



wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 08:39 pm BST

PDB ID : 6FTI / pdb_00006fti
EMDB ID : EMD-4316
Title : Cryo-EM Structure of the Mammalian Oligosaccharyltransferase Bound to Sec61 and the Programmed 80S Ribosome
Authors : Braunger, K.; Becker, T.; Beckmann, R.
Deposited on : 2018-02-22
Resolution : 4.20 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.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

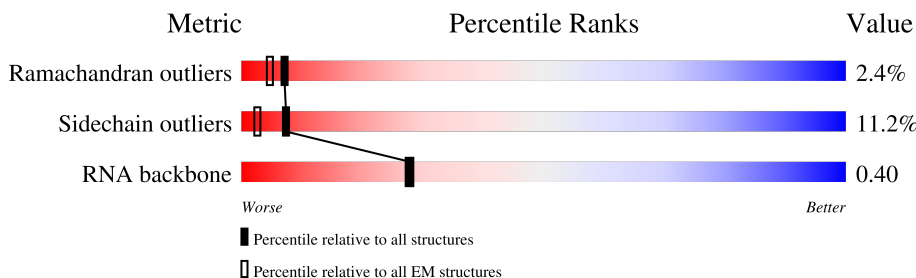
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	244	
2	B	394	
3	C	362	
4	D	292	
5	E	248	
6	F	225	
7	G	241	
8	H	190	

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Mol	Chain	Length	Quality of chain
9	I	213	
10	J	169	
11	L	210	
12	M	138	
13	N	203	
14	O	199	
15	P	153	
16	Q	187	
17	R	180	
18	S	175	
19	T	159	
20	U	99	
21	V	131	
22	W	63	
23	X	119	
24	Y	134	
25	Z	135	
26	a	147	
27	b	75	
28	c	94	
29	d	107	
30	e	128	
31	f	109	
32	g	114	
33	h	122	

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Mol	Chain	Length	Quality of chain
34	i	102	
35	j	86	
36	k	69	
37	l	50	
38	m	52	
39	n	23	
40	o	104	
41	p	91	
42	r	136	
43	s	198	
44	t	163	
45	q	76	
46	u	3662	
47	v	120	
48	w	156	
49	x	461	
50	y	62	
51	z	29	
52	1	162	
53	2	60	
54	3	120	
55	4	34	
56	5	705	
57	6	109	
58	7	25	

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Mol	Chain	Length	Quality of chain
59	8	80	 100%
60	0	24	 100%
61	K	8	 25% 25% 75%

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 153850 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 uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	244	Total	C	N	O	S	0	0
			1868	1171	382	309	6		

- Molecule 2 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	394	Total	C	N	O	S	0	0
			3148	2007	591	537	13		

- Molecule 3 is a protein called Ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	362	Total	C	N	O	S	0	0
			2884	1814	578	478	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	362	LYS	SER	conflict	UNP G1SVW5
C	363	SER	ASP	conflict	UNP G1SVW5

- Molecule 4 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	292	Total	C	N	O	S	0	0
			2386	1509	437	426	14		

- Molecule 5 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	236	Total	C	N	O	S	0	0
			1898	1215	362	318	3		

- Molecule 6 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	175	ALA	THR	conflict	UNP G1SV32
F	185	GLY	ASN	conflict	UNP G1SV32
F	202	ARG	HIS	conflict	UNP G1SV32
F	233	GLU	GLY	conflict	UNP G1SV32

- Molecule 7 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	241	Total	C	N	O	S	0	0
			1934	1233	371	326	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	191	GLY	CYS	conflict	UNP G1STW0

- Molecule 8 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 9 is a protein called Ribosomal protein L10 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	204	Total	C	N	O	S	0	0
			1655	1051	319	272	13		

- Molecule 10 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	169	Total	C	N	O	S	0	0
			1353	855	252	240	6		

- Molecule 11 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	210	Total	C	N	O	S	0	0
			1703	1065	354	280	4		

- Molecule 12 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 13 is a protein called Ribosomal protein L15.

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

- Molecule 14 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	199	Total	C	N	O	S	0	0
			1638	1056	321	256	5		

- Molecule 15 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	54	GLN	LYS	conflict	UNP G1TVT6

- Molecule 16 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	187	Total	C	N	O	S	0	0
			1506	941	311	249	5		

- Molecule 17 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 18 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	175	Total	C	N	O	S	0	0
			1454	925	284	235	10		

- Molecule 19 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 20 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

- Molecule 21 is a protein called uL14.

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

- Molecule 22 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	63	Total	C	N	O	S	0	0
			528	337	103	85	3		

- Molecule 23 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 24 is a protein called Ribosomal protein L26.

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

- Molecule 25 is a protein called 60S ribosomal protein L27.

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

- Molecule 26 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 27 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	75	Total	C	N	O	S	0	0
			609	378	130	98	3		

- Molecule 28 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	94	Total	C	N	O	S	0	0
			732	465	130	131	6		

- Molecule 29 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 30 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 31 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 32 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 33 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 34 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 35 is a protein called Ribosomal protein L37.

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

- Molecule 36 is a protein called eL38.

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

- Molecule 37 is a protein called eL39.

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

- Molecule 38 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 39 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	23	Total	C	N	O	S	0	0
			222	134	61	25	2		

- Molecule 40 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 41 is a protein called Ribosomal protein L37a.

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

- Molecule 42 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	r	136	Total	C	N	O	S	0	0
			1094	676	229	183	6		

- Molecule 43 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	198	Total	C	N	O	S	0	0
			1523	969	265	280	9		

- Molecule 44 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	163	Total	C	N	O	S	0	0
			1238	773	230	230	5		

- Molecule 45 is a RNA chain called p-Site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 46 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	u	3662	Total	C	N	O	P	0	0
			78486	34947	14363	25515	3661		

- Molecule 47 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 48 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	w	156	Total	C	N	O	P	0	0
			3314	1480	585	1094	155		

- Molecule 49 is a protein called Protein transport protein Sec61 subunit alpha isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	426	Total	C	N	O	S	0	0
			3313	2181	535	576	21		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	145	SER	ALA	conflict	UNP P38377

- Molecule 50 is a protein called Protein transport protein Sec61 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	y	62	Total	C	N	O	S	0	0
			494	326	86	79	3		

- Molecule 51 is a protein called Protein transport protein Sec61 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	z	29	Total	C	N	O	S	0	0
			229	157	36	34	2		

- Molecule 52 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1,RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1	162	Total	C	N	O		0	0
			885	553	165	167			

- Molecule 53 is a protein called TMEM258.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2	60	Total	C	N	O		0	0
			300	180	60	60			

- Molecule 54 is a protein called Oligosaccharyltransferase complex subunit OSTC.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3	120	Total	C	N	O	S	0	0
			802	529	130	136	7		

- Molecule 55 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4	34	Total	C	N	O	S	0	0
			268	180	41	45	2		

- Molecule 56 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	5	644	Total	C	N	O	S	0	0
			5090	3331	819	904	36		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	88	LEU	ILE	conflict	UNP F1PJP5

- Molecule 57 is a protein called DAD1.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	6	97	Total	C	N	O	0	0
			485	291	97	97		

- Molecule 58 is a protein called OST48.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	7	25	Total	C	N	O	0	0
			125	75	25	25		

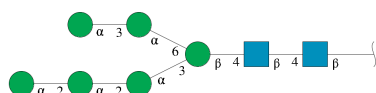
- Molecule 59 is a protein called RPN1.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	8	80	Total	C	N	O	0	0
			400	240	80	80		

- Molecule 60 is a protein called Unidentified TM.

Mol	Chain	Residues	Atoms				AltConf	Trace
60	0	24	Total	C	N	O	0	0
			120	72	24	24		

- Molecule 61 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
61	K	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 62 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
62	B	1	Total	Mg	0
			1	1	
62	I	1	Total	Mg	0
			1	1	

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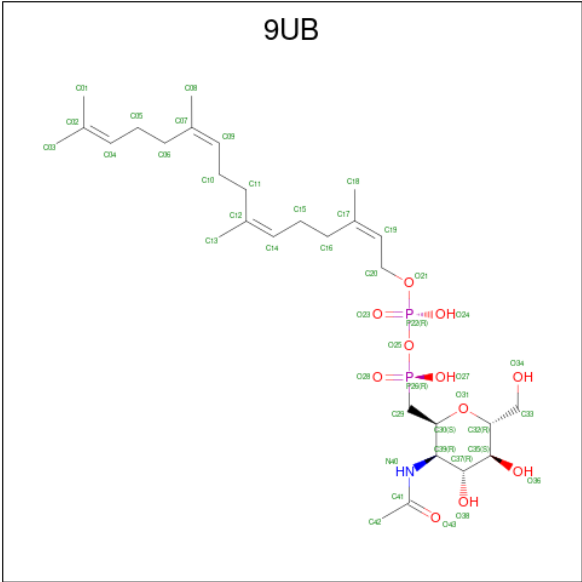
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Mol	Chain	Residues	Atoms		AltConf
62	P	1	Total 1	Mg 1	0
62	V	1	Total 1	Mg 1	0
62	a	1	Total 1	Mg 1	0
62	e	1	Total 1	Mg 1	0
62	g	1	Total 1	Mg 1	0
62	u	145	Total 145	Mg 145	0
62	v	5	Total 5	Mg 5	0
62	w	2	Total 2	Mg 2	0

- Molecule 63 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
63	g	1	Total 1	Zn 1	0
63	j	1	Total 1	Zn 1	0
63	m	1	Total 1	Zn 1	0
63	o	1	Total 1	Zn 1	0
63	p	1	Total 1	Zn 1	0

- Molecule 64 is [(2 {S},3 {R},4 {R},5 {S},6 {R})-3-acetamido-6-(hydroxymethyl)-4,5-bis(oxidanyl)oxan-2-yl]methyl-[oxidanyl-[(2 {Z},6 {Z},10 {Z})-3,7,11,15-tetramethylhexadeca-2,6,10,14-tetraenoxy]phosphoryl]oxy-phosphinic acid (CCD ID: 9UB) (formula: C₂₉H₅₁NO₁₁P₂).

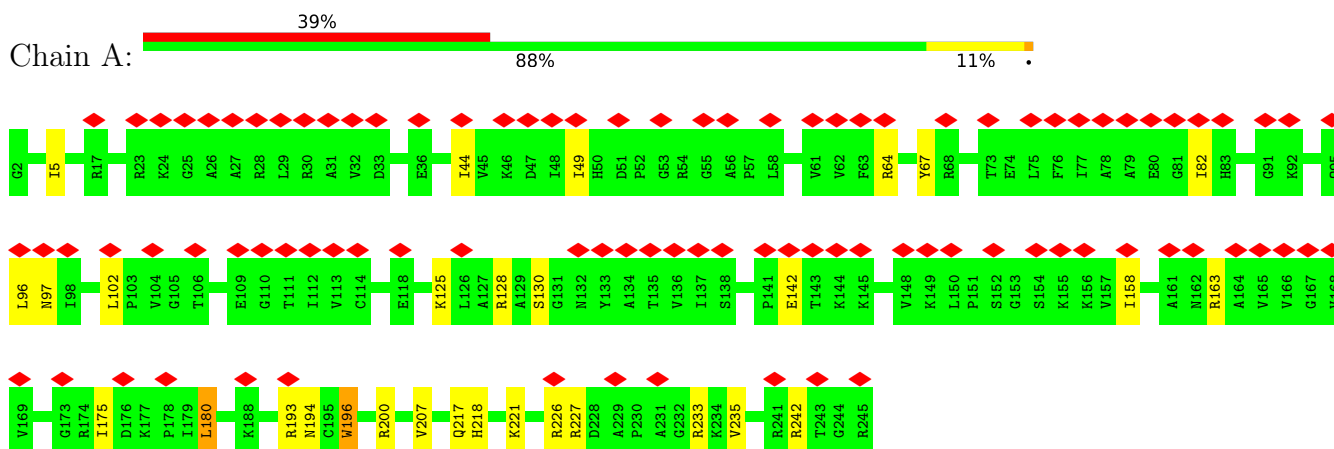


Mol	Chain	Residues	Atoms					AltConf
64	5	1	Total	C	N	O	P	0
			43	29	1	11	2	

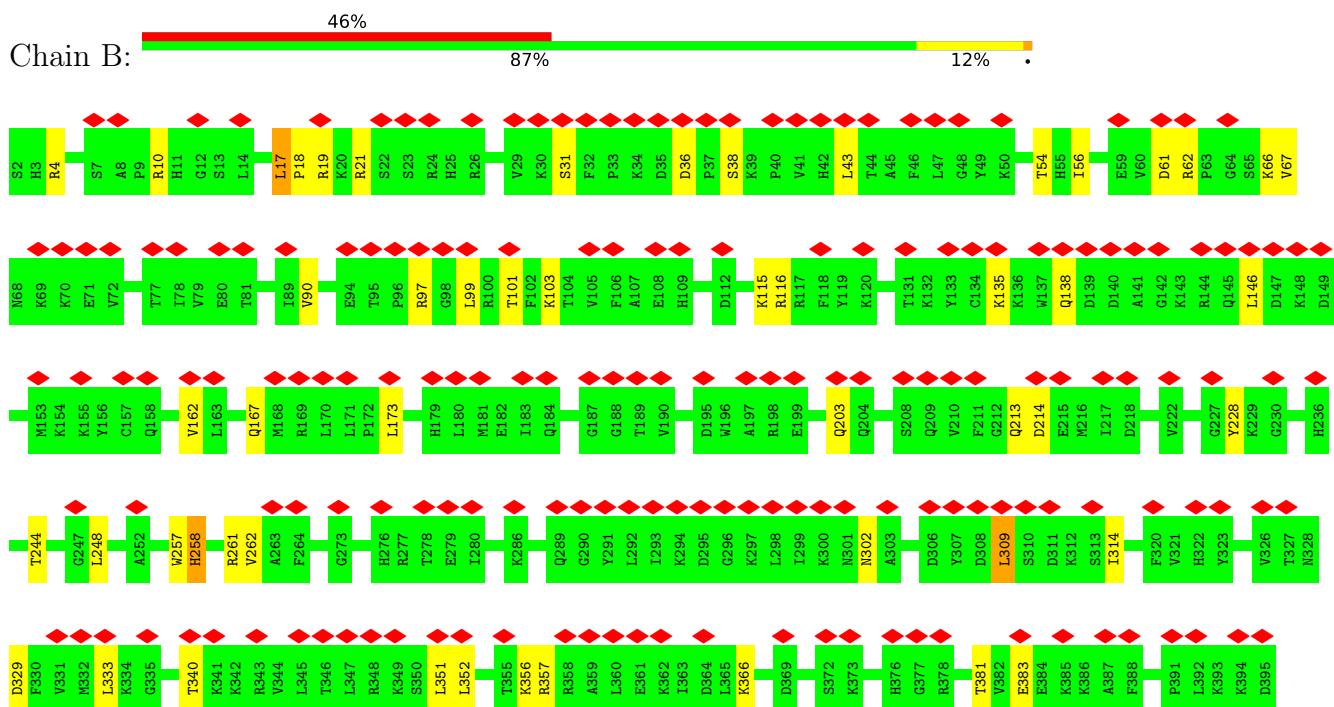
3 Residue-property plots

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

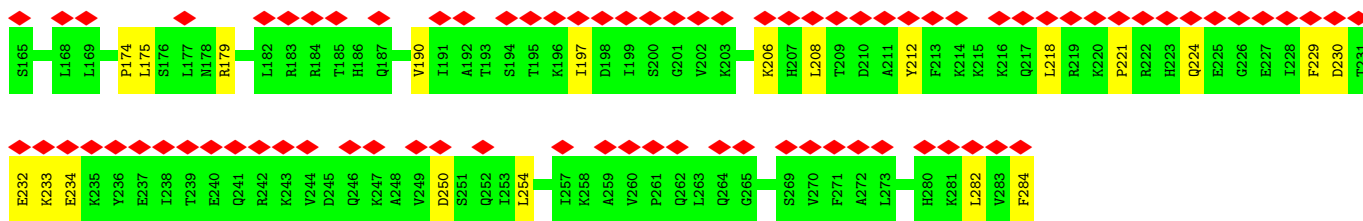
• Molecule 1: uL2



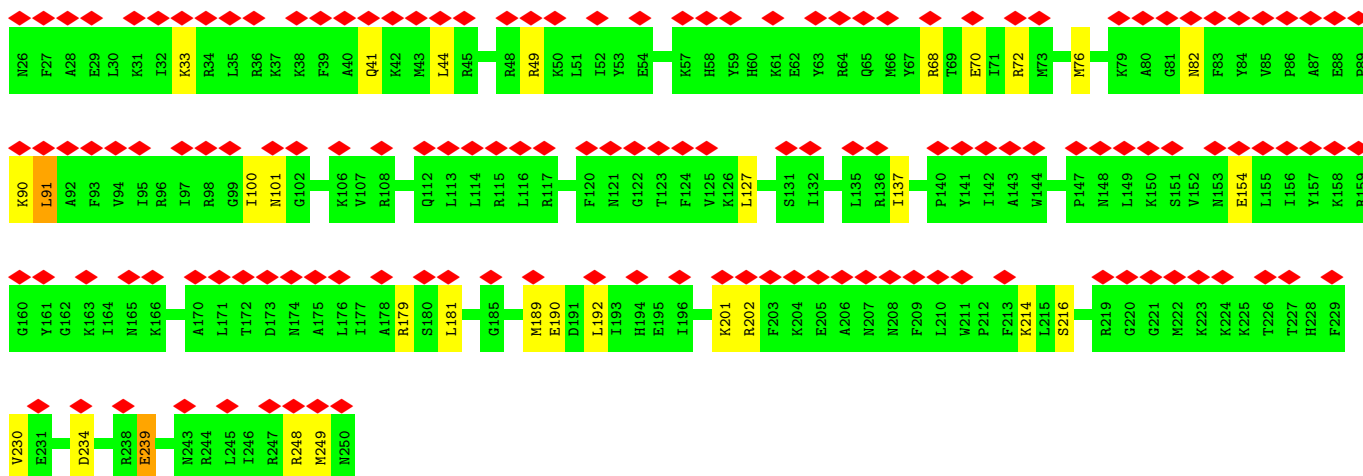
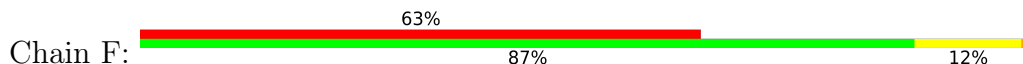
• Molecule 2: uL3



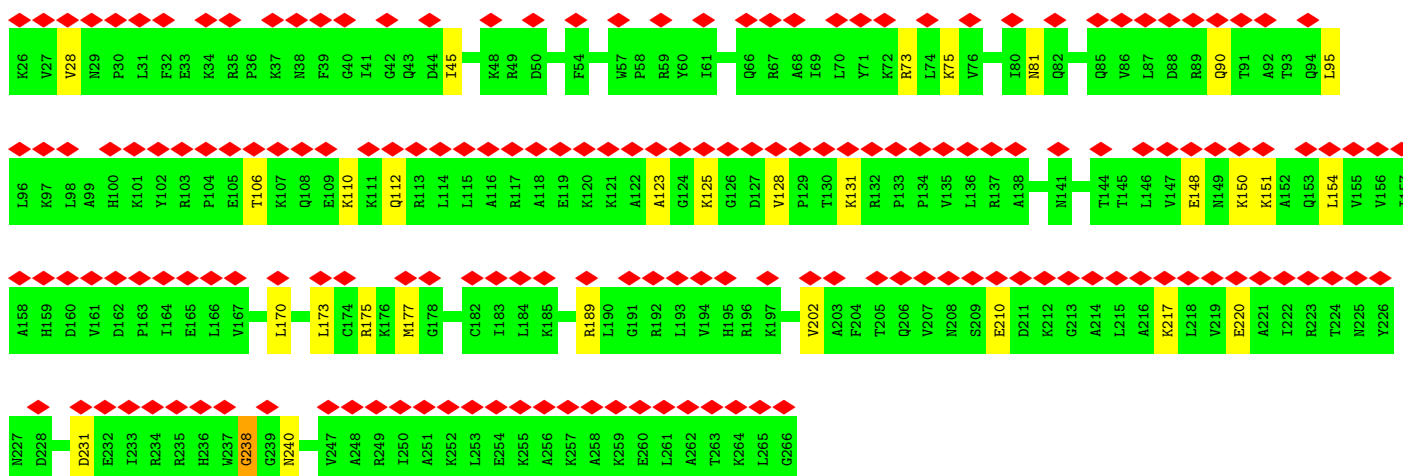
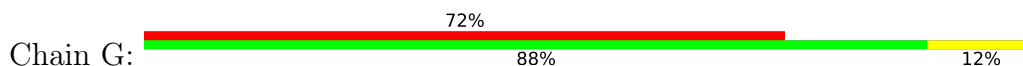
• Molecule 3: Ribosomal protein L4



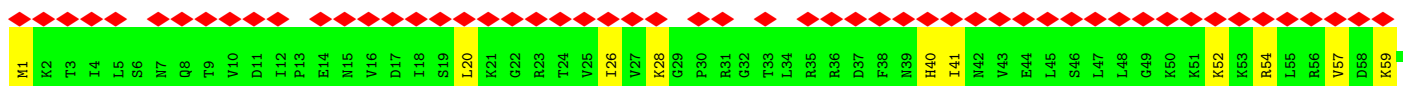
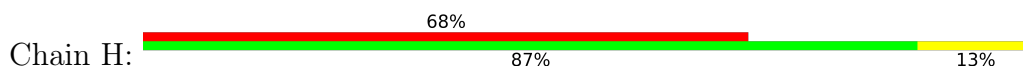
• Molecule 6: uL30

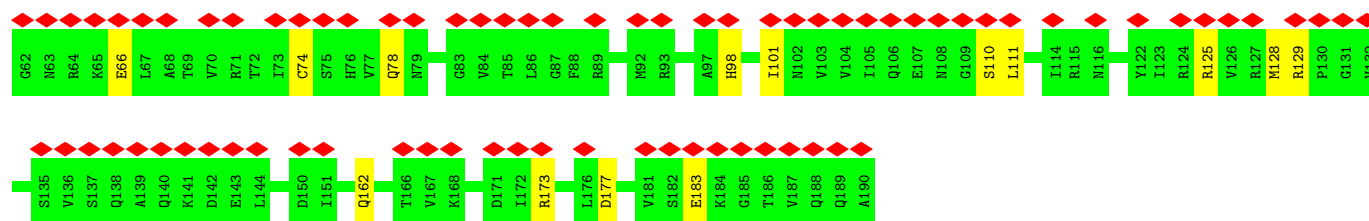


• Molecule 7: eL8

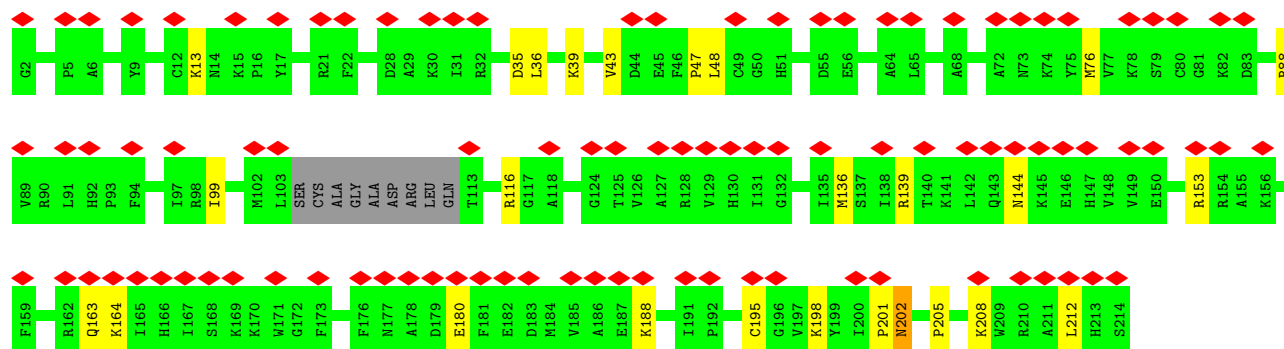
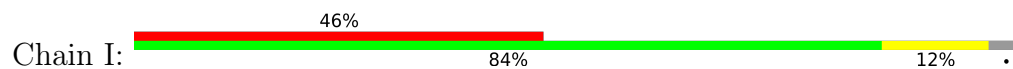


• Molecule 8: uL6

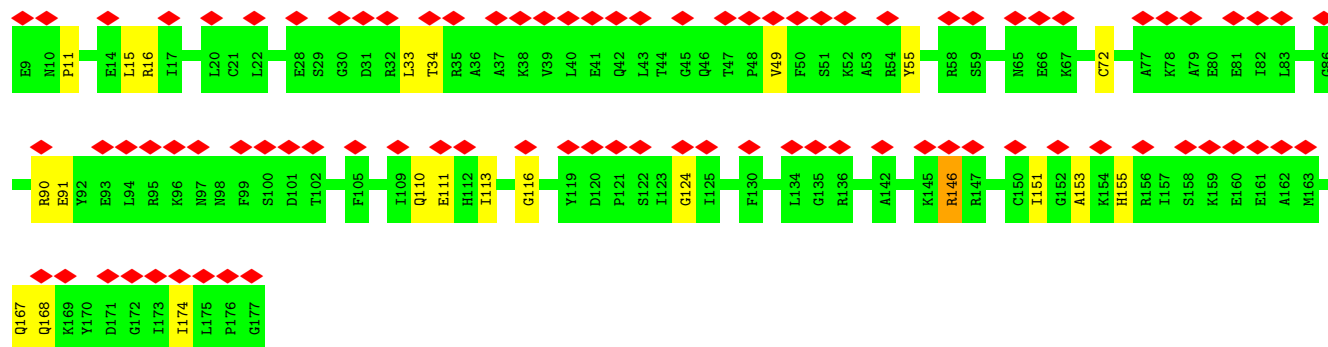
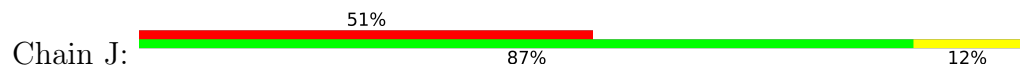




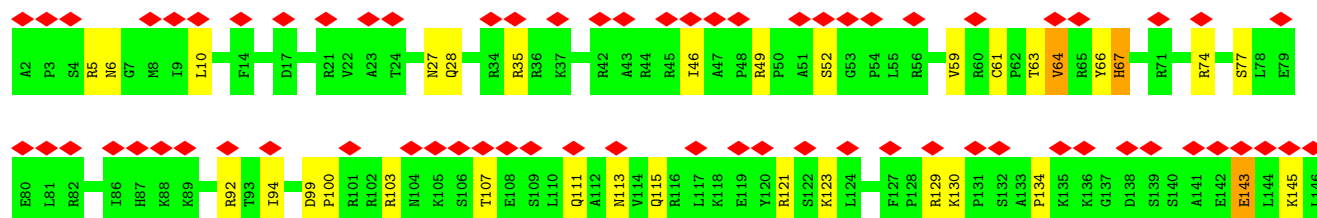
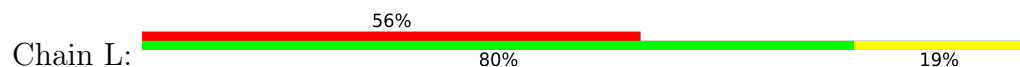
• Molecule 9: Ribosomal protein L10 (Predicted)

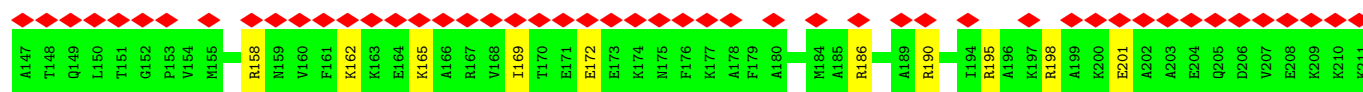


• Molecule 10: Ribosomal protein L11

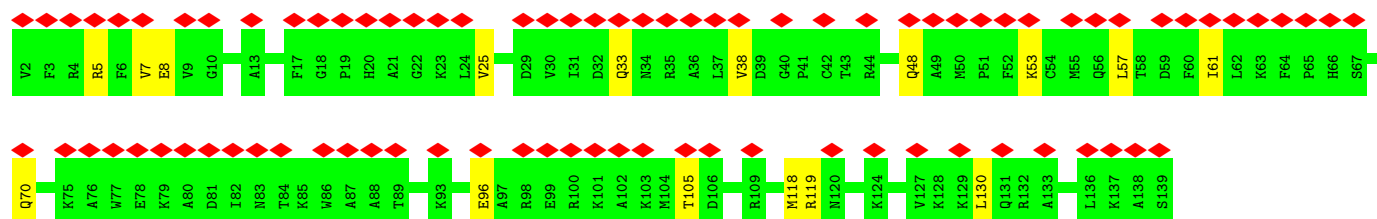
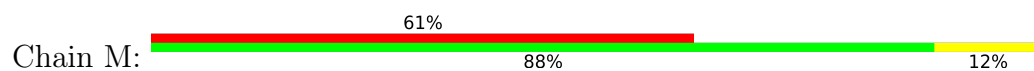


• Molecule 11: eL13

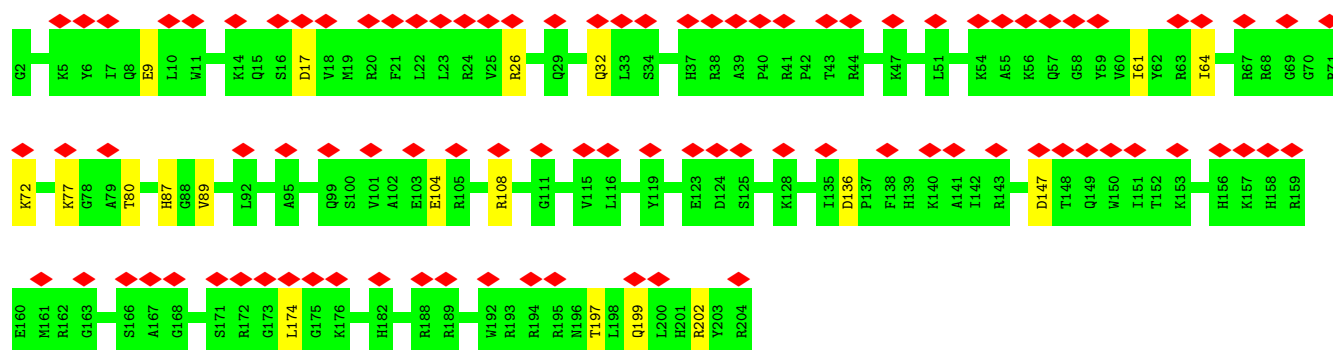
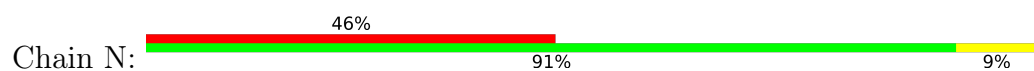




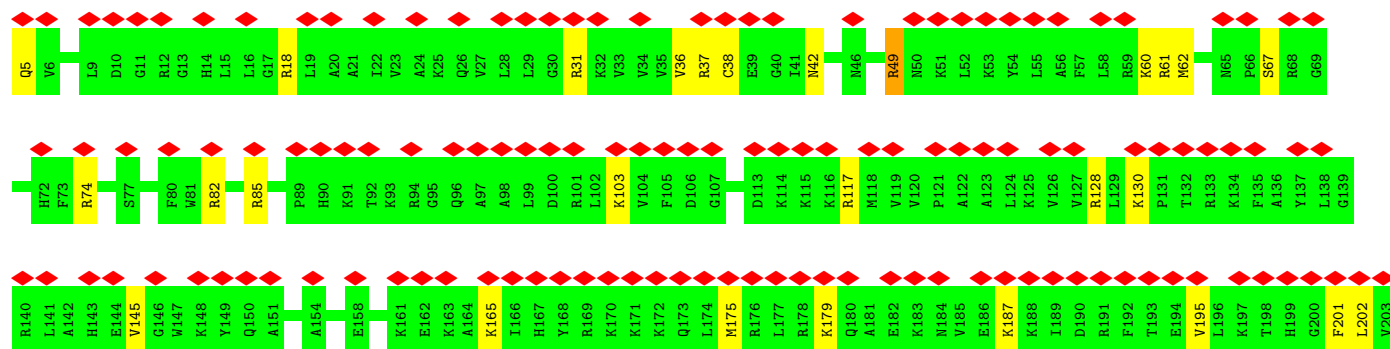
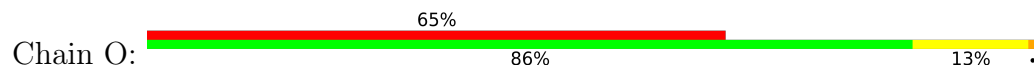
• Molecule 12: Ribosomal protein L14



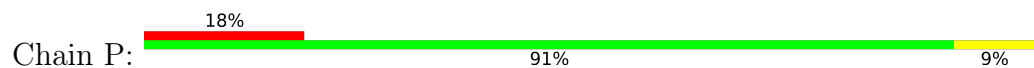
• Molecule 13: Ribosomal protein L15

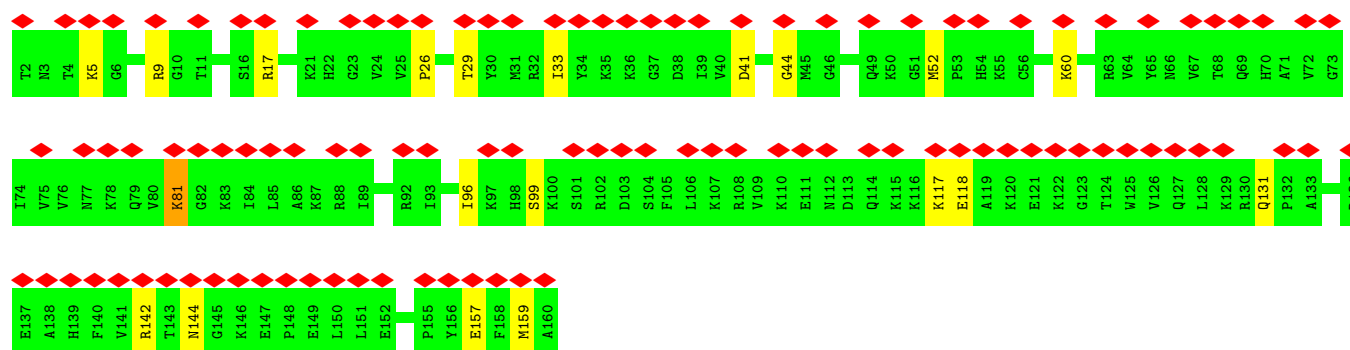
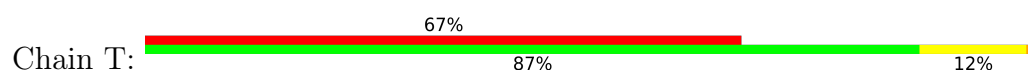


• Molecule 14: uL13

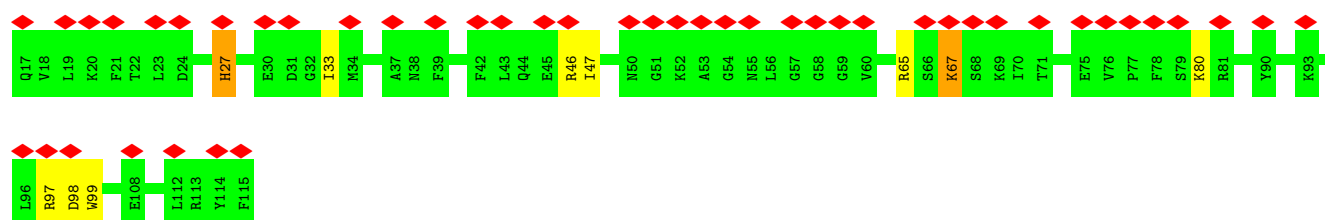
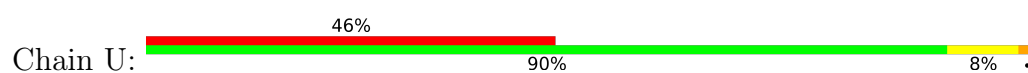


• Molecule 15: uL22

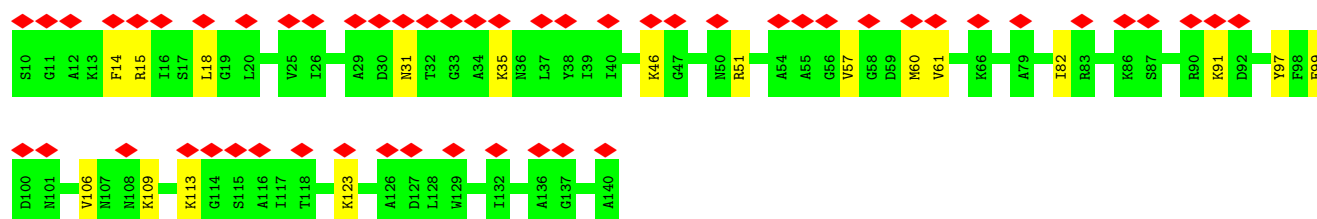
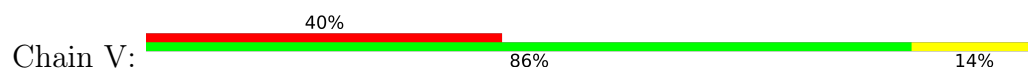




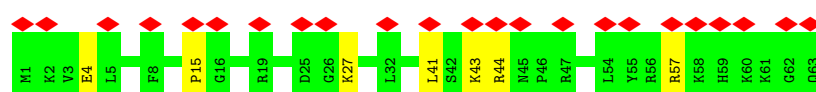
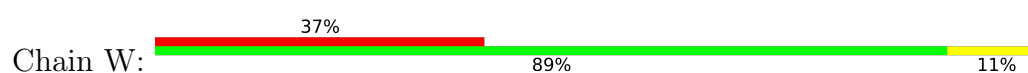
• Molecule 20: eL22



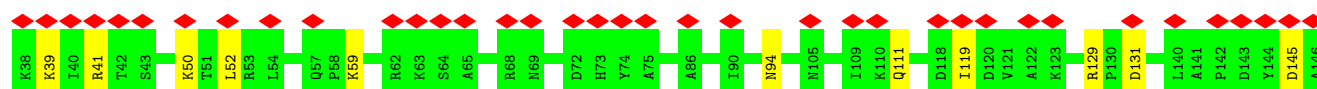
• Molecule 21: uL14

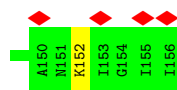


• Molecule 22: Ribosomal protein L24

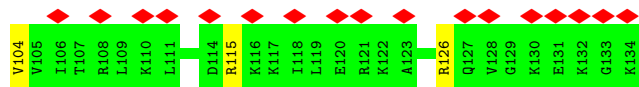
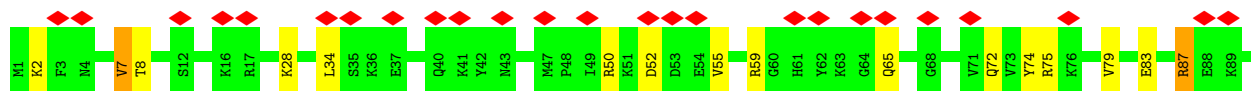
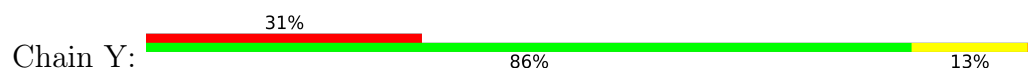


• Molecule 23: uL23

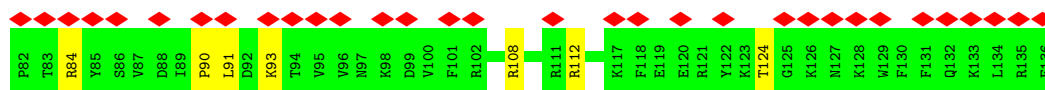
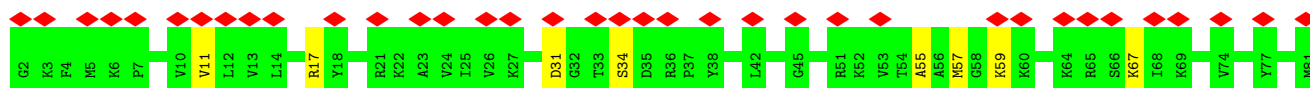
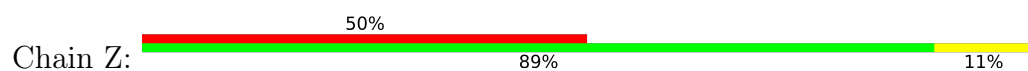




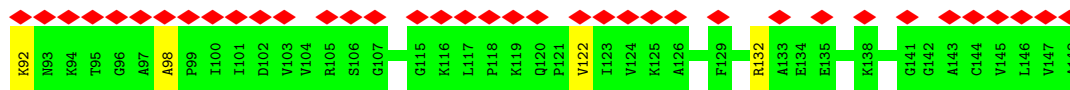
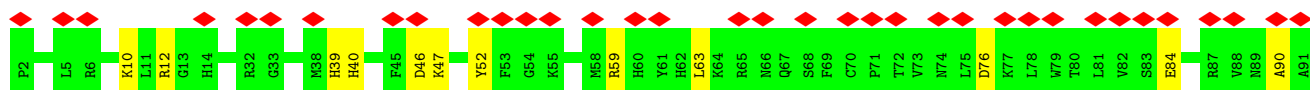
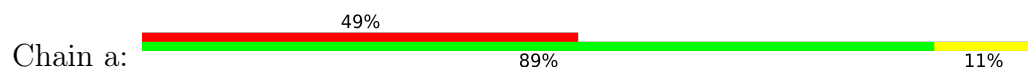
• Molecule 24: Ribosomal protein L26



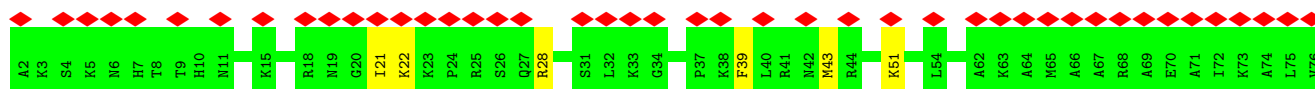
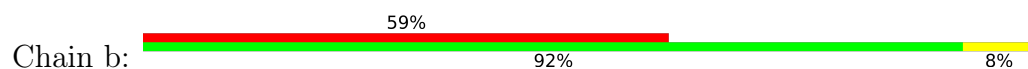
• Molecule 25: 60S ribosomal protein L27



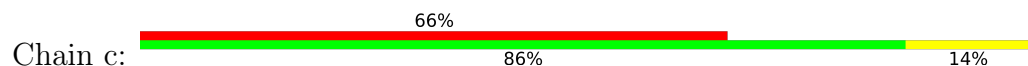
• Molecule 26: uL15

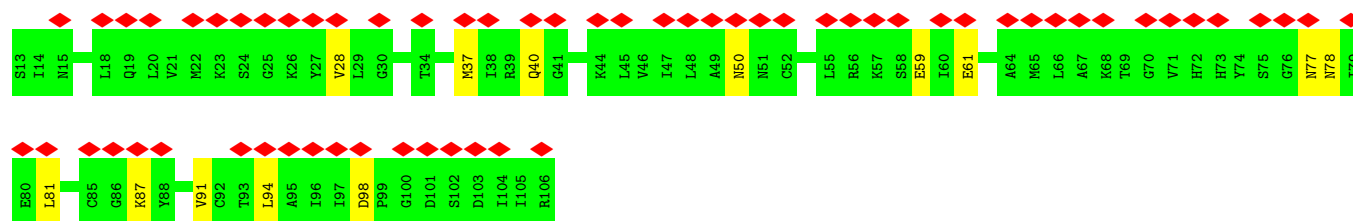


• Molecule 27: 60S ribosomal protein L29

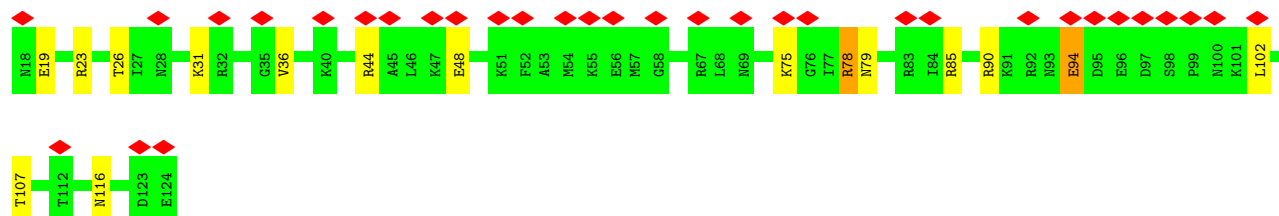
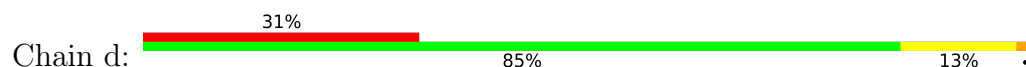


• Molecule 28: eL30

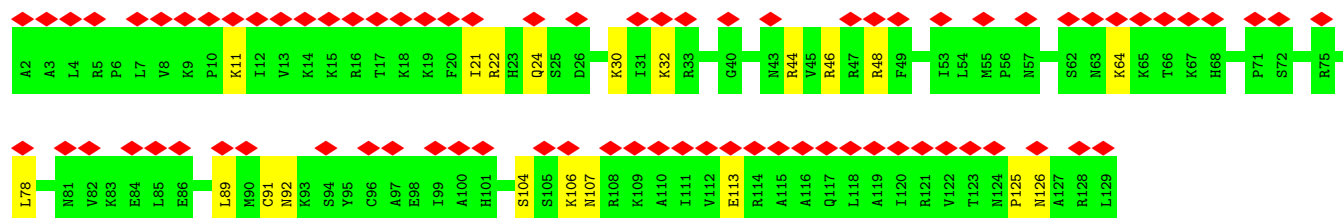
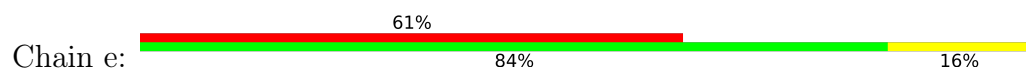




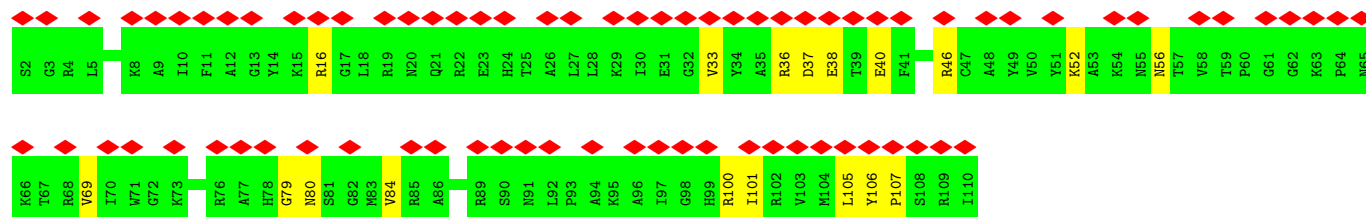
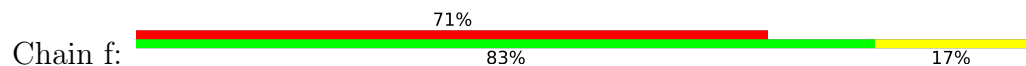
• Molecule 29: eL31



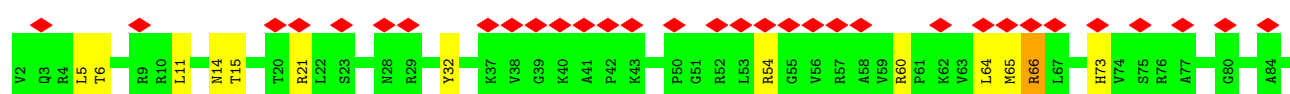
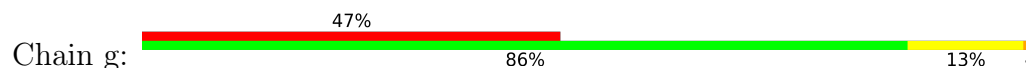
• Molecule 30: eL32

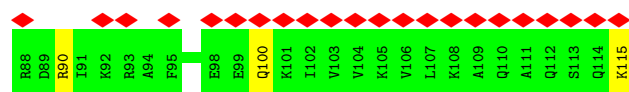


• Molecule 31: eL33

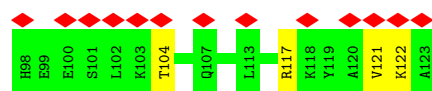
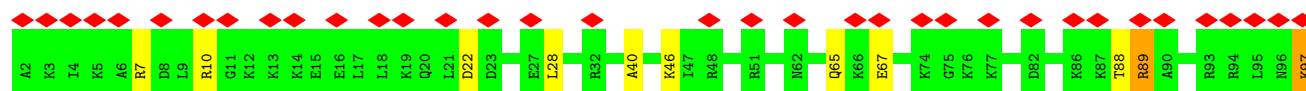
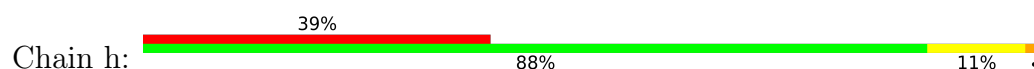


• Molecule 32: eL34

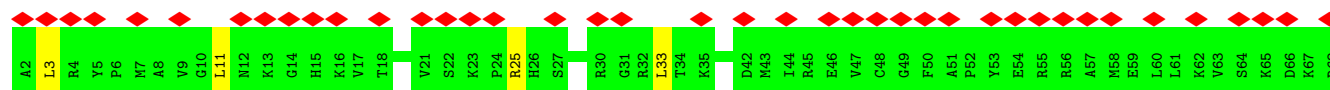
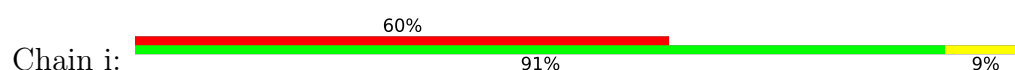




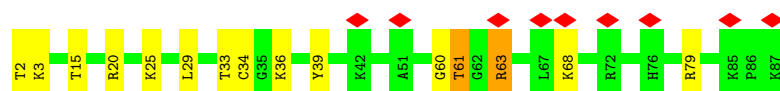
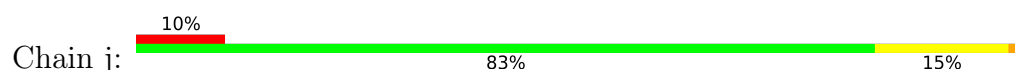
• Molecule 33: uL29



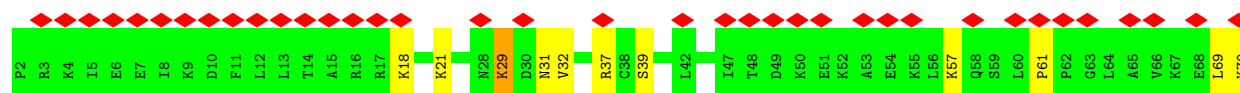
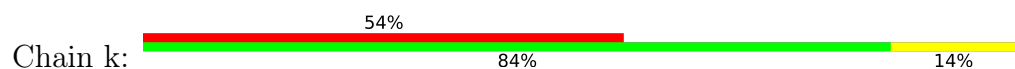
• Molecule 34: 60S ribosomal protein L36



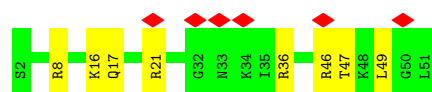
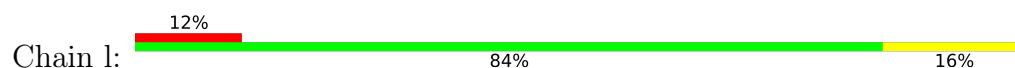
• Molecule 35: Ribosomal protein L37



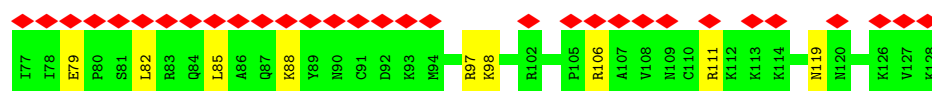
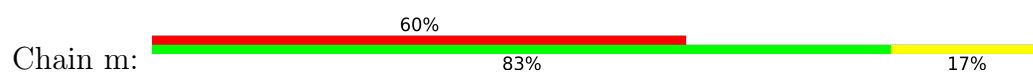
• Molecule 36: eL38



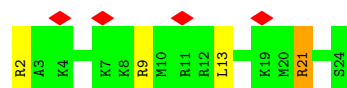
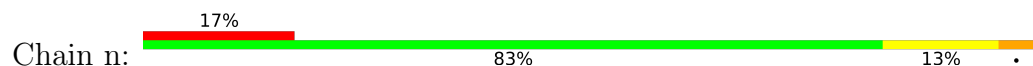
• Molecule 37: eL39



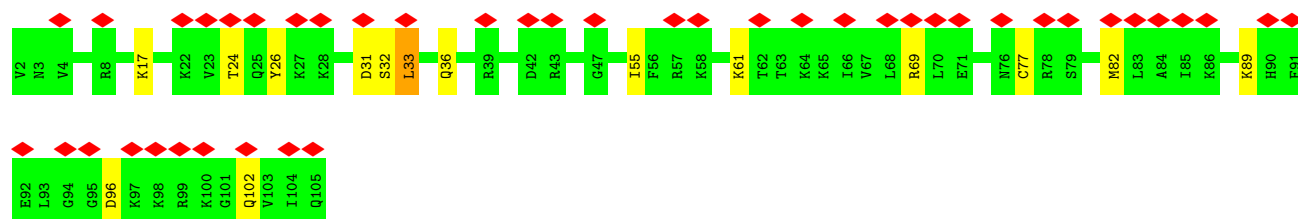
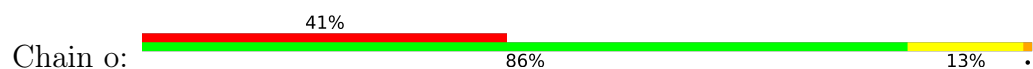
• Molecule 38: eL40



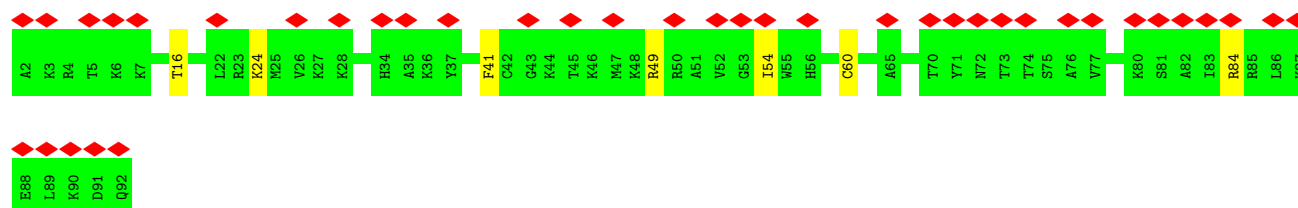
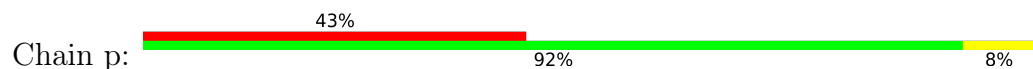
• Molecule 39: 60s ribosomal protein l41



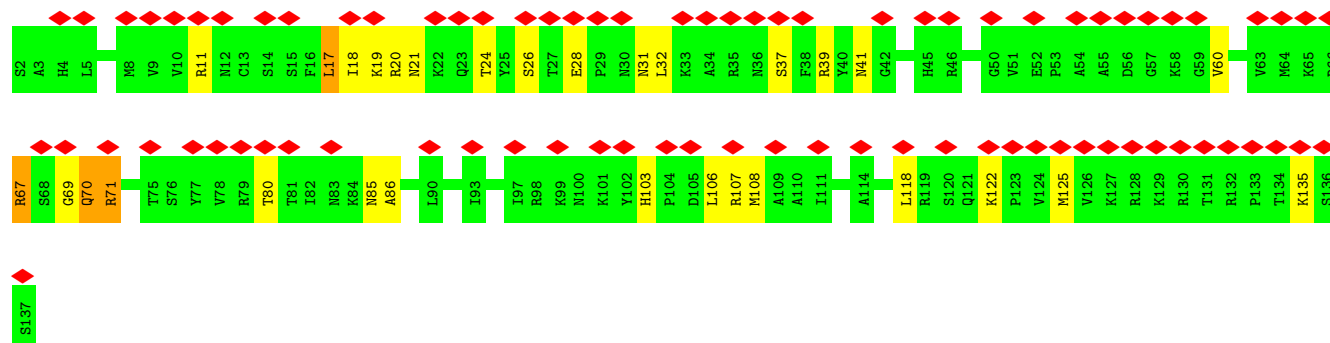
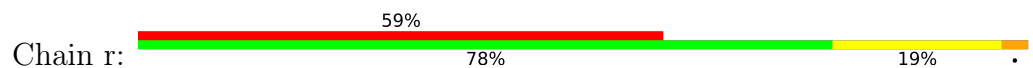
• Molecule 40: eL42



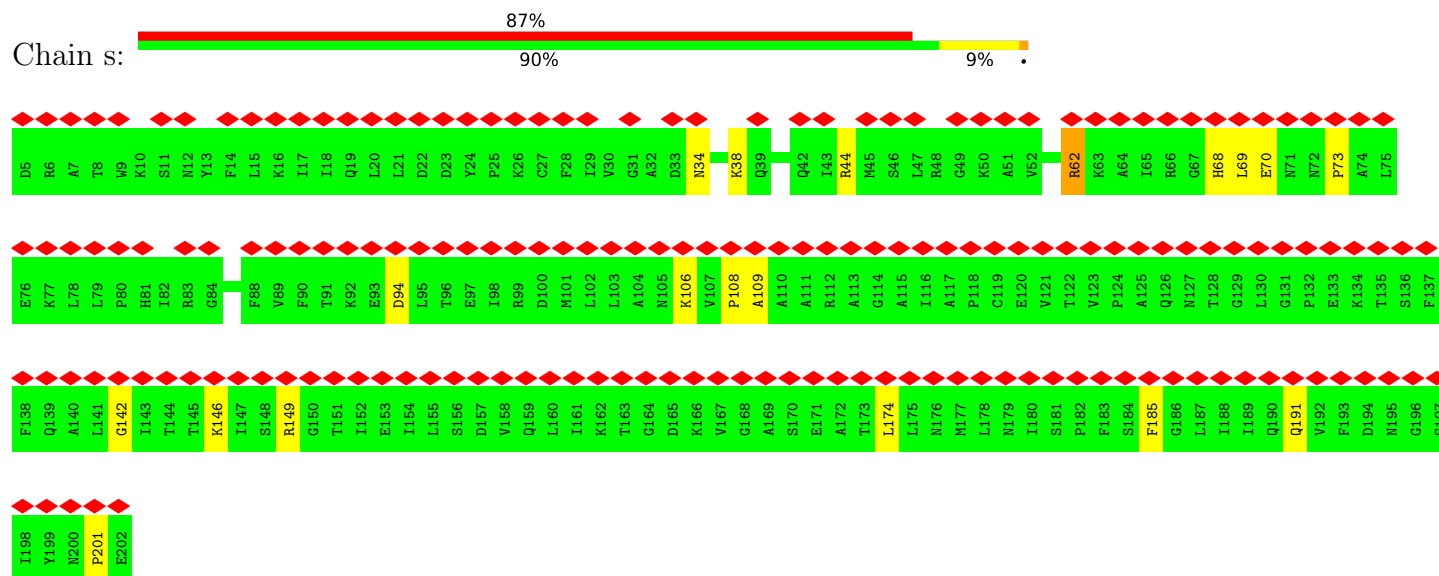
• Molecule 41: Ribosomal protein L37a



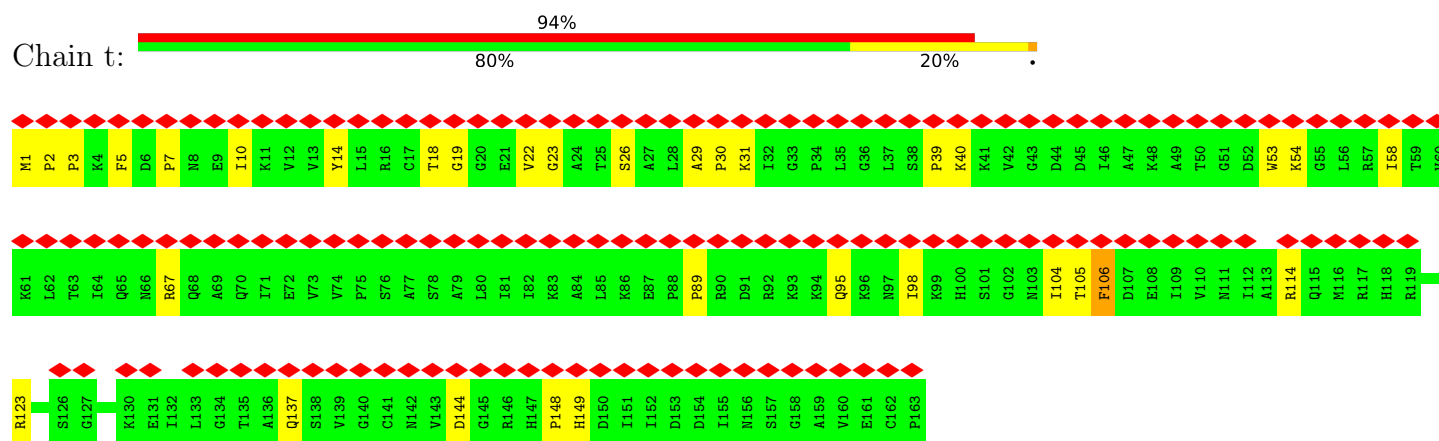
• Molecule 42: eL28



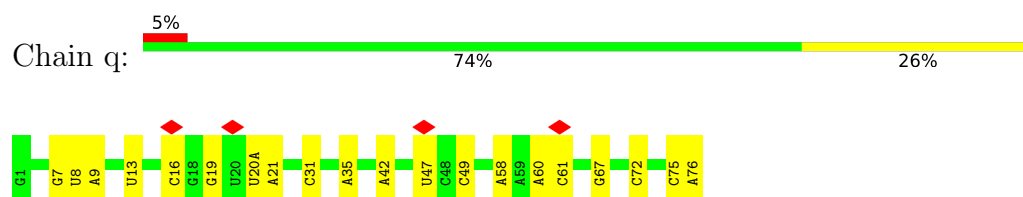
- Molecule 43: 60S acidic ribosomal protein P0



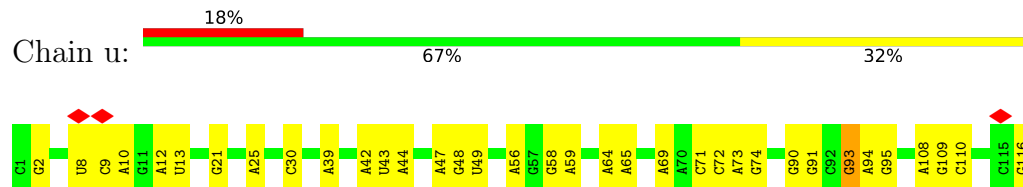
- Molecule 44: Ribosomal protein L12



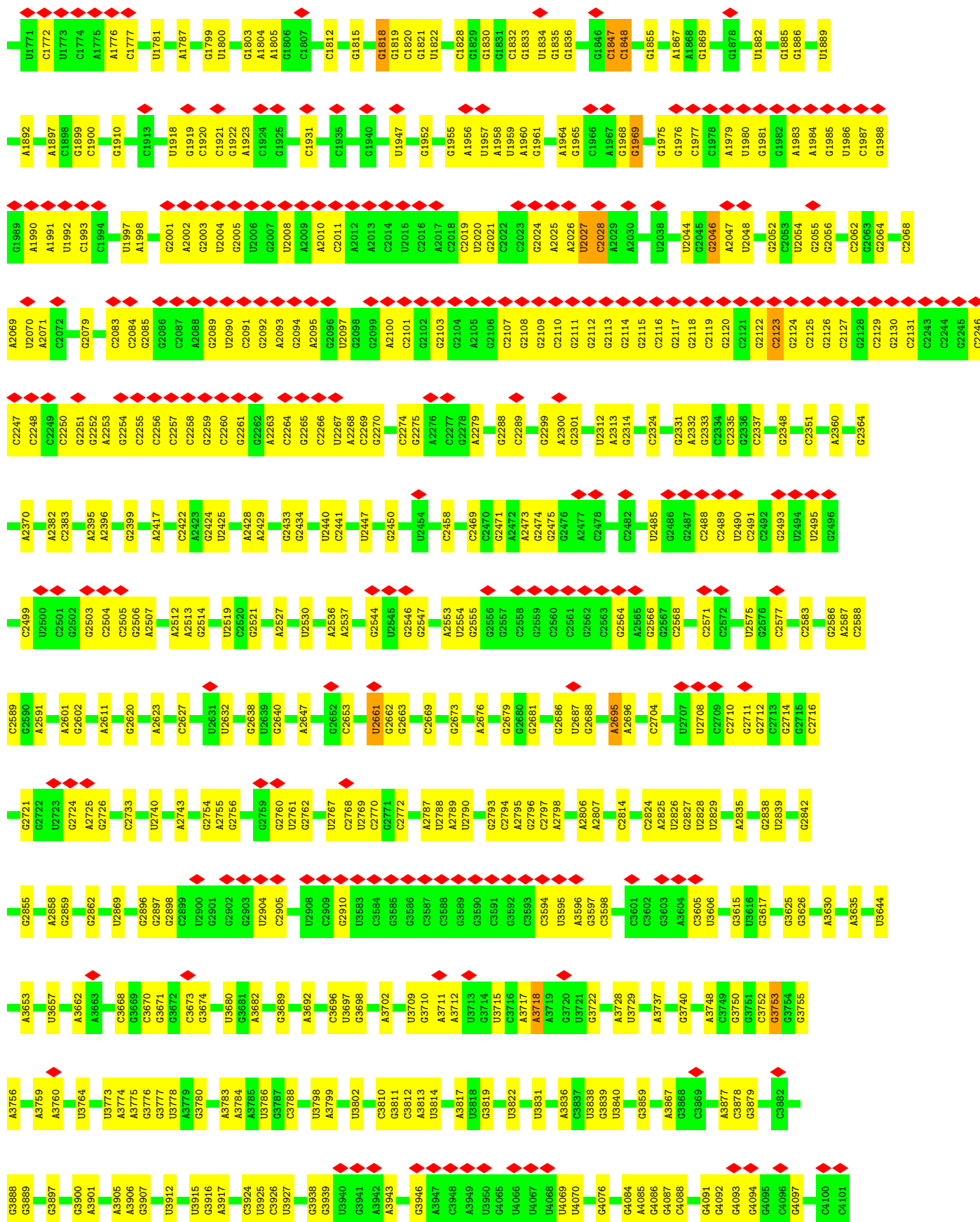
- Molecule 45: p-Site tRNA

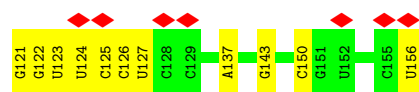


- Molecule 46: 28S rRNA

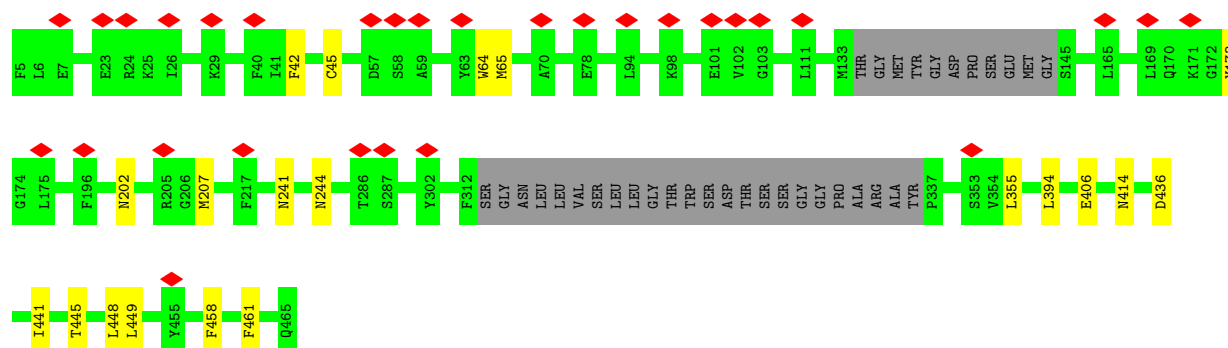
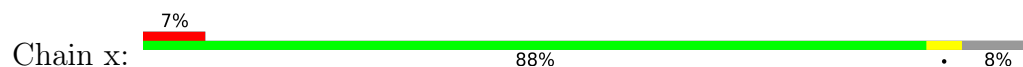




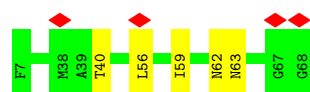
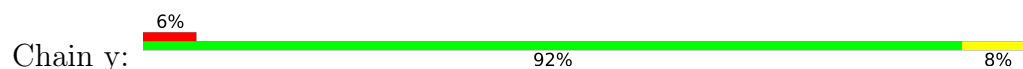




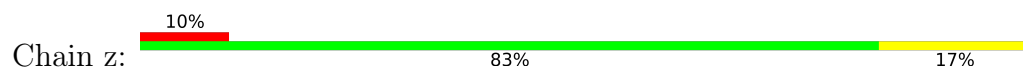
- Molecule 49: Protein transport protein Sec61 subunit alpha isoform 1



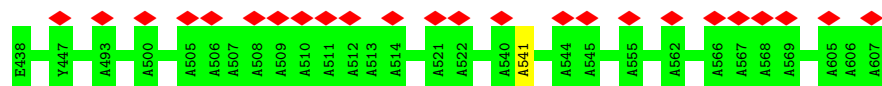
- Molecule 50: Protein transport protein Sec61 subunit gamma



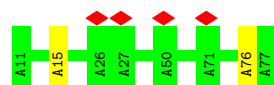
- Molecule 51: Protein transport protein Sec61 subunit beta



- Molecule 52: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1,RPN1

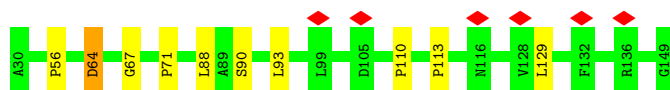


- Molecule 53: TMEM258




- Molecule 54: Oligosaccharyltransferase complex subunit OSTC

Chain 3:  5% 92% 8% .




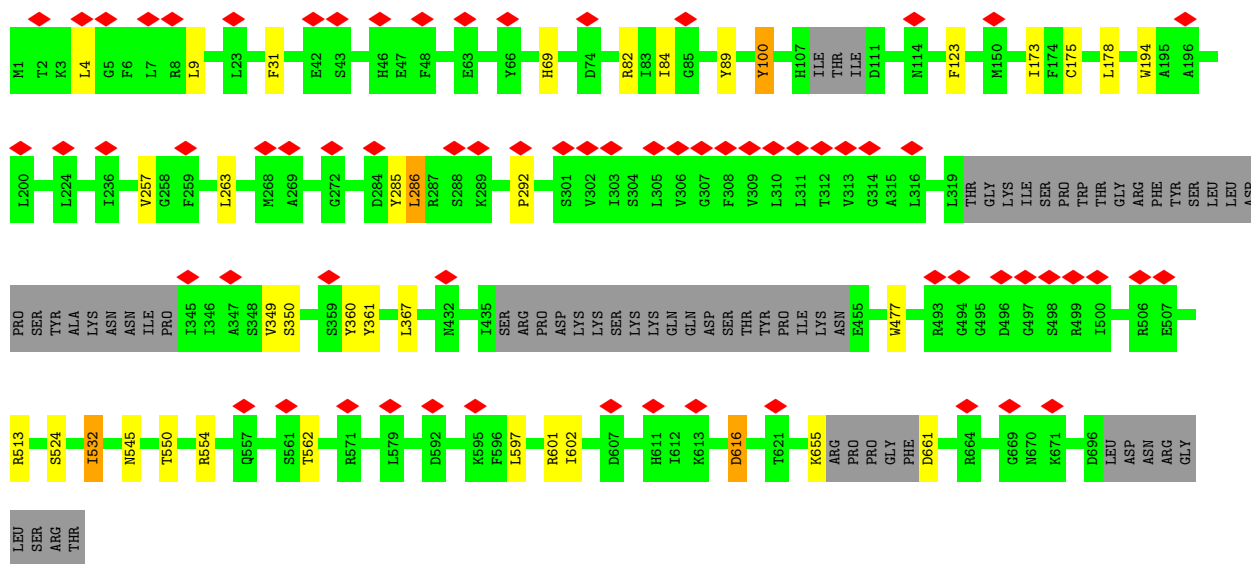
- Molecule 55: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 4

Chain 4:  91% 9%




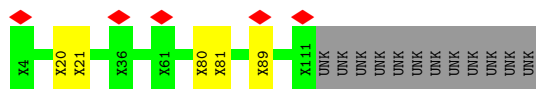
- Molecule 56: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3A

Chain 5:  10% 86% 5% . 9%



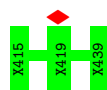
- Molecule 57: DAD1

Chain 6:  5% 84% 5% 11%



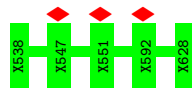
- Molecule 58: OST48

Chain 7:  100%



- Molecule 59: RPN1

Chain 8:  100%



- Molecule 60: Unidentified TM

Chain 0:  100%

There are no outlier residues recorded for this chain.

- Molecule 61: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  25% 75%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	188900	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 ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.373	Depositor
Minimum map value	-0.224	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	596.2, 596.2, 596.2	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1924, 1.1924, 1.1924	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, ZN, NAG, BMA, 9UB, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.46	0/1906	0.79	0/2556
2	B	0.40	0/3216	0.78	1/4311 (0.0%)
3	C	0.43	0/2938	0.80	5/3946 (0.1%)
4	D	0.37	0/2432	0.70	1/3257 (0.0%)
5	E	0.46	0/1936	0.82	2/2600 (0.1%)
6	F	0.40	0/1905	0.75	1/2539 (0.0%)
7	G	0.38	0/1967	0.73	1/2647 (0.0%)
8	H	0.37	0/1535	0.71	0/2063
9	I	0.41	0/1693	0.69	0/2260
10	J	0.38	0/1376	0.73	0/1841
11	L	0.41	0/1734	0.79	0/2317
12	M	0.38	0/1158	0.74	0/1547
13	N	0.43	0/1746	0.83	0/2338
14	O	0.40	0/1671	0.77	0/2234
15	P	0.42	0/1268	0.75	0/1701
16	Q	0.41	0/1530	0.81	1/2041 (0.0%)
17	R	0.41	0/1524	0.79	0/2013
18	S	0.40	0/1493	0.85	3/2002 (0.1%)
19	T	0.41	0/1326	0.72	0/1770
20	U	0.41	0/822	0.68	0/1103
21	V	0.40	0/993	0.73	0/1332
22	W	0.48	0/541	0.83	1/720 (0.1%)
23	X	0.42	0/993	0.74	0/1334
24	Y	0.37	0/1132	0.80	2/1504 (0.1%)
25	Z	0.40	0/1130	0.72	0/1507
26	a	0.40	0/1191	0.79	0/1590
27	b	0.44	0/619	0.73	0/818
28	c	0.36	0/742	0.69	0/996
29	d	0.38	0/903	0.81	1/1216 (0.1%)
30	e	0.47	0/1071	0.85	0/1429
31	f	0.52	0/895	0.87	0/1198
32	g	0.42	0/916	0.81	1/1220 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.36	0/1021	0.77	1/1348 (0.1%)
34	i	0.40	0/841	0.82	2/1112 (0.2%)
35	j	0.46	0/720	0.94	1/952 (0.1%)
36	k	0.37	0/575	0.69	0/761
37	l	0.50	0/454	0.84	0/599
38	m	0.37	0/435	0.76	0/575
39	n	0.41	0/223	0.92	1/284 (0.4%)
40	o	0.39	0/864	0.75	0/1140
41	p	0.42	0/718	0.71	0/953
42	r	0.46	0/1110	0.77	1/1484 (0.1%)
43	s	0.38	0/1547	0.58	0/2088
44	t	0.41	0/1257	0.69	0/1697
45	q	0.27	0/1805	0.72	0/2809
46	u	0.41	11/87790 (0.0%)	0.80	94/136937 (0.1%)
47	v	0.31	0/2858	0.69	0/4455
48	w	0.36	0/3701	0.74	0/5766
49	x	0.51	0/3383	0.79	3/4584 (0.1%)
50	y	0.49	0/504	0.76	1/673 (0.1%)
51	z	0.42	0/236	0.74	0/321
52	1	0.31	0/889	0.49	0/1237
53	2	0.35	0/298	0.53	0/414
54	3	0.58	0/815	0.89	5/1107 (0.5%)
55	4	0.52	0/273	0.66	0/371
56	5	0.66	5/5224 (0.1%)	0.86	17/7093 (0.2%)
All	All	0.42	16/163843 (0.0%)	0.79	146/240710 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	4
3	C	0	2
4	D	0	1
5	E	0	1
7	G	0	1
9	I	0	2
11	L	0	3
17	R	0	1
18	S	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
19	T	0	1
20	U	0	1
24	Y	0	1
31	f	0	1
42	r	0	2
46	u	0	1
49	x	0	2
53	2	0	1
54	3	0	2
56	5	0	6
57	6	0	5
All	All	0	41

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	u	680	G	O3'-P	-33.63	1.20	1.61
46	u	692	A	O3'-P	32.98	2.00	1.61
46	u	1965	G	O3'-P	-23.04	1.33	1.61
46	u	472	C	O3'-P	-19.63	1.37	1.61
56	5	545	ASN	C-N	-18.33	0.91	1.34

The worst 5 of 146 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	5	545	ASN	C-N-CA	-16.90	79.46	121.70
46	u	462	G	P-O3'-C3'	-16.27	100.18	119.70
56	5	545	ASN	O-C-N	14.86	146.47	122.70
46	u	680	G	O3'-P-O5'	14.37	131.31	104.00
56	5	545	ASN	CA-C-N	-13.09	88.39	117.20

There are no chirality outliers.

5 of 41 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	TRP	Peptide
2	B	17	LEU	Peptide
2	B	257	TRP	Peptide
2	B	258	HIS	Peptide
2	B	351	LEU	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	
1	A	242/244 (99%)	209 (86%)	28 (12%)	5 (2%)	5	32
2	B	392/394 (100%)	345 (88%)	42 (11%)	5 (1%)	10	42
3	C	360/362 (99%)	322 (89%)	27 (8%)	11 (3%)	3	25
4	D	290/292 (99%)	262 (90%)	25 (9%)	3 (1%)	13	48
5	E	232/248 (94%)	179 (77%)	36 (16%)	17 (7%)	1	13
6	F	223/225 (99%)	204 (92%)	17 (8%)	2 (1%)	14	50
7	G	239/241 (99%)	203 (85%)	31 (13%)	5 (2%)	5	32
8	H	188/190 (99%)	166 (88%)	19 (10%)	3 (2%)	8	38
9	I	200/213 (94%)	181 (90%)	15 (8%)	4 (2%)	6	34
10	J	167/169 (99%)	147 (88%)	13 (8%)	7 (4%)	2	20
11	L	208/210 (99%)	180 (86%)	16 (8%)	12 (6%)	1	16
12	M	136/138 (99%)	123 (90%)	12 (9%)	1 (1%)	19	56
13	N	201/203 (99%)	181 (90%)	20 (10%)	0	100	100
14	O	197/199 (99%)	184 (93%)	12 (6%)	1 (0%)	25	62
15	P	151/153 (99%)	135 (89%)	16 (11%)	0	100	100
16	Q	185/187 (99%)	169 (91%)	14 (8%)	2 (1%)	12	46
17	R	178/180 (99%)	166 (93%)	9 (5%)	3 (2%)	7	37
18	S	173/175 (99%)	157 (91%)	12 (7%)	4 (2%)	5	31
19	T	157/159 (99%)	139 (88%)	15 (10%)	3 (2%)	6	35
20	U	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	2	21
21	V	129/131 (98%)	115 (89%)	13 (10%)	1 (1%)	16	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	W	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	8	38
23	X	117/119 (98%)	109 (93%)	6 (5%)	2 (2%)	7	37
24	Y	132/134 (98%)	114 (86%)	17 (13%)	1 (1%)	16	54
25	Z	133/135 (98%)	113 (85%)	13 (10%)	7 (5%)	1	18
26	a	145/147 (99%)	122 (84%)	19 (13%)	4 (3%)	4	27
27	b	73/75 (97%)	67 (92%)	5 (7%)	1 (1%)	9	40
28	c	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
29	d	105/107 (98%)	91 (87%)	13 (12%)	1 (1%)	13	48
30	e	126/128 (98%)	115 (91%)	6 (5%)	5 (4%)	2	21
31	f	107/109 (98%)	94 (88%)	8 (8%)	5 (5%)	2	19
32	g	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	14	50
33	h	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	3	24
34	i	100/102 (98%)	92 (92%)	6 (6%)	2 (2%)	6	34
35	j	84/86 (98%)	71 (84%)	8 (10%)	5 (6%)	1	16
36	k	67/69 (97%)	56 (84%)	7 (10%)	4 (6%)	1	16
37	l	48/50 (96%)	40 (83%)	7 (15%)	1 (2%)	5	32
38	m	50/52 (96%)	44 (88%)	6 (12%)	0	100	100
39	n	21/23 (91%)	21 (100%)	0	0	100	100
40	o	102/104 (98%)	92 (90%)	7 (7%)	3 (3%)	3	26
41	p	89/91 (98%)	80 (90%)	8 (9%)	1 (1%)	12	46
42	r	132/136 (97%)	113 (86%)	12 (9%)	7 (5%)	1	18
43	s	196/198 (99%)	164 (84%)	22 (11%)	10 (5%)	1	18
44	t	161/163 (99%)	102 (63%)	33 (20%)	26 (16%)	0	3
49	x	420/461 (91%)	373 (89%)	46 (11%)	1 (0%)	44	77
50	y	60/62 (97%)	52 (87%)	8 (13%)	0	100	100
51	z	27/29 (93%)	25 (93%)	1 (4%)	1 (4%)	2	22
52	1	158/162 (98%)	151 (96%)	6 (4%)	1 (1%)	22	59
53	2	56/60 (93%)	53 (95%)	2 (4%)	1 (2%)	7	36
54	3	118/120 (98%)	99 (84%)	18 (15%)	1 (1%)	16	54
55	4	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
56	5	632/705 (90%)	538 (85%)	88 (14%)	6 (1%)	14	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	8221/8466 (97%)	7225 (88%)	801 (10%)	195 (2%)	7	30

5 of 195 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	TRP
3	C	273	LEU
5	E	91	PRO
5	E	95	ASP
5	E	118	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/187 (100%)	161 (86%)	26 (14%)	3	15
2	B	336/342 (98%)	291 (87%)	45 (13%)	3	16
3	C	302/302 (100%)	260 (86%)	42 (14%)	3	15
4	D	247/247 (100%)	218 (88%)	29 (12%)	4	18
5	E	208/221 (94%)	185 (89%)	23 (11%)	5	20
6	F	194/195 (100%)	165 (85%)	29 (15%)	2	14
7	G	206/206 (100%)	182 (88%)	24 (12%)	4	18
8	H	169/169 (100%)	148 (88%)	21 (12%)	4	17
9	I	174/180 (97%)	153 (88%)	21 (12%)	4	18
10	J	142/142 (100%)	126 (89%)	16 (11%)	4	19
11	L	176/176 (100%)	145 (82%)	31 (18%)	1	10
12	M	117/117 (100%)	102 (87%)	15 (13%)	3	17
13	N	171/171 (100%)	152 (89%)	19 (11%)	5	20
14	O	171/171 (100%)	144 (84%)	27 (16%)	2	13
15	P	134/134 (100%)	120 (90%)	14 (10%)	5	22
16	Q	163/163 (100%)	145 (89%)	18 (11%)	5	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	R	159/159 (100%)	140 (88%)	19 (12%)	4	18
18	S	156/156 (100%)	132 (85%)	24 (15%)	2	13
19	T	139/139 (100%)	122 (88%)	17 (12%)	4	18
20	U	89/89 (100%)	82 (92%)	7 (8%)	10	32
21	V	101/101 (100%)	84 (83%)	17 (17%)	1	11
22	W	55/55 (100%)	50 (91%)	5 (9%)	7	26
23	X	107/107 (100%)	97 (91%)	10 (9%)	7	25
24	Y	124/124 (100%)	107 (86%)	17 (14%)	3	16
25	Z	117/117 (100%)	109 (93%)	8 (7%)	13	36
26	a	119/119 (100%)	107 (90%)	12 (10%)	6	22
27	b	62/62 (100%)	57 (92%)	5 (8%)	9	31
28	c	79/79 (100%)	66 (84%)	13 (16%)	2	11
29	d	98/98 (100%)	82 (84%)	16 (16%)	2	11
30	e	114/114 (100%)	99 (87%)	15 (13%)	3	16
31	f	88/88 (100%)	76 (86%)	12 (14%)	3	16
32	g	98/98 (100%)	83 (85%)	15 (15%)	2	13
33	h	109/109 (100%)	97 (89%)	12 (11%)	5	20
34	i	86/86 (100%)	81 (94%)	5 (6%)	17	40
35	j	73/73 (100%)	62 (85%)	11 (15%)	2	13
36	k	64/64 (100%)	56 (88%)	8 (12%)	3	17
37	l	47/47 (100%)	40 (85%)	7 (15%)	2	14
38	m	48/48 (100%)	39 (81%)	9 (19%)	1	8
39	n	22/22 (100%)	18 (82%)	4 (18%)	1	9
40	o	92/92 (100%)	79 (86%)	13 (14%)	3	15
41	p	74/74 (100%)	68 (92%)	6 (8%)	9	31
42	r	120/120 (100%)	96 (80%)	24 (20%)	1	7
43	s	166/166 (100%)	156 (94%)	10 (6%)	16	40
44	t	136/136 (100%)	128 (94%)	8 (6%)	16	40
49	x	360/388 (93%)	346 (96%)	14 (4%)	27	50
50	y	53/53 (100%)	49 (92%)	4 (8%)	11	33
51	z	26/26 (100%)	22 (85%)	4 (15%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	1	20/20 (100%)	20 (100%)	0	100	100
54	3	61/101 (60%)	58 (95%)	3 (5%)	21	44
55	4	30/30 (100%)	27 (90%)	3 (10%)	6	23
56	5	528/615 (86%)	512 (97%)	16 (3%)	36	57
All	All	6917/7098 (97%)	6144 (89%)	773 (11%)	7	20

5 of 773 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	U	67	LYS
30	e	24	GLN
21	V	82	ILE
20	U	65	ARG
25	Z	67	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
55	4	12	ASN
56	5	217	ASN
56	5	531	GLN
56	5	222	HIS
56	5	168	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
45	q	74/76 (97%)	20 (27%)	0
46	u	3643/3662 (99%)	1188 (32%)	0
47	v	119/120 (99%)	19 (15%)	0
48	w	155/156 (99%)	52 (33%)	0
All	All	3991/4014 (99%)	1279 (32%)	0

5 of 1279 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
45	q	7	G
45	q	8	U

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Mol	Chain	Res	Type
45	q	9	A
45	q	13	U
45	q	16	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

8 monosaccharides 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	$\# Z > 2$
61	NAG	K	1	61,56	14,14,15	0.49	0	17,19,21	0.63	0
61	NAG	K	2	61	14,14,15	0.24	0	17,19,21	0.53	0
61	BMA	K	3	61	11,11,12	0.67	0	15,15,17	0.87	1 (6%)
61	MAN	K	4	61	11,11,12	0.82	0	15,15,17	1.66	2 (13%)
61	MAN	K	5	61	11,11,12	0.71	0	15,15,17	1.25	2 (13%)
61	MAN	K	6	61	11,11,12	0.93	1 (9%)	15,15,17	0.99	2 (13%)
61	MAN	K	7	61	11,11,12	1.26	1 (9%)	15,15,17	1.28	2 (13%)
61	MAN	K	8	61	11,11,12	0.68	0	15,15,17	1.04	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	NAG	K	1	61,56	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	NAG	K	2	61	-	1/6/23/26	0/1/1/1
61	BMA	K	3	61	-	2/2/19/22	0/1/1/1
61	MAN	K	4	61	-	0/2/19/22	0/1/1/1
61	MAN	K	5	61	-	1/2/19/22	0/1/1/1
61	MAN	K	6	61	-	0/2/19/22	0/1/1/1
61	MAN	K	7	61	-	0/2/19/22	0/1/1/1
61	MAN	K	8	61	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	K	7	MAN	C2-C3	2.49	1.56	1.52
61	K	6	MAN	O5-C1	-2.14	1.40	1.43

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	K	4	MAN	C1-O5-C5	4.42	118.18	112.19
61	K	4	MAN	O2-C2-C3	-3.76	102.61	110.14
61	K	7	MAN	C1-O5-C5	3.19	116.51	112.19
61	K	5	MAN	O2-C2-C3	-3.07	104.00	110.14
61	K	5	MAN	C1-O5-C5	3.00	116.25	112.19

There are no chirality outliers.

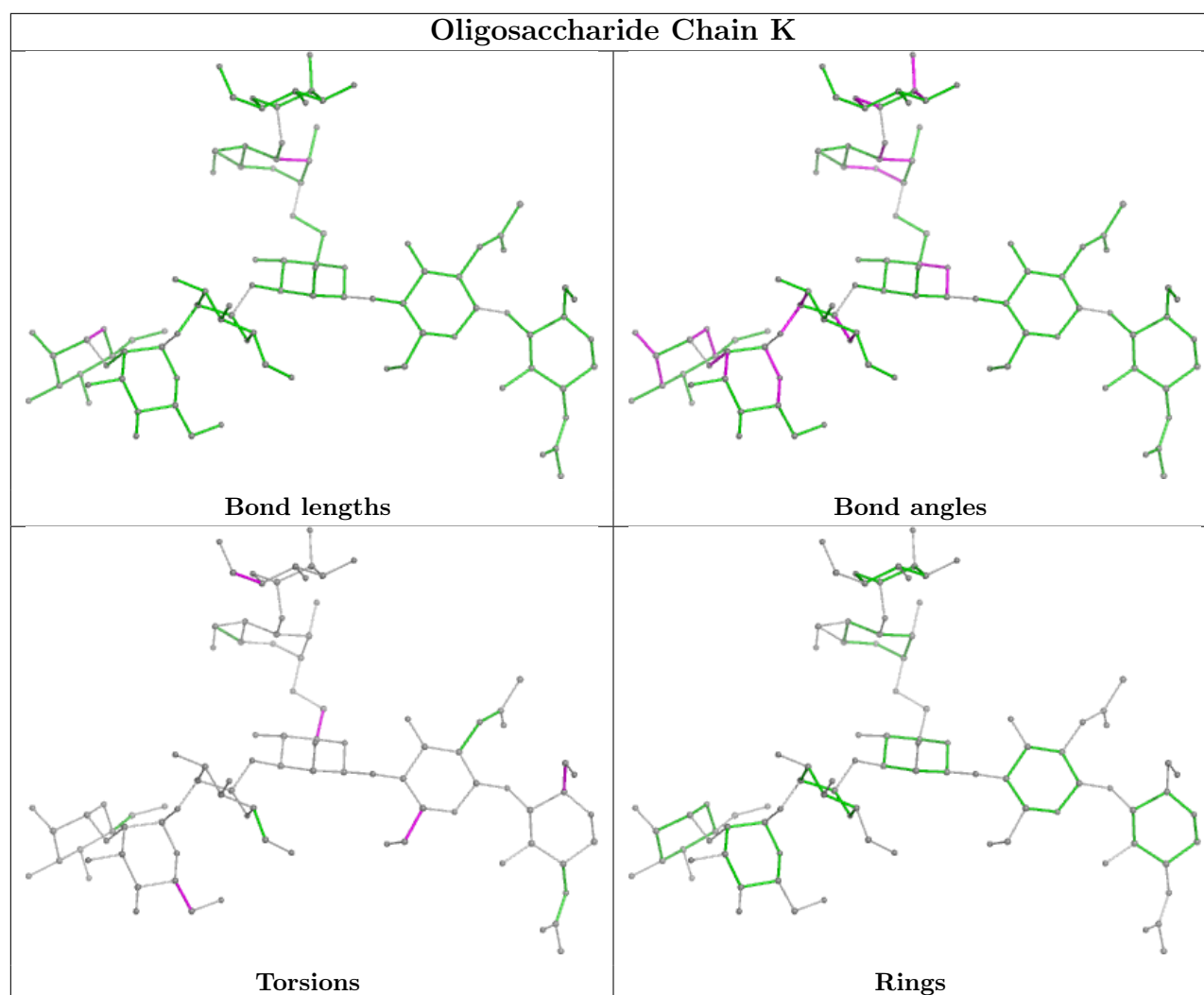
5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	K	3	BMA	C4-C5-C6-O6
61	K	3	BMA	O5-C5-C6-O6
61	K	8	MAN	O5-C5-C6-O6
61	K	8	MAN	C4-C5-C6-O6
61	K	1	NAG	C4-C5-C6-O6

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 oligosaccharide.



5.6 Ligand geometry [i](#)

Of 165 ligands modelled in this entry, 164 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
64	9UB	5	809	56	41,43,43	2.31	9 (21%)	47,59,59	1.65	13 (27%)

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
64	9UB	5	809	56	-	4/39/62/62	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	5	809	9UB	P26-O25	8.13	1.67	1.58
64	5	809	9UB	P26-C29	7.17	1.91	1.80
64	5	809	9UB	C37-C39	-3.64	1.46	1.53
64	5	809	9UB	C41-N40	3.36	1.45	1.34
64	5	809	9UB	C06-C07	3.00	1.57	1.51

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	5	809	9UB	C18-C17-C16	4.24	122.40	115.27
64	5	809	9UB	C20-C19-C17	-3.50	119.98	126.04
64	5	809	9UB	C01-C02-C03	2.70	120.57	114.60
64	5	809	9UB	C39-N40-C41	-2.61	116.82	123.18
64	5	809	9UB	C32-O31-C30	2.60	117.70	113.16

There are no chirality outliers.

All (4) torsion outliers are listed below:

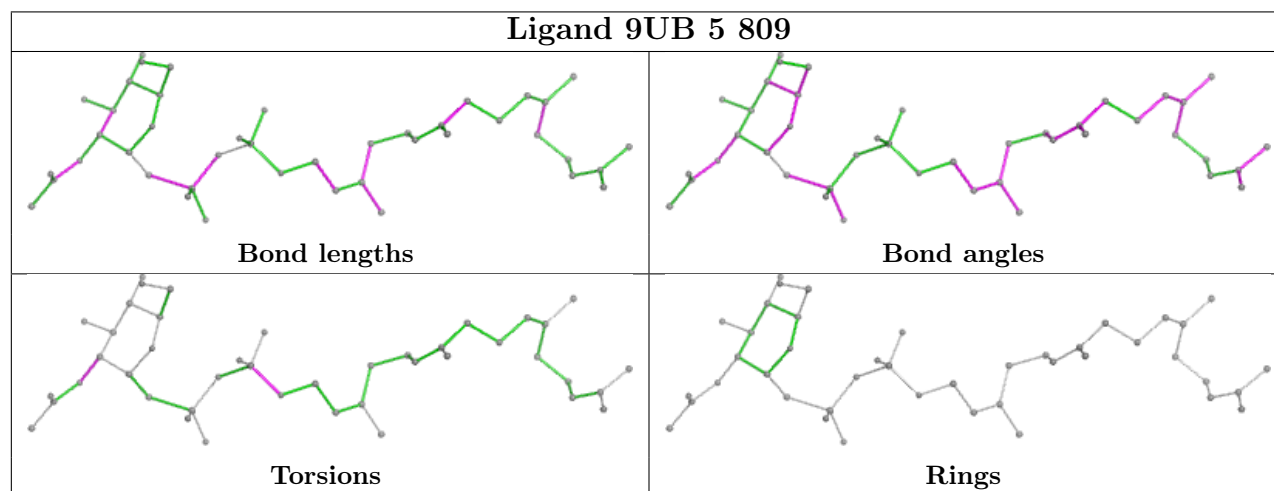
Mol	Chain	Res	Type	Atoms
64	5	809	9UB	C20-O21-P22-O25
64	5	809	9UB	C20-O21-P22-O23
64	5	809	9UB	C20-O21-P22-O24
64	5	809	9UB	C30-C39-N40-C41

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
46	u	21
56	5	4
59	8	2
57	6	2
52	1	1
53	2	1
45	q	1
42	r	1

The worst 5 of 33 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	u	4776:G	O3'	4859:C	P	17.95
1	u	757:G	O3'	906:C	P	17.49
1	u	519:C	O3'	642:G	P	16.73
1	u	2910:G	O3'	3583:U	P	16.46
1	8	566:UNK	C	577:UNK	N	15.56

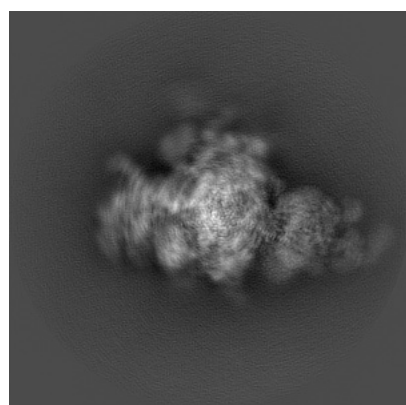
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4316. These allow visual inspection of the internal detail of the map and identification of artifacts.

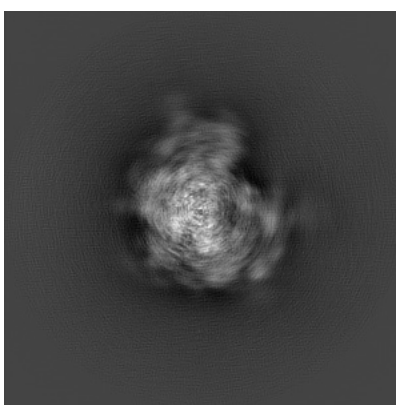
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

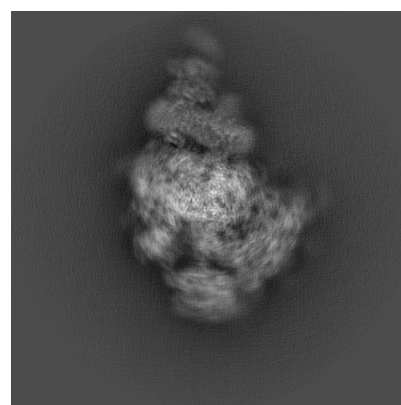
6.1.1 Primary map



X



Y

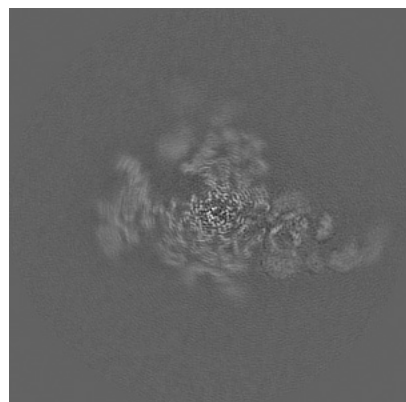


Z

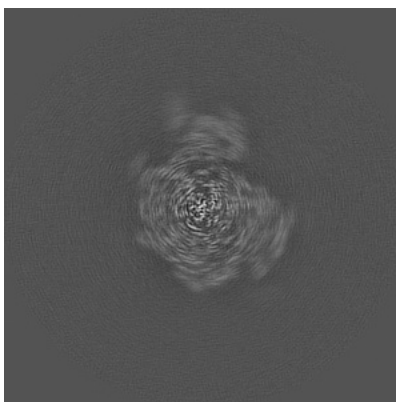
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

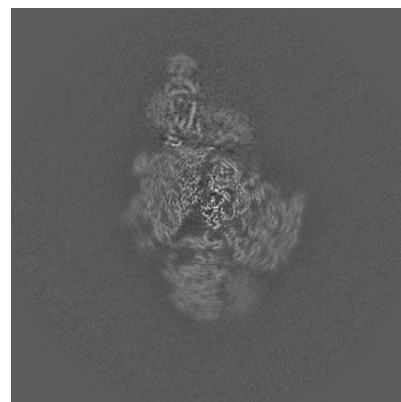
6.2.1 Primary map



X Index: 250



Y Index: 250

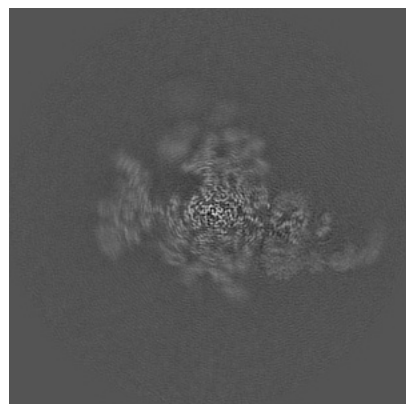


Z Index: 250

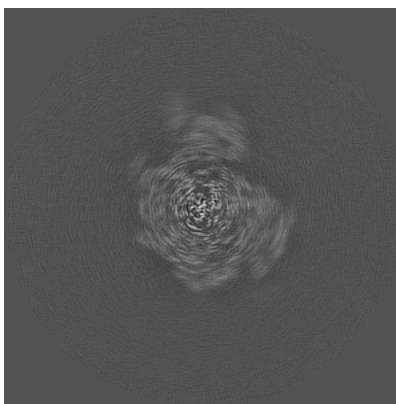
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

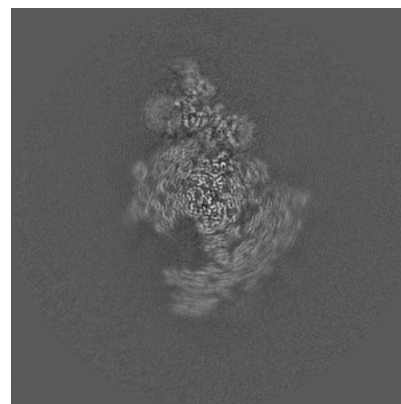
6.3.1 Primary map



X Index: 253



Y Index: 250

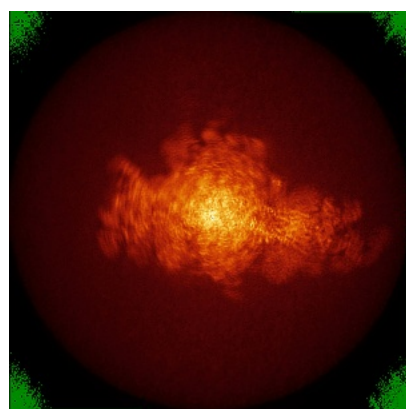


Z Index: 235

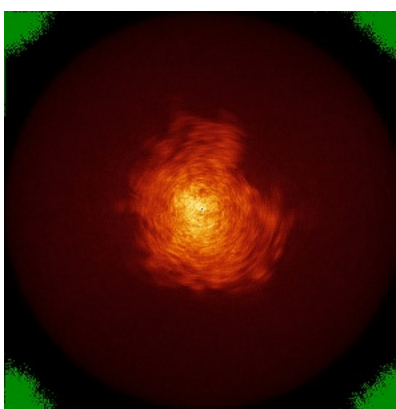
The images above show the largest variance slices of the map in three orthogonal directions.

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

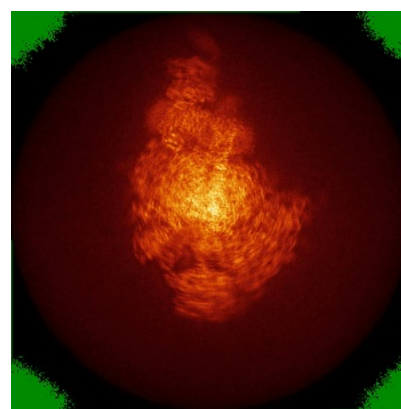
6.4.1 Primary map



X



Y

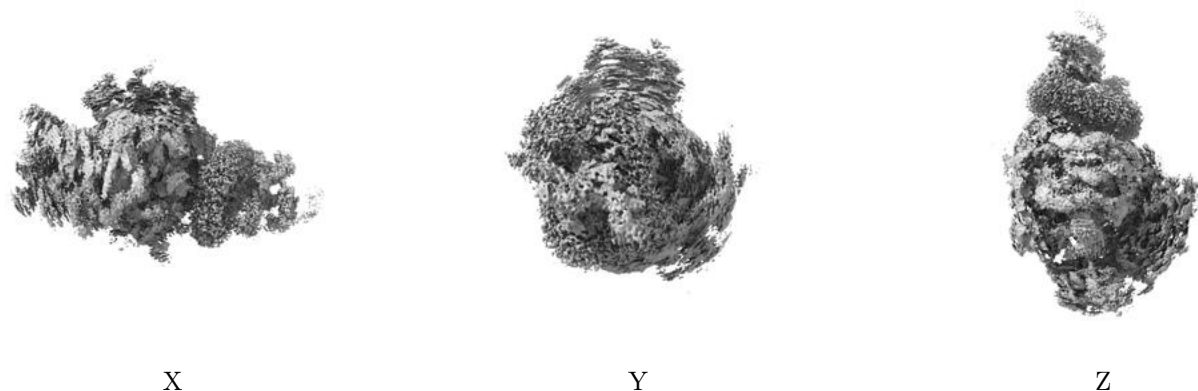


Z

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

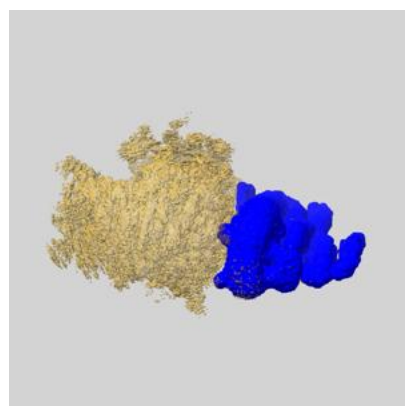
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

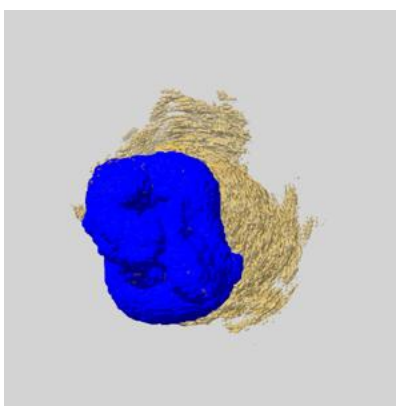
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

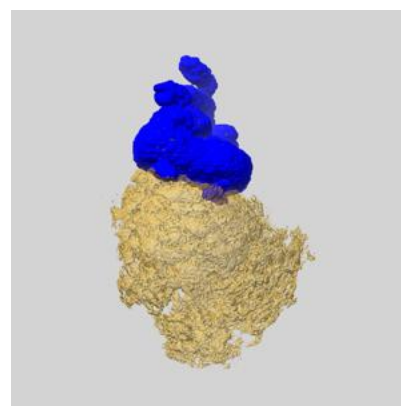
6.6.1 emd_4316_msk_1.map [i](#)



X



Y

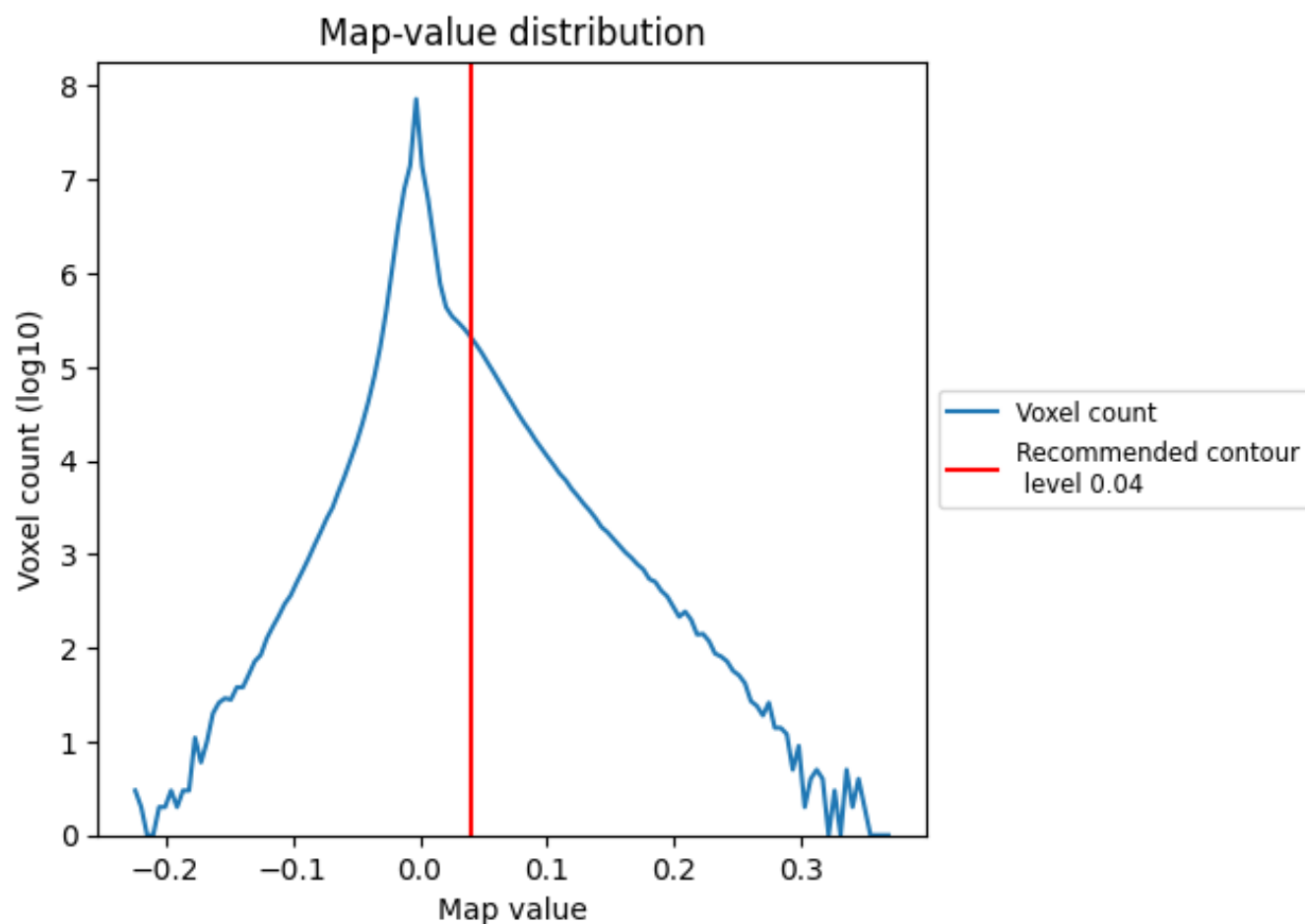


Z

7 Map analysis [i](#)

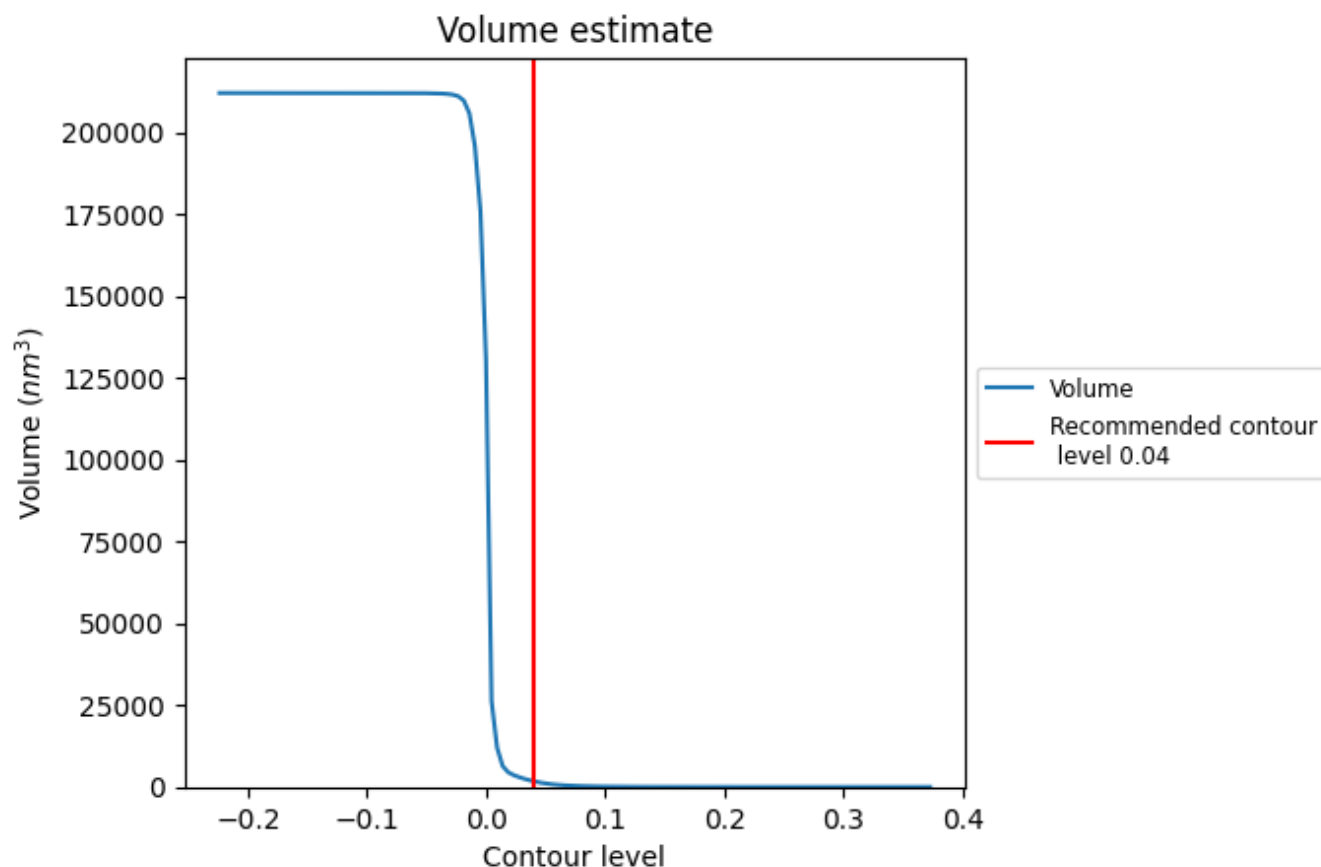
This section contains the results of statistical analysis of the map.

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.

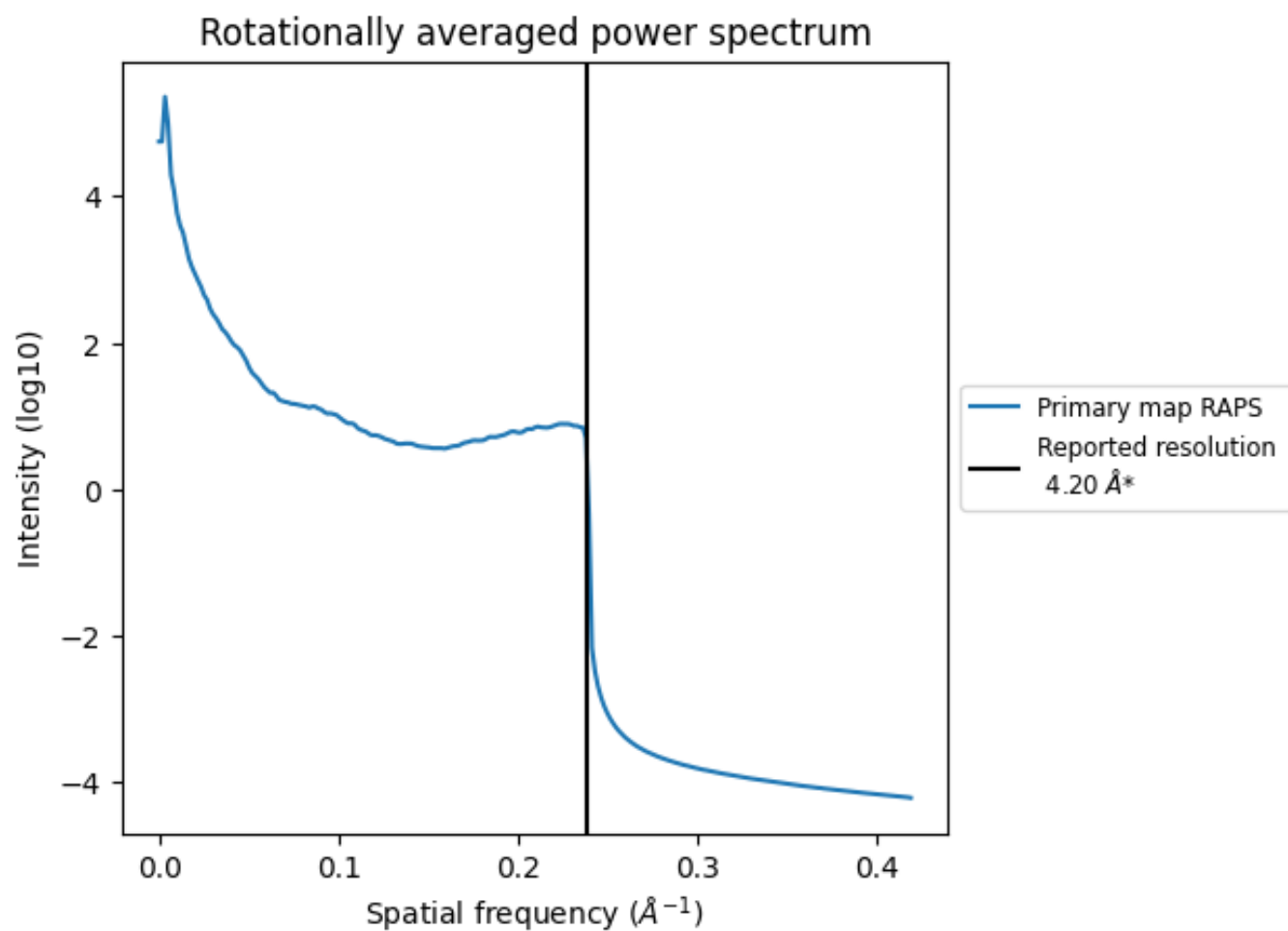
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1751 nm³; this corresponds to an approximate mass of 1581 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 0.238 Å⁻¹

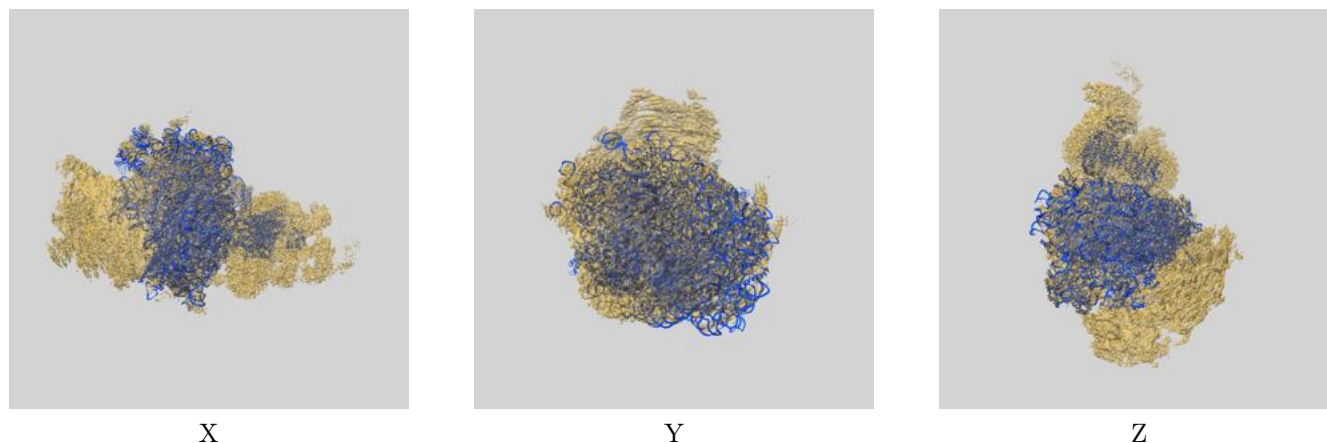
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

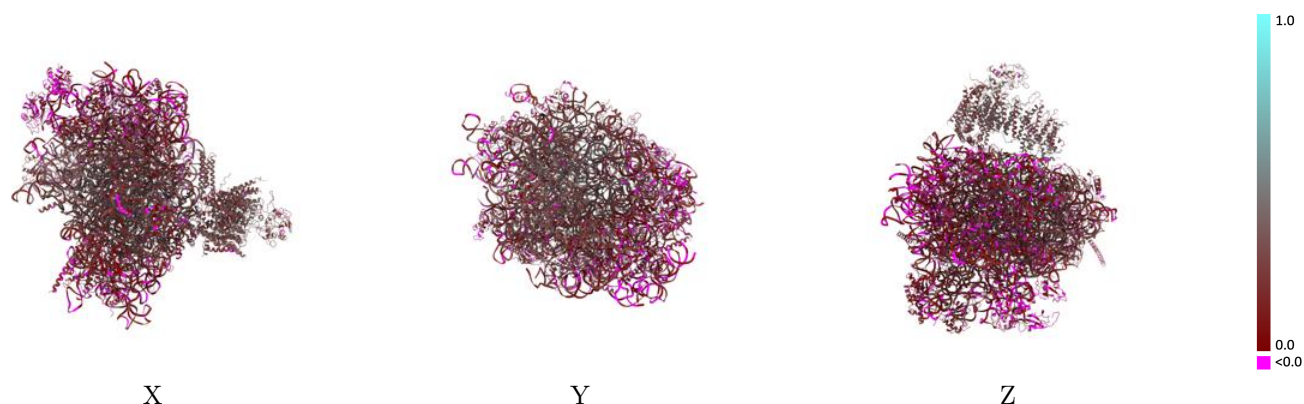
This section contains information regarding the fit between EMDB map EMD-4316 and PDB model 6FTI. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



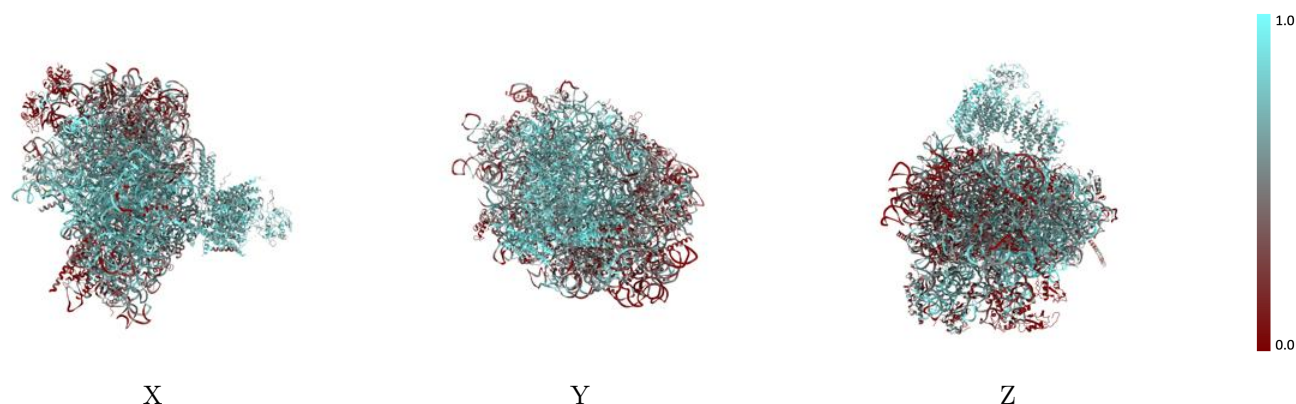
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



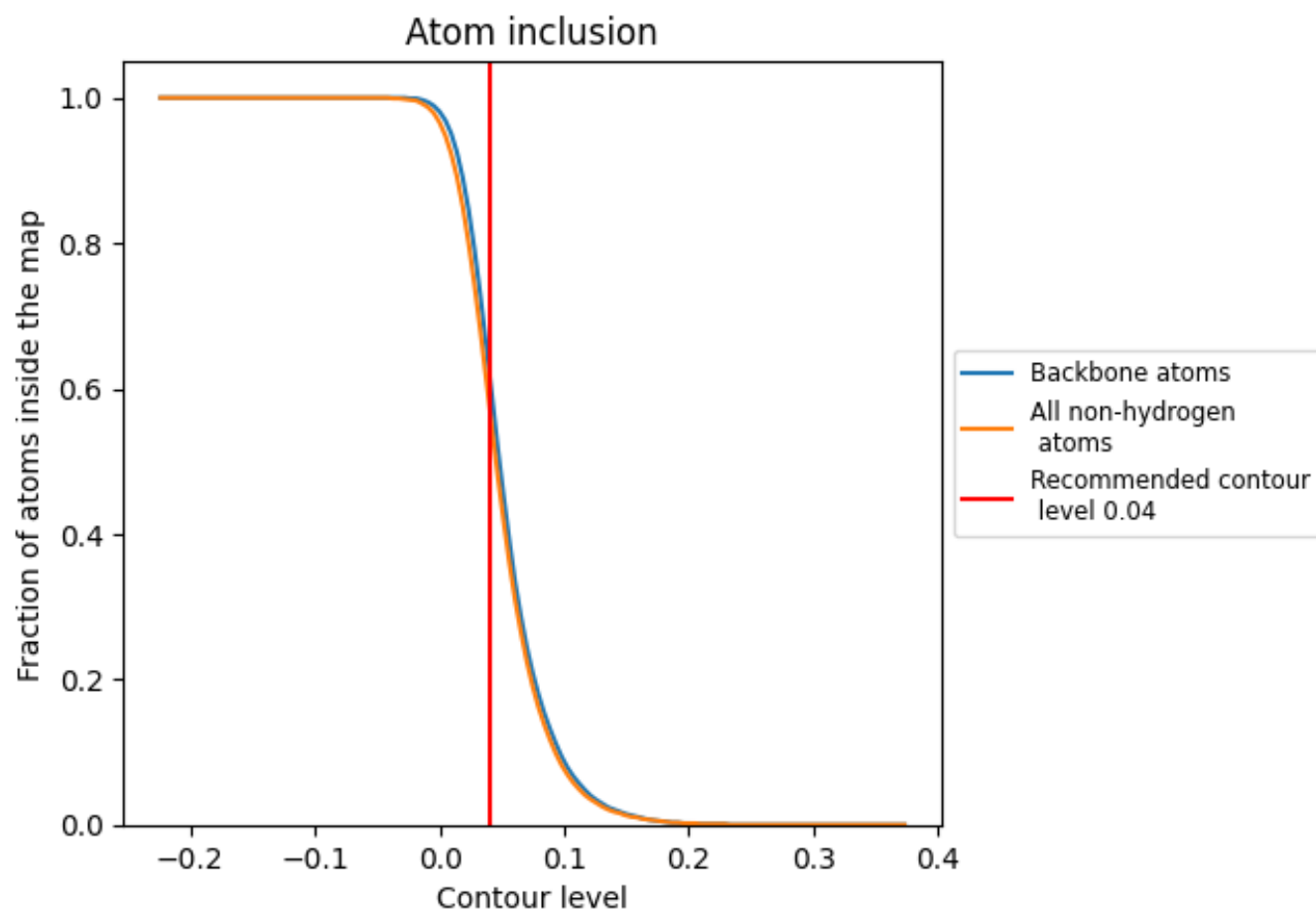
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 58% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5760	 0.2070
0	 0.8170	 0.3480
1	 0.7260	 0.2410
2	 0.8400	 0.2790
3	 0.7390	 0.3310
4	 0.7410	 0.3220
5	 0.6880	 0.3080
6	 0.8720	 0.2940
7	 0.8640	 0.2860
8	 0.8820	 0.2950
A	 0.4870	 0.2520
B	 0.4490	 0.1910
C	 0.4050	 0.2000
D	 0.3950	 0.1370
E	 0.2730	 0.1120
F	 0.3230	 0.1360
G	 0.2490	 0.1090
H	 0.2700	 0.1090
I	 0.4260	 0.1720
J	 0.4260	 0.1720
K	 0.5210	 0.1890
L	 0.3800	 0.1800
M	 0.3510	 0.1240
N	 0.4650	 0.2230
O	 0.2970	 0.1450
P	 0.5970	 0.2860
Q	 0.3590	 0.1780
R	 0.4910	 0.2130
S	 0.3090	 0.1340
T	 0.2870	 0.1650
U	 0.4440	 0.1620
V	 0.4720	 0.2200
W	 0.4950	 0.2140
X	 0.4970	 0.2450
Y	 0.4900	 0.2310



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Chain	Atom inclusion	Q-score
Z	 0.3930	 0.1430
a	 0.4030	 0.1980
b	 0.3730	 0.1800
c	 0.3450	 0.1750
d	 0.5430	 0.2490
e	 0.3460	 0.2080
f	 0.3090	 0.1400
g	 0.4350	 0.2320
h	 0.4780	 0.2080
i	 0.3570	 0.1600
j	 0.6720	 0.3330
k	 0.3840	 0.1590
l	 0.6900	 0.3540
m	 0.3650	 0.1260
n	 0.5420	 0.2860
o	 0.4710	 0.2160
p	 0.4490	 0.2210
q	 0.7230	 0.2410
r	 0.3680	 0.1290
s	 0.1290	 0.0120
t	 0.0700	 0.0310
u	 0.6650	 0.2130
v	 0.7190	 0.1710
w	 0.7570	 0.2540
x	 0.7050	 0.3250
y	 0.7040	 0.3160
z	 0.6310	 0.2730