



## wwPDB EM Validation Summary Report ⓘ

Jun 25, 2026 – 09:18 AM EDT

PDB ID : 7UCK / pdb\_00007uck  
EMDB ID : EMD-26445  
Title : 80S translation initiation complex with ac4c(-1) mRNA and Harringtonine  
Authors : Yang, R.; Arango, D.; Sturgill, D.; Oberdoerffer, S.  
Deposited on : 2022-03-16  
Resolution : 2.80 Å(reported)

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

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

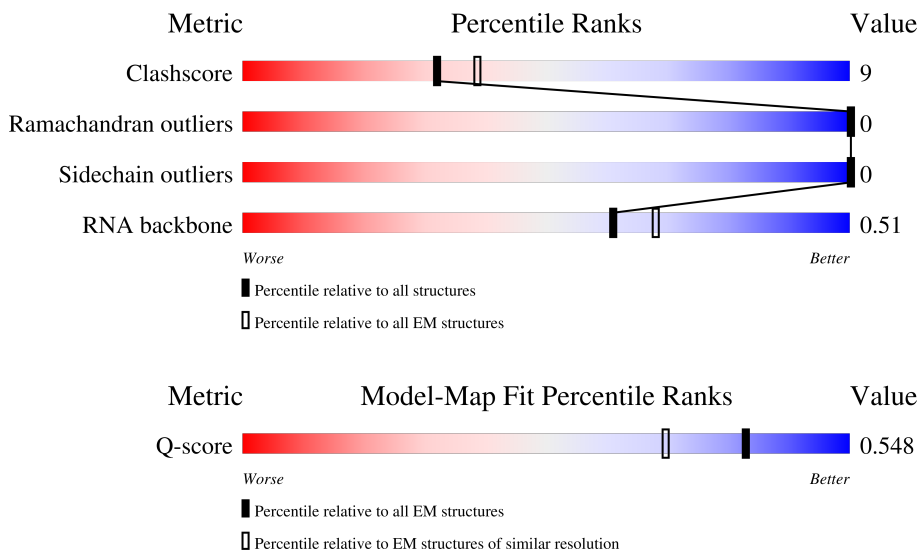
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 Å.

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





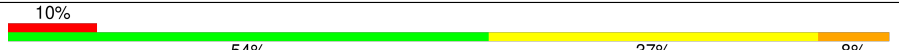
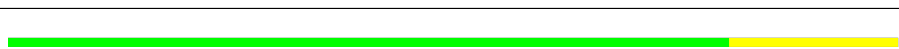

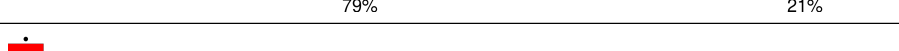
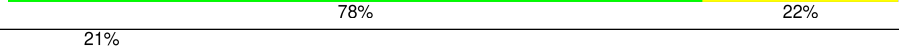





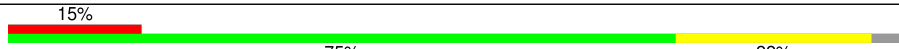


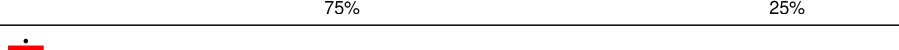








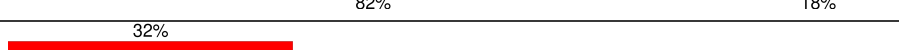
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 ( 2.30 - 3.30 )

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	2	76	
2	1	6	
3	5	3546	

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Mol	Chain	Length	Quality of chain
4	7	120	
5	8	156	
6	9	1698	
7	A	248	
8	B	394	
9	C	360	
10	D	291	
11	E	251	
12	F	225	
13	G	234	
14	H	190	
15	I	213	
16	J	170	
17	L	210	
18	M	138	
19	N	203	
20	O	199	
21	P	153	
22	Q	187	
23	R	180	
24	S	176	
25	T	159	
26	U	98	
27	V	131	
28	W	121	

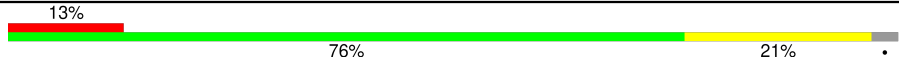
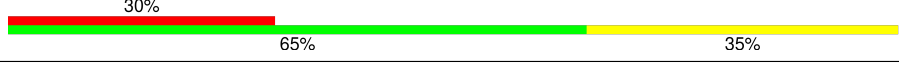
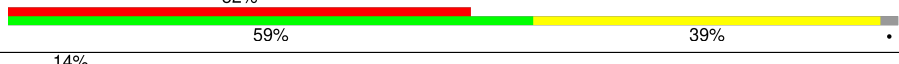


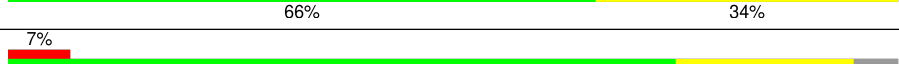
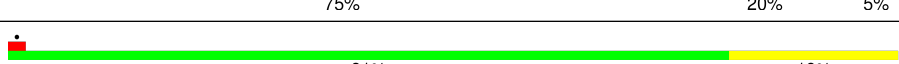
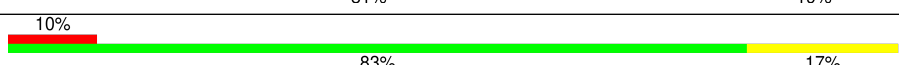
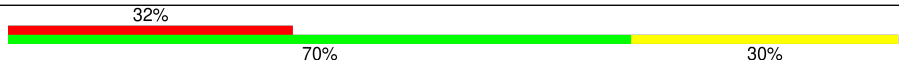

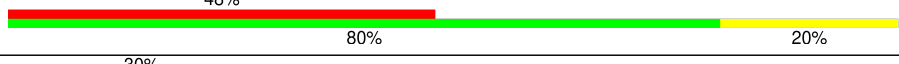
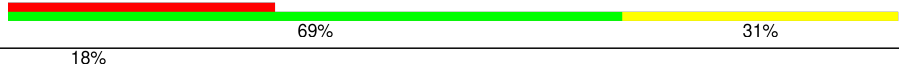
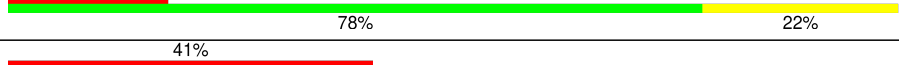

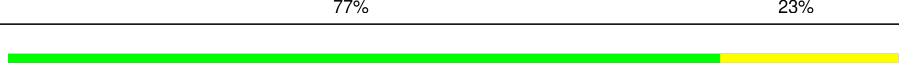










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Mol	Chain	Length	Quality of chain
29	X	118	13% 76% 24%
30	Y	134	22% 66% 34%
31	Z	135	16% 69% 31%
32	a	147	• 82% 18%
33	b	116	16% 75% 15% 10%
34	c	98	9% 74% 26%
35	d	107	12% 81% 19%
36	e	128	• 89% 11%
37	f	109	• 79% 21%
38	g	114	11% 86% 14%
39	h	122	17% 77% 23%
40	i	102	15% 75% 25%
41	j	86	• 79% 21%
42	k	69	51% 71% 29%
43	l	50	78% 22%
44	m	51	16% 69% 31%
45	n	25	80% 20%
46	o	103	10% 83% 17%
47	p	91	• 86% 14%
48	r	124	6% 79% 21%
49	AA	217	18% 79% 21%
50	BB	213	17% 71% 29%
51	CC	221	9% 73% 27%
52	DD	228	20% 81% 19%
53	EE	262	5% 78% 22%


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Mol	Chain	Length	Quality of chain
54	FF	191	
55	GG	237	
56	HH	189	
57	II	206	
58	JJ	185	
59	KK	96	
60	LL	151	
61	NN	149	
62	OO	136	
63	PP	120	
64	QQ	142	
65	RR	132	
66	SS	144	
67	TT	141	
68	UU	100	
69	VV	83	
70	WW	129	
71	XX	141	
72	YY	124	
73	ZZ	75	
74	Aa	101	
75	Bb	83	
76	Cc	62	
77	Dd	55	
78	Ee	55	

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Mol	Chain	Length	Quality of chain
79	Gg	313	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into three segments: a red segment on the left labeled '59%', a green segment in the middle labeled '65%', and a yellow segment on the right labeled '35%'. The segments are stacked horizontally, with the red segment starting from the left and ending at 59%, the green segment starting at 59% and ending at 65%, and the yellow segment starting at 65% and ending at 35%.</p>

## 2 Entry composition

There are 82 unique types of molecules in this entry. The entry contains 210046 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	72	1552	694	289	498	71	0	0

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	1	6	133	60	25	42	6	0	0

- Molecule 3 is a RNA chain called 28s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	5	3546	76153	33978	13919	24710	3546	0	0

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	7	120	2558	1141	456	842	119	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	2	U	N	conflict	GB X06789.1
7	36	C	N	conflict	GB X06789.1
7	102	U	N	conflict	GB X06789.1
7	112	U	N	conflict	GB X06789.1
7	114	U	N	conflict	GB X06789.1
7	119	U	C	conflict	GB X06789.1
7	120	U	N	conflict	GB X06789.1

- Molecule 5 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	8	151	Total	C	N	O	P	0	0
			3209	1433	564	1062	150		

- Molecule 6 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	9	1698	Total	C	N	O	P	0	0
			36291	16217	6509	11868	1697		

- Molecule 7 is a protein called 60S ribosomal protein L8.

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

- Molecule 8 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

- Molecule 9 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	360	Total	C	N	O	S	0	0
			2870	1806	575	475	14		

- Molecule 10 is a protein called Ribosomal\_L18\_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	291	Total	C	N	O	S	0	0
			2381	1506	436	425	14		

- Molecule 11 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 12 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	F	225	1875	1205	358	303	9	0	0

- Molecule 13 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	G	227	1837	1172	354	307	4	0	0

- Molecule 14 is a protein called 60S ribosomal protein L9.

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

- Molecule 15 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	I	205	1664	1056	321	274	13	0	0

- Molecule 16 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	J	170	1362	861	254	241	6	0	0

- Molecule 17 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	L	210	1702	1065	354	279	4	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	46	ILE	-	insertion	UNP G1TPV0
L	47	ALA	-	insertion	UNP G1TPV0
L	48	PRO	-	insertion	UNP G1TPV0
L	49	ARG	-	insertion	UNP G1TPV0
L	50	PRO	-	insertion	UNP G1TPV0
L	51	ALA	-	insertion	UNP G1TPV0

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Chain	Residue	Modelled	Actual	Comment	Reference
L	52	ALA	-	insertion	UNP G1TPV0
L	53	GLY	-	insertion	UNP G1TPV0
L	54	PRO	-	insertion	UNP G1TPV0

- Molecule 18 is a protein called 60S ribosomal protein L14.

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

- Molecule 19 is a protein called 60S ribosomal protein L15.

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

- Molecule 20 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	O	199	1630	1051	319	255	5	0	0

- Molecule 21 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	P	153	1242	777	241	215	9	0	0

- Molecule 22 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Q	187	1515	946	315	250	4	0	0

- Molecule 23 is a protein called 60S ribosomal protein L19.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	38	ARG	HIS	conflict	UNP G1TYL6
R	151	ARG	HIS	conflict	UNP G1TYL6

- Molecule 24 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	S	176	1462	930	285	236	11	0	0

- Molecule 25 is a protein called 60S ribosomal protein L21.

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

- Molecule 26 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	U	98	800	514	139	145	2	0	0

- Molecule 27 is a protein called 60S ribosomal protein L23.

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

- Molecule 28 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	W	106	860	538	174	144	4	0	0

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

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

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

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

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

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

- Molecule 32 is a protein called 60S ribosomal protein L27a.

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

- Molecule 33 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	b	104	848	527	189	129	3	0	0

- Molecule 34 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	c	98	761	481	134	140	6	0	0

- Molecule 35 is a protein called 60S ribosomal protein L31.

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

- Molecule 36 is a protein called 60S ribosomal protein L32.

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

- Molecule 37 is a protein called 60S ribosomal protein L35a.

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

- Molecule 38 is a protein called 60S ribosomal protein L34.

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

- Molecule 39 is a protein called 60S ribosomal protein L35.

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

- Molecule 40 is a protein called 60S ribosomal protein L36.

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

- Molecule 41 is a protein called 60S ribosomal protein L37.

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

- Molecule 42 is a protein called 60S ribosomal protein L38.

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

- Molecule 43 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 44 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	51	Total	C	N	O	S	0	0
			420	261	88	65	6		

- Molecule 45 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 46 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	103	Total	C	N	O	S	0	0
			842	528	172	136	6		

- Molecule 47 is a protein called 60S ribosomal protein L37a.

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

- Molecule 48 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 49 is a protein called 40S\_SA\_C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AA	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

- Molecule 50 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BB	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 51 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	CC	221	1716	1111	295	301	9	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	73	MET	VAL	conflict	UNP G1TUT9
CC	101	SER	ALA	conflict	UNP G1TUT9
CC	119	GLY	ALA	conflict	UNP G1TUT9
CC	194	ARG	HIS	conflict	UNP G1TUT9
CC	215	MET	LEU	conflict	UNP G1TUT9
CC	227	ARG	TRP	conflict	UNP G1TUT9
CC	228	GLY	SER	conflict	UNP G1TUT9

- Molecule 52 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	DD	228	1768	1126	318	316	8	0	0

- Molecule 53 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	EE	262	2076	1324	386	358	8	0	0

- Molecule 54 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	FF	185	1471	921	277	266	7	0	0

- Molecule 55 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	GG	237	1923	1200	387	329	7	0	0

- Molecule 56 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	HH	185	1488	952	271	264	1	0	0

- Molecule 57 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	II	203	1668	1047	328	288	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
II	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 58 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	JJ	185	1525	969	306	248	2	0	0

- Molecule 59 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	KK	96	810	530	143	131	6	0	0

- Molecule 60 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	LL	143	1175	749	222	198	6	0	0

- Molecule 61 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	NN	149	1202	770	228	203	1	0	0

- Molecule 62 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	OO	136	1016	621	199	190	6	0	0

- Molecule 63 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	PP	120	997	635	187	168	7	0	0

- Molecule 64 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	QQ	142	1128	717	213	195	3	0	0

- Molecule 65 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	RR	132	1068	670	199	195	4	0	0

- Molecule 66 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	SS	144	1190	746	241	202	1	0	0

- Molecule 67 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	TT	141	1097	688	211	195	3	0	0

- Molecule 68 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	UU	100	795	498	152	141	4	0	0

- Molecule 69 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	VV	83	636	393	117	121	5	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
VV	3	ASN	SER	conflict	UNP G1TM82
VV	4	ASP	ASN	conflict	UNP G1TM82
VV	33	GLN	PRO	conflict	UNP G1TM82
VV	50	PHE	SER	conflict	UNP G1TM82
VV	75	ALA	SER	conflict	UNP G1TM82
VV	76	ASP	HIS	conflict	UNP G1TM82
VV	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 70 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	WW	129	1034	659	193	176	6	0	0

- Molecule 71 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	XX	141	1098	693	219	183	3	0	0

- Molecule 72 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	YY	124	1011	640	198	168	5	0	0

- Molecule 73 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	ZZ	75	598	382	111	104	1	0	0

- Molecule 74 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	Aa	101	814	507	170	132	5	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	28	ARG	CYS	conflict	UNP G1TFE8
Aa	56	ALA	VAL	conflict	UNP G1TFE8

- Molecule 75 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	Bb	83	651	408	121	115	7	0	0

- Molecule 76 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	Cc	62	488	297	97	92	2	0	0

- Molecule 77 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	Dd	55	459	286	94	74	5	0	0

- Molecule 78 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	Ee	55	443	274	97	71	1	0	0

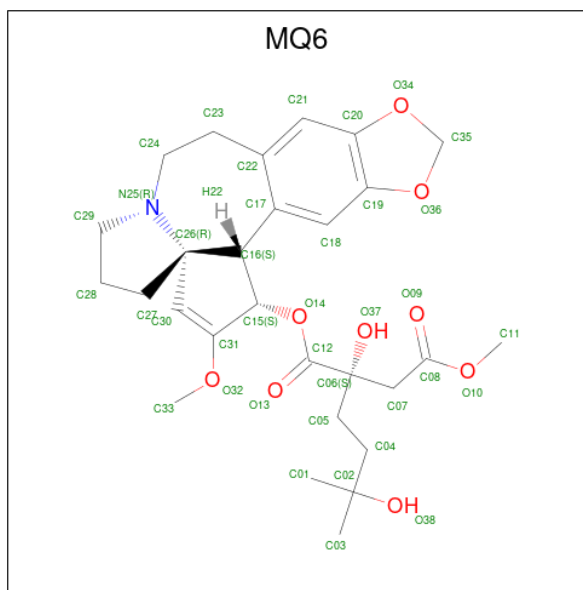
- Molecule 79 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	Gg	313	2436	1535	424	465	12	0	0

- Molecule 80 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
80	5	196	Total Mg 196 196	0
80	7	7	Total Mg 7 7	0
80	8	8	Total Mg 8 8	0
80	9	78	Total Mg 78 78	0
80	A	1	Total Mg 1 1	0
80	I	1	Total Mg 1 1	0
80	P	1	Total Mg 1 1	0
80	V	1	Total Mg 1 1	0
80	a	1	Total Mg 1 1	0
80	g	1	Total Mg 1 1	0
80	j	1	Total Mg 1 1	0
80	LL	1	Total Mg 1 1	0

- Molecule 81 is Harringtonine (CCD ID: MQ6) (formula:  $C_{28}H_{37}NO_9$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
81	5	1	38	28	1	9	0

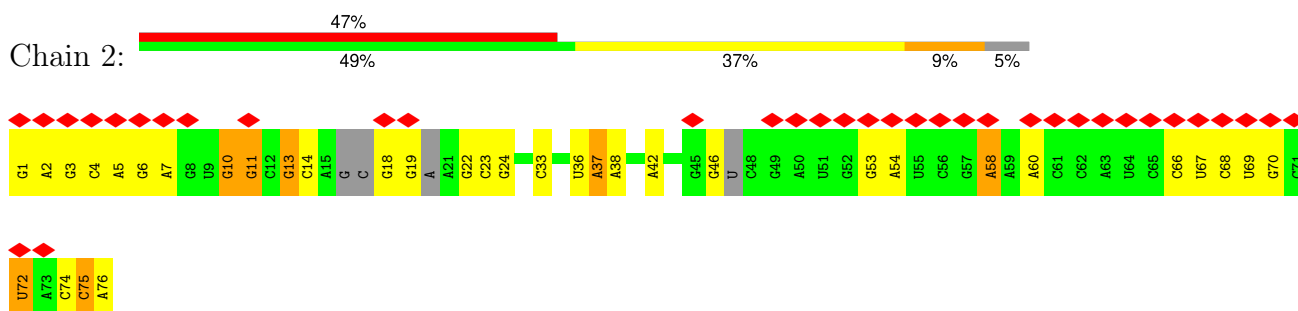
- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
82	g	1	1	1	0
82	j	1	1	1	0
82	m	1	1	1	0
82	o	1	1	1	0
82	p	1	1	1	0
82	Aa	1	1	1	0
82	Dd	1	1	1	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.

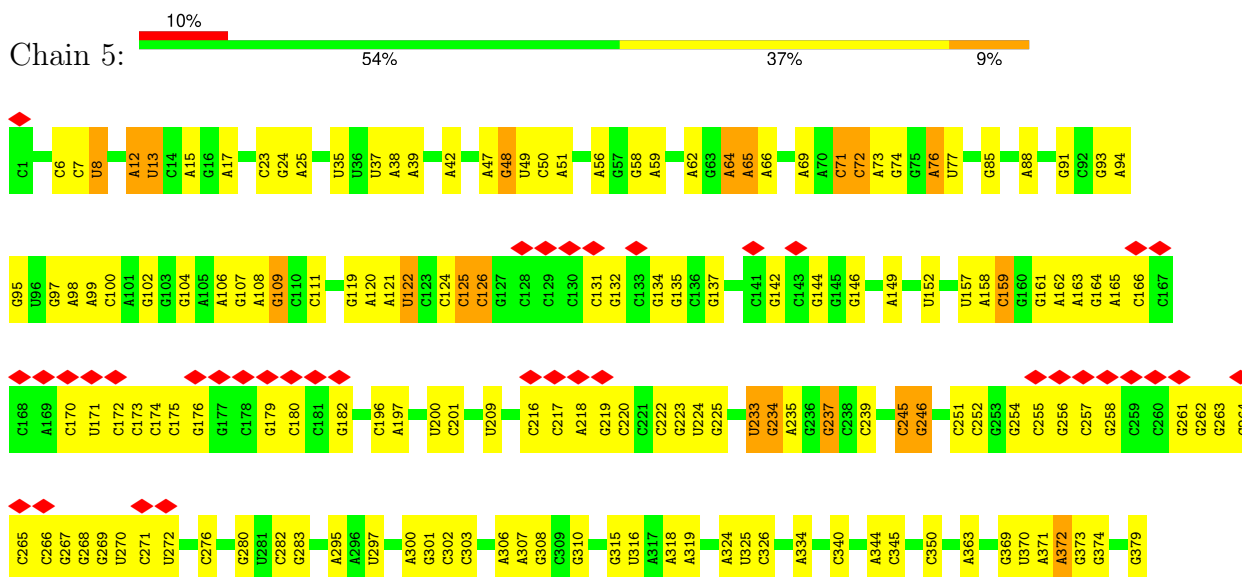
- Molecule 1: P-site tRNA



- Molecule 2: mRNA

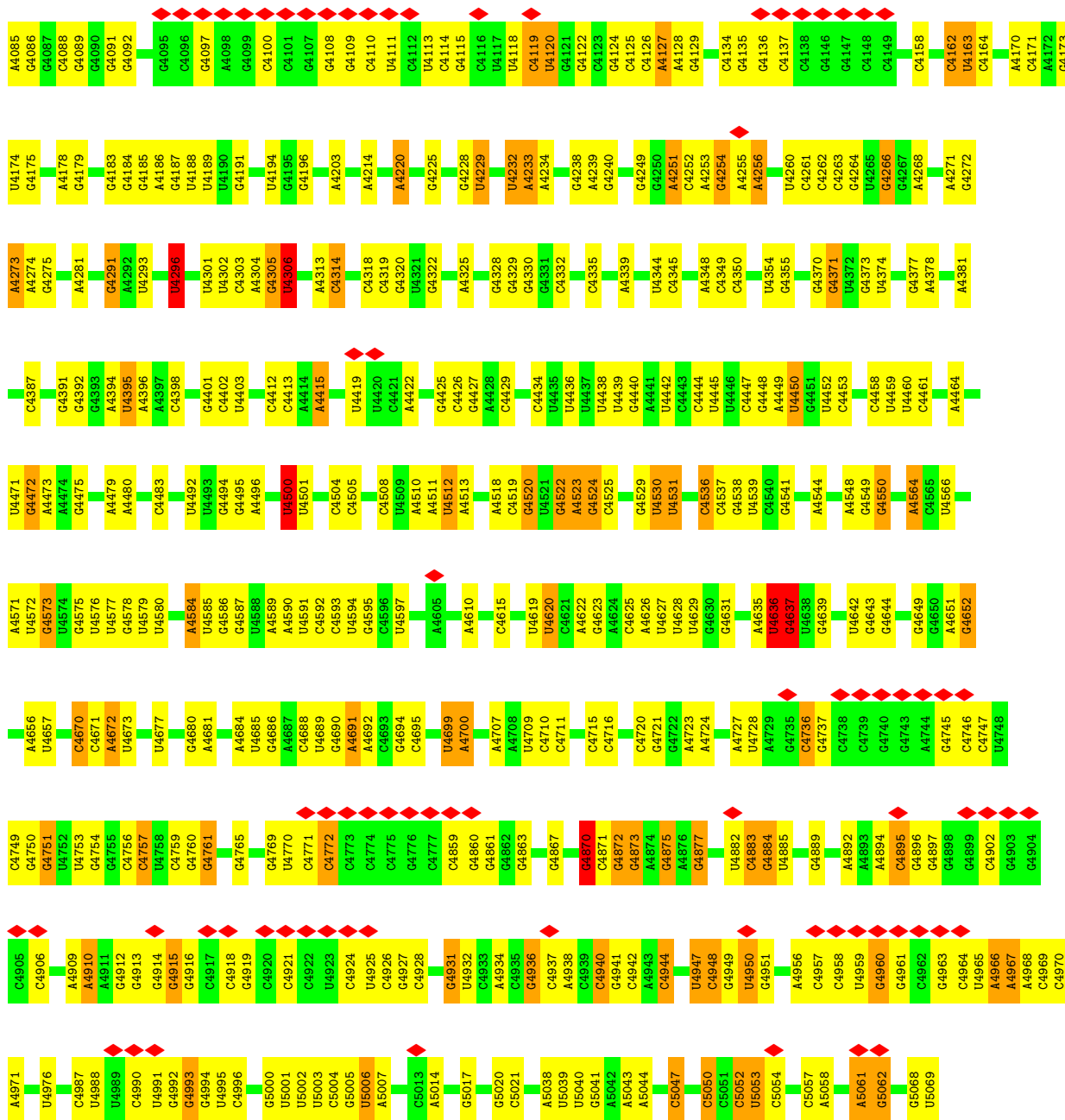


- Molecule 3: 28s rRNA

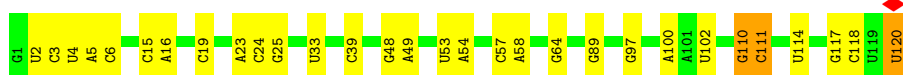




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G3046	A2047	U2048	G2049	G2050	C2051	G2052	G2055	A2056	A2057	G2058	C2059	G2060	G2063	C2068	A2069	C2072	C2073	G2076	G2079	U2080	C2081	G2082	G2083	U2084	G2089	U2090	C2091	G2092	G2093	A2094	G2095	G2096	A2097	G2098	C2099	A2100	G2101	G2102	A2105	G2106	A2107	G2108	A2109	G2110	U2111	C2258	G2259	C2260	G2261	G2262	A2209	A2230	C2231	U2232	A2233	G2234	A2235	G2236	C2237	A2238	G2239	A2240	A2241	G2242	C2243	G2244	A2245	G2246	C2247	A2248	G2249	C2250	A2251	G2252	C2253	A2254	G2255	C2256	A2257	G2258	C2259	A2260	G2261	C2262	A2263	G2264	C2265	A2266	G2267	C2268	A2269	G2270	C2271	A2272	G2273	C2274	A2275	G2276	C2277	A2278	G2279	C2280	A2281	G2282	C2283	A2284	G2285	C2286	A2287	G2288	C2289	A2290	G2291	C2292	A2293	G2294	C2295	A2296	G2297	C2298	A2299	G2300	C2301	A2302	G2303	C2304	A2305	G2306	C2307	A2308	G2309	C2310	A2311	G2312	C2313	A2314	G2315	C2316	A2317	G2318	C2319	A2320	G2321	C2322	A2323	G2324	C2325	A2326	G2327	C2328	A2329	G2330	C2331	A2332	G2333	C2334	A2335	G2336	C2337	A2338	G2339	C2340	A2341	G2342	C2343	A2344	G2345	C2346	A2347	G2348	C2349	A2350	G2351	C2352	A2353	G2354	C2355	A2356	G2357	C2358	A2359	G2360	C2361	A2362	G2363	C2364	A2365	G2366	C2367	A2368	G2369	C2370	A2371	G2372	C2373	A2374	G2375	C2376	A2377	G2378	C2379	A2380	G2381	C2382	A2383	G2384	C2385	A2386	G2387	C2388	A2389	G2390	C2391	A2392	G2393	C2394	A2395	G2396	C2397	A2398	G2399	C2400	A2401	G2402	C2403	A2404	G2405	C2406	A2407	G2408	C2409	A2410	G2411	C2412	A2413	G2414	C2415	A2416	G2417	C2418	A2419	G2420	C2421	A2422	G2423	C2424	A2425	G2426	C2427	A2428	G2429	C2430	A2431	G2432	C2433	A2434	G2435	C2436	A2437	G2438	C2439	A2440	G2441	C2442	A2443	G2444	C2445	A2446	G2447	C2448	A2449	G2450	C2451	A2452	G2453	C2454	A2455	G2456	C2457	A2458	G2459	C2460	A2461	G2462	C2463	A2464	G2465	C2466	A2467	G2468	C2469	A2469	G2470	C2471	A2472	G2473	C2474	A2475	G2476	C2477	A2478	G2479	C2480	A2481	G2482	C2483	A2484	G2485	C2486	A2487	G2488	C2489	A2490	G2491	C2492	A2493	G2494	C2495	A2496	G2497	C2498	A2499	G2500	C2501	A2502	G2503	C2504	A2505	G2506	C2507	A2508	G2509	C2510	A2511	G2512	C2513	A2514	G2515	C2516	A2517	G2518	C2519	A2520	G2521	C2522	A2523	G2524	C2525	A2526	G2527	C2528	A2529	G2530	C2531	A2532	G2533	C2534	A2535	G2536	C2537	A2538	G2539	C2540	A2541	G2542	C2543	A2544	G2545	C2546	A2547	G2548	C2549	A2550	G2551	C2552	A2553	G2554	C2555	A2556	G2557	C2558	A2559	G2560	C2561	A2562	G2563	C2564	A2565	G2566	C2567	A2568	G2569	C2570	A2571	G2572	C2573	A2574	G2575	C2576	A2577	G2578	C2579	A2580	G2581	C2582	A2583	G2584	C2585	A2586	G2587	C2588	A2589	G2590	C2591	A2592	G2593	C2594	A2595	G2596	C2597	A2598	G2599	C2600	A2601	G2602	C2603	A2604	G2605	C2606	A2607	G2608	C2609	A2610	G2611	C2612	A2613	G2614	C2615	A2616	G2617	C2618	A2619	G2620	C2621	A2622	G2623	C2624	A2625	G2626	C2627	A2628	G2629	C2630	A2631	G2632	C2633	A2634	G2635	C2636	A2637	G2638	C2639	A2640	G2641	C2642	A2643	G2644	C2645	A2646	G2647	C2648	A2649	G2650	C2651	A2652	G2653	C2654	A2655	G2656	C2657	A2658	G2659	C2660	A2661	G2662	C2663	A2664	G2665	C2666	A2667	G2668	C2669	A2669	G2670	C2671	A2672	G2673	C2674	A2675	G2676	C2677	A2678	G2679	C2680	A2681	G2682	C2683	A2684	G2685	C2686	A2687	G2688	C2689	A2689	G2690	C2691	A2692	G2693	C2694	A2695	G2696	C2697	A2698	G2699	C2700	A2701	G2702	C2703	A2704	G2705	C2706	A2707	G2708	C2709	A2710	G2711	C2712	A2713	G2714	C2715	A2716	G2717	C2718	A2719	G2720	C2721	A2722	G2723	C2724	A2725	G2726	C2727	A2728	G2729	C2730	A2731	G2732	C2733	A2734	G2735	C2736	A2737	G2738	C2739	A2740	G2741	C2742	A2743	G2744	C2745	A2746	G2747	C2748	A2749	G2750	C2751	A2752	G2753	C2754	A2755	G2756	A2757	G2758	C2759	A2760	G2761	C2762	A2763	G2764	A2765	G2766	C2767	A2768	G2769	C2770	A2771	G2772	C2773	A2774	G2775	C2776	A2777	G2778	C2779	A2779	G2780	C2781	A2782	G2783	C2784	A2785	G2786	C2787	A2788	G2789	C2790	A2791	G2792	C2793	A2794	G2795	C2796	A2797	G2798	C2799	A2800	G2801	C2802	A2803	G2804	C2805	A2806	G2807	C2808	A2809	G2810	C2811	A2812	G2813	C2814	A2815	G2816	C2817	A2818	G2819	C2820	A2821	G2822	C2823	A2824	G2825	C2826	A2827	G2828	C2829	A2829	G2830	C2831	A2832	G2833	C2834	A2835	G2836	C2837	A2838	G2839	C2840	A2841	G2842	C2843	A2844	G2845	C2846	A2847	G2848	C2849	A2850	G2851	C2852	A2853	G2854	C2855	A2856	G2857	C2858	A2859	G2860	C2861	A2862	G2863	C2864	A2865	G2866	C2867	A2868	G2869	C2870	A2871	G2872	C2873	A2874	G2875	C2876	A2877	G2878	C2879	A2880	G2881	C2882	A2883	G2884	C2885	A2886	G2887	C2888	A2889	G2890	C2891	A2892	G2893	C2894	A2895	G2896	C2897	A2898	G2899	C2900	A2901	G2902	C2903	A2904	G2905	C2906	A2907	G2908	C2909	A2910	G2911	C2912	A2913	G2914	C2915	A2916	G2917	C2918	A2919	G2920	C2921	A2922	G2923	C2924	A2925	G2926	C2927	A2928	G2929	C2930	A2931	G2932	C2933	A2934	G2935	C2936	A2937	G2938	C2939	A2940	G2941	C2942	A2943	G2944	C2945	A2946	G2947	C2948	A2949	G2950	C2951	A2952	G2953	C2954	A2955	G2956	C2957	A2958	G2959	C2960	A2961	G2962	C2963	A2964	G2965	C2966	A2967	G2968	C2969	A2970	G2971	C2972	A2973	G2974	C2975	A2976	G2977	C2978	A2979	G2980	C2981	A2982	G2983	C2984	A2985	G2986	C2987	A2988	G2989	C2990	A2991	G2992	C2993	A2994	G2995	C2996	A2997	G2998	C2999	A3000	G3001	C3002	A3003	G3004	C3005	A3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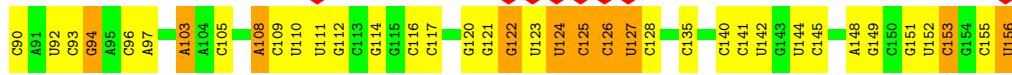
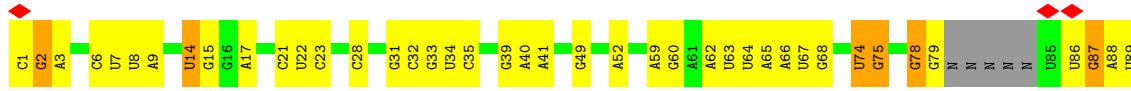


● Molecule 4: 5S rRNA

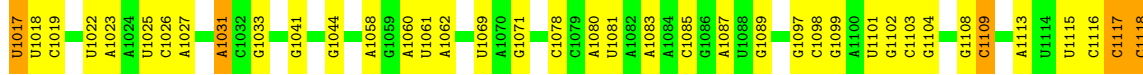
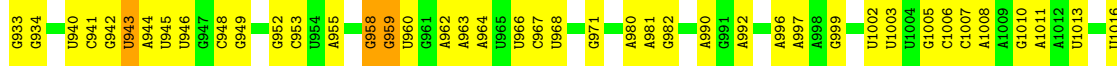
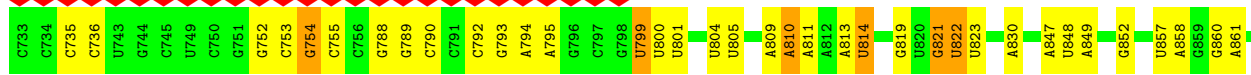
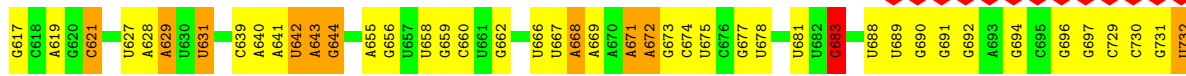
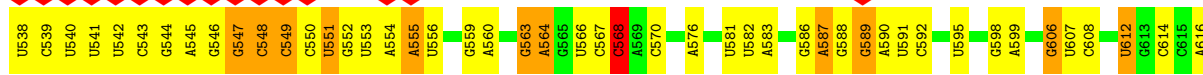
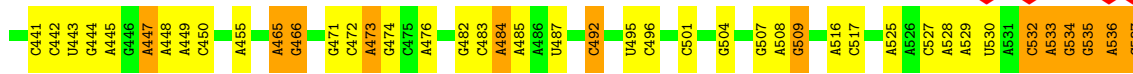
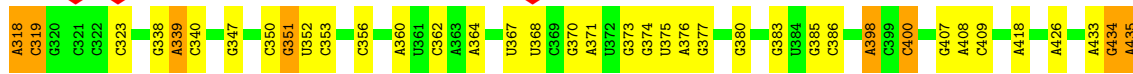
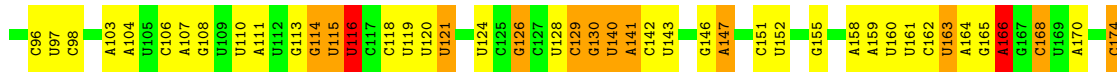
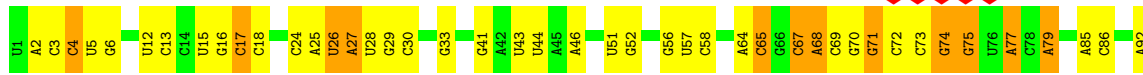


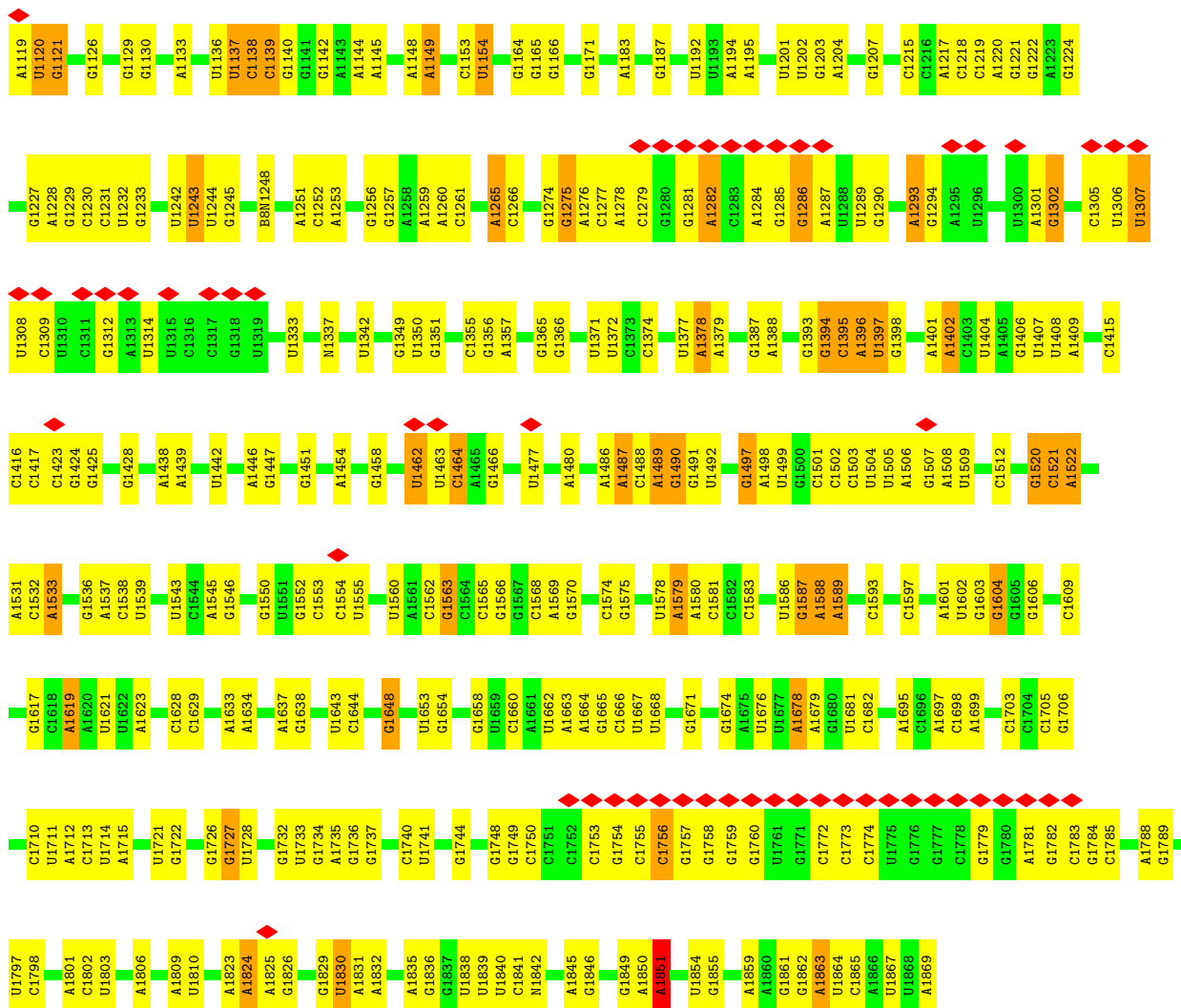
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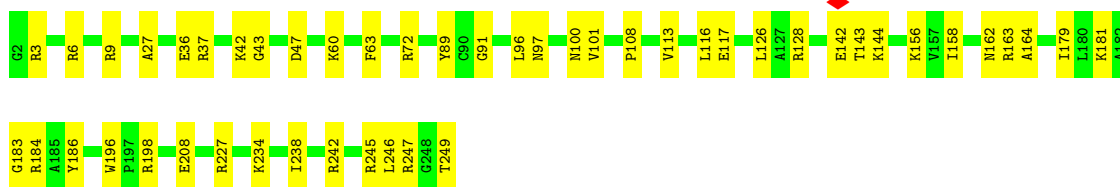
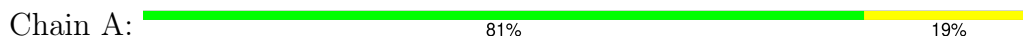


• Molecule 6: 18S rRNA

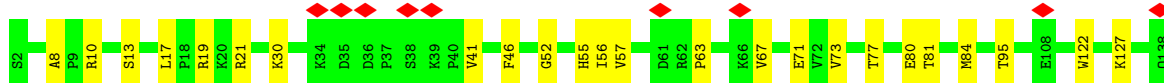
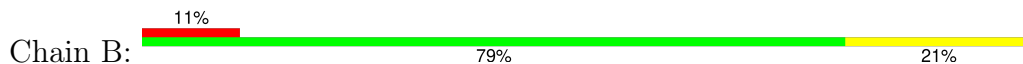


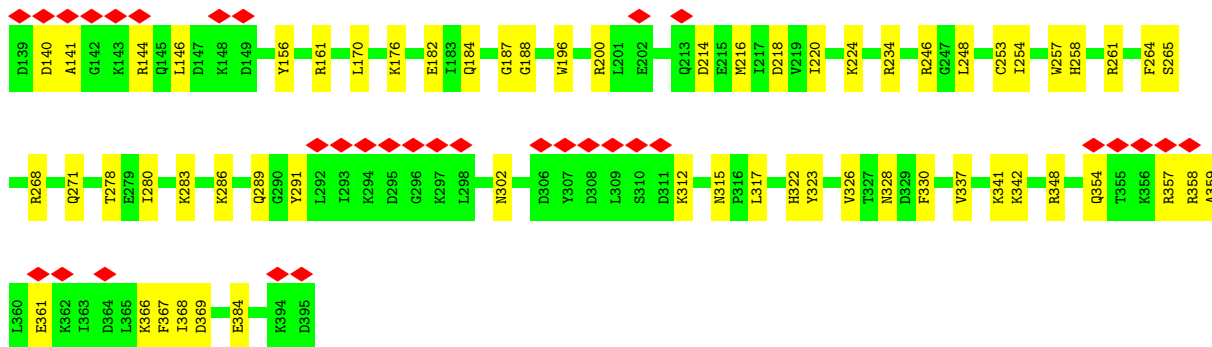


• Molecule 7: 60S ribosomal protein L8

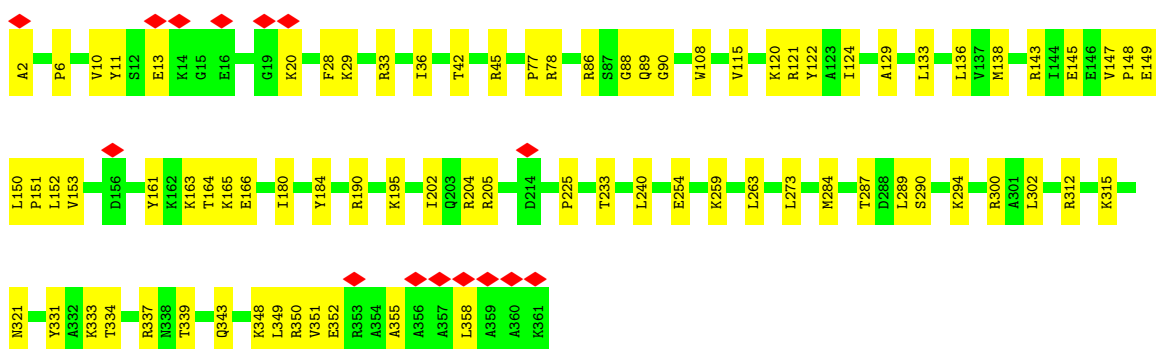
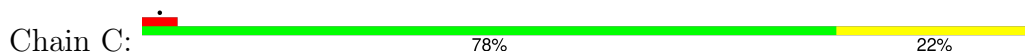


• Molecule 8: 60S ribosomal protein L3

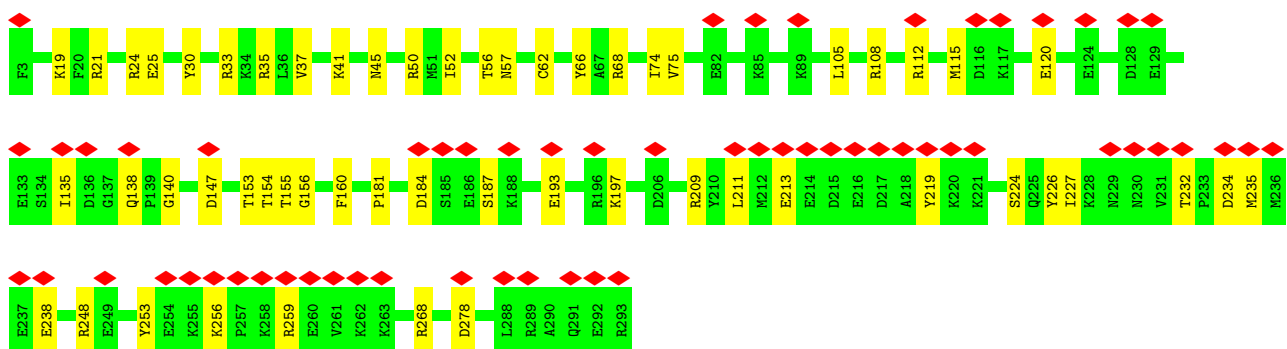
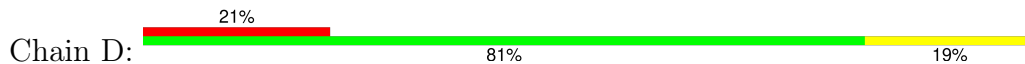




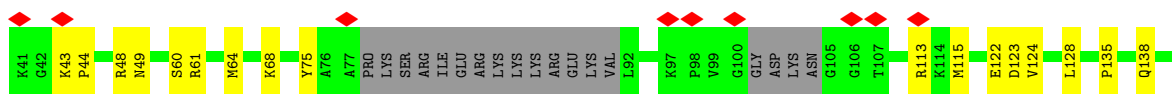
• Molecule 9: 60S ribosomal protein L4

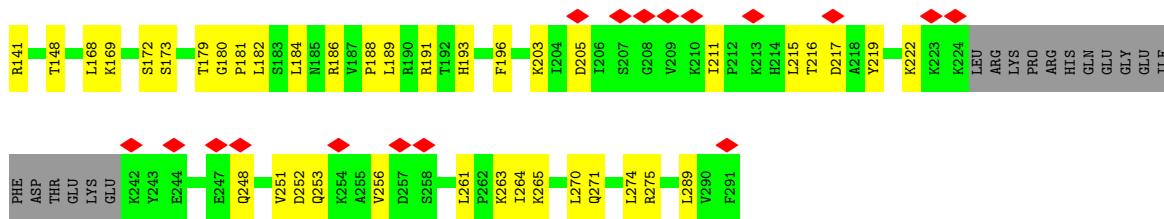


• Molecule 10: Ribosomal\_L18\_c domain-containing protein



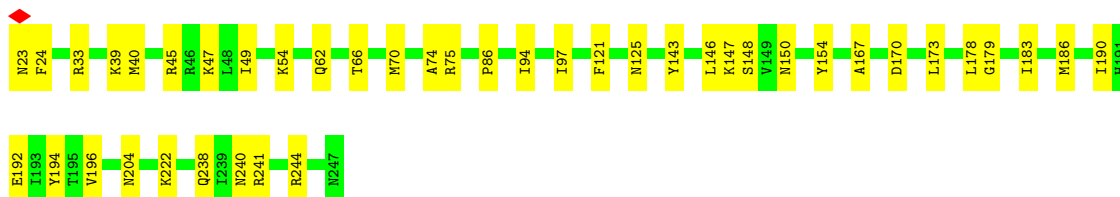
• Molecule 11: 60S ribosomal protein L6





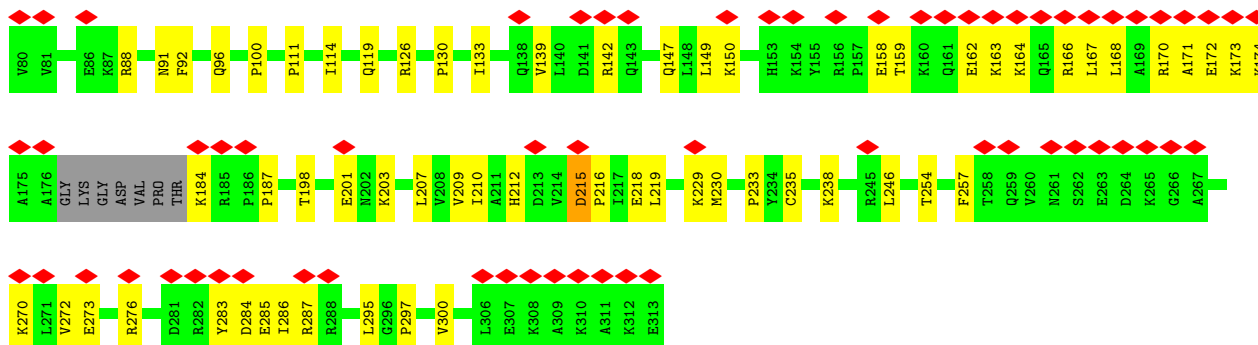
- Molecule 12: 60S ribosomal protein L7

Chain F: 81% 19%



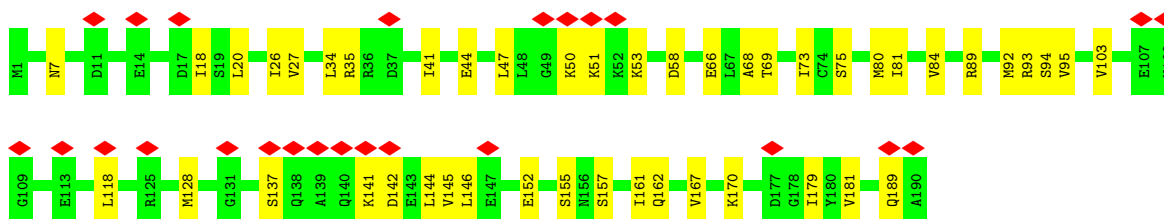
- Molecule 13: 60S ribosomal protein L7a

Chain G: 27% 71% 2%



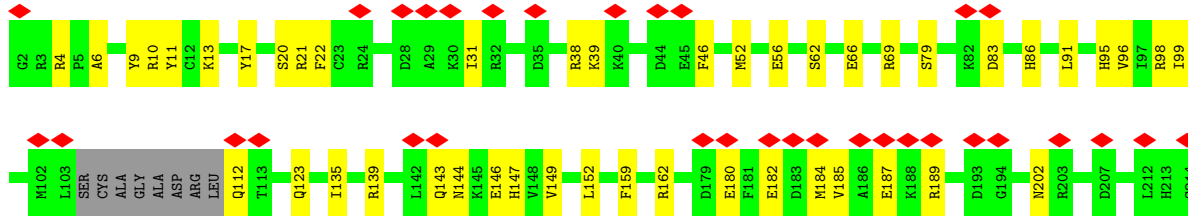
- Molecule 14: 60S ribosomal protein L9

Chain H: 13% 76% 11%

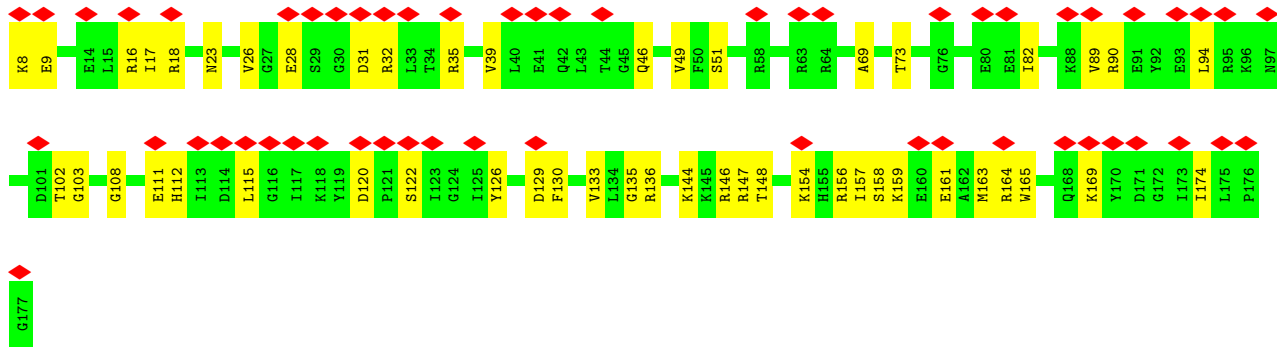


- Molecule 15: Ribosomal protein L10

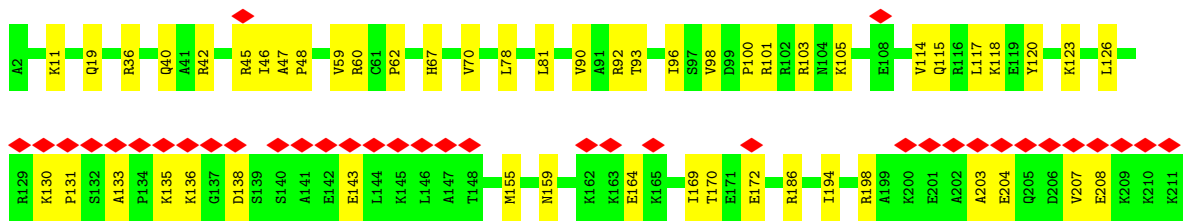
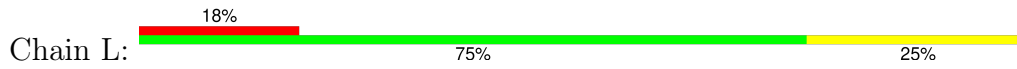
Chain I: 15% 75% 10%



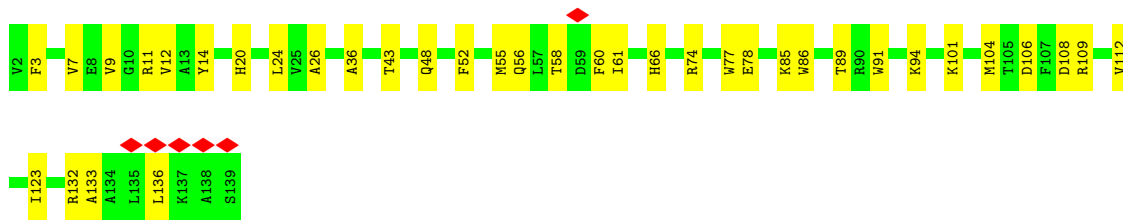
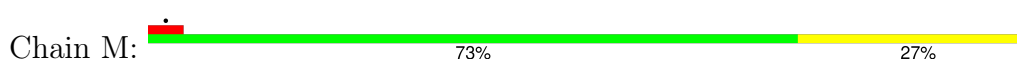
• Molecule 16: 60S ribosomal protein L11



• Molecule 17: 60S ribosomal protein L13

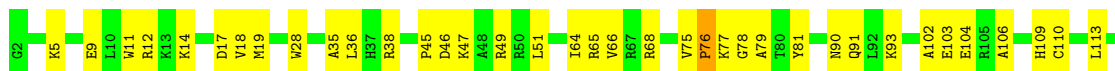


• Molecule 18: 60S ribosomal protein L14

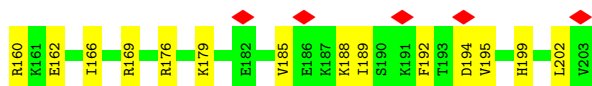
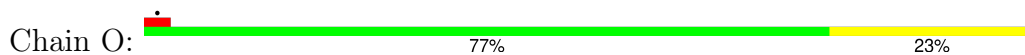


• Molecule 19: 60S ribosomal protein L15

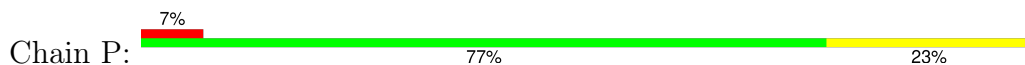




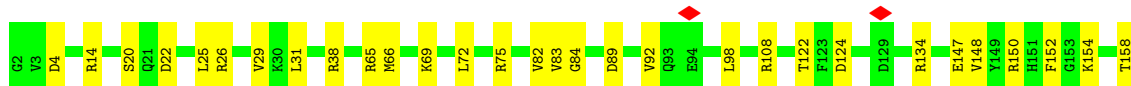
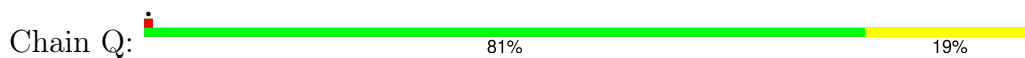
• Molecule 20: 60S ribosomal protein L13a



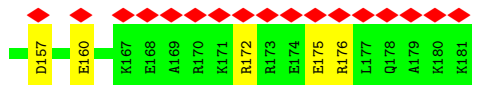
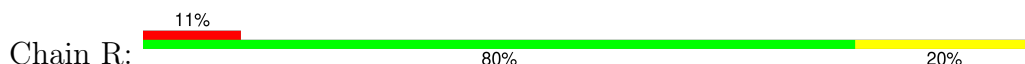
• Molecule 21: 60S ribosomal protein L17



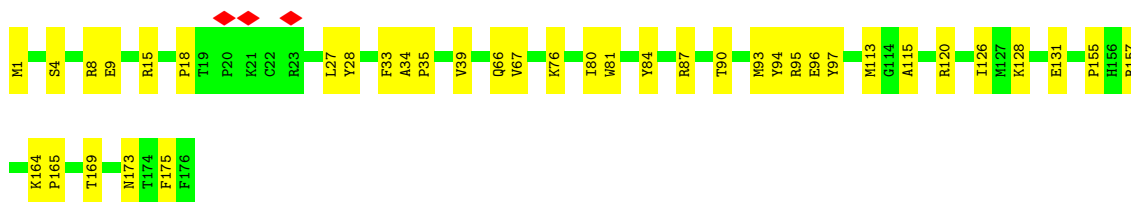
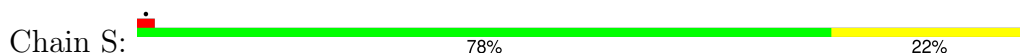
• Molecule 22: 60S ribosomal protein L18



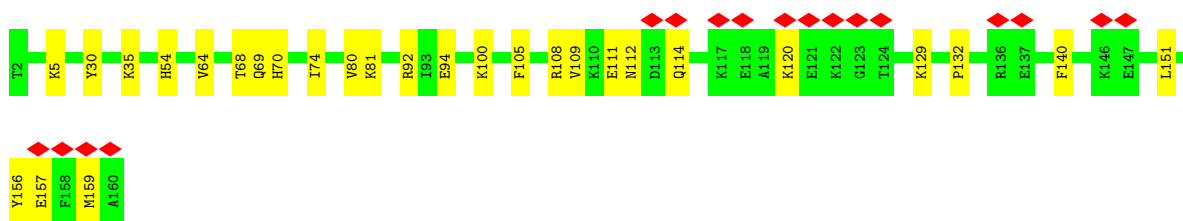
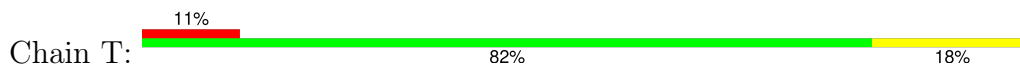
• Molecule 23: 60S ribosomal protein L19



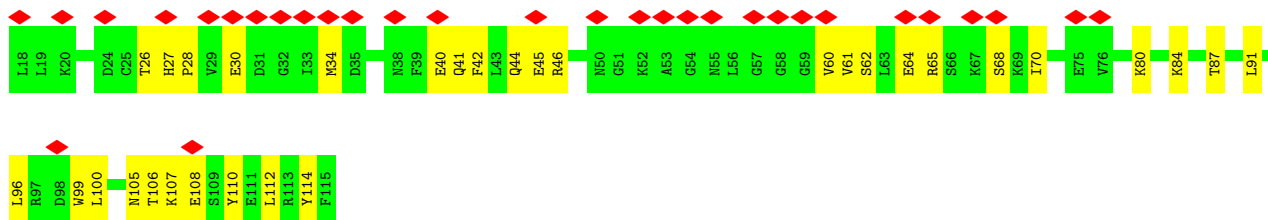
• Molecule 24: 60S ribosomal protein L18a



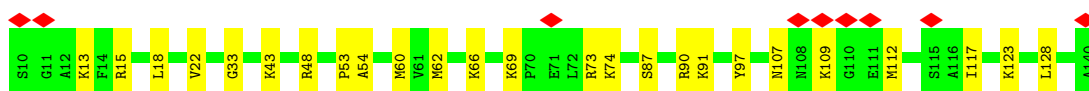
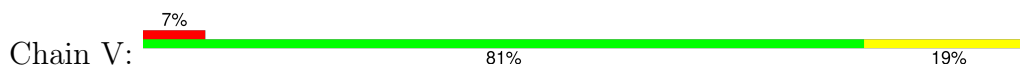
• Molecule 25: 60S ribosomal protein L21



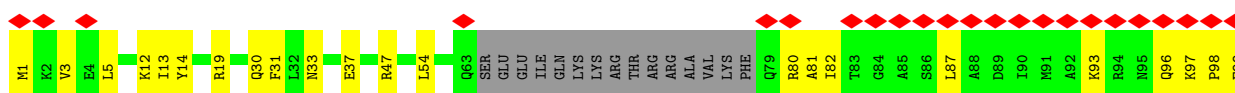
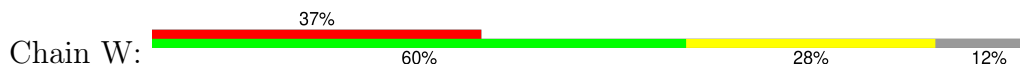
• Molecule 26: 60S ribosomal protein L22

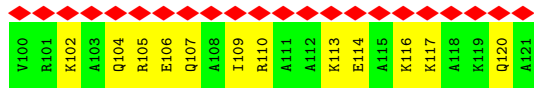


• Molecule 27: 60S ribosomal protein L23

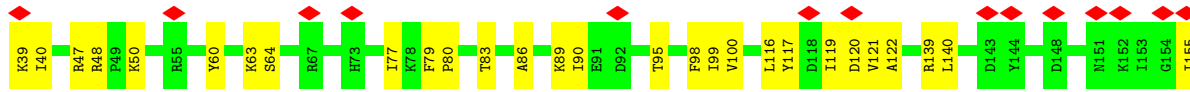
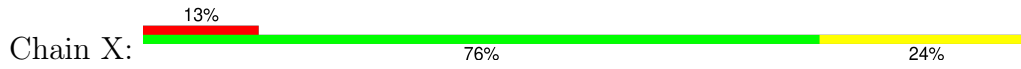


• Molecule 28: Ribosomal protein L24

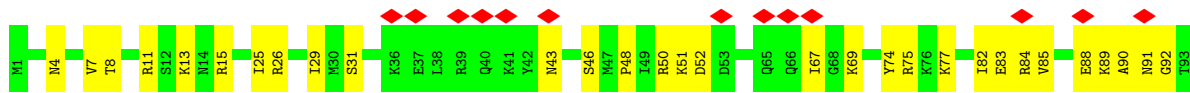




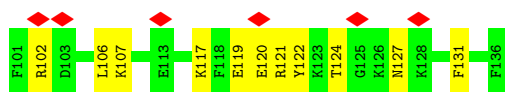
• Molecule 29: 60S ribosomal protein L23a



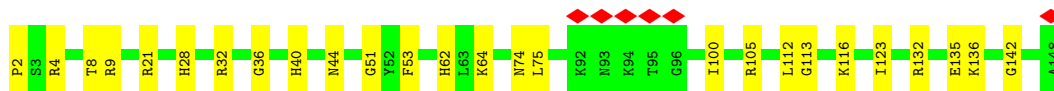
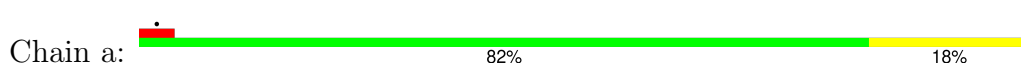
• Molecule 30: 60S ribosomal protein L26



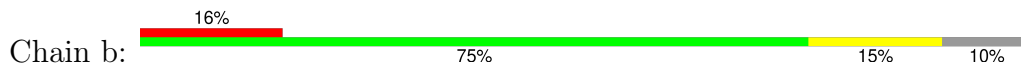
• Molecule 31: 60S ribosomal protein L27

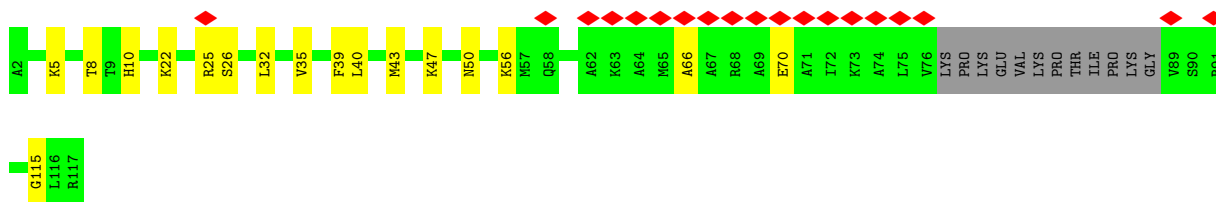


• Molecule 32: 60S ribosomal protein L27a

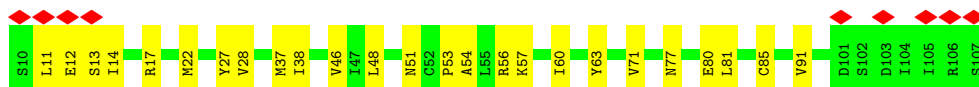
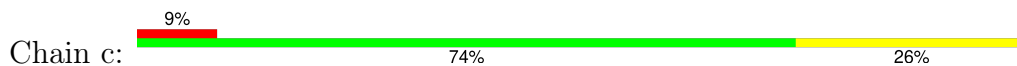


• Molecule 33: 60S ribosomal protein L29

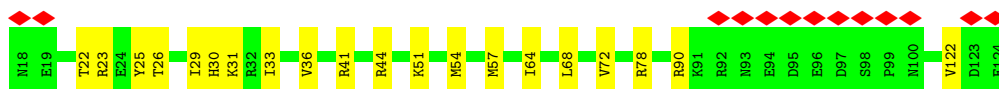
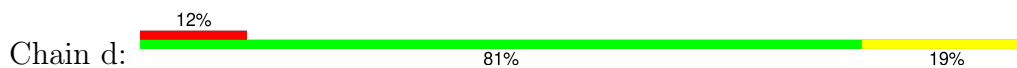




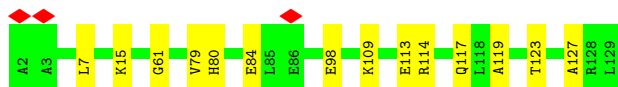
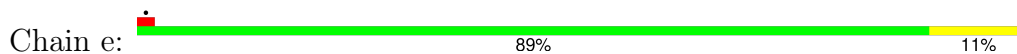
- Molecule 34: 60S ribosomal protein L30



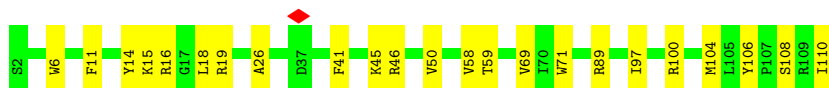
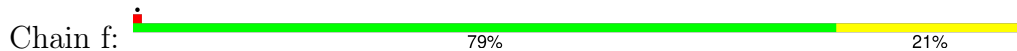
- Molecule 35: 60S ribosomal protein L31



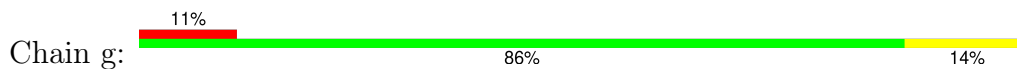
- Molecule 36: 60S ribosomal protein L32



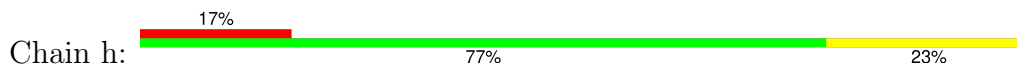
- Molecule 37: 60S ribosomal protein L35a

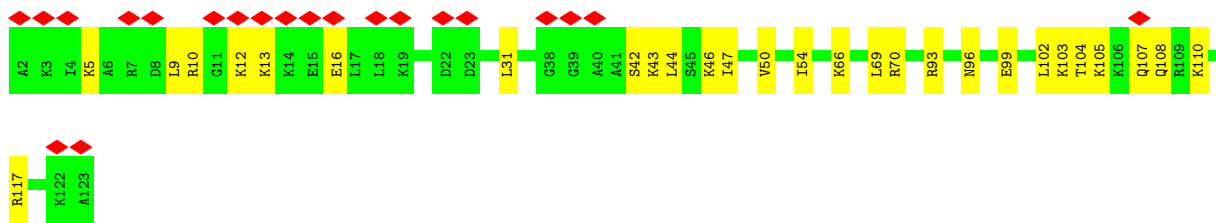


- Molecule 38: 60S ribosomal protein L34

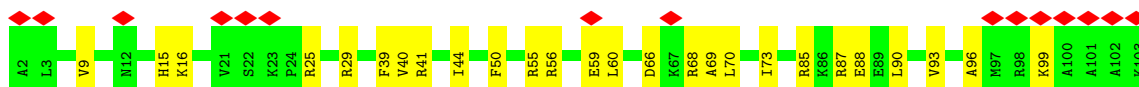
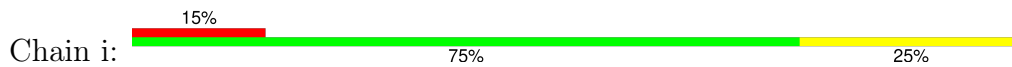


- Molecule 39: 60S ribosomal protein L35

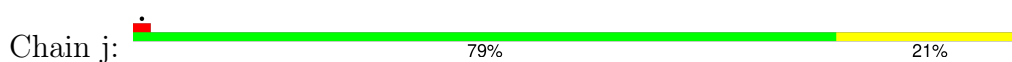




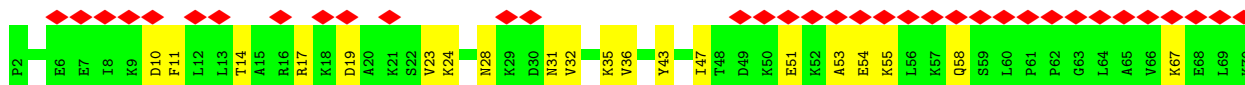
- Molecule 40: 60S ribosomal protein L36



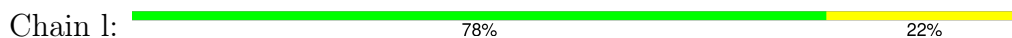
- Molecule 41: 60S ribosomal protein L37



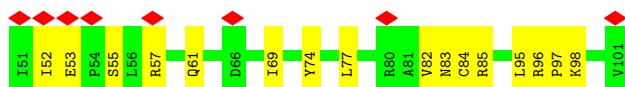
- Molecule 42: 60S ribosomal protein L38



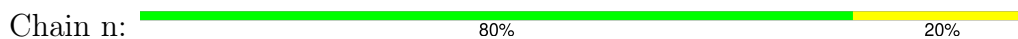
- Molecule 43: 60S ribosomal protein L39



- Molecule 44: 60S ribosomal protein L40

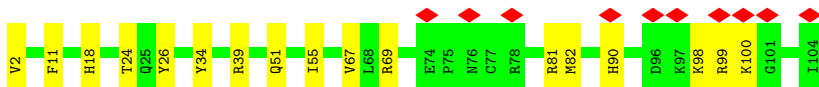
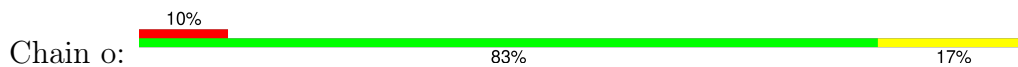


- Molecule 45: eL41

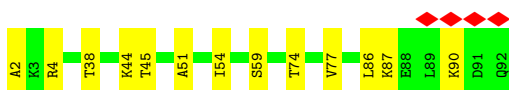
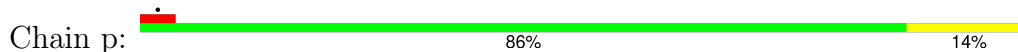




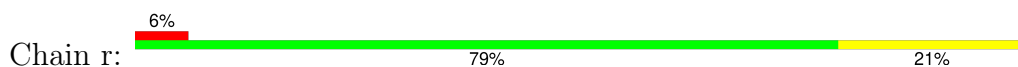
- Molecule 46: 60S ribosomal protein L36a



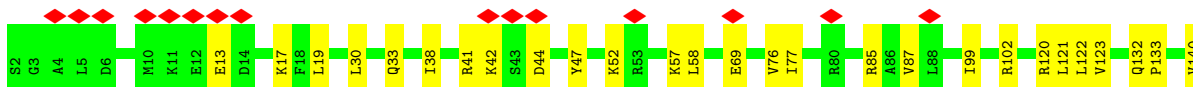
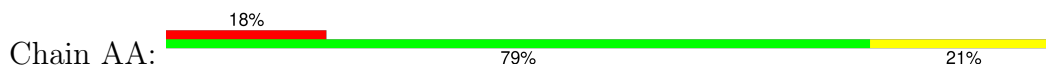
- Molecule 47: 60S ribosomal protein L37a



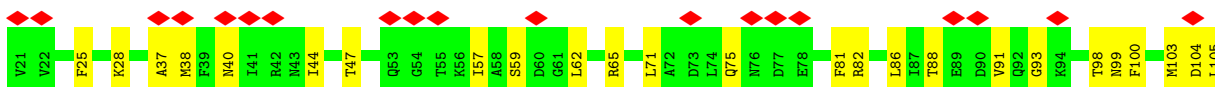
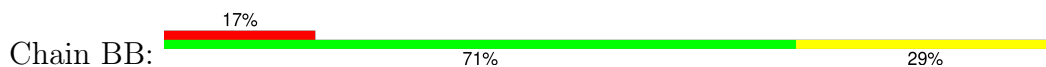
- Molecule 48: 60S ribosomal protein L28

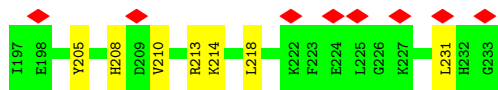


- Molecule 49: 40S\_SA\_C domain-containing protein

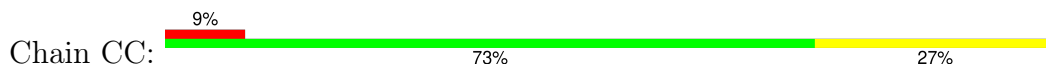


- Molecule 50: 40S ribosomal protein S3a

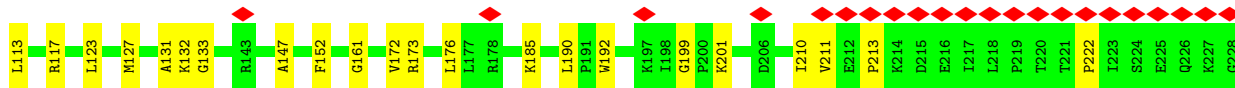
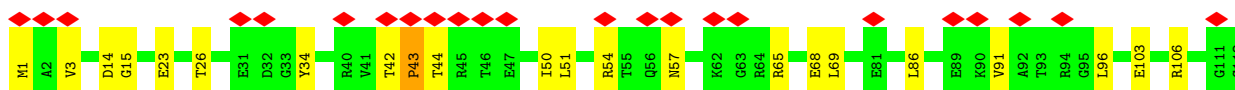
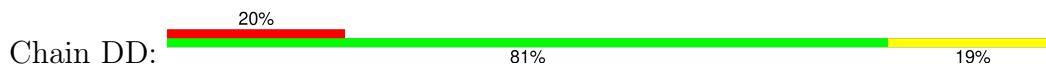




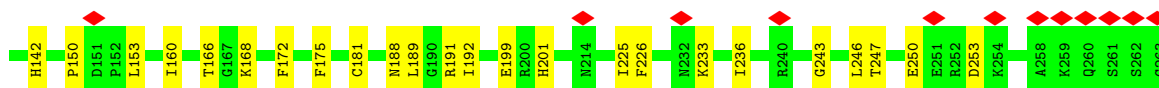
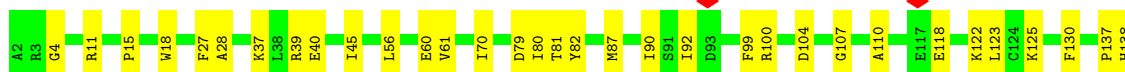
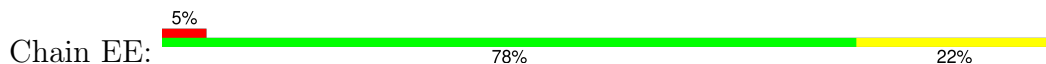
- Molecule 51: 40S ribosomal protein S2



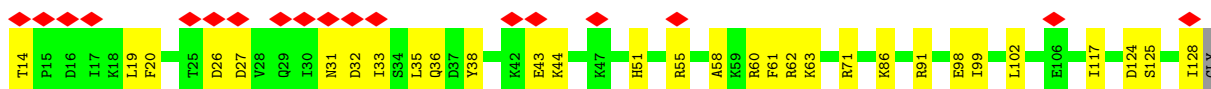
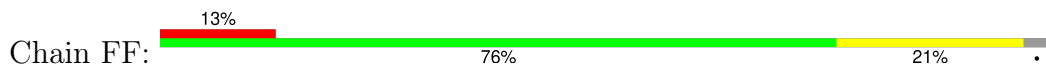
- Molecule 52: 40S ribosomal protein S3



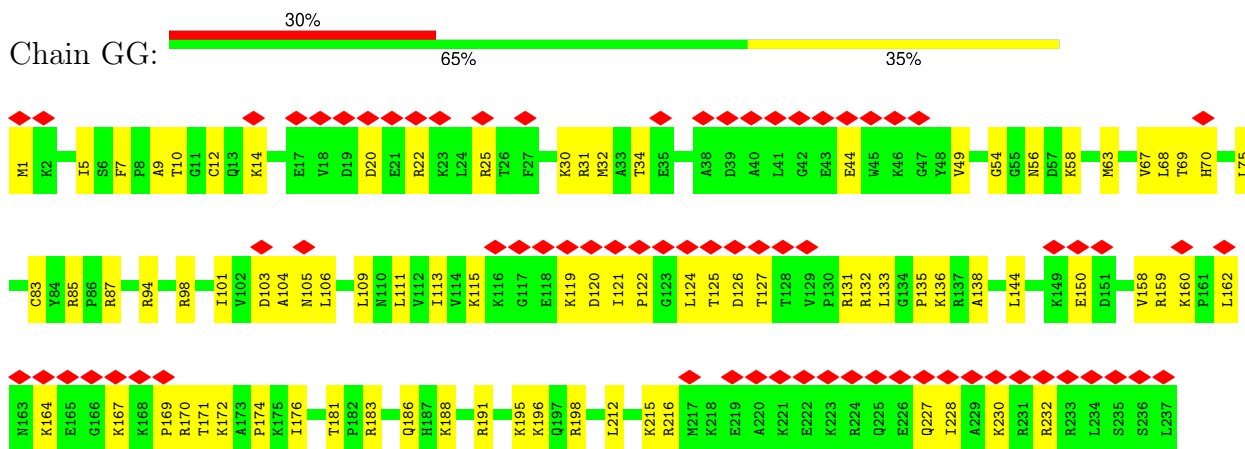
- Molecule 53: 40S ribosomal protein S4



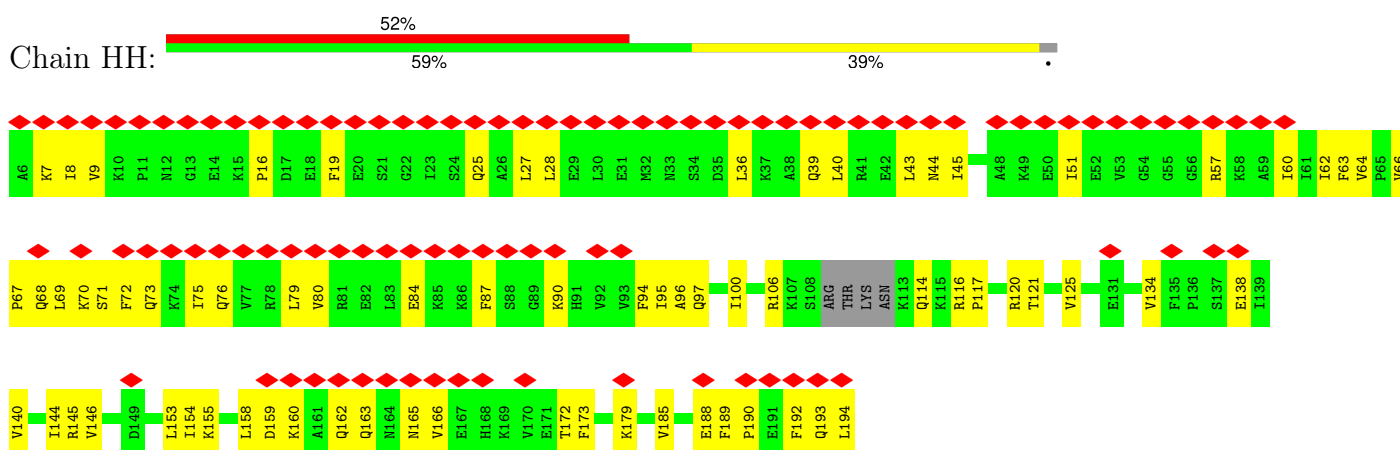
- Molecule 54: Ribosomal protein S5



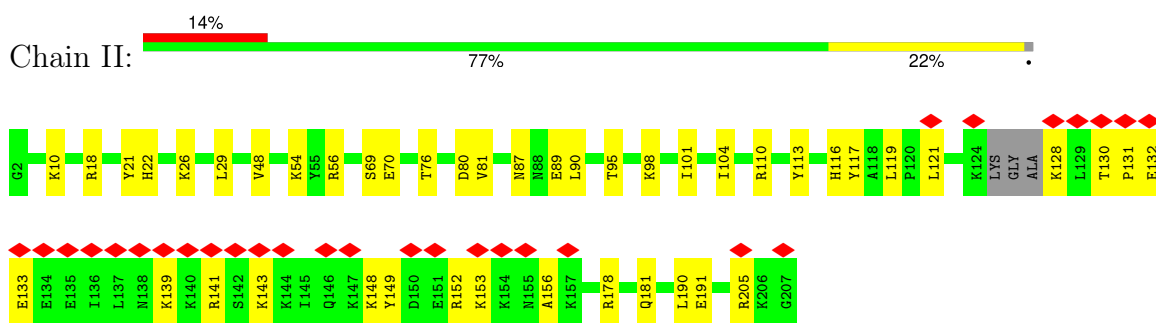
- Molecule 55: 40S ribosomal protein S6



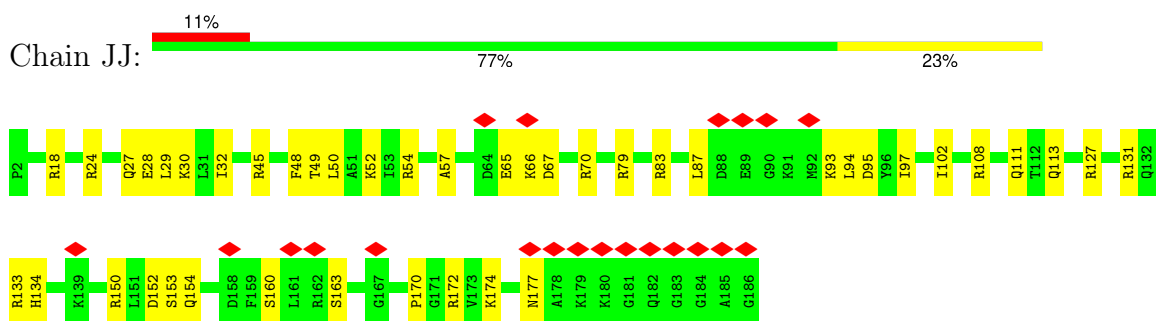
• Molecule 56: 40S ribosomal protein S7



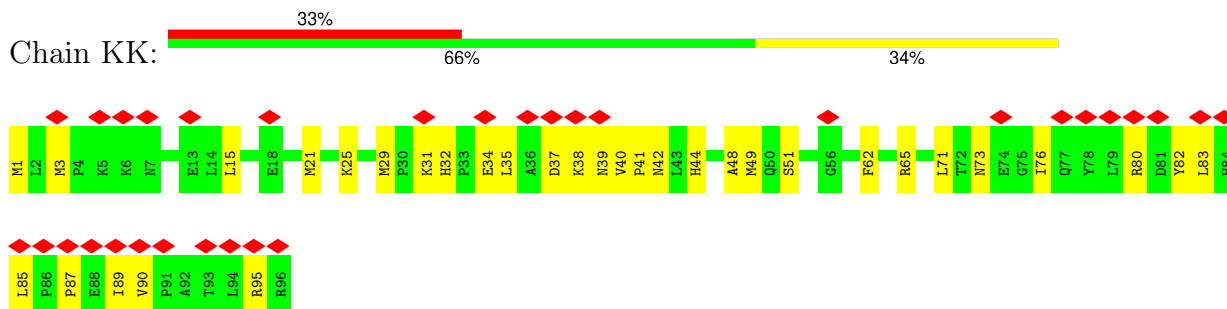
• Molecule 57: 40S ribosomal protein S8



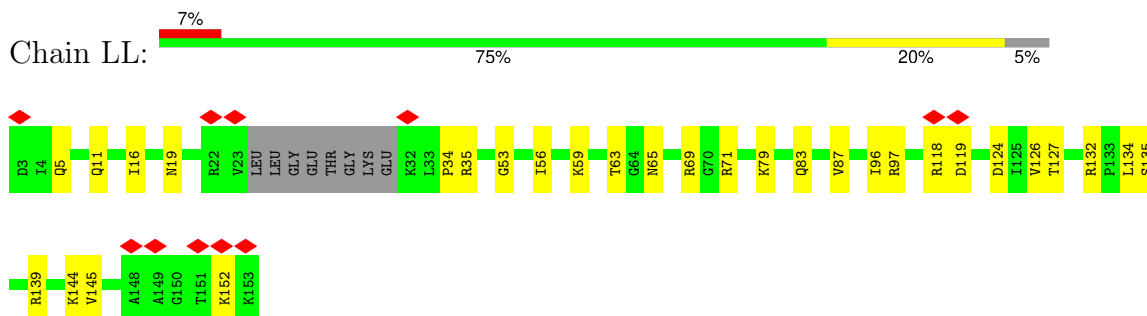
• Molecule 58: 40S ribosomal protein S9



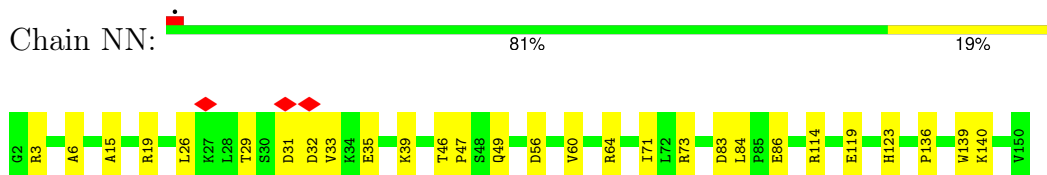
- Molecule 59: 40S ribosomal protein S10



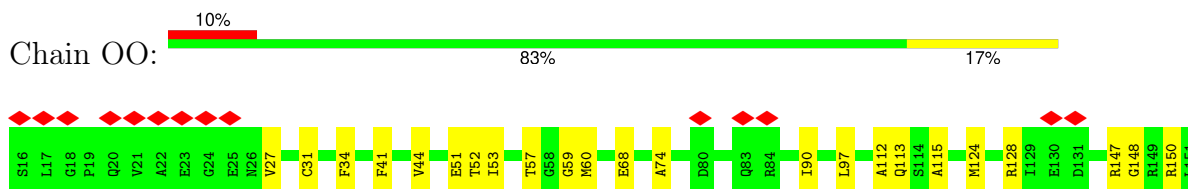
- Molecule 60: 40S ribosomal protein S11



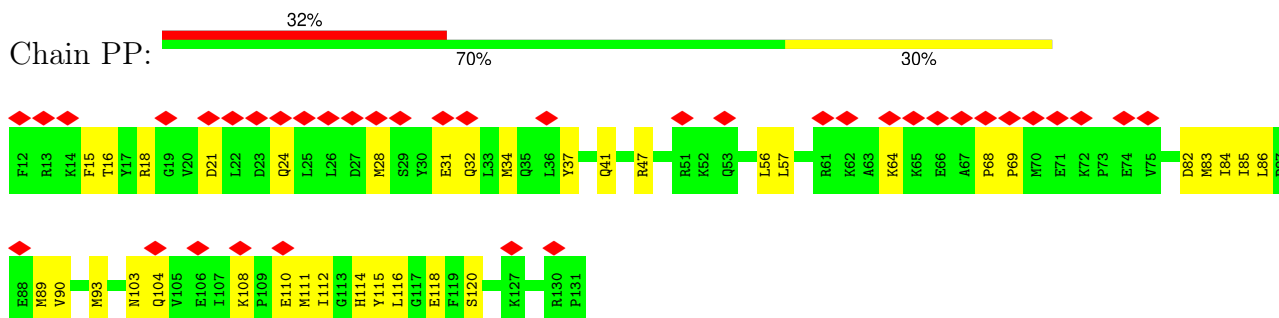
- Molecule 61: 40S ribosomal protein S13



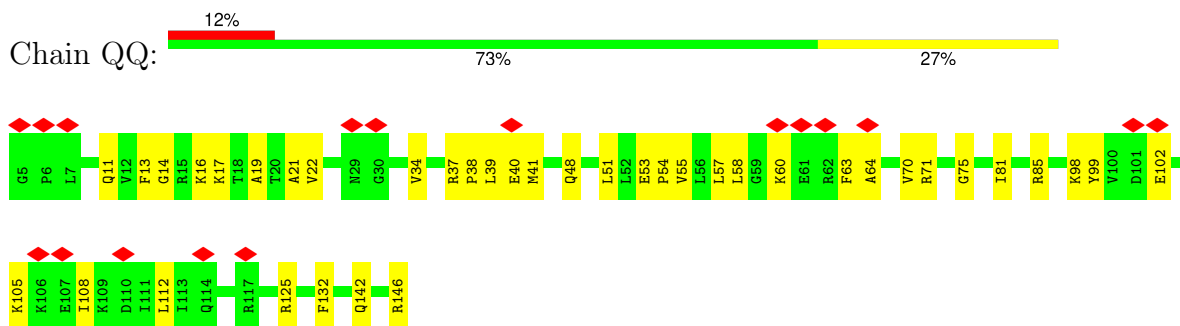
- Molecule 62: 40S ribosomal protein S14



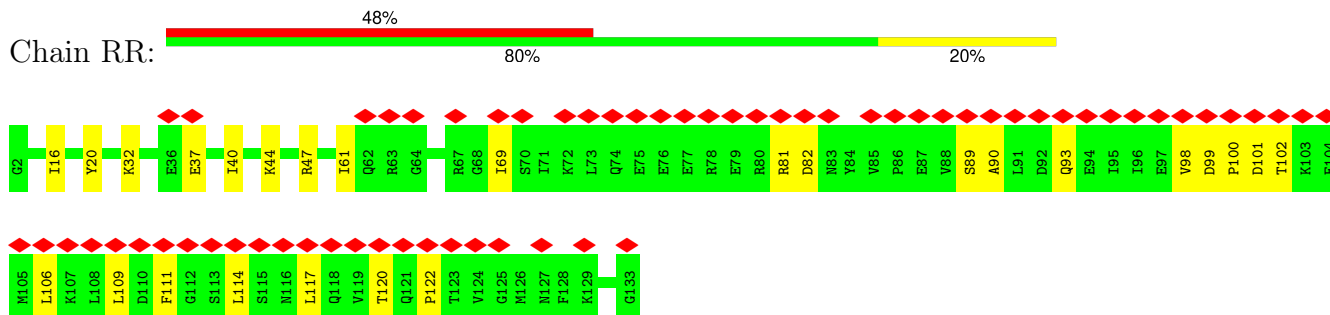
- Molecule 63: 40S ribosomal protein S15



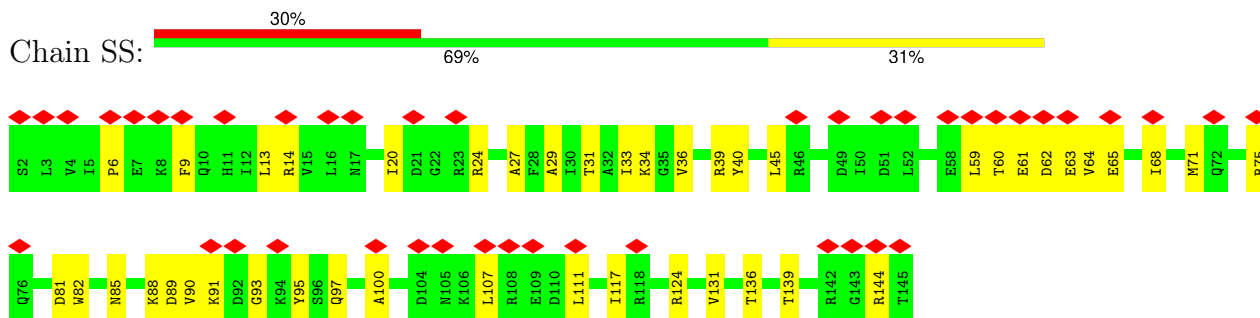
- Molecule 64: 40S ribosomal protein S16



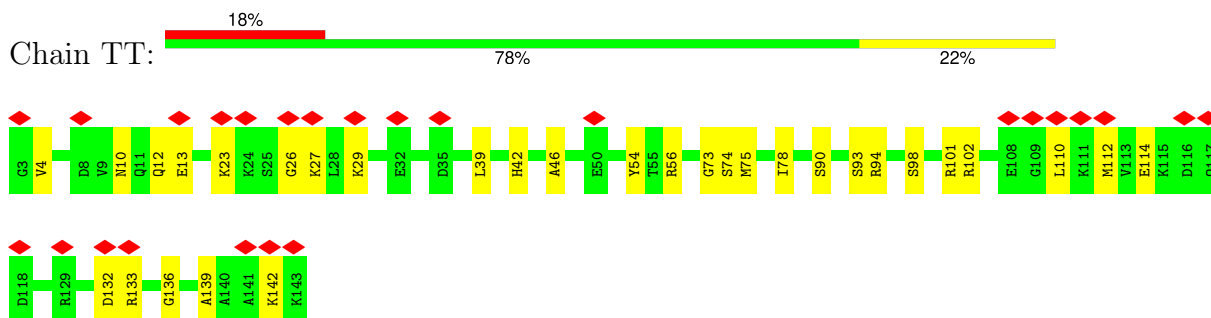
- Molecule 65: 40S ribosomal protein S17



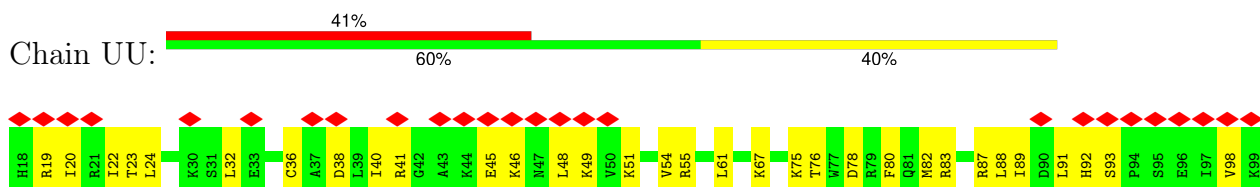
- Molecule 66: 40S ribosomal protein S18

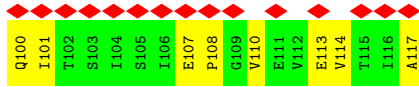


- Molecule 67: 40S ribosomal protein S19

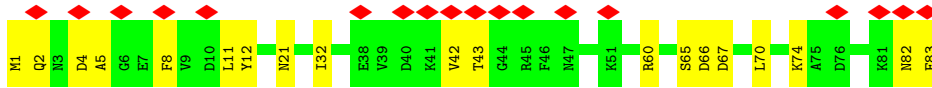
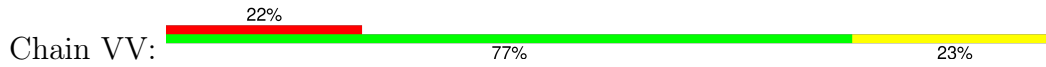


- Molecule 68: 40S ribosomal protein S20

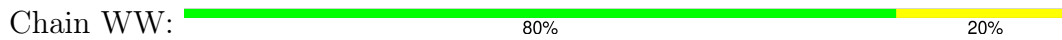




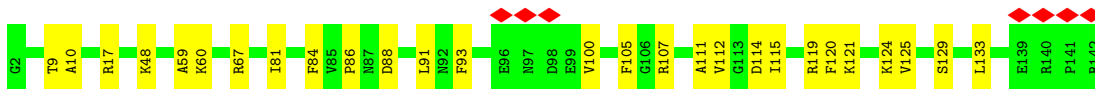
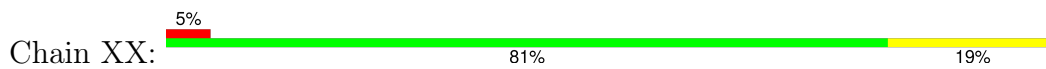
- Molecule 69: eS21



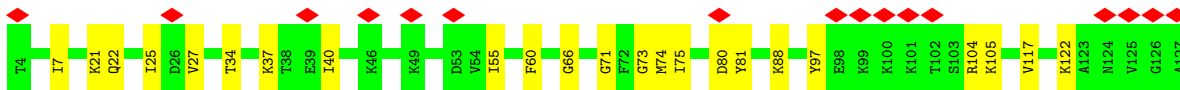
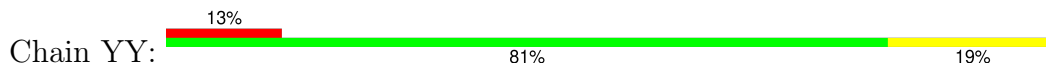
- Molecule 70: 40S ribosomal protein S15a



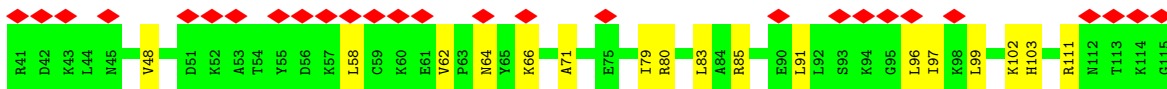
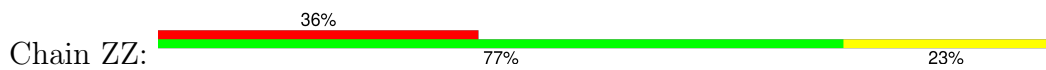
- Molecule 71: 40S ribosomal protein S23



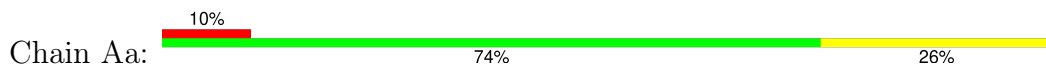
- Molecule 72: 40S ribosomal protein S24



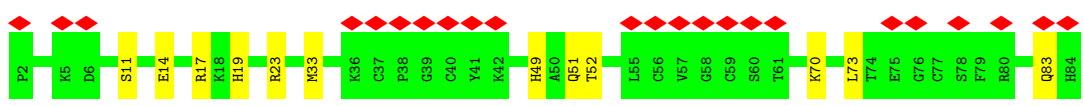
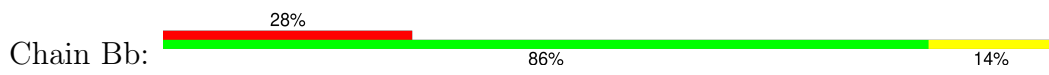
- Molecule 73: 40S ribosomal protein S25



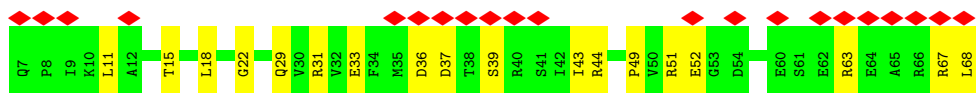
- Molecule 74: eS26



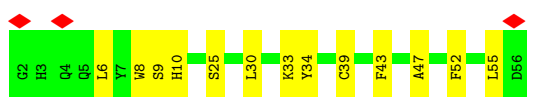
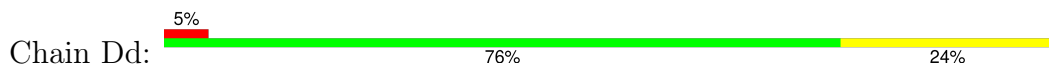
- Molecule 75: 40S ribosomal protein S27



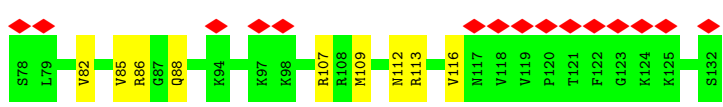
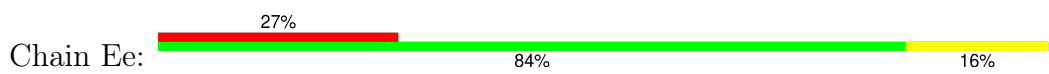
• Molecule 76: 40S ribosomal protein S28



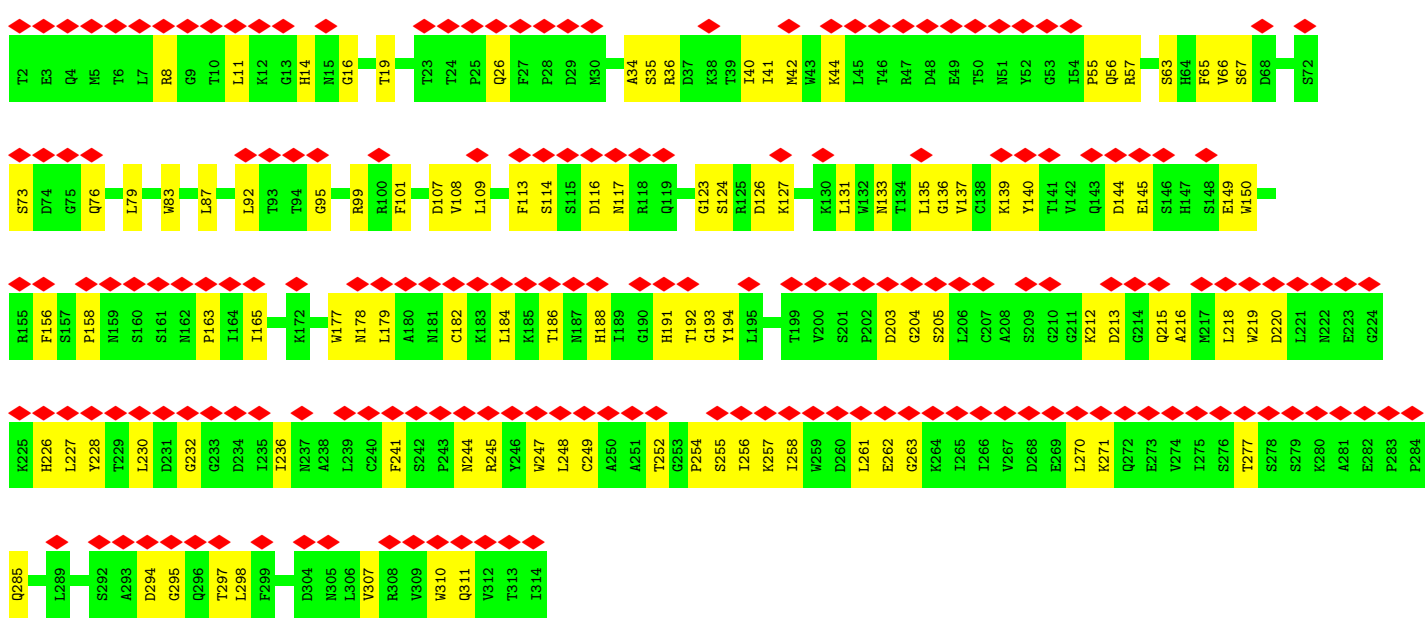
• Molecule 77: 40S ribosomal protein S29



• Molecule 78: 40S ribosomal protein S30



• Molecule 79: Receptor of activated protein C kinase 1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	107057	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.197	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.037	Depositor
Map size ( $\text{\AA}$ )	651.84, 651.84, 651.84	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.358, 1.358, 1.358	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: B8N, 2MG, B8K, MLZ, MHG, OMG, 4AC, 5MU, E6G, B9H, P7G, 5MC, MMX, MA6, E7G, A2M, 6MZ, OMU, B8T, B9B, T6A, BGH, M7A, MG, MQ6, B8W, B8Q, 7MG, 1MA, PSU, I4U, ZN, P4U, OMC, B8H, UR3

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	2	0.18	1/1698 (0.1%)	0.28	0/2640
2	1	0.12	0/122	0.22	0/186
3	5	0.18	1/82609 (0.0%)	0.30	0/128762
4	7	0.14	0/2858	0.24	0/4455
5	8	0.17	0/3559	0.25	0/5543
6	9	0.18	0/39730	0.30	0/61898
7	A	0.18	0/1936	0.40	0/2596
8	B	0.18	0/3240	0.38	0/4339
9	C	0.18	0/2913	0.35	0/3913
10	D	0.15	0/2427	0.34	0/3250
11	E	0.15	0/1762	0.35	0/2362
12	F	0.18	0/1911	0.37	0/2549
13	G	0.19	0/1868	0.43	0/2514
14	H	0.18	0/1535	0.43	0/2063
15	I	0.16	0/1702	0.34	0/2272
16	J	0.17	0/1385	0.46	0/1852
17	L	0.17	0/1733	0.39	0/2316
18	M	0.20	0/1158	0.43	0/1547
19	N	0.20	0/1746	0.38	0/2338
20	O	0.20	0/1662	0.39	0/2222
21	P	0.18	0/1268	0.41	0/1700
22	Q	0.18	0/1539	0.41	1/2054 (0.0%)
23	R	0.18	0/1524	0.42	0/2013
24	S	0.17	0/1501	0.36	0/2012
25	T	0.17	0/1326	0.35	0/1770
26	U	0.18	0/814	0.53	0/1092
27	V	0.15	0/993	0.32	0/1332
28	W	0.19	0/873	0.51	0/1158
29	X	0.15	0/984	0.37	0/1323
30	Y	0.18	0/1132	0.38	0/1504

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	Z	0.15	0/1130	0.33	0/1507
32	a	0.18	0/1191	0.35	0/1590
33	b	0.16	0/861	0.34	0/1138
34	c	0.17	0/771	0.40	0/1034
35	d	0.16	0/903	0.35	0/1216
36	e	0.18	0/1071	0.34	0/1429
37	f	0.17	0/895	0.36	0/1198
38	g	0.16	0/916	0.34	0/1220
39	h	0.16	0/1021	0.40	0/1348
40	i	0.14	0/841	0.36	0/1112
41	j	0.17	0/720	0.38	0/952
42	k	0.17	0/575	0.37	0/761
43	l	0.19	0/459	0.40	0/608
44	m	0.16	0/415	0.44	0/550
45	n	0.25	0/240	0.57	0/305
46	o	0.15	0/855	0.31	0/1128
47	p	0.15	0/718	0.33	0/953
48	r	0.17	0/1010	0.35	0/1354
49	AA	0.15	0/1747	0.30	0/2374
50	BB	0.16	0/1756	0.33	0/2350
51	CC	0.19	0/1753	0.37	0/2369
52	DD	0.14	0/1796	0.36	1/2417 (0.0%)
53	EE	0.16	0/2118	0.33	0/2849
54	FF	0.13	0/1492	0.32	0/2005
55	GG	0.15	0/1946	0.34	1/2590 (0.0%)
56	HH	0.15	0/1510	0.35	0/2022
57	II	0.17	0/1696	0.35	0/2261
58	JJ	0.17	0/1550	0.33	0/2069
59	KK	0.15	0/834	0.33	0/1125
60	LL	0.19	0/1195	0.36	0/1597
61	NN	0.16	0/1226	0.34	0/1649
62	OO	0.16	0/1029	0.34	0/1380
63	PP	0.20	0/1017	0.39	0/1358
64	QQ	0.14	0/1146	0.33	0/1534
65	RR	0.15	0/1082	0.35	0/1452
66	SS	0.16	0/1208	0.38	0/1618
67	TT	0.14	0/1115	0.29	0/1493
68	UU	0.15	0/805	0.38	0/1081
69	VV	0.15	0/643	0.31	0/860
70	WW	0.21	0/1051	0.39	0/1406
71	XX	0.17	0/1116	0.38	0/1490
72	YY	0.17	0/1028	0.35	0/1366
73	ZZ	0.13	0/604	0.38	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
74	Aa	0.16	0/828	0.36	0/1109
75	Bb	0.15	0/665	0.33	0/891
76	Cc	0.16	0/490	0.39	0/656
77	Dd	0.14	0/470	0.28	0/623
78	Ee	0.12	0/447	0.30	0/587
79	Gg	0.15	0/2493	0.38	0/3394
All	All	0.17	2/221956 (0.0%)	0.32	3/325763 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	G	0	1
19	N	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	37	T6A	O3'-P	5.20	1.61	1.56
3	5	3785	A2M	O3'-P	5.09	1.61	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	DD	43	PRO	CA-N-CD	-7.55	101.44	112.00
22	Q	83	VAL	N-CA-C	-5.38	107.12	111.91
55	GG	169	PRO	CA-N-CD	-5.14	104.80	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	G	215	ASP	Peptide
19	N	76	PRO	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	1552	0	793	32	0
2	1	133	0	68	1	0
3	5	76153	0	38232	993	0
4	7	2558	0	1296	23	0
5	8	3209	0	1631	58	0
6	9	36291	0	18318	464	0
7	A	1898	0	1993	40	0
8	B	3172	0	3310	68	0
9	C	2870	0	3045	61	0
10	D	2381	0	2414	43	0
11	E	1729	0	1887	52	0
12	F	1875	0	1995	36	0
13	G	1837	0	1977	46	0
14	H	1516	0	1596	38	0
15	I	1664	0	1711	33	0
16	J	1362	0	1399	36	0
17	L	1702	0	1820	44	0
18	M	1137	0	1209	27	0
19	N	1701	0	1749	51	0
20	O	1630	0	1778	35	0
21	P	1242	0	1274	22	0
22	Q	1515	0	1634	29	0
23	R	1508	0	1664	26	0
24	S	1462	0	1508	26	0
25	T	1298	0	1366	26	0
26	U	800	0	825	21	0
27	V	979	0	1039	16	0
28	W	860	0	903	35	0
29	X	967	0	1040	20	0
30	Y	1115	0	1205	36	0
31	Z	1107	0	1182	28	0
32	a	1162	0	1209	24	0
33	b	848	0	920	11	0
34	c	761	0	794	17	0
35	d	888	0	930	13	0
36	e	1053	0	1147	9	0
37	f	876	0	912	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	g	906	0	998	12	0
39	h	1013	0	1147	22	0
40	i	830	0	916	22	0
41	j	705	0	737	13	0
42	k	569	0	637	16	0
43	l	447	0	480	9	0
44	m	420	0	453	14	0
45	n	239	0	289	4	0
46	o	842	0	912	11	0
47	p	708	0	756	9	0
48	r	994	0	1051	20	0
49	AA	1710	0	1708	37	0
50	BB	1729	0	1803	41	0
51	CC	1716	0	1806	52	0
52	DD	1768	0	1866	32	0
53	EE	2076	0	2177	39	0
54	FF	1471	0	1522	33	0
55	GG	1923	0	2089	64	0
56	HH	1488	0	1582	52	0
57	II	1668	0	1750	31	0
58	JJ	1525	0	1640	33	0
59	KK	810	0	836	26	0
60	LL	1175	0	1249	24	0
61	NN	1202	0	1289	20	0
62	OO	1016	0	1039	18	0
63	PP	997	0	1045	28	0
64	QQ	1128	0	1195	33	0
65	RR	1068	0	1121	20	0
66	SS	1190	0	1249	34	0
67	TT	1097	0	1132	22	0
68	UU	795	0	862	30	0
69	VV	636	0	637	15	0
70	WW	1034	0	1080	22	0
71	XX	1098	0	1167	21	0
72	YY	1011	0	1083	18	0
73	ZZ	598	0	656	13	0
74	Aa	814	0	863	19	0
75	Bb	651	0	672	8	0
76	Cc	488	0	514	15	0
77	Dd	459	0	449	9	0
78	Ee	443	0	492	8	0
79	Gg	2436	0	2393	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	5	196	0	0	0	0
80	7	7	0	0	0	0
80	8	8	0	0	0	0
80	9	78	0	0	0	0
80	A	1	0	0	0	0
80	I	1	0	0	0	0
80	LL	1	0	0	0	0
80	P	1	0	0	0	0
80	V	1	0	0	0	0
80	a	1	0	0	0	0
80	g	1	0	0	0	0
80	j	1	0	0	0	0
81	5	38	0	0	0	0
82	Aa	1	0	0	0	0
82	Dd	1	0	0	0	0
82	g	1	0	0	0	0
82	j	1	0	0	0	0
82	m	1	0	0	0	0
82	o	1	0	0	0	0
82	p	1	0	0	0	0
All	All	210046	0	155115	3102	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 3102 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:4296:B8H:C5	3:5:4296:B8H:C4	1.81	1.53
3:5:3762:B8H:C4	3:5:3762:B8H:C5	1.82	1.52
3:5:1860:B8H:C4	3:5:1860:B8H:C5	1.81	1.52
3:5:2007:G:H21	3:5:2012:A:N6	1.53	1.06
3:5:2007:G:N2	3:5:2012:A:H62	1.53	1.05

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	A	246/248 (99%)	228 (93%)	18 (7%)	0	100	100
8	B	392/394 (100%)	378 (96%)	14 (4%)	0	100	100
9	C	357/360 (99%)	347 (97%)	10 (3%)	0	100	100
10	D	289/291 (99%)	280 (97%)	9 (3%)	0	100	100
11	E	208/251 (83%)	198 (95%)	10 (5%)	0	100	100
12	F	223/225 (99%)	211 (95%)	12 (5%)	0	100	100
13	G	223/234 (95%)	215 (96%)	8 (4%)	0	100	100
14	H	188/190 (99%)	177 (94%)	11 (6%)	0	100	100
15	I	201/213 (94%)	195 (97%)	6 (3%)	0	100	100
16	J	168/170 (99%)	163 (97%)	5 (3%)	0	100	100
17	L	208/210 (99%)	200 (96%)	8 (4%)	0	100	100
18	M	136/138 (99%)	128 (94%)	8 (6%)	0	100	100
19	N	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
20	O	197/199 (99%)	194 (98%)	3 (2%)	0	100	100
21	P	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
22	Q	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
23	R	178/180 (99%)	171 (96%)	7 (4%)	0	100	100
24	S	174/176 (99%)	167 (96%)	7 (4%)	0	100	100
25	T	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
26	U	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
27	V	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
28	W	102/121 (84%)	99 (97%)	3 (3%)	0	100	100
29	X	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
30	Y	132/134 (98%)	131 (99%)	1 (1%)	0	100	100
31	Z	133/135 (98%)	130 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	a	145/147 (99%)	140 (97%)	5 (3%)	0	100	100
33	b	100/116 (86%)	97 (97%)	3 (3%)	0	100	100
34	c	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
35	d	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
36	e	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
37	f	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
38	g	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
39	h	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
40	i	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
41	j	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
42	k	67/69 (97%)	67 (100%)	0	0	100	100
43	l	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
44	m	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
45	n	23/25 (92%)	23 (100%)	0	0	100	100
46	o	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
47	p	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
48	r	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
49	AA	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
50	BB	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
51	CC	219/221 (99%)	210 (96%)	9 (4%)	0	100	100
52	DD	226/228 (99%)	220 (97%)	6 (3%)	0	100	100
53	EE	260/262 (99%)	255 (98%)	5 (2%)	0	100	100
54	FF	181/191 (95%)	166 (92%)	15 (8%)	0	100	100
55	GG	235/237 (99%)	229 (97%)	6 (3%)	0	100	100
56	HH	181/189 (96%)	171 (94%)	10 (6%)	0	100	100
57	II	199/206 (97%)	190 (96%)	9 (4%)	0	100	100
58	JJ	183/185 (99%)	178 (97%)	5 (3%)	0	100	100
59	KK	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
60	LL	139/151 (92%)	134 (96%)	5 (4%)	0	100	100
61	NN	147/149 (99%)	145 (99%)	2 (1%)	0	100	100
62	OO	134/136 (98%)	132 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	PP	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
64	QQ	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
65	RR	130/132 (98%)	129 (99%)	1 (1%)	0	100	100
66	SS	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
67	TT	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
68	UU	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
69	VV	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
70	WW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
71	XX	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
72	YY	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
73	ZZ	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
74	Aa	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
75	Bb	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
76	Cc	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
77	Dd	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
78	Ee	53/55 (96%)	53 (100%)	0	0	100	100
79	Gg	311/313 (99%)	293 (94%)	18 (6%)	0	100	100
All	All	10973/11241 (98%)	10587 (96%)	386 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
7	A	190/190 (100%)	190 (100%)	0	100	100
8	B	342/342 (100%)	342 (100%)	0	100	100
9	C	299/299 (100%)	299 (100%)	0	100	100
10	D	247/247 (100%)	247 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	E	190/223 (85%)	190 (100%)	0	100	100
12	F	196/196 (100%)	196 (100%)	0	100	100
13	G	196/201 (98%)	196 (100%)	0	100	100
14	H	169/169 (100%)	169 (100%)	0	100	100
15	I	175/180 (97%)	175 (100%)	0	100	100
16	J	143/143 (100%)	143 (100%)	0	100	100
17	L	175/175 (100%)	175 (100%)	0	100	100
18	M	117/117 (100%)	117 (100%)	0	100	100
19	N	171/171 (100%)	171 (100%)	0	100	100
20	O	171/171 (100%)	171 (100%)	0	100	100
21	P	134/134 (100%)	134 (100%)	0	100	100
22	Q	164/164 (100%)	164 (100%)	0	100	100
23	R	159/159 (100%)	159 (100%)	0	100	100
24	S	157/157 (100%)	157 (100%)	0	100	100
25	T	139/139 (100%)	139 (100%)	0	100	100
26	U	88/88 (100%)	88 (100%)	0	100	100
27	V	101/101 (100%)	101 (100%)	0	100	100
28	W	86/100 (86%)	86 (100%)	0	100	100
29	X	106/106 (100%)	106 (100%)	0	100	100
30	Y	124/124 (100%)	124 (100%)	0	100	100
31	Z	117/117 (100%)	117 (100%)	0	100	100
32	a	119/119 (100%)	119 (100%)	0	100	100
33	b	84/95 (88%)	84 (100%)	0	100	100
34	c	84/84 (100%)	84 (100%)	0	100	100
35	d	98/98 (100%)	98 (100%)	0	100	100
36	e	114/114 (100%)	114 (100%)	0	100	100
37	f	88/88 (100%)	88 (100%)	0	100	100
38	g	98/98 (100%)	98 (100%)	0	100	100
39	h	109/109 (100%)	109 (100%)	0	100	100
40	i	86/86 (100%)	86 (100%)	0	100	100
41	j	73/73 (100%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	k	64/64 (100%)	64 (100%)	0	100	100
43	l	47/47 (100%)	47 (100%)	0	100	100
44	m	46/46 (100%)	46 (100%)	0	100	100
45	n	24/24 (100%)	24 (100%)	0	100	100
46	o	91/91 (100%)	91 (100%)	0	100	100
47	p	74/74 (100%)	74 (100%)	0	100	100
48	r	108/108 (100%)	108 (100%)	0	100	100
49	AA	180/181 (99%)	180 (100%)	0	100	100
50	BB	194/194 (100%)	194 (100%)	0	100	100
51	CC	187/187 (100%)	187 (100%)	0	100	100
52	DD	190/190 (100%)	190 (100%)	0	100	100
53	EE	224/224 (100%)	224 (100%)	0	100	100
54	FF	158/161 (98%)	158 (100%)	0	100	100
55	GG	207/207 (100%)	207 (100%)	0	100	100
56	HH	165/169 (98%)	165 (100%)	0	100	100
57	II	177/178 (99%)	177 (100%)	0	100	100
58	JJ	161/161 (100%)	161 (100%)	0	100	100
59	KK	87/87 (100%)	87 (100%)	0	100	100
60	LL	130/136 (96%)	130 (100%)	0	100	100
61	NN	130/130 (100%)	130 (100%)	0	100	100
62	OO	106/106 (100%)	106 (100%)	0	100	100
63	PP	109/109 (100%)	109 (100%)	0	100	100
64	QQ	117/117 (100%)	117 (100%)	0	100	100
65	RR	119/119 (100%)	119 (100%)	0	100	100
66	SS	125/125 (100%)	125 (100%)	0	100	100
67	TT	111/111 (100%)	111 (100%)	0	100	100
68	UU	92/92 (100%)	92 (100%)	0	100	100
69	VV	67/67 (100%)	67 (100%)	0	100	100
70	WW	112/112 (100%)	112 (100%)	0	100	100
71	XX	113/113 (100%)	113 (100%)	0	100	100
72	YY	107/107 (100%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	ZZ	66/66 (100%)	66 (100%)	0	100	100
74	Aa	88/88 (100%)	88 (100%)	0	100	100
75	Bb	75/75 (100%)	75 (100%)	0	100	100
76	Cc	55/55 (100%)	55 (100%)	0	100	100
77	Dd	48/48 (100%)	48 (100%)	0	100	100
78	Ee	46/46 (100%)	46 (100%)	0	100	100
79	Gg	272/272 (100%)	272 (100%)	0	100	100
All	All	9581/9664 (99%)	9581 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
36	e	52	GLN
76	Cc	45	ASN
50	BB	40	ASN
76	Cc	29	GLN
64	QQ	86	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	68/76 (89%)	11 (16%)	0
2	1	5/6 (83%)	1 (20%)	0
3	5	3524/3546 (99%)	694 (19%)	55 (1%)
4	7	119/120 (99%)	10 (8%)	0
5	8	149/156 (95%)	29 (19%)	1 (0%)
6	9	1687/1698 (99%)	330 (19%)	18 (1%)
All	All	5552/5602 (99%)	1075 (19%)	74 (1%)

5 of 1075 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	10	G
1	2	11	G
1	2	13	G
1	2	14	C

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Mol	Chain	Res	Type
1	2	19	G

5 of 74 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	9	110	U
6	9	1489	A
6	9	434	G
6	9	752	G
3	5	1370	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
6	MA6	9	1851	6	23,26,27	1.64	5 (21%)	33,38,41	3.83	14 (42%)
3	B9B	5	1574	3,80	25,28,29	1.79	6 (24%)	35,40,43	5.26	14 (40%)
3	7MG	5	2522	3	23,26,27	3.47	10 (43%)	27,39,42	2.20	9 (33%)
3	OMU	5	4620	3	19,22,23	3.03	8 (42%)	25,31,34	1.78	4 (16%)
3	PSU	5	3729	3	18,21,22	1.12	1 (5%)	21,30,33	1.95	5 (23%)
3	PSU	5	4403	3	18,21,22	1.10	1 (5%)	21,30,33	1.81	5 (23%)
2	4AC	1	45	2	21,24,25	3.28	9 (42%)	28,34,37	1.15	4 (14%)
3	1MA	5	4415	3	21,25,26	3.11	6 (28%)	30,37,40	2.34	8 (26%)
3	A2M	5	2363	3,80	22,25,26	3.22	10 (45%)	30,36,39	2.90	10 (33%)
3	OMC	5	2422	3,80	19,22,23	3.02	8 (42%)	25,31,34	0.75	0
6	OMC	9	174	6	19,22,23	3.01	8 (42%)	25,31,34	0.73	0
6	OMG	9	644	6	23,26,27	2.34	8 (34%)	32,38,41	1.91	9 (28%)
3	7MG	5	1605	3	23,26,27	3.48	10 (43%)	27,39,42	2.17	9 (33%)
3	A2M	5	3825	3	22,25,26	3.22	10 (45%)	30,36,39	2.90	10 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	A2M	9	27	6,80	22,25,26	3.21	10 (45%)	30,36,39	2.91	11 (36%)
3	OMU	5	4306	3	19,22,23	3.00	8 (42%)	25,31,34	1.82	5 (20%)
3	OMG	5	4494	3	23,26,27	2.36	8 (34%)	32,38,41	1.93	8 (25%)
3	OMG	5	4370	3	23,26,27	2.36	9 (39%)	32,38,41	1.87	8 (25%)
3	OMG	5	4637	3	23,26,27	2.38	8 (34%)	32,38,41	1.92	9 (28%)
3	A2M	5	4571	3	22,25,26	3.22	10 (45%)	30,36,39	2.90	10 (33%)
3	OMG	5	2424	3	23,26,27	2.38	8 (34%)	32,38,41	1.88	7 (21%)
6	OMG	9	683	6	23,26,27	2.35	8 (34%)	32,38,41	1.93	8 (25%)
3	B8K	5	3897	3	24,28,29	3.18	11 (45%)	29,42,45	2.36	11 (37%)
6	M7A	9	1806	6	19,25,26	1.64	2 (10%)	25,37,40	4.09	8 (32%)
6	B8Q	9	1219	6,80	18,22,23	2.96	4 (22%)	21,32,35	2.32	7 (33%)
3	B8W	5	2380	3	23,26,27	2.81	5 (21%)	33,38,41	2.89	15 (45%)
3	PSU	5	4628	3	18,21,22	1.12	1 (5%)	21,30,33	1.96	5 (23%)
3	B8W	5	4129	3	23,26,27	2.87	5 (21%)	33,38,41	2.73	17 (51%)
3	A2M	5	1524	3	22,25,26	3.24	10 (45%)	30,36,39	2.94	12 (40%)
3	UR3	5	4530	3	19,22,23	2.85	7 (36%)	26,32,35	1.63	3 (11%)
6	OMU	9	116	6	19,22,23	3.06	8 (42%)	25,31,34	1.81	6 (24%)
3	B8W	5	4529	3,80	23,26,27	2.87	5 (21%)	33,38,41	2.80	15 (45%)
6	PSU	9	119	6	18,21,22	1.02	1 (5%)	21,30,33	1.76	4 (19%)
6	MMX	9	568	6	20,23,24	3.83	5 (25%)	21,33,36	2.90	5 (23%)
3	2MG	5	4872	3	23,26,27	2.80	9 (39%)	33,38,41	2.61	15 (45%)
3	PSU	5	1683	3	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)
3	OMC	5	4536	3	19,22,23	2.98	8 (42%)	25,31,34	0.80	0
3	OMG	5	3792	3	23,26,27	2.36	8 (34%)	32,38,41	1.91	9 (28%)
3	2MG	5	1517	3	23,26,27	2.81	8 (34%)	33,38,41	2.37	11 (33%)
3	PSU	5	4450	3,80	18,21,22	1.09	2 (11%)	21,30,33	2.03	5 (23%)
3	P7G	5	3880	3	24,28,29	3.62	11 (45%)	25,41,44	1.34	2 (8%)
6	6MZ	9	1832	6,80	22,25,26	2.43	4 (18%)	29,36,39	3.39	11 (37%)
9	MLZ	C	333	9	8,9,10	0.84	0	4,9,11	0.70	0
3	PSU	5	1582	3	18,21,22	1.04	1 (5%)	21,30,33	1.69	4 (19%)
3	OMC	5	2804	3	19,22,23	2.96	8 (42%)	25,31,34	0.70	0
3	PSU	5	4531	3	18,21,22	1.09	1 (5%)	21,30,33	1.91	5 (23%)
6	PSU	9	612	6	18,21,22	1.10	1 (5%)	21,30,33	1.97	6 (28%)
6	A2M	9	484	6	22,25,26	3.23	10 (45%)	30,36,39	2.98	11 (36%)
3	M7A	5	4564	3	19,25,26	1.60	2 (10%)	25,37,40	4.23	8 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	B8W	5	4185	3	23,26,27	2.82	5 (21%)	33,38,41	2.78	16 (48%)
6	PSU	9	823	6	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)
3	OMG	5	4623	3	23,26,27	2.34	8 (34%)	32,38,41	1.93	8 (25%)
6	PSU	9	822	6	18,21,22	1.12	1 (5%)	21,30,33	1.96	5 (23%)
3	E7G	5	2297	3	24,27,28	3.57	11 (45%)	28,40,43	2.30	9 (32%)
6	A2M	9	1031	6	22,25,26	3.23	9 (40%)	30,36,39	3.00	11 (36%)
3	PSU	5	4500	3	18,21,22	1.10	1 (5%)	21,30,33	1.92	6 (28%)
6	B8N	9	1248	6	25,29,30	3.38	7 (28%)	28,42,45	2.00	7 (25%)
3	PSU	5	1677	3	18,21,22	1.09	1 (5%)	21,30,33	1.91	5 (23%)
3	OMG	5	373	3	23,26,27	2.34	8 (34%)	32,38,41	1.90	8 (25%)
6	MA6	9	1850	6	23,26,27	1.64	5 (21%)	33,38,41	3.70	13 (39%)
3	PSU	5	4293	3	18,21,22	1.09	1 (5%)	21,30,33	1.95	5 (23%)
6	4AC	9	1337	6	21,24,25	3.19	9 (42%)	28,34,37	1.11	4 (14%)
3	OMG	5	4196	3	23,26,27	2.35	8 (34%)	32,38,41	1.93	9 (28%)
3	OMG	5	1522	3	23,26,27	2.33	9 (39%)	32,38,41	1.84	8 (25%)
3	B8T	5	4671	3	19,22,23	3.61	8 (42%)	25,31,34	0.90	1 (4%)
3	1MA	5	1322	3,80	21,25,26	3.05	6 (28%)	30,37,40	2.20	7 (23%)
3	B8W	5	4472	3	23,26,27	2.85	5 (21%)	33,38,41	2.69	15 (45%)
3	P4U	5	1348	3	21,24,25	3.41	8 (38%)	28,33,36	1.57	2 (7%)
3	A2M	5	1871	3,80	22,25,26	3.22	10 (45%)	30,36,39	2.94	11 (36%)
3	2MG	5	729	3	23,26,27	2.88	8 (34%)	33,38,41	2.21	7 (21%)
3	B8Q	5	1456	3	18,22,23	2.89	6 (33%)	21,32,35	1.91	4 (19%)
3	A2M	5	3867	3	22,25,26	3.21	10 (45%)	30,36,39	2.93	11 (36%)
3	P7G	5	1909	3	24,28,29	3.70	11 (45%)	25,41,44	1.29	2 (8%)
44	MLZ	m	72	44	8,9,10	0.79	0	4,9,11	0.61	0
3	OMG	5	2364	3	23,26,27	2.32	9 (39%)	32,38,41	1.86	8 (25%)
3	OMC	5	3887	3	19,22,23	3.00	8 (42%)	25,31,34	0.77	0
3	6MZ	5	4220	3	22,25,26	2.47	4 (18%)	29,36,39	3.45	12 (41%)
3	OMC	5	2365	3	19,22,23	2.97	8 (42%)	25,31,34	0.76	0
3	B9H	5	2786	3	21,25,26	3.03	4 (19%)	22,35,38	1.47	3 (13%)
3	PSU	5	4442	3	18,21,22	1.07	1 (5%)	21,30,33	1.92	5 (23%)
6	5MU	9	814	6	19,22,23	4.97	7 (36%)	27,32,35	3.55	10 (37%)
3	5MC	5	4335	3	19,22,23	3.87	8 (42%)	26,32,35	1.08	2 (7%)
1	T6A	2	37	1	31,34,35	1.75	8 (25%)	43,49,52	2.01	10 (23%)
3	A2M	5	2401	3,80	22,25,26	3.24	10 (45%)	30,36,39	2.97	11 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	B8H	5	3762	3	19,22,23	6.83	6 (31%)	21,32,35	2.51	5 (23%)
3	E6G	5	4355	3	24,27,28	2.06	4 (16%)	34,39,42	3.02	16 (47%)
6	A2M	9	1678	6	22,25,26	3.17	9 (40%)	30,36,39	2.97	10 (33%)
6	OMU	9	121	6	19,22,23	3.05	8 (42%)	25,31,34	1.84	4 (16%)
6	4AC	9	1842	6	21,24,25	3.17	10 (47%)	28,34,37	1.05	4 (14%)
3	I4U	5	4194	3	20,24,25	3.40	8 (40%)	27,34,37	2.16	2 (7%)
3	OMG	5	1883	3	23,26,27	2.35	9 (39%)	32,38,41	1.93	8 (25%)
6	OMC	9	1710	6	19,22,23	3.02	8 (42%)	25,31,34	0.76	0
6	PSU	9	1081	6	18,21,22	1.04	1 (5%)	21,30,33	1.82	5 (23%)
3	OMC	5	3909	3	19,22,23	3.00	8 (42%)	25,31,34	0.96	1 (4%)
6	OMC	9	517	6	19,22,23	3.02	8 (42%)	25,31,34	0.77	0
3	PSU	5	4636	3	18,21,22	1.12	1 (5%)	21,30,33	2.03	6 (28%)
6	A2M	9	159	6	22,25,26	3.23	10 (45%)	30,36,39	2.97	11 (36%)
6	UR3	9	1830	6	19,22,23	2.92	7 (36%)	26,32,35	1.72	4 (15%)
3	OMC	5	3869	3	19,22,23	3.01	8 (42%)	25,31,34	0.75	0
3	OMG	5	4870	3	23,26,27	2.37	9 (39%)	32,38,41	1.86	8 (25%)
3	OMG	5	2773	3	23,26,27	2.37	9 (39%)	32,38,41	1.86	8 (25%)
3	A2M	5	398	3	22,25,26	3.23	9 (40%)	30,36,39	2.91	10 (33%)
3	B9B	5	2754	3,80	25,28,29	1.79	6 (24%)	35,40,43	5.49	13 (37%)
3	OMC	5	3701	3,80	19,22,23	2.99	8 (42%)	25,31,34	0.72	0
3	BGH	5	3899	3,80	25,29,30	4.50	18 (72%)	30,43,46	2.48	13 (43%)
3	A2M	5	1326	3	22,25,26	3.21	10 (45%)	30,36,39	2.90	10 (33%)
3	PSU	5	2508	3	18,21,22	1.07	1 (5%)	21,30,33	1.89	5 (23%)
3	UR3	5	4597	3	19,22,23	2.90	6 (31%)	26,32,35	1.53	3 (11%)
3	OMG	5	2050	3	23,26,27	2.35	9 (39%)	32,38,41	1.86	8 (25%)
3	B8H	5	4296	3	19,22,23	6.85	6 (31%)	21,32,35	2.51	5 (23%)
3	I4U	5	1659	3	20,24,25	3.43	8 (40%)	27,34,37	2.00	2 (7%)
3	B8K	5	4690	3	24,28,29	3.27	11 (45%)	29,42,45	2.45	11 (37%)
3	5MC	5	4447	3	19,22,23	3.76	8 (42%)	26,32,35	1.08	1 (3%)
6	PSU	9	1243	6	18,21,22	1.10	1 (5%)	21,30,33	1.89	4 (19%)
3	A2M	5	3718	3	22,25,26	3.24	10 (45%)	30,36,39	2.86	11 (36%)
3	A2M	5	3723	3	22,25,26	3.21	10 (45%)	30,36,39	2.91	10 (33%)
3	OMG	5	1316	3	23,26,27	2.33	9 (39%)	32,38,41	1.88	8 (25%)
3	A2M	5	1534	3,80	22,25,26	3.23	10 (45%)	30,36,39	2.96	11 (36%)
3	5MC	5	3782	3	19,22,23	3.79	8 (42%)	26,32,35	1.04	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	UR3	5	1866	3	19,22,23	2.86	6 (31%)	26,32,35	1.57	3 (11%)
3	5MU	5	4083	3	19,22,23	4.97	7 (36%)	27,32,35	3.61	10 (37%)
3	PSU	5	3715	3	18,21,22	1.09	1 (5%)	21,30,33	1.89	4 (19%)
3	OMC	5	2861	3	19,22,23	3.00	8 (42%)	25,31,34	0.75	0
6	A2M	9	668	6,80	22,25,26	3.25	10 (45%)	30,36,39	2.99	11 (36%)
3	MHG	5	4371	3	29,32,33	3.55	11 (37%)	34,46,49	2.45	11 (32%)
3	E7G	5	1797	3	24,27,28	3.60	11 (45%)	28,40,43	2.33	9 (32%)
6	OMG	9	509	6,80	23,26,27	2.34	8 (34%)	32,38,41	1.88	8 (25%)
6	5MC	9	1374	6	19,22,23	3.80	8 (42%)	26,32,35	1.02	2 (7%)
3	7MG	5	4550	3	23,26,27	3.46	10 (43%)	27,39,42	2.11	9 (33%)
6	OMC	9	1703	6	19,22,23	3.01	8 (42%)	25,31,34	0.75	0
6	A2M	9	166	6	22,25,26	3.24	10 (45%)	30,36,39	2.93	13 (43%)
3	A2M	5	3785	3	22,25,26	3.23	10 (45%)	30,36,39	3.06	14 (46%)
3	B9B	5	237	3	25,28,29	1.80	6 (24%)	35,40,43	5.23	12 (34%)
3	B8T	5	4483	3	19,22,23	3.60	8 (42%)	25,31,34	0.91	1 (4%)
5	OMU	8	14	5,3	19,22,23	3.07	8 (42%)	25,31,34	1.81	5 (20%)
3	PSU	5	3764	3	18,21,22	1.12	1 (5%)	21,30,33	1.84	4 (19%)
3	A2M	5	4523	3,80	22,25,26	3.22	10 (45%)	30,36,39	2.97	11 (36%)
3	B8H	5	1860	3	19,22,23	6.84	6 (31%)	21,32,35	2.48	5 (23%)
3	OMG	5	1625	3,80	23,26,27	2.37	8 (34%)	32,38,41	1.94	9 (28%)

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
6	MA6	9	1851	6	-	2/11/29/30	0/3/3/3
3	B9B	5	1574	3,80	-	3/11/29/30	0/3/3/3
3	7MG	5	2522	3	-	0/7/37/38	0/3/3/3
3	OMU	5	4620	3	-	0/9/27/28	0/2/2/2
3	PSU	5	3729	3	-	2/7/25/26	0/2/2/2
3	PSU	5	4403	3	-	3/7/25/26	0/2/2/2
2	4AC	1	45	2	-	0/11/29/30	0/2/2/2
3	1MA	5	4415	3	-	1/7/25/26	0/3/3/3
3	A2M	5	2363	3,80	-	1/9/27/28	0/3/3/3
3	OMC	5	2422	3,80	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OMC	9	174	6	-	1/9/27/28	0/2/2/2
6	OMG	9	644	6	-	2/9/27/28	0/3/3/3
3	7MG	5	1605	3	-	0/7/37/38	0/3/3/3
3	A2M	5	3825	3	-	0/9/27/28	0/3/3/3
6	A2M	9	27	6,80	-	1/9/27/28	0/3/3/3
3	OMU	5	4306	3	-	1/9/27/28	0/2/2/2
3	OMG	5	4494	3	-	1/9/27/28	0/3/3/3
3	OMG	5	4370	3	-	1/9/27/28	0/3/3/3
3	OMG	5	4637	3	-	2/9/27/28	0/3/3/3
3	A2M	5	4571	3	-	0/9/27/28	0/3/3/3
3	OMG	5	2424	3	-	2/9/27/28	0/3/3/3
6	OMG	9	683	6	-	2/9/27/28	0/3/3/3
3	B8K	5	3897	3	-	3/11/41/42	0/3/3/3
6	M7A	9	1806	6	-	0/7/37/38	0/3/3/3
6	B8Q	9	1219	6,80	-	2/7/42/43	0/2/2/2
3	B8W	5	2380	3	-	4/9/27/28	0/3/3/3
3	PSU	5	4628	3	-	0/7/25/26	0/2/2/2
3	B8W	5	4129	3	-	2/9/27/28	0/3/3/3
3	A2M	5	1524	3	-	2/9/27/28	0/3/3/3
3	UR3	5	4530	3	-	2/7/25/26	0/2/2/2
6	OMU	9	116	6	-	3/9/27/28	0/2/2/2
3	B8W	5	4529	3,80	-	2/9/27/28	0/3/3/3
6	PSU	9	119	6	-	0/7/25/26	0/2/2/2
6	MMX	9	568	6	-	4/9/44/45	0/2/2/2
3	2MG	5	4872	3	-	1/9/27/28	0/3/3/3
3	PSU	5	1683	3	-	0/7/25/26	0/2/2/2
3	OMC	5	4536	3	-	0/9/27/28	0/2/2/2
3	OMG	5	3792	3	-	2/9/27/28	0/3/3/3
3	2MG	5	1517	3	-	0/9/27/28	0/3/3/3
3	PSU	5	4450	3,80	-	1/7/25/26	0/2/2/2
3	P7G	5	3880	3	-	4/10/40/41	0/3/3/3
6	6MZ	9	1832	6,80	-	2/9/27/28	0/3/3/3
9	MLZ	C	333	9	-	1/7/8/10	-
3	PSU	5	1582	3	-	1/7/25/26	0/2/2/2
3	OMC	5	2804	3	-	0/9/27/28	0/2/2/2
3	PSU	5	4531	3	-	2/7/25/26	0/2/2/2
6	PSU	9	612	6	-	0/7/25/26	0/2/2/2
6	A2M	9	484	6	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	M7A	5	4564	3	-	0/7/37/38	0/3/3/3
3	B8W	5	4185	3	-	2/9/27/28	0/3/3/3
6	PSU	9	823	6	-	0/7/25/26	0/2/2/2
3	OMG	5	4623	3	-	0/9/27/28	0/3/3/3
6	PSU	9	822	6	-	0/7/25/26	0/2/2/2
3	E7G	5	2297	3	-	1/9/39/40	0/3/3/3
6	A2M	9	1031	6	-	1/9/27/28	0/3/3/3
3	PSU	5	4500	3	-	3/7/25/26	0/2/2/2
6	B8N	9	1248	6	-	1/16/34/35	0/2/2/2
3	PSU	5	1677	3	-	3/7/25/26	0/2/2/2
3	OMG	5	373	3	-	1/9/27/28	0/3/3/3
6	MA6	9	1850	6	-	0/11/29/30	0/3/3/3
3	PSU	5	4293	3	-	0/7/25/26	0/2/2/2
6	4AC	9	1337	6	-	1/11/29/30	0/2/2/2
3	OMG	5	4196	3	-	1/9/27/28	0/3/3/3
3	OMG	5	1522	3	-	0/9/27/28	0/3/3/3
3	B8T	5	4671	3	-	1/7/27/28	0/2/2/2
3	1MA	5	1322	3,80	-	0/7/25/26	0/3/3/3
3	B8W	5	4472	3	-	2/9/27/28	0/3/3/3
3	P4U	5	1348	3	-	4/10/29/30	0/2/2/2
3	A2M	5	1871	3,80	-	0/9/27/28	0/3/3/3
3	2MG	5	729	3	-	0/9/27/28	0/3/3/3
3	B8Q	5	1456	3	-	0/7/42/43	0/2/2/2
3	A2M	5	3867	3	-	3/9/27/28	0/3/3/3
3	P7G	5	1909	3	-	2/10/40/41	0/3/3/3
44	MLZ	m	72	44	-	4/7/8/10	-
3	OMG	5	2364	3	-	2/9/27/28	0/3/3/3
3	OMC	5	3887	3	-	1/9/27/28	0/2/2/2
3	6MZ	5	4220	3	-	1/9/27/28	0/3/3/3
3	OMC	5	2365	3	-	0/9/27/28	0/2/2/2
3	B9H	5	2786	3	-	2/12/47/48	0/2/2/2
3	PSU	5	4442	3	-	0/7/25/26	0/2/2/2
6	5MU	9	814	6	-	1/7/25/26	0/2/2/2
3	5MC	5	4335	3	-	0/7/25/26	0/2/2/2
1	T6A	2	37	1	-	2/23/41/42	0/3/3/3
3	A2M	5	2401	3,80	-	0/9/27/28	0/3/3/3
3	B8H	5	3762	3	-	2/7/25/26	0/2/2/2
3	E6G	5	4355	3	-	4/10/28/29	0/3/3/3
6	A2M	9	1678	6	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OMU	9	121	6	-	1/9/27/28	0/2/2/2
6	4AC	9	1842	6	-	0/11/29/30	0/2/2/2
3	I4U	5	4194	3	-	1/9/29/30	0/2/2/2
3	OMG	5	1883	3	-	1/9/27/28	0/3/3/3
6	OMC	9	1710	6	-	0/9/27/28	0/2/2/2
6	PSU	9	1081	6	-	1/7/25/26	0/2/2/2
3	OMC	5	3909	3	-	2/9/27/28	0/2/2/2
6	OMC	9	517	6	-	1/9/27/28	0/2/2/2
3	PSU	5	4636	3	-	4/7/25/26	0/2/2/2
6	A2M	9	159	6	-	2/9/27/28	0/3/3/3
6	UR3	9	1830	6	-	2/7/25/26	0/2/2/2
3	OMC	5	3869	3	-	0/9/27/28	0/2/2/2
3	OMG	5	4870	3	-	3/9/27/28	0/3/3/3
3	OMG	5	2773	3	-	0/9/27/28	0/3/3/3
3	A2M	5	398	3	-	2/9/27/28	0/3/3/3
3	B9B	5	2754	3,80	-	4/11/29/30	0/3/3/3
3	OMC	5	3701	3,80	-	4/9/27/28	0/2/2/2
3	BGH	5	3899	3,80	-	0/13/43/44	0/3/3/3
3	A2M	5	1326	3	-	2/9/27/28	0/3/3/3
3	PSU	5	2508	3	-	0/7/25/26	0/2/2/2
3	UR3	5	4597	3	-	0/7/25/26	0/2/2/2
3	OMG	5	2050	3	-	0/9/27/28	0/3/3/3
3	B8H	5	4296	3	-	2/7/25/26	0/2/2/2
3	I4U	5	1659	3	-	0/9/29/30	0/2/2/2
3	B8K	5	4690	3	-	0/11/41/42	0/3/3/3
3	5MC	5	4447	3	-	0/7/25/26	0/2/2/2
6	PSU	9	1243	6	-	2/7/25/26	0/2/2/2
3	A2M	5	3718	3	-	1/9/27/28	0/3/3/3
3	A2M	5	3723	3	-	1/9/27/28	0/3/3/3
3	OMG	5	1316	3	-	1/9/27/28	0/3/3/3
3	A2M	5	1534	3,80	-	1/9/27/28	0/3/3/3
3	5MC	5	3782	3	-	0/7/25/26	0/2/2/2
3	UR3	5	1866	3	-	0/7/25/26	0/2/2/2
3	5MU	5	4083	3	-	0/7/25/26	0/2/2/2
3	PSU	5	3715	3	-	0/7/25/26	0/2/2/2
3	OMC	5	2861	3	-	1/9/27/28	0/2/2/2
6	A2M	9	668	6,80	-	3/9/27/28	0/3/3/3
3	MHG	5	4371	3	-	6/16/46/47	0/3/3/3
3	E7G	5	1797	3	-	2/9/39/40	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OMG	9	509	6,80	-	0/9/27/28	0/3/3/3
6	5MC	9	1374	6	-	0/7/25/26	0/2/2/2
3	7MG	5	4550	3	-	0/7/37/38	0/3/3/3
6	OMC	9	1703	6	-	2/9/27/28	0/2/2/2
6	A2M	9	166	6	-	2/9/27/28	0/3/3/3
3	A2M	5	3785	3	-	4/9/27/28	0/3/3/3
3	B9B	5	237	3	-	5/11/29/30	0/3/3/3
3	B8T	5	4483	3	-	0/7/27/28	0/2/2/2
5	OMU	8	14	5,3	-	1/9/27/28	0/2/2/2
3	PSU	5	3764	3	-	2/7/25/26	0/2/2/2
3	A2M	5	4523	3,80	-	0/9/27/28	0/3/3/3
3	B8H	5	1860	3	-	2/7/25/26	0/2/2/2
3	OMG	5	1625	3,80	-	1/9/27/28	0/3/3/3

The worst 5 of 956 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5	4296	B8H	C6-C5	-16.57	1.11	1.35
3	5	1860	B8H	C6-C5	-16.55	1.11	1.35
3	5	3762	B8H	C6-C5	-16.37	1.11	1.35
3	5	4296	B8H	C4-N3	-15.63	1.09	1.38
3	5	1860	B8H	C4-N3	-15.60	1.09	1.38

The worst 5 of 967 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	2754	B9B	O6-C6-C5	21.64	145.31	116.73
3	5	1574	B9B	O6-C6-C5	20.67	144.03	116.73
3	5	237	B9B	O6-C6-C5	20.33	143.58	116.73
3	5	2754	B9B	O6-C6-N1	-20.10	93.18	120.02
3	5	1574	B9B	O6-C6-N1	-19.23	94.34	120.02

There are no chirality outliers.

5 of 180 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	333	MLZ	CD-CE-NZ-CM
3	5	237	B9B	C5-C6-O6-C61
3	5	237	B9B	N1-C6-O6-C61
3	5	237	B9B	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	5	237	B9B	O4'-C4'-C5'-O5'

There are no ring outliers.

62 monomers are involved in 83 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	9	1851	MA6	1	0
3	5	1574	B9B	1	0
3	5	2522	7MG	1	0
3	5	4620	OMU	2	0
3	5	4415	1MA	1	0
3	5	2363	A2M	1	0
6	9	174	OMC	1	0
6	9	644	OMG	1	0
3	5	1605	7MG	1	0
3	5	3825	A2M	1	0
6	9	27	A2M	1	0
3	5	4306	OMU	1	0
3	5	4637	OMG	2	0
3	5	2424	OMG	1	0
6	9	683	OMG	1	0
3	5	3897	B8K	2	0
3	5	1524	A2M	1	0
6	9	116	OMU	2	0
6	9	568	MMX	1	0
3	5	4872	2MG	1	0
3	5	1683	PSU	3	0
3	5	4536	OMC	1	0
3	5	4450	PSU	1	0
9	C	333	MLZ	1	0
6	9	612	PSU	1	0
6	9	484	A2M	1	0
3	5	4564	M7A	1	0
6	9	1031	A2M	1	0
3	5	4500	PSU	1	0
3	5	4472	B8W	2	0
3	5	1871	A2M	1	0
3	5	729	2MG	2	0
3	5	1456	B8Q	1	0
3	5	3867	A2M	2	0
3	5	4220	6MZ	1	0
6	9	814	5MU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	37	T6A	3	0
3	5	3762	B8H	1	0
6	9	1678	A2M	2	0
6	9	121	OMU	2	0
3	5	3909	OMC	1	0
3	5	4636	PSU	1	0
6	9	1830	UR3	1	0
3	5	4870	OMG	1	0
3	5	2773	OMG	1	0
3	5	398	A2M	1	0
3	5	2754	B9B	1	0
3	5	1326	A2M	2	0
3	5	4296	B8H	1	0
3	5	3718	A2M	3	0
3	5	3723	A2M	4	0
3	5	1316	OMG	1	0
3	5	1534	A2M	1	0
3	5	1866	UR3	1	0
3	5	4083	5MU	1	0
6	9	509	OMG	1	0
3	5	4550	7MG	1	0
6	9	166	A2M	1	0
3	5	3785	A2M	2	0
5	8	14	OMU	2	0
3	5	4523	A2M	1	0
3	5	1860	B8H	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 304 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
81	MQ6	5	5294	-	40,42,42	1.27	5 (12%)	40,65,65	2.64	9 (22%)

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
81	MQ6	5	5294	-	-	14/26/73/73	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	5	5294	MQ6	O37-C06	-3.48	1.36	1.43
81	5	5294	MQ6	O14-C12	2.40	1.38	1.34
81	5	5294	MQ6	C30-C31	2.16	1.35	1.32
81	5	5294	MQ6	C17-C16	2.11	1.54	1.51
81	5	5294	MQ6	C24-C23	-2.05	1.49	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	5	5294	MQ6	O37-C06-C05	-12.42	89.01	108.88
81	5	5294	MQ6	O37-C06-C07	6.16	123.42	109.38
81	5	5294	MQ6	O14-C12-C06	4.87	120.18	111.24
81	5	5294	MQ6	C23-C22-C21	-3.49	111.78	119.35
81	5	5294	MQ6	C28-C29-N25	2.58	107.64	103.94

There are no chirality outliers.

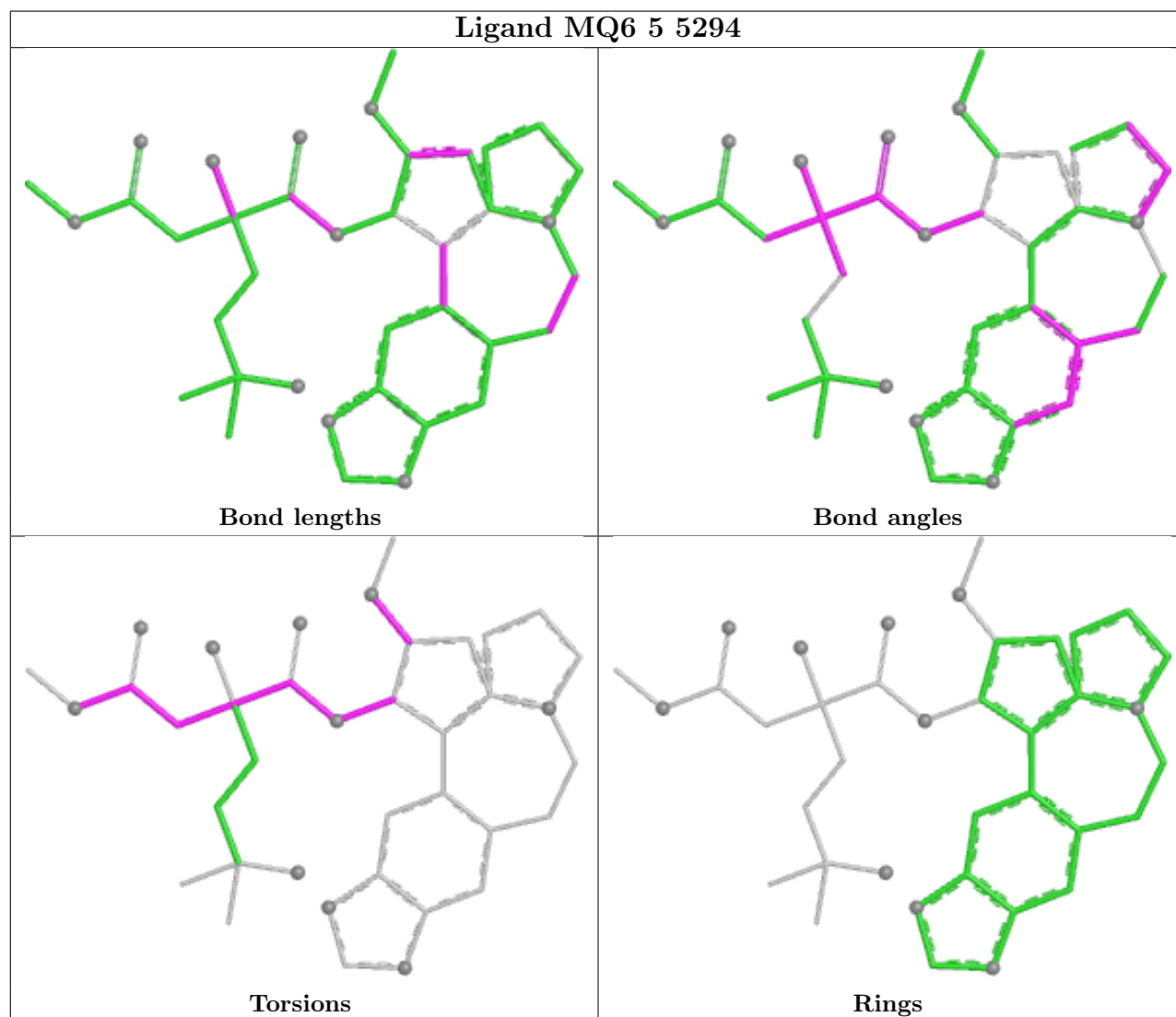
5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	5	5294	MQ6	C31-C15-O14-C12
81	5	5294	MQ6	C07-C06-C12-O13
81	5	5294	MQ6	C07-C06-C12-O14
81	5	5294	MQ6	C06-C12-O14-C15
81	5	5294	MQ6	C30-C31-O32-C33

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	5	24
6	9	11

The worst 5 of 35 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	41.43
1	5	1252:C	O3'	1271:G	P	35.31
1	5	1219:G	O3'	1233:G	P	20.31
1	5	4101:C	O3'	4107:G	P	17.50
1	5	1407:G	O3'	1410:C	P	17.49

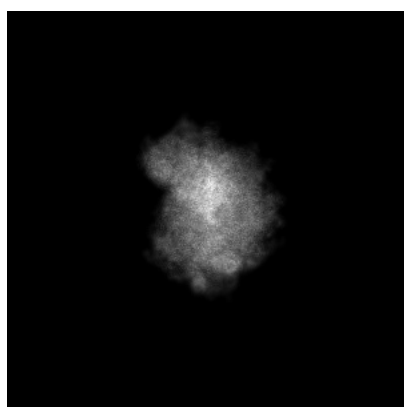
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26445. These allow visual inspection of the internal detail of the map and identification of artifacts.

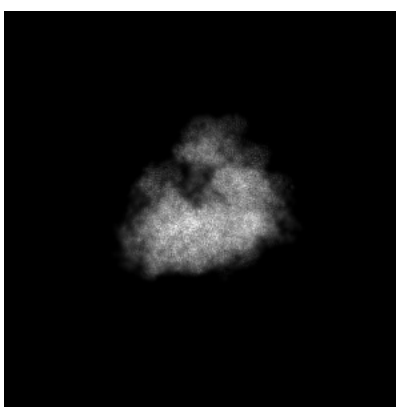
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

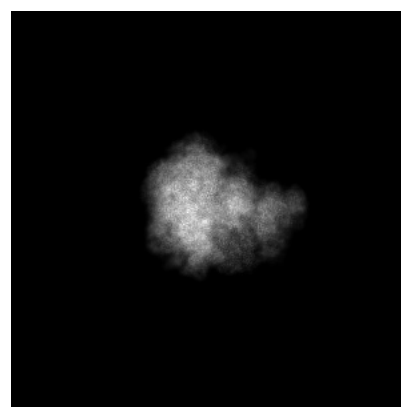
#### 6.1.1 Primary map



X



Y

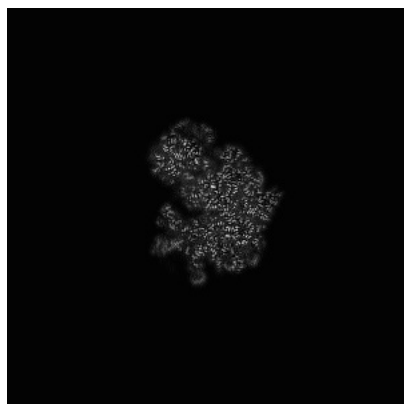


Z

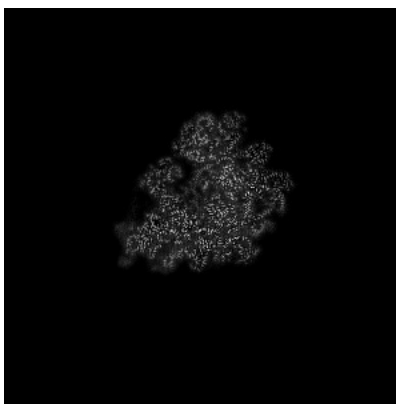
The images above show the map projected in three orthogonal directions.

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

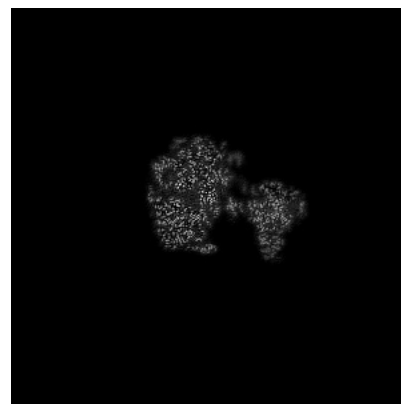
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

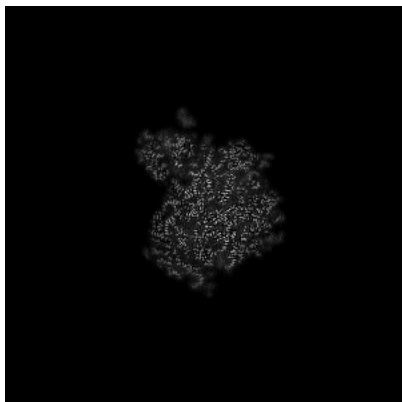


Z Index: 240

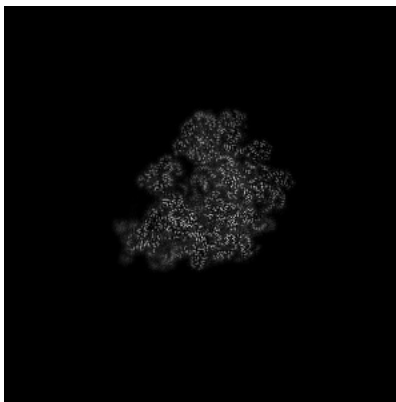
The images above show central slices of the map in three orthogonal directions.

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

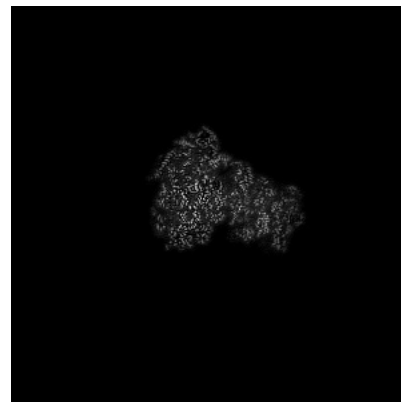
### 6.3.1 Primary map



X Index: 221



Y Index: 242

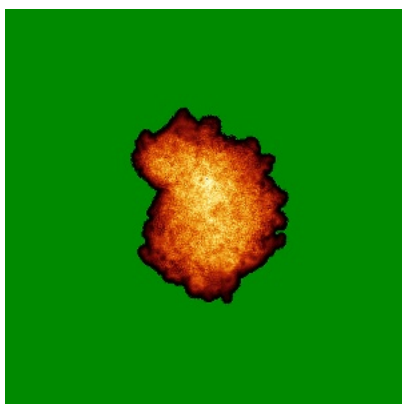


Z Index: 255

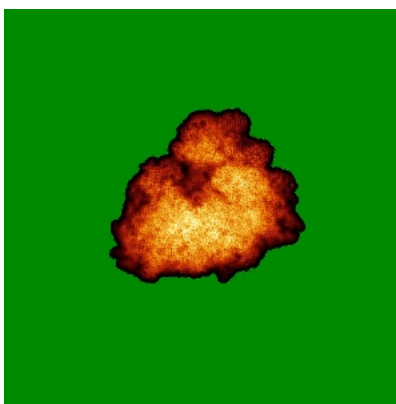
The images above show the largest variance slices of the map in three orthogonal directions.

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

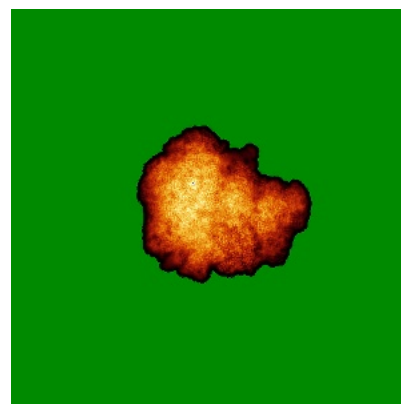
### 6.4.1 Primary map



X



Y

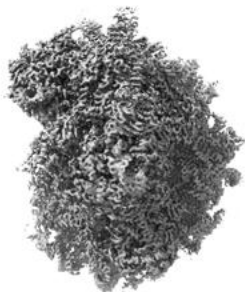


Z

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

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

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.037. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

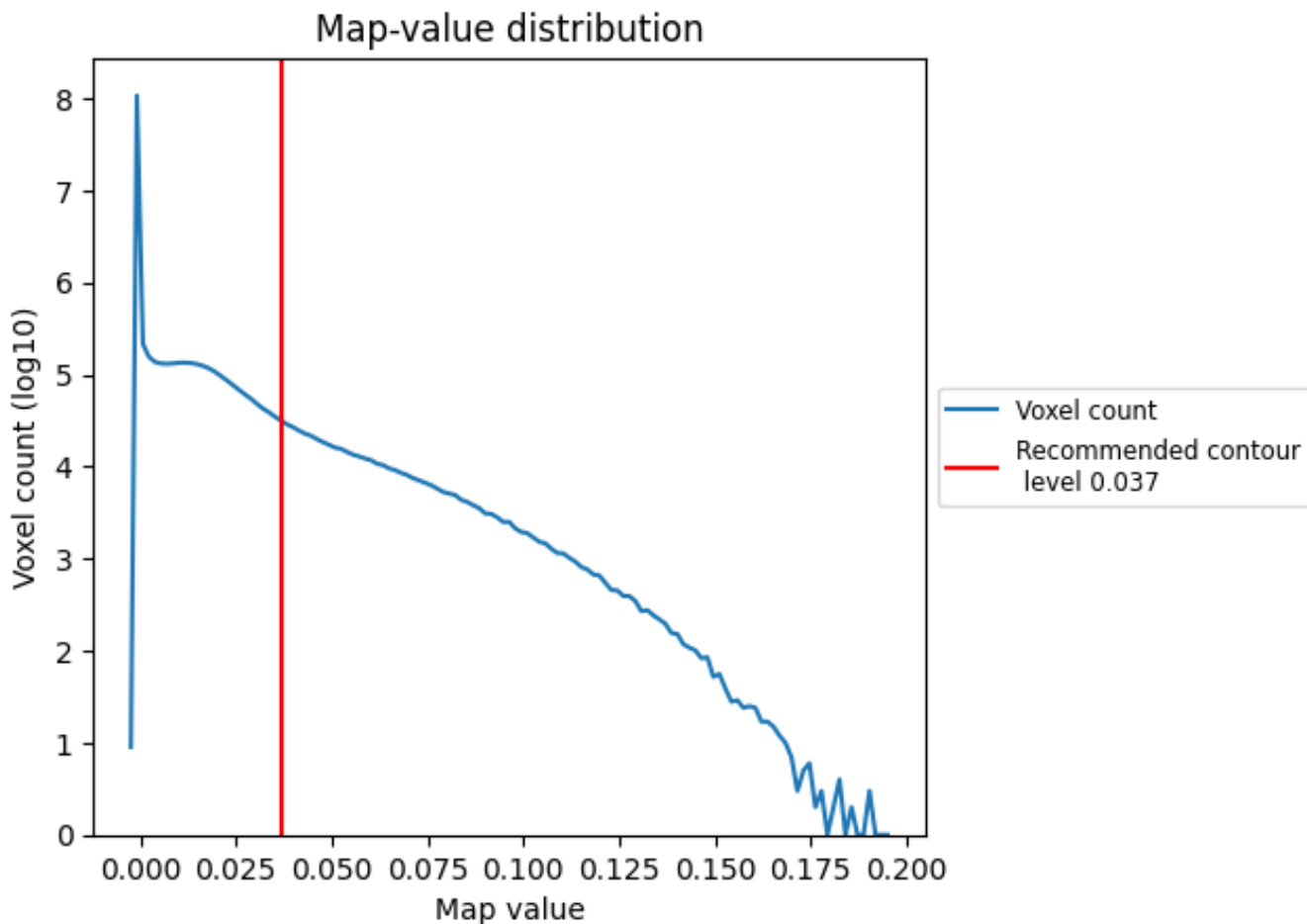
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

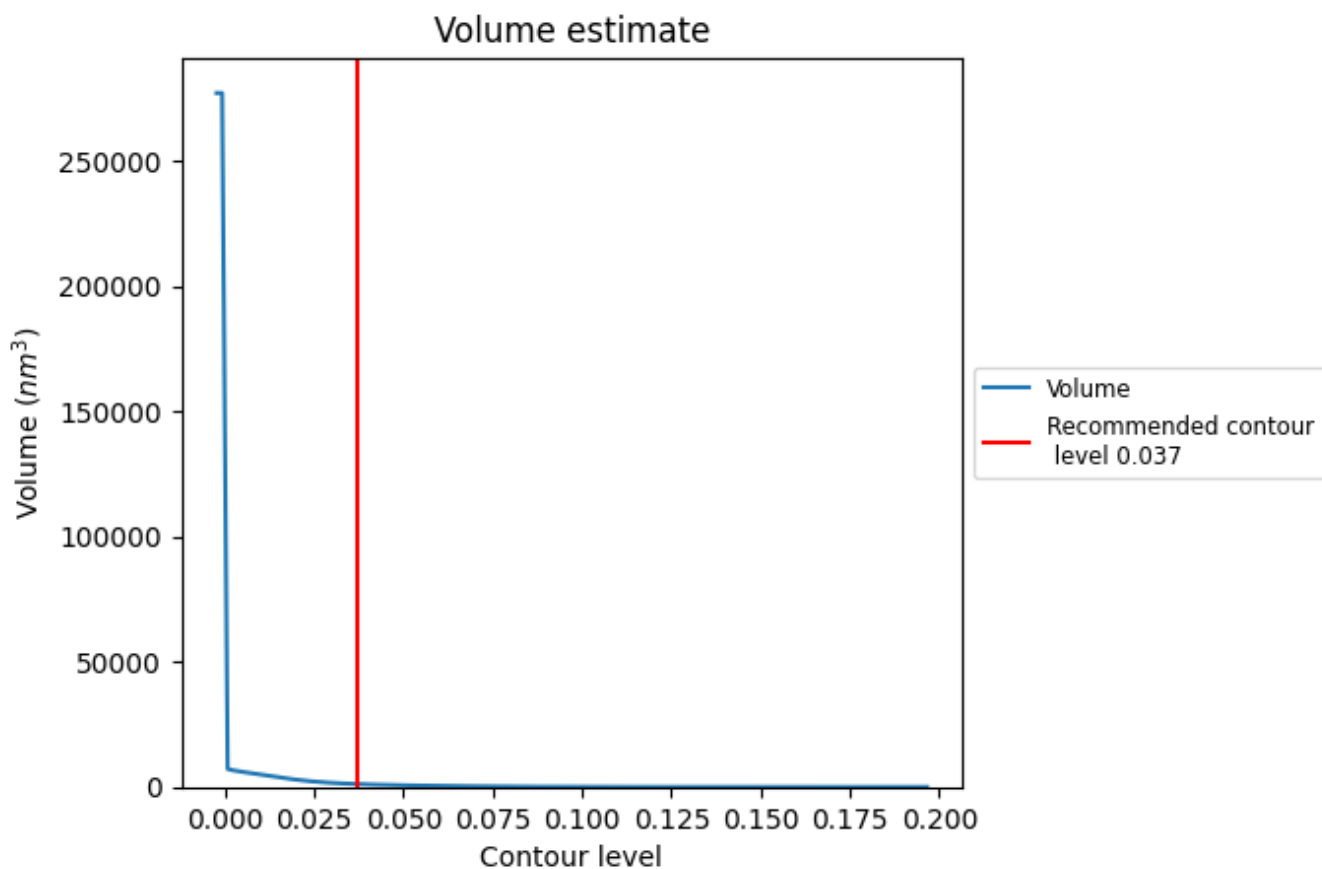
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

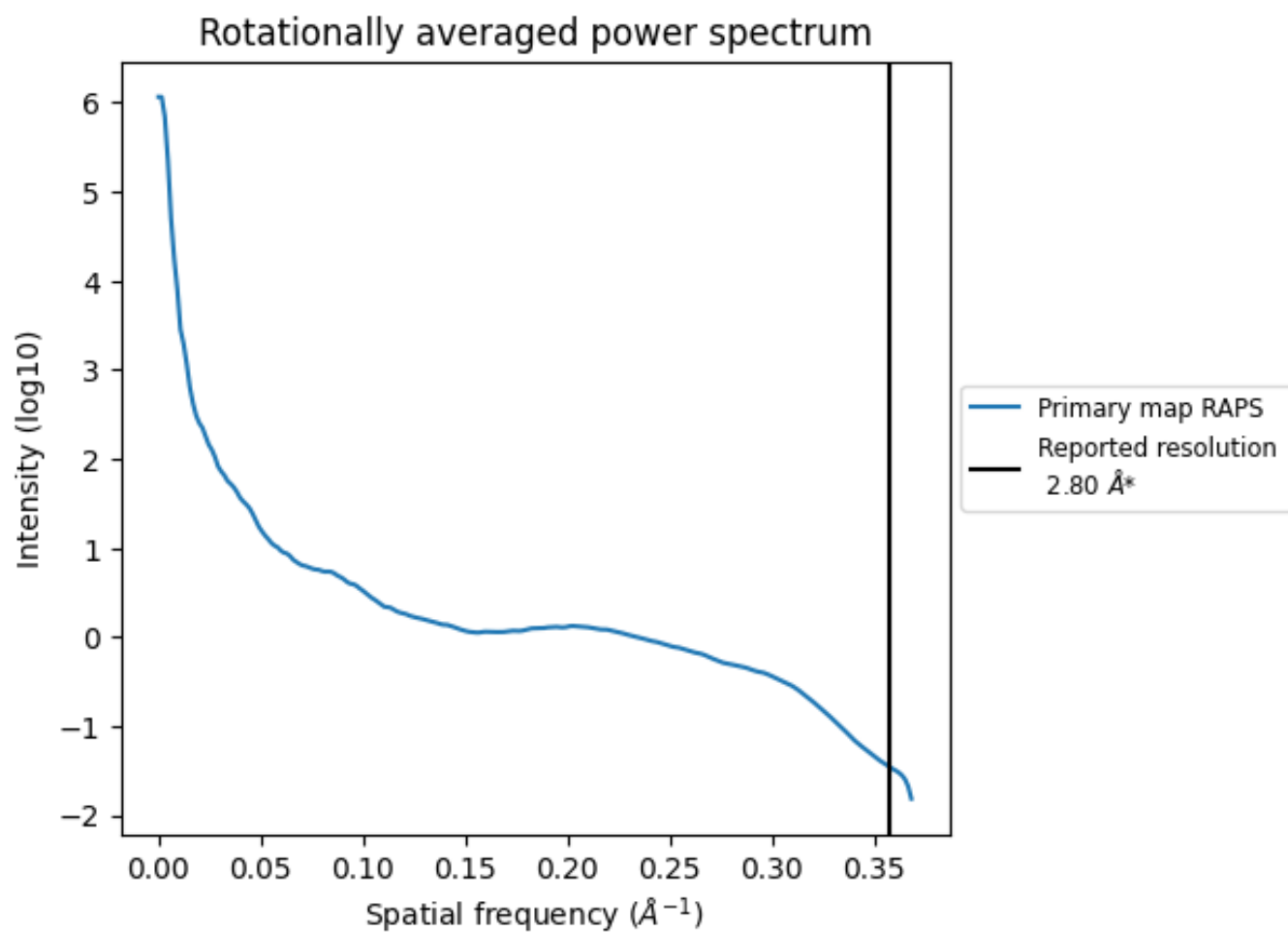
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1162  $\text{nm}^3$ ; this corresponds to an approximate mass of 1050 kDa.

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

### 7.3 Rotationally averaged power spectrum i



\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

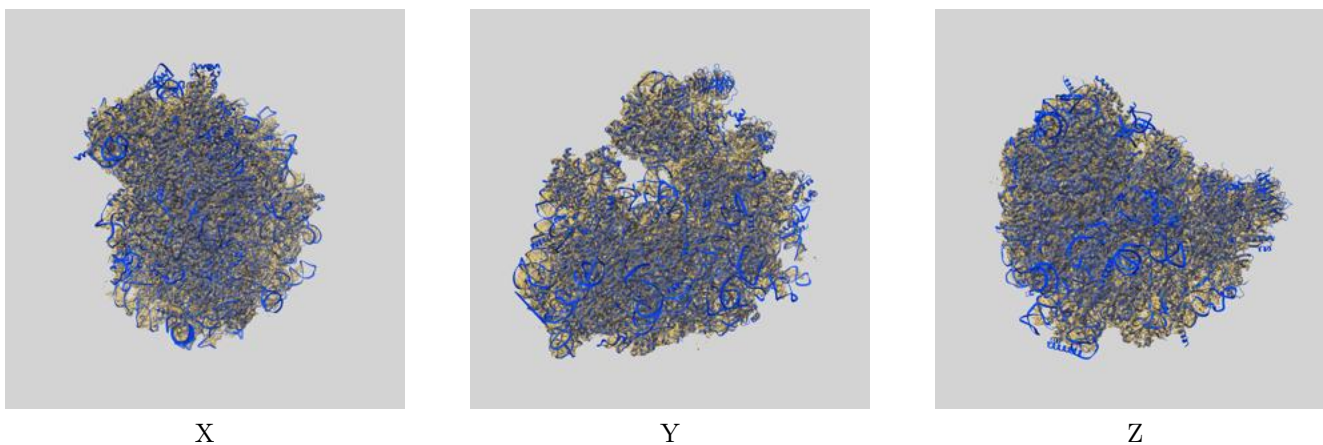
## 8 Fourier-Shell correlation

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

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

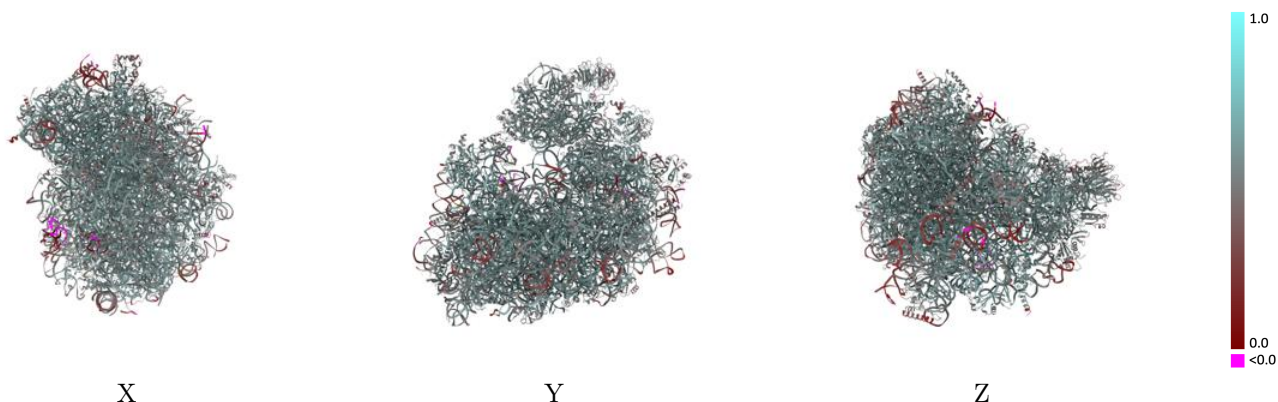
This section contains information regarding the fit between EMDB map EMD-26445 and PDB model 7UCK. Per-residue inclusion information can be found in section 3 on page 22.

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



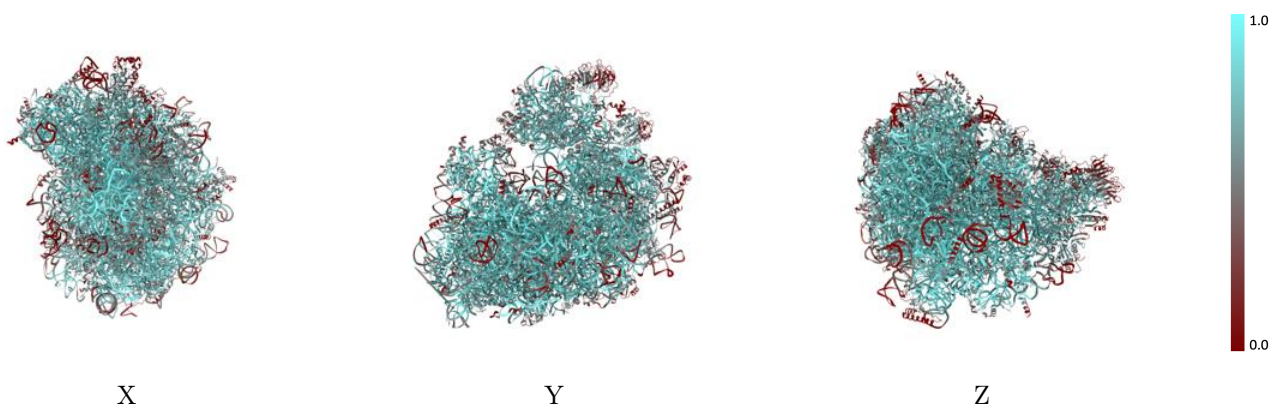
The images above show the 3D surface view of the map at the recommended contour level 0.037 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



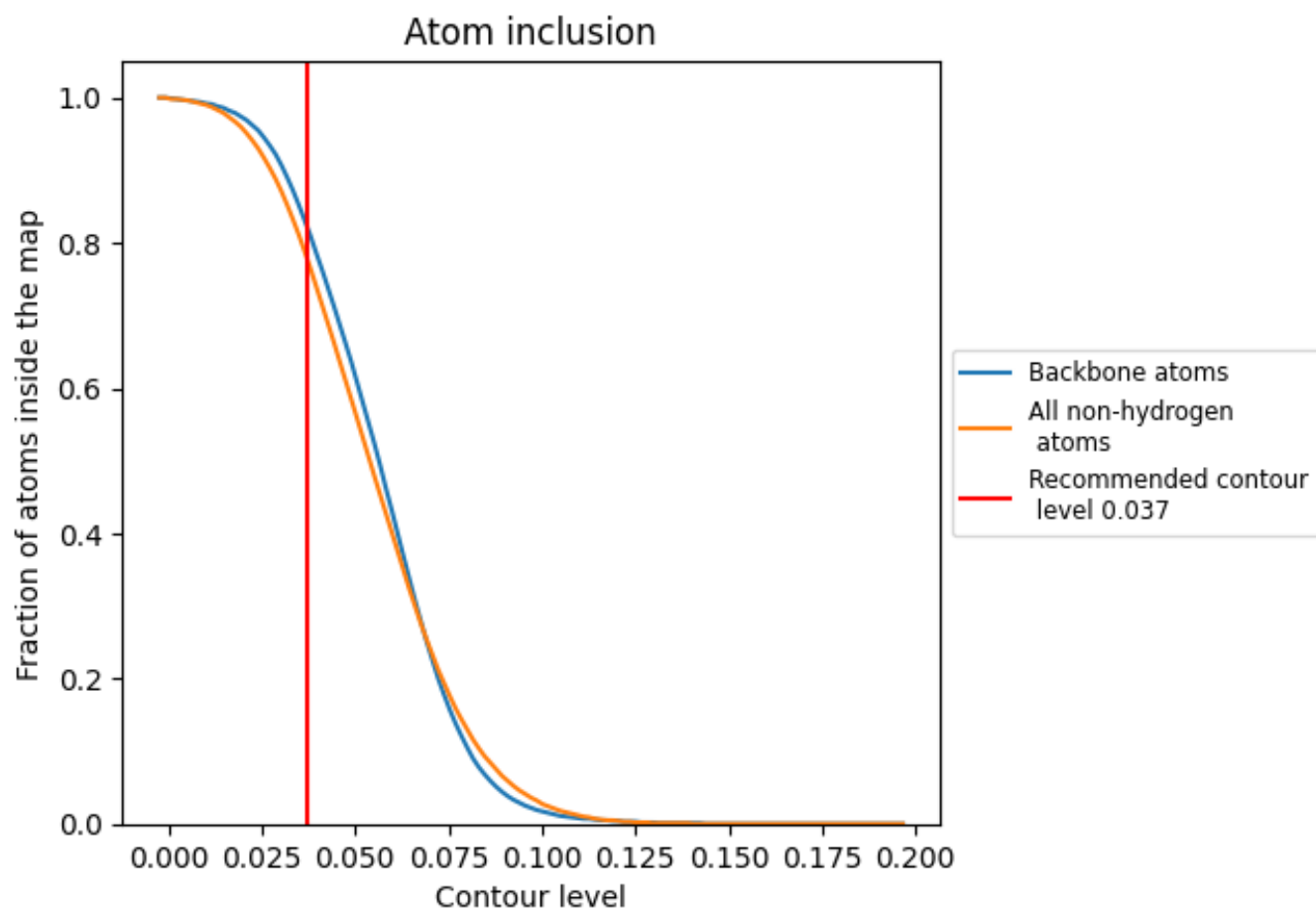
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.037).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 78% 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 (0.037) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7810	 0.5480
1	 0.9170	 0.5710
2	 0.4110	 0.5020
5	 0.8450	 0.5480
7	 0.9200	 0.5820
8	 0.8760	 0.5650
9	 0.8550	 0.5460
A	 0.8750	 0.5890
AA	 0.5810	 0.5490
Aa	 0.7760	 0.5540
B	 0.7290	 0.5740
BB	 0.6570	 0.5410
Bb	 0.5670	 0.5220
C	 0.8220	 0.5720
CC	 0.7270	 0.5640
Cc	 0.5130	 0.4950
D	 0.6320	 0.5460
DD	 0.5910	 0.5160
Dd	 0.8390	 0.5710
E	 0.7140	 0.5420
EE	 0.7840	 0.5690
Ee	 0.5750	 0.5190
F	 0.8690	 0.5750
FF	 0.6510	 0.5330
G	 0.5690	 0.5200
GG	 0.5460	 0.4980
Gg	 0.3380	 0.4730
H	 0.6070	 0.5480
HH	 0.3700	 0.4780
I	 0.6420	 0.5480
II	 0.7610	 0.5540
J	 0.5230	 0.5080
JJ	 0.7540	 0.5570
KK	 0.5340	 0.4910
L	 0.6920	 0.5400






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Chain	Atom inclusion	Q-score
LL	0.8160	0.5770
M	0.7560	0.5510
N	0.9090	0.5940
NN	0.7920	0.5700
O	0.8140	0.5680
OO	0.7130	0.5460
P	0.7850	0.5790
PP	0.5230	0.5030
Q	0.8700	0.5930
QQ	0.7080	0.5370
R	0.7610	0.5420
RR	0.4210	0.5000
S	0.8200	0.5780
SS	0.5770	0.5160
T	0.7650	0.5560
TT	0.6660	0.5380
U	0.5400	0.5040
UU	0.5030	0.4950
V	0.7220	0.5730
VV	0.5920	0.5590
W	0.5160	0.4740
WW	0.8260	0.5840
X	0.6660	0.5450
XX	0.7820	0.5750
Y	0.6420	0.5410
YY	0.6530	0.5350
Z	0.6530	0.5460
ZZ	0.4490	0.5020
a	0.8650	0.6000
b	0.6970	0.5320
c	0.6910	0.5390
d	0.6980	0.5630
e	0.8580	0.5920
f	0.8930	0.5900
g	0.8020	0.5640
h	0.6180	0.5280
i	0.6680	0.5350
j	0.9140	0.5980
k	0.4520	0.5000
l	0.8270	0.5740
m	0.7100	0.5630
n	0.9130	0.5840

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Chain	Atom inclusion	Q-score
o	 0.7530	 0.5730
p	 0.8010	 0.5630
r	 0.8140	 0.5810