



## Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 01:17 am GMT

PDB ID : 6FTJ  
EMDB ID : EMD-4317  
Title : Cryo-EM Structure of the Mammalian Oligosaccharyltransferase Bound to Sec61 and the Non-programmed 80S Ribosome  
Authors : Braunger, K.; Becker, T.; Beckmann, R.  
Deposited on : 2018-02-22  
Resolution : 4.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

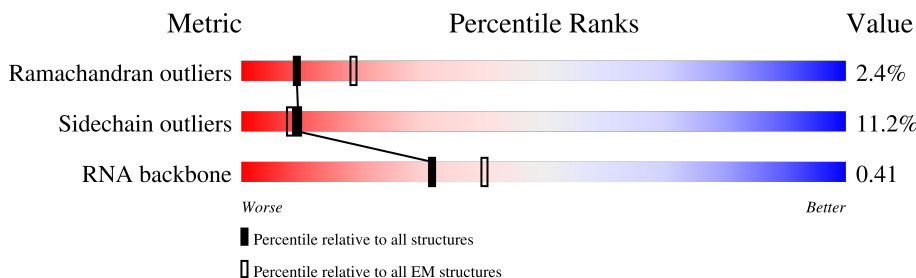
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 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 4.70 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  $\geq 3$ , 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	62% 84% 12%
10	J	169	54% 87% 12%
11	L	210	61% 80% 19%
12	M	138	68% 88% 12%
13	N	203	57% 91% 9%
14	O	199	75% 86% 13%
15	P	153	30% 91% 9%
16	Q	187	61% 89% 11%
17	R	180	49% 88% 12%
18	S	175	74% 83% 17%
19	T	159	76% 87% 12%
20	U	99	46% 90% 8%
21	V	131	62% 86% 14%
22	W	63	52% 89% 11%
23	X	119	48% 90% 10%
24	Y	134	49% 86% 13%
25	Z	135	58% 89% 11%
26	a	147	69% 89% 11%
27	b	75	63% 92% 8%
28	c	94	59% 86% 14%
29	d	107	43% 85% 13%
30	e	128	72% 84% 16%
31	f	109	83% 83% 17%
32	g	114	68% 86% 13%
33	h	122	42% 88% 11%


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Mol	Chain	Length	Quality of chain
34	i	102	64% 91% 9%
35	j	86	24% 83% 15%
36	k	69	67% 84% 14%
37	l	50	20% 84% 16%
38	m	52	69% 83% 17%
39	n	23	57% 83% 13%
40	o	104	46% 86% 13%
41	p	91	60% 92% 8%
42	r	136	61% 78% 19%
43	s	198	84% 90% 9%
44	t	163	86% 80% 20%
45	u	3662	20% 67% 32%
46	v	120	8% 84% 16%
47	w	156	11% 67% 33%
48	x	426	26% 95% 5%
49	y	62	26% 92% 8%
50	z	29	69% 83% 17%
51	1	162	28% 99%
52	2	60	15% 98%
53	3	120	31% 92% 8%
54	4	34	9% 91% 9%
55	5	696	21% 87% 5% 7%
56	6	97	5% 95% 5%
57	7	25	8% 100%
58	8	80	16% 100%

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Mol	Chain	Length	Quality of chain
59	K	8	 <p>A horizontal bar chart showing the quality of chain for Mol 59, Chain K, Length 8. The bar is divided into three segments: a green segment representing 25%, a red segment representing 38%, and a yellow segment representing 75%.</p>

## 2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 152111 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
			Total	C	N	O	S		
1	A	244	1868	1171	382	309	6	0	0

- Molecule 2 is a protein called uL3.

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

- Molecule 3 is a protein called Ribosomal protein L4.

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

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
			Total	C	N	O	S		
4	D	292	2386	1509	437	426	14	0	0

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

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

- Molecule 6 is a protein called U130.

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

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 uL8.

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

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
			Total	C	N	O	S		
8	H	190	1516	954	284	272	6	0	0

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

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

- Molecule 10 is a protein called Ribosomal protein L11.

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

- Molecule 11 is a protein called eL13.

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

- Molecule 12 is a protein called Ribosomal protein L14.

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

- Molecule 13 is a protein called Ribosomal protein L15.

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

- Molecule 14 is a protein called uL13.

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

- Molecule 15 is a protein called uL22.

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

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
			Total	C	N	O	S		
16	Q	187	1506	941	311	249	5	0	0

- Molecule 17 is a protein called eL19.



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

- Molecule 18 is a protein called eL20.

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

- Molecule 19 is a protein called eL21.

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

- Molecule 20 is a protein called Ribosomal protein L22.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	32	GLY	ARG	conflict	UNP G1TSG1
U	36	ALA	GLU	conflict	UNP G1TSG1
U	39	PHE	SER	conflict	UNP G1TSG1
U	54	GLY	ARG	conflict	UNP G1TSG1
U	60	VAL	ALA	conflict	UNP G1TSG1
U	97	ARG	HIS	conflict	UNP G1TSG1

- Molecule 21 is a protein called uL14.

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

- Molecule 22 is a protein called Ribosomal protein L24.

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

- Molecule 23 is a protein called uL23.

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

- Molecule 24 is a protein called Ribosomal protein L26.

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

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

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

- Molecule 26 is a protein called uL15.

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

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

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

- Molecule 28 is a protein called eL30.

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

- Molecule 29 is a protein called eL31.

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

- 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 28S rRNA.

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

- Molecule 46 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 47 is a RNA chain called 5.8S ribosomal RNA.

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

- Molecule 48 is a protein called Protein transport protein Sec61 subunit alpha isoform 1.

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

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	?	-	THR	deletion	UNP P38377
x	?	-	GLY	deletion	UNP P38377
x	?	-	MET	deletion	UNP P38377
x	?	-	TYR	deletion	UNP P38377
x	?	-	GLY	deletion	UNP P38377
x	?	-	ASP	deletion	UNP P38377
x	?	-	PRO	deletion	UNP P38377
x	?	-	SER	deletion	UNP P38377
x	?	-	GLU	deletion	UNP P38377
x	?	-	MET	deletion	UNP P38377
x	?	-	GLY	deletion	UNP P38377
x	145	SER	ALA	conflict	UNP P38377
x	?	-	SER	deletion	UNP P38377

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Chain	Residue	Modelled	Actual	Comment	Reference
x	?	-	GLY	deletion	UNP P38377
x	?	-	ASN	deletion	UNP P38377
x	?	-	LEU	deletion	UNP P38377
x	?	-	LEU	deletion	UNP P38377
x	?	-	VAL	deletion	UNP P38377
x	?	-	SER	deletion	UNP P38377
x	?	-	LEU	deletion	UNP P38377
x	?	-	LEU	deletion	UNP P38377
x	?	-	GLY	deletion	UNP P38377
x	?	-	THR	deletion	UNP P38377
x	?	-	TRP	deletion	UNP P38377
x	?	-	SER	deletion	UNP P38377
x	?	-	ASP	deletion	UNP P38377
x	?	-	THR	deletion	UNP P38377
x	?	-	SER	deletion	UNP P38377
x	?	-	SER	deletion	UNP P38377
x	?	-	GLY	deletion	UNP P38377
x	?	-	GLY	deletion	UNP P38377
x	?	-	PRO	deletion	UNP P38377
x	?	-	ALA	deletion	UNP P38377
x	?	-	ARG	deletion	UNP P38377
x	?	-	ALA	deletion	UNP P38377
x	?	-	TYR	deletion	UNP P38377

- Molecule 49 is a protein called Protein transport protein Sec61 subunit gamma.

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

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

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

- Molecule 51 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1,RPN1.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	1	162	Total	C	N	O	0	0
			882	550	165	167		

- Molecule 52 is a protein called TMEM258.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	2	60	300	180	60	60	0	0

- Molecule 53 is a protein called Oligosaccharyltransferase complex subunit OSTC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	3	120	802	529	130	136	7	0	0

- Molecule 54 is a protein called OST4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	4	34	268	180	41	45	2	0	0

- Molecule 55 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	5	644	5090	3331	819	904	36	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 56 is a protein called DAD1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
56	6	97	485	291	97	97	0	0

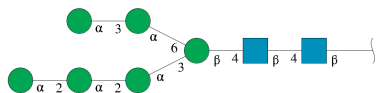
- Molecule 57 is a protein called OST48.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
57	7	25	125	75	25	25	0	0

- Molecule 58 is a protein called RPN2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
58	8	80	400	240	80	80	0	0

- Molecule 59 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
			Total	C	N	O		
59	K	8	94	52	2	40	0	0

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

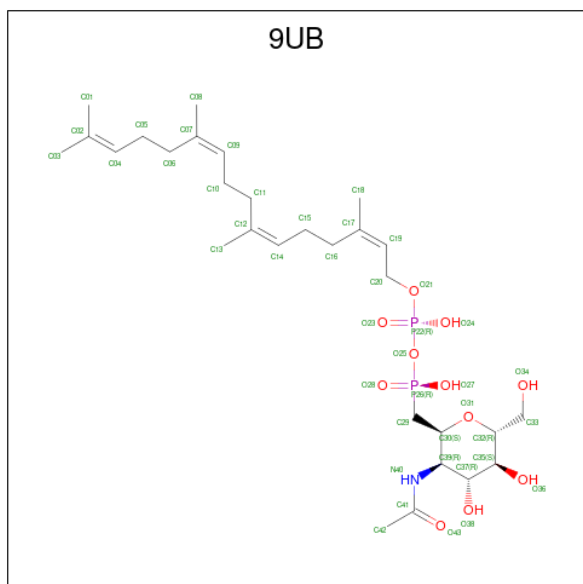
Mol	Chain	Residues	Atoms		AltConf
60	B	1	Total	Mg	0
			1	1	
60	I	1	Total	Mg	0
			1	1	
60	P	1	Total	Mg	0
			1	1	
60	V	1	Total	Mg	0
			1	1	
60	a	1	Total	Mg	0
			1	1	
60	e	1	Total	Mg	0
			1	1	
60	g	1	Total	Mg	0
			1	1	
60	u	145	Total	Mg	0
			145	145	
60	v	5	Total	Mg	0
			5	5	
60	w	2	Total	Mg	0
			2	2	

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).



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

- Molecule 62 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 (three-letter code: 9UB) (formula:  $C_{29}H_{51}NO_{11}P_2$ ).

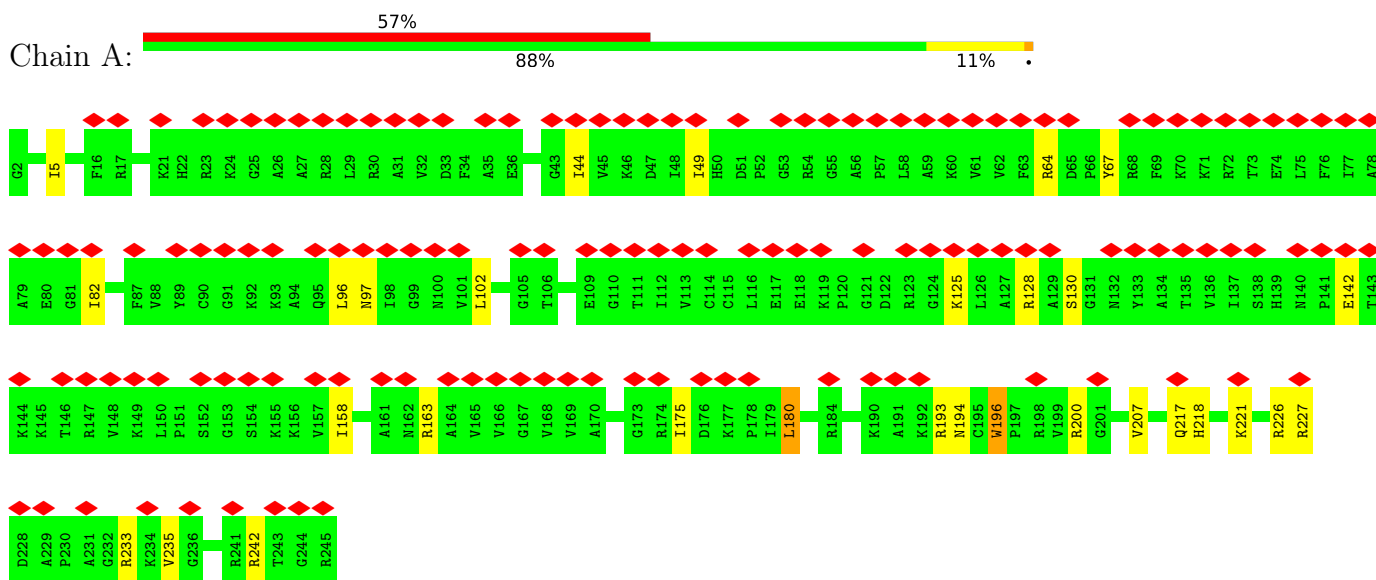


Mol	Chain	Residues	Atoms	AltConf
62	5	1	Total C N O P 43 29 1 11 2	0

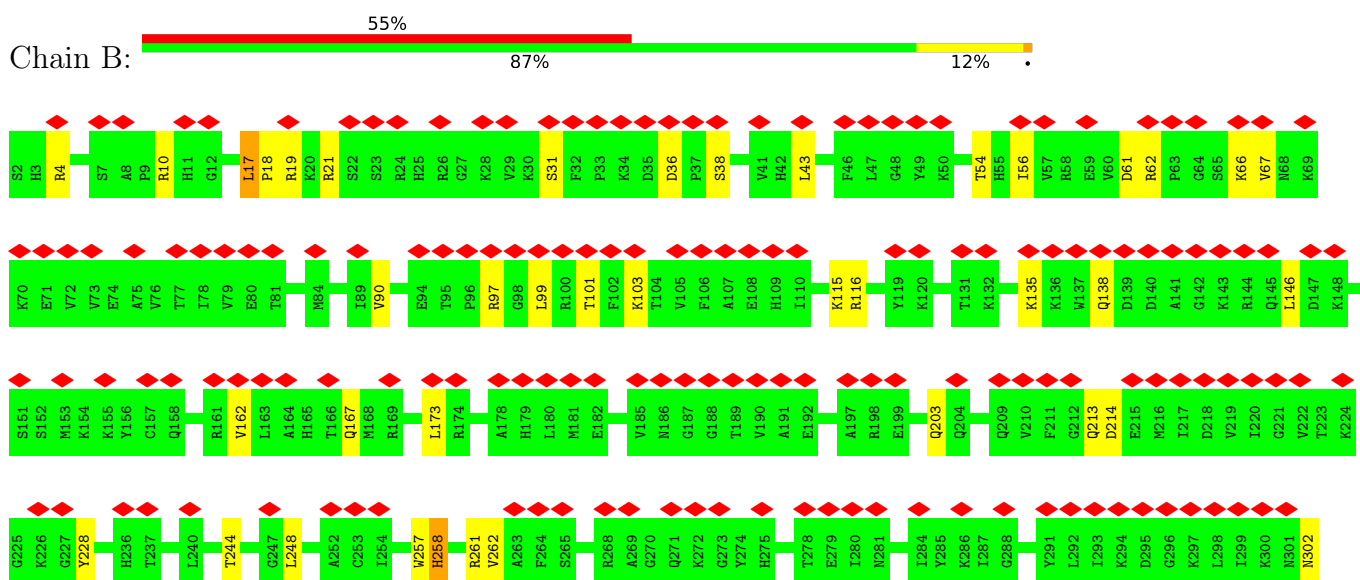
### 3 Residue-property plots [i](#)

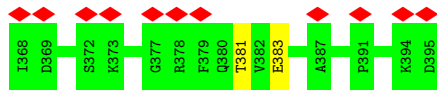
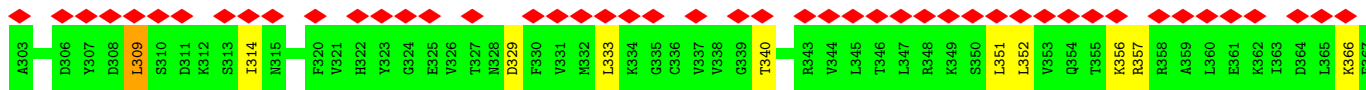
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: uL2

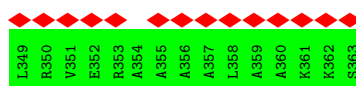
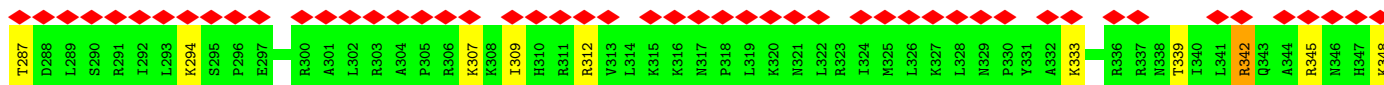
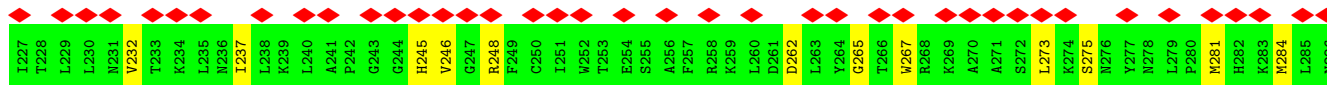
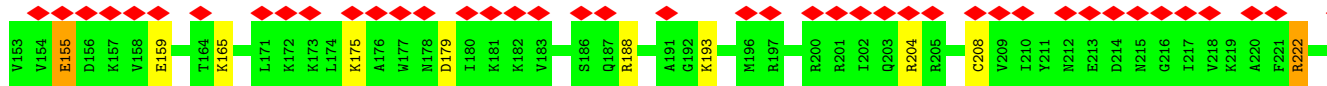
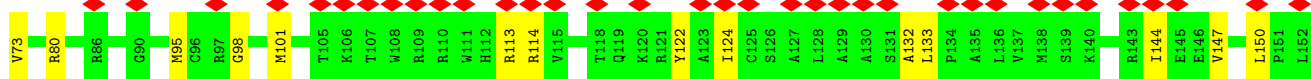
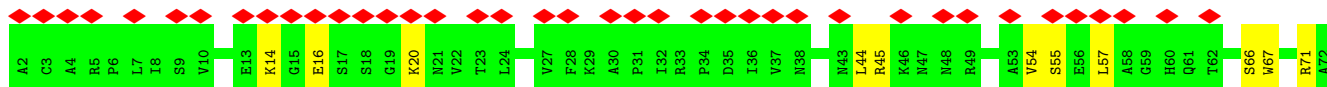
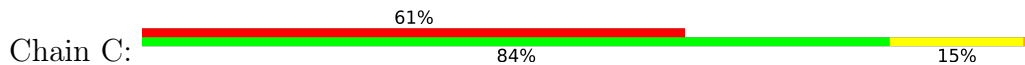


- Molecule 2: uL3

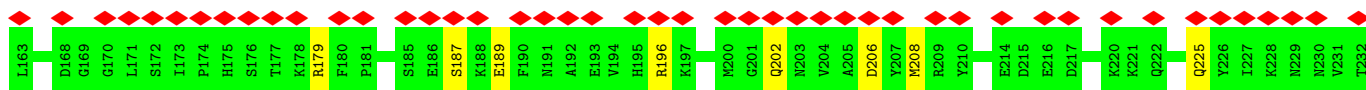
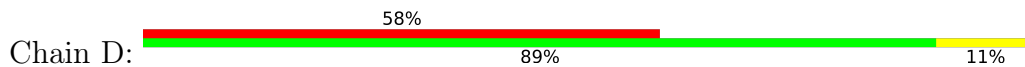


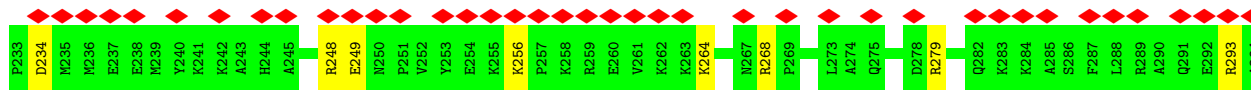


• Molecule 3: Ribosomal protein L4

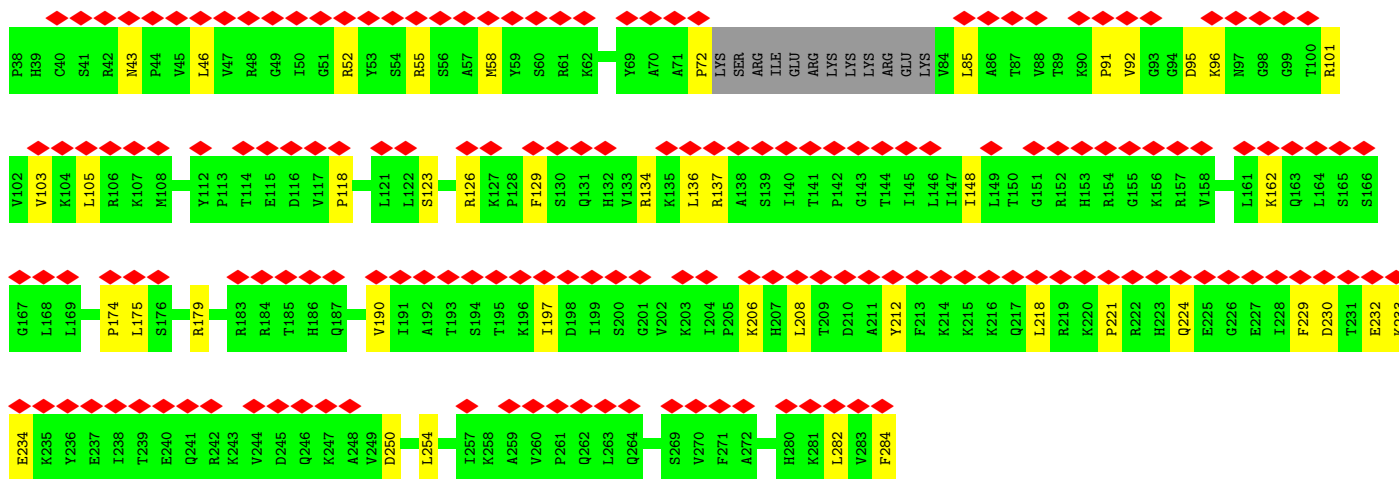
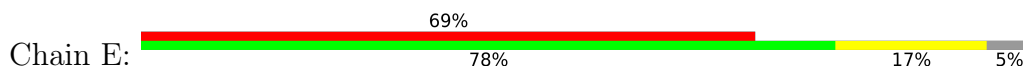


• Molecule 4: 60S ribosomal protein L5

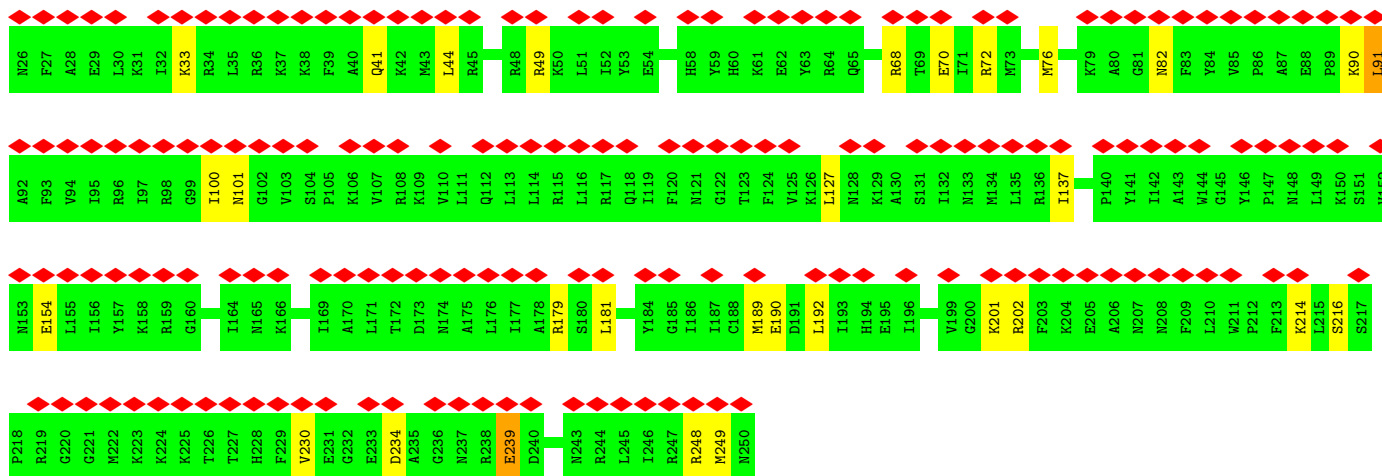
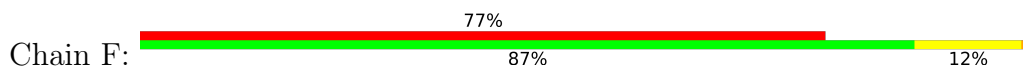




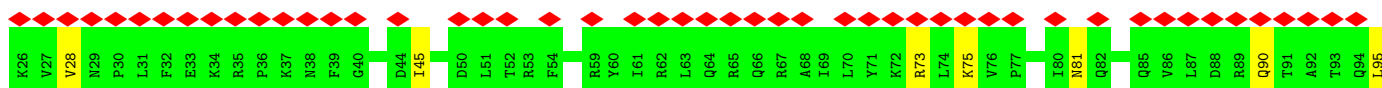
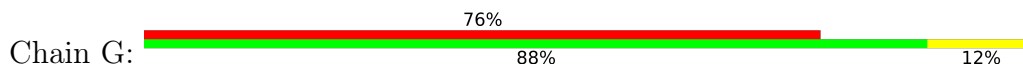
- Molecule 5: 60S ribosomal protein L6

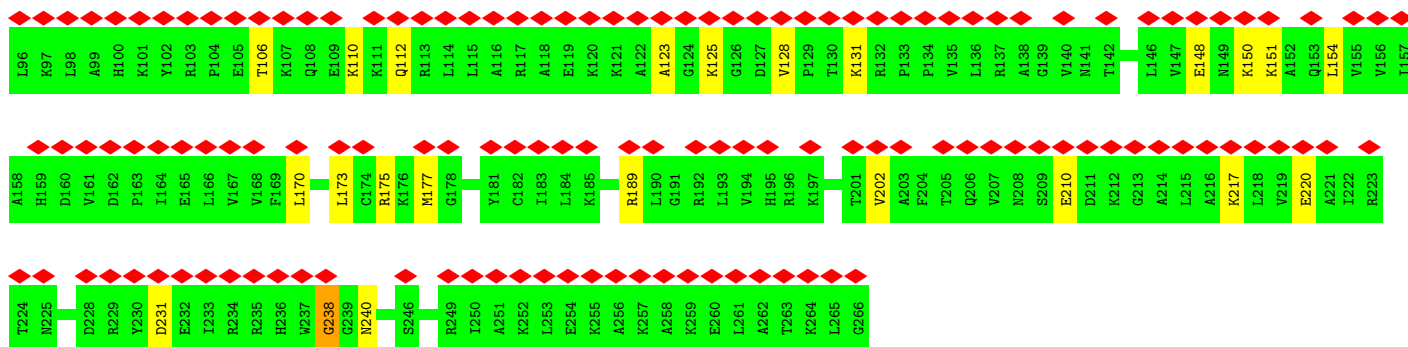


- Molecule 6: U130

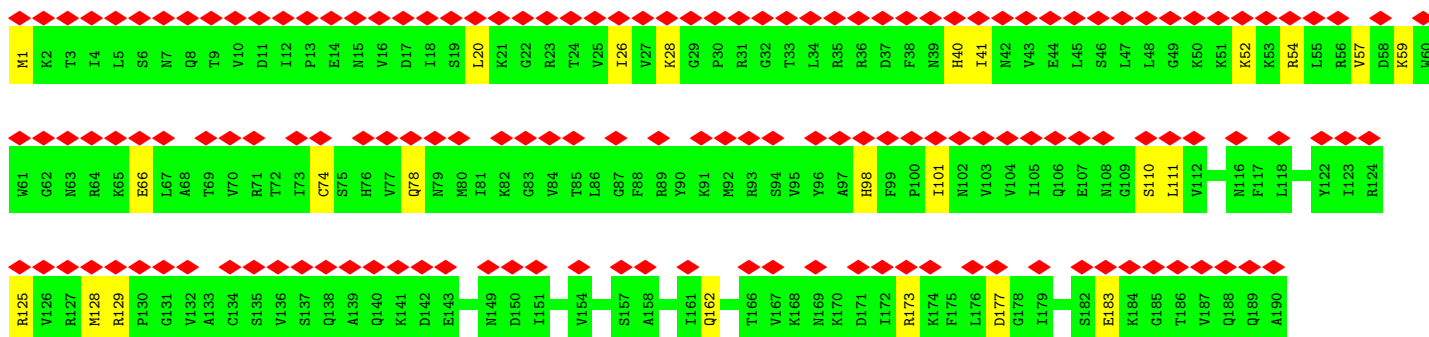
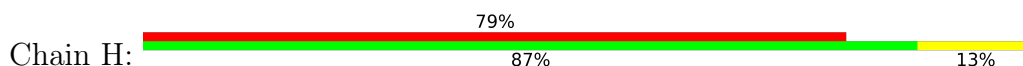


- Molecule 7: uL8

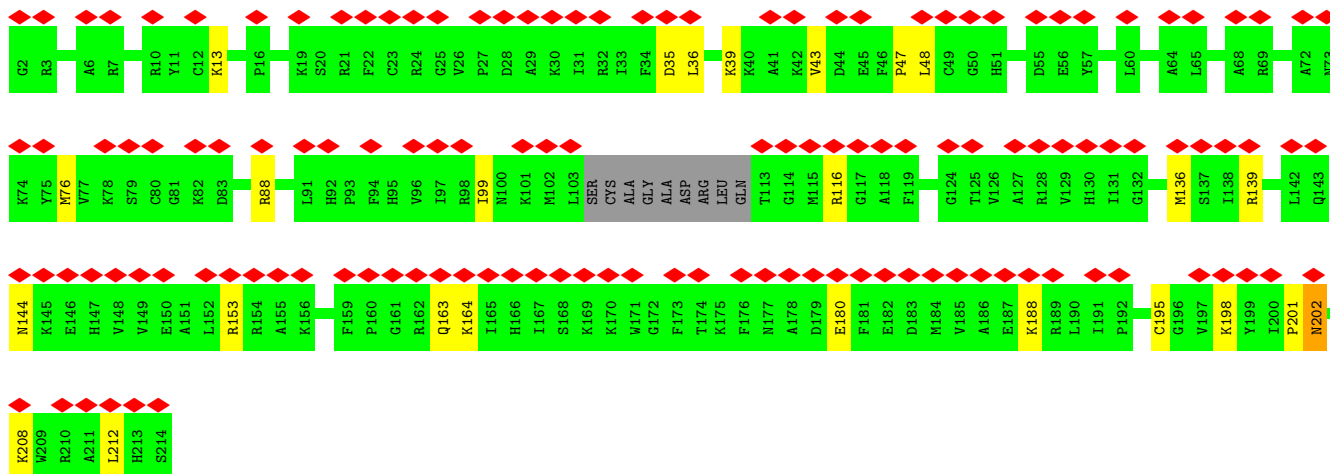
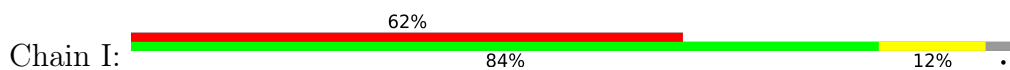




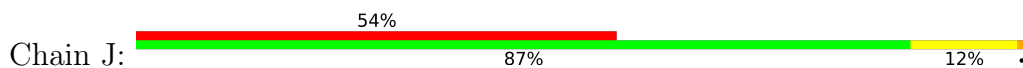
- Molecule 8: uL6

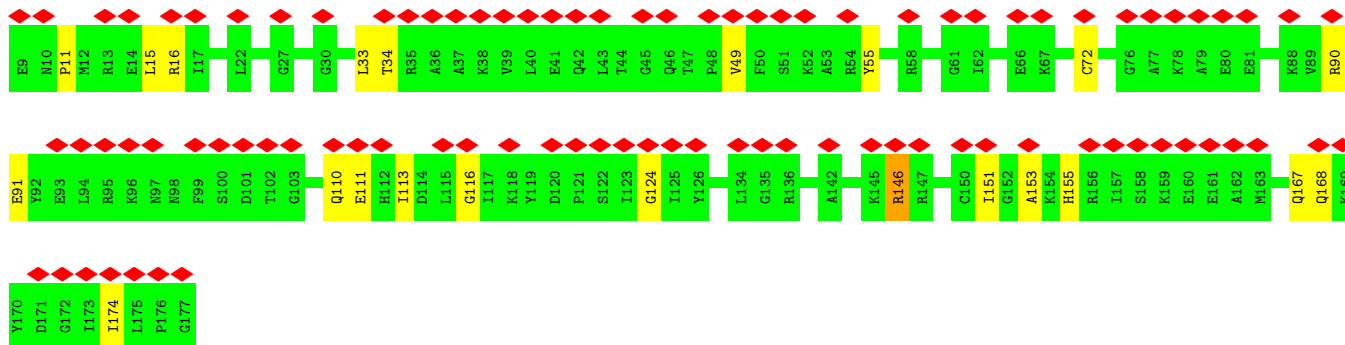


- Molecule 9: Ribosomal protein L10 (Predicted)

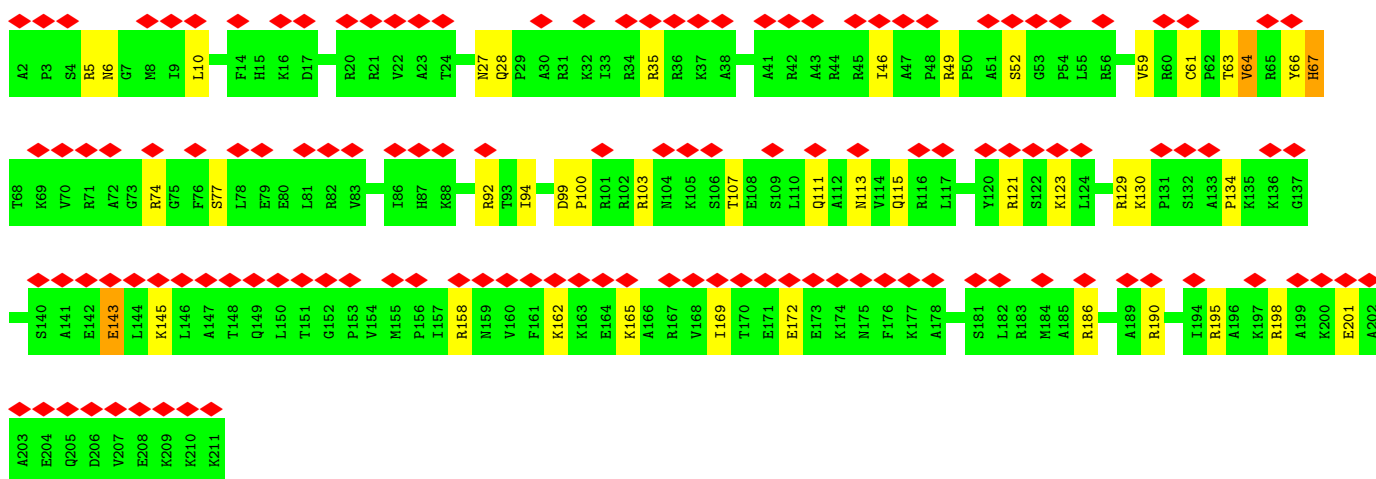
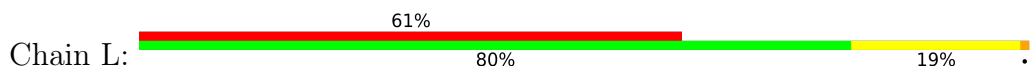


- Molecule 10: Ribosomal protein L11

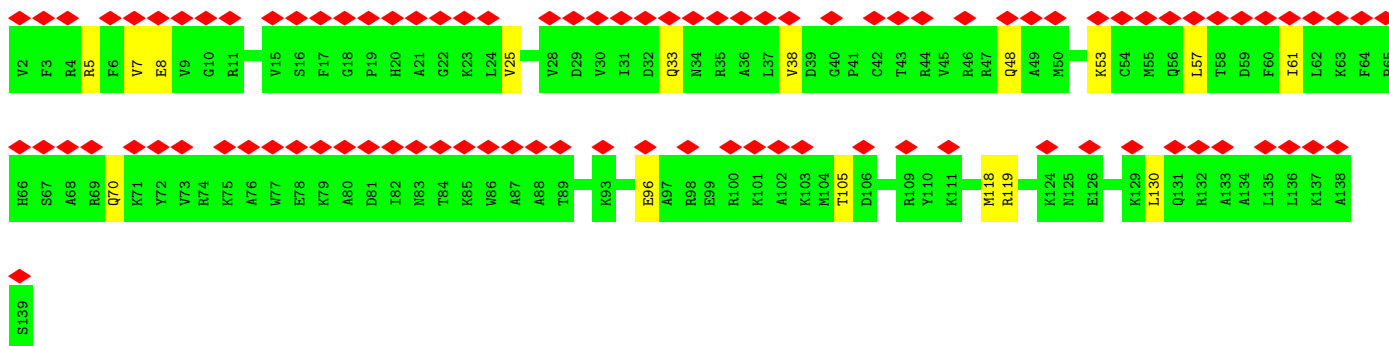
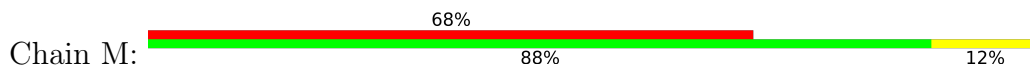




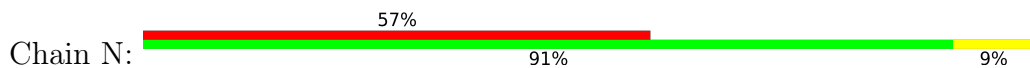
• Molecule 11: eL13

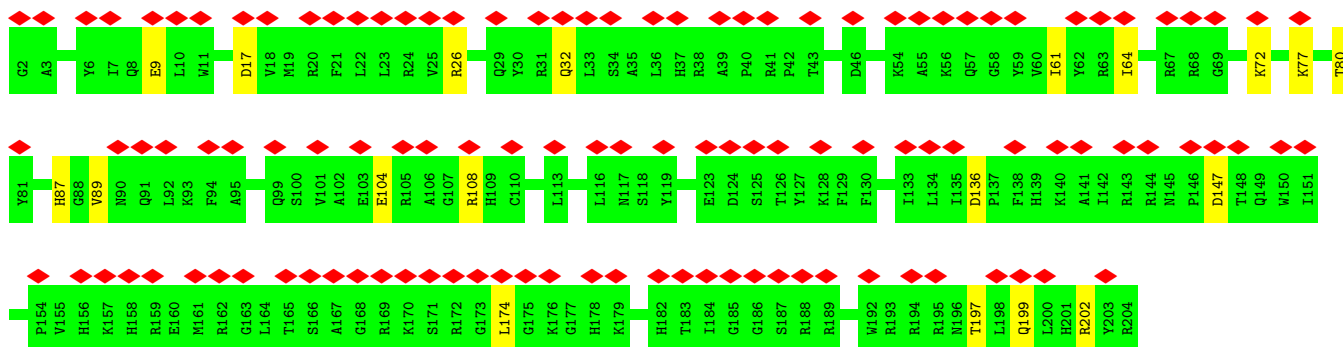


• Molecule 12: Ribosomal protein L14

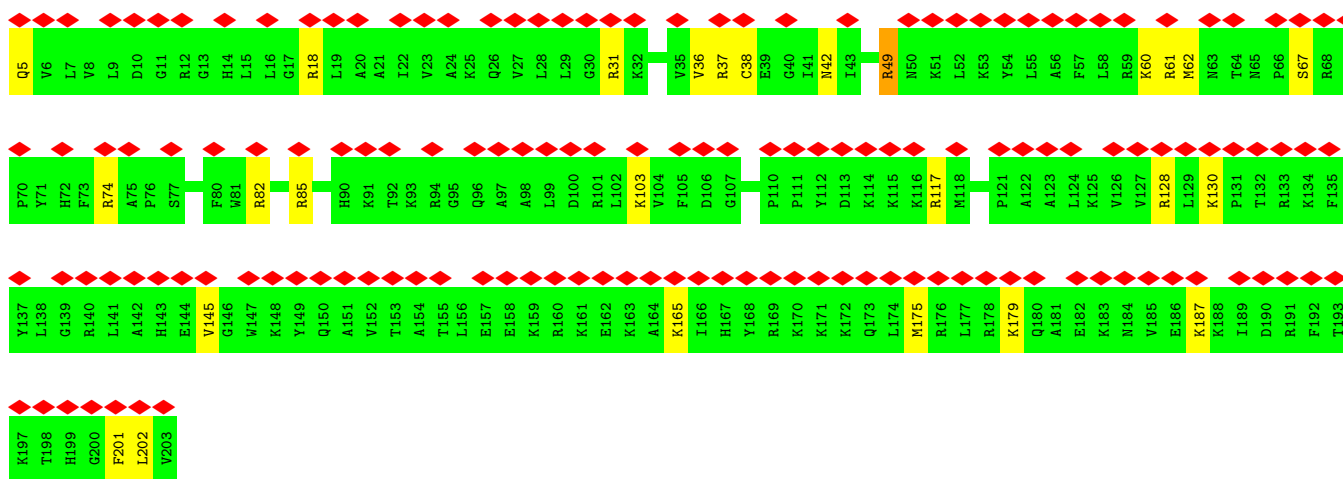
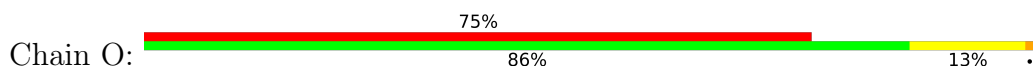


• Molecule 13: Ribosomal protein L15

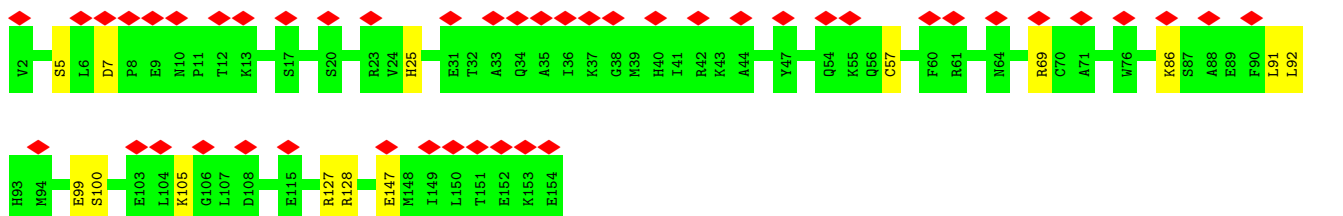
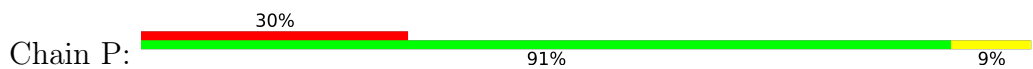




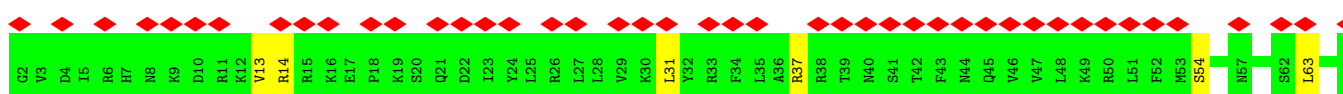
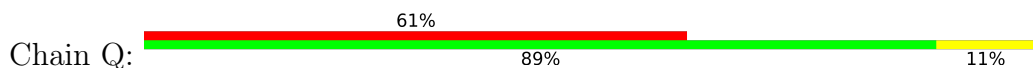
• Molecule 14: uL13

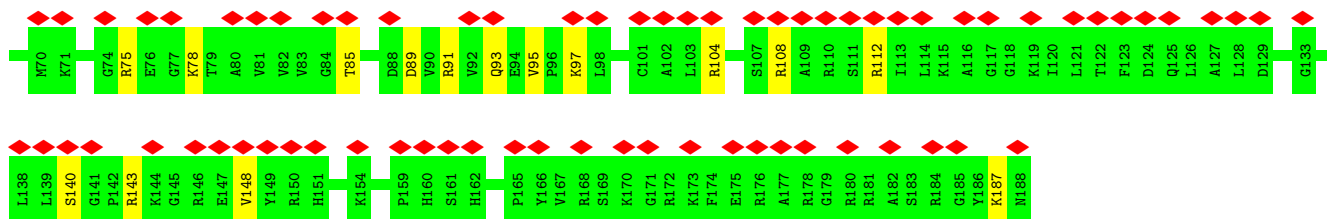


• Molecule 15: uL22

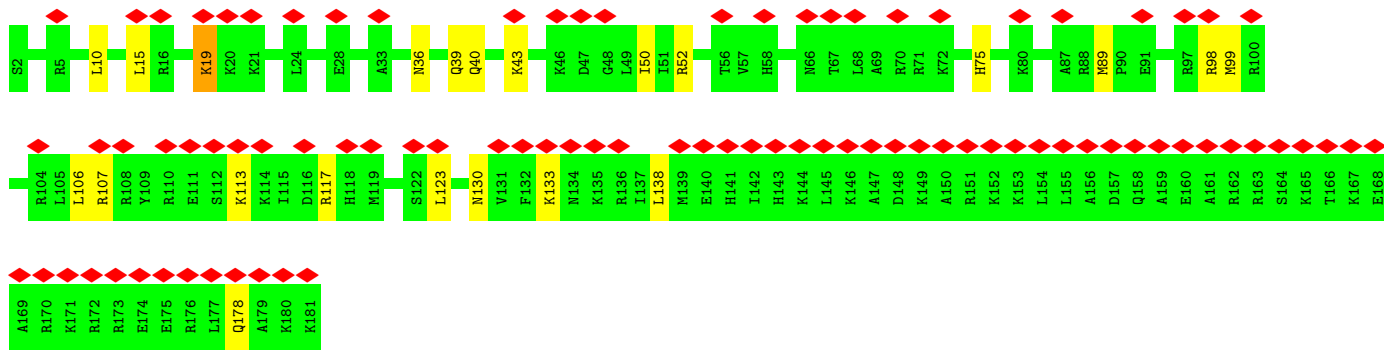
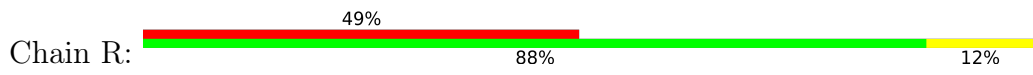


• Molecule 16: uL14

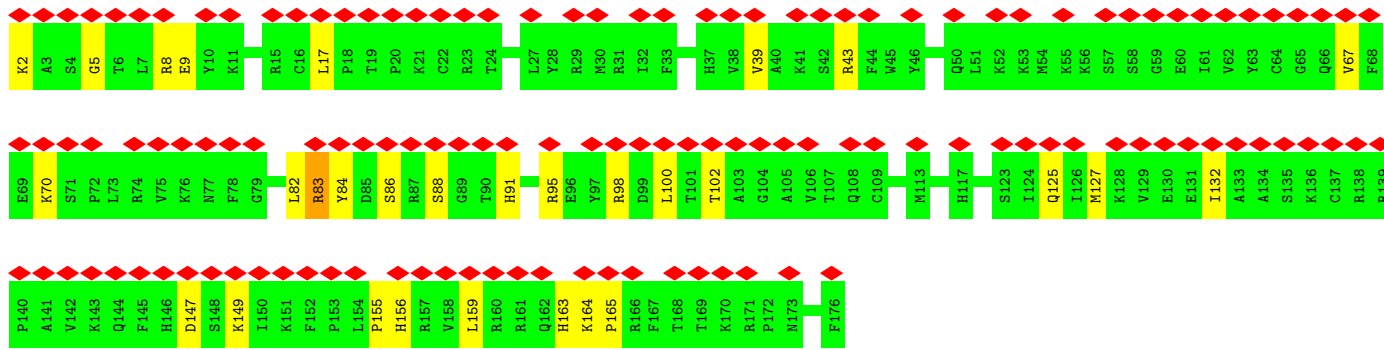
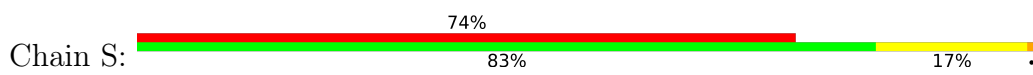




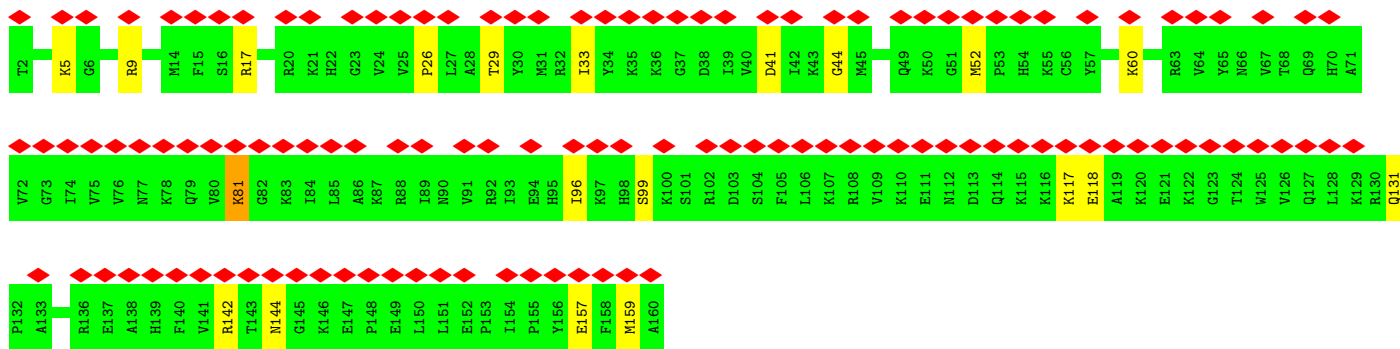
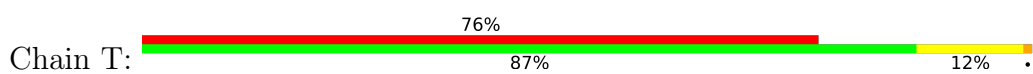
• Molecule 17: eL19



• Molecule 18: eL20

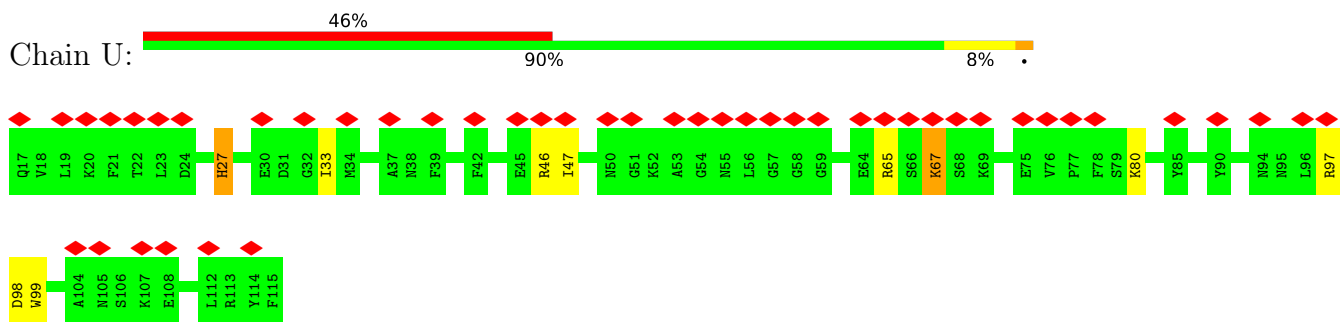


• Molecule 19: eL21

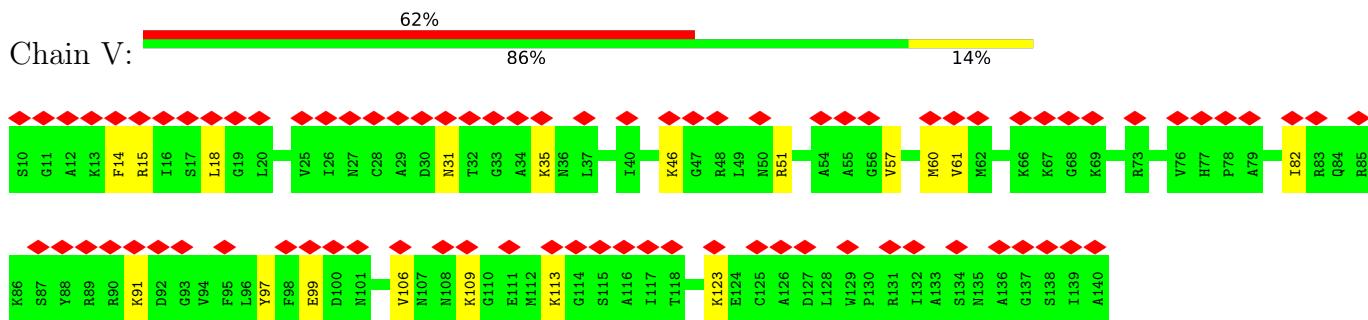




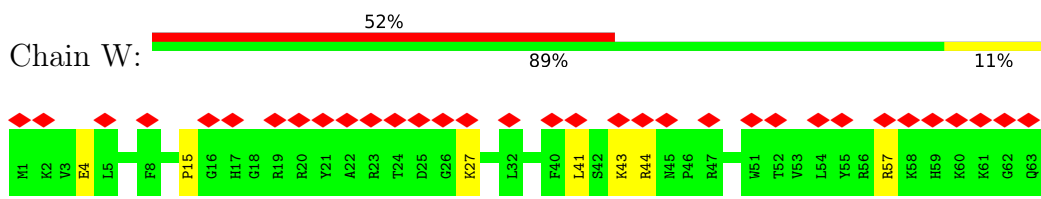
• Molecule 20: Ribosomal protein L22



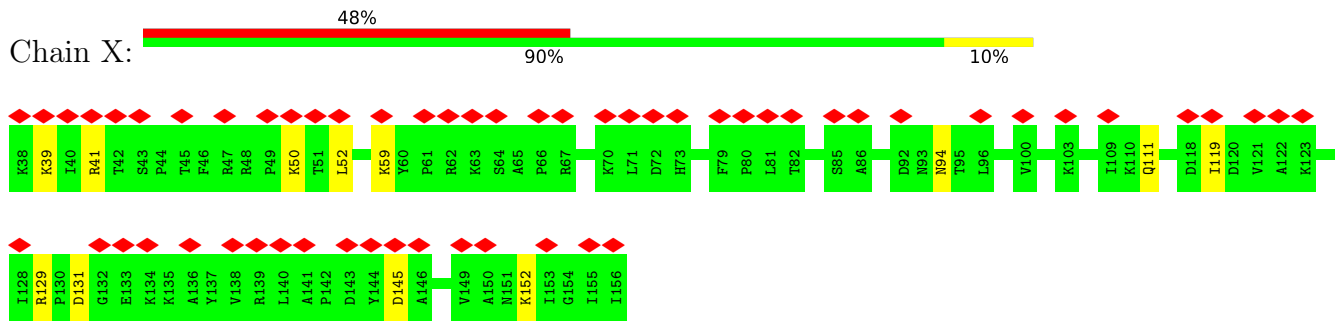
• Molecule 21: uL14



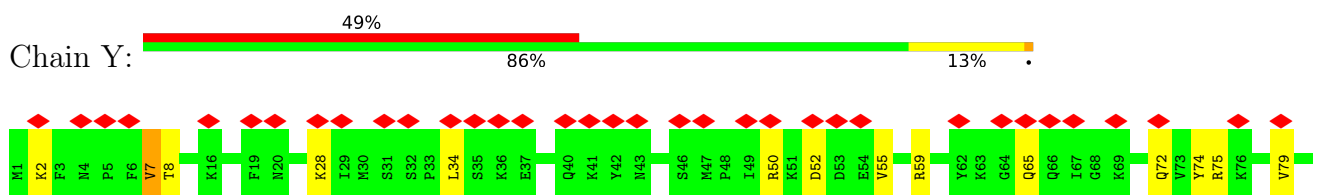
• Molecule 22: Ribosomal protein L24

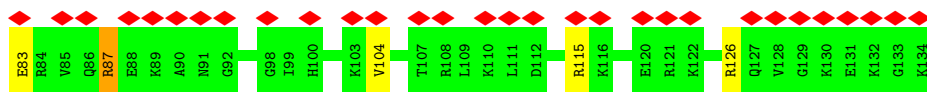


• Molecule 23: uL23

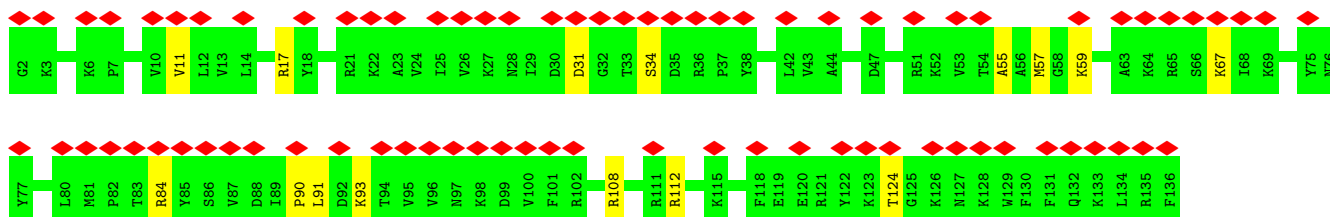
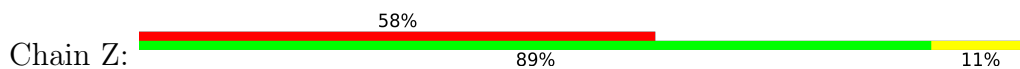


• Molecule 24: Ribosomal protein L26

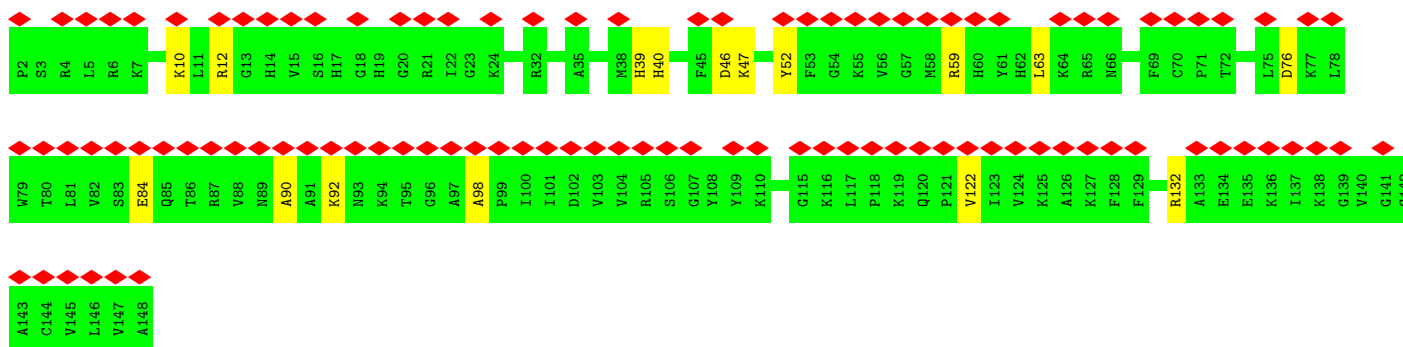
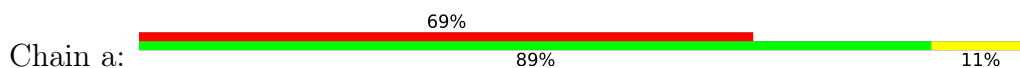




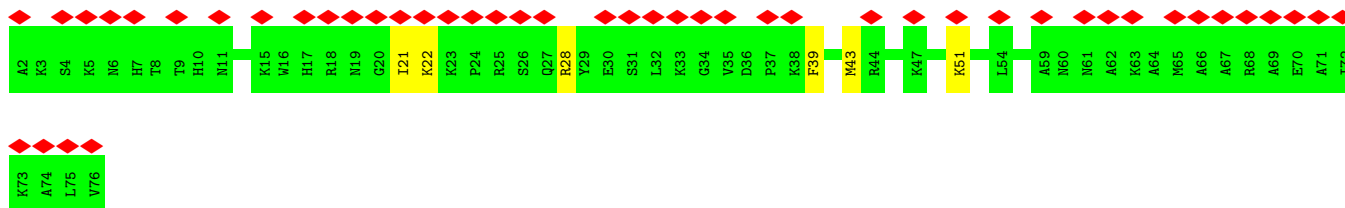
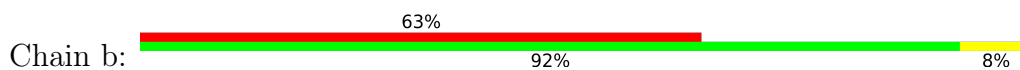
- Molecule 25: 60S ribosomal protein L27



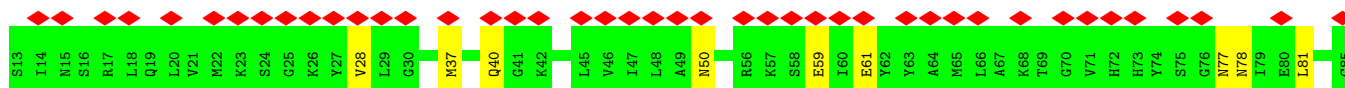
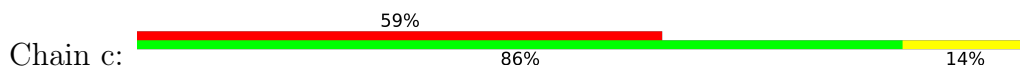
- Molecule 26: uL15

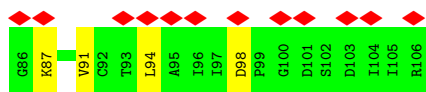


- Molecule 27: 60S ribosomal protein L29

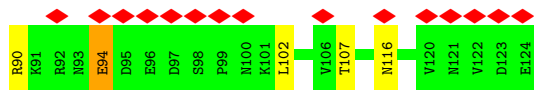
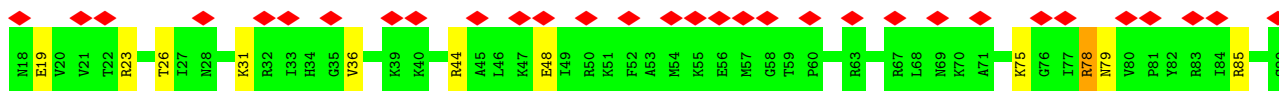
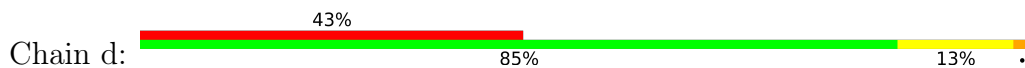


- Molecule 28: eL30

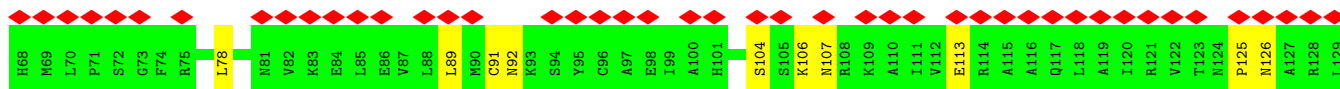
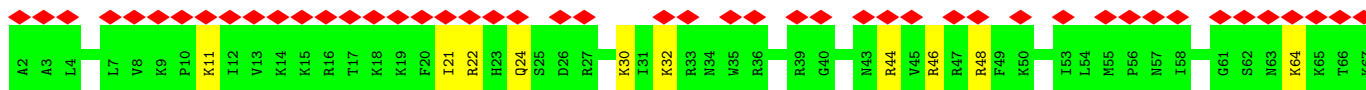
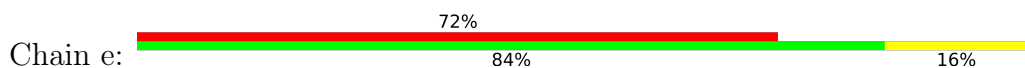




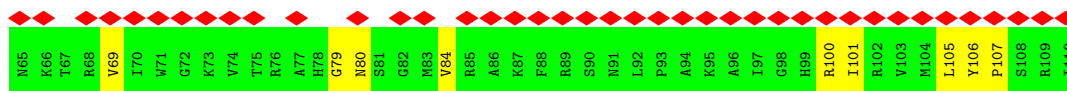
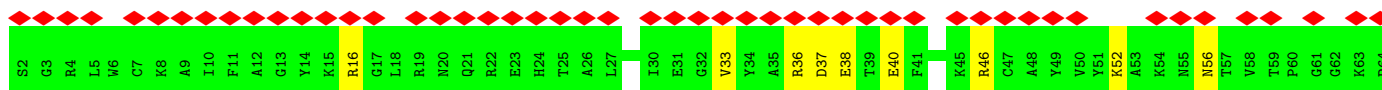
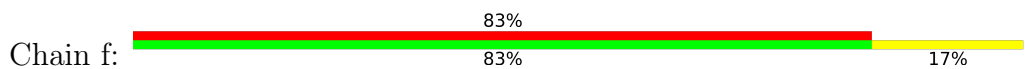
• Molecule 29: eL31



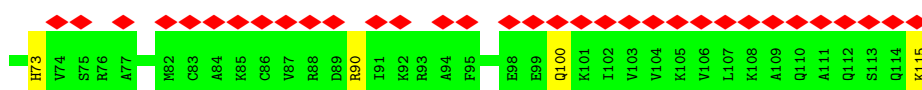
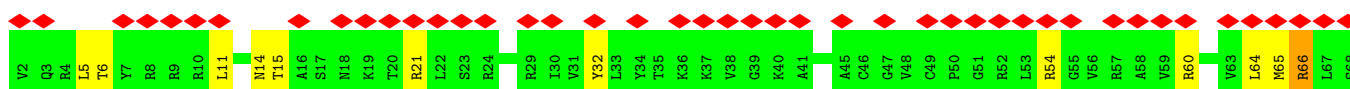
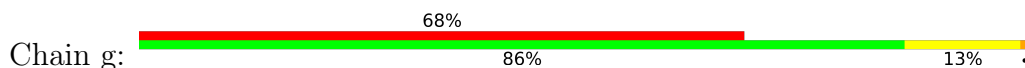
• Molecule 30: eL32



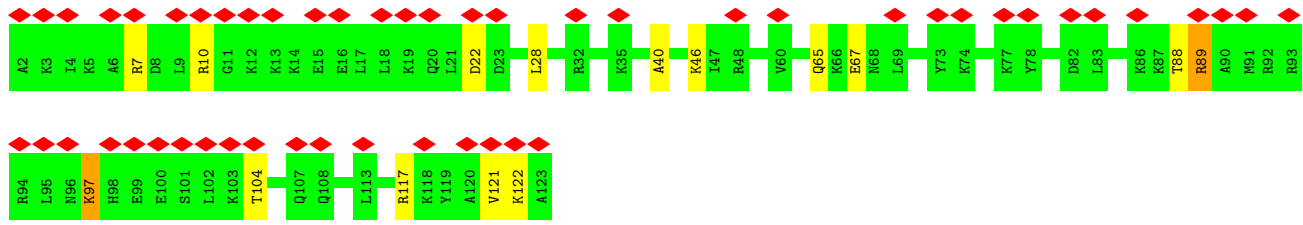
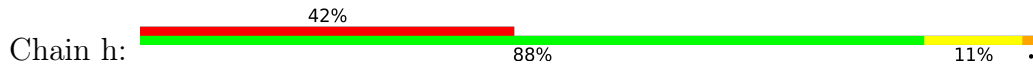
• Molecule 31: eL33



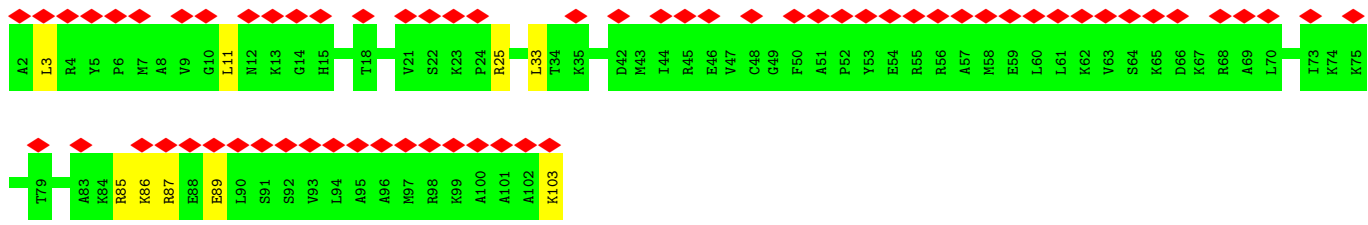
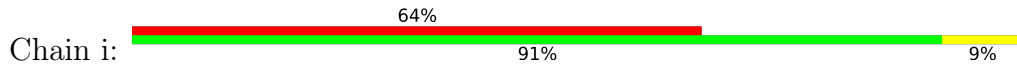
• Molecule 32: eL34



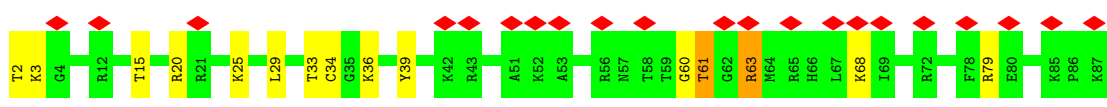
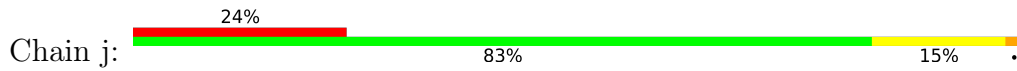
• Molecule 33: uL29



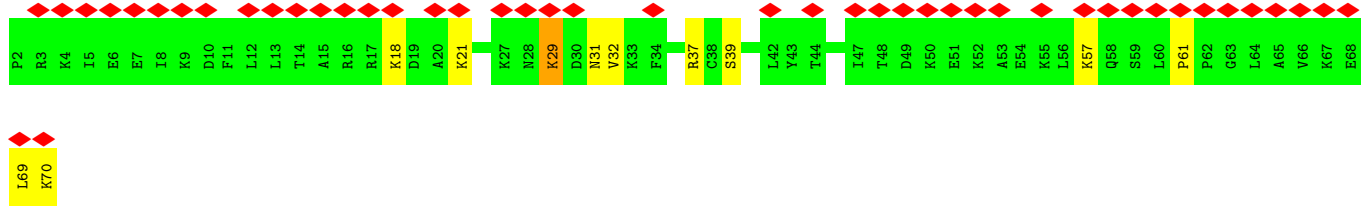
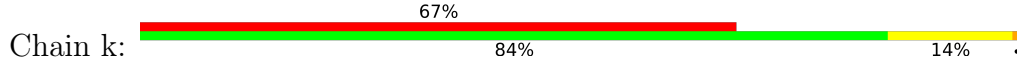
• Molecule 34: 60S ribosomal protein L36



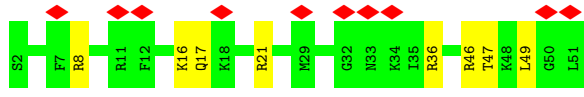
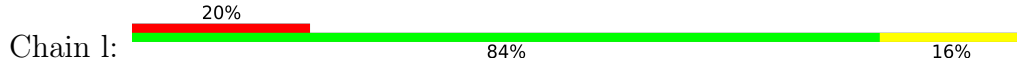
• Molecule 35: Ribosomal protein L37



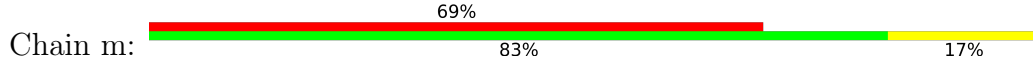
• Molecule 36: eL38

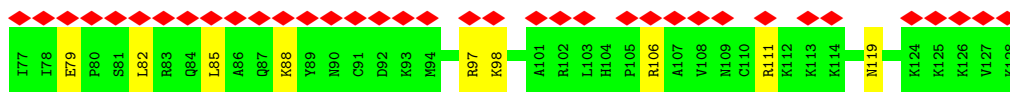


• Molecule 37: eL39

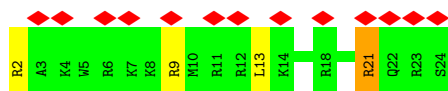
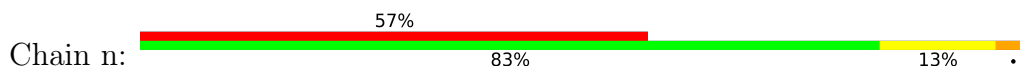


• Molecule 38: eL40

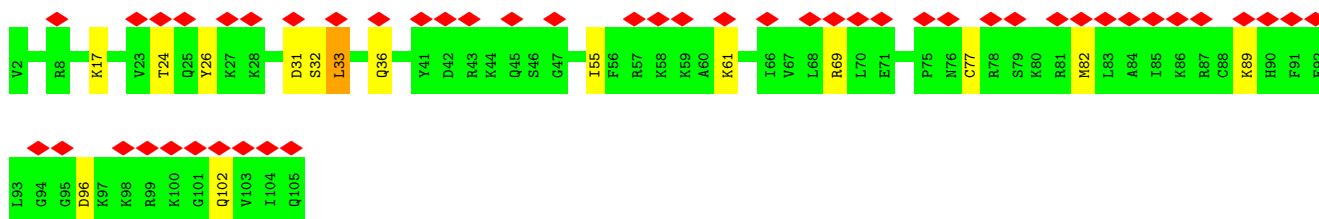
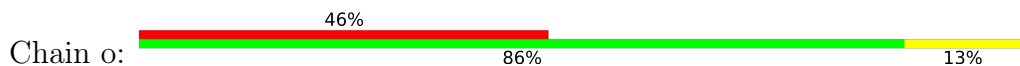




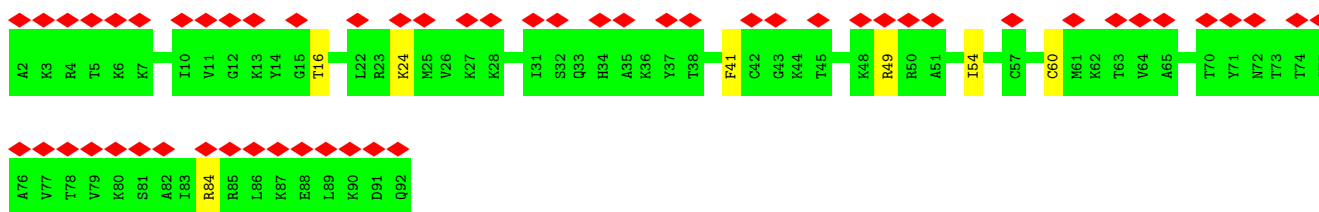
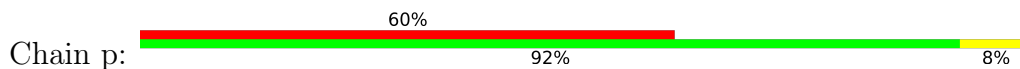
- Molecule 39: 60s ribosomal protein l41



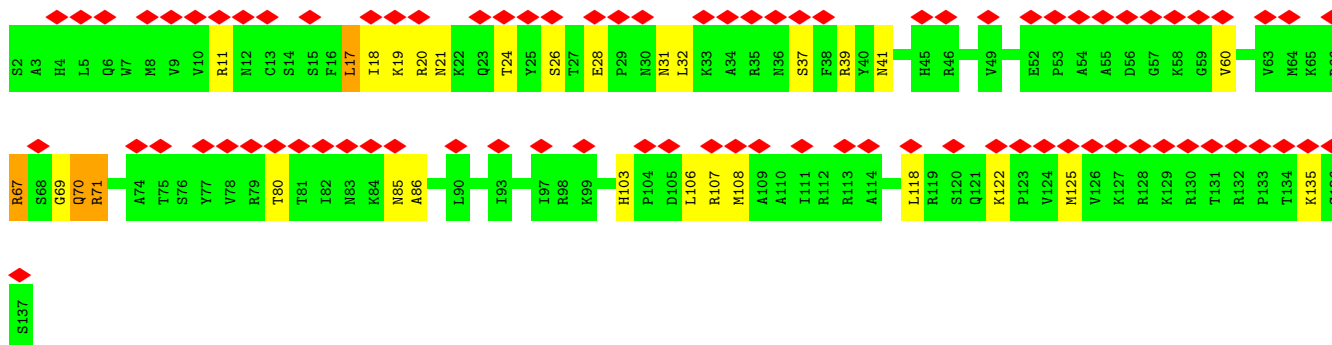
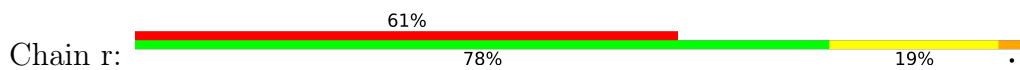
- Molecule 40: eL42



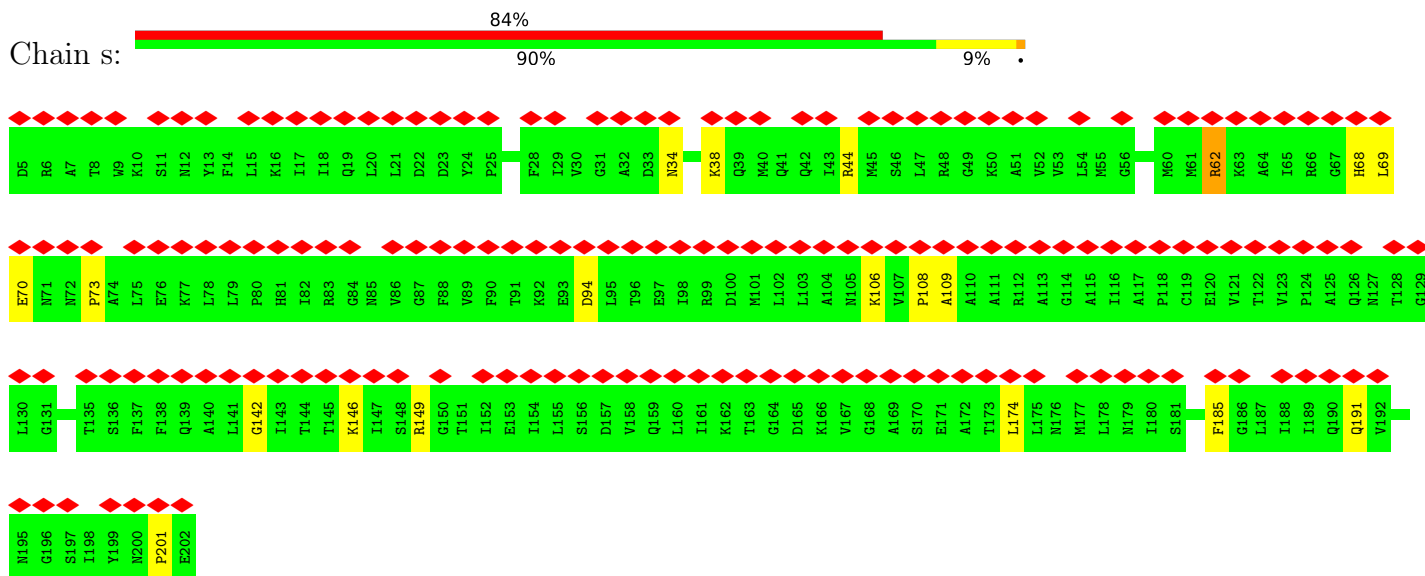
- Molecule 41: Ribosomal protein L37a



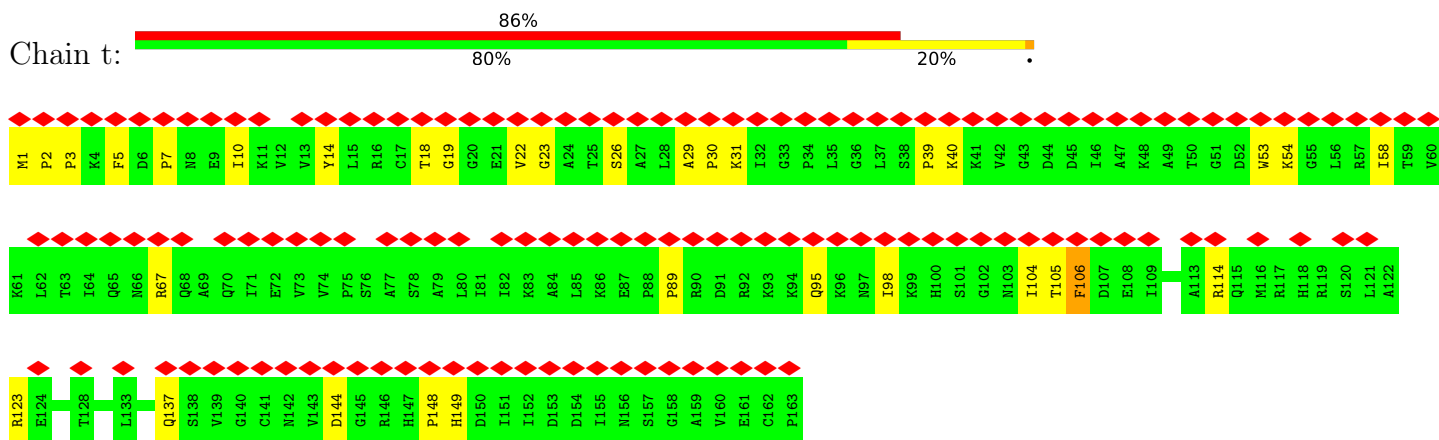
- Molecule 42: eL28



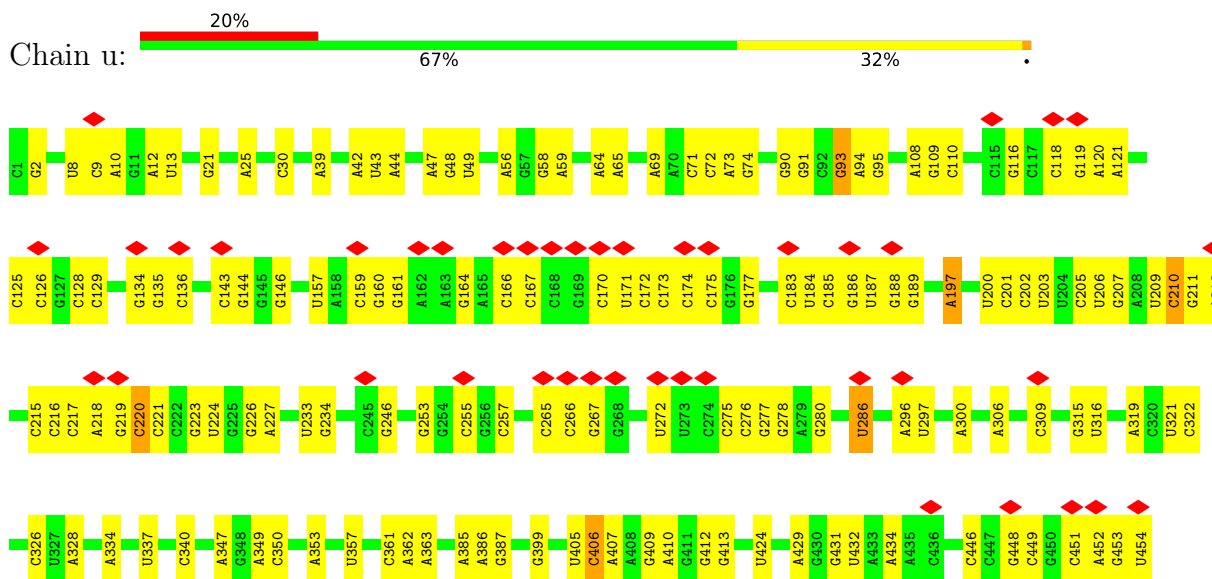
- Molecule 43: 60S acidic ribosomal protein P0



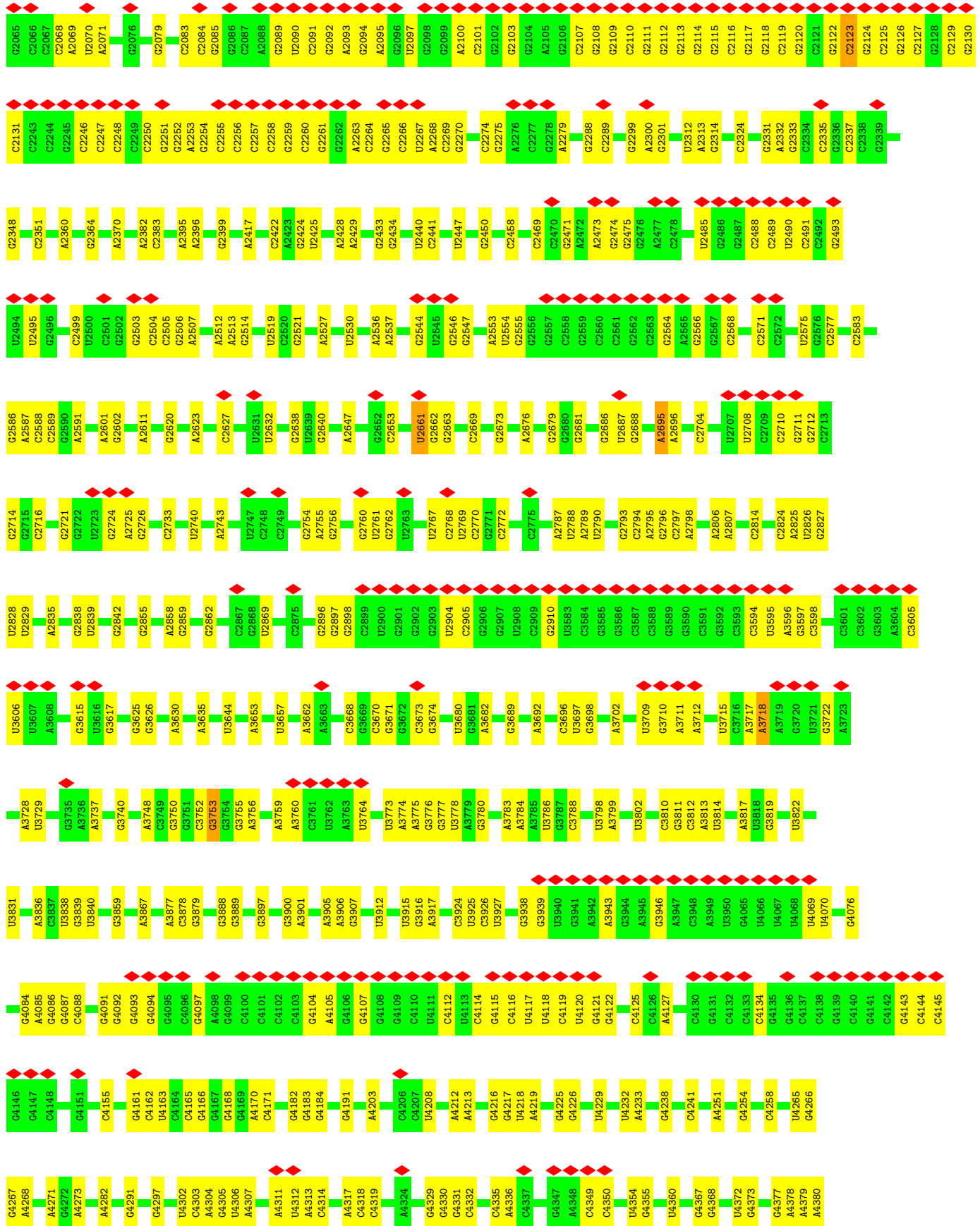
• Molecule 44: Ribosomal protein L12



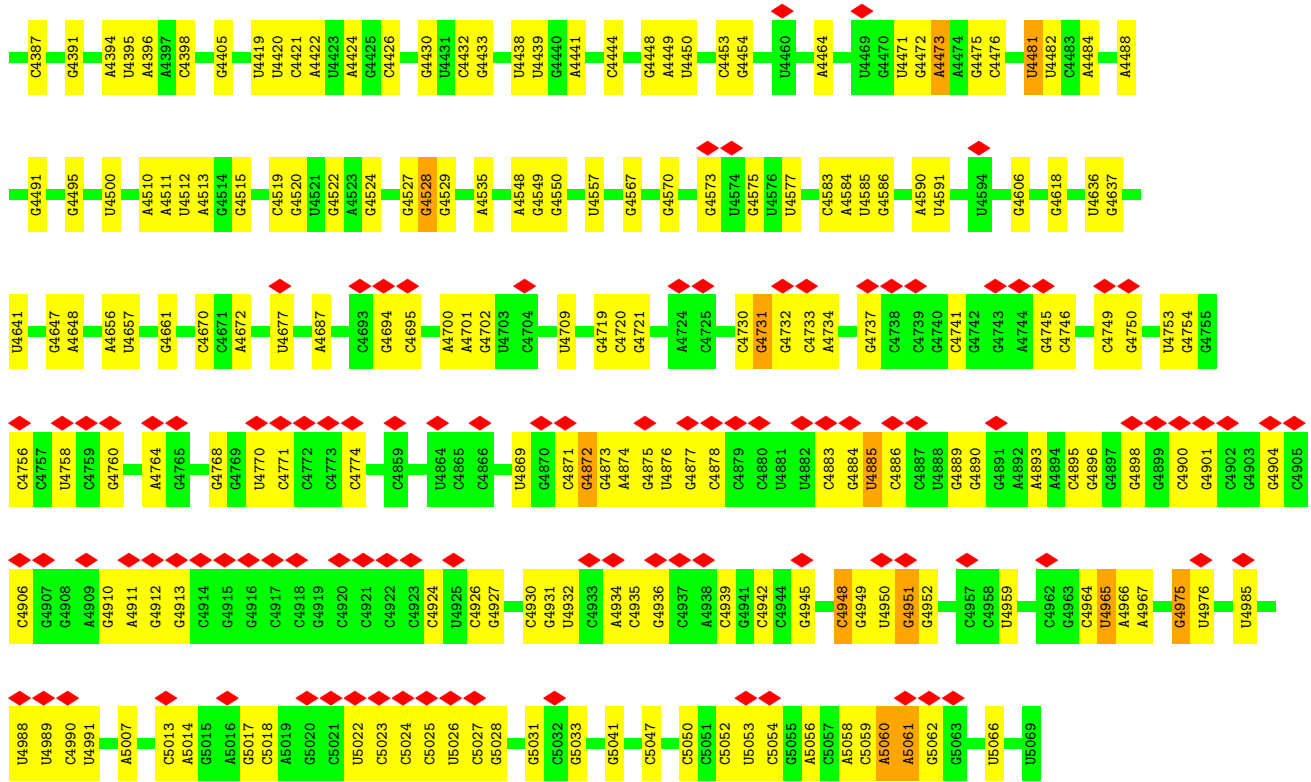
• Molecule 45: 28S rRNA



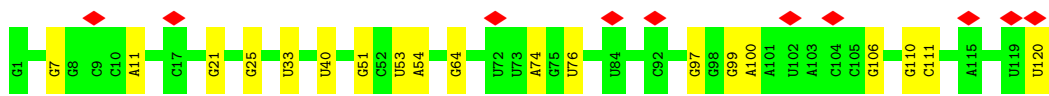
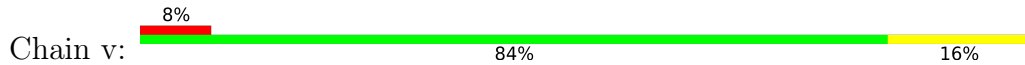




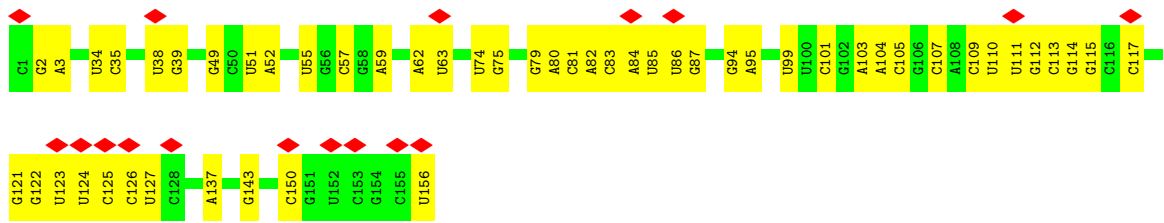




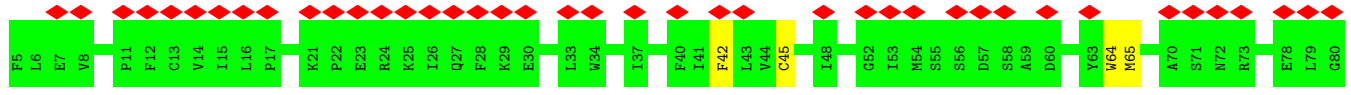
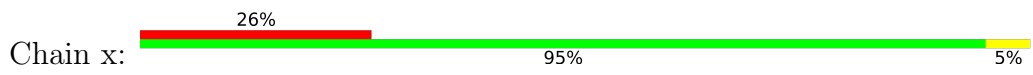
• Molecule 46: 5S ribosomal RNA

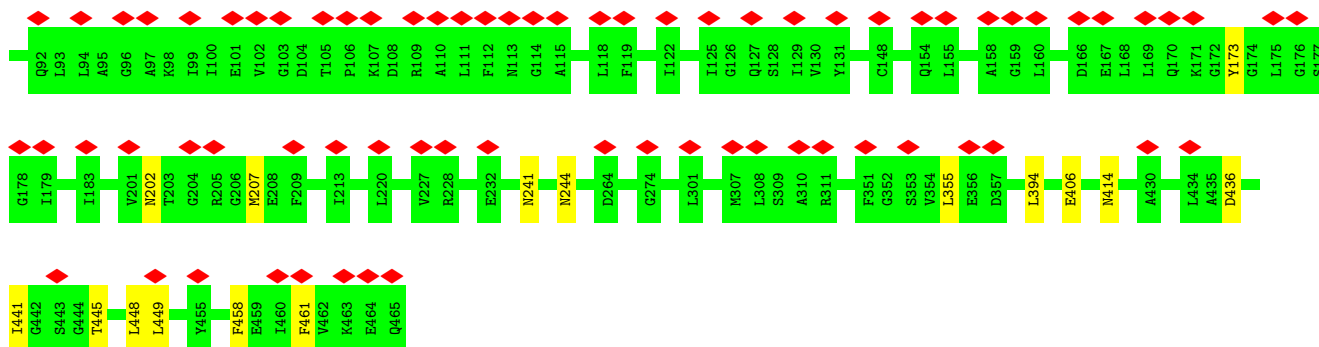


• Molecule 47: 5.8S ribosomal RNA

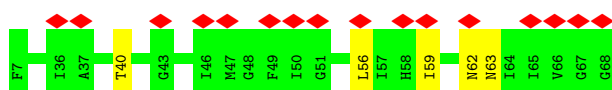
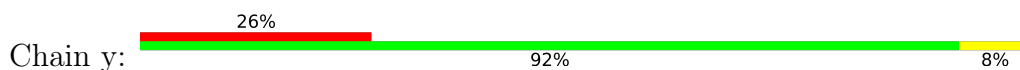


• Molecule 48: Protein transport protein Sec61 subunit alpha isoform 1

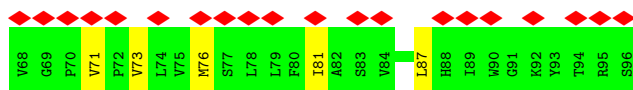
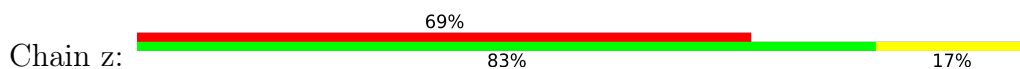




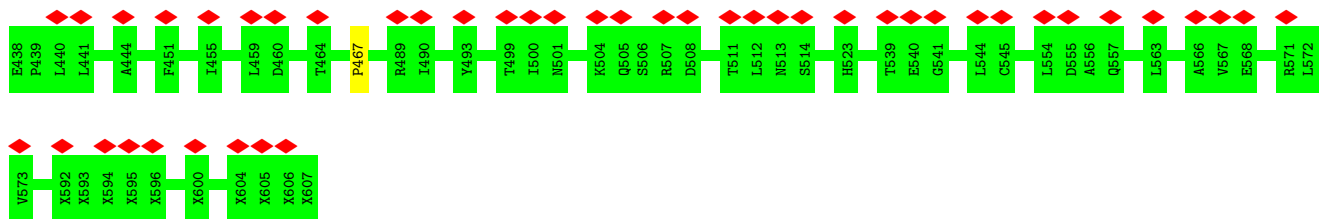
- Molecule 49: Protein transport protein Sec61 subunit gamma



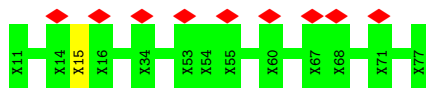
- Molecule 50: Protein transport protein Sec61 subunit beta



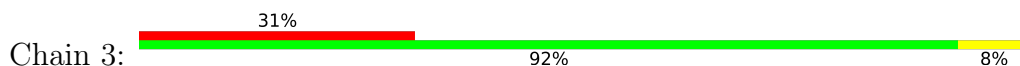
- Molecule 51: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1, RPN1

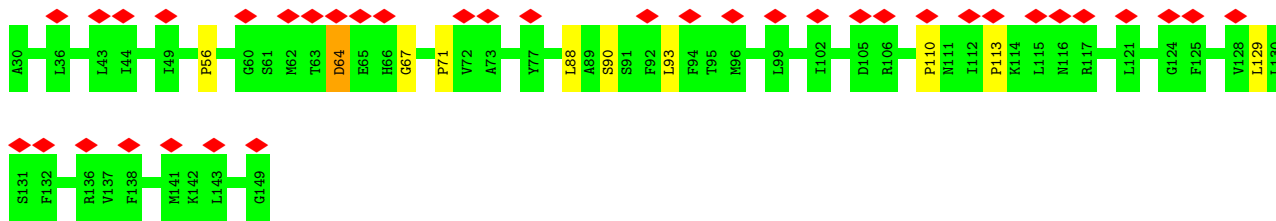


- Molecule 52: TMEM258

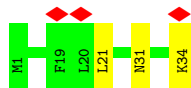
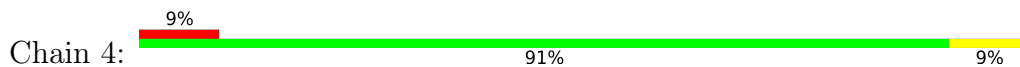


- Molecule 53: Oligosaccharyltransferase complex subunit OSTC

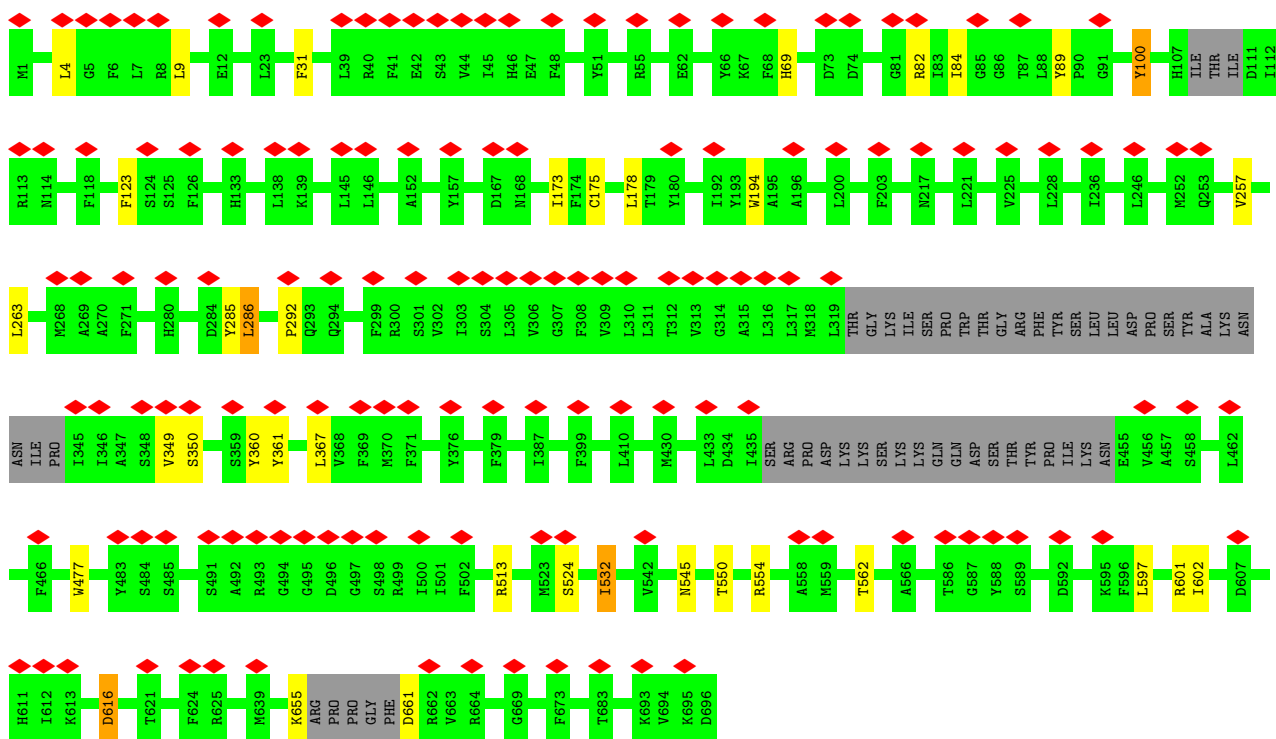
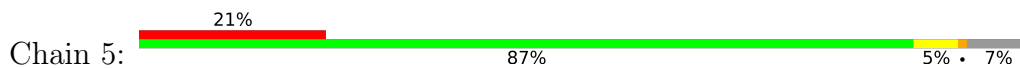




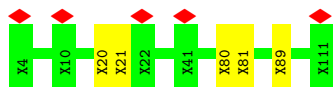
• Molecule 54: OST4



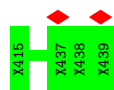
• Molecule 55: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3A



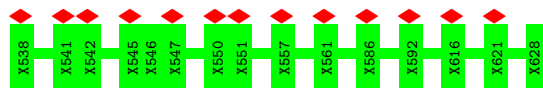
• Molecule 56: DAD1



• Molecule 57: OST48



- Molecule 58: RPN2



- Molecule 59: 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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90895	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	0.291	Depositor
Minimum map value	-0.169	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	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: MG, BMA, ZN, NAG, MAN, 9UB

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	u	0.41	11/87790 (0.0%)	0.80	94/136937 (0.1%)
46	v	0.31	0/2858	0.69	0/4455
47	w	0.36	0/3701	0.74	0/5766
48	x	0.52	0/3383	0.79	3/4584 (0.1%)
49	y	0.49	0/504	0.76	1/673 (0.1%)
50	z	0.42	0/236	0.74	0/321
51	1	0.39	0/757	0.53	1/1052 (0.1%)
53	3	0.57	0/815	0.89	5/1107 (0.5%)
54	4	0.52	0/273	0.66	0/371
55	5	0.66	5/5224 (0.1%)	0.86	17/7093 (0.2%)
All	All	0.42	16/161608 (0.0%)	0.79	147/237302 (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
19	T	0	1
20	U	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
24	Y	0	1
31	f	0	1
42	r	0	2
45	u	0	1
48	x	0	2
52	2	0	1
53	3	0	2
55	5	0	6
56	6	0	5
All	All	0	41

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	u	680	G	O3'-P	-33.63	1.20	1.61
45	u	692	A	O3'-P	32.98	2.00	1.61
45	u	1965	G	O3'-P	-23.04	1.33	1.61
45	u	472	C	O3'-P	-19.63	1.37	1.61
55	5	545	ASN	C-N	-18.35	0.91	1.34
55	5	550	THR	C-N	-16.38	0.96	1.34
45	u	197	A	O3'-P	13.18	1.76	1.61
55	5	513	ARG	C-N	10.49	1.58	1.34
45	u	462	G	O3'-P	-9.24	1.50	1.61
55	5	194	TRP	CB-CG	-7.09	1.37	1.50
45	u	223	G	O3'-P	-6.55	1.53	1.61
45	u	207	G	O3'-P	-6.23	1.53	1.61
45	u	1847	C	O3'-P	-6.12	1.53	1.61
45	u	957	G	O3'-P	5.59	1.67	1.61
55	5	477	TRP	CB-CG	-5.33	1.40	1.50
45	u	1358	G	O3'-P	5.09	1.67	1.61

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	5	545	ASN	C-N-CA	-16.91	79.43	121.70
45	u	462	G	P-O3'-C3'	-16.27	100.18	119.70
55	5	545	ASN	O-C-N	14.89	146.53	122.70
45	u	680	G	O3'-P-O5'	14.37	131.31	104.00
55	5	545	ASN	CA-C-N	-13.11	88.36	117.20
45	u	3753	G	N9-C1'-C2'	-11.93	98.49	114.00
45	u	197	A	P-O3'-C3'	11.51	133.51	119.70
45	u	220	C	N1-C1'-C2'	-11.09	99.58	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	u	3718	A	N9-C1'-C2'	-10.28	100.64	114.00
55	5	550	THR	O-C-N	-10.25	106.30	122.70
45	u	1358	G	C4'-C3'-O3'	10.20	133.39	113.00
45	u	1357	C	C4'-C3'-O3'	9.69	132.38	113.00
55	5	513	ARG	O-C-N	-9.14	108.08	122.70
24	Y	87	ARG	NE-CZ-NH2	9.13	124.86	120.30
45	u	223	G	P-O3'-C3'	9.04	130.55	119.70
45	u	692	A	P-O3'-C3'	8.98	130.48	119.70
48	x	449	LEU	CA-CB-CG	-8.96	94.69	115.30
45	u	4975	G	C2'-C3'-O3'	8.96	129.20	109.50
22	W	44	ARG	NE-CZ-NH1	8.60	124.60	120.30
45	u	90	G	C2'-C3'-O3'	8.39	127.95	109.50
45	u	4528	G	C2'-C3'-O3'	8.35	127.88	109.50
45	u	3888	G	C2'-C3'-O3'	8.31	127.78	109.50
45	u	1969	G	N9-C1'-C2'	-8.26	102.91	112.00
45	u	4948	C	C2'-C3'-O3'	8.05	127.22	109.50
18	S	83	ARG	NE-CZ-NH2	7.99	124.30	120.30
45	u	220	C	C2'-C3'-O3'	7.99	127.08	109.50
45	u	1211	G	C2'-C3'-O3'	7.96	127.00	109.50
45	u	3697	U	C2'-C3'-O3'	7.91	126.91	109.50
35	j	63	ARG	NE-CZ-NH1	7.88	124.24	120.30
45	u	1455	G	C2'-C3'-O3'	7.77	126.59	109.50
45	u	2858	A	N9-C1'-C2'	-7.63	103.60	112.00
3	C	342	ARG	NE-CZ-NH1	7.62	124.11	120.30
45	u	2858	A	C4'-C3'-O3'	7.62	128.24	113.00
45	u	1292	C	C2'-C3'-O3'	7.53	126.06	109.50
45	u	3718	A	C4'-C3'-O3'	7.50	127.99	113.00
55	5	532	ILE	O-C-N	-7.49	110.72	122.70
45	u	275	C	C2'-C3'-O3'	7.35	125.66	109.50
45	u	5060	A	C2'-C3'-O3'	7.33	125.62	109.50
45	u	125	C	C2'-C3'-O3'	7.33	125.61	109.50
45	u	2797	C	N1-C1'-C2'	-7.28	103.99	112.00
45	u	1477	C	C2'-C3'-O3'	7.28	125.52	109.50
45	u	5061	A	C2'-C3'-O3'	7.20	125.34	109.50
45	u	47	A	C4'-C3'-O3'	7.19	127.38	113.00
45	u	2027	U	N1-C1'-C2'	-7.16	104.12	112.00
45	u	2695	A	C2'-C3'-O3'	7.15	125.22	109.50
45	u	5059	C	C2'-C3'-O3'	7.15	125.22	109.50
45	u	406	C	C2'-C3'-O3'	7.14	125.20	109.50
55	5	550	THR	C-N-CA	7.04	139.30	121.70
55	5	550	THR	CA-C-N	7.02	132.65	117.20
55	5	350	SER	C-N-CA	-7.01	104.18	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	u	209	U	O4'-C1'-N1	6.97	113.78	108.20
45	u	1485	C	C2'-C3'-O3'	6.93	124.78	113.70
45	u	462	G	OP1-P-O3'	-6.80	90.23	105.20
45	u	1279	A	C2'-C3'-O3'	6.79	124.57	113.70
45	u	2046	G	C2'-C3'-O3'	6.78	124.54	113.70
45	u	1236	C	C2'-C3'-O3'	6.71	124.43	113.70
45	u	977	C	C2'-C3'-O3'	6.68	124.39	113.70
45	u	692	A	OP1-P-O3'	6.67	119.88	105.20
55	5	257	VAL	N-CA-C	-6.67	93.01	111.00
45	u	4885	U	C2'-C3'-O3'	6.66	124.36	113.70
45	u	93	G	C4'-C3'-O3'	6.65	126.30	113.00
45	u	1818	G	C2'-C3'-O3'	6.54	124.16	113.70
34	i	25	ARG	NE-CZ-NH1	6.50	123.55	120.30
45	u	209	U	C4'-C3'-O3'	6.44	125.89	113.00
45	u	2083	C	C4'-C3'-O3'	6.42	125.85	113.00
4	D	22	ARG	NE-CZ-NH1	6.41	123.51	120.30
45	u	93	G	N9-C1'-C2'	-6.39	104.97	112.00
45	u	3657	U	C2'-C3'-O3'	6.38	123.90	113.70
45	u	680	G	OP2-P-O3'	-6.33	91.28	105.20
5	E	208	LEU	CA-CB-CG	6.33	129.85	115.30
45	u	1474	C	C2'-C3'-O3'	6.31	123.80	113.70
48	x	448	LEU	CA-CB-CG	6.30	129.78	115.30
45	u	1398	A	C2'-C3'-O3'	6.28	123.74	113.70
45	u	1500	A	C2'-C3'-O3'	6.26	123.72	113.70
45	u	1969	G	C4'-C3'-O3'	6.24	125.48	113.00
45	u	2123	C	C2'-C3'-O3'	6.23	123.67	113.70
45	u	1380	G	N9-C1'-C2'	6.20	122.06	114.00
45	u	1239	C	C2'-C3'-O3'	6.20	123.61	113.70
45	u	2632	U	N1-C1'-C2'	6.17	122.02	114.00
45	u	1072	C	N1-C1'-C2'	6.08	121.90	114.00
55	5	349	VAL	N-CA-C	-6.07	94.60	111.00
45	u	1672	U	N1-C1'-C2'	6.04	121.85	114.00
53	3	71	PRO	N-CA-CB	6.02	110.52	103.30
45	u	1848	C	C2'-C3'-O3'	6.00	123.30	113.70
45	u	462	G	O3'-P-O5'	5.96	115.31	104.00
45	u	1390	G	C2'-C3'-O3'	5.93	123.19	113.70
29	d	78	ARG	NE-CZ-NH1	5.92	123.26	120.30
34	i	85	ARG	NE-CZ-NH1	5.91	123.26	120.30
55	5	513	ARG	CA-C-N	5.90	130.18	117.20
45	u	1696	C	C2'-C3'-O3'	5.89	123.13	113.70
45	u	1965	G	P-O3'-C3'	5.86	126.73	119.70
51	1	467	PRO	N-CA-CB	5.83	110.30	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	104	ARG	NE-CZ-NH1	5.81	123.21	120.30
5	E	72	PRO	N-CA-CB	5.80	110.26	103.30
45	u	978	G	C2'-C3'-O3'	5.80	122.97	113.70
49	y	56	LEU	CA-CB-CG	5.79	128.61	115.30
45	u	4951	G	C2'-C3'-O3'	5.78	122.95	113.70
45	u	4872	G	C2'-C3'-O3'	5.78	122.94	113.70
45	u	1329	G	C2'-C3'-O3'	5.76	122.92	113.70
45	u	4975	G	C4'-C3'-O3'	-5.73	97.36	109.40
53	3	110	PRO	N-CA-CB	5.67	110.10	103.30
3	C	98	GLY	N-CA-C	-5.64	99.01	113.10
18	S	83	ARG	NE-CZ-NH1	-5.62	117.49	120.30
53	3	56	PRO	N-CA-CB	5.55	109.96	103.30
6	F	91	LEU	CA-CB-CG	5.55	128.06	115.30
55	5	286	LEU	C-N-CA	-5.52	107.89	121.70
2	B	36	ASP	C-N-CD	5.52	140.00	128.40
45	u	687	U	N1-C1'-C2'	-5.48	105.97	112.00
45	u	4473	A	N9-C1'-C2'	5.46	121.10	114.00
45	u	2054	U	N1-C1'-C2'	5.46	121.10	114.00
53	3	113	PRO	N-CA-CB	5.46	109.85	103.30
45	u	979	C	C2'-C3'-O3'	5.45	122.43	113.70
45	u	210	C	N1-C1'-C2'	5.44	121.08	114.00
45	u	2028	C	N1-C1'-C2'	-5.43	106.03	112.00
45	u	957	G	P-O3'-C3'	5.38	126.16	119.70
45	u	1365	C	C4'-C3'-O3'	5.38	123.77	113.00
55	5	292	PRO	N-CA-CB	5.37	109.74	103.30
45	u	215	C	C4'-C3'-O3'	-5.36	98.14	109.40
24	Y	75	ARG	NE-CZ-NH1	5.35	122.97	120.30
45	u	212	A	N9-C1'-C2'	5.35	120.95	114.00
55	5	4	LEU	CA-CB-CG	5.33	127.55	115.30
45	u	486	C	C2'-C3'-O3'	5.30	122.18	113.70
45	u	1266	G	C2'-C3'-O3'	5.29	122.17	113.70
33	h	22	ASP	CB-CG-OD2	5.28	123.05	118.30
55	5	513	ARG	C-N-CA	5.26	134.85	121.70
3	C	262	ASP	CB-CG-OD2	5.25	123.02	118.30
45	u	3715	U	N1-C1'-C2'	-5.24	106.23	112.00
45	u	2586	G	N9-C1'-C2'	5.23	120.80	114.00
18	S	83	ARG	CG-CD-NE	5.22	122.76	111.80
45	u	223	G	N9-C1'-C2'	-5.20	106.28	112.00
53	3	129	LEU	CA-CB-CG	5.17	127.19	115.30
7	G	231	ASP	CB-CG-OD2	5.15	122.93	118.30
45	u	2661	U	C2'-C3'-O3'	5.13	121.91	113.70
32	g	66	ARG	NE-CZ-NH1	5.12	122.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	r	17	LEU	CA-CB-CG	5.11	127.06	115.30
45	u	4731	G	N9-C1'-C2'	5.10	120.63	114.00
45	u	4481	U	C5'-C4'-O4'	5.09	115.21	109.10
55	5	100	TYR	CA-CB-CG	5.09	123.07	113.40
45	u	4965	U	C2'-C3'-O3'	5.07	121.81	113.70
39	n	21	ARG	NE-CZ-NH2	-5.06	117.77	120.30
45	u	1755	C	C2'-C3'-O3'	5.06	121.79	113.70
48	x	394	LEU	CA-CB-CG	-5.05	103.68	115.30
45	u	680	G	P-O3'-C3'	-5.04	113.65	119.70
3	C	67	TRP	N-CA-C	-5.03	97.42	111.00
3	C	45	ARG	NE-CZ-NH1	5.01	122.81	120.30
45	u	286	U	N1-C1'-C2'	5.00	120.50	114.00
45	u	2246	C	C2'-C3'-O3'	5.00	121.71	113.70

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
52	2	15	UNK	Peptide
53	3	64	ASP	Peptide
53	3	67	GLY	Peptide
55	5	100	TYR	Peptide
55	5	263	LEU	Peptide
55	5	532	ILE	Mainchain
55	5	616	ASP	Peptide
55	5	655	LYS	Peptide
55	5	69	HIS	Peptide
56	6	20	UNK	Peptide
56	6	21	UNK	Peptide
56	6	80	UNK	Peptide
56	6	81	UNK	Peptide
56	6	89	UNK	Peptide
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
3	C	245	HIS	Peptide
3	C	339	THR	Peptide
4	D	36	LEU	Peptide
5	E	123	SER	Peptide
7	G	238	GLY	Peptide

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Mol	Chain	Res	Type	Group
9	I	188	LYS	Peptide
9	I	202	ASN	Peptide
11	L	27	ASN	Peptide
11	L	46	ILE	Peptide
11	L	66	TYR	Peptide
17	R	19	LYS	Peptide
18	S	163	HIS	Peptide
18	S	164	LYS	Peptide
19	T	26	PRO	Peptide
20	U	27	HIS	Peptide
24	Y	7	VAL	Peptide
31	f	105	LEU	Peptide
42	r	106	LEU	Peptide
42	r	70	GLN	Peptide
45	u	2793	G	Sidechain
48	x	173	TYR	Peptide
48	x	42	PHE	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%)	7	38
2	B	392/394 (100%)	345 (88%)	42 (11%)	5 (1%)	12	48
3	C	360/362 (99%)	322 (89%)	27 (8%)	11 (3%)	4	30
4	D	290/292 (99%)	262 (90%)	25 (9%)	3 (1%)	15	54
5	E	232/248 (94%)	179 (77%)	36 (16%)	17 (7%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	223/225 (99%)	204 (92%)	17 (8%)	2 (1%)	17	56
7	G	239/241 (99%)	203 (85%)	31 (13%)	5 (2%)	7	38
8	H	188/190 (99%)	166 (88%)	19 (10%)	3 (2%)	9	45
9	I	200/213 (94%)	181 (90%)	15 (8%)	4 (2%)	7	40
10	J	167/169 (99%)	147 (88%)	13 (8%)	7 (4%)	3	25
11	L	208/210 (99%)	180 (86%)	16 (8%)	12 (6%)	1	20
12	M	136/138 (99%)	123 (90%)	12 (9%)	1 (1%)	22	62
13	N	201/203 (99%)	181 (90%)	20 (10%)	0	100	100
14	O	197/199 (99%)	184 (93%)	12 (6%)	1 (0%)	29	68
15	P	151/153 (99%)	135 (89%)	16 (11%)	0	100	100
16	Q	185/187 (99%)	169 (91%)	14 (8%)	2 (1%)	14	52
17	R	178/180 (99%)	166 (93%)	9 (5%)	3 (2%)	9	43
18	S	173/175 (99%)	157 (91%)	12 (7%)	4 (2%)	6	36
19	T	157/159 (99%)	139 (88%)	15 (10%)	3 (2%)	8	40
20	U	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	3	25
21	V	129/131 (98%)	115 (89%)	13 (10%)	1 (1%)	19	60
22	W	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	9	45
23	X	117/119 (98%)	109 (93%)	6 (5%)	2 (2%)	9	43
24	Y	132/134 (98%)	114 (86%)	17 (13%)	1 (1%)	19	60
25	Z	133/135 (98%)	113 (85%)	13 (10%)	7 (5%)	2	21
26	a	145/147 (99%)	122 (84%)	19 (13%)	4 (3%)	5	33
27	b	73/75 (97%)	67 (92%)	5 (7%)	1 (1%)	11	47
28	c	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
29	d	105/107 (98%)	91 (87%)	13 (12%)	1 (1%)	15	54
30	e	126/128 (98%)	115 (91%)	6 (5%)	5 (4%)	3	25
31	f	107/109 (98%)	94 (88%)	8 (8%)	5 (5%)	2	23
32	g	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	17	56
33	h	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	4	29
34	i	100/102 (98%)	92 (92%)	6 (6%)	2 (2%)	7	40
35	j	84/86 (98%)	71 (84%)	8 (10%)	5 (6%)	1	19
36	k	67/69 (97%)	56 (84%)	7 (10%)	4 (6%)	1	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	l	48/50 (96%)	40 (83%)	7 (15%)	1 (2%)	7	38
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%)	4	32
41	p	89/91 (98%)	80 (90%)	8 (9%)	1 (1%)	14	52
42	r	132/136 (97%)	113 (86%)	12 (9%)	7 (5%)	2	21
43	s	196/198 (99%)	164 (84%)	22 (11%)	10 (5%)	2	22
44	t	161/163 (99%)	102 (63%)	33 (20%)	26 (16%)	0	4
48	x	420/426 (99%)	373 (89%)	46 (11%)	1 (0%)	47	81
49	y	60/62 (97%)	52 (87%)	8 (13%)	0	100	100
50	z	27/29 (93%)	25 (93%)	1 (4%)	1 (4%)	3	27
51	1	134/162 (83%)	129 (96%)	5 (4%)	0	100	100
53	3	118/120 (98%)	99 (84%)	18 (15%)	1 (1%)	19	60
54	4	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
55	5	632/696 (91%)	538 (85%)	88 (14%)	6 (1%)	17	56
All	All	8141/8362 (97%)	7150 (88%)	798 (10%)	193 (2%)	9	35

All (193) 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	E	175	LEU
5	E	221	PRO
7	G	45	ILE
7	G	128	VAL
8	H	40	HIS
8	H	110	SER
9	I	47	PRO
11	L	64	VAL
11	L	67	HIS
17	R	36	ASN
18	S	165	PRO
20	U	47	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	Z	84	ARG
26	a	90	ALA
29	d	94	GLU
30	e	92	ASN
31	f	80	ASN
33	h	7	ARG
36	k	61	PRO
40	o	32	SER
42	r	86	ALA
43	s	62	ARG
43	s	201	PRO
44	t	29	ALA
44	t	30	PRO
44	t	31	LYS
44	t	53	TRP
44	t	89	PRO
44	t	144	ASP
44	t	148	PRO
44	t	149	HIS
48	x	445	THR
55	5	84	ILE
55	5	89	TYR
1	A	217	GLN
2	B	38	SER
2	B	302	ASN
3	C	73	VAL
3	C	155	GLU
3	C	275	SER
4	D	187	SER
5	E	85	LEU
5	E	92	VAL
5	E	174	PRO
5	E	234	GLU
10	J	116	GLY
10	J	155	HIS
11	L	63	THR
11	L	143	GLU
11	L	172	GLU
17	R	130	ASN
18	S	88	SER
19	T	81	LYS
20	U	98	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
23	X	131	ASP
25	Z	34	SER
26	a	76	ASP
30	e	44	ARG
34	i	11	LEU
35	j	36	LYS
35	j	39	TYR
42	r	67	ARG
42	r	71	ARG
43	s	70	GLU
43	s	106	LYS
43	s	109	ALA
44	t	5	PHE
44	t	26	SER
44	t	39	PRO
44	t	58	ILE
44	t	106	PHE
55	5	360	TYR
55	5	361	TYR
2	B	18	PRO
3	C	16	GLU
3	C	132	ALA
3	C	248	ARG
5	E	96	LYS
5	E	179	ARG
5	E	232	GLU
6	F	239	GLU
9	I	205	PRO
10	J	11	PRO
10	J	146	ARG
16	Q	14	ARG
17	R	19	LYS
21	V	14	PHE
25	Z	55	ALA
25	Z	124	THR
26	a	92	LYS
30	e	125	PRO
30	e	126	ASN
31	f	37	ASP
31	f	79	GLY
33	h	97	LYS
34	i	3	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	k	32	VAL
37	l	47	THR
42	r	19	LYS
42	r	85	ASN
43	s	69	LEU
43	s	108	PRO
43	s	142	GLY
44	t	54	LYS
44	t	67	ARG
44	t	105	THR
44	t	137	GLN
53	3	64	ASP
55	5	661	ASP
1	A	180	LEU
2	B	54	THR
5	E	129	PHE
5	E	224	GLN
8	H	101	ILE
11	L	5	ARG
11	L	52	SER
19	T	29	THR
24	Y	83	GLU
25	Z	31	ASP
26	a	98	ALA
30	e	89	LEU
32	g	65	MET
33	h	89	ARG
36	k	29	LYS
41	p	41	PHE
44	t	2	PRO
44	t	18	THR
1	A	130	SER
2	B	309	LEU
4	D	20	PHE
5	E	218	LEU
5	E	229	PHE
7	G	123	ALA
7	G	125	LYS
10	J	153	ALA
11	L	6	ASN
11	L	103	ARG
16	Q	148	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
20	U	27	HIS
25	Z	91	LEU
31	f	107	PRO
33	h	40	ALA
35	j	34	CYS
35	j	61	THR
36	k	21	LYS
40	o	77	CYS
42	r	11	ARG
43	s	34	ASN
44	t	7	PRO
55	5	616	ASP
1	A	67	TYR
3	C	222	ARG
3	C	309	ILE
10	J	124	GLY
11	L	100	PRO
11	L	169	ILE
14	O	49	ARG
18	S	5	GLY
20	U	67	LYS
22	W	15	PRO
31	f	106	TYR
35	j	60	GLY
40	o	33	LEU
44	t	10	ILE
44	t	19	GLY
44	t	22	VAL
3	C	133	LEU
9	I	99	ILE
27	b	21	ILE
43	s	73	PRO
4	D	125	VAL
11	L	134	PRO
25	Z	90	PRO
3	C	265	GLY
5	E	103	VAL
6	F	230	VAL
7	G	238	GLY
9	I	201	PRO
19	T	44	GLY
10	J	174	ILE

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Mol	Chain	Res	Type
12	M	7	VAL
18	S	155	PRO
44	t	3	PRO
44	t	98	ILE
23	X	119	ILE
42	r	69	GLY
44	t	23	GLY
50	z	71	VAL

### 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
1	A	187/187 (100%)	161 (86%)	26 (14%)	3 19
2	B	336/342 (98%)	291 (87%)	45 (13%)	4 20
3	C	302/302 (100%)	260 (86%)	42 (14%)	3 19
4	D	247/247 (100%)	218 (88%)	29 (12%)	5 23
5	E	208/221 (94%)	185 (89%)	23 (11%)	6 25
6	F	194/195 (100%)	165 (85%)	29 (15%)	3 16
7	G	206/206 (100%)	182 (88%)	24 (12%)	5 23
8	H	169/169 (100%)	148 (88%)	21 (12%)	4 21
9	I	174/180 (97%)	153 (88%)	21 (12%)	5 22
10	J	142/142 (100%)	126 (89%)	16 (11%)	6 24
11	L	176/176 (100%)	145 (82%)	31 (18%)	2 12
12	M	117/117 (100%)	102 (87%)	15 (13%)	4 21
13	N	171/171 (100%)	152 (89%)	19 (11%)	6 25
14	O	171/171 (100%)	144 (84%)	27 (16%)	2 15
15	P	134/134 (100%)	120 (90%)	14 (10%)	7 27
16	Q	163/163 (100%)	145 (89%)	18 (11%)	6 25
17	R	159/159 (100%)	140 (88%)	19 (12%)	5 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	S	156/156 (100%)	132 (85%)	24 (15%)	2	16
19	T	139/139 (100%)	122 (88%)	17 (12%)	5	22
20	U	89/89 (100%)	82 (92%)	7 (8%)	12	38
21	V	101/101 (100%)	84 (83%)	17 (17%)	2	13
22	W	55/55 (100%)	50 (91%)	5 (9%)	9	32
23	X	107/107 (100%)	97 (91%)	10 (9%)	9	30
24	Y	124/124 (100%)	107 (86%)	17 (14%)	3	19
25	Z	117/117 (100%)	109 (93%)	8 (7%)	16	42
26	a	119/119 (100%)	107 (90%)	12 (10%)	7	27
27	b	62/62 (100%)	57 (92%)	5 (8%)	11	37
28	c	79/79 (100%)	66 (84%)	13 (16%)	2	14
29	d	98/98 (100%)	82 (84%)	16 (16%)	2	14
30	e	114/114 (100%)	99 (87%)	15 (13%)	4	20
31	f	88/88 (100%)	76 (86%)	12 (14%)	3	19
32	g	98/98 (100%)	83 (85%)	15 (15%)	2	16
33	h	109/109 (100%)	97 (89%)	12 (11%)	6	25
34	i	86/86 (100%)	81 (94%)	5 (6%)	20	47
35	j	73/73 (100%)	62 (85%)	11 (15%)	3	16
36	k	64/64 (100%)	56 (88%)	8 (12%)	4	21
37	l	47/47 (100%)	40 (85%)	7 (15%)	3	16
38	m	48/48 (100%)	39 (81%)	9 (19%)	1	10
39	n	22/22 (100%)	18 (82%)	4 (18%)	1	11
40	o	92/92 (100%)	79 (86%)	13 (14%)	3	18
41	p	74/74 (100%)	68 (92%)	6 (8%)	11	37
42	r	120/120 (100%)	96 (80%)	24 (20%)	1	8
43	s	166/166 (100%)	156 (94%)	10 (6%)	19	46
44	t	136/136 (100%)	128 (94%)	8 (6%)	19	47
48	x	360/362 (99%)	346 (96%)	14 (4%)	32	57
49	y	53/53 (100%)	49 (92%)	4 (8%)	13	40
50	z	26/26 (100%)	22 (85%)	4 (15%)	2	16
51	1	20/122 (16%)	20 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	3	61/101 (60%)	58 (95%)	3 (5%)	25	51
54	4	30/30 (100%)	27 (90%)	3 (10%)	7	28
55	5	528/607 (87%)	512 (97%)	16 (3%)	41	63
All	All	6917/7166 (96%)	6144 (89%)	773 (11%)	9	24

All (773) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	44	ILE
1	A	49	ILE
1	A	64	ARG
1	A	82	ILE
1	A	96	LEU
1	A	97	ASN
1	A	102	LEU
1	A	125	LYS
1	A	128	ARG
1	A	142	GLU
1	A	158	ILE
1	A	163	ARG
1	A	175	ILE
1	A	180	LEU
1	A	193	ARG
1	A	194	ASN
1	A	200	ARG
1	A	207	VAL
1	A	218	HIS
1	A	221	LYS
1	A	226	ARG
1	A	227	ARG
1	A	233	ARG
1	A	235	VAL
1	A	242	ARG
2	B	4	ARG
2	B	10	ARG
2	B	17	LEU
2	B	19	ARG
2	B	21	ARG
2	B	31	SER
2	B	43	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	56	ILE
2	B	61	ASP
2	B	62	ARG
2	B	66	LYS
2	B	67	VAL
2	B	90	VAL
2	B	97	ARG
2	B	99	LEU
2	B	101	THR
2	B	103	LYS
2	B	115	LYS
2	B	116	ARG
2	B	135	LYS
2	B	138	GLN
2	B	146	LEU
2	B	162	VAL
2	B	167	GLN
2	B	173	LEU
2	B	203	GLN
2	B	213	GLN
2	B	214	ASP
2	B	228	TYR
2	B	244	THR
2	B	248	LEU
2	B	258	HIS
2	B	261	ARG
2	B	262	VAL
2	B	309	LEU
2	B	314	ILE
2	B	329	ASP
2	B	333	LEU
2	B	340	THR
2	B	352	LEU
2	B	356	LYS
2	B	357	ARG
2	B	366	LYS
2	B	381	THR
2	B	383	GLU
3	C	14	LYS
3	C	20	LYS
3	C	44	LEU
3	C	54	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	55	SER
3	C	57	LEU
3	C	66	SER
3	C	71	ARG
3	C	80	ARG
3	C	95	MET
3	C	101	MET
3	C	113	ARG
3	C	114	ARG
3	C	122	TYR
3	C	124	ILE
3	C	144	ILE
3	C	147	VAL
3	C	150	LEU
3	C	155	GLU
3	C	159	GLU
3	C	165	LYS
3	C	175	LYS
3	C	179	ASP
3	C	188	ARG
3	C	193	LYS
3	C	204	ARG
3	C	208	CYS
3	C	222	ARG
3	C	232	VAL
3	C	237	ILE
3	C	246	VAL
3	C	267	TRP
3	C	281	MET
3	C	284	MET
3	C	287	THR
3	C	294	LYS
3	C	307	LYS
3	C	312	ARG
3	C	333	LYS
3	C	342	ARG
3	C	345	ARG
3	C	348	LYS
4	D	4	VAL
4	D	22	ARG
4	D	33	ARG
4	D	37	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	D	50	ARG
4	D	66	TYR
4	D	89	LYS
4	D	94	ASN
4	D	104	LEU
4	D	110	LEU
4	D	111	ASN
4	D	124	GLU
4	D	128	ASP
4	D	152	ARG
4	D	179	ARG
4	D	189	GLU
4	D	196	ARG
4	D	202	GLN
4	D	206	ASP
4	D	208	MET
4	D	225	GLN
4	D	234	ASP
4	D	248	ARG
4	D	249	GLU
4	D	256	LYS
4	D	264	LYS
4	D	268	ARG
4	D	279	ARG
4	D	293	ARG
5	E	43	ASN
5	E	46	LEU
5	E	52	ARG
5	E	55	ARG
5	E	58	MET
5	E	101	ARG
5	E	105	LEU
5	E	126	ARG
5	E	134	ARG
5	E	136	LEU
5	E	137	ARG
5	E	148	ILE
5	E	162	LYS
5	E	190	VAL
5	E	197	ILE
5	E	206	LYS
5	E	212	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	E	230	ASP
5	E	233	LYS
5	E	250	ASP
5	E	254	LEU
5	E	282	LEU
5	E	284	PHE
6	F	33	LYS
6	F	41	GLN
6	F	44	LEU
6	F	49	ARG
6	F	68	ARG
6	F	70	GLU
6	F	72	ARG
6	F	76	MET
6	F	82	ASN
6	F	90	LYS
6	F	91	LEU
6	F	100	ILE
6	F	101	ASN
6	F	127	LEU
6	F	137	ILE
6	F	154	GLU
6	F	179	ARG
6	F	181	LEU
6	F	189	MET
6	F	190	GLU
6	F	192	LEU
6	F	201	LYS
6	F	202	ARG
6	F	214	LYS
6	F	216	SER
6	F	234	ASP
6	F	239	GLU
6	F	248	ARG
6	F	249	MET
7	G	28	VAL
7	G	73	ARG
7	G	75	LYS
7	G	81	ASN
7	G	90	GLN
7	G	95	LEU
7	G	106	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	G	110	LYS
7	G	112	GLN
7	G	131	LYS
7	G	148	GLU
7	G	150	LYS
7	G	151	LYS
7	G	154	LEU
7	G	170	LEU
7	G	173	LEU
7	G	175	ARG
7	G	177	MET
7	G	189	ARG
7	G	202	VAL
7	G	210	GLU
7	G	217	LYS
7	G	220	GLU
7	G	240	ASN
8	H	1	MET
8	H	20	LEU
8	H	26	ILE
8	H	28	LYS
8	H	41	ILE
8	H	52	LYS
8	H	54	ARG
8	H	57	VAL
8	H	59	LYS
8	H	66	GLU
8	H	74	CYS
8	H	78	GLN
8	H	98	HIS
8	H	111	LEU
8	H	125	ARG
8	H	128	MET
8	H	129	ARG
8	H	162	GLN
8	H	173	ARG
8	H	177	ASP
8	H	183	GLU
9	I	13	LYS
9	I	35	ASP
9	I	36	LEU
9	I	39	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	I	43	VAL
9	I	48	LEU
9	I	76	MET
9	I	88	ARG
9	I	116	ARG
9	I	136	MET
9	I	139	ARG
9	I	144	ASN
9	I	153	ARG
9	I	163	GLN
9	I	164	LYS
9	I	180	GLU
9	I	195	CYS
9	I	198	LYS
9	I	202	ASN
9	I	208	LYS
9	I	212	LEU
10	J	15	LEU
10	J	16	ARG
10	J	33	LEU
10	J	34	THR
10	J	49	VAL
10	J	55	TYR
10	J	72	CYS
10	J	90	ARG
10	J	91	GLU
10	J	110	GLN
10	J	111	GLU
10	J	113	ILE
10	J	146	ARG
10	J	151	ILE
10	J	167	GLN
10	J	168	GLN
11	L	10	LEU
11	L	28	GLN
11	L	35	ARG
11	L	49	ARG
11	L	59	VAL
11	L	61	CYS
11	L	64	VAL
11	L	67	HIS
11	L	74	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	L	77	SER
11	L	92	ARG
11	L	94	ILE
11	L	99	ASP
11	L	107	THR
11	L	111	GLN
11	L	113	ASN
11	L	115	GLN
11	L	121	ARG
11	L	123	LYS
11	L	129	ARG
11	L	130	LYS
11	L	143	GLU
11	L	145	LYS
11	L	158	ARG
11	L	162	LYS
11	L	165	LYS
11	L	186	ARG
11	L	190	ARG
11	L	195	ARG
11	L	198	ARG
11	L	201	GLU
12	M	5	ARG
12	M	8	GLU
12	M	25	VAL
12	M	33	GLN
12	M	38	VAL
12	M	48	GLN
12	M	53	LYS
12	M	57	LEU
12	M	61	ILE
12	M	70	GLN
12	M	96	GLU
12	M	105	THR
12	M	118	MET
12	M	119	ARG
12	M	130	LEU
13	N	9	GLU
13	N	17	ASP
13	N	26	ARG
13	N	32	GLN
13	N	61	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
13	N	64	ILE
13	N	72	LYS
13	N	77	LYS
13	N	80	THR
13	N	87	HIS
13	N	89	VAL
13	N	104	GLU
13	N	108	ARG
13	N	136	ASP
13	N	147	ASP
13	N	174	LEU
13	N	197	THR
13	N	199	GLN
13	N	202	ARG
14	O	5	GLN
14	O	18	ARG
14	O	31	ARG
14	O	36	VAL
14	O	37	ARG
14	O	38	CYS
14	O	42	ASN
14	O	49	ARG
14	O	60	LYS
14	O	61	ARG
14	O	62	MET
14	O	67	SER
14	O	74	ARG
14	O	82	ARG
14	O	85	ARG
14	O	103	LYS
14	O	117	ARG
14	O	128	ARG
14	O	130	LYS
14	O	145	VAL
14	O	165	LYS
14	O	175	MET
14	O	179	LYS
14	O	187	LYS
14	O	195	VAL
14	O	201	PHE
14	O	202	LEU
15	P	5	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	P	7	ASP
15	P	25	HIS
15	P	57	CYS
15	P	69	ARG
15	P	86	LYS
15	P	91	LEU
15	P	92	LEU
15	P	99	GLU
15	P	100	SER
15	P	105	LYS
15	P	127	ARG
15	P	128	ARG
15	P	147	GLU
16	Q	13	VAL
16	Q	31	LEU
16	Q	37	ARG
16	Q	54	SER
16	Q	63	LEU
16	Q	75	ARG
16	Q	78	LYS
16	Q	85	THR
16	Q	89	ASP
16	Q	91	ARG
16	Q	93	GLN
16	Q	95	VAL
16	Q	97	LYS
16	Q	108	ARG
16	Q	112	ARG
16	Q	140	SER
16	Q	143	ARG
16	Q	187	LYS
17	R	10	LEU
17	R	15	LEU
17	R	39	GLN
17	R	40	GLN
17	R	43	LYS
17	R	50	ILE
17	R	52	ARG
17	R	75	HIS
17	R	89	MET
17	R	98	ARG
17	R	99	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	R	106	LEU
17	R	107	ARG
17	R	113	LYS
17	R	117	ARG
17	R	123	LEU
17	R	133	LYS
17	R	138	LEU
17	R	178	GLN
18	S	2	LYS
18	S	8	ARG
18	S	9	GLU
18	S	17	LEU
18	S	39	VAL
18	S	43	ARG
18	S	67	VAL
18	S	70	LYS
18	S	82	LEU
18	S	83	ARG
18	S	84	TYR
18	S	86	SER
18	S	91	HIS
18	S	95	ARG
18	S	98	ARG
18	S	100	LEU
18	S	102	THR
18	S	125	GLN
18	S	127	MET
18	S	132	ILE
18	S	147	ASP
18	S	149	LYS
18	S	156	HIS
18	S	159	LEU
19	T	5	LYS
19	T	9	ARG
19	T	17	ARG
19	T	33	ILE
19	T	41	ASP
19	T	52	MET
19	T	60	LYS
19	T	81	LYS
19	T	96	ILE
19	T	99	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
19	T	117	LYS
19	T	118	GLU
19	T	131	GLN
19	T	142	ARG
19	T	144	ASN
19	T	157	GLU
19	T	159	MET
20	U	33	ILE
20	U	46	ARG
20	U	65	ARG
20	U	67	LYS
20	U	80	LYS
20	U	97	ARG
20	U	99	TRP
21	V	15	ARG
21	V	18	LEU
21	V	31	ASN
21	V	35	LYS
21	V	46	LYS
21	V	51	ARG
21	V	57	VAL
21	V	60	MET
21	V	61	VAL
21	V	82	ILE
21	V	91	LYS
21	V	97	TYR
21	V	99	GLU
21	V	106	VAL
21	V	109	LYS
21	V	113	LYS
21	V	123	LYS
22	W	4	GLU
22	W	27	LYS
22	W	41	LEU
22	W	43	LYS
22	W	57	ARG
23	X	39	LYS
23	X	41	ARG
23	X	50	LYS
23	X	52	LEU
23	X	59	LYS
23	X	94	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
23	X	111	GLN
23	X	129	ARG
23	X	145	ASP
23	X	152	LYS
24	Y	2	LYS
24	Y	7	VAL
24	Y	8	THR
24	Y	28	LYS
24	Y	34	LEU
24	Y	50	ARG
24	Y	52	ASP
24	Y	55	VAL
24	Y	59	ARG
24	Y	65	GLN
24	Y	72	GLN
24	Y	74	TYR
24	Y	79	VAL
24	Y	87	ARG
24	Y	104	VAL
24	Y	115	ARG
24	Y	126	ARG
25	Z	11	VAL
25	Z	17	ARG
25	Z	57	MET
25	Z	59	LYS
25	Z	67	LYS
25	Z	93	LYS
25	Z	108	ARG
25	Z	112	ARG
26	a	10	LYS
26	a	12	ARG
26	a	39	HIS
26	a	40	HIS
26	a	46	ASP
26	a	47	LYS
26	a	52	TYR
26	a	59	ARG
26	a	63	LEU
26	a	84	GLU
26	a	122	VAL
26	a	132	ARG
27	b	22	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	b	28	ARG
27	b	39	PHE
27	b	43	MET
27	b	51	LYS
28	c	28	VAL
28	c	37	MET
28	c	40	GLN
28	c	50	ASN
28	c	59	GLU
28	c	61	GLU
28	c	77	ASN
28	c	78	ASN
28	c	81	LEU
28	c	87	LYS
28	c	91	VAL
28	c	94	LEU
28	c	98	ASP
29	d	19	GLU
29	d	23	ARG
29	d	26	THR
29	d	31	LYS
29	d	36	VAL
29	d	44	ARG
29	d	48	GLU
29	d	75	LYS
29	d	78	ARG
29	d	79	ASN
29	d	85	ARG
29	d	90	ARG
29	d	94	GLU
29	d	102	LEU
29	d	107	THR
29	d	116	ASN
30	e	11	LYS
30	e	21	ILE
30	e	22	ARG
30	e	24	GLN
30	e	30	LYS
30	e	32	LYS
30	e	46	ARG
30	e	48	ARG
30	e	64	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
30	e	78	LEU
30	e	91	CYS
30	e	104	SER
30	e	106	LYS
30	e	107	ASN
30	e	113	GLU
31	f	16	ARG
31	f	33	VAL
31	f	36	ARG
31	f	38	GLU
31	f	40	GLU
31	f	46	ARG
31	f	52	LYS
31	f	56	ASN
31	f	69	VAL
31	f	84	VAL
31	f	100	ARG
31	f	101	ILE
32	g	5	LEU
32	g	6	THR
32	g	11	LEU
32	g	14	ASN
32	g	15	THR
32	g	21	ARG
32	g	32	TYR
32	g	54	ARG
32	g	60	ARG
32	g	64	LEU
32	g	66	ARG
32	g	73	HIS
32	g	90	ARG
32	g	100	GLN
32	g	115	LYS
33	h	10	ARG
33	h	28	LEU
33	h	46	LYS
33	h	65	GLN
33	h	67	GLU
33	h	88	THR
33	h	89	ARG
33	h	97	LYS
33	h	104	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
33	h	117	ARG
33	h	121	VAL
33	h	122	LYS
34	i	33	LEU
34	i	86	LYS
34	i	87	ARG
34	i	89	GLU
34	i	103	LYS
35	j	2	THR
35	j	3	LYS
35	j	15	THR
35	j	20	ARG
35	j	25	LYS
35	j	29	LEU
35	j	33	THR
35	j	61	THR
35	j	63	ARG
35	j	68	LYS
35	j	79	ARG
36	k	18	LYS
36	k	29	LYS
36	k	31	ASN
36	k	37	ARG
36	k	39	SER
36	k	57	LYS
36	k	69	LEU
36	k	70	LYS
37	l	8	ARG
37	l	16	LYS
37	l	17	GLN
37	l	21	ARG
37	l	36	ARG
37	l	46	ARG
37	l	49	LEU
38	m	79	GLU
38	m	82	LEU
38	m	85	LEU
38	m	88	LYS
38	m	97	ARG
38	m	98	LYS
38	m	106	ARG
38	m	111	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
38	m	119	ASN
39	n	2	ARG
39	n	9	ARG
39	n	13	LEU
39	n	21	ARG
40	o	17	LYS
40	o	24	THR
40	o	26	TYR
40	o	31	ASP
40	o	33	LEU
40	o	36	GLN
40	o	55	ILE
40	o	61	LYS
40	o	69	ARG
40	o	82	MET
40	o	89	LYS
40	o	96	ASP
40	o	102	GLN
41	p	16	THR
41	p	24	LYS
41	p	49	ARG
41	p	54	ILE
41	p	60	CYS
41	p	84	ARG
42	r	17	LEU
42	r	18	ILE
42	r	20	ARG
42	r	21	ASN
42	r	24	THR
42	r	26	SER
42	r	28	GLU
42	r	31	ASN
42	r	32	LEU
42	r	37	SER
42	r	39	ARG
42	r	41	ASN
42	r	60	VAL
42	r	67	ARG
42	r	70	GLN
42	r	71	ARG
42	r	80	THR
42	r	103	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
42	r	107	ARG
42	r	108	MET
42	r	118	LEU
42	r	122	LYS
42	r	125	MET
42	r	135	LYS
43	s	38	LYS
43	s	44	ARG
43	s	62	ARG
43	s	68	HIS
43	s	94	ASP
43	s	146	LYS
43	s	149	ARG
43	s	174	LEU
43	s	185	PHE
43	s	191	GLN
44	t	1	MET
44	t	14	TYR
44	t	40	LYS
44	t	95	GLN
44	t	104	ILE
44	t	106	PHE
44	t	114	ARG
44	t	123	ARG
48	x	45	CYS
48	x	64	TRP
48	x	65	MET
48	x	202	ASN
48	x	207	MET
48	x	241	ASN
48	x	244	ASN
48	x	355	LEU
48	x	406	GLU
48	x	414	ASN
48	x	436	ASP
48	x	441	ILE
48	x	458	PHE
48	x	461	PHE
49	y	40	THR
49	y	59	ILE
49	y	62	ASN
49	y	63	ASN

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Mol	Chain	Res	Type
50	z	73	VAL
50	z	76	MET
50	z	81	ILE
50	z	87	LEU
53	3	88	LEU
53	3	90	SER
53	3	93	LEU
54	4	21	LEU
54	4	31	ASN
54	4	34	LYS
55	5	9	LEU
55	5	31	PHE
55	5	82	ARG
55	5	123	PHE
55	5	173	ILE
55	5	175	CYS
55	5	178	LEU
55	5	285	TYR
55	5	286	LEU
55	5	367	LEU
55	5	524	SER
55	5	554	ARG
55	5	562	THR
55	5	597	LEU
55	5	601	ARG
55	5	602	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
2	B	68	ASN
5	E	217	GLN
7	G	29	ASN
14	O	96	GLN
42	r	121	GLN
48	x	202	ASN
48	x	241	ASN
48	x	244	ASN
48	x	300	ASN
48	x	414	ASN
48	x	465	GLN

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Mol	Chain	Res	Type
49	y	63	ASN
54	4	12	ASN
55	5	46	HIS
55	5	168	ASN
55	5	217	ASN
55	5	222	HIS
55	5	352	HIS
55	5	531	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
45	u	3643/3662 (99%)	1188 (32%)	0
46	v	119/120 (99%)	19 (15%)	0
47	w	155/156 (99%)	52 (33%)	0
All	All	3917/3938 (99%)	1259 (32%)	0

All (1259) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
45	u	2	G
45	u	8	U
45	u	9	C
45	u	10	A
45	u	12	A
45	u	13	U
45	u	21	G
45	u	25	A
45	u	30	C
45	u	39	A
45	u	42	A
45	u	43	U
45	u	44	A
45	u	48	G
45	u	49	U
45	u	56	A
45	u	58	G
45	u	59	A
45	u	64	A
45	u	65	A
45	u	69	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	71	C
45	u	72	C
45	u	73	A
45	u	74	G
45	u	91	G
45	u	93	G
45	u	94	A
45	u	95	G
45	u	108	A
45	u	109	G
45	u	110	C
45	u	116	G
45	u	118	C
45	u	119	G
45	u	120	A
45	u	121	A
45	u	126	C
45	u	128	C
45	u	129	C
45	u	134	G
45	u	135	G
45	u	136	C
45	u	143	C
45	u	144	G
45	u	146	G
45	u	157	U
45	u	159	C
45	u	160	G
45	u	161	G
45	u	164	G
45	u	166	C
45	u	167	C
45	u	170	C
45	u	171	U
45	u	172	C
45	u	173	C
45	u	174	C
45	u	175	C
45	u	177	G
45	u	183	C
45	u	184	U
45	u	185	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	186	G
45	u	187	U
45	u	188	G
45	u	189	G
45	u	197	A
45	u	200	U
45	u	201	C
45	u	202	C
45	u	203	U
45	u	205	C
45	u	206	U
45	u	210	C
45	u	211	G
45	u	216	C
45	u	217	C
45	u	218	A
45	u	219	G
45	u	220	C
45	u	221	C
45	u	224	U
45	u	226	G
45	u	227	A
45	u	233	U
45	u	234	G
45	u	246	G
45	u	253	G
45	u	255	C
45	u	257	C
45	u	265	C
45	u	266	C
45	u	267	G
45	u	272	U
45	u	276	C
45	u	277	G
45	u	278	G
45	u	280	G
45	u	286	U
45	u	296	A
45	u	297	U
45	u	300	A
45	u	306	A
45	u	309	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	315	G
45	u	316	U
45	u	319	A
45	u	321	U
45	u	322	C
45	u	326	C
45	u	328	A
45	u	334	A
45	u	337	U
45	u	340	C
45	u	347	A
45	u	349	A
45	u	350	C
45	u	353	A
45	u	357	U
45	u	361	C
45	u	362	A
45	u	363	A
45	u	385	A
45	u	386	A
45	u	387	G
45	u	399	G
45	u	405	U
45	u	406	C
45	u	407	A
45	u	409	G
45	u	410	A
45	u	412	G
45	u	413	G
45	u	424	U
45	u	429	A
45	u	431	G
45	u	432	U
45	u	434	A
45	u	446	C
45	u	448	G
45	u	449	C
45	u	451	C
45	u	452	A
45	u	453	G
45	u	454	U
45	u	455	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	458	C
45	u	466	A
45	u	467	U
45	u	468	U
45	u	469	C
45	u	470	A
45	u	471	A
45	u	473	C
45	u	485	C
45	u	486	C
45	u	487	G
45	u	498	C
45	u	499	G
45	u	500	G
45	u	501	C
45	u	502	C
45	u	503	C
45	u	504	G
45	u	506	C
45	u	509	A
45	u	510	U
45	u	513	U
45	u	514	U
45	u	515	C
45	u	519	C
45	u	649	A
45	u	654	C
45	u	655	C
45	u	663	G
45	u	664	G
45	u	665	C
45	u	666	G
45	u	667	A
45	u	668	C
45	u	681	G
45	u	682	G
45	u	683	C
45	u	684	G
45	u	685	C
45	u	686	A
45	u	687	U
45	u	689	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	690	C
45	u	692	A
45	u	694	C
45	u	695	G
45	u	696	C
45	u	697	G
45	u	701	G
45	u	703	G
45	u	707	C
45	u	718	C
45	u	721	G
45	u	722	G
45	u	724	C
45	u	728	U
45	u	729	G
45	u	730	G
45	u	737	C
45	u	742	G
45	u	745	G
45	u	746	A
45	u	747	A
45	u	748	G
45	u	749	G
45	u	756	G
45	u	911	U
45	u	914	U
45	u	915	A
45	u	917	A
45	u	918	G
45	u	919	C
45	u	920	C
45	u	925	C
45	u	927	G
45	u	928	C
45	u	929	A
45	u	930	G
45	u	931	C
45	u	932	A
45	u	933	G
45	u	934	C
45	u	935	A
45	u	936	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	937	U
45	u	938	C
45	u	939	G
45	u	940	C
45	u	942	G
45	u	943	A
45	u	944	A
45	u	945	U
45	u	946	C
45	u	947	C
45	u	957	G
45	u	958	G
45	u	960	A
45	u	961	G
45	u	962	C
45	u	963	G
45	u	964	A
45	u	965	G
45	u	966	A
45	u	967	C
45	u	968	C
45	u	969	C
45	u	970	G
45	u	971	U
45	u	972	C
45	u	973	G
45	u	976	G
45	u	977	C
45	u	978	G
45	u	979	C
45	u	982	U
45	u	983	C
45	u	984	C
45	u	989	U
45	u	990	C
45	u	992	C
45	u	1051	G
45	u	1070	G
45	u	1072	C
45	u	1073	G
45	u	1075	G
45	u	1076	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	1083	U
45	u	1097	C
45	u	1175	A
45	u	1176	C
45	u	1177	U
45	u	1181	C
45	u	1182	C
45	u	1183	C
45	u	1193	C
45	u	1204	C
45	u	1209	U
45	u	1211	G
45	u	1212	G
45	u	1214	C
45	u	1215	C
45	u	1219	G
45	u	1221	G
45	u	1222	A
45	u	1233	G
45	u	1234	G
45	u	1235	G
45	u	1236	C
45	u	1237	C
45	u	1238	A
45	u	1239	C
45	u	1240	G
45	u	1241	C
45	u	1242	G
45	u	1243	C
45	u	1244	G
45	u	1245	C
45	u	1255	A
45	u	1256	G
45	u	1259	G
45	u	1266	G
45	u	1267	C
45	u	1268	G
45	u	1269	G
45	u	1270	A
45	u	1272	C
45	u	1273	G
45	u	1274	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	1275	G
45	u	1279	A
45	u	1280	C
45	u	1281	G
45	u	1285	U
45	u	1286	C
45	u	1287	G
45	u	1288	G
45	u	1289	C
45	u	1293	G
45	u	1294	A
45	u	1295	C
45	u	1296	G
45	u	1297	U
45	u	1301	C
45	u	1303	A
45	u	1304	C
45	u	1313	C
45	u	1326	A
45	u	1330	A
45	u	1337	A
45	u	1344	C
45	u	1354	A
45	u	1358	G
45	u	1364	U
45	u	1365	C
45	u	1366	G
45	u	1367	C
45	u	1368	A
45	u	1369	C
45	u	1370	G
45	u	1371	A
45	u	1372	A
45	u	1376	C
45	u	1377	G
45	u	1378	C
45	u	1379	C
45	u	1380	G
45	u	1381	U
45	u	1387	A
45	u	1390	G
45	u	1394	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	1397	A
45	u	1398	A
45	u	1399	G
45	u	1407	C
45	u	1408	G
45	u	1409	C
45	u	1410	U
45	u	1411	C
45	u	1413	C
45	u	1414	C
45	u	1416	G
45	u	1418	C
45	u	1420	A
45	u	1421	G
45	u	1429	C
45	u	1432	G
45	u	1435	G
45	u	1436	C
45	u	1439	C
45	u	1440	U
45	u	1441	C
45	u	1442	C
45	u	1445	U
45	u	1446	C
45	u	1448	G
45	u	1449	C
45	u	1455	G
45	u	1456	C
45	u	1457	G
45	u	1475	G
45	u	1477	C
45	u	1478	C
45	u	1481	C
45	u	1482	G
45	u	1483	C
45	u	1484	G
45	u	1485	C
45	u	1486	C
45	u	1489	G
45	u	1497	A
45	u	1498	G
45	u	1501	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	1502	G
45	u	1504	G
45	u	1514	U
45	u	1516	G
45	u	1518	A
45	u	1523	A
45	u	1524	A
45	u	1533	A
45	u	1534	A
45	u	1547	A
45	u	1563	A
45	u	1564	A
45	u	1566	C
45	u	1568	C
45	u	1578	U
45	u	1582	U
45	u	1586	G
45	u	1591	U
45	u	1592	G
45	u	1596	U
45	u	1602	U
45	u	1612	G
45	u	1613	A
45	u	1614	C
45	u	1624	G
45	u	1625	G
45	u	1631	A
45	u	1633	G
45	u	1634	A
45	u	1636	U
45	u	1638	A
45	u	1641	G
45	u	1654	G
45	u	1655	C
45	u	1656	U
45	u	1661	C
45	u	1670	G
45	u	1676	C
45	u	1677	U
45	u	1691	G
45	u	1692	C
45	u	1696	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	1697	G
45	u	1698	C
45	u	1699	A
45	u	1719	A
45	u	1720	C
45	u	1721	G
45	u	1722	C
45	u	1724	G
45	u	1725	U
45	u	1733	G
45	u	1734	G
45	u	1735	U
45	u	1742	A
45	u	1746	A
45	u	1750	G
45	u	1753	G
45	u	1754	U
45	u	1755	C
45	u	1756	U
45	u	1757	U
45	u	1758	G
45	u	1760	G
45	u	1761	G
45	u	1764	G
45	u	1767	A
45	u	1768	C
45	u	1772	C
45	u	1776	A
45	u	1777	C
45	u	1781	U
45	u	1787	A
45	u	1799	G
45	u	1800	U
45	u	1803	G
45	u	1804	A
45	u	1805	A
45	u	1812	C
45	u	1815	G
45	u	1818	G
45	u	1819	G
45	u	1820	C
45	u	1821	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	1822	U
45	u	1828	C
45	u	1830	G
45	u	1832	C
45	u	1833	G
45	u	1834	U
45	u	1835	G
45	u	1836	G
45	u	1847	C
45	u	1848	C
45	u	1855	G
45	u	1867	A
45	u	1869	G
45	u	1882	U
45	u	1885	G
45	u	1886	G
45	u	1889	U
45	u	1892	A
45	u	1897	A
45	u	1899	G
45	u	1900	C
45	u	1910	G
45	u	1918	U
45	u	1919	G
45	u	1920	C
45	u	1921	C
45	u	1922	G
45	u	1923	A
45	u	1931	C
45	u	1947	U
45	u	1952	G
45	u	1955	G
45	u	1956	A
45	u	1957	U
45	u	1958	A
45	u	1959	U
45	u	1960	A
45	u	1961	G
45	u	1964	A
45	u	1968	G
45	u	1969	G
45	u	1975	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	1976	G
45	u	1977	C
45	u	1979	A
45	u	1980	U
45	u	1981	G
45	u	1983	A
45	u	1984	A
45	u	1985	G
45	u	1986	U
45	u	1987	C
45	u	1988	G
45	u	1990	A
45	u	1991	A
45	u	1992	U
45	u	1993	C
45	u	1997	U
45	u	1998	A
45	u	2001	G
45	u	2002	A
45	u	2003	G
45	u	2004	U
45	u	2005	G
45	u	2008	U
45	u	2010	A
45	u	2011	C
45	u	2019	C
45	u	2020	U
45	u	2021	G
45	u	2024	G
45	u	2025	A
45	u	2026	A
45	u	2027	U
45	u	2028	C
45	u	2044	U
45	u	2046	G
45	u	2047	A
45	u	2048	U
45	u	2052	G
45	u	2055	G
45	u	2056	G
45	u	2062	C
45	u	2064	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	2068	C
45	u	2069	A
45	u	2070	U
45	u	2071	A
45	u	2079	G
45	u	2084	C
45	u	2085	G
45	u	2089	G
45	u	2090	U
45	u	2091	C
45	u	2092	G
45	u	2093	A
45	u	2094	G
45	u	2095	A
45	u	2097	U
45	u	2100	A
45	u	2101	C
45	u	2103	G
45	u	2107	C
45	u	2108	G
45	u	2109	G
45	u	2110	C
45	u	2111	G
45	u	2112	G
45	u	2113	G
45	u	2114	G
45	u	2115	G
45	u	2116	C
45	u	2117	G
45	u	2118	G
45	u	2119	C
45	u	2120	G
45	u	2122	G
45	u	2123	C
45	u	2124	G
45	u	2125	C
45	u	2126	G
45	u	2127	C
45	u	2129	C
45	u	2130	G
45	u	2131	C
45	u	2247	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	2248	C
45	u	2250	C
45	u	2251	G
45	u	2252	G
45	u	2253	A
45	u	2254	G
45	u	2255	C
45	u	2256	C
45	u	2257	C
45	u	2258	C
45	u	2259	G
45	u	2260	C
45	u	2261	G
45	u	2263	A
45	u	2264	C
45	u	2265	G
45	u	2266	C
45	u	2267	U
45	u	2268	A
45	u	2269	C
45	u	2270	G
45	u	2274	C
45	u	2275	G
45	u	2279	A
45	u	2288	G
45	u	2289	C
45	u	2299	G
45	u	2300	A
45	u	2301	G
45	u	2312	U
45	u	2313	A
45	u	2314	G
45	u	2324	C
45	u	2331	G
45	u	2332	A
45	u	2333	G
45	u	2335	C
45	u	2337	C
45	u	2348	G
45	u	2351	C
45	u	2360	A
45	u	2364	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	2370	A
45	u	2382	A
45	u	2383	C
45	u	2395	A
45	u	2396	A
45	u	2399	G
45	u	2417	A
45	u	2422	C
45	u	2424	G
45	u	2425	U
45	u	2428	A
45	u	2429	A
45	u	2433	G
45	u	2434	G
45	u	2440	U
45	u	2441	C
45	u	2447	U
45	u	2450	G
45	u	2458	C
45	u	2469	C
45	u	2471	G
45	u	2473	A
45	u	2474	G
45	u	2475	G
45	u	2485	U
45	u	2488	C
45	u	2489	C
45	u	2490	U
45	u	2491	C
45	u	2493	G
45	u	2495	U
45	u	2499	C
45	u	2503	G
45	u	2504	C
45	u	2505	C
45	u	2506	G
45	u	2507	A
45	u	2512	A
45	u	2513	A
45	u	2514	G
45	u	2519	U
45	u	2521	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	2527	A
45	u	2530	U
45	u	2536	A
45	u	2537	A
45	u	2544	G
45	u	2546	G
45	u	2547	G
45	u	2553	A
45	u	2554	U
45	u	2555	G
45	u	2564	G
45	u	2566	G
45	u	2568	C
45	u	2571	C
45	u	2575	U
45	u	2577	C
45	u	2583	C
45	u	2587	A
45	u	2588	C
45	u	2589	C
45	u	2591	A
45	u	2601	A
45	u	2602	G
45	u	2611	A
45	u	2620	G
45	u	2623	A
45	u	2627	C
45	u	2638	G
45	u	2640	G
45	u	2647	A
45	u	2653	C
45	u	2661	U
45	u	2662	G
45	u	2663	G
45	u	2669	C
45	u	2673	G
45	u	2676	A
45	u	2679	G
45	u	2681	G
45	u	2686	G
45	u	2687	U
45	u	2688	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	2695	A
45	u	2696	A
45	u	2704	C
45	u	2708	U
45	u	2710	C
45	u	2711	G
45	u	2712	G
45	u	2714	G
45	u	2716	C
45	u	2721	G
45	u	2724	G
45	u	2725	A
45	u	2726	G
45	u	2733	C
45	u	2740	U
45	u	2743	A
45	u	2754	G
45	u	2755	A
45	u	2756	G
45	u	2760	G
45	u	2761	U
45	u	2762	G
45	u	2767	U
45	u	2768	C
45	u	2769	U
45	u	2770	C
45	u	2772	C
45	u	2787	A
45	u	2788	U
45	u	2789	A
45	u	2790	U
45	u	2794	C
45	u	2795	A
45	u	2796	G
45	u	2798	A
45	u	2806	A
45	u	2807	A
45	u	2814	C
45	u	2824	C
45	u	2825	A
45	u	2826	U
45	u	2827	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	2828	U
45	u	2829	U
45	u	2835	A
45	u	2838	G
45	u	2839	U
45	u	2842	G
45	u	2855	G
45	u	2859	G
45	u	2862	G
45	u	2869	U
45	u	2896	G
45	u	2897	G
45	u	2898	G
45	u	2904	U
45	u	2905	C
45	u	2910	G
45	u	3594	C
45	u	3595	U
45	u	3596	A
45	u	3597	G
45	u	3598	C
45	u	3605	C
45	u	3606	U
45	u	3615	G
45	u	3617	G
45	u	3625	G
45	u	3626	G
45	u	3630	A
45	u	3635	A
45	u	3644	U
45	u	3653	A
45	u	3662	A
45	u	3668	C
45	u	3670	C
45	u	3671	G
45	u	3673	C
45	u	3674	G
45	u	3680	U
45	u	3682	A
45	u	3689	G
45	u	3692	A
45	u	3696	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	3698	G
45	u	3702	A
45	u	3709	U
45	u	3710	G
45	u	3711	A
45	u	3712	A
45	u	3717	A
45	u	3718	A
45	u	3722	G
45	u	3728	A
45	u	3729	U
45	u	3737	A
45	u	3740	G
45	u	3748	A
45	u	3750	G
45	u	3752	C
45	u	3753	G
45	u	3755	G
45	u	3756	A
45	u	3759	A
45	u	3760	A
45	u	3764	U
45	u	3773	U
45	u	3774	A
45	u	3775	A
45	u	3776	G
45	u	3777	G
45	u	3778	U
45	u	3780	G
45	u	3783	A
45	u	3784	A
45	u	3786	U
45	u	3788	C
45	u	3798	U
45	u	3799	A
45	u	3802	U
45	u	3810	C
45	u	3811	G
45	u	3812	C
45	u	3813	A
45	u	3814	U
45	u	3817	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	3819	G
45	u	3822	U
45	u	3831	U
45	u	3836	A
45	u	3838	U
45	u	3839	G
45	u	3840	U
45	u	3859	G
45	u	3867	A
45	u	3877	A
45	u	3878	C
45	u	3879	G
45	u	3889	G
45	u	3897	G
45	u	3900	G
45	u	3901	A
45	u	3905	A
45	u	3906	A
45	u	3907	G
45	u	3912	U
45	u	3915	U
45	u	3916	G
45	u	3917	A
45	u	3924	C
45	u	3925	U
45	u	3926	C
45	u	3927	U
45	u	3938	G
45	u	3939	G
45	u	3943	A
45	u	3946	G
45	u	4069	U
45	u	4070	U
45	u	4076	G
45	u	4084	G
45	u	4085	A
45	u	4086	G
45	u	4087	G
45	u	4088	C
45	u	4091	G
45	u	4092	G
45	u	4093	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	4094	G
45	u	4097	G
45	u	4104	G
45	u	4105	A
45	u	4107	G
45	u	4112	C
45	u	4114	C
45	u	4115	G
45	u	4116	C
45	u	4117	U
45	u	4118	U
45	u	4119	C
45	u	4120	U
45	u	4121	G
45	u	4122	G
45	u	4125	C
45	u	4127	A
45	u	4134	C
45	u	4143	G
45	u	4144	C
45	u	4145	C
45	u	4155	C
45	u	4161	G
45	u	4162	C
45	u	4163	U
45	u	4165	C
45	u	4166	G
45	u	4168	G
45	u	4170	A
45	u	4171	C
45	u	4182	G
45	u	4183	G
45	u	4184	G
45	u	4191	G
45	u	4203	A
45	u	4208	U
45	u	4212	A
45	u	4213	A
45	u	4216	G
45	u	4217	G
45	u	4218	U
45	u	4219	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	4225	G
45	u	4226	G
45	u	4229	U
45	u	4232	U
45	u	4233	A
45	u	4238	G
45	u	4241	C
45	u	4251	A
45	u	4254	G
45	u	4258	C
45	u	4265	U
45	u	4266	G
45	u	4267	G
45	u	4268	A
45	u	4271	A
45	u	4273	A
45	u	4282	A
45	u	4291	G
45	u	4297	G
45	u	4302	U
45	u	4303	C
45	u	4304	A
45	u	4305	G
45	u	4306	U
45	u	4307	A
45	u	4311	A
45	u	4312	U
45	u	4313	A
45	u	4314	C
45	u	4317	A
45	u	4318	C
45	u	4319	C
45	u	4329	G
45	u	4330	G
45	u	4331	G
45	u	4332	C
45	u	4335	C
45	u	4336	A
45	u	4349	C
45	u	4350	C
45	u	4354	U
45	u	4355	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	4360	U
45	u	4367	G
45	u	4368	G
45	u	4372	U
45	u	4373	G
45	u	4377	G
45	u	4378	A
45	u	4379	A
45	u	4380	A
45	u	4387	C
45	u	4391	G
45	u	4394	A
45	u	4395	U
45	u	4396	A
45	u	4398	C
45	u	4405	G
45	u	4419	U
45	u	4420	U
45	u	4421	C
45	u	4422	A
45	u	4424	A
45	u	4426	C
45	u	4430	G
45	u	4432	C
45	u	4433	G
45	u	4438	U
45	u	4439	U
45	u	4441	A
45	u	4444	C
45	u	4448	G
45	u	4449	A
45	u	4450	U
45	u	4453	C
45	u	4454	G
45	u	4464	A
45	u	4471	U
45	u	4472	G
45	u	4473	A
45	u	4475	G
45	u	4476	C
45	u	4481	U
45	u	4482	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	4484	A
45	u	4488	A
45	u	4491	G
45	u	4495	G
45	u	4500	U
45	u	4510	A
45	u	4511	A
45	u	4512	U
45	u	4513	A
45	u	4515	G
45	u	4519	C
45	u	4520	G
45	u	4522	G
45	u	4524	G
45	u	4527	G
45	u	4528	G
45	u	4529	G
45	u	4535	A
45	u	4548	A
45	u	4549	G
45	u	4550	G
45	u	4557	U
45	u	4567	G
45	u	4570	G
45	u	4573	G
45	u	4575	G
45	u	4577	U
45	u	4583	C
45	u	4584	A
45	u	4585	U
45	u	4586	G
45	u	4590	A
45	u	4591	U
45	u	4606	G
45	u	4618	G
45	u	4636	U
45	u	4637	G
45	u	4641	U
45	u	4647	G
45	u	4648	A
45	u	4656	A
45	u	4657	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	4661	G
45	u	4670	C
45	u	4672	A
45	u	4677	U
45	u	4687	A
45	u	4694	G
45	u	4695	C
45	u	4700	A
45	u	4701	A
45	u	4702	G
45	u	4709	U
45	u	4719	G
45	u	4720	C
45	u	4721	G
45	u	4730	C
45	u	4731	G
45	u	4732	G
45	u	4733	C
45	u	4734	A
45	u	4737	G
45	u	4741	C
45	u	4745	G
45	u	4746	C
45	u	4749	C
45	u	4750	G
45	u	4753	U
45	u	4754	G
45	u	4756	C
45	u	4758	U
45	u	4760	G
45	u	4764	A
45	u	4768	G
45	u	4770	U
45	u	4771	C
45	u	4774	C
45	u	4869	U
45	u	4871	C
45	u	4872	G
45	u	4873	G
45	u	4874	A
45	u	4875	G
45	u	4876	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	4877	G
45	u	4878	C
45	u	4883	C
45	u	4884	G
45	u	4885	U
45	u	4886	C
45	u	4889	G
45	u	4890	G
45	u	4893	A
45	u	4895	C
45	u	4896	G
45	u	4898	G
45	u	4900	C
45	u	4901	G
45	u	4904	G
45	u	4906	C
45	u	4910	G
45	u	4911	A
45	u	4912	G
45	u	4913	G
45	u	4924	C
45	u	4926	C
45	u	4927	G
45	u	4930	C
45	u	4931	G
45	u	4932	U
45	u	4934	A
45	u	4935	C
45	u	4936	G
45	u	4939	C
45	u	4942	C
45	u	4945	G
45	u	4948	C
45	u	4949	G
45	u	4950	U
45	u	4951	G
45	u	4952	G
45	u	4959	U
45	u	4964	C
45	u	4965	U
45	u	4966	A
45	u	4967	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	u	4975	G
45	u	4976	U
45	u	4985	U
45	u	4988	U
45	u	4989	U
45	u	4990	C
45	u	4991	U
45	u	5007	A
45	u	5013	C
45	u	5014	A
45	u	5017	G
45	u	5018	C
45	u	5022	U
45	u	5023	C
45	u	5024	C
45	u	5025	C
45	u	5026	U
45	u	5027	C
45	u	5028	G
45	u	5031	G
45	u	5033	G
45	u	5041	G
45	u	5047	C
45	u	5050	C
45	u	5052	C
45	u	5053	U
45	u	5054	C
45	u	5056	A
45	u	5058	A
45	u	5060	A
45	u	5061	A
45	u	5062	G
45	u	5066	U
46	v	7	G
46	v	11	A
46	v	21	G
46	v	25	G
46	v	33	U
46	v	40	U
46	v	51	G
46	v	53	U
46	v	54	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
46	v	64	G
46	v	74	A
46	v	76	U
46	v	97	G
46	v	99	G
46	v	100	A
46	v	106	G
46	v	110	G
46	v	111	C
46	v	120	U
47	w	2	G
47	w	3	A
47	w	34	U
47	w	35	C
47	w	38	U
47	w	39	G
47	w	49	G
47	w	51	U
47	w	52	A
47	w	55	U
47	w	57	C
47	w	59	A
47	w	62	A
47	w	63	U
47	w	74	U
47	w	75	G
47	w	79	G
47	w	80	A
47	w	81	C
47	w	82	A
47	w	83	C
47	w	84	A
47	w	85	U
47	w	86	U
47	w	87	G
47	w	94	G
47	w	95	A
47	w	99	U
47	w	101	C
47	w	103	A
47	w	104	A
47	w	105	C

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Mol	Chain	Res	Type
47	w	107	C
47	w	109	C
47	w	110	U
47	w	111	U
47	w	112	G
47	w	113	C
47	w	114	G
47	w	115	G
47	w	117	C
47	w	121	G
47	w	122	G
47	w	123	U
47	w	124	U
47	w	125	C
47	w	126	C
47	w	127	U
47	w	137	A
47	w	143	G
47	w	150	C
47	w	156	U

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	$\# Z  > 2$
59	NAG	K	1	59,55	14,14,15	0.49	0	17,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
59	NAG	K	2	59	14,14,15	0.24	0	17,19,21	0.53	0
59	BMA	K	3	59	11,11,12	0.67	0	15,15,17	0.88	1 (6%)
59	MAN	K	4	59	11,11,12	0.82	0	15,15,17	1.66	2 (13%)
59	MAN	K	5	59	11,11,12	0.71	0	15,15,17	1.25	2 (13%)
59	MAN	K	6	59	11,11,12	0.92	1 (9%)	15,15,17	0.99	2 (13%)
59	MAN	K	7	59	11,11,12	1.26	1 (9%)	15,15,17	1.29	2 (13%)
59	MAN	K	8	59	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
59	NAG	K	1	59,55	-	2/6/23/26	0/1/1/1
59	NAG	K	2	59	-	1/6/23/26	0/1/1/1
59	BMA	K	3	59	-	2/2/19/22	0/1/1/1
59	MAN	K	4	59	-	0/2/19/22	0/1/1/1
59	MAN	K	5	59	-	1/2/19/22	0/1/1/1
59	MAN	K	6	59	-	0/2/19/22	0/1/1/1
59	MAN	K	7	59	-	0/2/19/22	0/1/1/1
59	MAN	K	8	59	-	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)
59	K	7	MAN	C2-C3	2.51	1.56	1.52
59	K	6	MAN	O5-C1	-2.12	1.40	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	K	4	MAN	C1-O5-C5	4.40	118.15	112.19
59	K	4	MAN	O2-C2-C3	-3.75	102.62	110.14
59	K	7	MAN	C1-O5-C5	3.21	116.55	112.19
59	K	5	MAN	O2-C2-C3	-3.06	104.02	110.14
59	K	5	MAN	C1-O5-C5	3.01	116.27	112.19
59	K	8	MAN	C1-O5-C5	2.80	115.98	112.19
59	K	7	MAN	O3-C3-C2	2.54	114.86	109.99
59	K	6	MAN	O2-C2-C3	-2.48	105.16	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	K	8	MAN	O2-C2-C3	-2.19	105.76	110.14
59	K	3	BMA	C1-O5-C5	2.12	115.07	112.19
59	K	6	MAN	C1-O5-C5	2.04	114.96	112.19

There are no chirality outliers.

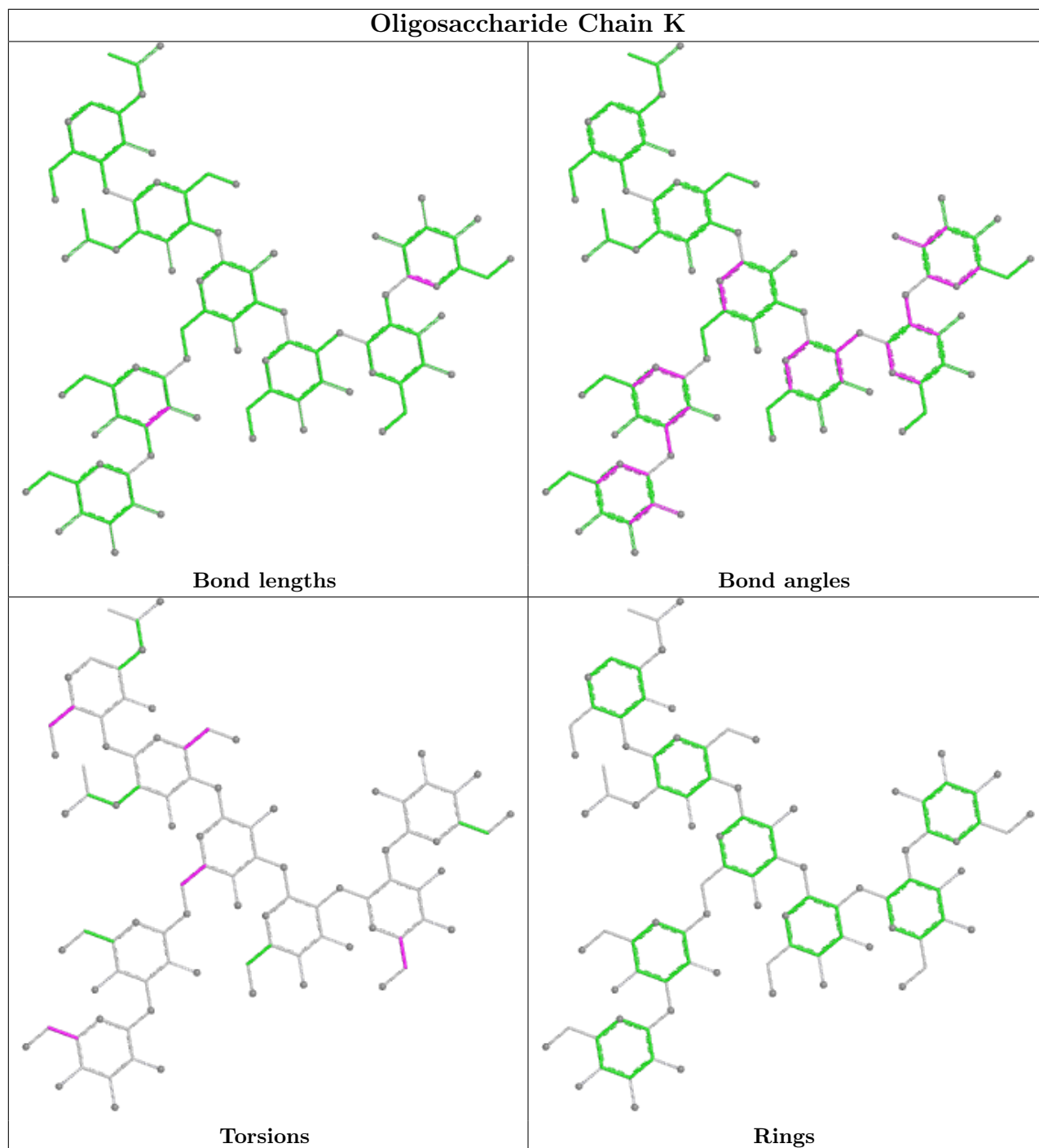
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	K	3	BMA	C4-C5-C6-O6
59	K	3	BMA	O5-C5-C6-O6
59	K	8	MAN	O5-C5-C6-O6
59	K	8	MAN	C4-C5-C6-O6
59	K	1	NAG	C4-C5-C6-O6
59	K	1	NAG	O5-C5-C6-O6
59	K	5	MAN	O5-C5-C6-O6
59	K	2	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	$\# Z  > 2$
62	9UB	5	809	55	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
62	9UB	5	809	55	-	4/39/62/62	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	5	809	9UB	P26-O25	8.10	1.67	1.58
62	5	809	9UB	P26-C29	7.18	1.91	1.80
62	5	809	9UB	C37-C39	-3.65	1.46	1.53
62	5	809	9UB	C41-N40	3.35	1.45	1.34
62	5	809	9UB	C06-C07	2.98	1.57	1.51
62	5	809	9UB	C11-C12	2.68	1.56	1.51
62	5	809	9UB	C16-C17	2.37	1.56	1.51
62	5	809	9UB	C18-C17	2.32	1.56	1.50
62	5	809	9UB	C20-C19	2.05	1.55	1.49

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	5	809	9UB	C18-C17-C16	4.23	122.39	115.27
62	5	809	9UB	C20-C19-C17	-3.49	120.01	126.04
62	5	809	9UB	C01-C02-C03	2.72	120.61	114.60
62	5	809	9UB	C32-O31-C30	2.61	117.72	113.16
62	5	809	9UB	C39-N40-C41	-2.61	116.83	123.18
62	5	809	9UB	O31-C32-C35	2.44	114.12	109.69
62	5	809	9UB	O27-P26-C29	2.41	111.04	105.72
62	5	809	9UB	C08-C07-C06	2.37	119.26	115.27
62	5	809	9UB	C15-C14-C12	-2.29	122.14	127.66
62	5	809	9UB	C10-C09-C07	-2.28	122.18	127.66
62	5	809	9UB	C18-C17-C19	-2.23	117.95	123.68
62	5	809	9UB	C13-C12-C11	2.21	118.99	115.27
62	5	809	9UB	C33-C32-C35	-2.16	107.95	113.00

There are no chirality outliers.

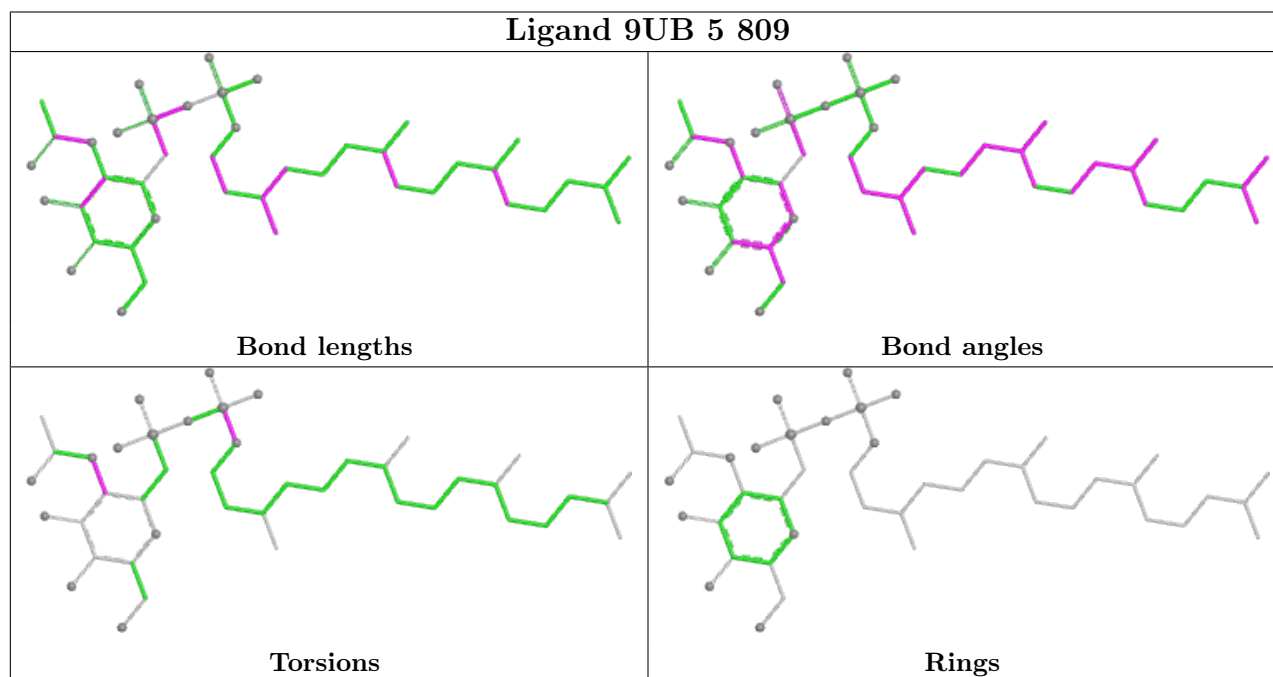
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	5	809	9UB	C20-O21-P22-O25
62	5	809	9UB	C20-O21-P22-O23
62	5	809	9UB	C20-O21-P22-O24
62	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
45	u	21
55	5	4
58	8	2
56	6	2
48	x	2
51	1	1
52	2	1
42	r	1

All 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
1	1	573:VAL	C	582:UNK	N	15.25
1	u	2131:C	O3'	2243:C	P	14.50
1	u	3950:U	O3'	4065:G	P	14.39
1	u	997:C	O3'	1047:C	P	13.95
1	6	46:UNK	C	53:UNK	N	13.30
1	2	42:UNK	C	50:UNK	N	12.33
1	8	598:UNK	C	600:UNK	N	11.54
1	6	82:UNK	C	88:UNK	N	10.20
1	x	312:PHE	C	337:PRO	N	9.61
1	u	1051:G	O3'	1064:G	P	8.98
1	x	133:MET	C	145:SER	N	8.39
1	u	1222:A	O3'	1232:G	P	5.15
1	u	2016:C	O3'	2017:A	P	4.53
1	u	1100:U	O3'	1167:C	P	4.42
1	u	1699:A	O3'	1718:C	P	4.00
1	r	121:GLN	C	122:LYS	N	2.97
1	u	1840:G	O3'	1842:G	P	2.91
1	u	4939:C	O3'	4941:G	P	2.80

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	502:PHE	C	503:ASP	N	2.78
1	u	4942:C	O3'	4944:C	P	2.73
1	u	1823:G	O3'	1825:A	P	2.56
1	5	590:SER	C	591:ASP	N	2.33
1	u	692:A	O3'	693:C	P	2.00
1	u	197:A	O3'	198:A	P	1.77
1	u	472:C	O3'	473:C	P	1.37
1	u	1965:G	O3'	1966:C	P	1.33
1	u	680:G	O3'	681:G	P	1.20
1	5	550:THR	C	551:HIS	N	0.96
1	5	545:ASN	C	546:THR	N	0.91

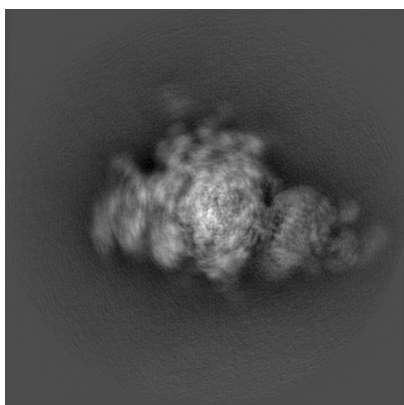
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4317. These allow visual inspection of the internal detail of the map and identification of artifacts.

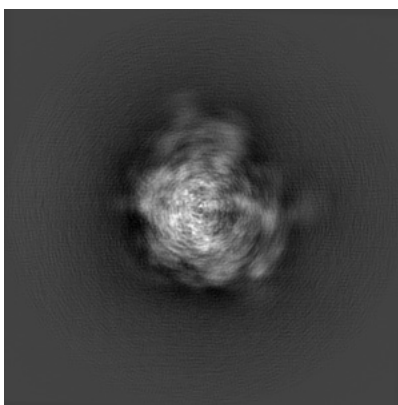
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

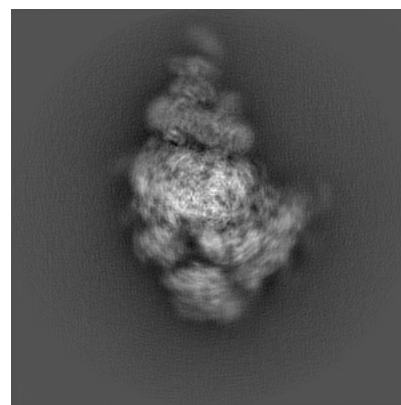
#### 6.1.1 Primary map



X



Y

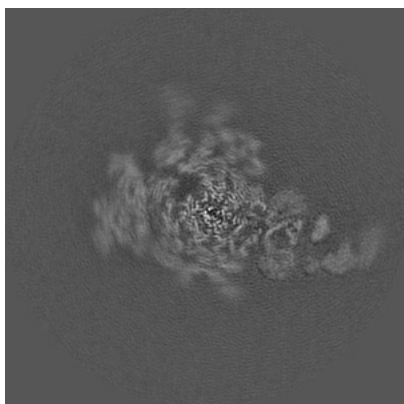


Z

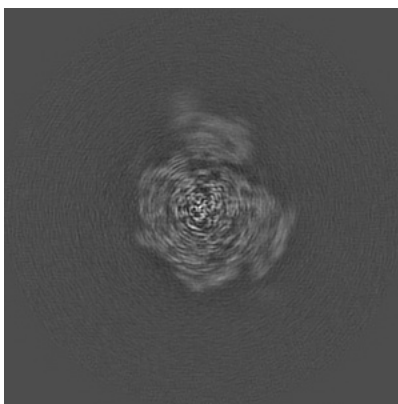
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

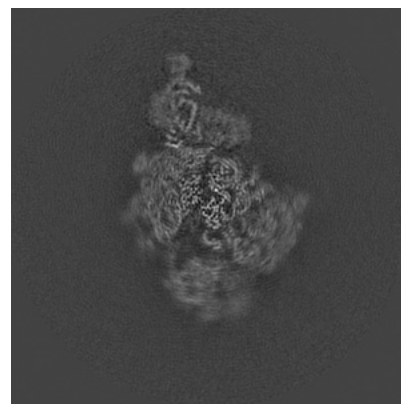
#### 6.2.1 Primary map



X Index: 250



Y Index: 250

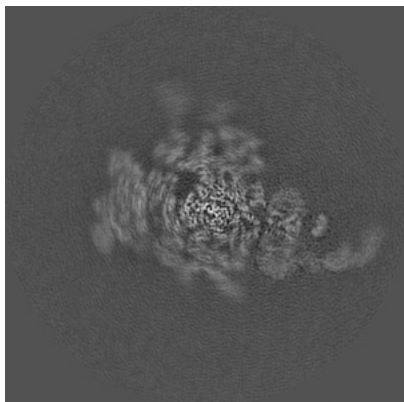


Z Index: 250

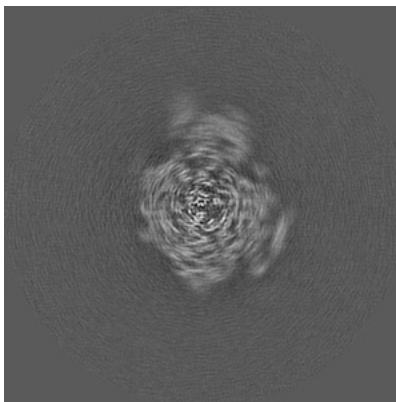
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

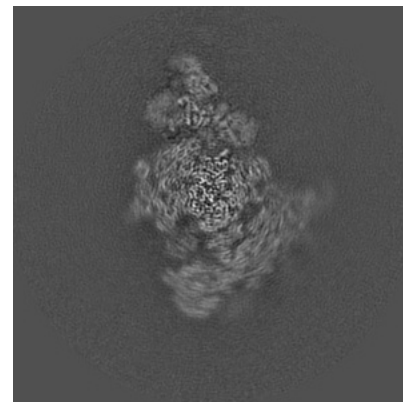
### 6.3.1 Primary map



X Index: 253



Y Index: 245



Z Index: 235

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

## 6.4 Orthogonal surface views [i](#)

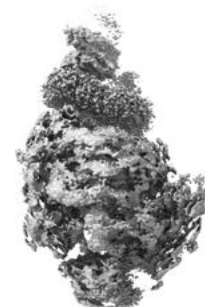
### 6.4.1 Primary map



X



Y



Z

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.



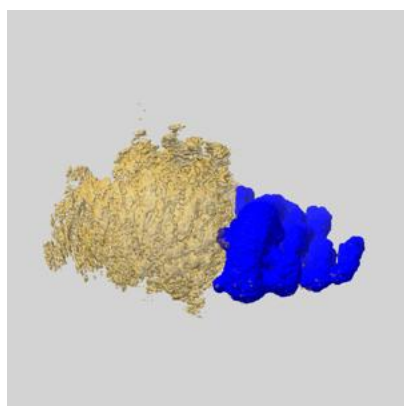
## 6.5 Mask visualisation [i](#)

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

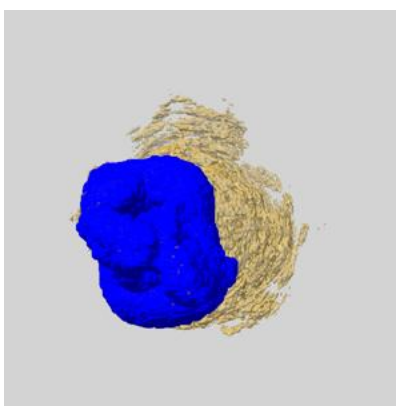
A mask typically either:

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

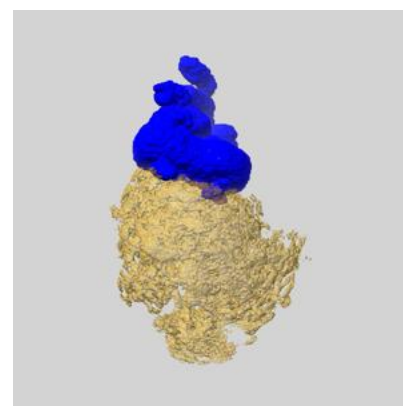
### 6.5.1 emd\_4317\_msk\_1.map [i](#)



X



Y

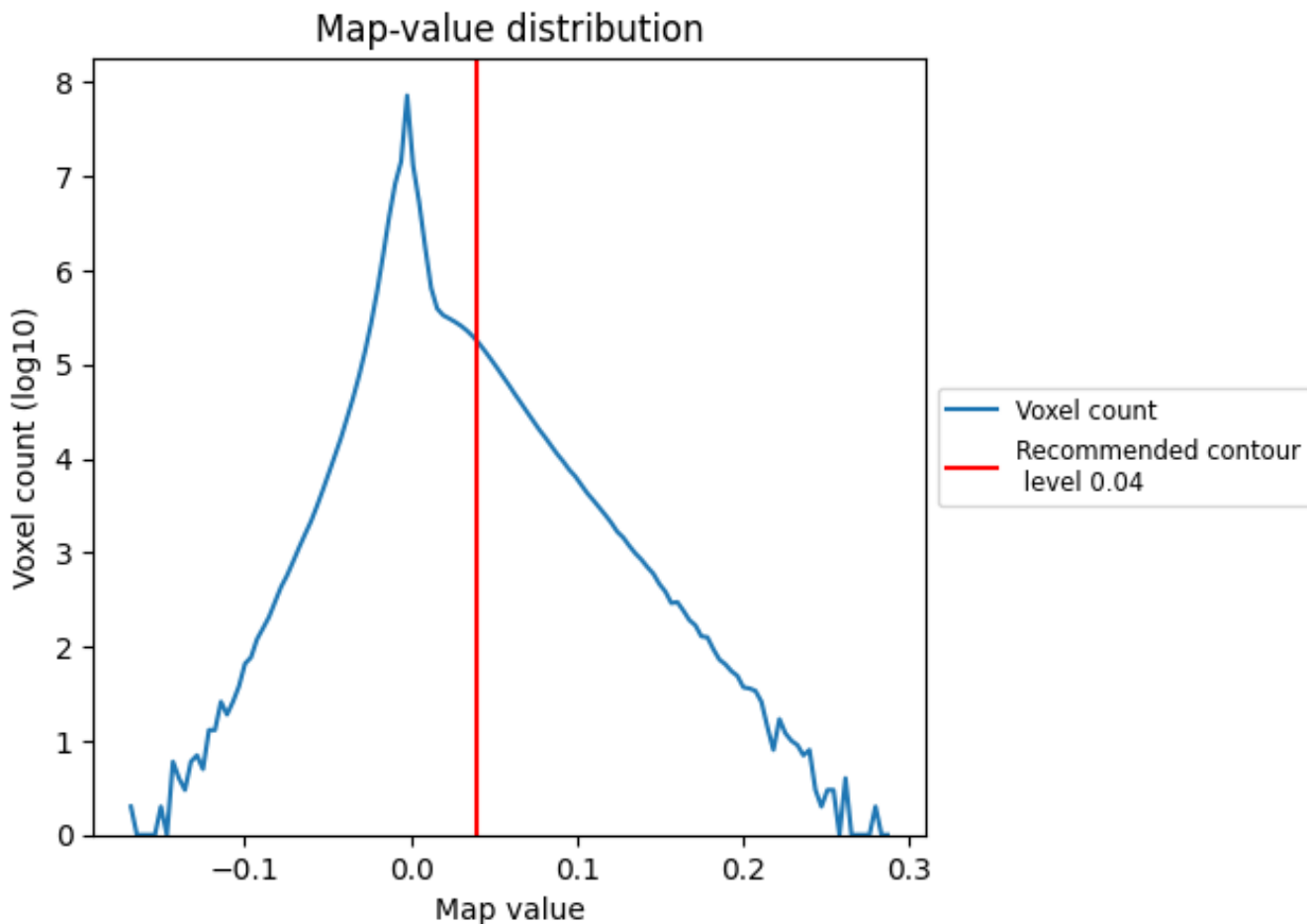


Z

## 7 Map analysis [i](#)

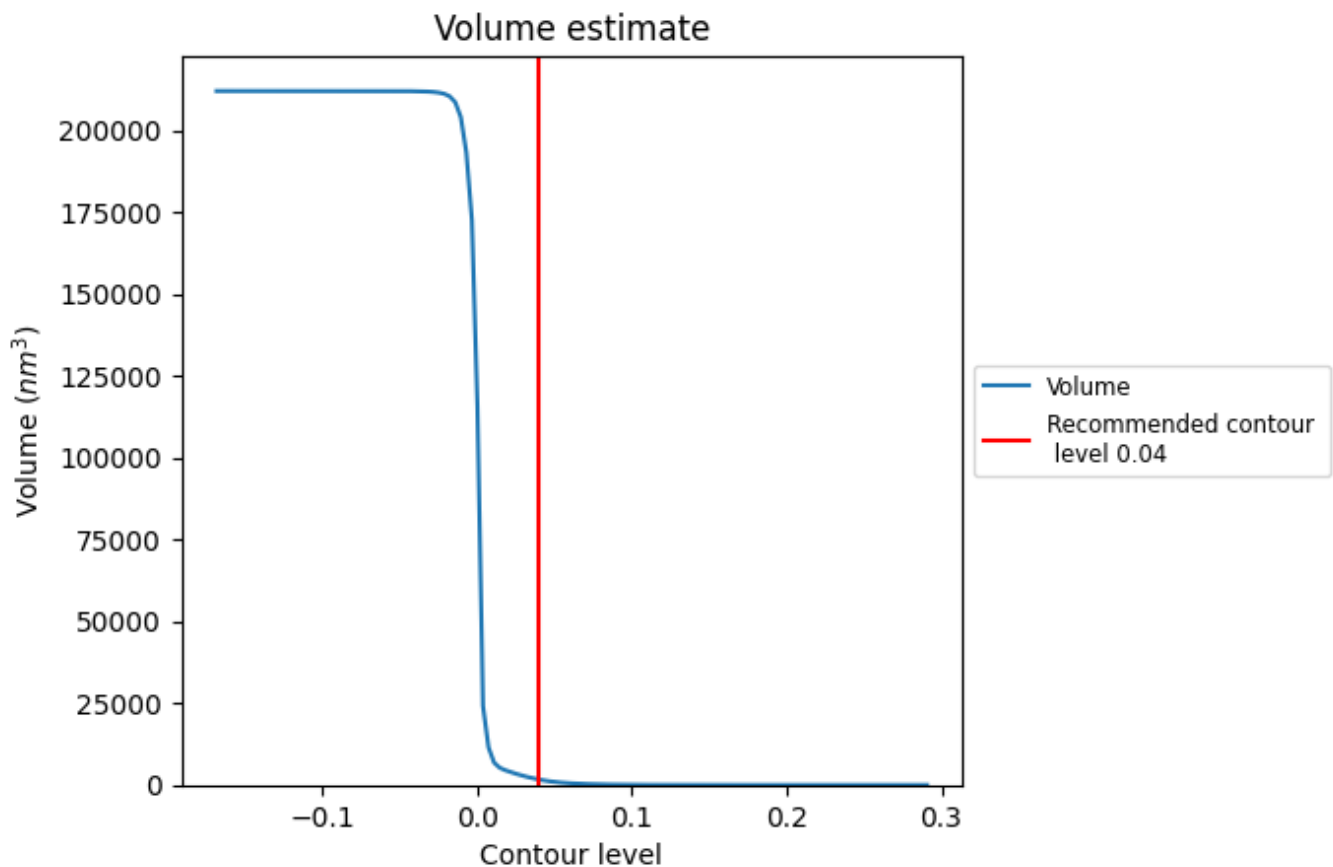
This section contains the results of statistical analysis of the map.

### 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.

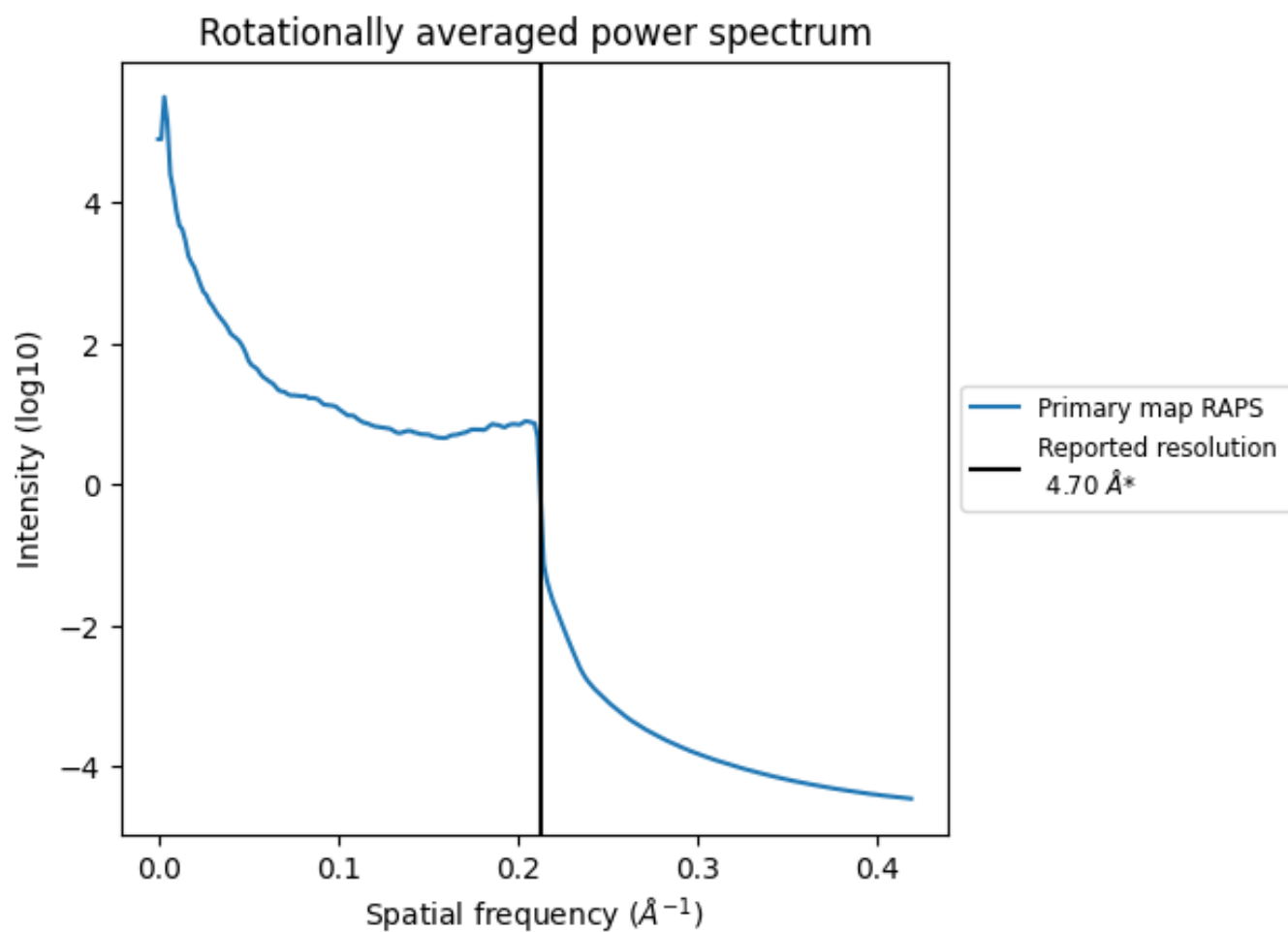
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1641  $\text{nm}^3$ ; this corresponds to an approximate mass of 1482 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 0.213 Å<sup>-1</sup>

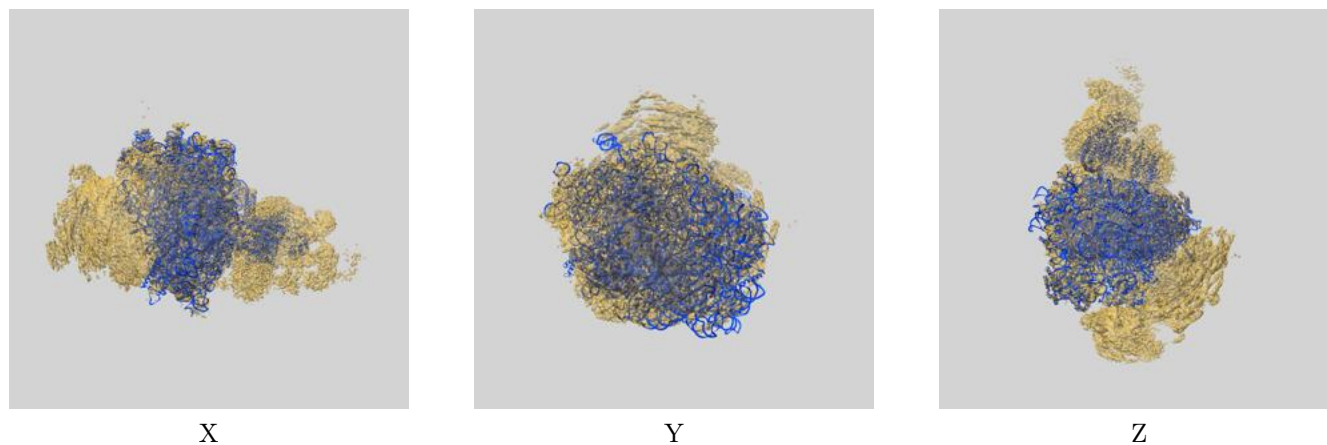
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

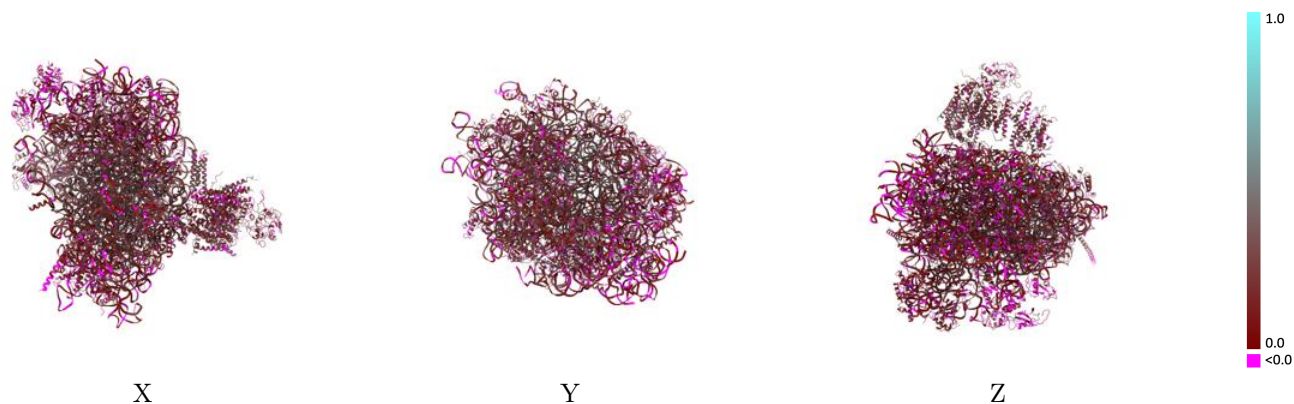
This section contains information regarding the fit between EMDB map EMD-4317 and PDB model 6FTJ. Per-residue inclusion information can be found in section 3 on page 18.

### 9.1 Map-model overlay [i](#)



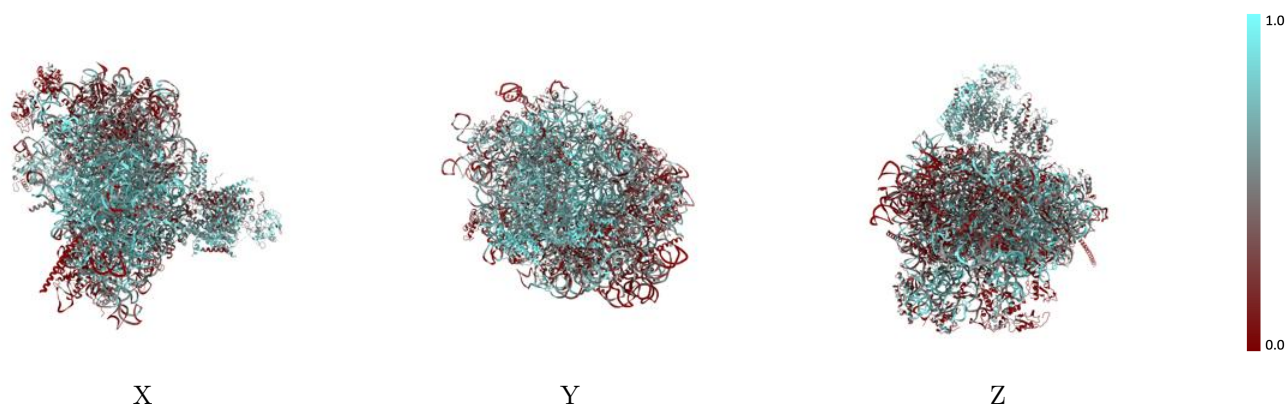
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



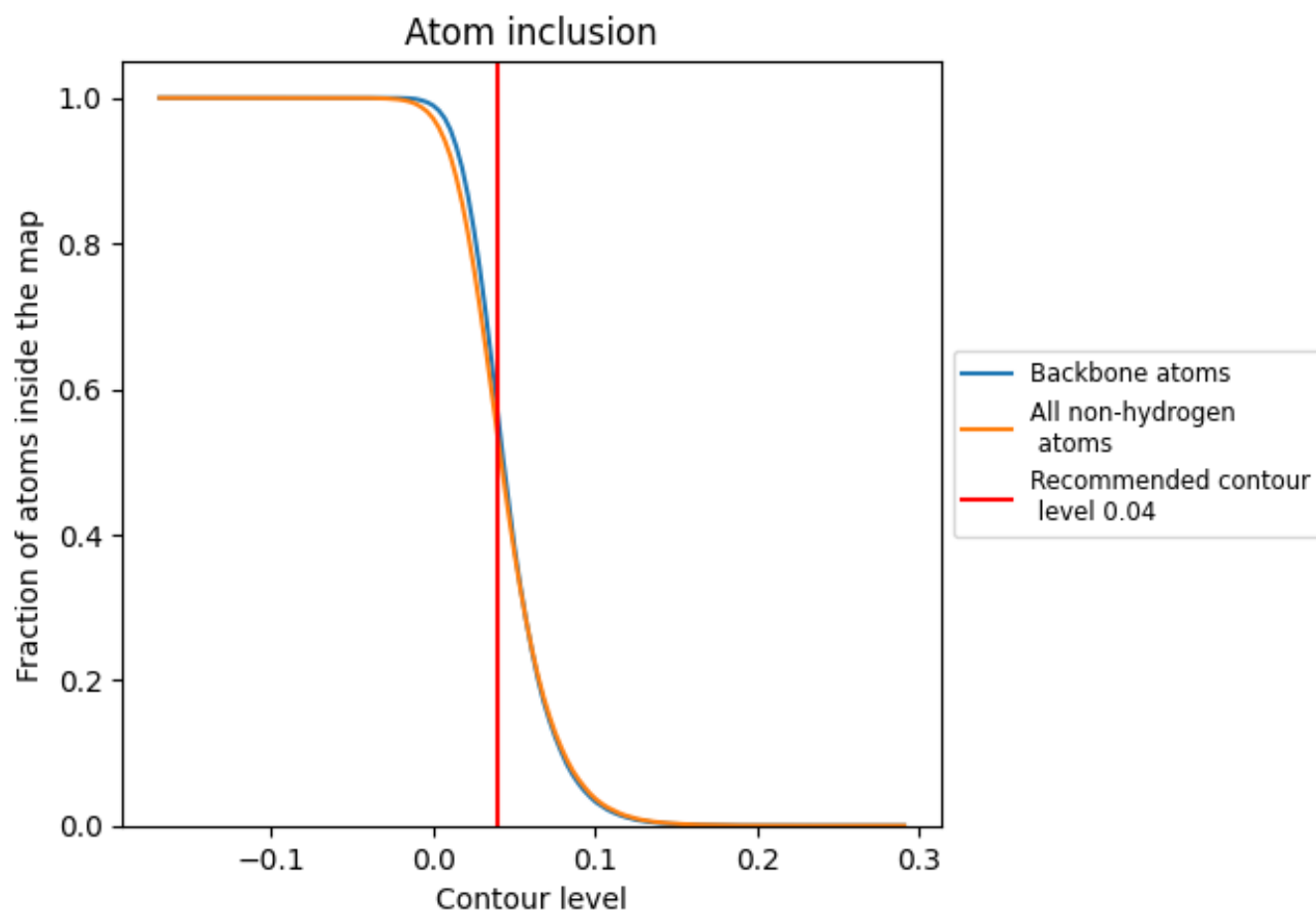
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 57% of all backbone atoms, 53% 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	 0.5344	 0.1740
1	 0.6549	 0.1980
2	 0.7600	 0.2210
3	 0.5738	 0.1750
4	 0.6090	 0.2080
5	 0.5847	 0.1790
6	 0.8474	 0.2550
7	 0.8160	 0.2140
8	 0.7775	 0.2330
A	 0.3641	 0.1920
B	 0.3704	 0.1570
C	 0.3318	 0.1680
D	 0.3634	 0.1080
E	 0.2454	 0.0940
F	 0.2584	 0.1230
G	 0.2181	 0.1030
H	 0.2084	 0.0760
I	 0.3288	 0.1670
J	 0.3872	 0.1220
K	 0.5213	 0.1490
L	 0.3223	 0.1430
M	 0.2966	 0.1060
N	 0.3926	 0.1800
O	 0.2382	 0.1060
P	 0.5145	 0.2280
Q	 0.3306	 0.1600
R	 0.3907	 0.1490
S	 0.2486	 0.1080
T	 0.2312	 0.1230
U	 0.4114	 0.1380
V	 0.3351	 0.1830
W	 0.3929	 0.1850
X	 0.4089	 0.1880
Y	 0.4174	 0.1650
Z	 0.3625	 0.1310



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Chain	Atom inclusion	Q-score
a	0.3012	0.1530
b	0.3339	0.1360
c	0.3161	0.1520
d	0.4644	0.2090
e	0.2436	0.1380
f	0.1829	0.0770
g	0.3031	0.1600
h	0.4392	0.1690
i	0.3367	0.1670
j	0.5721	0.2520
k	0.2998	0.1370
l	0.5579	0.2660
m	0.2524	0.0870
n	0.4527	0.1880
o	0.4213	0.1890
p	0.3222	0.1620
r	0.3349	0.1260
s	0.1439	0.0380
t	0.1176	0.0100
u	0.6529	0.1930
v	0.7113	0.1640
w	0.7425	0.2300
x	0.5500	0.1930
y	0.5617	0.1960
z	0.2622	0.0520