



wwPDB EM Validation Summary Report ⓘ

Nov 6, 2023 – 11:08 AM JST

PDB ID : 8IDT
EMDB ID : EMD-35370
Title : human nuclear pre-60S ribosomal particle - State G
Authors : Zhang, Y.; Gao, N.
Deposited on : 2023-02-14
Resolution : 2.80 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:

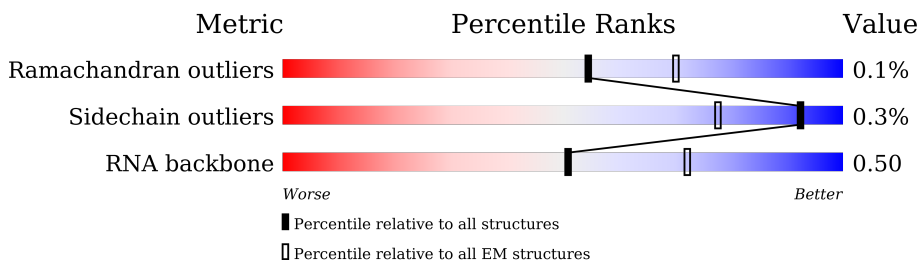
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	5	120	
2	6	245	
3	7	163	
4	8	156	
5	9	134	
6	B	403	
7	C	159	
8	D	427	

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Mol	Chain	Length	Quality of chain
9	E	115	23% 85% 15%
10	F	117	7% 93% 7%
11	G	266	18% 90% 9%
12	H	123	98% ..
13	I	192	7% 97% ..
14	K	105	6% 97% .
15	L	148	97% ..
16	M	97	89% 11%
17	N	178	56% 91% 7%
18	O	70	34% 99% .
19	P	51	96% ..
20	Q	211	7% 99% .
21	S	215	60% 37%
22	U	204	98% .
23	V	203	99% .
24	W	106	10% 94% 5%
25	X	92	14% 99% .
26	Z	188	99% .
27	a	196	76% 24%
28	b	176	100%
29	c	160	96% ..
30	e	140	93% 6%
31	g	156	75% 24%
32	h	145	92% 8%
33	i	136	16% 96% ..

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Mol	Chain	Length	Quality of chain
34	l	137	91% 9%
35	m	257	95%
36	n	110	95%
37	o	288	12% 80% 18%
38	p	248	90% 9%
39	r	297	31% 98%
40	A	731	17% 41% 58%
41	R	203	26% 74% 25%
42	J	239	91% 92% 7%
43	T	99	15% 49% 49%
44	2	5054	9% 44% 23% 30%
45	y	165	100% 98%
46	4	634	26% 94%
47	d	128	5% 80% 19%
48	j	125	9% 88% 11%
49	k	135	96%
50	Y	184	8% 90% 9%
51	z	129	22% 50% 48%

2 Entry composition [i](#)

There are 55 unique types of molecules in this entry. The entry contains 147681 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 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	5	120	2558	1141	456	842	119	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	9	97	793	484	171	134	4	0	0

- Molecule 6 is a protein called 60S ribosomal protein L3.

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

- Molecule 7 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	93	764	476	167	117	4	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	G	241	1935	1233	374	324	4	1	0

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

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

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

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

- Molecule 14 is a protein called 60S ribosomal protein L36.

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

- Molecule 15 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	L	147	1162	736	237	186	3	0	0

- Molecule 16 is a protein called 60S ribosomal protein L37.

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

- Molecule 17 is a protein called 60S ribosomal protein L11.

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

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

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

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

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

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

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

- 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 L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	101	Total	C	N	O	S	0	0
			827	517	170	134	6		

- Molecule 25 is a protein called 60S ribosomal protein L37a.

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

- Molecule 26 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 27 is a protein called 60S ribosomal protein L19.

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

- Molecule 28 is a protein called 60S ribosomal protein L18a.

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

- Molecule 29 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	c	155	1264	801	248	210	5	0	0

- Molecule 30 is a protein called 60S ribosomal protein L23.

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

- Molecule 31 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	g	118	967	618	181	167	1	0	0

- Molecule 32 is a protein called 60S ribosomal protein L26.

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

- Molecule 33 is a protein called 60S ribosomal protein L27.

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

- Molecule 34 is a protein called 60S ribosomal protein L28.

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

- Molecule 35 is a protein called 60S ribosomal protein L8.

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

- Molecule 36 is a protein called 60S ribosomal protein L35a.

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

- Molecule 37 is a protein called 60S ribosomal protein L6.

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

- Molecule 38 is a protein called 60S ribosomal protein L7.

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

- Molecule 39 is a protein called 60S ribosomal protein L5.

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

- Molecule 40 is a protein called G Protein Nucleolar 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A	307	Total	C	N	O	S	0	0
			2460	1576	419	457	8		

- Molecule 41 is a protein called Translation machinery-associated protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	R	153	Total	C	N	O	S	0	0
			1296	810	248	233	5		

- Molecule 42 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	J	223	1809	1140	309	349	11	0	0

- Molecule 43 is a protein called Leydig cell tumor 10 kDa protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	T	50	393	247	82	63	1	0	0

- Molecule 44 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
44	2	3524	75681	33754	13848	24556	3523	0	0

- Molecule 45 is a protein called 60S ribosomal protein L12.

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

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

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

- Molecule 47 is a protein called 60S ribosomal protein L22.

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

- Molecule 48 is a protein called 60S ribosomal protein L31.

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

- Molecule 49 is a protein called 60S ribosomal protein L32.

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

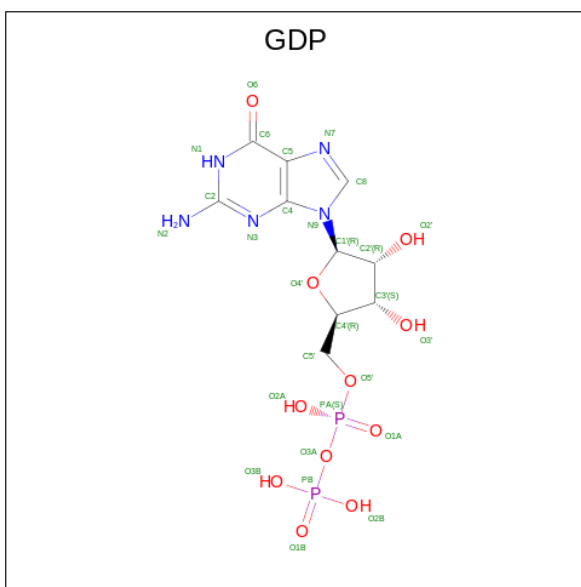
- Molecule 50 is a protein called 60S ribosomal protein L17.

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

- Molecule 51 is a protein called Protein LLP homolog.

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

- Molecule 52 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
52	A	1	28	10	5	11	2	0

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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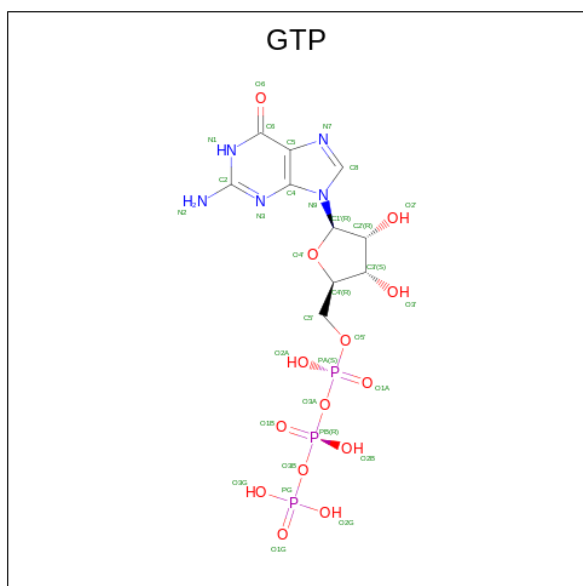
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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
53	4	1	1	1	0

- Molecule 54 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
54	A	1	1	1	0

- Molecule 55 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

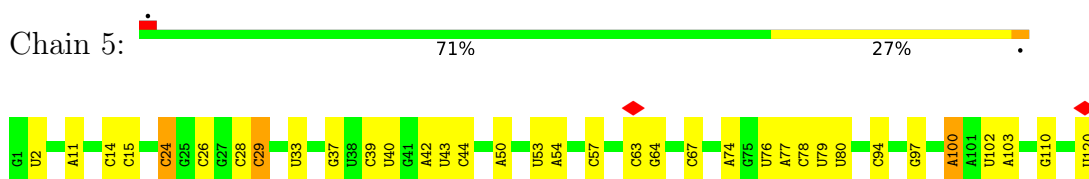


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
55	4	1	32	10	5	14	3	0

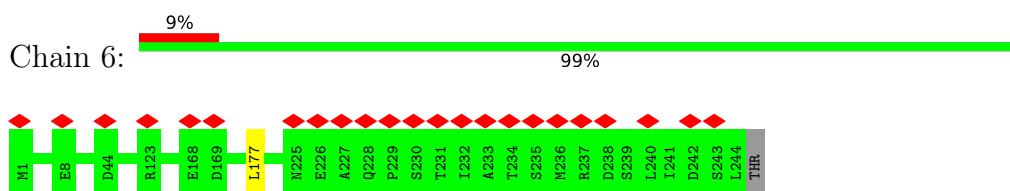
3 Residue-property plots [i](#)

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

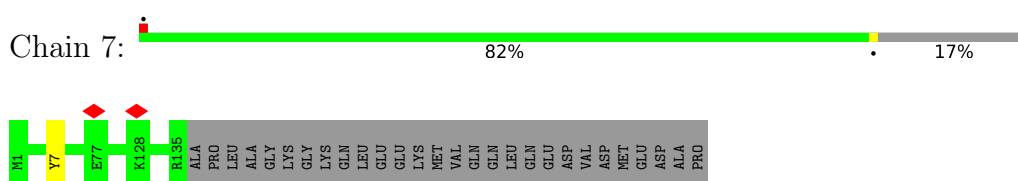
- Molecule 1: 5S rRNA



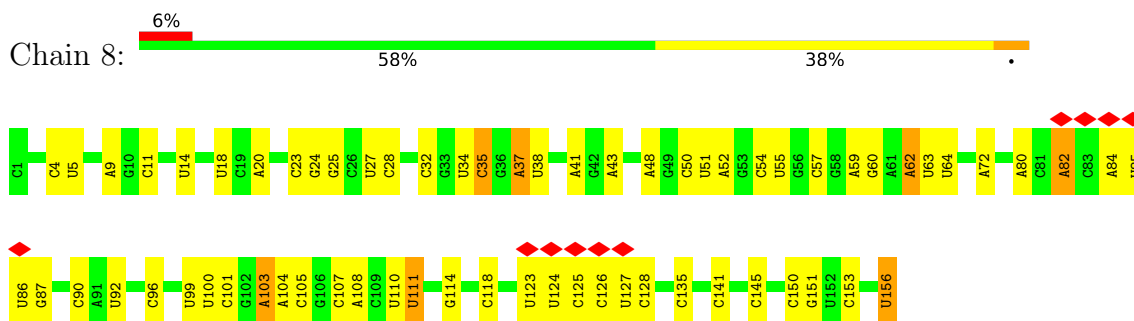
- Molecule 2: Eukaryotic translation initiation factor 6



- Molecule 3: Probable ribosome biogenesis protein RLP24

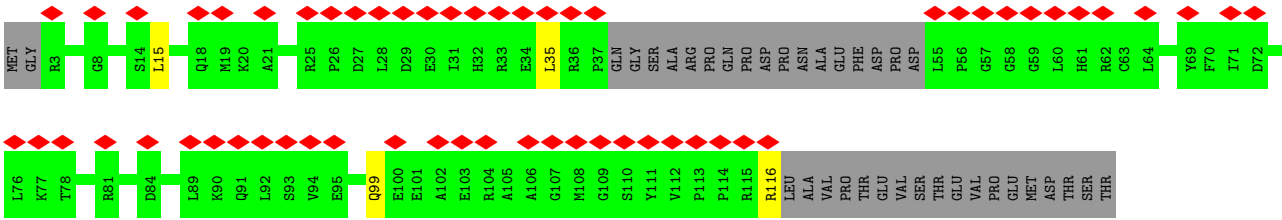


- Molecule 4: 5.8S rRNA

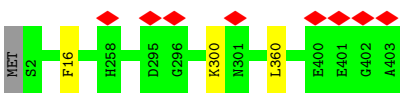


- Molecule 5: Zinc finger protein 593

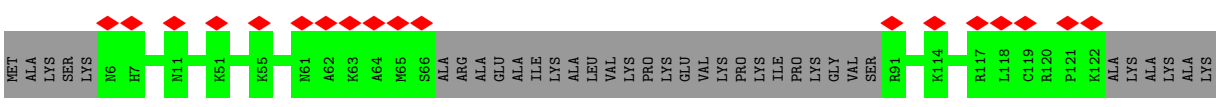




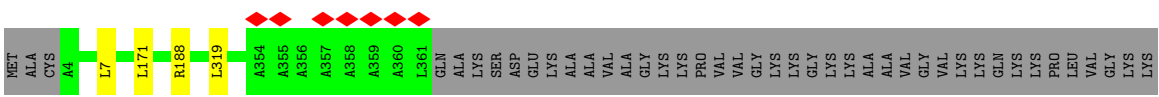
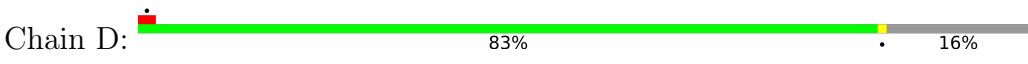
• Molecule 6: 60S ribosomal protein L3



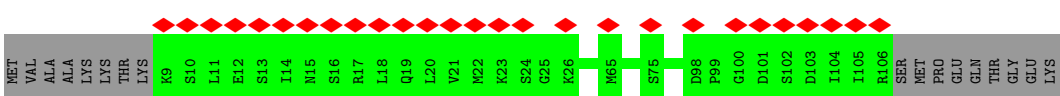
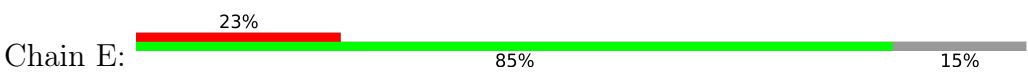
• Molecule 7: 60S ribosomal protein L29



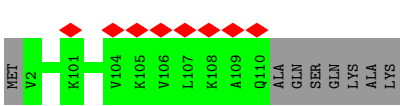
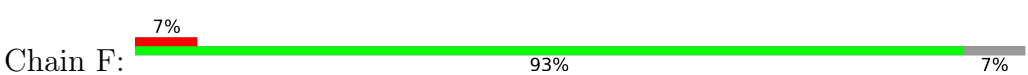
• Molecule 8: 60S ribosomal protein L4



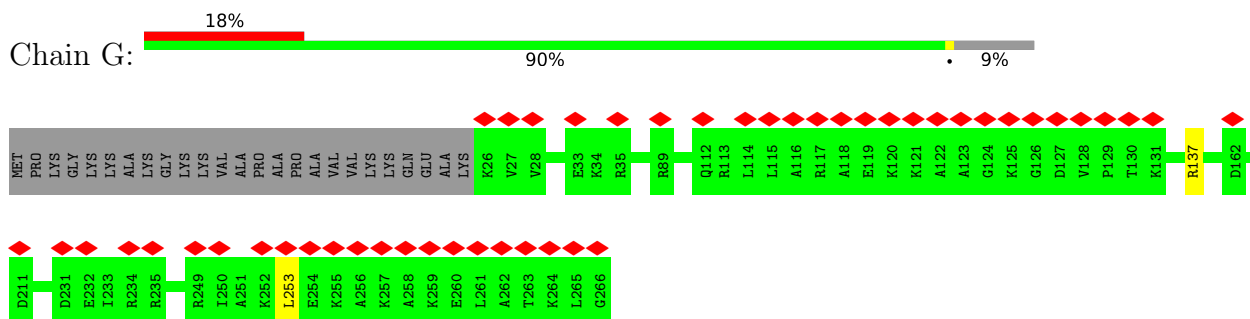
• Molecule 9: 60S ribosomal protein L30



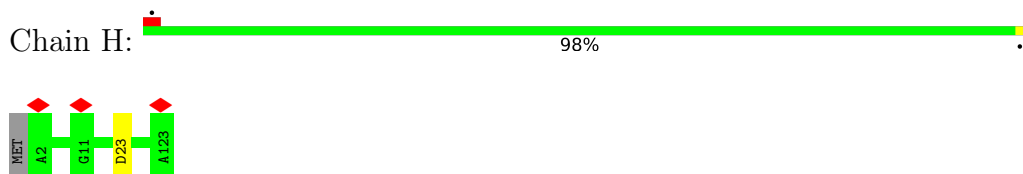
• Molecule 10: 60S ribosomal protein L34



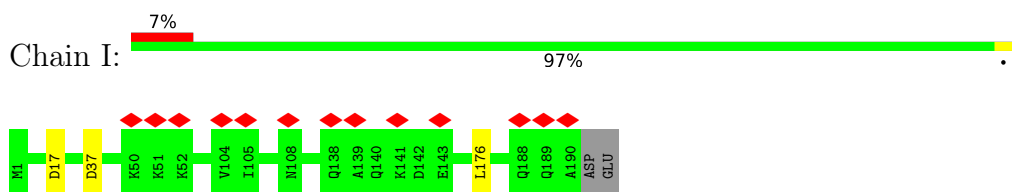
- Molecule 11: 60S ribosomal protein L7a



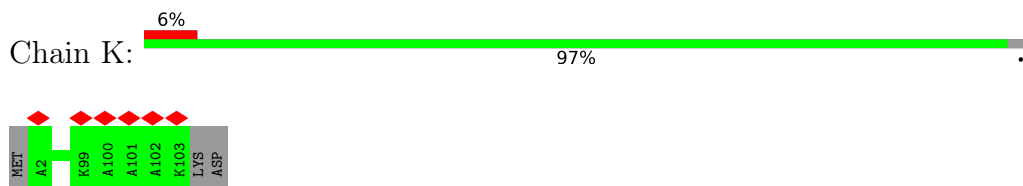
- Molecule 12: 60S ribosomal protein L35



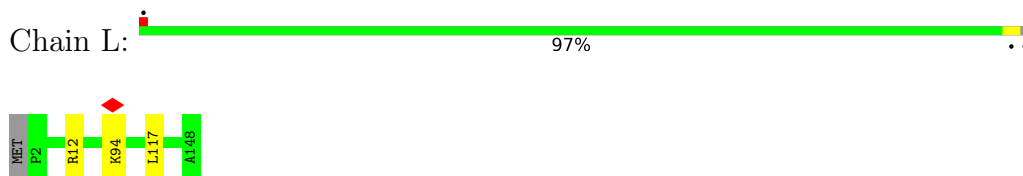
- Molecule 13: 60S ribosomal protein L9



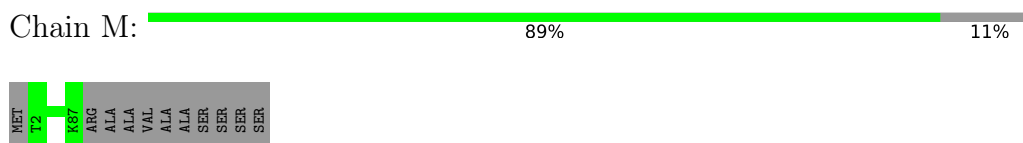
- Molecule 14: 60S ribosomal protein L36



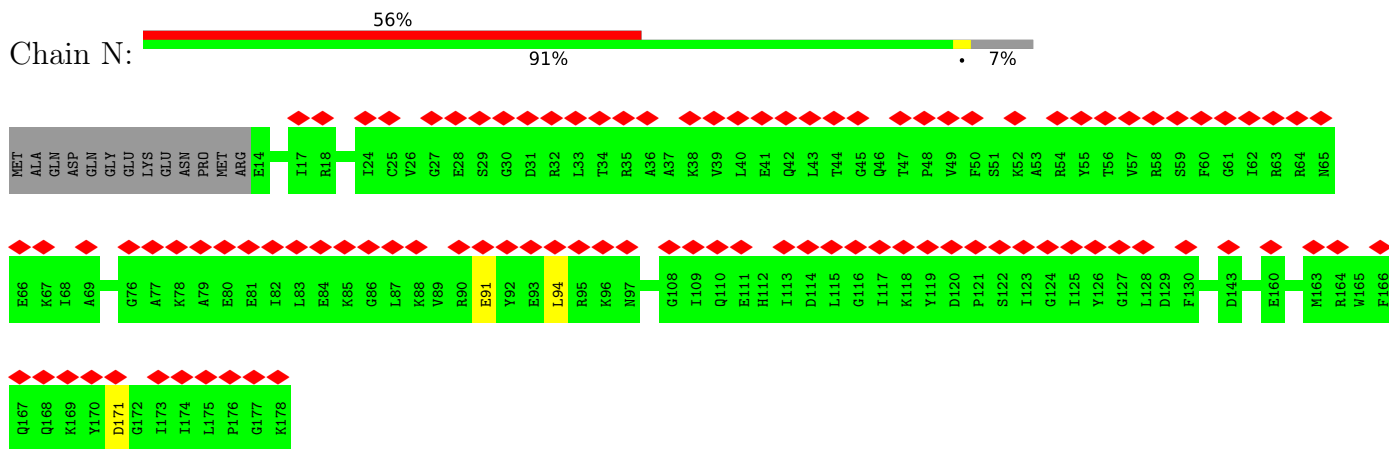
- Molecule 15: 60S ribosomal protein L27a



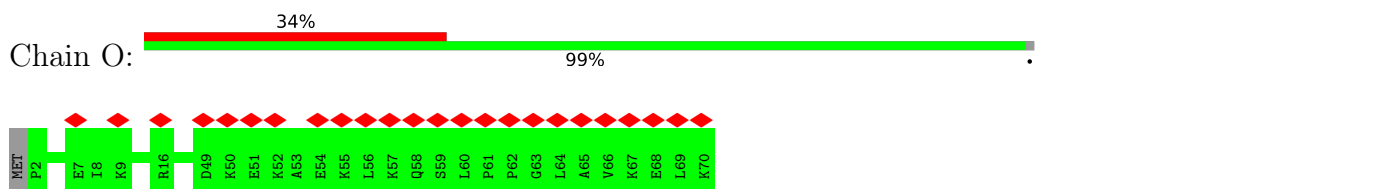
- Molecule 16: 60S ribosomal protein L37



- Molecule 17: 60S ribosomal protein L11



• Molecule 18: 60S ribosomal protein L38



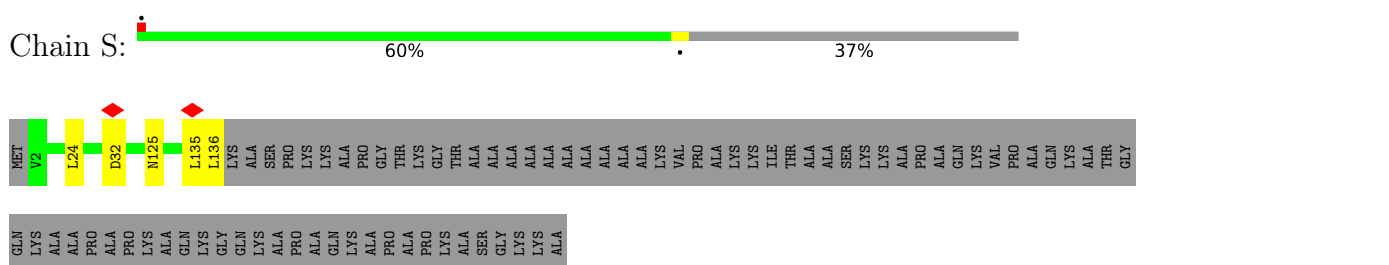
• Molecule 19: 60S ribosomal protein L39



• Molecule 20: 60S ribosomal protein L13

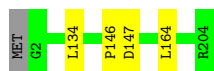


• Molecule 21: 60S ribosomal protein L14

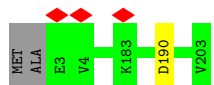


• Molecule 22: 60S ribosomal protein L15

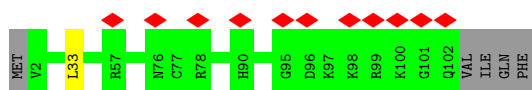




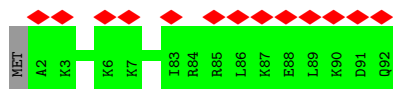
- Molecule 23: 60S ribosomal protein L13a



- Molecule 24: 60S ribosomal protein L36a



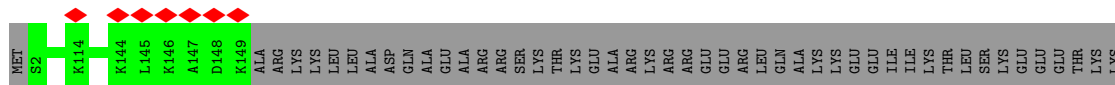
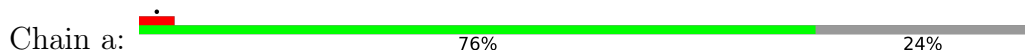
- Molecule 25: 60S ribosomal protein L37a



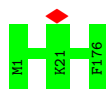
- Molecule 26: 60S ribosomal protein L18



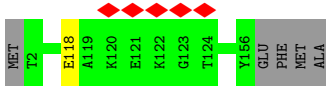
- Molecule 27: 60S ribosomal protein L19



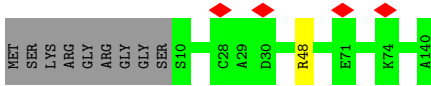
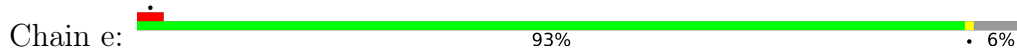
- Molecule 28: 60S ribosomal protein L18a



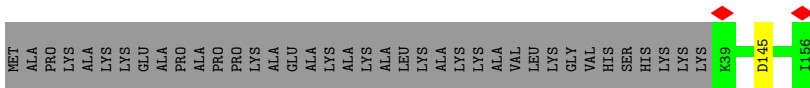
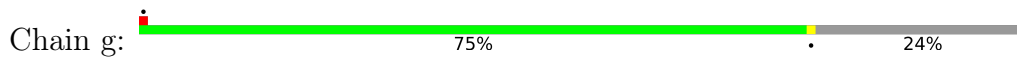
- Molecule 29: 60S ribosomal protein L21



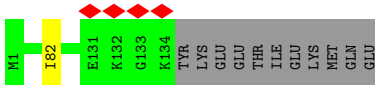
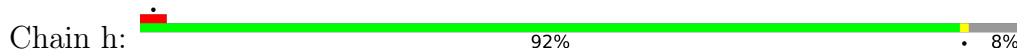
- Molecule 30: 60S ribosomal protein L23



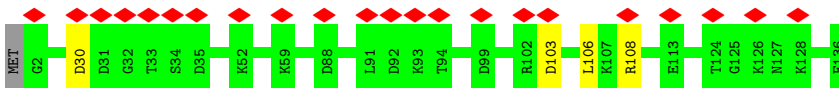
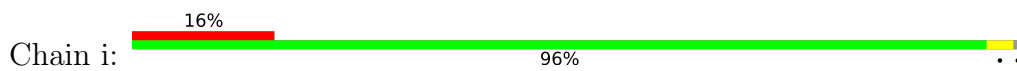
- Molecule 31: 60S ribosomal protein L23a



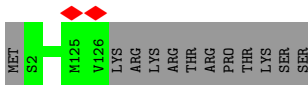
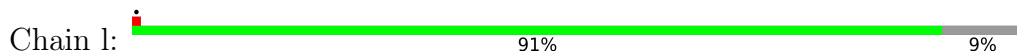
- Molecule 32: 60S ribosomal protein L26



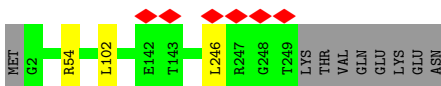
- Molecule 33: 60S ribosomal protein L27



- Molecule 34: 60S ribosomal protein L28




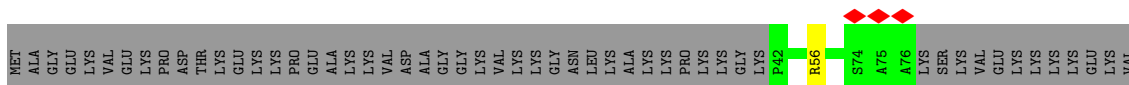
- Molecule 35: 60S ribosomal protein L8



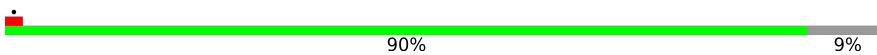
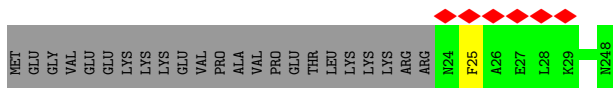
● Molecule 36: 60S ribosomal protein L35a

Chain n:  95%

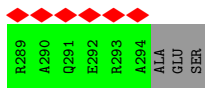
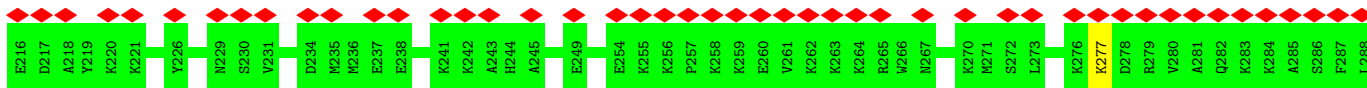
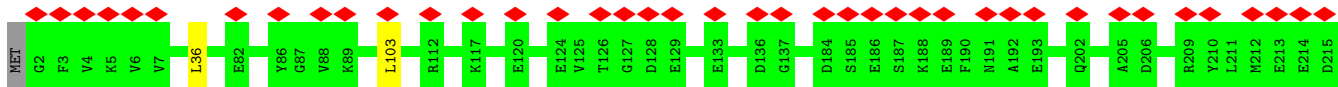
● Molecule 37: 60S ribosomal protein L6

Chain o:  12% 80% 18%

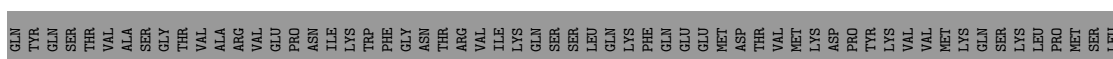
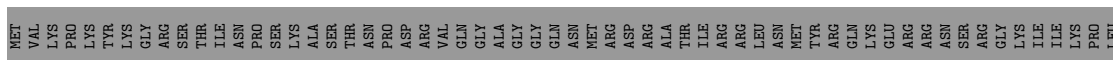
● Molecule 38: 60S ribosomal protein L7

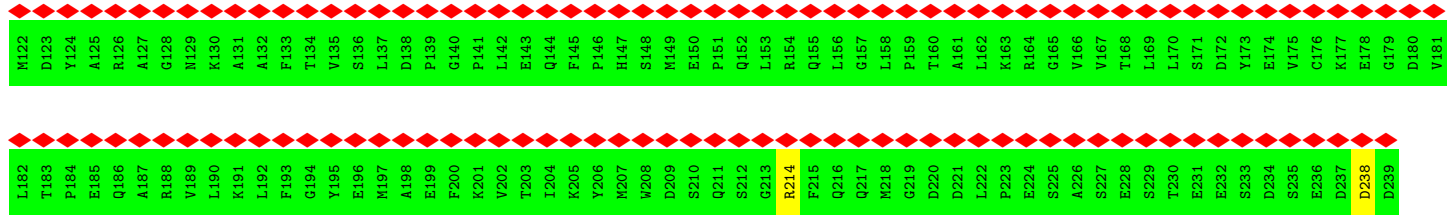
Chain p:  90% 9%

● Molecule 39: 60S ribosomal protein L5

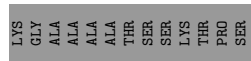
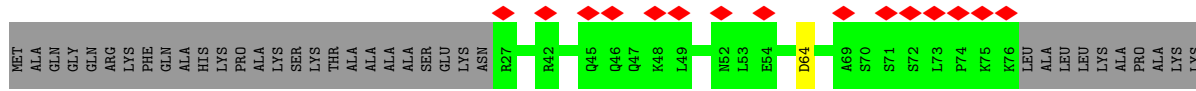
Chain r:  31% 98%

● Molecule 40: G Protein Nucleolar 2

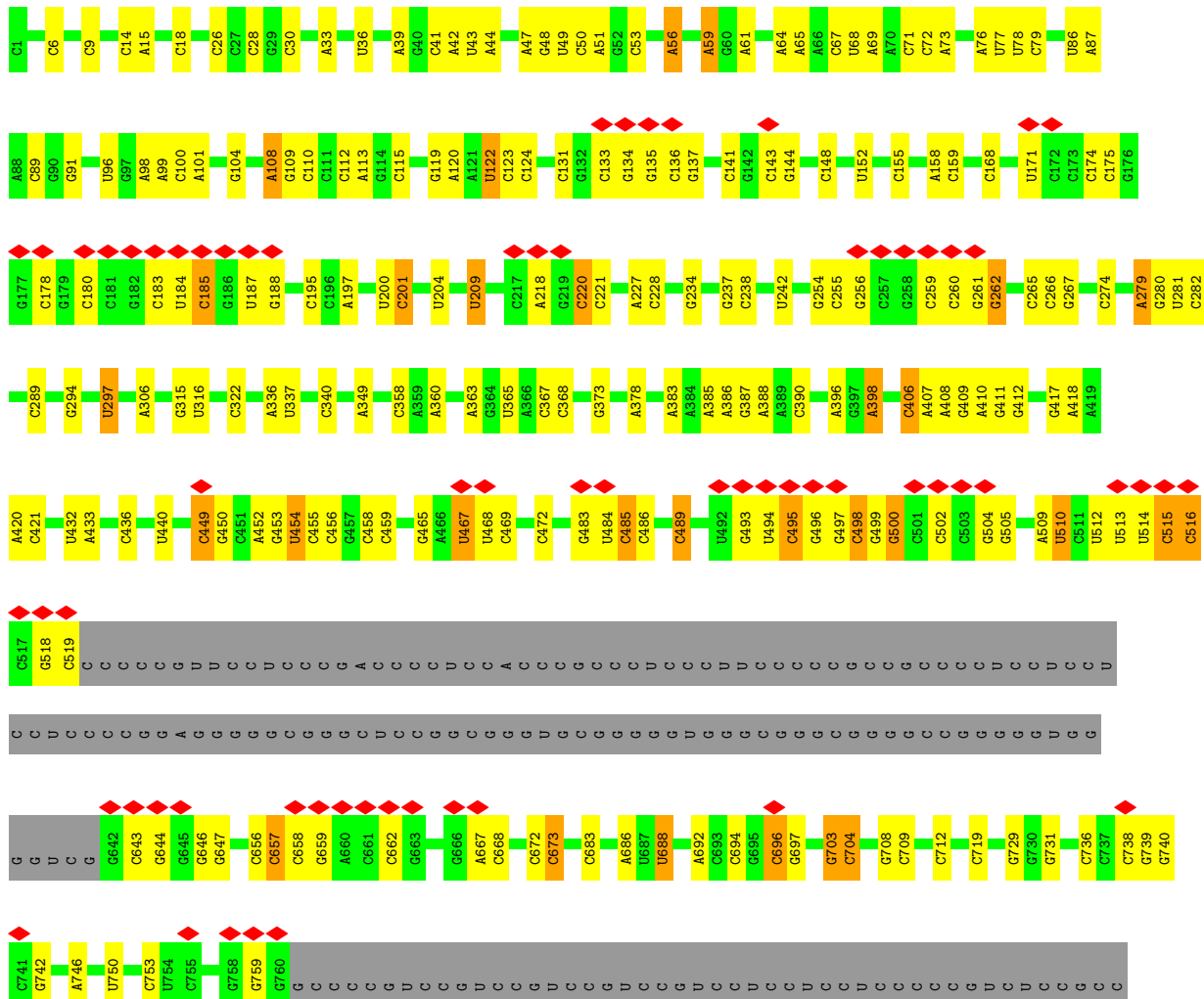
Chain A:  17% 41% 58%

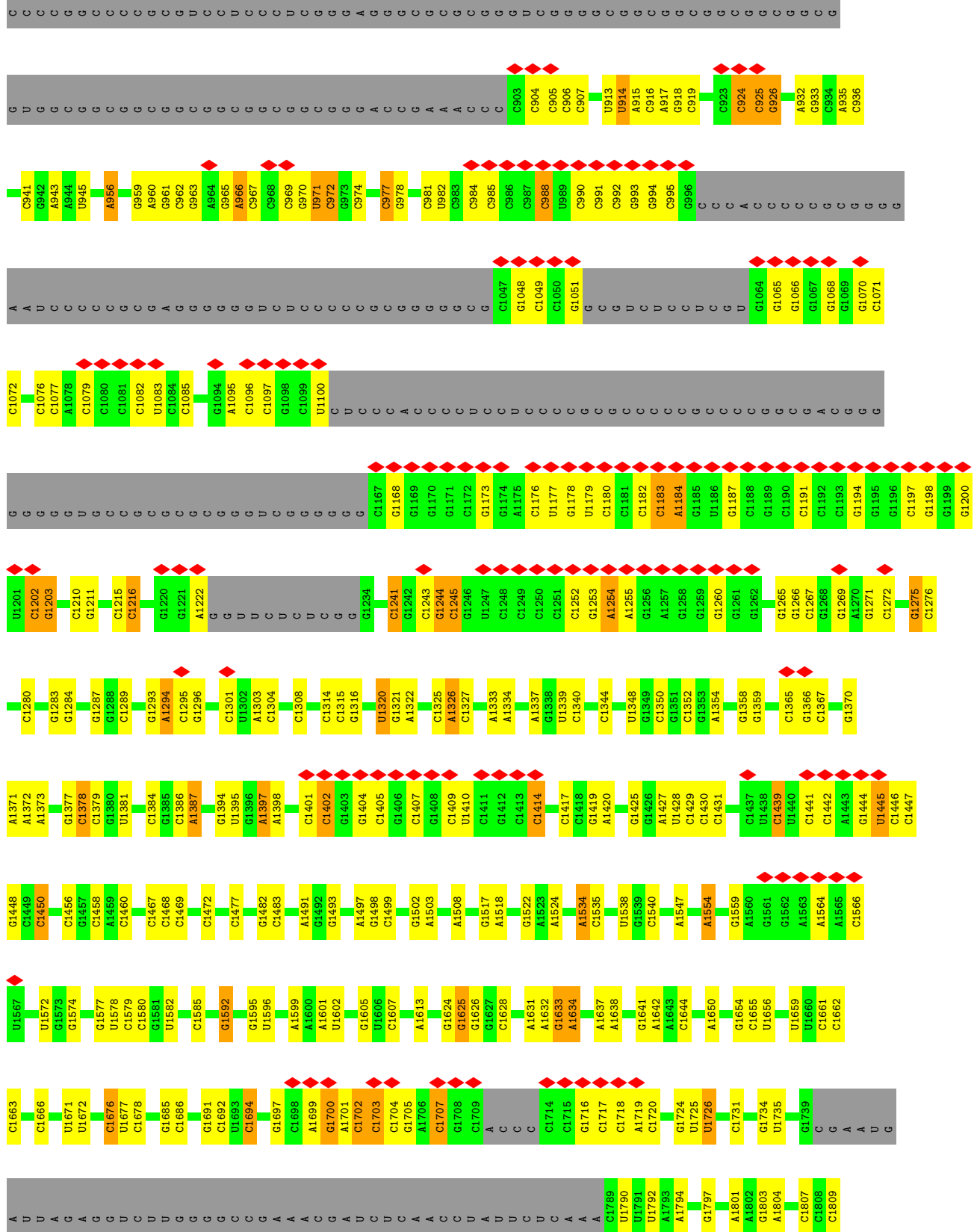


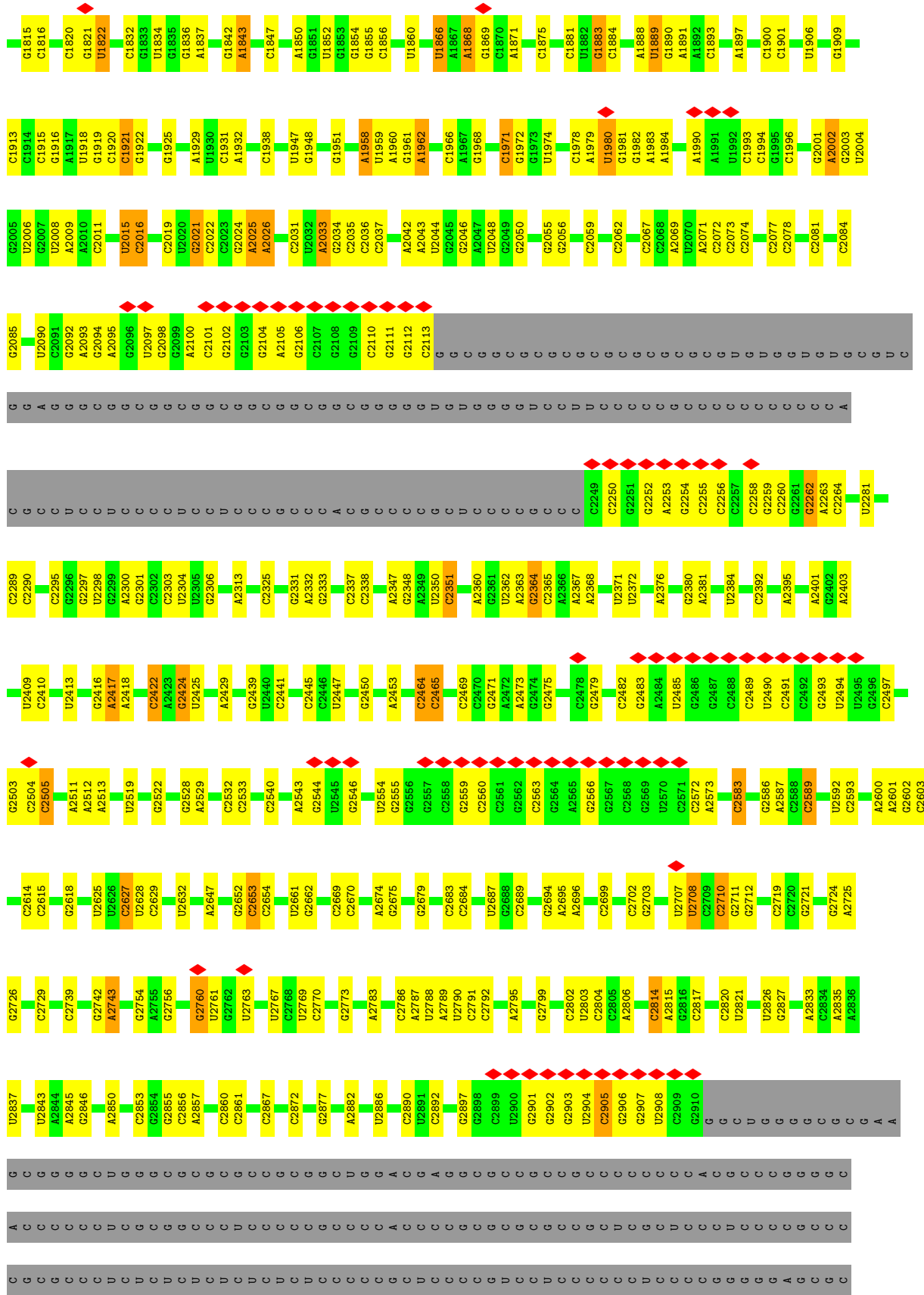
• Molecule 43: Leydig cell tumor 10 kDa protein homolog

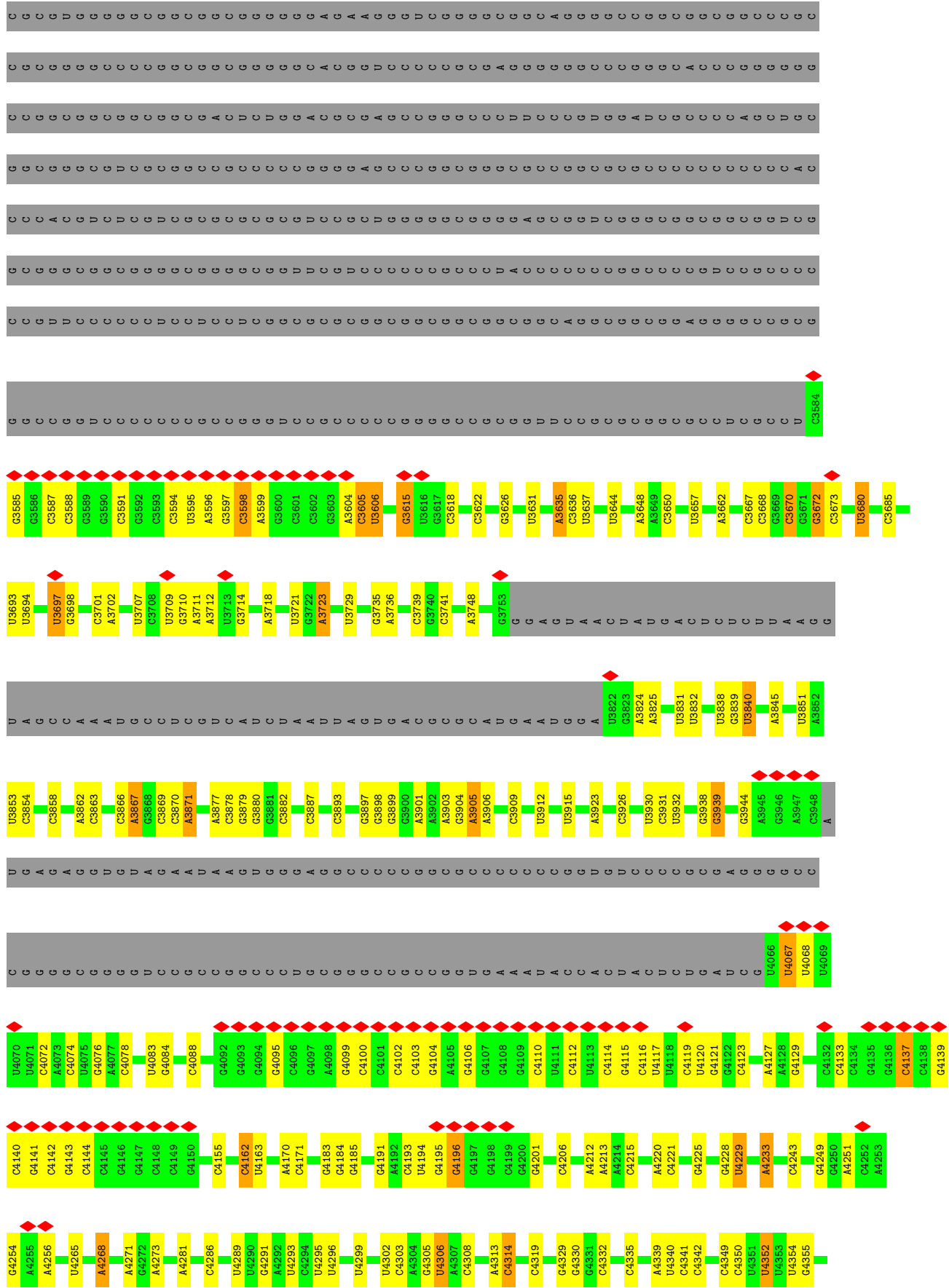


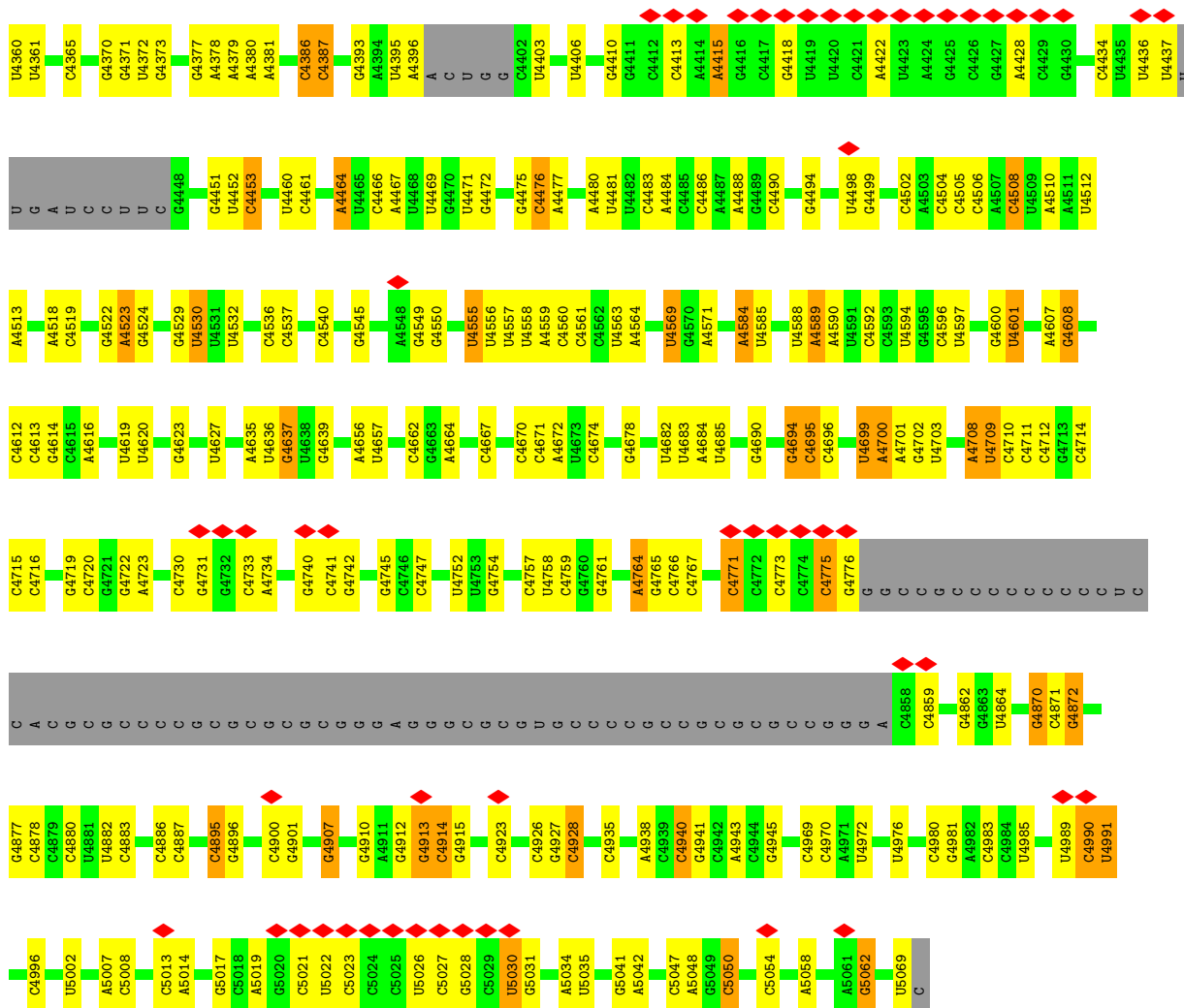
• Molecule 44: 28S rRNA



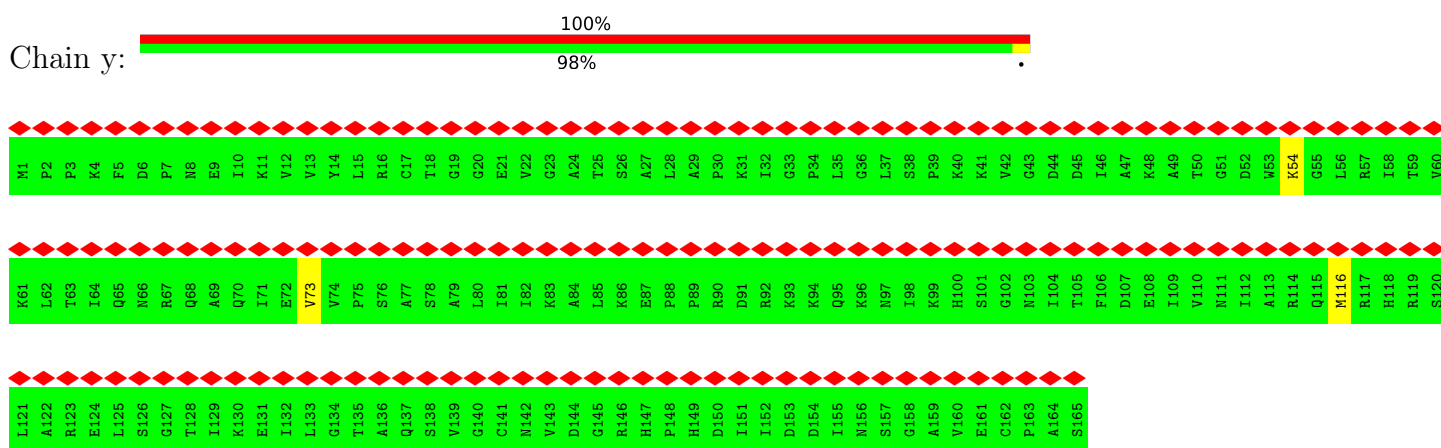






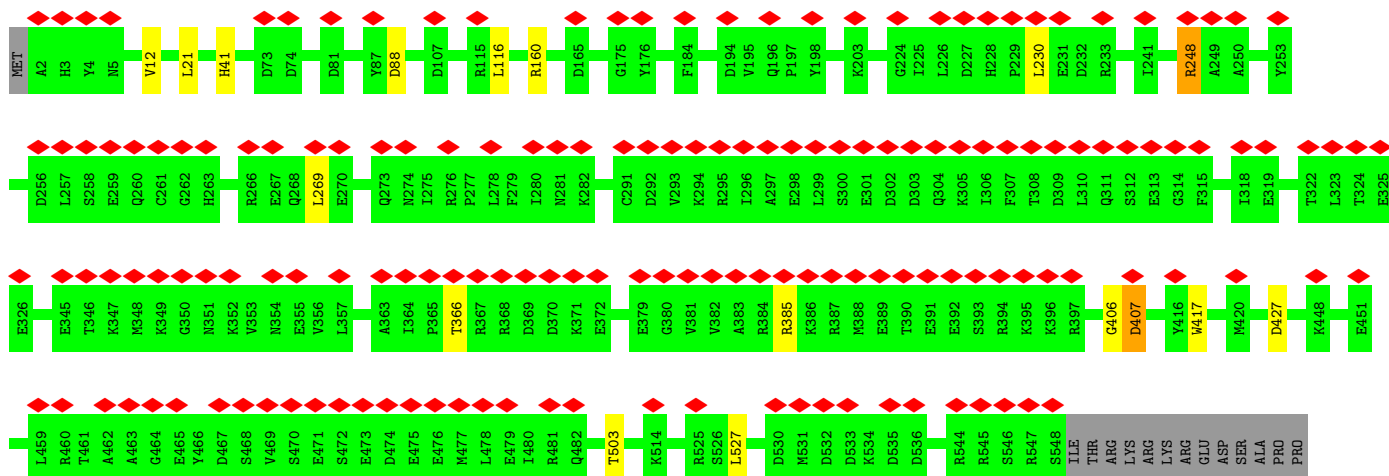


• Molecule 45: 60S ribosomal protein L12

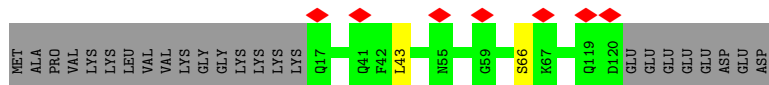
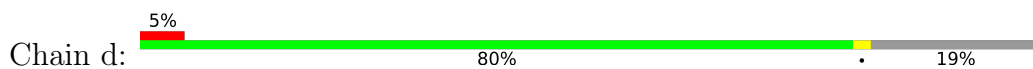


• Molecule 46: GTP-binding protein 4

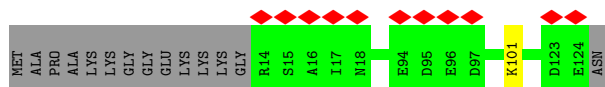
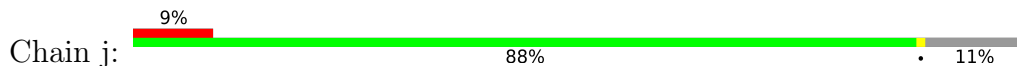




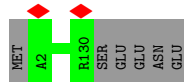
- Molecule 47: 60S ribosomal protein L22



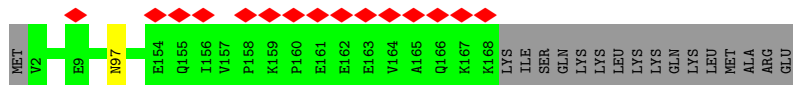
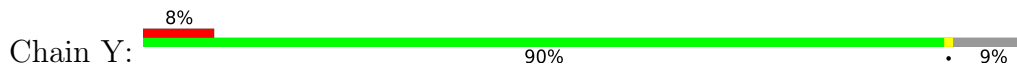
- Molecule 48: 60S ribosomal protein L31



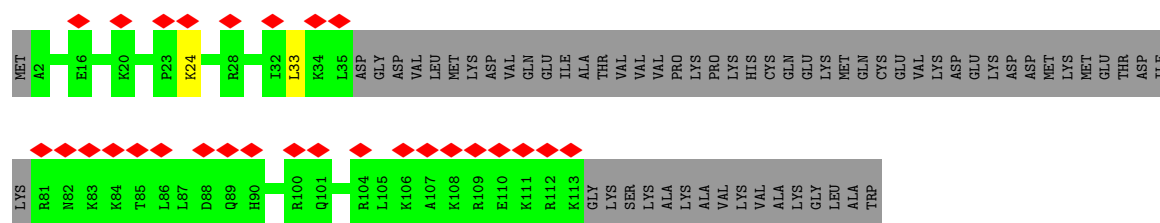
- Molecule 49: 60S ribosomal protein L32



- Molecule 50: 60S ribosomal protein L17



- Molecule 51: Protein LLP homolog



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	175116	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	0.312	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.045	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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, B9H, K, UR3, I4U, 5MU, E7G, P7G, B8K, 1MA, B8H, B8T, 6MZ, OMG, GTP, B9B, OMU, B8W, MG, B8Q, 5MC, 7MG, A2M, M7A, P4U, GDP, BGH, E6G, MHG, 2MG

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	5	0.45	0/2858	1.37	46/4455 (1.0%)
2	6	0.35	0/1877	0.74	1/2554 (0.0%)
3	7	0.39	0/1181	0.75	1/1563 (0.1%)
4	8	0.52	0/3679	1.44	74/5732 (1.3%)
5	9	0.32	0/808	0.83	2/1076 (0.2%)
6	B	0.33	0/3315	0.71	1/4435 (0.0%)
7	C	0.29	0/777	0.67	0/1026
8	D	0.33	0/2907	0.78	4/3905 (0.1%)
9	E	0.30	0/774	0.65	0/1038
10	F	0.30	0/878	0.73	0/1170
11	G	0.34	0/1971	0.71	1/2651 (0.0%)
12	H	0.32	0/1023	0.68	1/1351 (0.1%)
13	I	0.34	0/1537	0.79	3/2066 (0.1%)
14	K	0.31	0/843	0.67	0/1115
15	L	0.31	0/1191	0.69	2/1591 (0.1%)
16	M	0.35	0/720	0.74	0/952
17	N	0.37	0/1341	0.81	2/1793 (0.1%)
18	O	0.32	0/575	0.69	0/761
19	P	0.32	0/454	0.72	0/599
20	Q	0.35	0/1732	0.75	1/2315 (0.0%)
21	S	0.36	0/1133	0.76	4/1516 (0.3%)
22	U	0.31	0/1746	0.73	4/2338 (0.2%)
23	V	0.34	0/1682	0.66	1/2250 (0.0%)
24	W	0.31	0/840	0.73	1/1107 (0.1%)
25	X	0.30	0/718	0.63	0/953
26	Z	0.31	0/1537	0.72	0/2052
27	a	0.31	0/1255	0.70	0/1662
28	b	0.34	0/1501	0.66	0/2013
29	c	0.36	0/1291	0.72	1/1725 (0.1%)
30	e	0.38	0/993	0.71	0/1332
31	g	0.30	0/984	0.66	1/1323 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	h	0.35	0/1132	0.72	1/1504 (0.1%)
33	i	0.40	0/1130	0.82	3/1507 (0.2%)
34	l	0.31	0/1017	0.70	0/1364
35	m	0.34	0/1936	0.76	2/2596 (0.1%)
36	n	0.31	0/895	0.79	4/1198 (0.3%)
37	o	0.34	0/1935	0.78	1/2596 (0.0%)
38	p	0.37	0/1916	0.74	1/2553 (0.0%)
39	r	0.33	0/2428	0.71	2/3252 (0.1%)
40	A	0.31	0/2515	0.58	2/3403 (0.1%)
41	R	0.35	0/1317	0.63	0/1757
42	J	0.36	0/1844	0.71	2/2476 (0.1%)
43	T	0.31	0/396	0.77	1/522 (0.2%)
44	2	0.48	3/82562 (0.0%)	1.39	1341/128718 (1.0%)
45	y	0.31	0/1269	0.74	2/1712 (0.1%)
46	4	0.36	0/5099	0.79	13/6840 (0.2%)
47	d	0.38	0/864	0.81	2/1160 (0.2%)
48	j	0.32	0/933	0.70	0/1256
49	k	0.31	0/1082	0.70	0/1443
50	Y	0.31	0/1383	0.62	0/1856
51	z	0.33	0/587	0.75	1/767 (0.1%)
All	All	0.43	3/156361 (0.0%)	1.18	1529/228899 (0.7%)

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
6	B	0	1
17	N	0	1
20	Q	0	1
35	m	0	1
36	n	0	1
42	J	0	1
46	4	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	1929	A	N9-C4	5.71	1.41	1.37
44	2	1632	A	N9-C4	5.13	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	485	C	N1-C2	5.03	1.45	1.40

The worst 5 of 1529 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	485	C	C2-N1-C1'	14.98	135.28	118.80
44	2	495	C	N1-C2-O2	13.24	126.85	118.90
44	2	495	C	C2-N1-C1'	12.95	133.05	118.80
44	2	4502	C	N1-C2-O2	12.46	126.38	118.90
44	2	753	C	N1-C2-O2	12.38	126.33	118.90

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	B	16	PHE	Peptide
17	N	94	LEU	Peptide
20	Q	154	VAL	Peptide
35	m	54	ARG	Peptide
36	n	106	TYR	Peptide

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
2	6	242/245 (99%)	227 (94%)	15 (6%)	0	100 100
3	7	133/163 (82%)	129 (97%)	4 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	9	93/134 (69%)	81 (87%)	11 (12%)	1 (1%)	14	41
6	B	401/403 (100%)	382 (95%)	19 (5%)	0	100	100
7	C	89/159 (56%)	86 (97%)	3 (3%)	0	100	100
8	D	356/427 (83%)	335 (94%)	21 (6%)	0	100	100
9	E	96/115 (84%)	94 (98%)	2 (2%)	0	100	100
10	F	107/117 (92%)	104 (97%)	3 (3%)	0	100	100
11	G	240/266 (90%)	231 (96%)	9 (4%)	0	100	100
12	H	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
13	I	188/192 (98%)	179 (95%)	9 (5%)	0	100	100
14	K	100/105 (95%)	93 (93%)	7 (7%)	0	100	100
15	L	145/148 (98%)	137 (94%)	8 (6%)	0	100	100
16	M	84/97 (87%)	79 (94%)	5 (6%)	0	100	100
17	N	163/178 (92%)	147 (90%)	16 (10%)	0	100	100
18	O	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
19	P	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
20	Q	208/211 (99%)	193 (93%)	15 (7%)	0	100	100
21	S	133/215 (62%)	125 (94%)	8 (6%)	0	100	100
22	U	201/204 (98%)	192 (96%)	9 (4%)	0	100	100
23	V	199/203 (98%)	192 (96%)	7 (4%)	0	100	100
24	W	99/106 (93%)	95 (96%)	4 (4%)	0	100	100
25	X	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
26	Z	185/188 (98%)	179 (97%)	6 (3%)	0	100	100
27	a	146/196 (74%)	142 (97%)	4 (3%)	0	100	100
28	b	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
29	c	153/160 (96%)	148 (97%)	5 (3%)	0	100	100
30	e	129/140 (92%)	117 (91%)	12 (9%)	0	100	100
31	g	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
32	h	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
33	i	133/136 (98%)	124 (93%)	9 (7%)	0	100	100
34	l	123/137 (90%)	115 (94%)	8 (6%)	0	100	100
35	m	246/257 (96%)	221 (90%)	25 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	n	107/110 (97%)	103 (96%)	3 (3%)	1 (1%)	17	46
37	o	231/288 (80%)	214 (93%)	17 (7%)	0	100	100
38	p	224/248 (90%)	216 (96%)	8 (4%)	0	100	100
39	r	291/297 (98%)	279 (96%)	12 (4%)	0	100	100
40	A	305/731 (42%)	300 (98%)	4 (1%)	1 (0%)	41	72
41	R	151/203 (74%)	148 (98%)	2 (1%)	1 (1%)	22	53
42	J	221/239 (92%)	206 (93%)	15 (7%)	0	100	100
43	T	48/99 (48%)	48 (100%)	0	0	100	100
45	y	163/165 (99%)	158 (97%)	5 (3%)	0	100	100
46	4	607/634 (96%)	559 (92%)	44 (7%)	4 (1%)	22	53
47	d	102/128 (80%)	95 (93%)	7 (7%)	0	100	100
48	j	109/125 (87%)	104 (95%)	5 (5%)	0	100	100
49	k	127/135 (94%)	121 (95%)	6 (5%)	0	100	100
50	Y	165/184 (90%)	158 (96%)	7 (4%)	0	100	100
51	z	63/129 (49%)	59 (94%)	3 (5%)	1 (2%)	9	31
All	All	8052/9430 (85%)	7638 (95%)	405 (5%)	9 (0%)	54	81

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
36	n	106	TYR
5	9	99	GLN
51	z	24	LYS
40	A	160	MET
46	4	88	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	6	212/213 (100%)	212 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	7	126/149 (85%)	126 (100%)	0	100	100
5	9	82/114 (72%)	81 (99%)	1 (1%)	71	92
6	B	349/349 (100%)	348 (100%)	1 (0%)	92	98
7	C	78/126 (62%)	78 (100%)	0	100	100
8	D	298/348 (86%)	297 (100%)	1 (0%)	92	98
9	E	83/97 (86%)	83 (100%)	0	100	100
10	F	94/100 (94%)	94 (100%)	0	100	100
11	G	204/223 (92%)	202 (99%)	2 (1%)	76	93
12	H	109/110 (99%)	109 (100%)	0	100	100
13	I	169/171 (99%)	169 (100%)	0	100	100
14	K	86/89 (97%)	86 (100%)	0	100	100
15	L	120/121 (99%)	119 (99%)	1 (1%)	81	94
16	M	73/80 (91%)	73 (100%)	0	100	100
17	N	138/149 (93%)	138 (100%)	0	100	100
18	O	64/65 (98%)	64 (100%)	0	100	100
19	P	47/48 (98%)	46 (98%)	1 (2%)	53	84
20	Q	176/177 (99%)	176 (100%)	0	100	100
21	S	115/161 (71%)	114 (99%)	1 (1%)	78	94
22	U	171/172 (99%)	171 (100%)	0	100	100
23	V	173/174 (99%)	173 (100%)	0	100	100
24	W	89/94 (95%)	89 (100%)	0	100	100
25	X	74/75 (99%)	74 (100%)	0	100	100
26	Z	164/165 (99%)	164 (100%)	0	100	100
27	a	133/175 (76%)	133 (100%)	0	100	100
28	b	157/157 (100%)	157 (100%)	0	100	100
29	c	136/140 (97%)	136 (100%)	0	100	100
30	e	101/107 (94%)	100 (99%)	1 (1%)	76	93
31	g	106/133 (80%)	106 (100%)	0	100	100
32	h	124/135 (92%)	124 (100%)	0	100	100
33	i	117/118 (99%)	116 (99%)	1 (1%)	78	94
34	l	109/121 (90%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	m	190/199 (96%)	190 (100%)	0	100	100
36	n	88/89 (99%)	88 (100%)	0	100	100
37	o	208/252 (82%)	205 (99%)	3 (1%)	67	90
38	p	195/215 (91%)	195 (100%)	0	100	100
39	r	246/250 (98%)	245 (100%)	1 (0%)	91	97
40	A	272/654 (42%)	271 (100%)	1 (0%)	91	97
41	R	141/184 (77%)	140 (99%)	1 (1%)	84	95
42	J	199/214 (93%)	197 (99%)	2 (1%)	76	93
43	T	43/76 (57%)	43 (100%)	0	100	100
45	y	137/137 (100%)	136 (99%)	1 (1%)	84	95
46	4	554/574 (96%)	552 (100%)	2 (0%)	91	97
47	d	94/115 (82%)	94 (100%)	0	100	100
48	j	101/110 (92%)	100 (99%)	1 (1%)	76	93
49	k	115/121 (95%)	115 (100%)	0	100	100
50	Y	147/163 (90%)	146 (99%)	1 (1%)	84	95
51	z	61/115 (53%)	61 (100%)	0	100	100
All	All	7068/8124 (87%)	7045 (100%)	23 (0%)	92	98

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	A	428	ARG
42	J	214	ARG
42	J	118	LYS
45	y	54	LYS
19	P	21	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
15	L	66	ASN
28	b	77	ASN
35	m	215	ASN
42	J	50	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	119/120 (99%)	16 (13%)	0
4	8	155/156 (99%)	31 (20%)	0
44	2	3481/5054 (68%)	776 (22%)	15 (0%)
All	All	3755/5330 (70%)	823 (21%)	15 (0%)

5 of 823 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	11	A
1	5	24	C
1	5	29	C
1	5	33	U
1	5	37	G

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
44	2	2760	G
44	2	4699	U
44	2	3596	A
44	2	4913	G
44	2	4498	U

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

80 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
44	OMC	2	4536	44	19,22,23	3.00	8 (42%)	26,31,34	1.15	3 (11%)
44	7MG	2	1605	44	22,26,27	3.79	10 (45%)	29,39,42	1.96	8 (27%)
44	OMG	2	2424	44	18,26,27	2.85	8 (44%)	19,38,41	1.49	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	OMG	2	4870	44	18,26,27	2.87	8 (44%)	19,38,41	1.58	4 (21%)
44	A2M	2	3825	44	18,25,26	3.61	8 (44%)	18,36,39	3.37	3 (16%)
44	2MG	2	729	44	18,26,27	2.62	6 (33%)	16,38,41	1.38	3 (18%)
44	OMG	2	1625	44	18,26,27	2.87	8 (44%)	19,38,41	1.42	4 (21%)
44	A2M	2	3723	44	18,25,26	3.57	8 (44%)	18,36,39	3.41	4 (22%)
44	M7A	2	4564	44	20,25,26	1.98	3 (15%)	28,37,40	3.90	6 (21%)
44	5MC	2	4335	44	18,22,23	3.56	7 (38%)	26,32,35	1.07	2 (7%)
44	OMU	2	4306	44	19,22,23	3.02	8 (42%)	26,31,34	1.70	4 (15%)
44	B8K	2	4690	44	24,28,29	3.31	12 (50%)	30,42,45	2.64	12 (40%)
44	B9B	2	2754	44	21,28,29	2.02	3 (14%)	23,40,43	6.49	4 (17%)
44	UR3	2	4597	44	19,22,23	2.76	6 (31%)	26,32,35	2.11	6 (23%)
44	E7G	2	1797	44	24,27,28	4.04	11 (45%)	30,40,43	2.29	10 (33%)
44	UR3	2	4530	44	19,22,23	2.87	7 (36%)	26,32,35	1.34	2 (7%)
44	A2M	2	1534	44	18,25,26	3.60	8 (44%)	18,36,39	3.62	4 (22%)
44	OMG	2	2773	44	18,26,27	2.85	8 (44%)	19,38,41	1.47	5 (26%)
44	7MG	2	2522	44	22,26,27	3.67	10 (45%)	29,39,42	2.00	9 (31%)
44	OMC	2	2861	44	19,22,23	3.03	8 (42%)	26,31,34	1.06	2 (7%)
44	A2M	2	3867	44	18,25,26	3.61	8 (44%)	18,36,39	3.42	4 (22%)
44	B8H	2	4296	44	19,22,23	6.77	6 (31%)	22,32,35	2.30	5 (22%)
44	B8W	2	4472	44	18,26,27	2.12	2 (11%)	21,38,41	2.63	7 (33%)
44	B8T	2	4671	44	19,22,23	3.55	8 (42%)	26,31,34	0.97	1 (3%)
44	OMG	2	4370	44	18,26,27	2.81	8 (44%)	19,38,41	1.50	5 (26%)
44	OMC	2	3909	44	19,22,23	3.04	8 (42%)	26,31,34	1.23	3 (11%)
44	A2M	2	2401	44	18,25,26	3.60	8 (44%)	18,36,39	3.39	3 (16%)
44	OMG	2	1316	44	18,26,27	2.80	8 (44%)	19,38,41	1.62	5 (26%)
44	A2M	2	4571	44	18,25,26	3.59	8 (44%)	18,36,39	3.40	4 (22%)
44	BGH	2	3899	44	25,29,30	4.56	17 (68%)	31,43,46	2.61	12 (38%)
44	UR3	2	1866	44	19,22,23	2.91	6 (31%)	26,32,35	1.31	2 (7%)
44	A2M	2	398	44	18,25,26	3.59	8 (44%)	18,36,39	3.47	4 (22%)
44	6MZ	2	4220	44	18,25,26	1.89	3 (16%)	16,36,39	3.68	3 (18%)
44	2MG	2	4872	44	18,26,27	2.54	6 (33%)	16,38,41	1.80	4 (25%)
44	E7G	2	2297	44	24,27,28	3.93	11 (45%)	30,40,43	2.14	9 (30%)
44	OMG	2	4196	44	18,26,27	2.96	7 (38%)	19,38,41	1.65	6 (31%)
44	OMG	2	1883	44	18,26,27	2.82	8 (44%)	19,38,41	1.56	6 (31%)
4	OMU	8	14	4,44	19,22,23	2.91	8 (42%)	26,31,34	1.80	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	2MG	2	1517	44	18,26,27	2.68	6 (33%)	16,38,41	1.57	3 (18%)
44	OMC	2	2804	44	19,22,23	2.94	8 (42%)	26,31,34	1.22	3 (11%)
44	OMC	2	2422	44,50	19,22,23	2.98	8 (42%)	26,31,34	1.10	2 (7%)
44	A2M	2	1524	44	18,25,26	3.61	8 (44%)	18,36,39	3.42	4 (22%)
44	5MU	2	4083	44	19,22,23	7.23	8 (42%)	28,32,35	3.38	10 (35%)
44	OMC	2	3887	44	19,22,23	3.03	8 (42%)	26,31,34	0.92	1 (3%)
44	B8H	2	1860	44	19,22,23	6.75	6 (31%)	22,32,35	2.28	5 (22%)
44	B8W	2	4129	44	18,26,27	2.11	2 (11%)	21,38,41	2.49	8 (38%)
44	B8W	2	4185	44	18,26,27	2.11	2 (11%)	21,38,41	2.48	7 (33%)
44	1MA	2	4415	44	16,25,26	4.35	5 (31%)	18,37,40	1.69	3 (16%)
44	OMG	2	2364	44	18,26,27	2.78	8 (44%)	19,38,41	1.56	5 (26%)
44	P7G	2	1909	44	24,28,29	3.96	11 (45%)	27,41,44	1.59	4 (14%)
44	E6G	2	4355	44	20,27,28	2.77	3 (15%)	22,39,42	3.04	7 (31%)
44	B8T	2	4483	44	19,22,23	3.64	8 (42%)	26,31,34	1.31	3 (11%)
44	B8K	2	3897	44	24,28,29	3.41	11 (45%)	30,42,45	2.54	11 (36%)
44	OMC	2	3869	44	19,22,23	3.04	8 (42%)	26,31,34	1.63	5 (19%)
44	B9B	2	1574	44	21,28,29	1.94	3 (14%)	23,40,43	6.41	5 (21%)
44	OMG	2	1522	44	18,26,27	2.76	8 (44%)	19,38,41	1.51	5 (26%)
44	7MG	2	4550	44	22,26,27	3.84	10 (45%)	29,39,42	1.96	9 (31%)
44	B9B	2	237	44	21,28,29	1.97	3 (14%)	23,40,43	6.57	5 (21%)
44	B8W	2	4529	44	18,26,27	2.13	2 (11%)	21,38,41	2.69	7 (33%)
44	OMC	2	3701	44	19,22,23	2.98	8 (42%)	26,31,34	0.82	0
44	A2M	2	3718	44	18,25,26	3.59	8 (44%)	18,36,39	3.42	4 (22%)
44	OMC	2	2365	44	19,22,23	2.91	8 (42%)	26,31,34	0.82	0
44	MHG	2	4371	44	29,32,33	3.94	11 (37%)	34,46,49	2.32	12 (35%)
44	P7G	2	3880	44	24,28,29	4.04	11 (45%)	27,41,44	1.53	4 (14%)
44	OMG	2	4637	44	18,26,27	2.78	8 (44%)	19,38,41	1.56	5 (26%)
44	B9H	2	2786	44	20,25,26	3.35	4 (20%)	22,35,38	2.75	7 (31%)
44	B8W	2	2380	44	18,26,27	2.03	2 (11%)	21,38,41	2.36	6 (28%)
44	OMU	2	4620	44	19,22,23	2.94	8 (42%)	26,31,34	1.67	5 (19%)
44	A2M	2	4523	44	18,25,26	3.57	8 (44%)	18,36,39	3.39	4 (22%)
44	OMG	2	2050	44	18,26,27	2.77	8 (44%)	19,38,41	1.55	5 (26%)
44	OMG	2	4494	44	18,26,27	2.87	8 (44%)	19,38,41	1.46	4 (21%)
44	2MG	2	978	44	18,26,27	2.68	6 (33%)	16,38,41	1.41	4 (25%)
44	OMG	2	4623	44	18,26,27	2.72	8 (44%)	19,38,41	1.58	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	I4U	2	1659	44	21,24,25	3.50	9 (42%)	27,34,37	1.31	2 (7%)
44	B8Q	2	1456	44	17,22,23	2.97	5 (29%)	22,32,35	2.39	6 (27%)
44	A2M	2	1326	44	18,25,26	3.69	9 (50%)	18,36,39	3.50	4 (22%)
44	OMG	2	373	44	18,26,27	2.85	8 (44%)	19,38,41	1.66	5 (26%)
44	A2M	2	2363	44	18,25,26	3.59	8 (44%)	18,36,39	3.38	4 (22%)
44	A2M	2	1871	44	18,25,26	3.58	8 (44%)	18,36,39	3.40	3 (16%)
44	P4U	2	1348	44	21,24,25	3.52	8 (38%)	27,33,36	1.09	2 (7%)

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
44	OMC	2	4536	44	-	0/9/27/28	0/2/2/2
44	7MG	2	1605	44	-	0/7/37/38	0/3/3/3
44	OMG	2	2424	44	-	2/5/27/28	0/3/3/3
44	OMG	2	4870	44	-	3/5/27/28	0/3/3/3
44	A2M	2	3825	44	-	0/5/27/28	0/3/3/3
44	2MG	2	729	44	-	1/5/27/28	0/3/3/3
44	OMG	2	1625	44	-	2/5/27/28	0/3/3/3
44	A2M	2	3723	44	-	2/5/27/28	0/3/3/3
44	M7A	2	4564	44	-	0/7/37/38	0/3/3/3
44	5MC	2	4335	44	-	0/7/25/26	0/2/2/2
44	OMU	2	4306	44	-	0/9/27/28	0/2/2/2
44	B8K	2	4690	44	-	1/11/41/42	0/3/3/3
44	B9B	2	2754	44	-	3/7/29/30	0/3/3/3
44	UR3	2	4597	44	-	0/7/25/26	0/2/2/2
44	E7G	2	1797	44	-	2/9/39/40	0/3/3/3
44	UR3	2	4530	44	-	0/7/25/26	0/2/2/2
44	A2M	2	1534	44	-	1/5/27/28	0/3/3/3
44	OMG	2	2773	44	-	1/5/27/28	0/3/3/3
44	7MG	2	2522	44	-	0/7/37/38	0/3/3/3
44	OMC	2	2861	44	-	0/9/27/28	0/2/2/2
44	A2M	2	3867	44	-	2/5/27/28	0/3/3/3
44	B8H	2	4296	44	-	2/7/25/26	0/2/2/2
44	B8W	2	4472	44	-	1/5/27/28	0/3/3/3
44	B8T	2	4671	44	-	0/7/27/28	0/2/2/2
44	OMG	2	4370	44	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	OMC	2	3909	44	-	0/9/27/28	0/2/2/2
44	A2M	2	2401	44	-	1/5/27/28	0/3/3/3
44	OMG	2	1316	44	-	1/5/27/28	0/3/3/3
44	A2M	2	4571	44	-	0/5/27/28	0/3/3/3
44	BGH	2	3899	44	-	0/13/43/44	0/3/3/3
44	UR3	2	1866	44	-	2/7/25/26	0/2/2/2
44	A2M	2	398	44	-	2/5/27/28	0/3/3/3
44	6MZ	2	4220	44	-	0/5/27/28	0/3/3/3
44	2MG	2	4872	44	-	2/5/27/28	0/3/3/3
44	E7G	2	2297	44	-	1/9/39/40	0/3/3/3
44	OMG	2	4196	44	-	2/5/27/28	0/3/3/3
44	OMG	2	1883	44	-	2/5/27/28	0/3/3/3
4	OMU	8	14	4,44	-	1/9/27/28	0/2/2/2
44	2MG	2	1517	44	-	3/5/27/28	0/3/3/3
44	OMC	2	2804	44	-	0/9/27/28	0/2/2/2
44	OMC	2	2422	44,50	-	1/9/27/28	0/2/2/2
44	A2M	2	1524	44	-	2/5/27/28	0/3/3/3
44	5MU	2	4083	44	-	0/7/25/26	0/2/2/2
44	OMC	2	3887	44	-	1/9/27/28	0/2/2/2
44	B8H	2	1860	44	-	0/7/25/26	0/2/2/2
44	B8W	2	4129	44	-	2/5/27/28	0/3/3/3
44	B8W	2	4185	44	-	2/5/27/28	0/3/3/3
44	1MA	2	4415	44	-	3/3/25/26	0/3/3/3
44	OMG	2	2364	44	-	2/5/27/28	0/3/3/3
44	P7G	2	1909	44	-	2/10/40/41	0/3/3/3
44	E6G	2	4355	44	-	2/6/28/29	0/3/3/3
44	B8T	2	4483	44	-	0/7/27/28	0/2/2/2
44	B8K	2	3897	44	-	3/11/41/42	0/3/3/3
44	OMC	2	3869	44	-	5/9/27/28	0/2/2/2
44	B9B	2	1574	44	-	3/7/29/30	0/3/3/3
44	OMG	2	1522	44	-	0/5/27/28	0/3/3/3
44	7MG	2	4550	44	-	0/7/37/38	0/3/3/3
44	B9B	2	237	44	-	5/7/29/30	0/3/3/3
44	B8W	2	4529	44	-	0/5/27/28	0/3/3/3
44	OMC	2	3701	44	-	4/9/27/28	0/2/2/2
44	A2M	2	3718	44	-	0/5/27/28	0/3/3/3
44	OMC	2	2365	44	-	0/9/27/28	0/2/2/2
44	MHG	2	4371	44	-	3/16/46/47	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	P7G	2	3880	44	-	4/10/40/41	0/3/3/3
44	OMG	2	4637	44	-	3/5/27/28	0/3/3/3
44	B9H	2	2786	44	-	1/12/47/48	0/2/2/2
44	B8W	2	2380	44	-	2/5/27/28	0/3/3/3
44	OMU	2	4620	44	-	0/9/27/28	0/2/2/2
44	A2M	2	4523	44	-	3/5/27/28	0/3/3/3
44	OMG	2	2050	44	-	0/5/27/28	0/3/3/3
44	OMG	2	4494	44	-	0/5/27/28	0/3/3/3
44	2MG	2	978	44	-	0/5/27/28	0/3/3/3
44	OMG	2	4623	44	-	0/5/27/28	0/3/3/3
44	I4U	2	1659	44	-	2/9/29/30	0/2/2/2
44	B8Q	2	1456	44	-	0/7/42/43	0/2/2/2
44	A2M	2	1326	44	-	3/5/27/28	0/3/3/3
44	OMG	2	373	44	-	1/5/27/28	0/3/3/3
44	A2M	2	2363	44	-	0/5/27/28	0/3/3/3
44	A2M	2	1871	44	-	0/5/27/28	0/3/3/3
44	P4U	2	1348	44	-	2/10/29/30	0/2/2/2

The worst 5 of 590 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	4083	5MU	C4-C5	20.75	1.79	1.44
44	2	4296	B8H	C6-C5	-16.42	1.11	1.34
44	2	1860	B8H	C6-C5	-16.38	1.11	1.34
44	2	4415	1MA	C2-N3	16.04	1.48	1.29
44	2	4083	5MU	C6-N1	15.93	1.65	1.38

The worst 5 of 389 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	2	237	B9B	O6-C6-N1	-29.95	94.27	120.12
44	2	2754	B9B	O6-C6-N1	-29.72	94.47	120.12
44	2	1574	B9B	O6-C6-N1	-29.42	94.72	120.12
44	2	4564	M7A	C5-C6-N6	13.78	147.27	123.74
44	2	4220	6MZ	C1'-N9-C4	-12.45	104.76	126.64

There are no chirality outliers.

5 of 101 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	8	14	OMU	C1'-C2'-O2'-CM2
44	2	237	B9B	C5-C6-O6-C61
44	2	237	B9B	N1-C6-O6-C61
44	2	237	B9B	C3'-C4'-C5'-O5'
44	2	237	B9B	O4'-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 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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$
52	GDP	A	801	53,54	24,30,30	1.20	2 (8%)	30,47,47	1.41	5 (16%)
55	GTP	4	701	46,53	26,34,34	1.12	2 (7%)	32,54,54	1.64	7 (21%)

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
52	GDP	A	801	53,54	-	2/12/32/32	0/3/3/3
55	GTP	4	701	46,53	-	2/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	4	701	GTP	C5-C6	-3.90	1.39	1.47
52	A	801	GDP	C6-N1	-3.47	1.32	1.37
52	A	801	GDP	C2'-C1'	-2.22	1.50	1.53
55	4	701	GTP	C2-N3	2.14	1.38	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	A	801	GDP	PA-O3A-PB	-3.52	120.74	132.83
55	4	701	GTP	C5-C6-N1	3.50	120.14	113.95
55	4	701	GTP	C3'-C2'-C1'	3.38	106.06	100.98
52	A	801	GDP	C3'-C2'-C1'	3.26	105.89	100.98
55	4	701	GTP	C2-N1-C6	-3.03	119.51	125.10

There are no chirality outliers.

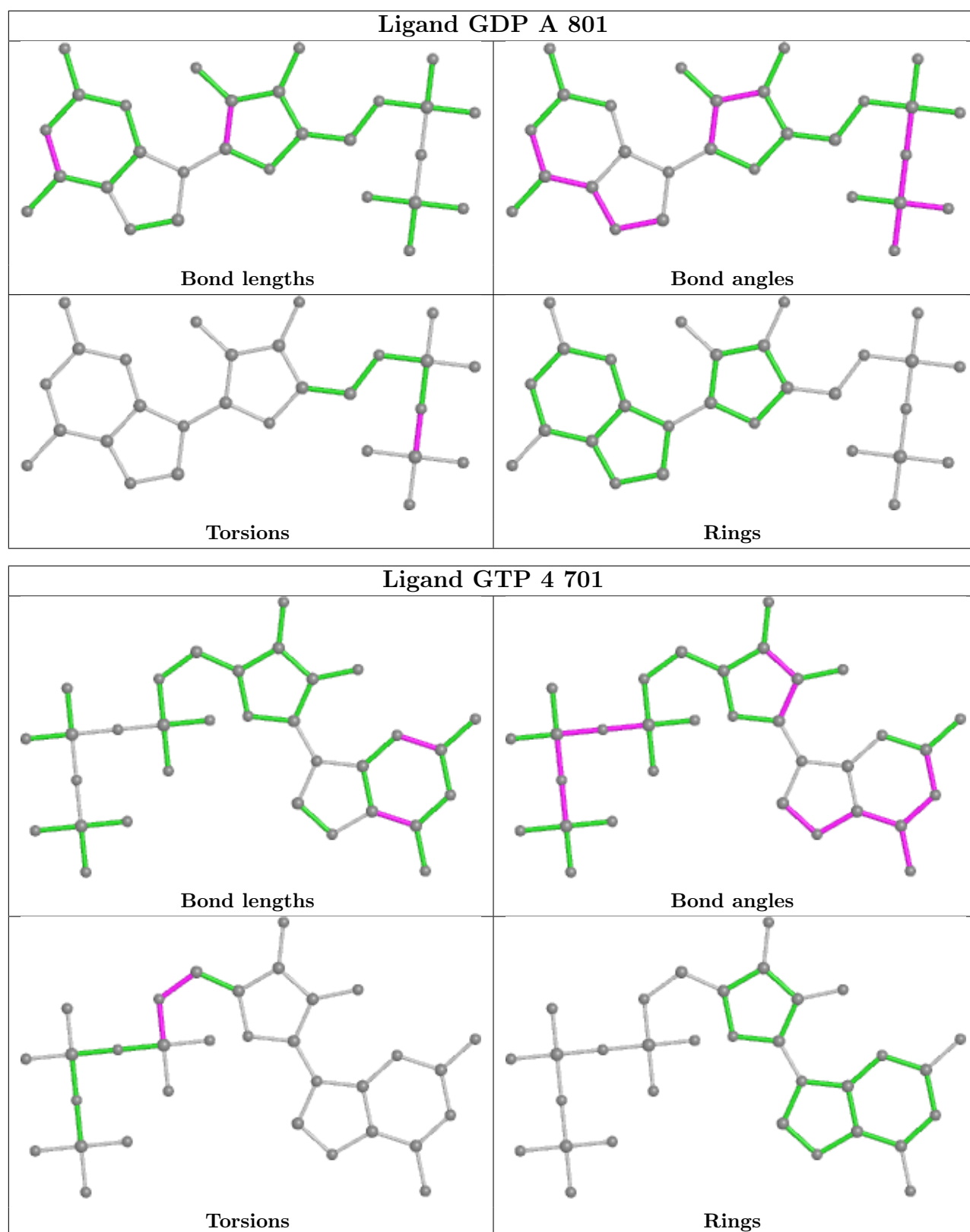
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	A	801	GDP	PA-O3A-PB-O2B
55	4	701	GTP	C4'-C5'-O5'-PA
52	A	801	GDP	PA-O3A-PB-O1B
55	4	701	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

There are no chain breaks in this entry.

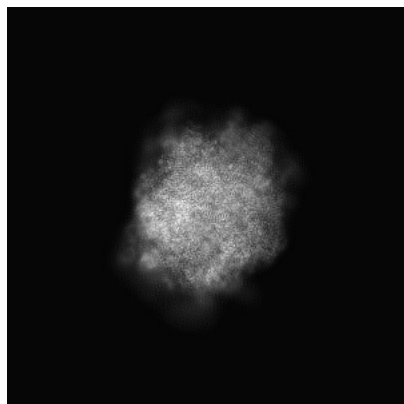
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35370. These allow visual inspection of the internal detail of the map and identification of artifacts.

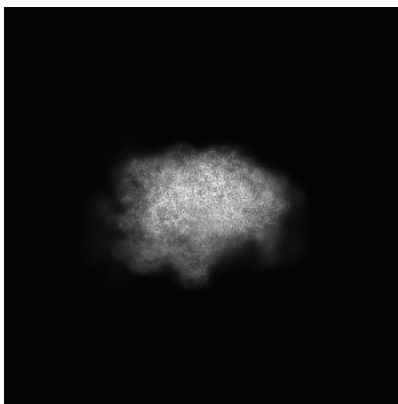
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

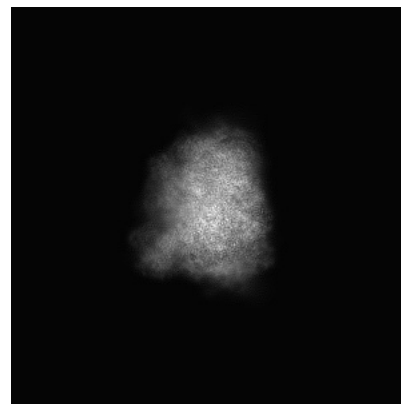
6.1.1 Primary map



X

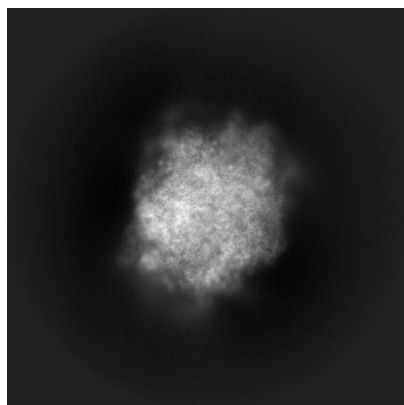


Y

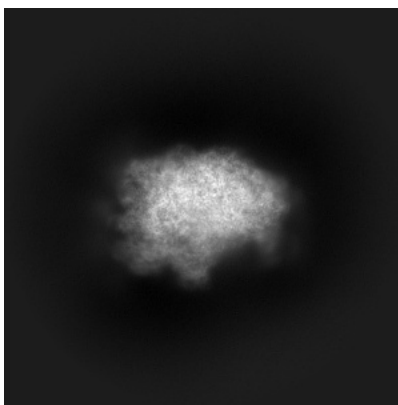


Z

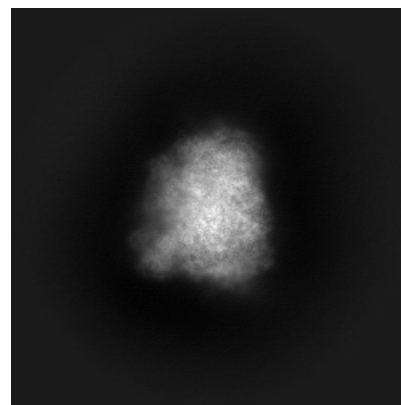
6.1.2 Raw map



X



Y

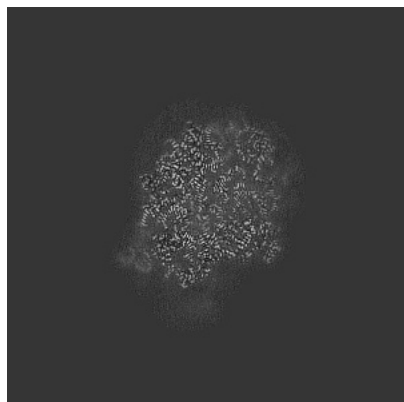


Z

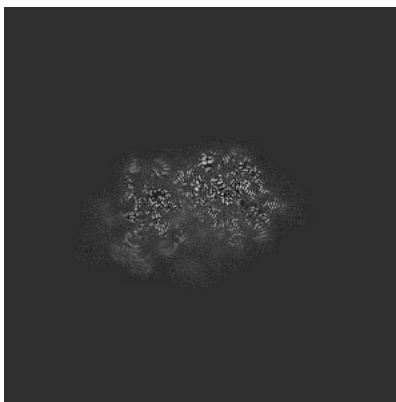
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

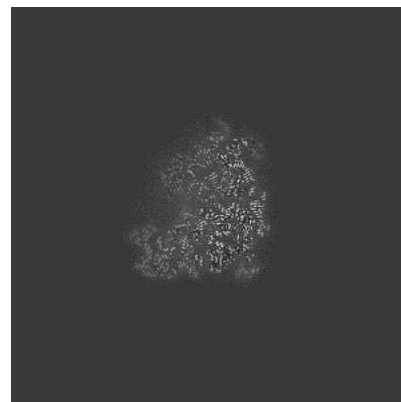
6.2.1 Primary map



X Index: 200

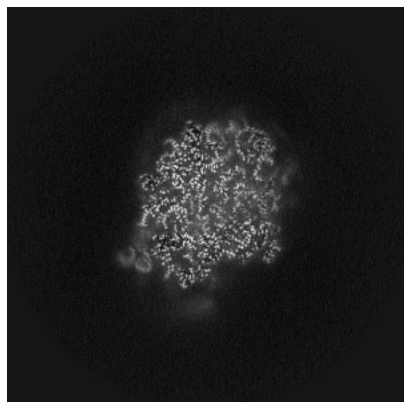


Y Index: 200

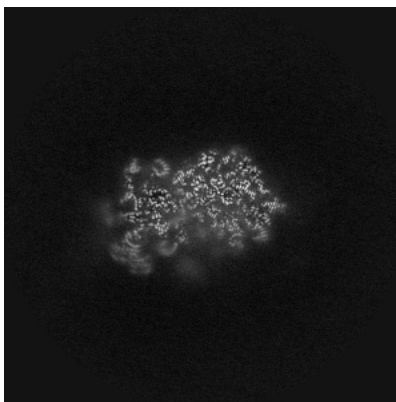


Z Index: 200

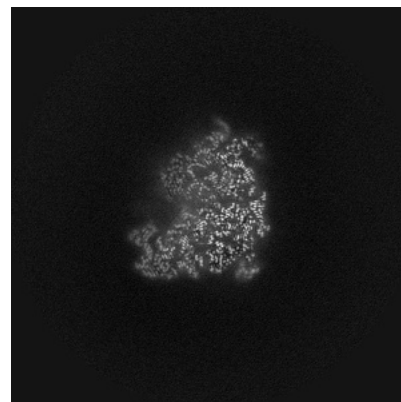
6.2.2 Raw map



X Index: 200



Y Index: 200

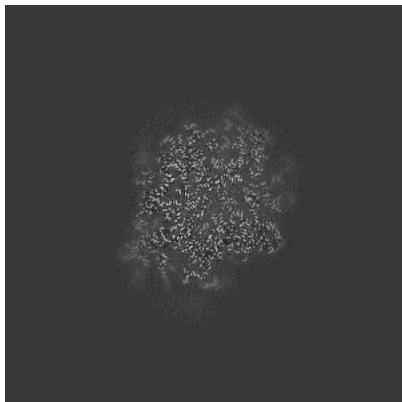


Z Index: 200

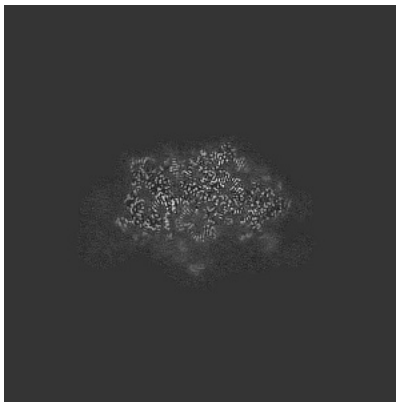
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

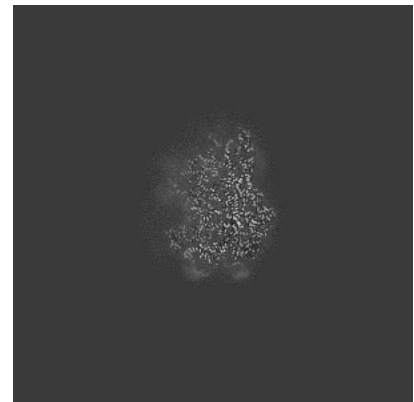
6.3.1 Primary map



X Index: 206

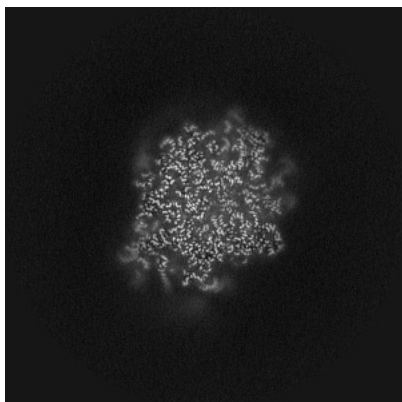


Y Index: 182

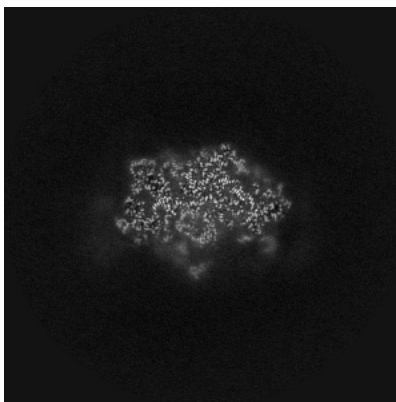


Z Index: 215

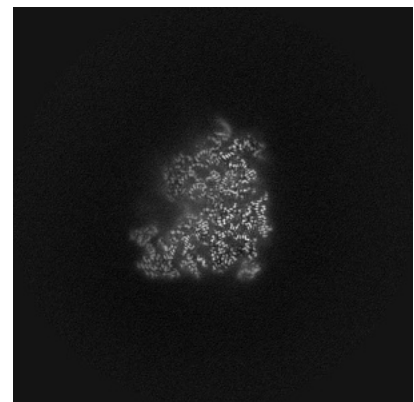
6.3.2 Raw map



X Index: 206



Y Index: 181

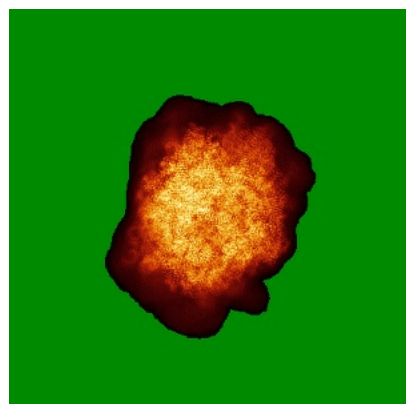


Z Index: 201

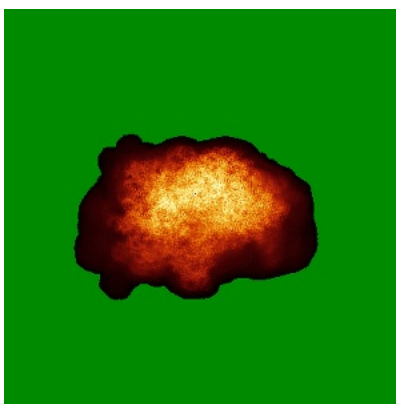
The images above show the largest variance slices of the map in three orthogonal directions.

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

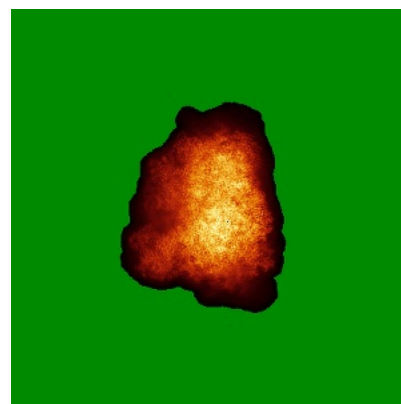
6.4.1 Primary map



X

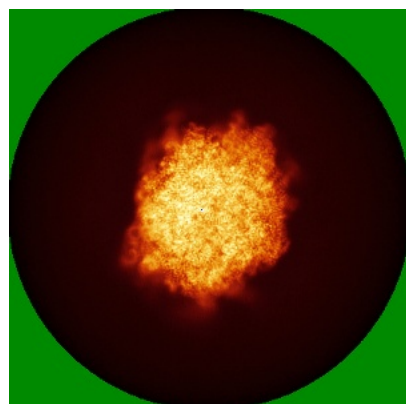


Y

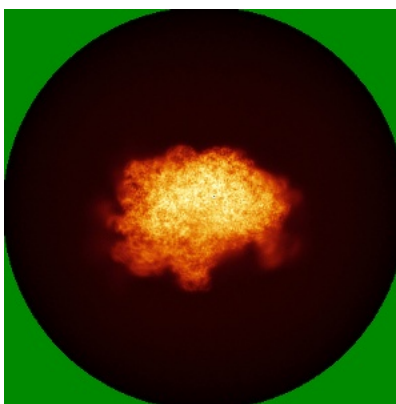


Z

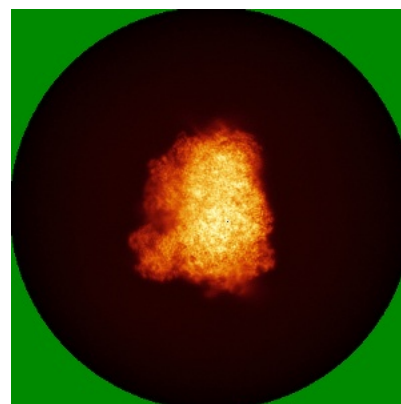
6.4.2 Raw map



X



Y



Z

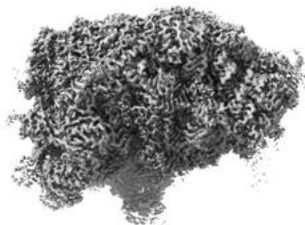
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



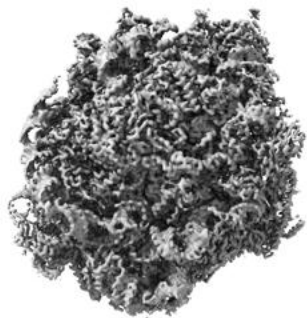
Y



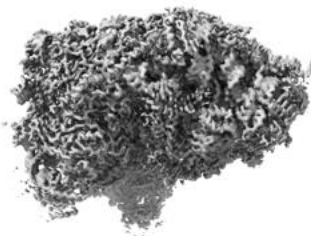
Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

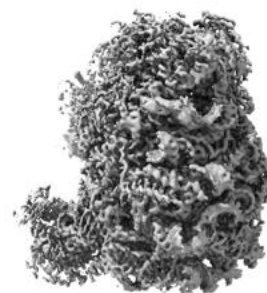
6.5.2 Raw map



X



Y



Z

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

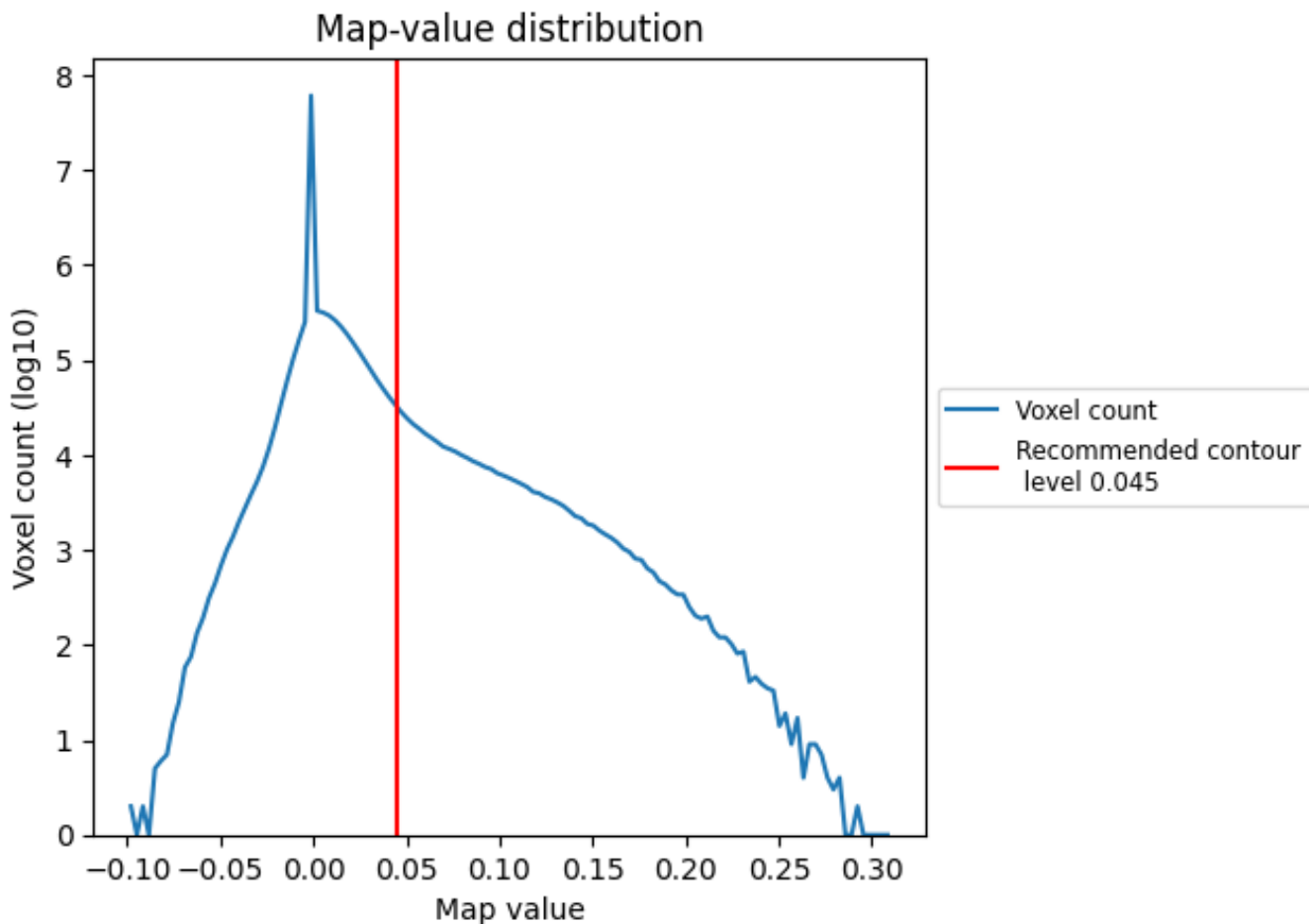
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

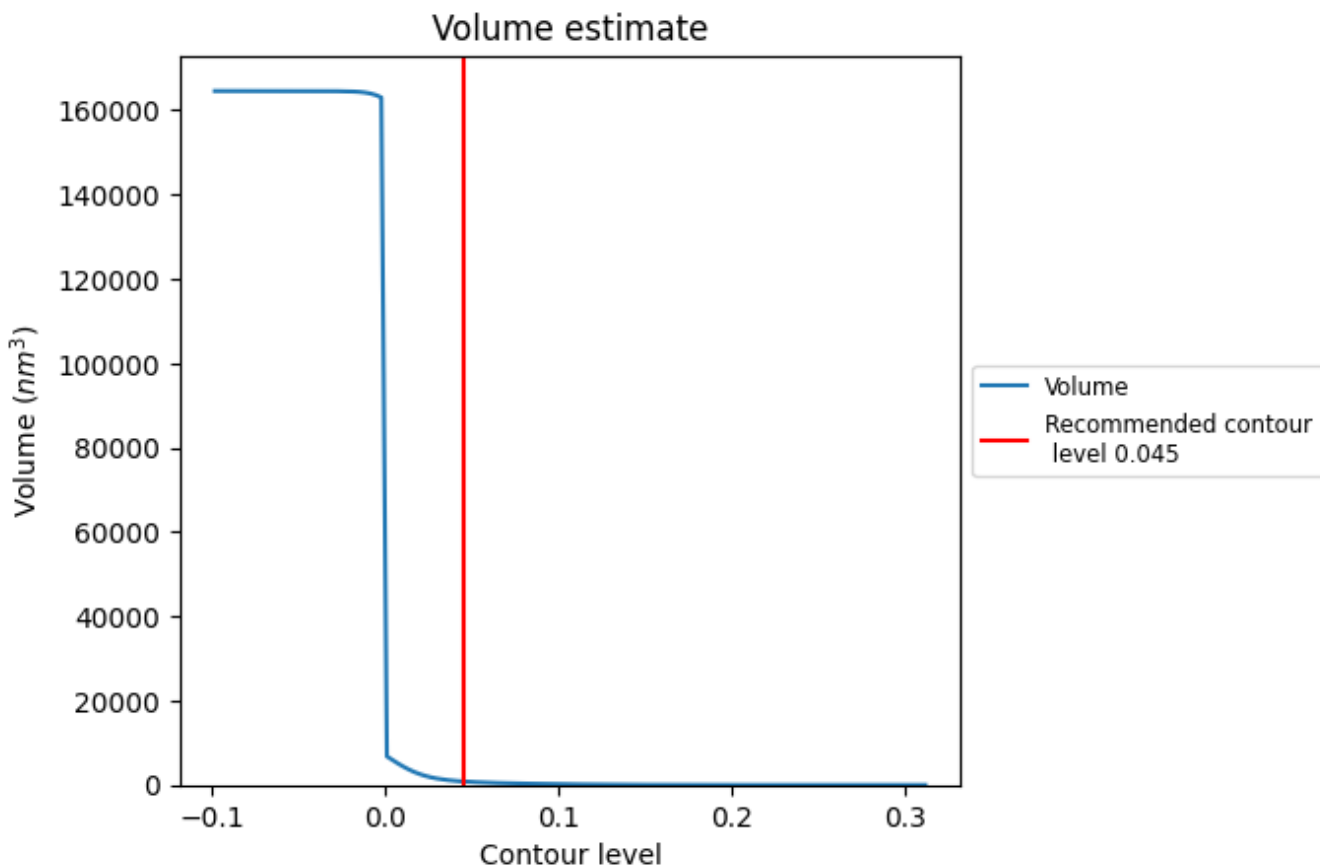
This section contains the results of statistical analysis of the map.

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.

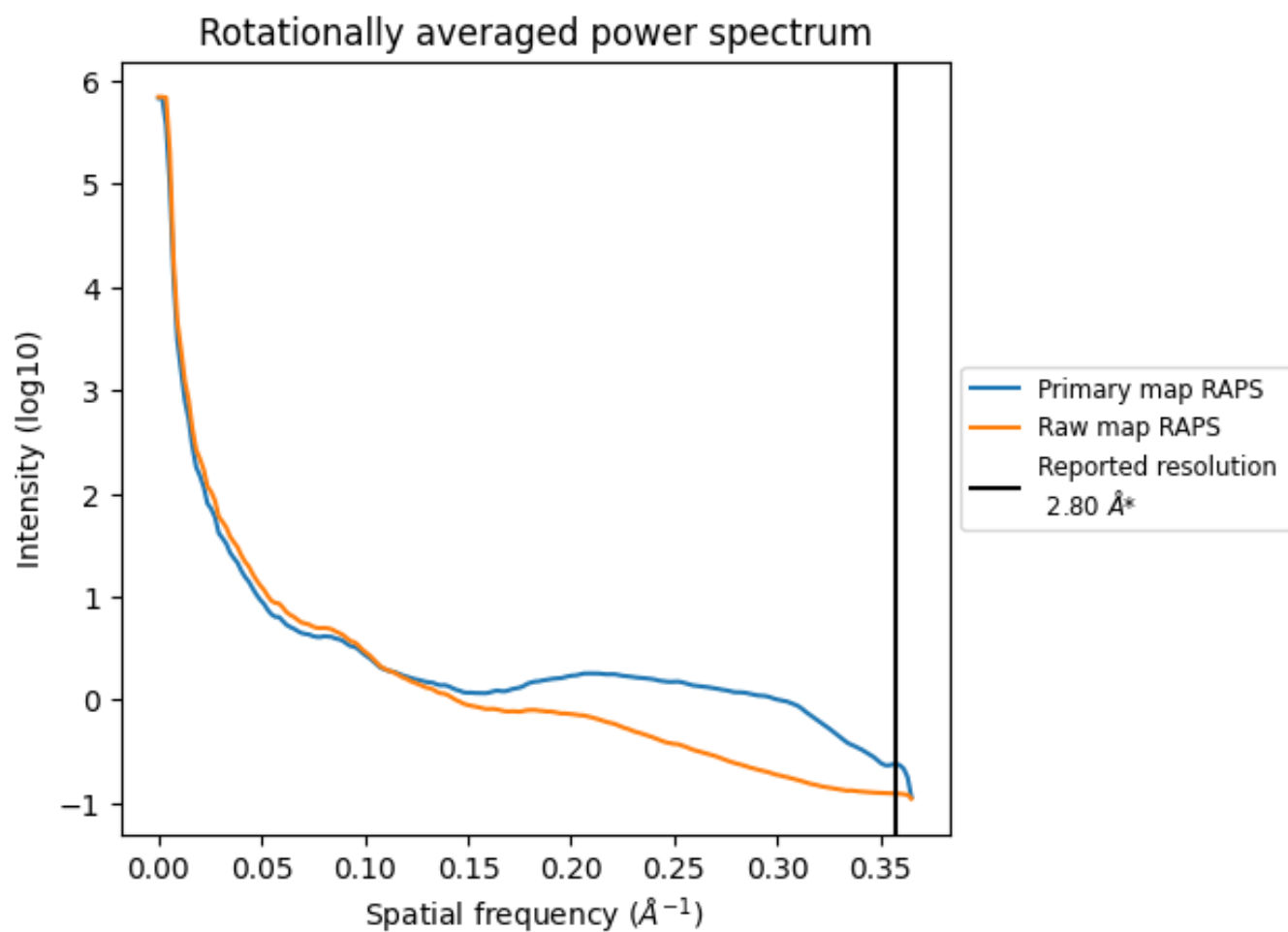
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 836 nm³; this corresponds to an approximate mass of 755 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

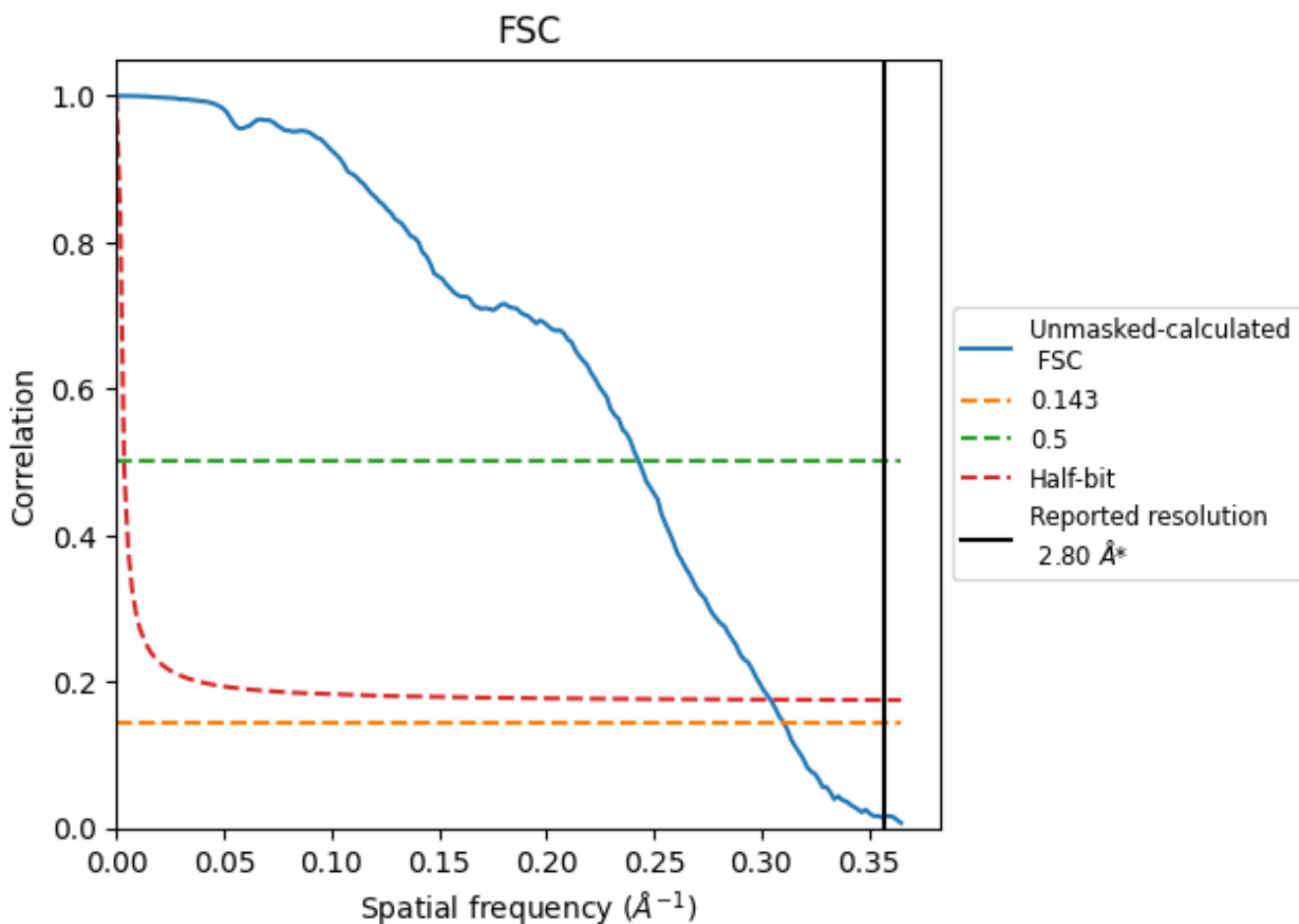


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357\AA^{-1}

8.2 Resolution estimates [i](#)

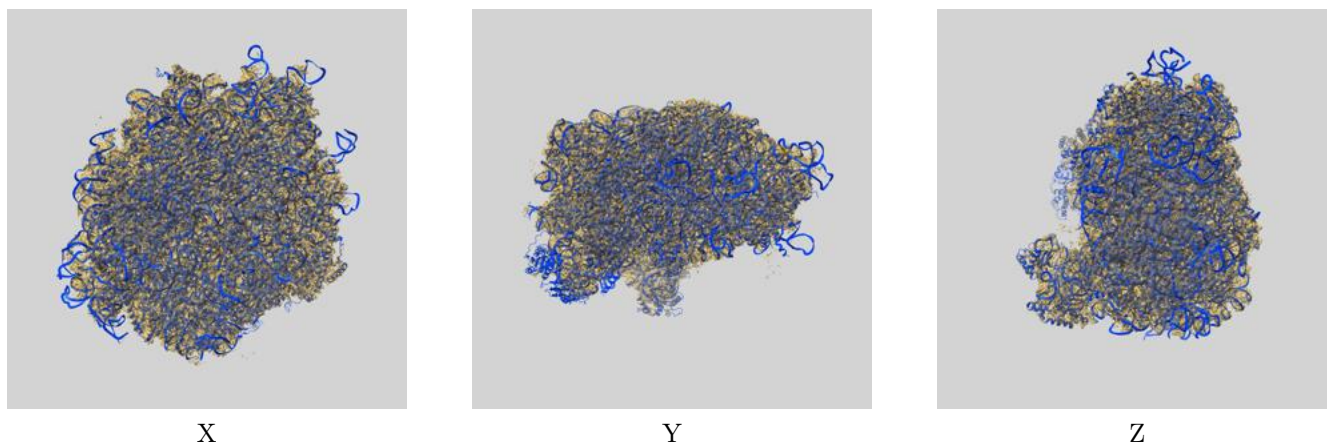
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.22	4.12	3.29

*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 3.22 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

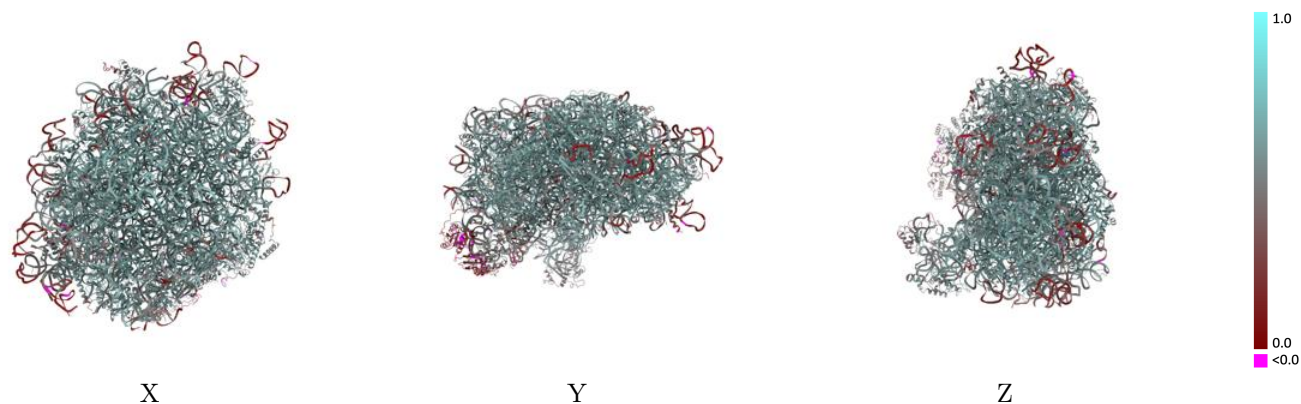
This section contains information regarding the fit between EMDB map EMD-35370 and PDB model 8IDT. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



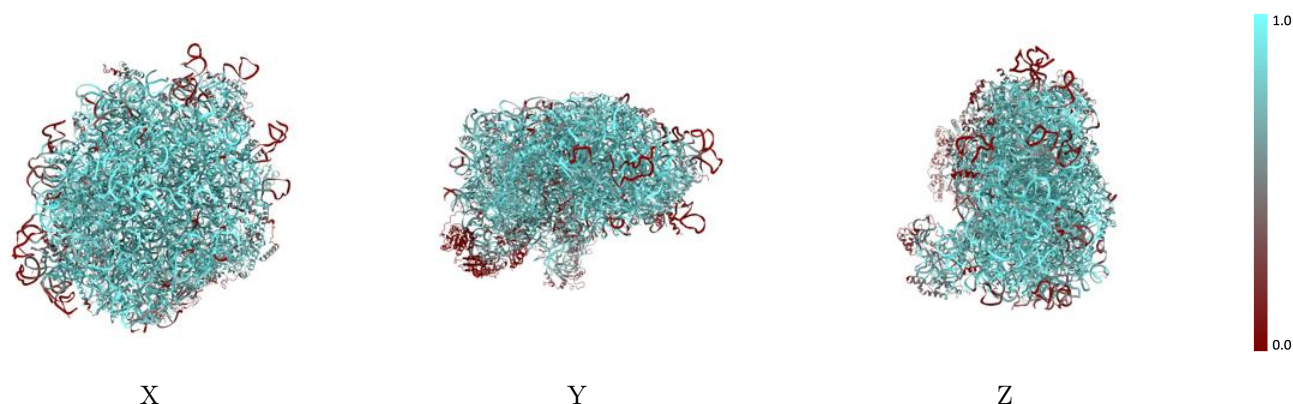
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



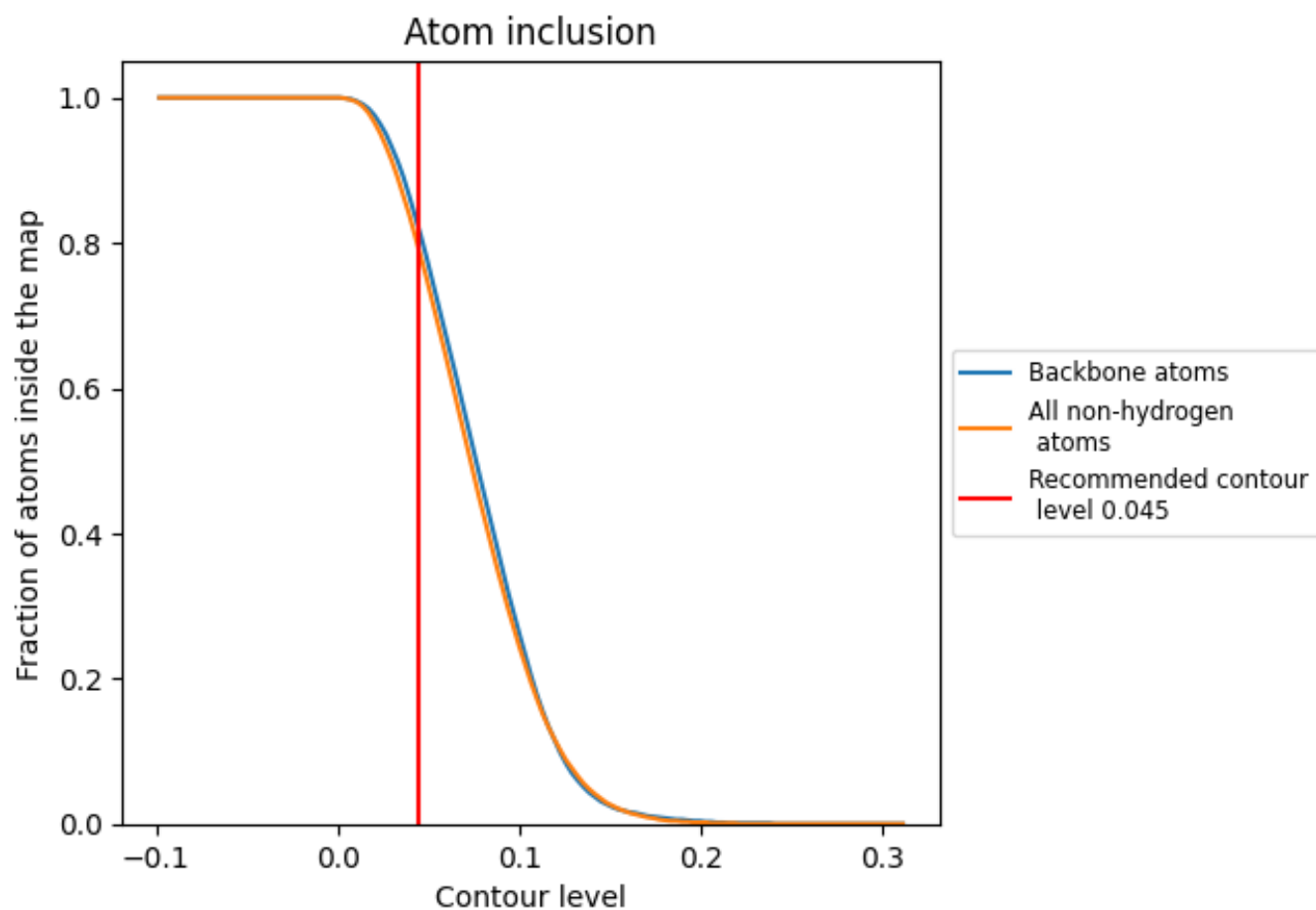
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 79% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7910	 0.5500
2	 0.8320	 0.5460
4	 0.6000	 0.4920
5	 0.8910	 0.5750
6	 0.7140	 0.5450
7	 0.8060	 0.5820
8	 0.9220	 0.5940
9	 0.3770	 0.4980
A	 0.4620	 0.5310
B	 0.8960	 0.6100
C	 0.6720	 0.5150
D	 0.9220	 0.6120
E	 0.5600	 0.5360
F	 0.8450	 0.5860
G	 0.6810	 0.5200
H	 0.8420	 0.5950
I	 0.7840	 0.5710
J	 0.0470	 0.1950
K	 0.8180	 0.5860
L	 0.9260	 0.6220
M	 0.9520	 0.6190
N	 0.3540	 0.4200
O	 0.6140	 0.5230
P	 0.9690	 0.6220
Q	 0.8290	 0.5770
R	 0.4980	 0.5180
S	 0.8750	 0.5950
T	 0.5200	 0.5110
U	 0.9620	 0.6320
V	 0.9120	 0.6080
W	 0.7270	 0.5800
X	 0.7280	 0.5670
Y	 0.8490	 0.5990
Z	 0.9400	 0.6330
a	 0.8080	 0.5880



Continued on next page...

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Chain	Atom inclusion	Q-score
b	 0.9340	 0.6260
c	 0.8400	 0.5810
d	 0.7320	 0.5550
e	 0.8610	 0.5910
g	 0.8650	 0.6000
h	 0.8650	 0.5980
i	 0.6720	 0.5570
j	 0.8290	 0.5890
k	 0.9380	 0.6230
l	 0.9200	 0.6100
m	 0.8700	 0.5950
n	 0.9480	 0.6280
o	 0.7250	 0.5330
p	 0.9030	 0.6060
r	 0.5570	 0.5000
y	 0.0200	 0.2250
z	 0.4800	 0.4980