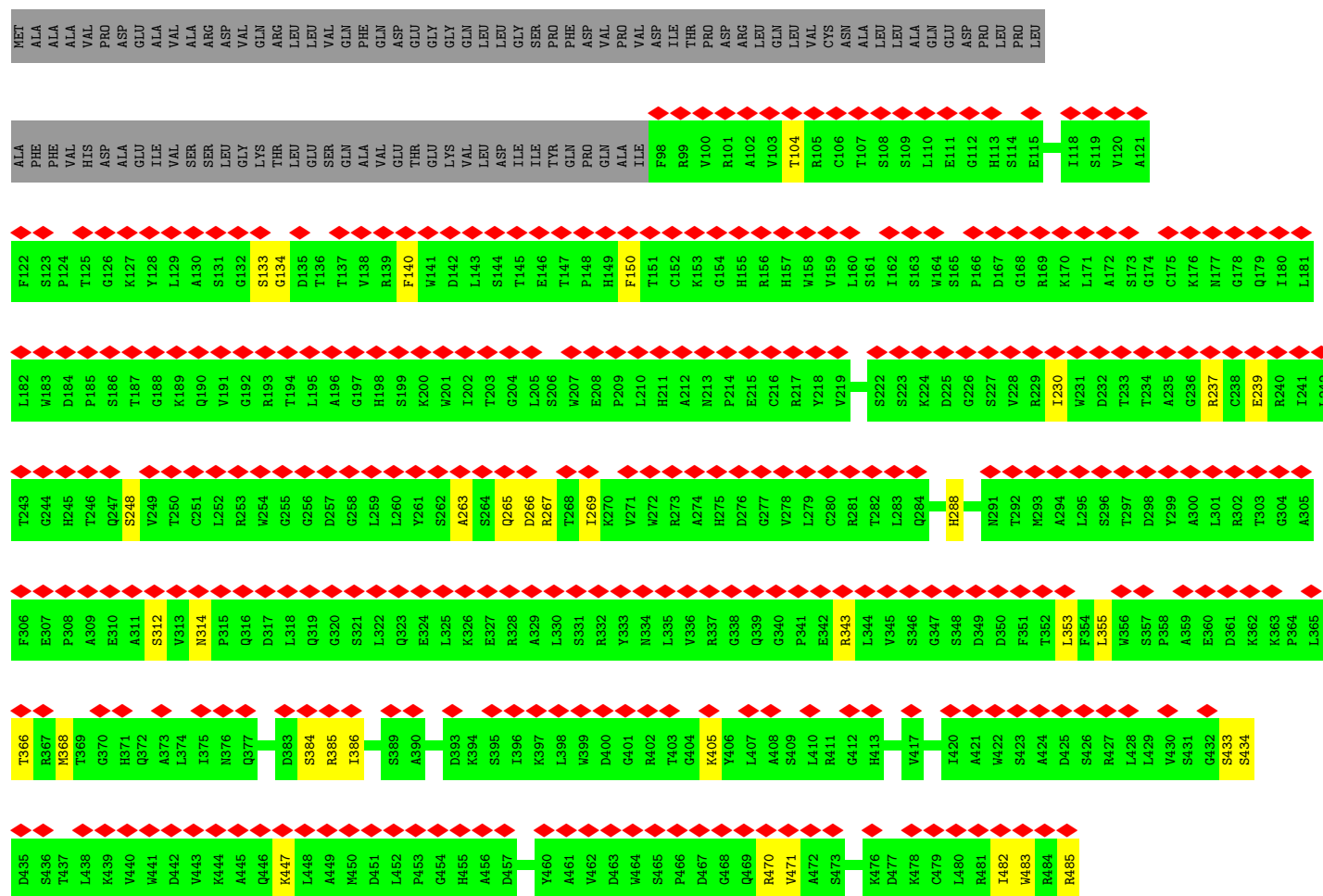
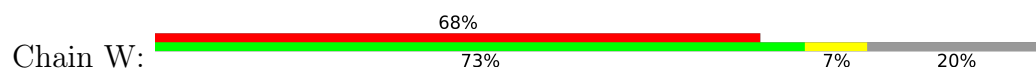


- Molecule 43: 60S ribosomal protein L5



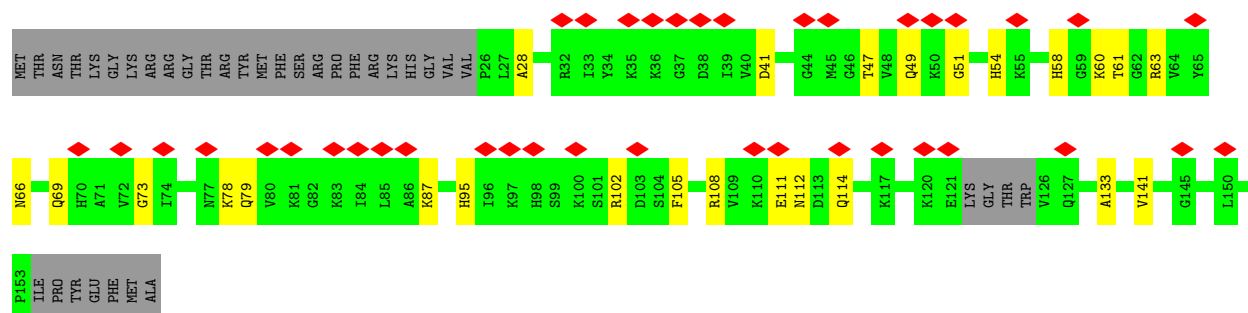


• Molecule 44: Notchless protein homolog 1

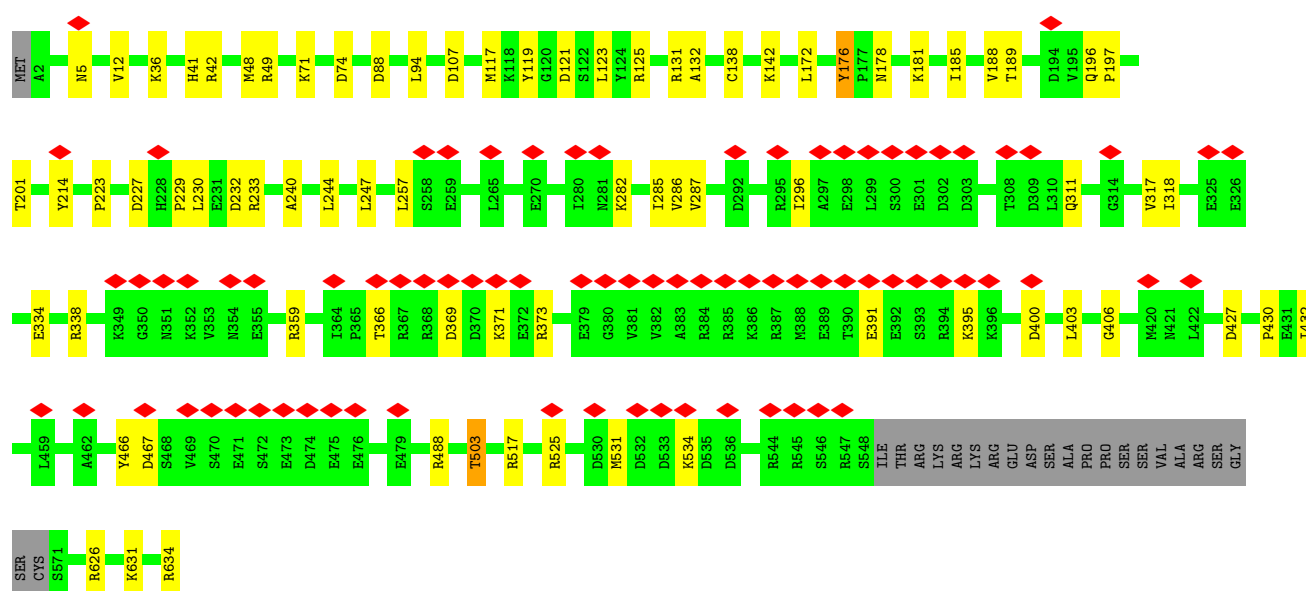
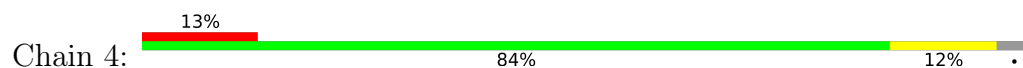


• Molecule 45: 60S ribosomal protein L21

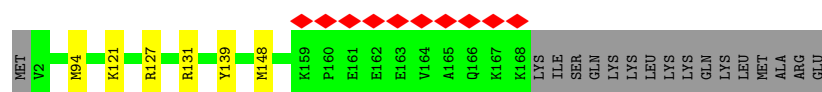
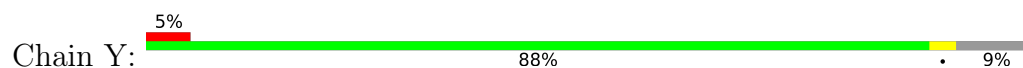




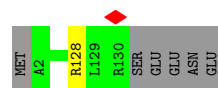
• Molecule 46: GTP-binding protein 4



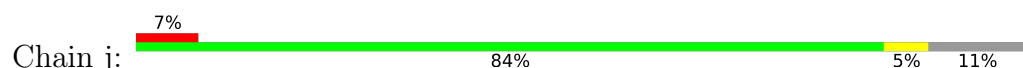
• Molecule 47: 60S ribosomal protein L17

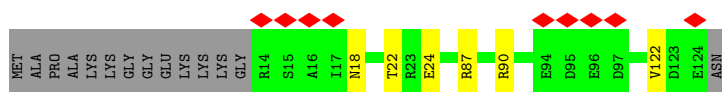


• Molecule 48: 60S ribosomal protein L32

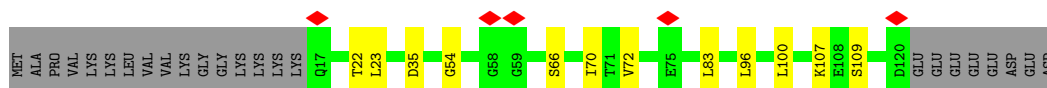


• Molecule 49: 60S ribosomal protein L31

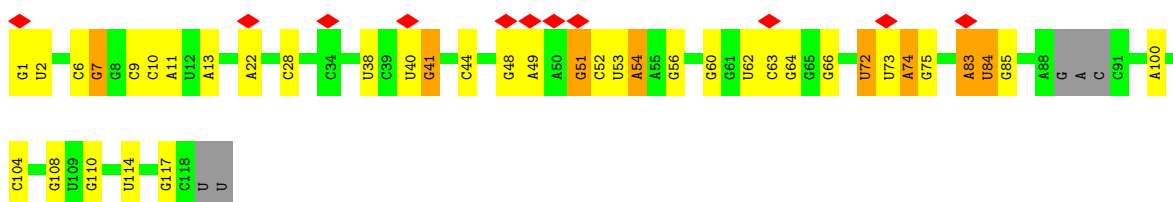




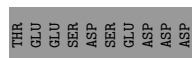
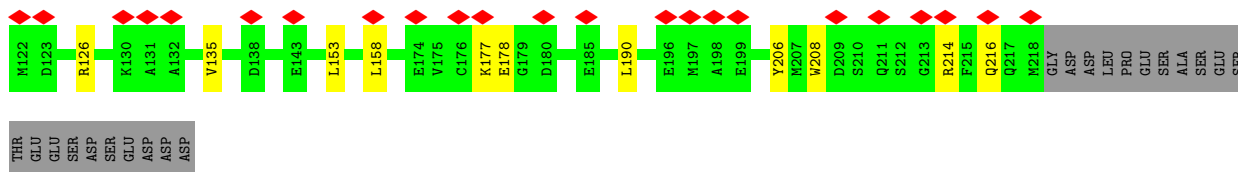
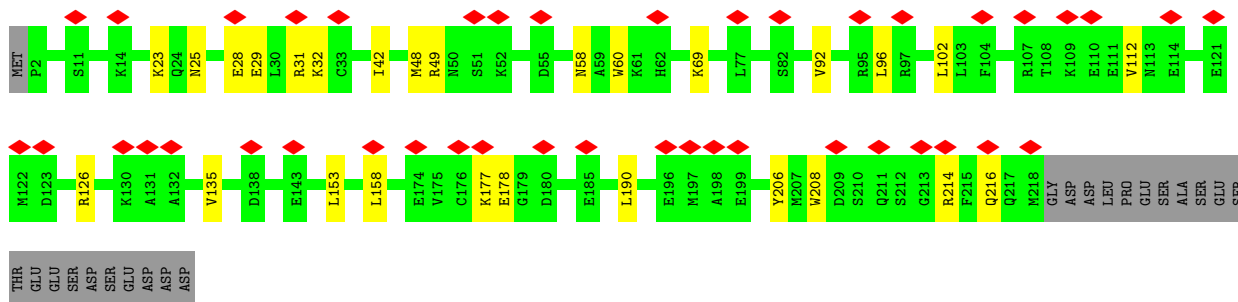
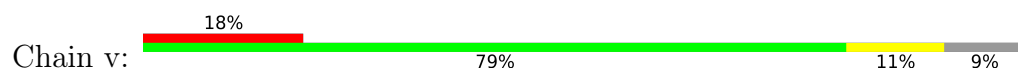
- Molecule 50: 60S ribosomal protein L22



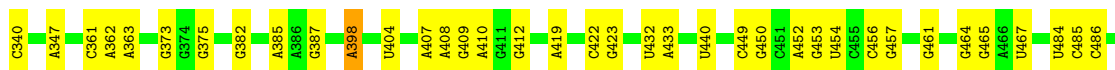
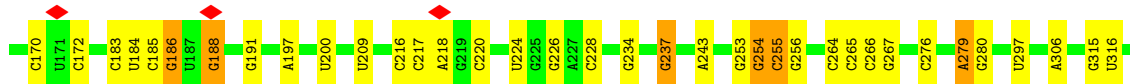
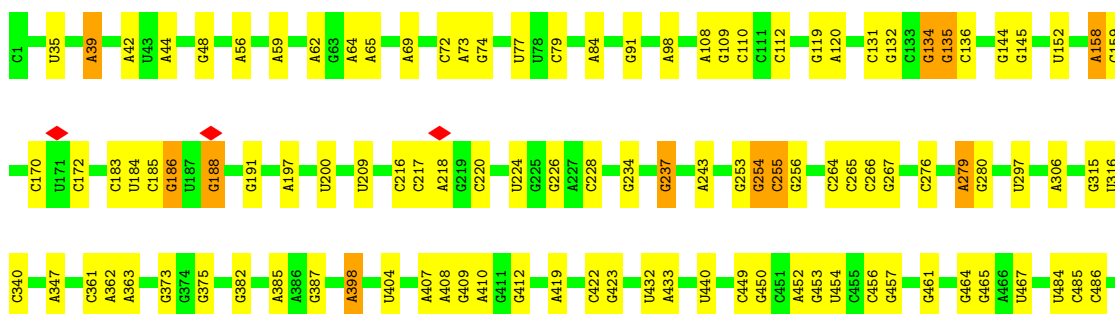
- Molecule 51: 5S rRNA



- Molecule 52: mRNA turnover protein 4 homolog

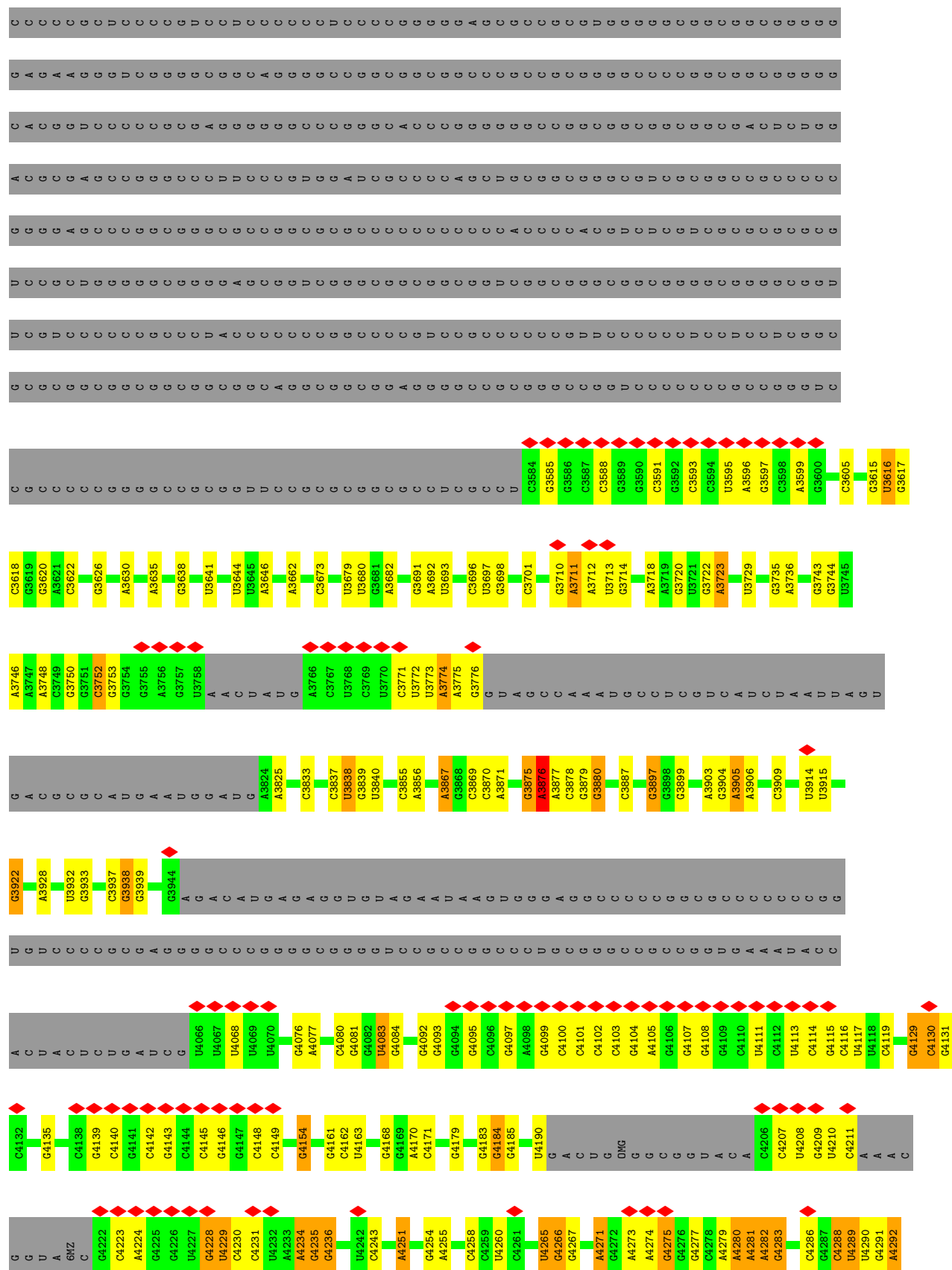


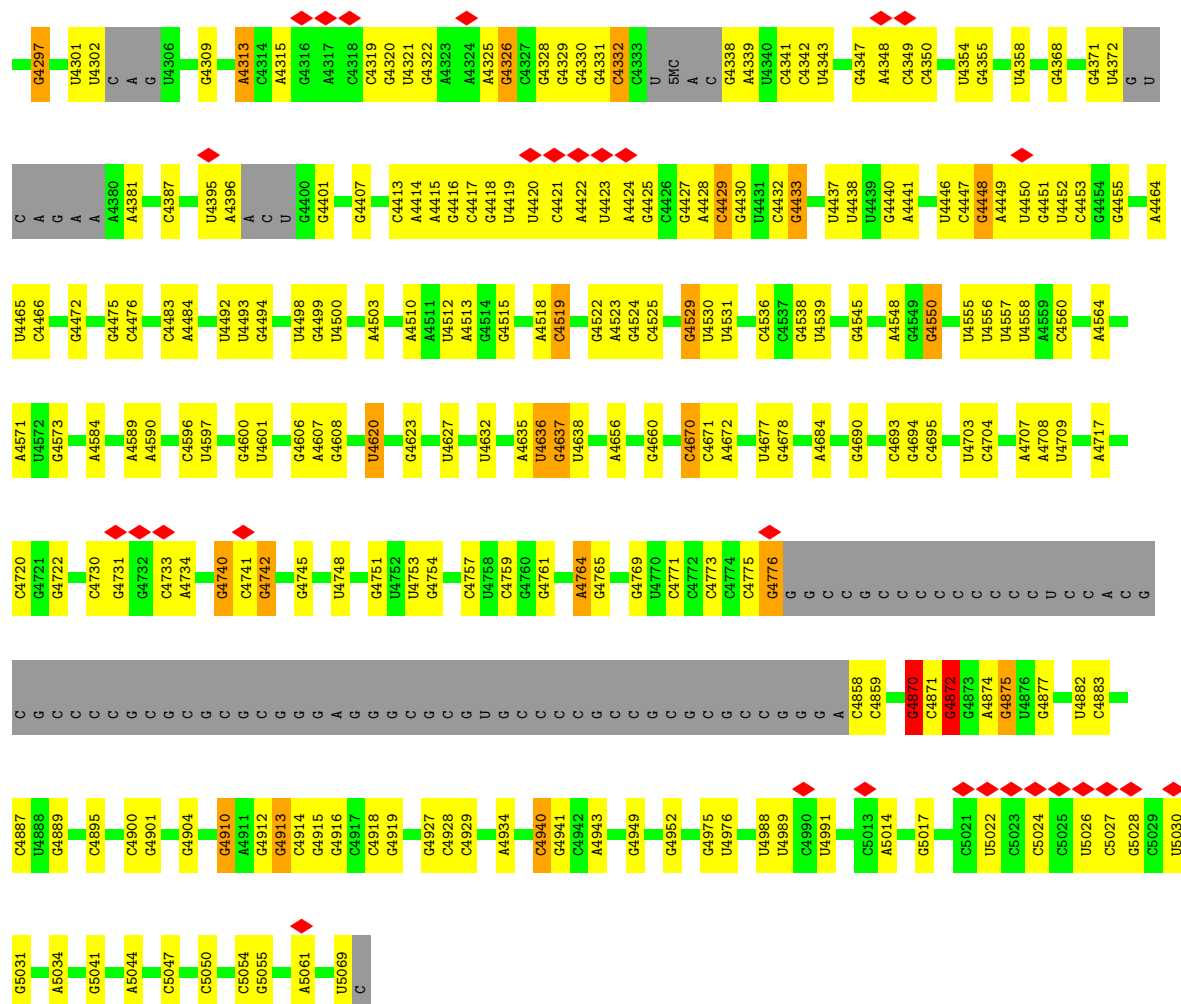
- Molecule 53: 28S rRNA











4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24229	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.8	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.205	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.031	Depositor
Map size (Å)	548.0, 548.0, 548.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	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, E7G, 2MG, P7G, B8T, OMU, GTP, P4U, B8Q, OMC, MG, 7MG, 5MU, I4U, UR3, B8K, B9H, BGH, B8W, M7A, B9B, OMG

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	N	0.37	1/2772 (0.0%)	0.72	0/3738
2	6	0.27	0/1877	0.66	0/2554
3	7	0.31	0/1181	0.64	0/1563
4	8	0.21	0/3679	0.38	0/5732
5	9	0.30	0/723	0.70	0/961
6	A	0.28	0/354	0.69	0/465
7	B	0.27	0/3315	0.66	4/4435 (0.1%)
8	D	0.27	0/2907	0.61	3/3905 (0.1%)
9	E	0.32	0/774	0.72	0/1038
10	F	0.26	0/878	0.56	0/1170
11	G	0.34	0/1960	0.70	2/2637 (0.1%)
12	H	0.31	0/1023	0.60	0/1351
13	I	0.29	0/1537	0.68	0/2066
14	J	0.24	0/1808	0.52	0/2414
15	K	0.29	0/843	0.68	0/1115
16	L	0.25	0/893	0.57	0/1193
17	M	0.27	0/720	0.61	0/952
18	O	0.28	0/575	0.65	0/761
19	P	0.26	0/454	0.54	0/599
20	Q	0.29	0/1732	0.62	0/2315
21	S	0.34	0/1133	0.72	2/1516 (0.1%)
22	U	0.42	1/1746 (0.1%)	0.79	6/2338 (0.3%)
23	V	0.29	0/1682	0.59	1/2250 (0.0%)
24	X	0.28	0/718	0.61	0/953
25	Z	0.24	0/1239	0.59	1/1658 (0.1%)
26	a	0.30	0/1255	0.74	4/1662 (0.2%)
27	b	0.26	0/1501	0.55	0/2013
28	e	0.26	0/993	0.63	0/1332
29	g	0.27	0/975	0.60	2/1312 (0.2%)
30	h	0.26	0/1132	0.59	0/1504
31	i	0.28	0/1130	0.66	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	l	0.26	0/1017	0.57	0/1364
33	m	0.29	0/1936	0.70	4/2596 (0.2%)
34	n	0.25	0/895	0.64	2/1198 (0.2%)
35	o	0.28	0/1935	0.71	2/2596 (0.1%)
36	p	0.34	0/1916	0.64	1/2553 (0.0%)
37	r	0.38	0/732	0.79	0/960
38	u	0.37	0/585	0.85	4/767 (0.5%)
39	w	0.28	0/3541	0.65	0/4775
40	y	0.37	0/1269	0.81	2/1712 (0.1%)
41	z	0.32	0/587	0.76	0/767
42	C	0.34	0/1341	0.84	3/1793 (0.2%)
43	R	0.34	0/2428	0.82	6/3252 (0.2%)
44	W	0.27	0/3093	0.66	2/4196 (0.0%)
45	T	0.31	0/1018	0.80	4/1357 (0.3%)
46	4	0.34	0/5099	0.82	13/6840 (0.2%)
47	Y	0.24	0/1383	0.56	0/1856
48	k	0.25	0/1082	0.59	0/1443
49	j	0.28	0/933	0.63	0/1256
50	d	0.35	0/864	0.88	4/1160 (0.3%)
51	3	0.24	0/2739	0.49	2/4266 (0.0%)
52	v	0.29	0/1806	0.68	0/2420
53	2	0.26	2/82131 (0.0%)	0.46	21/128040 (0.0%)
All	All	0.28	4/161839 (0.0%)	0.56	95/236176 (0.0%)

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	N	0	1
8	D	0	1
34	n	0	1
38	u	0	1
40	y	0	1
43	R	0	2
45	T	0	1
46	4	0	1
53	2	0	1
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	U	84	PRO	CG-CD	-12.94	1.06	1.50
53	2	3876	A	N9-C4	7.22	1.52	1.37
1	N	190	ARG	CA-C	6.92	1.62	1.52
53	2	3876	A	C1'-N9	5.56	1.55	1.47

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	U	84	PRO	N-CD-CG	-18.54	75.38	103.20
53	2	1871	A2M	OP2-P-O3'	-15.77	70.50	105.20
53	2	1871	A2M	OP1-P-O3'	14.46	137.01	105.20
53	2	1872	G	OP1-P-OP2	-13.41	79.36	119.60
22	U	84	PRO	CA-CB-CG	-11.79	82.11	104.50

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	D	231	ASN	Peptide
1	N	380	ASN	Peptide
34	n	106	TYR	Peptide
38	u	54	ALA	Peptide
40	y	55	GLY	Peptide

5.2 Too-close contacts

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	N	2719	0	2797	22	0
2	6	1852	0	1828	20	0
3	7	1159	0	1224	10	0
4	8	3315	0	1685	11	0
5	9	711	0	724	12	0
6	A	352	0	398	3	0
7	B	3244	0	3389	21	0
8	D	2853	0	3028	25	0
9	E	764	0	804	4	0
10	F	868	0	963	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	G	1927	0	2074	21	0
12	H	1015	0	1148	7	0
13	I	1518	0	1601	11	0
14	J	1772	0	1892	10	0
15	K	832	0	917	6	0
16	L	877	0	938	2	0
17	M	705	0	741	7	0
18	O	569	0	637	2	0
19	P	444	0	483	5	0
20	Q	1701	0	1818	9	0
21	S	1111	0	1174	8	0
22	U	1701	0	1749	13	0
23	V	1650	0	1794	13	0
24	X	708	0	760	8	0
25	Z	1223	0	1330	15	0
26	a	1239	0	1363	10	0
27	b	1461	0	1502	16	0
28	e	979	0	1039	11	0
29	g	958	0	1027	5	0
30	h	1115	0	1205	11	0
31	i	1107	0	1182	10	0
32	l	1002	0	1068	3	0
33	m	1898	0	1993	15	0
34	n	876	0	912	5	0
35	o	1897	0	2046	23	0
36	p	1878	0	2009	12	0
37	r	723	0	770	16	0
38	u	578	0	643	10	0
39	w	3472	0	3529	33	0
40	y	1250	0	1305	17	0
41	z	581	0	656	7	0
42	C	1319	0	1358	12	0
43	R	2382	0	2410	40	0
44	W	3018	0	2959	19	0
45	T	1001	0	1064	17	0
46	4	5016	0	5153	46	0
47	Y	1355	0	1389	5	0
48	k	1064	0	1160	1	0
49	j	918	0	964	3	0
50	d	850	0	868	6	0
51	3	2453	0	1243	19	0
52	v	1771	0	1810	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	2	75023	0	37751	304	0
54	w	32	0	12	0	0
55	w	1	0	0	0	0
All	All	152807	0	116286	731	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 3.

The worst 5 of 731 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)
53:2:4083:5MU:C5	53:2:4083:5MU:C4	1.79	1.64
40:y:121:LEU:HD22	52:v:58:ASN:ND2	1.46	1.29
43:R:19:LYS:NZ	53:2:4265:U:O4	1.78	1.17
45:T:49:GLN:NE2	53:2:4282:A:N3	2.06	1.02
53:2:4297:G:H1	53:2:4313:A:H2	0.98	0.96

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	N	324/687 (47%)	313 (97%)	11 (3%)	0	100	100
2	6	242/245 (99%)	227 (94%)	15 (6%)	0	100	100
3	7	133/163 (82%)	130 (98%)	3 (2%)	0	100	100
5	9	82/134 (61%)	75 (92%)	7 (8%)	0	100	100
6	A	41/159 (26%)	41 (100%)	0	0	100	100
7	B	401/403 (100%)	384 (96%)	17 (4%)	0	100	100
8	D	356/427 (83%)	335 (94%)	21 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	E	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
10	F	107/117 (92%)	105 (98%)	2 (2%)	0	100	100
11	G	239/266 (90%)	231 (97%)	8 (3%)	0	100	100
12	H	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
13	I	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
14	J	213/260 (82%)	208 (98%)	5 (2%)	0	100	100
15	K	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
16	L	108/148 (73%)	101 (94%)	7 (6%)	0	100	100
17	M	84/97 (87%)	79 (94%)	5 (6%)	0	100	100
18	O	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
19	P	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
20	Q	208/211 (99%)	198 (95%)	10 (5%)	0	100	100
21	S	133/215 (62%)	126 (95%)	7 (5%)	0	100	100
22	U	201/204 (98%)	190 (94%)	10 (5%)	1 (0%)	24	59
23	V	199/203 (98%)	191 (96%)	8 (4%)	0	100	100
24	X	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
25	Z	149/188 (79%)	147 (99%)	2 (1%)	0	100	100
26	a	146/196 (74%)	143 (98%)	3 (2%)	0	100	100
27	b	174/176 (99%)	167 (96%)	7 (4%)	0	100	100
28	e	129/140 (92%)	120 (93%)	9 (7%)	0	100	100
29	g	115/156 (74%)	111 (96%)	4 (4%)	0	100	100
30	h	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
31	i	133/136 (98%)	128 (96%)	4 (3%)	1 (1%)	16	50
32	l	123/137 (90%)	117 (95%)	6 (5%)	0	100	100
33	m	246/257 (96%)	224 (91%)	22 (9%)	0	100	100
34	n	107/110 (97%)	103 (96%)	4 (4%)	0	100	100
35	o	231/288 (80%)	217 (94%)	14 (6%)	0	100	100
36	p	224/248 (90%)	217 (97%)	7 (3%)	0	100	100
37	r	80/360 (22%)	76 (95%)	4 (5%)	0	100	100
38	u	64/549 (12%)	57 (89%)	5 (8%)	2 (3%)	3	22
39	w	427/731 (58%)	411 (96%)	13 (3%)	3 (1%)	18	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	y	163/165 (99%)	156 (96%)	7 (4%)	0	100	100
41	z	63/129 (49%)	63 (100%)	0	0	100	100
42	C	163/178 (92%)	152 (93%)	11 (7%)	0	100	100
43	R	291/297 (98%)	271 (93%)	17 (6%)	3 (1%)	12	45
44	W	386/485 (80%)	369 (96%)	16 (4%)	1 (0%)	36	68
45	T	120/160 (75%)	109 (91%)	11 (9%)	0	100	100
46	4	607/634 (96%)	558 (92%)	46 (8%)	3 (0%)	24	59
47	Y	165/184 (90%)	156 (94%)	9 (6%)	0	100	100
48	k	127/135 (94%)	121 (95%)	6 (5%)	0	100	100
49	j	109/125 (87%)	104 (95%)	5 (5%)	0	100	100
50	d	102/128 (80%)	92 (90%)	10 (10%)	0	100	100
52	v	215/239 (90%)	204 (95%)	11 (5%)	0	100	100
All	All	8770/11363 (77%)	8341 (95%)	415 (5%)	14 (0%)	44	73

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
38	u	55	PRO
44	W	267	ARG
38	u	14	THR
39	w	27	ALA
46	4	88	ASP

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	N	308/629 (49%)	308 (100%)	0	100	100
2	6	212/213 (100%)	212 (100%)	0	100	100
3	7	126/149 (85%)	126 (100%)	0	100	100
5	9	74/114 (65%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	A	34/126 (27%)	34 (100%)	0	100	100
7	B	349/349 (100%)	349 (100%)	0	100	100
8	D	298/348 (86%)	298 (100%)	0	100	100
9	E	83/97 (86%)	83 (100%)	0	100	100
10	F	94/100 (94%)	94 (100%)	0	100	100
11	G	203/223 (91%)	203 (100%)	0	100	100
12	H	109/110 (99%)	109 (100%)	0	100	100
13	I	169/171 (99%)	169 (100%)	0	100	100
14	J	191/228 (84%)	191 (100%)	0	100	100
15	K	86/89 (97%)	86 (100%)	0	100	100
16	L	94/121 (78%)	94 (100%)	0	100	100
17	M	73/80 (91%)	73 (100%)	0	100	100
18	O	64/65 (98%)	64 (100%)	0	100	100
19	P	47/48 (98%)	47 (100%)	0	100	100
20	Q	176/177 (99%)	176 (100%)	0	100	100
21	S	115/161 (71%)	115 (100%)	0	100	100
22	U	171/172 (99%)	171 (100%)	0	100	100
23	V	173/174 (99%)	173 (100%)	0	100	100
24	X	74/75 (99%)	74 (100%)	0	100	100
25	Z	136/165 (82%)	136 (100%)	0	100	100
26	a	133/175 (76%)	133 (100%)	0	100	100
27	b	157/157 (100%)	156 (99%)	1 (1%)	78	84
28	e	101/107 (94%)	101 (100%)	0	100	100
29	g	105/133 (79%)	105 (100%)	0	100	100
30	h	124/135 (92%)	124 (100%)	0	100	100
31	i	117/118 (99%)	117 (100%)	0	100	100
32	l	109/121 (90%)	109 (100%)	0	100	100
33	m	190/199 (96%)	190 (100%)	0	100	100
34	n	88/89 (99%)	88 (100%)	0	100	100
35	o	208/252 (82%)	208 (100%)	0	100	100
36	p	195/215 (91%)	195 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	r	76/312 (24%)	76 (100%)	0	100	100
38	u	62/485 (13%)	62 (100%)	0	100	100
39	w	385/654 (59%)	385 (100%)	0	100	100
40	y	137/137 (100%)	137 (100%)	0	100	100
41	z	61/115 (53%)	61 (100%)	0	100	100
42	C	138/149 (93%)	138 (100%)	0	100	100
43	R	246/250 (98%)	245 (100%)	1 (0%)	84	86
44	W	322/404 (80%)	322 (100%)	0	100	100
45	T	109/140 (78%)	109 (100%)	0	100	100
46	4	554/574 (96%)	554 (100%)	0	100	100
47	Y	147/163 (90%)	147 (100%)	0	100	100
48	k	115/121 (95%)	115 (100%)	0	100	100
49	j	101/110 (92%)	101 (100%)	0	100	100
50	d	94/115 (82%)	94 (100%)	0	100	100
52	v	194/214 (91%)	193 (100%)	1 (0%)	81	85
All	All	7727/9828 (79%)	7724 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	b	77	ASN
43	R	270	LYS
52	v	216	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
39	w	255	ASN
46	4	436	HIS
40	y	66	ASN
44	W	177	ASN
47	Y	133	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	8	155/156 (99%)	30 (19%)	0
51	3	113/120 (94%)	25 (22%)	2 (1%)
53	2	3472/5054 (68%)	869 (25%)	19 (0%)
All	All	3740/5330 (70%)	924 (24%)	21 (0%)

5 of 924 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	8	25	G
4	8	34	U
4	8	35	C
4	8	39	G
4	8	48	A

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	2	3905	A
53	2	4555	U
53	2	4913	G
53	2	4636	U
53	2	4415	A

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

68 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
53	OMU	2	4620	53	19,22,23	2.92	8 (42%)	26,31,34	1.70	5 (19%)
53	B8K	2	3897	53	24,28,29	3.44	11 (45%)	30,42,45	2.55	11 (36%)
53	OMC	2	2861	53	19,22,23	3.04	8 (42%)	26,31,34	1.18	3 (11%)
53	A2M	2	2363	53	22,25,26	3.20	9 (40%)	31,36,39	2.98	11 (35%)
53	BGH	2	3899	53	25,29,30	4.52	17 (68%)	31,43,46	2.59	11 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	OMC	2	2804	53	19,22,23	2.96	8 (42%)	26,31,34	0.76	0
53	OMC	2	3887	53	19,22,23	3.04	8 (42%)	26,31,34	1.06	2 (7%)
53	A2M	2	4523	53	22,25,26	3.18	9 (40%)	31,36,39	3.04	11 (35%)
53	5MU	2	4083	53	19,22,23	7.24	8 (42%)	28,32,35	3.38	10 (35%)
53	A2M	2	1524	53	22,25,26	3.18	9 (40%)	31,36,39	3.00	11 (35%)
53	A2M	2	2401	53	22,25,26	3.20	10 (45%)	31,36,39	2.97	11 (35%)
53	I4U	2	1659	53	21,24,25	3.51	9 (42%)	27,34,37	1.15	2 (7%)
53	A2M	2	1871	53	22,25,26	3.20	10 (45%)	31,36,39	3.13	12 (38%)
53	B8W	2	4472	53	23,26,27	2.80	5 (21%)	33,38,41	2.50	14 (42%)
53	OMG	2	2364	53	23,26,27	2.63	8 (34%)	33,38,41	2.76	10 (30%)
53	B8W	2	4185	53	23,26,27	2.73	6 (26%)	33,38,41	2.65	12 (36%)
53	A2M	2	3718	53	22,25,26	3.23	9 (40%)	31,36,39	2.84	10 (32%)
53	7MG	2	2522	53	22,26,27	3.73	10 (45%)	29,39,42	1.99	8 (27%)
53	B8T	2	4483	53	19,22,23	3.61	8 (42%)	26,31,34	1.45	5 (19%)
53	OMC	2	3701	53	19,22,23	3.02	8 (42%)	26,31,34	0.75	0
53	A2M	2	1534	53	22,25,26	3.20	9 (40%)	31,36,39	3.10	12 (38%)
53	B9B	2	1574	53	25,28,29	1.71	6 (24%)	35,40,43	5.16	11 (31%)
53	2MG	2	978	53	23,26,27	3.01	9 (39%)	32,38,41	2.23	9 (28%)
53	OMG	2	1883	53	23,26,27	2.68	8 (34%)	33,38,41	2.68	11 (33%)
53	UR3	2	4597	53	19,22,23	2.75	7 (36%)	26,32,35	1.91	4 (15%)
53	B8T	2	4671	53	19,22,23	3.57	8 (42%)	26,31,34	0.94	1 (3%)
53	B8W	2	4129	53	23,26,27	2.75	6 (26%)	33,38,41	2.75	12 (36%)
53	OMC	2	2365	53	19,22,23	2.90	8 (42%)	26,31,34	0.81	0
53	OMC	2	2422	53	19,22,23	2.99	8 (42%)	26,31,34	1.18	3 (11%)
53	OMC	2	4536	53	19,22,23	3.00	8 (42%)	26,31,34	1.08	2 (7%)
53	B8Q	2	1456	53	17,22,23	2.91	5 (29%)	22,32,35	2.24	6 (27%)
53	E7G	2	2297	53	24,27,28	3.89	11 (45%)	30,40,43	2.10	7 (23%)
53	OMG	2	4623	53	23,26,27	2.59	9 (39%)	33,38,41	2.72	13 (39%)
53	B8W	2	2380	53	23,26,27	2.70	5 (21%)	33,38,41	2.50	14 (42%)
53	OMG	2	2424	53	23,26,27	2.65	8 (34%)	33,38,41	2.72	9 (27%)
4	OMU	8	14	4,53	19,22,23	3.04	8 (42%)	26,31,34	1.74	5 (19%)
53	7MG	2	4550	53	22,26,27	3.85	10 (45%)	29,39,42	1.99	9 (31%)
53	OMG	2	373	53	23,26,27	2.66	9 (39%)	33,38,41	2.66	13 (39%)
53	B9B	2	237	53	25,28,29	1.72	6 (24%)	35,40,43	5.19	11 (31%)
53	B9H	2	2786	53	20,25,26	3.27	3 (15%)	22,35,38	2.36	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	UR3	2	4530	53	19,22,23	2.83	7 (36%)	26,32,35	1.33	3 (11%)
53	A2M	2	4571	53	22,25,26	3.21	9 (40%)	31,36,39	3.00	10 (32%)
53	2MG	2	729	53	23,26,27	2.92	8 (34%)	32,38,41	2.41	9 (28%)
53	OMG	2	1316	53	23,26,27	2.66	8 (34%)	33,38,41	2.75	12 (36%)
53	P4U	2	1348	53	21,24,25	3.48	8 (38%)	27,33,36	1.14	2 (7%)
53	7MG	2	1605	53	22,26,27	3.73	10 (45%)	29,39,42	2.01	10 (34%)
53	OMG	2	4494	53	23,26,27	2.73	8 (34%)	33,38,41	2.86	10 (30%)
53	OMG	2	4637	53	23,26,27	2.67	8 (34%)	33,38,41	2.80	10 (30%)
53	M7A	2	4564	53	20,25,26	1.99	3 (15%)	28,37,40	3.91	7 (25%)
53	B8K	2	4690	53	24,28,29	3.27	11 (45%)	30,42,45	2.57	11 (36%)
53	OMG	2	2773	53	23,26,27	2.70	8 (34%)	33,38,41	2.76	10 (30%)
53	A2M	2	1326	53	22,25,26	3.20	9 (40%)	31,36,39	2.98	10 (32%)
53	OMG	2	1522	53	23,26,27	2.63	8 (34%)	33,38,41	2.74	11 (33%)
53	P7G	2	1909	53	24,28,29	4.05	11 (45%)	27,41,44	1.50	3 (11%)
53	A2M	2	3723	53	22,25,26	3.15	9 (40%)	31,36,39	2.98	10 (32%)
53	OMG	2	1625	53	23,26,27	2.71	8 (34%)	33,38,41	2.76	10 (30%)
53	A2M	2	3825	53	22,25,26	3.18	9 (40%)	31,36,39	3.01	10 (32%)
53	OMC	2	3869	53	19,22,23	2.96	8 (42%)	26,31,34	0.93	1 (3%)
53	P7G	2	3880	53	24,28,29	4.01	11 (45%)	27,41,44	1.45	3 (11%)
53	OMG	2	4870	53	23,26,27	2.70	8 (34%)	33,38,41	2.94	10 (30%)
53	2MG	2	4872	53	23,26,27	2.85	9 (39%)	32,38,41	2.30	10 (31%)
53	B8W	2	4529	53	23,26,27	2.77	5 (21%)	33,38,41	2.57	13 (39%)
53	B9B	2	2754	53	25,28,29	1.75	5 (20%)	35,40,43	5.24	11 (31%)
53	A2M	2	398	53	22,25,26	3.22	9 (40%)	31,36,39	2.97	10 (32%)
53	A2M	2	3867	53	22,25,26	3.16	9 (40%)	31,36,39	3.07	10 (32%)
53	OMG	2	2050	53	23,26,27	2.64	8 (34%)	33,38,41	2.71	9 (27%)
53	2MG	2	1517	53	23,26,27	2.95	9 (39%)	32,38,41	2.26	9 (28%)
53	OMC	2	3909	53	19,22,23	3.13	8 (42%)	26,31,34	1.95	7 (26%)

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
53	OMU	2	4620	53	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	B8K	2	3897	53	-	3/11/41/42	0/3/3/3
53	OMC	2	2861	53	-	0/9/27/28	0/2/2/2
53	A2M	2	2363	53	-	0/9/27/28	0/3/3/3
53	BGH	2	3899	53	-	1/13/43/44	0/3/3/3
53	OMC	2	2804	53	-	0/9/27/28	0/2/2/2
53	OMC	2	3887	53	-	1/9/27/28	0/2/2/2
53	A2M	2	4523	53	-	1/9/27/28	0/3/3/3
53	5MU	2	4083	53	-	0/7/25/26	0/2/2/2
53	A2M	2	1524	53	-	1/9/27/28	0/3/3/3
53	A2M	2	2401	53	-	0/9/27/28	0/3/3/3
53	I4U	2	1659	53	-	2/9/29/30	0/2/2/2
53	A2M	2	1871	53	-	2/9/27/28	0/3/3/3
53	B8W	2	4472	53	-	2/9/27/28	0/3/3/3
53	OMG	2	2364	53	-	2/9/27/28	0/3/3/3
53	B8W	2	4185	53	-	0/9/27/28	0/3/3/3
53	A2M	2	3718	53	-	0/9/27/28	0/3/3/3
53	7MG	2	2522	53	-	0/7/37/38	0/3/3/3
53	B8T	2	4483	53	-	0/7/27/28	0/2/2/2
53	OMC	2	3701	53	-	2/9/27/28	0/2/2/2
53	A2M	2	1534	53	-	2/9/27/28	0/3/3/3
53	B9B	2	1574	53	-	4/11/29/30	0/3/3/3
53	2MG	2	978	53	-	0/9/27/28	0/3/3/3
53	OMG	2	1883	53	-	2/9/27/28	0/3/3/3
53	UR3	2	4597	53	-	0/7/25/26	0/2/2/2
53	B8T	2	4671	53	-	0/7/27/28	0/2/2/2
53	B8W	2	4129	53	-	4/9/27/28	0/3/3/3
53	OMC	2	2365	53	-	1/9/27/28	0/2/2/2
53	OMC	2	2422	53	-	1/9/27/28	0/2/2/2
53	OMC	2	4536	53	-	0/9/27/28	0/2/2/2
53	B8Q	2	1456	53	-	0/7/42/43	0/2/2/2
53	E7G	2	2297	53	-	1/9/39/40	0/3/3/3
53	OMG	2	4623	53	-	0/9/27/28	0/3/3/3
53	B8W	2	2380	53	-	3/9/27/28	0/3/3/3
53	OMG	2	2424	53	-	2/9/27/28	0/3/3/3
4	OMU	8	14	4,53	-	1/9/27/28	0/2/2/2
53	7MG	2	4550	53	-	2/7/37/38	0/3/3/3
53	OMG	2	373	53	-	1/9/27/28	0/3/3/3
53	B9B	2	237	53	-	4/11/29/30	0/3/3/3
53	B9H	2	2786	53	-	2/12/47/48	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	UR3	2	4530	53	-	0/7/25/26	0/2/2/2
53	A2M	2	4571	53	-	0/9/27/28	0/3/3/3
53	2MG	2	729	53	-	2/9/27/28	0/3/3/3
53	OMG	2	1316	53	-	0/9/27/28	0/3/3/3
53	P4U	2	1348	53	-	1/10/29/30	0/2/2/2
53	7MG	2	1605	53	-	0/7/37/38	0/3/3/3
53	OMG	2	4494	53	-	0/9/27/28	0/3/3/3
53	OMG	2	4637	53	-	4/9/27/28	0/3/3/3
53	M7A	2	4564	53	-	0/7/37/38	0/3/3/3
53	B8K	2	4690	53	-	0/11/41/42	0/3/3/3
53	OMG	2	2773	53	-	1/9/27/28	0/3/3/3
53	A2M	2	1326	53	-	0/9/27/28	0/3/3/3
53	OMG	2	1522	53	-	0/9/27/28	0/3/3/3
53	P7G	2	1909	53	-	2/10/40/41	0/3/3/3
53	A2M	2	3723	53	-	1/9/27/28	0/3/3/3
53	OMG	2	1625	53	-	2/9/27/28	0/3/3/3
53	A2M	2	3825	53	-	0/9/27/28	0/3/3/3
53	OMC	2	3869	53	-	2/9/27/28	0/2/2/2
53	P7G	2	3880	53	-	4/10/40/41	0/3/3/3
53	OMG	2	4870	53	-	2/9/27/28	0/3/3/3
53	2MG	2	4872	53	-	2/9/27/28	0/3/3/3
53	B8W	2	4529	53	-	4/9/27/28	0/3/3/3
53	B9B	2	2754	53	-	3/11/29/30	0/3/3/3
53	A2M	2	398	53	-	2/9/27/28	0/3/3/3
53	A2M	2	3867	53	-	3/9/27/28	0/3/3/3
53	OMG	2	2050	53	-	0/9/27/28	0/3/3/3
53	2MG	2	1517	53	-	3/9/27/28	0/3/3/3
53	OMC	2	3909	53	-	3/9/27/28	0/2/2/2

The worst 5 of 560 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2	4083	5MU	C4-C5	20.77	1.79	1.44
53	2	4083	5MU	C6-N1	16.04	1.65	1.38
53	2	4083	5MU	C6-C5	-11.52	1.15	1.34
53	2	4083	5MU	C4-N3	-11.04	1.18	1.38
53	2	1659	I4U	C4-N3	10.62	1.45	1.31

The worst 5 of 558 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	2	2754	B9B	O6-C6-C5	21.49	143.78	116.57
53	2	1574	B9B	O6-C6-C5	21.23	143.45	116.57
53	2	237	B9B	O6-C6-C5	21.10	143.28	116.57
53	2	2754	B9B	O6-C6-N1	-18.48	94.26	120.00
53	2	237	B9B	O6-C6-N1	-18.11	94.78	120.00

There are no chirality outliers.

5 of 88 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	8	14	OMU	C1'-C2'-O2'-CM2
53	2	237	B9B	C5-C6-O6-C61
53	2	237	B9B	N1-C6-O6-C61
53	2	237	B9B	C3'-C4'-C5'-O5'
53	2	237	B9B	O4'-C4'-C5'-O5'

There are no ring outliers.

16 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	2	4620	OMU	3	0
53	2	2363	A2M	1	0
53	2	4083	5MU	1	0
53	2	1871	A2M	1	0
53	2	2364	OMG	1	0
53	2	2522	7MG	1	0
53	2	1574	B9B	1	0
53	2	4129	B8W	1	0
53	2	1456	B8Q	1	0
53	2	729	2MG	1	0
53	2	1605	7MG	2	0
53	2	2773	OMG	1	0
53	2	3723	A2M	1	0
53	2	1625	OMG	1	0
53	2	4870	OMG	1	0
53	2	4872	2MG	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is 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	$\# Z > 2$
54	GTP	w	801	55	30,34,34	0.55	0	46,54,54	0.59	0

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
54	GTP	w	801	55	-	1/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

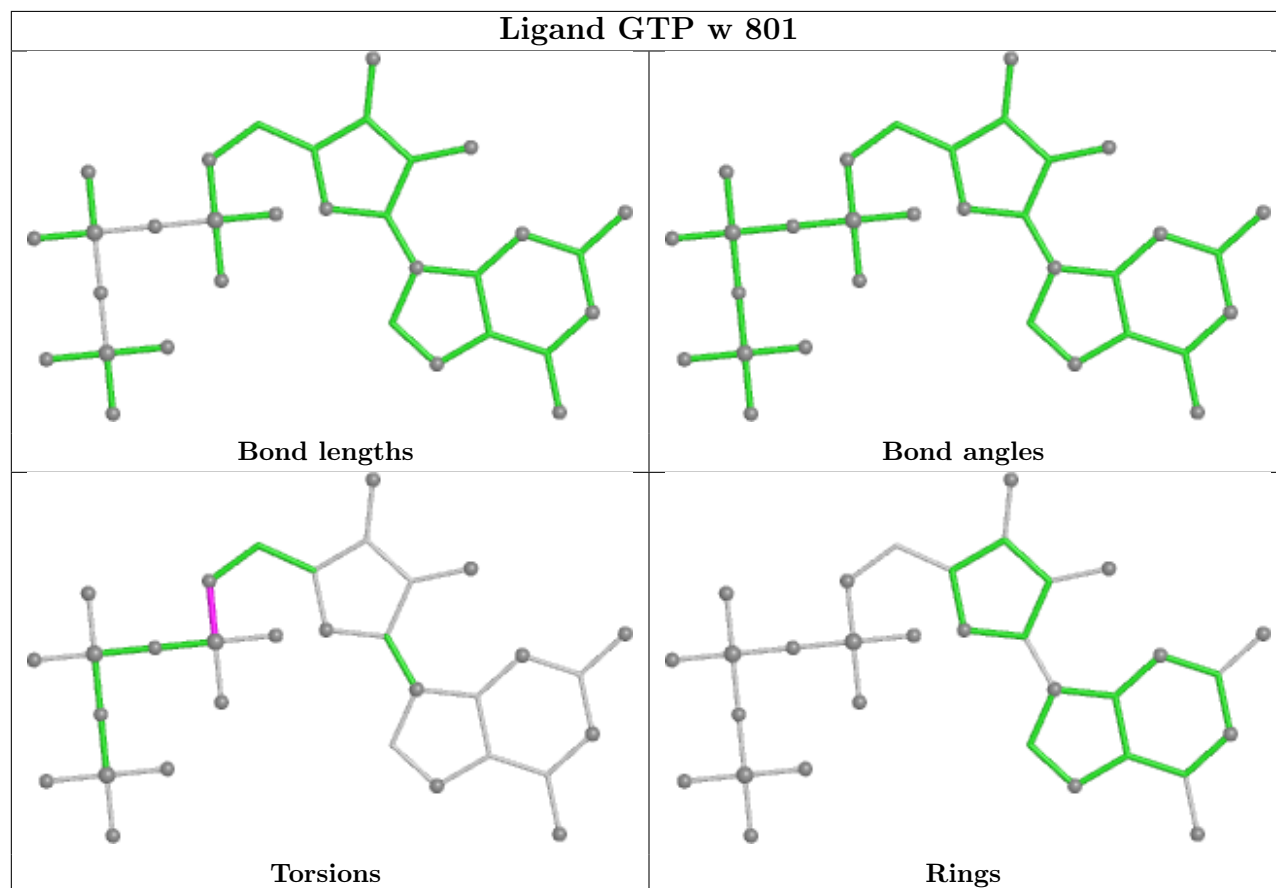
Mol	Chain	Res	Type	Atoms
54	w	801	GTP	C5'-O5'-PA-O1A

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](#)

There are no chain breaks in this entry.

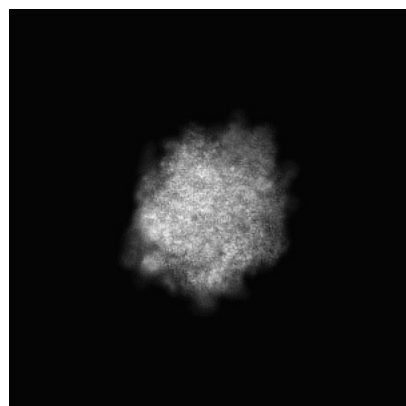
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35599. These allow visual inspection of the internal detail of the map and identification of artifacts.

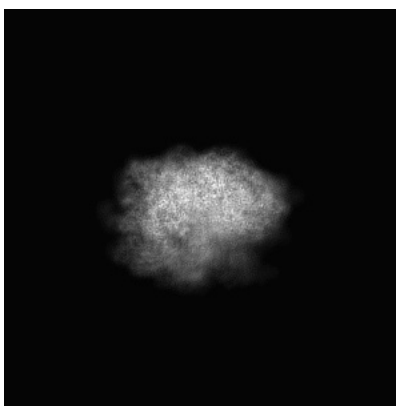
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

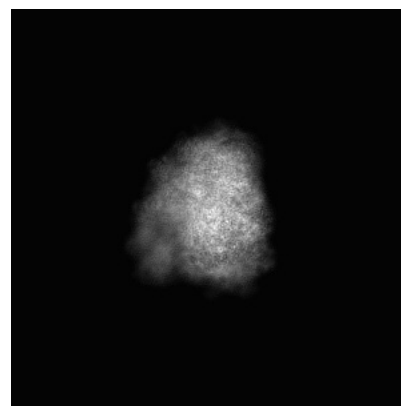
6.1.1 Primary map



X

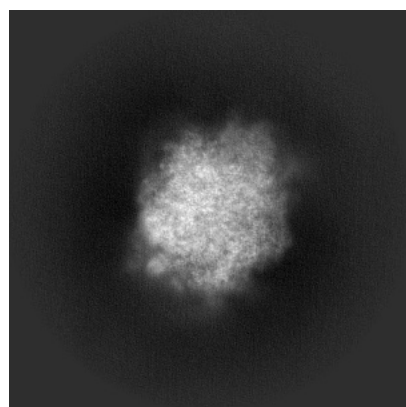


Y

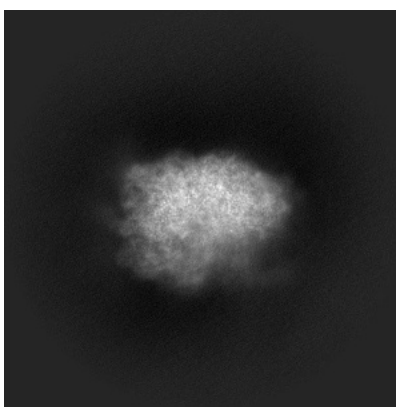


Z

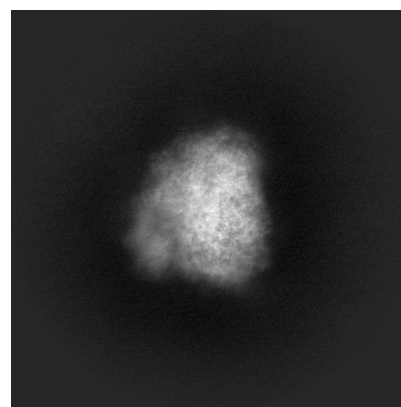
6.1.2 Raw map



X



Y

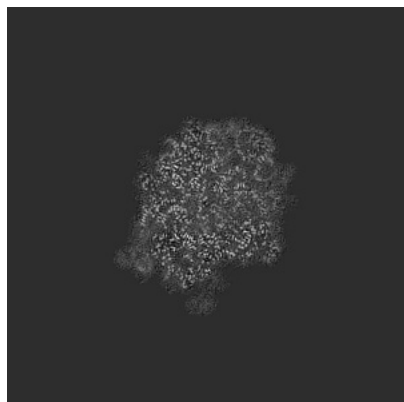


Z

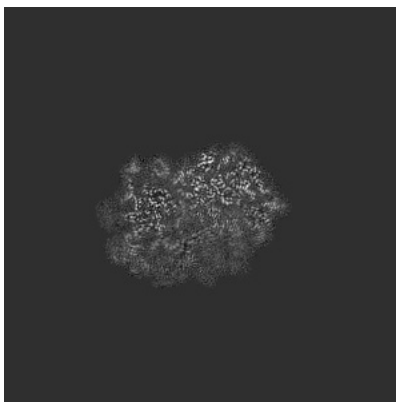
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

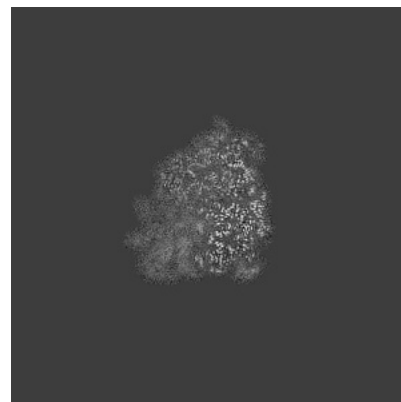
6.2.1 Primary map



X Index: 200

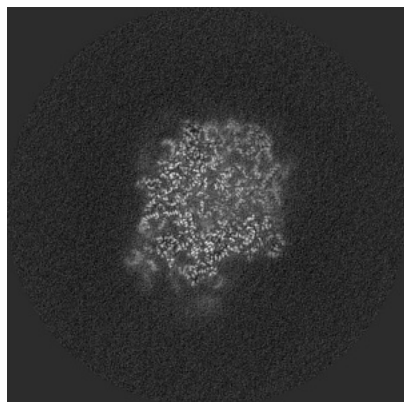


Y Index: 200

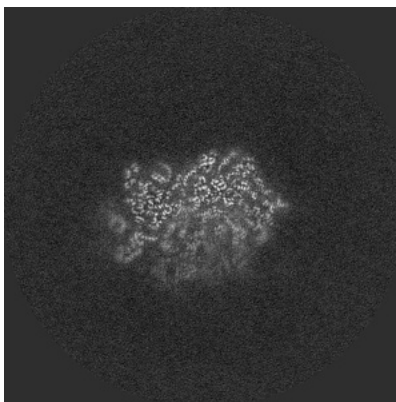


Z Index: 200

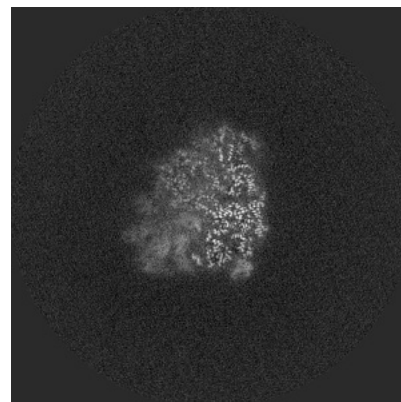
6.2.2 Raw map



X Index: 200



Y Index: 200

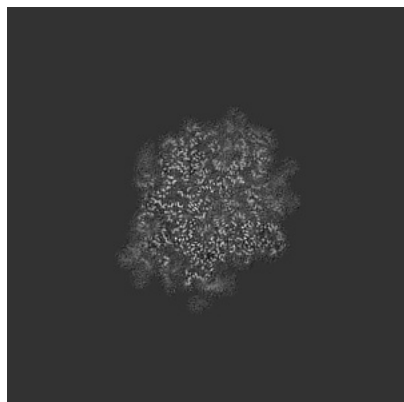


Z Index: 200

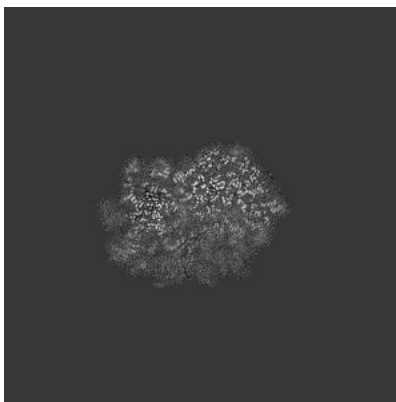
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

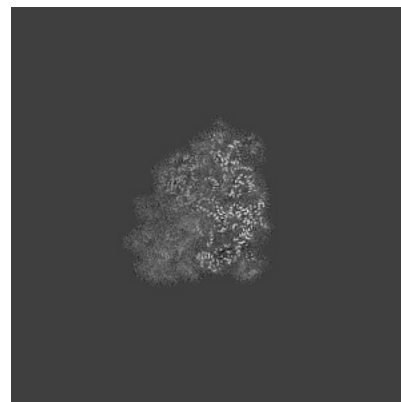
6.3.1 Primary map



X Index: 206

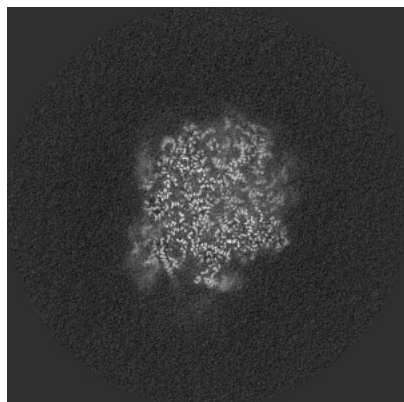


Y Index: 199

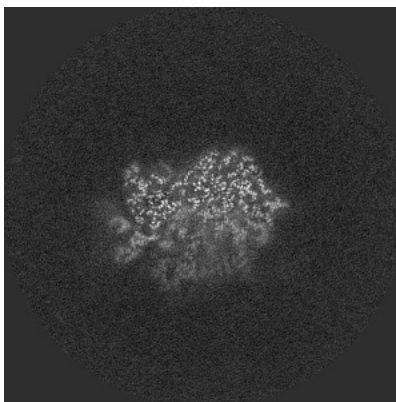


Z Index: 198

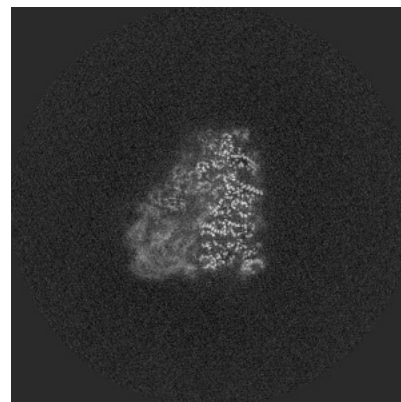
6.3.2 Raw map



X Index: 206



Y Index: 199

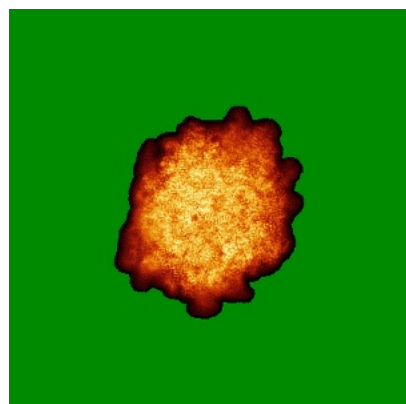


Z Index: 190

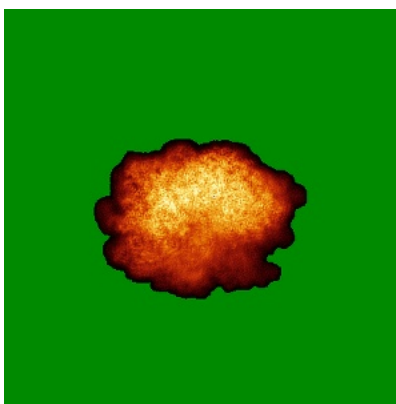
The images above show the largest variance slices of the map in three orthogonal directions.

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

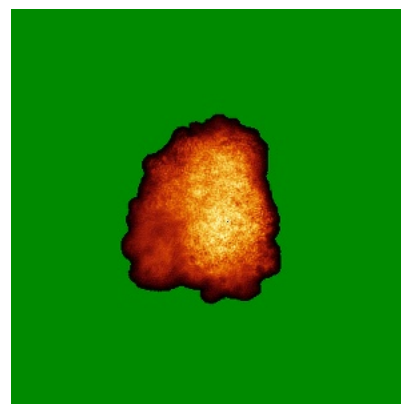
6.4.1 Primary map



X

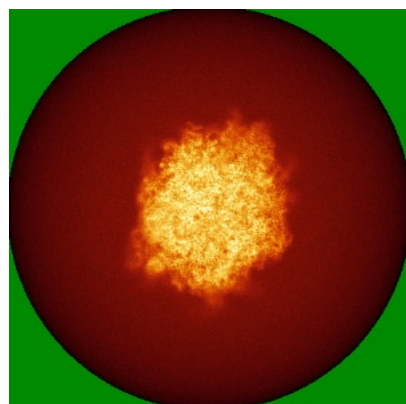


Y

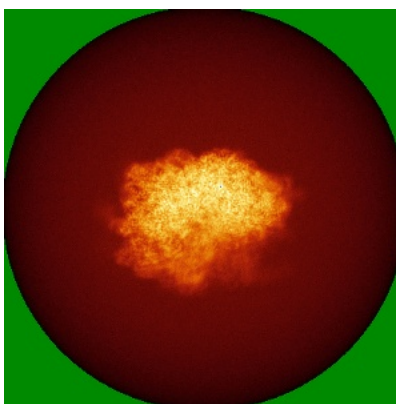


Z

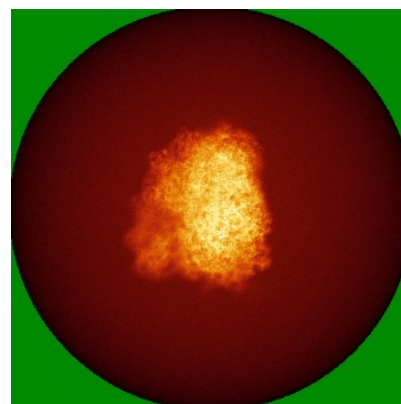
6.4.2 Raw map



X



Y

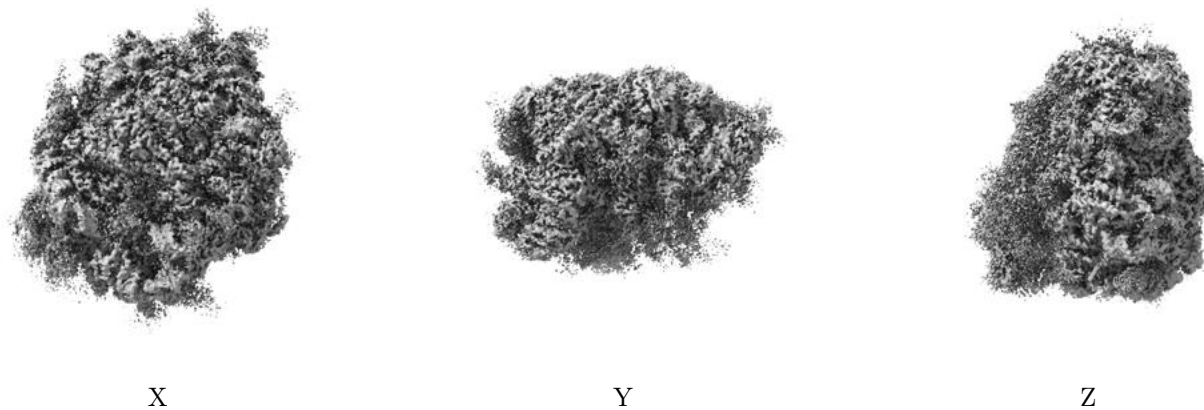


Z

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 0.031. 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.

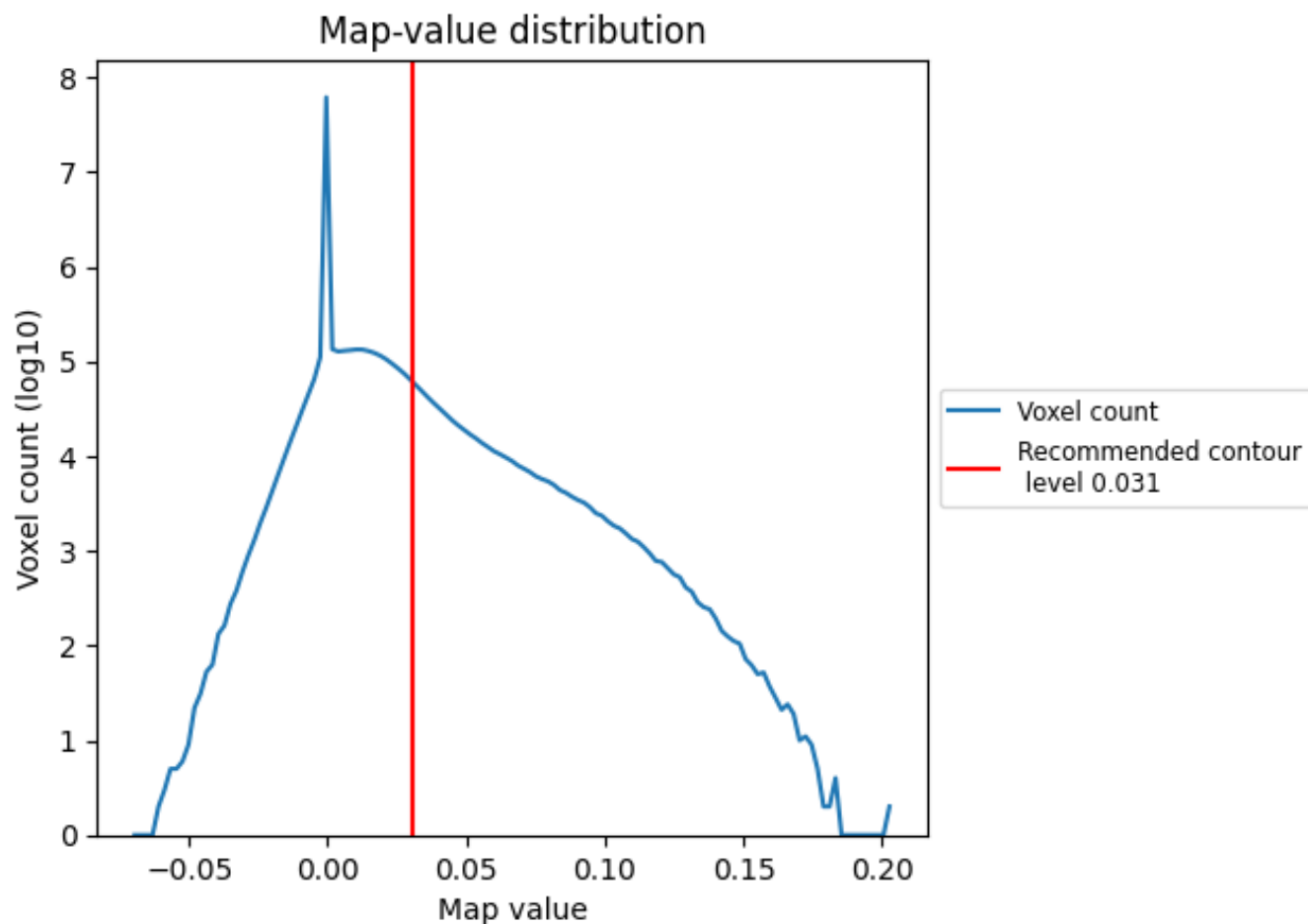
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

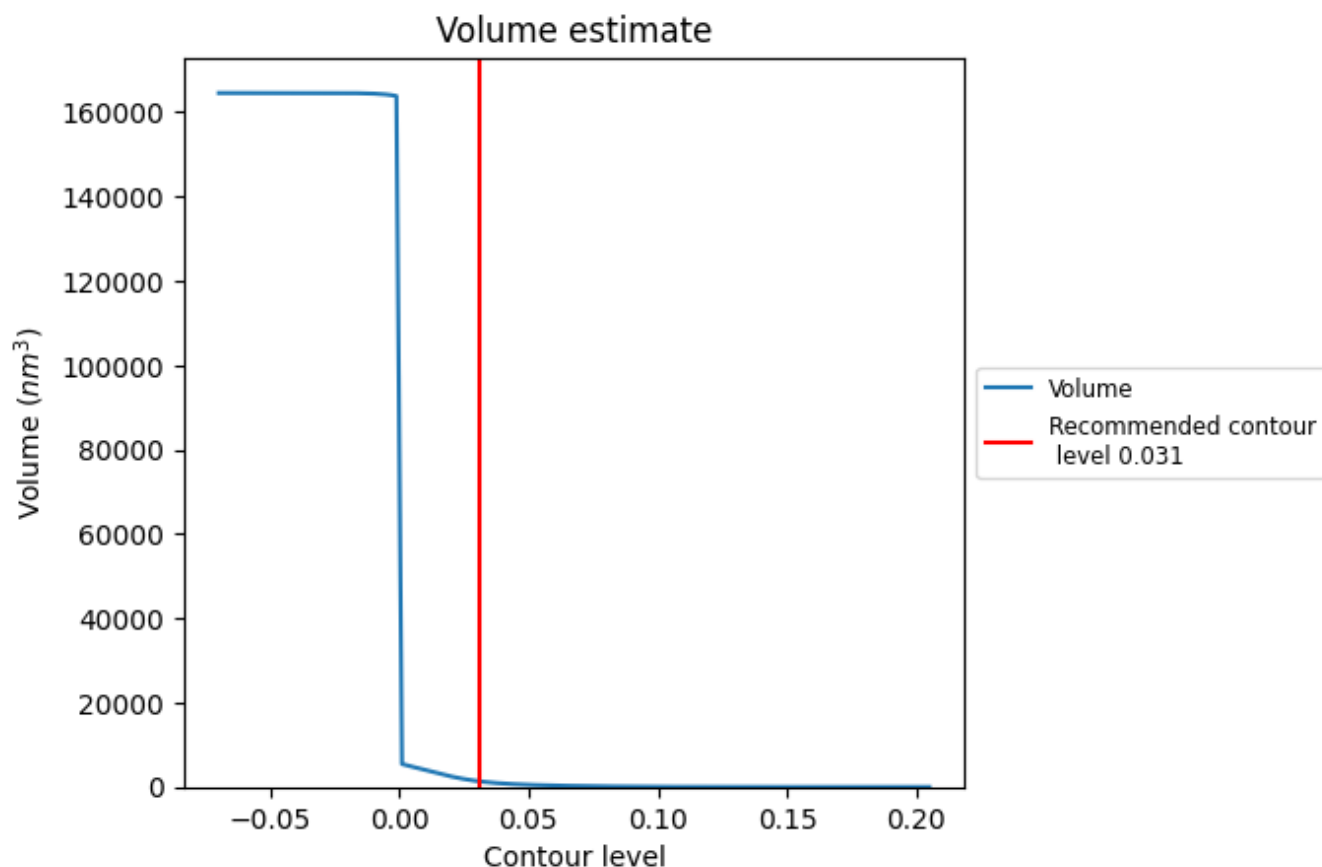
This section contains the results of statistical analysis of the map.

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.

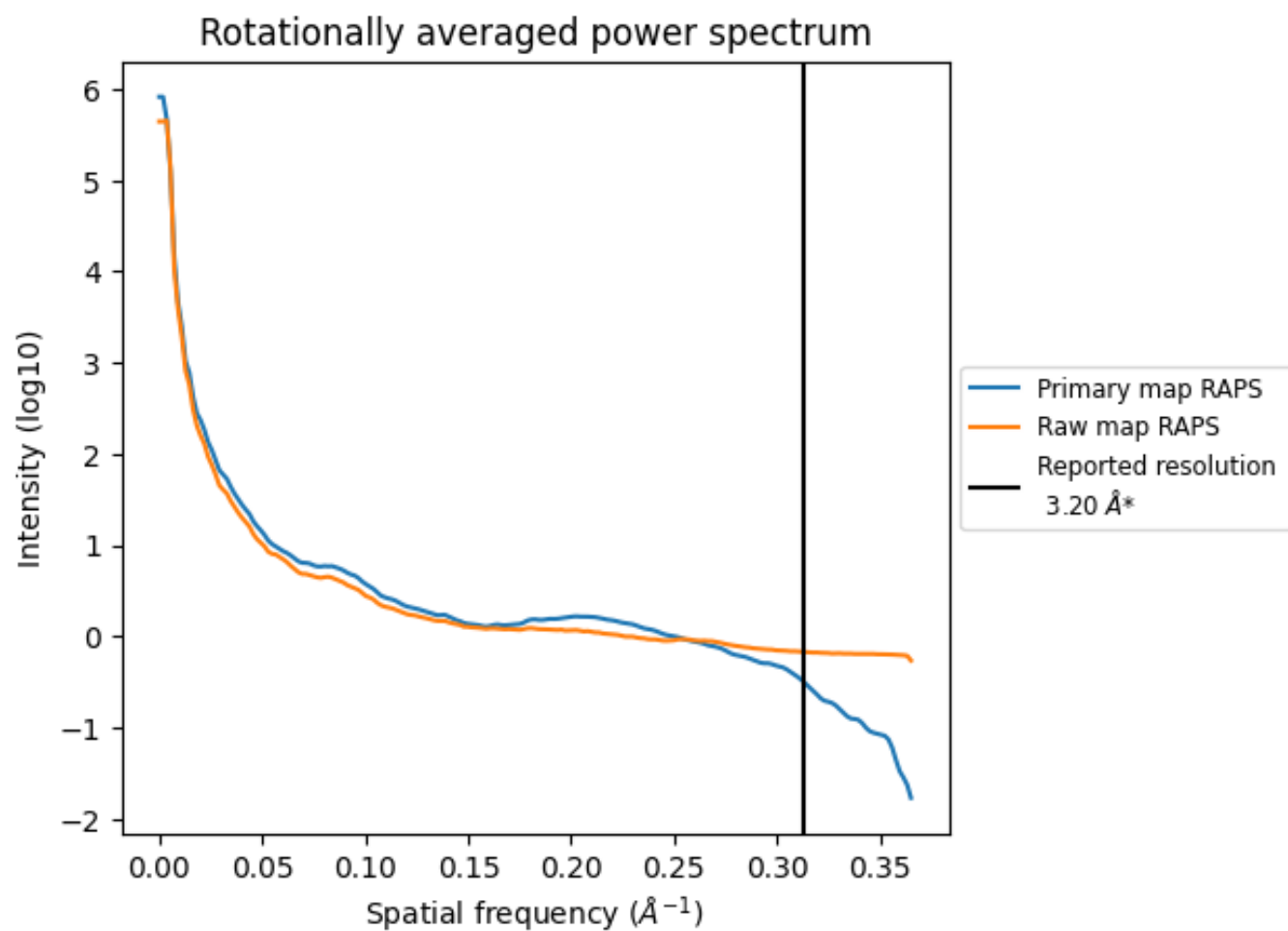
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1338 nm^3 ; this corresponds to an approximate mass of 1209 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 ⓘ

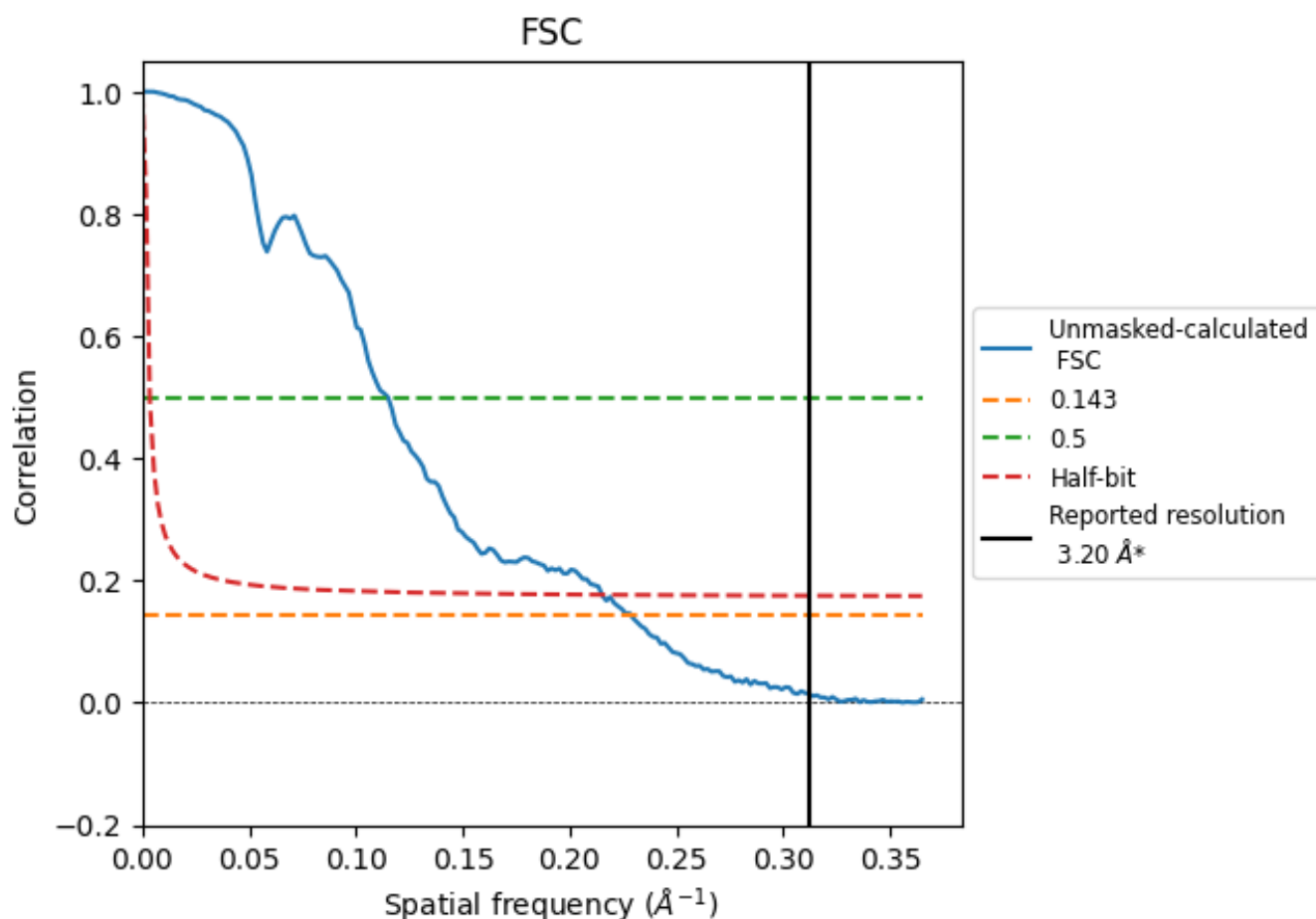


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

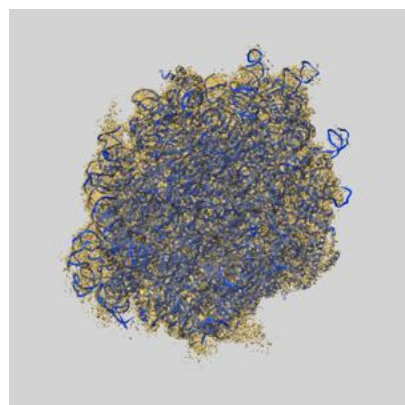
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.37	8.70	4.65

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.37 differs from the reported value 3.2 by more than 10 %

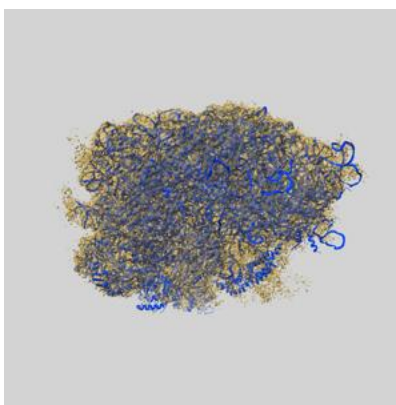
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35599 and PDB model 8INK. Per-residue inclusion information can be found in section [3](#) on page [14](#).

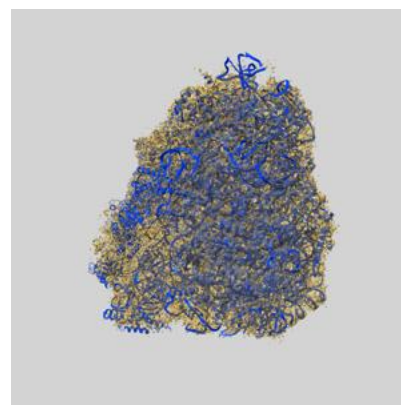
9.1 Map-model overlay [i](#)



X



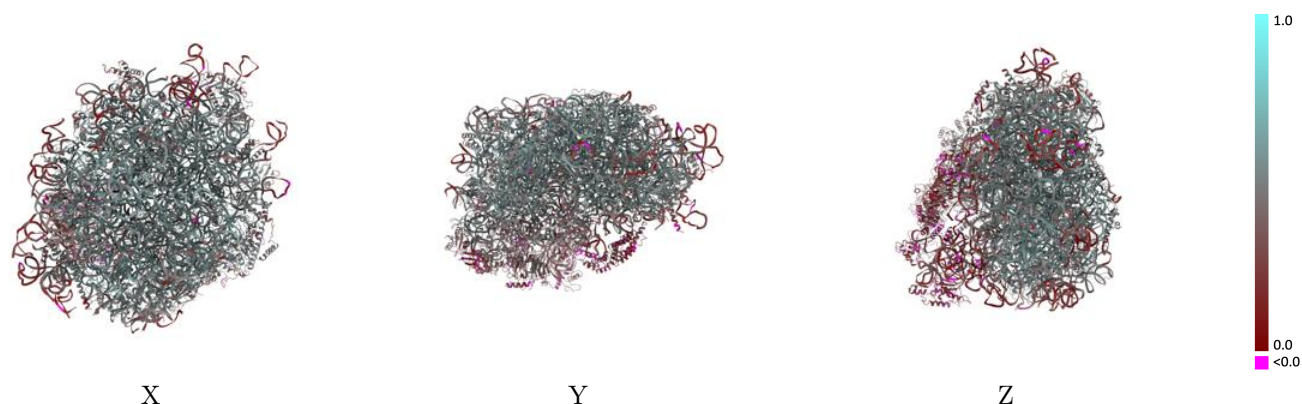
Y



Z

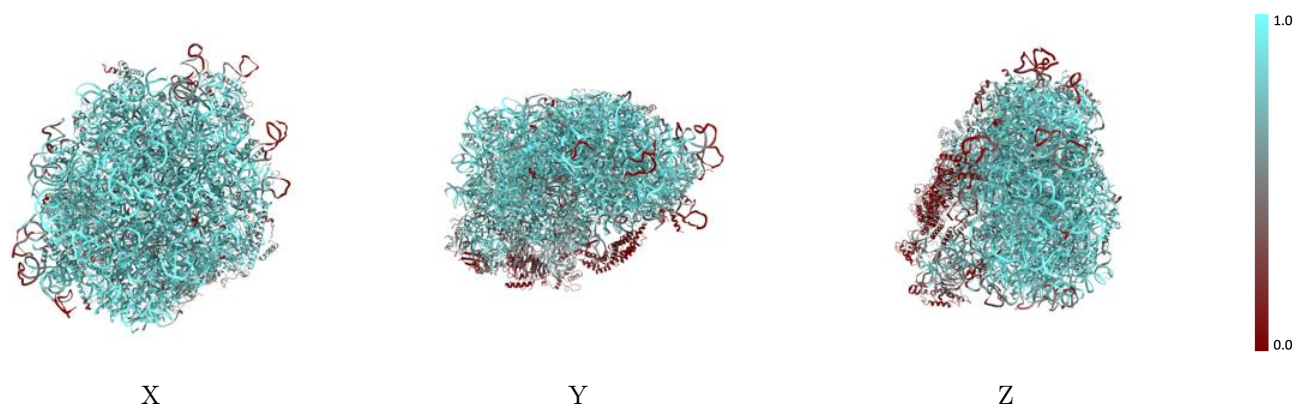
The images above show the 3D surface view of the map at the recommended contour level 0.031 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



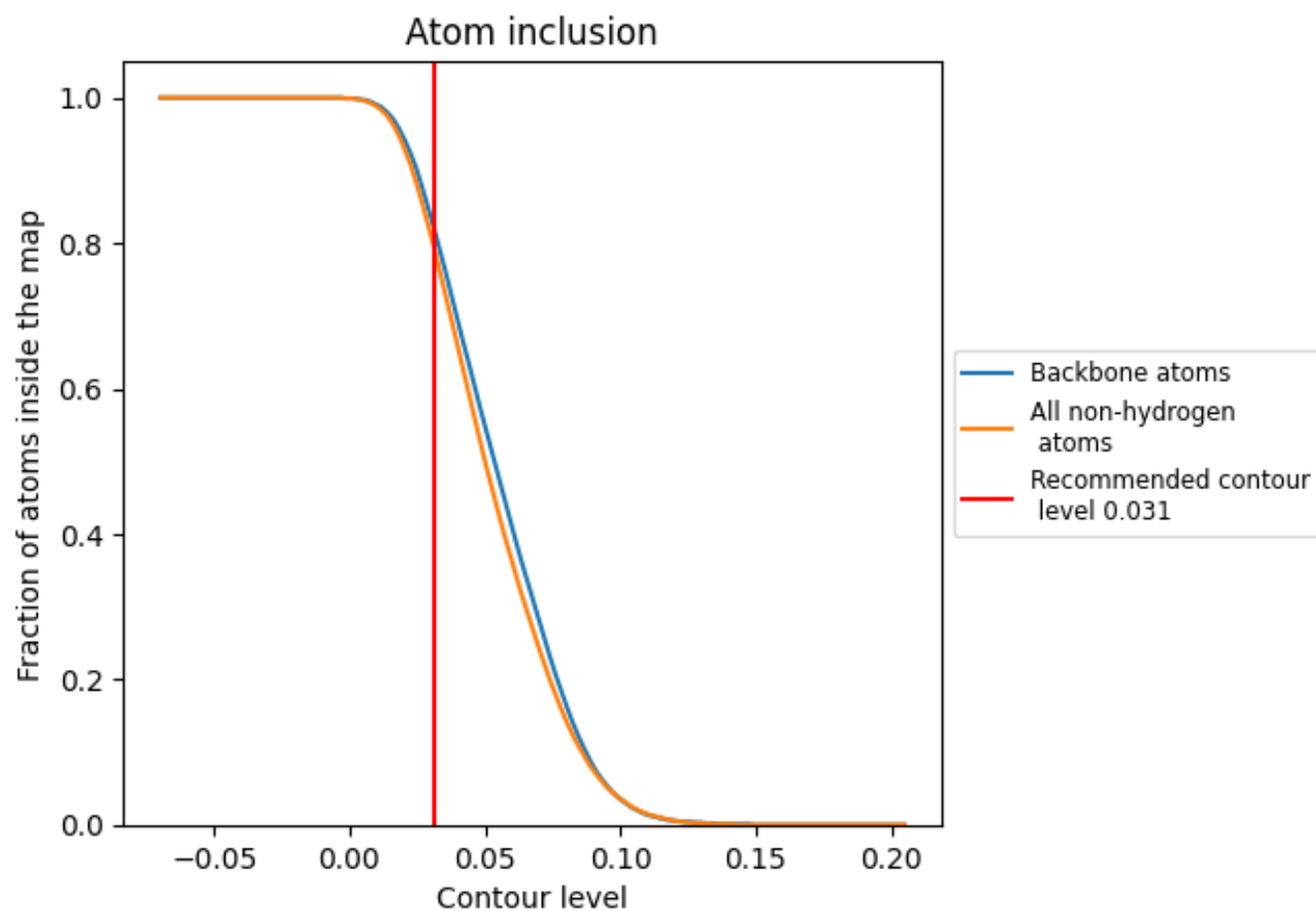
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.031).

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 80% 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 (0.031) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7980	 0.4550
2	 0.8700	 0.4640
3	 0.7720	 0.3080
4	 0.6970	 0.4290
6	 0.7670	 0.4760
7	 0.8480	 0.5120
8	 0.9440	 0.5160
9	 0.3710	 0.3610
A	 0.5840	 0.3760
B	 0.9010	 0.5380
C	 0.2590	 0.2110
D	 0.9200	 0.5410
E	 0.6010	 0.4300
F	 0.8510	 0.5030
G	 0.6830	 0.4300
H	 0.8720	 0.5090
I	 0.8350	 0.5060
J	 0.7950	 0.4750
K	 0.8060	 0.4710
L	 0.9230	 0.5400
M	 0.9520	 0.5520
N	 0.1090	 0.1830
O	 0.6970	 0.4580
P	 0.9720	 0.5530
Q	 0.8090	 0.4860
R	 0.2770	 0.1820
S	 0.8970	 0.5280
T	 0.5790	 0.2680
U	 0.9180	 0.5240
V	 0.9050	 0.5400
W	 0.1950	 0.3230
X	 0.7600	 0.4670
Y	 0.8670	 0.5310
Z	 0.9220	 0.5470
a	 0.8270	 0.4890



Continued on next page...

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Chain	Atom inclusion	Q-score
b	 0.9200	 0.5510
d	 0.7800	 0.4870
e	 0.8760	 0.5210
g	 0.8830	 0.5220
h	 0.8790	 0.5250
i	 0.7230	 0.4490
j	 0.8400	 0.5090
k	 0.9470	 0.5640
l	 0.9160	 0.5490
m	 0.8320	 0.4900
n	 0.9510	 0.5700
o	 0.7960	 0.4720
p	 0.9010	 0.5320
r	 0.3640	 0.3220
u	 0.5260	 0.3660
v	 0.6020	 0.4230
w	 0.7010	 0.4360
y	 0.3620	 0.2770
z	 0.6650	 0.4280