



wwPDB EM Validation Summary Report ⓘ

Dec 17, 2023 – 03:40 AM JST

PDB ID : 8JDL
EMDB ID : EMD-36180
Title : Structure of the Human cytoplasmic Ribosome with human tRNA
Tyr(GalQ34) and mRNA(UAU) (non-rotated state)
Authors : Ishiguro, K.; Yokoyama, T.; Shirouzu, M.; Suzuki, T.
Deposited on : 2023-05-14
Resolution : 2.42 Å(reported)
Based on initial model : 6Y0G

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

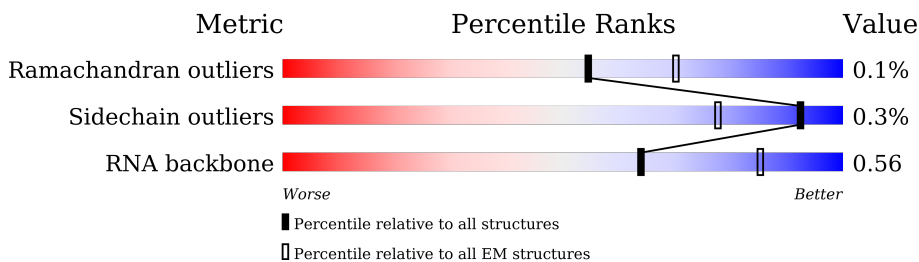
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.42 Å.

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



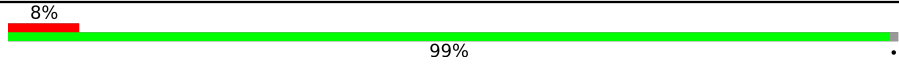
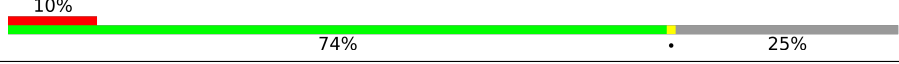
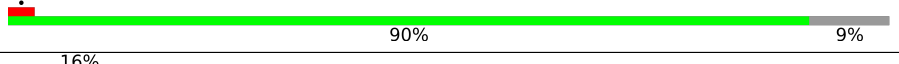

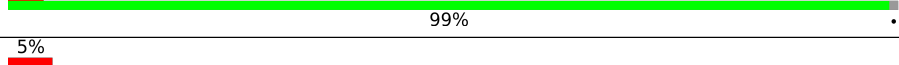
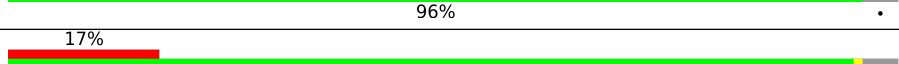
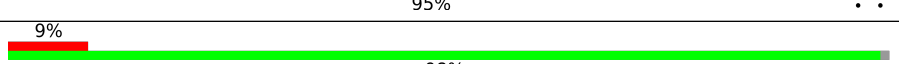
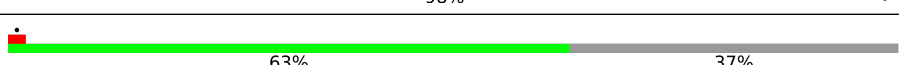
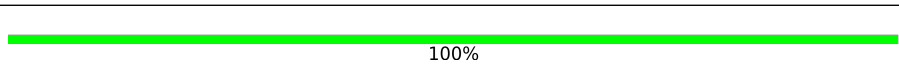
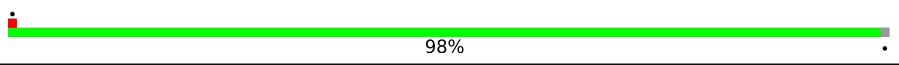

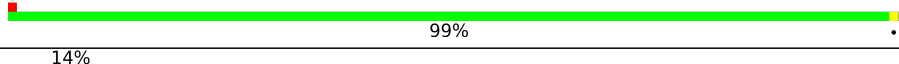
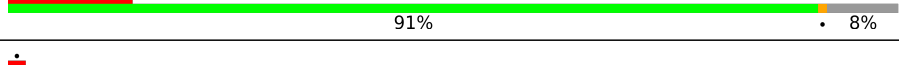
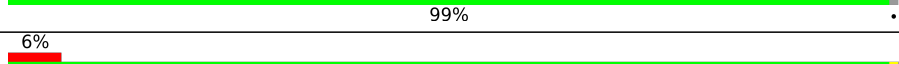
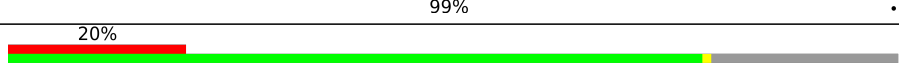
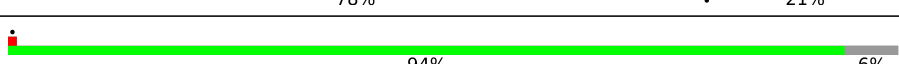
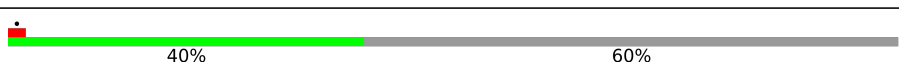

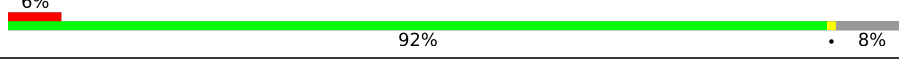
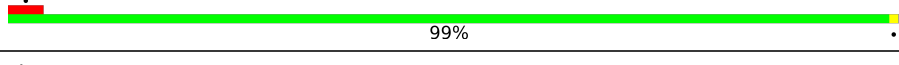
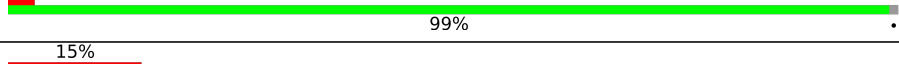




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	14	
2	B	76	
3	D	5070	
4	E	120	
5	F	156	
6	G	257	
7	H	403	
8	I	427	

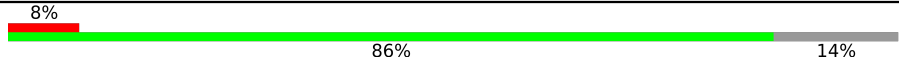
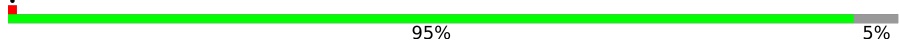
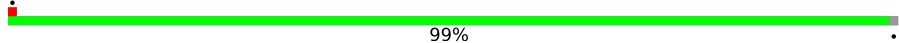
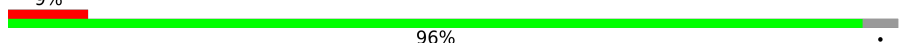
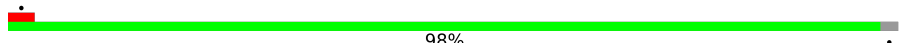
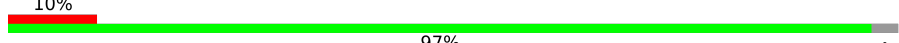


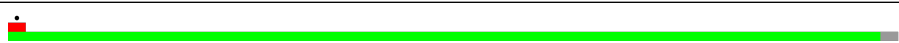

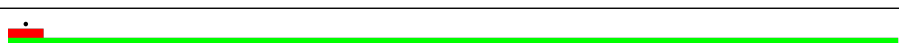

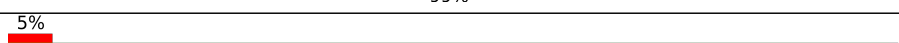
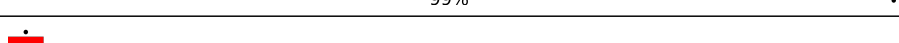
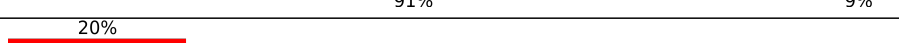
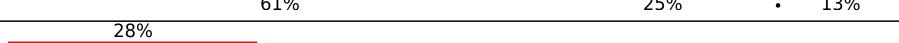
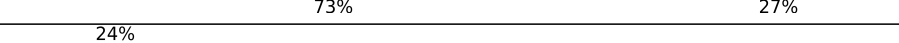
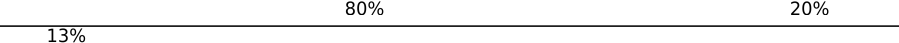
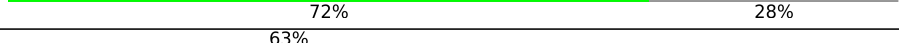

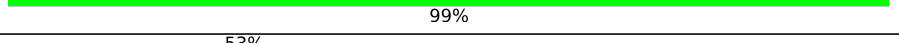
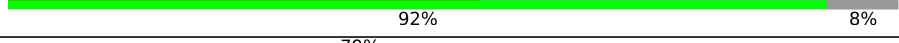
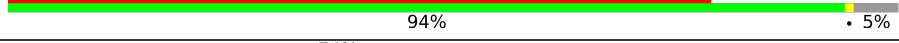
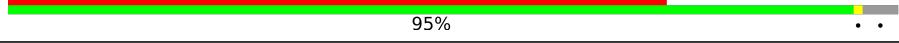
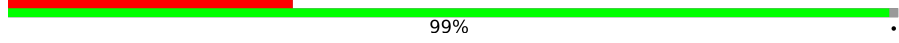
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Mol	Chain	Length	Quality of chain
9	J	297	 8% 99%
10	K	288	 10% 74% 25%
11	L	248	 90% 9%
12	M	266	 16% 85% 15%
13	N	192	 99%
14	O	214	 5% 96%
15	P	178	 17% 95%
16	Q	211	 9% 98%
17	R	215	 63% 37%
18	S	204	 100%
19	T	203	 98%
20	U	184	 85% 15%
21	V	188	 99%
22	W	196	 14% 91% 8%
23	X	176	 99%
24	Y	160	 6% 99%
25	Z	128	 20% 78% 21%
26	a	140	 94% 6%
27	b	157	 40% 60%
28	c	156	 77% 23%
29	d	145	 6% 92% 8%
30	e	136	 99%
31	f	148	 99%
32	g	159	 15% 64% 35%
33	h	115	 83% 16%

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Mol	Chain	Length	Quality of chain
34	i	125	
35	j	135	
36	k	110	
37	l	117	
38	m	123	
39	n	105	
40	o	97	
41	p	70	
42	q	51	
43	r	128	
44	s	25	
45	t	106	
46	u	92	
47	v	137	
48	w	1869	
49	x	295	
50	y	264	
51	z	293	
52	0	243	
53	1	263	
54	2	204	
55	3	249	
56	4	194	
57	5	208	
58	6	194	

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Mol	Chain	Length	Quality of chain
59	7	165	58% 58% 42%
60	8	158	15% 88% 10%
61	9	151	22% 99%
62	AA	151	15% 88% 11%
63	AB	145	87% 92% 8%
64	AC	146	65% 96% ..
65	AD	135	71% 96% ..
66	AE	152	72% 95% 5%
67	AF	145	71% 99%
68	AG	119	66% 86% 14%
69	AH	83	40% 100%
70	AI	130	7% 99%
71	AJ	143	17% 99%
72	AK	133	86% 92% 8%
73	AL	125	62% 69% 31%
74	AM	115	16% 86% 14%
75	AN	84	52% 98% ..
76	AO	69	52% 88% 12%
77	AP	56	27% 80% 20%
78	AQ	59	86% 93% ..
79	AR	317	98% 98%

2 Entry composition i

There are 82 unique types of molecules in this entry. The entry contains 207902 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 mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	11	226	102	31	82	11	0	0

- Molecule 2 is a RNA chain called tRNA (Tyr).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	76	1647	746	288	538	75	0	0

- Molecule 3 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	D	3512	75336	33585	13757	24482	3512	0	0

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

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

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

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

- Molecule 6 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	247	1891	1185	388	312	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	398	3211	2045	604	548	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	363	2884	1815	577	478	14	0	0

- Molecule 9 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	293	2379	1506	434	425	14	0	0

- Molecule 10 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	217	1751	1128	332	287	4	0	0

- Molecule 11 is a protein called 60S ribosomal protein L7.

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

- Molecule 12 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	227	1832	1168	352	308	4	0	0

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

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

- Molecule 14 is a protein called 60S ribosomal protein L10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	206	1660	1053	319	275	13	0	0

- Molecule 15 is a protein called 60S ribosomal protein L11.

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

- Molecule 16 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	208	1682	1052	348	278	4	0	0

- Molecule 17 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	R	136	1120	719	215	179	7	0	0

- Molecule 18 is a protein called 60S ribosomal protein L15.

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

- Molecule 19 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	T	200	1641	1058	320	258	5	0	0

- Molecule 20 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	U	157	1273	797	246	221	9	0	0

- Molecule 21 is a protein called 60S ribosomal protein L18.

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

- Molecule 22 is a protein called 60S ribosomal protein L19.

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

- Molecule 23 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 24 is a protein called 60S ribosomal protein L21.

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

- Molecule 25 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	101	Total	C	N	O	S	0	0
			821	526	143	150	2		

- Molecule 26 is a protein called 60S ribosomal protein L23.

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

- Molecule 27 is a protein called 60S ribosomal protein L24.

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

- Molecule 28 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	c	120	981	628	185	167	1	0	0

- Molecule 29 is a protein called 60S ribosomal protein L26.

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

- Molecule 30 is a protein called 60S ribosomal protein L27.

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

- Molecule 31 is a protein called 60S ribosomal protein L27a.

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

- Molecule 32 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	g	104	832	515	182	132	3	0	0

- Molecule 33 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	h	97	755	479	133	137	6	0	0

- Molecule 34 is a protein called 60S ribosomal protein L31.

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

- Molecule 35 is a protein called 60S ribosomal protein L32.

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

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

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

- Molecule 37 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	l	112	888	555	183	144	6	0	0

- Molecule 38 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	m	121	1010	638	204	167	1	0	0

- Molecule 39 is a protein called 60S ribosomal protein L36.

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

- Molecule 40 is a protein called 60S ribosomal protein L37.

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

- Molecule 41 is a protein called 60S ribosomal protein L38.

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

- Molecule 42 is a protein called 60S ribosomal protein L39.

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

- Molecule 43 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 44 is a protein called 60S ribosomal protein L41.

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

- Molecule 45 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	t	105	Total	C	N	O	S	0	0
			862	542	175	139	6		

- Molecule 46 is a protein called 60S ribosomal protein L37a.

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

- Molecule 47 is a protein called 60S ribosomal protein L28.

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

- Molecule 48 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	w	1634	Total	C	N	O	P	0	0
			34933	15622	6267	11411	1633		

- Molecule 49 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	215	Total	C	N	O	S	0	0
			1695	1077	297	313	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	y	212	Total	C	N	O	S	0	0
			1725	1096	308	307	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	z	212	Total	C	N	O	S	0	0
			1633	1059	279	285	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	0	212	Total	C	N	O	S	0	0
			1646	1050	299	290	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1	262	Total	C	N	O	S	0	0
			2070	1321	383	358	8		

- Molecule 54 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	187	Total	C	N	O	S	0	0
			1464	916	276	265	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
55	3	237	Total	C	N	O	S	0	0
			1917	1197	384	329	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4	187	Total	C	N	O	S	0	0
			1510	963	278	268	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	5	206	Total	C	N	O	S	0	0
			1674	1049	329	291	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
58	6	182	Total	C	N	O	S	0	0
			1506	959	300	245	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
59	7	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	8	142	Total	C	N	O	S	0	0
			1150	732	215	197	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
61	9	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AA	134	Total	C	N	O	S	0	0
			1002	612	197	187	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	AB	134	1103	703	208	185	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	AC	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	AD	131	1057	665	197	191	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	AE	144	1169	731	236	201	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	AF	143	1111	696	213	198	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	AG	102	799	501	153	141	4	0	0

- Molecule 69 is a protein called 40S ribosomal protein S21.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	AI	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	AJ	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	AK	123	1002	634	196	167	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	AL	86	680	436	127	116	1	0	0

- Molecule 74 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	AM	99	792	492	165	130	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	AN	83	643	402	119	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	AO	61	479	292	95	90	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	AP	45	370	228	77	60	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	AQ	57	452	279	99	73	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	AR	313	2436	1535	424	465	12	0	0

- Molecule 80 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

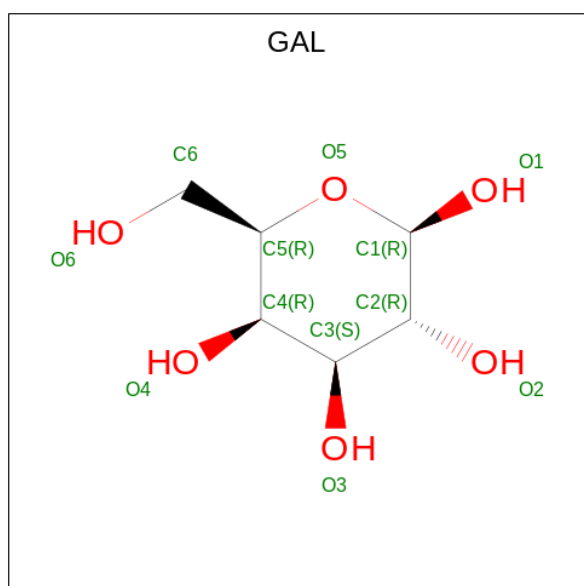
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
80	A	1	1	1	0
80	D	401	401	401	0
80	E	10	10	10	0
80	F	5	5	5	0
80	G	2	2	2	0
80	H	1	1	1	0
80	I	1	1	1	0
80	N	1	1	1	0
80	O	1	1	1	0
80	S	1	1	1	0
80	U	2	2	2	0
80	V	2	2	2	0

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Mol	Chain	Residues	Atoms	AltConf
80	X	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	k	1	Total Mg 1 1	0
80	l	1	Total Mg 1 1	0
80	w	100	Total Mg 100 100	0
80	8	1	Total Mg 1 1	0
80	AA	1	Total Mg 1 1	0
80	AF	1	Total Mg 1 1	0
80	AJ	1	Total Mg 1 1	0
80	AM	1	Total Mg 1 1	0

- Molecule 81 is beta-D-galactopyranose (three-letter code: GAL) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
81	B	1	Total	C	O	0
			11	6	5	

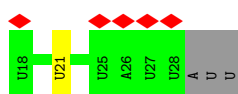
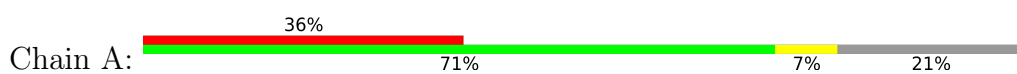
- Molecule 82 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
82	o	1	Total	Zn	0
			1	1	
82	r	1	Total	Zn	0
			1	1	
82	t	1	Total	Zn	0
			1	1	
82	u	1	Total	Zn	0
			1	1	
82	AM	1	Total	Zn	0
			1	1	
82	AP	1	Total	Zn	0
			1	1	

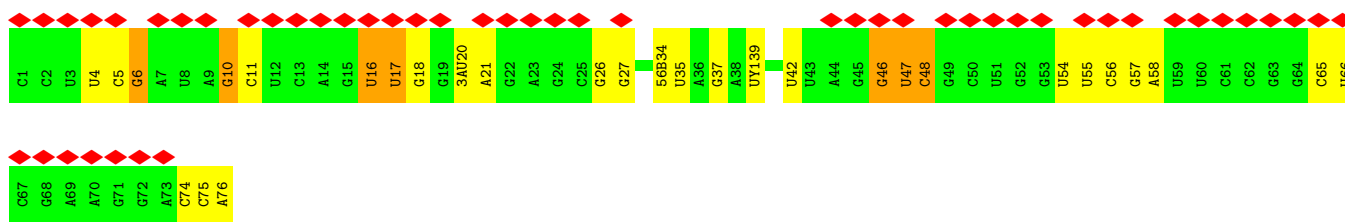
3 Residue-property plots i

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.

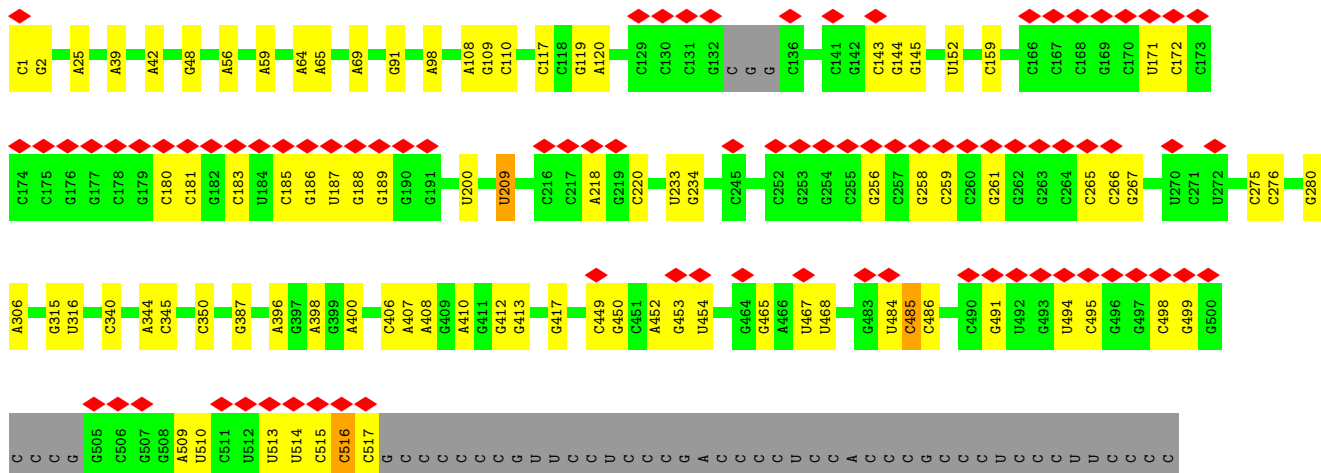
- Molecule 1: mRNA

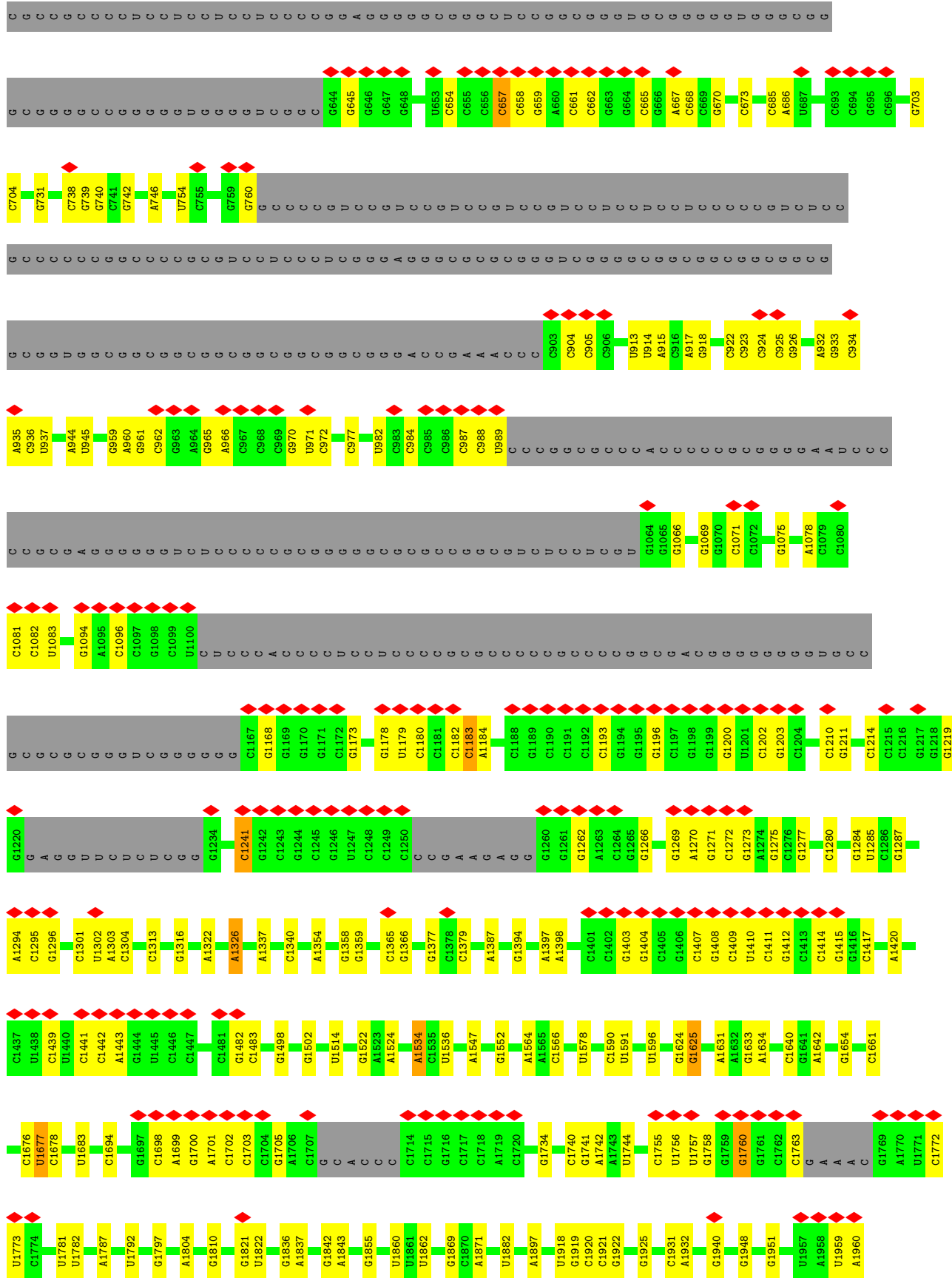


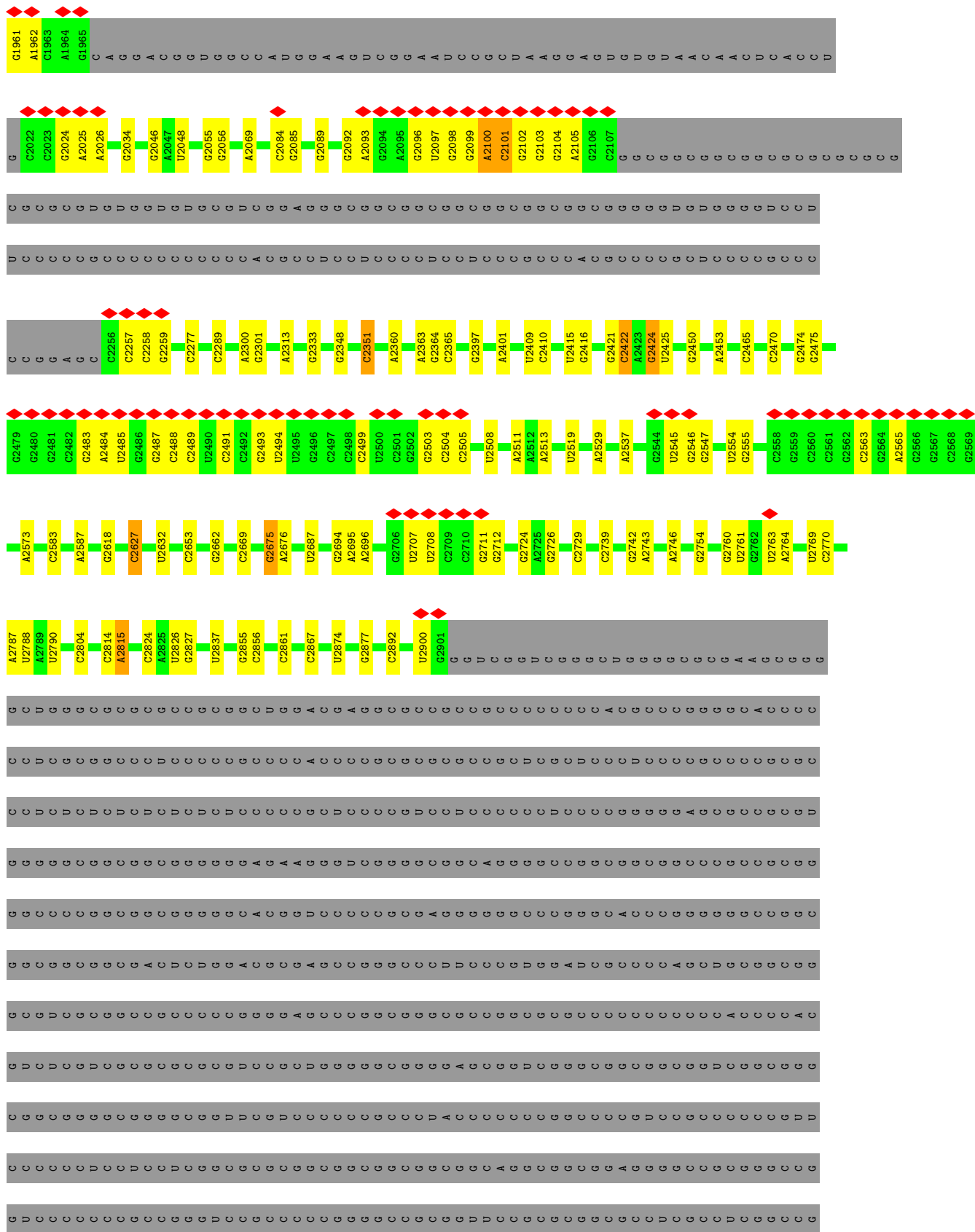
- Molecule 2: tRNA (Tyr)

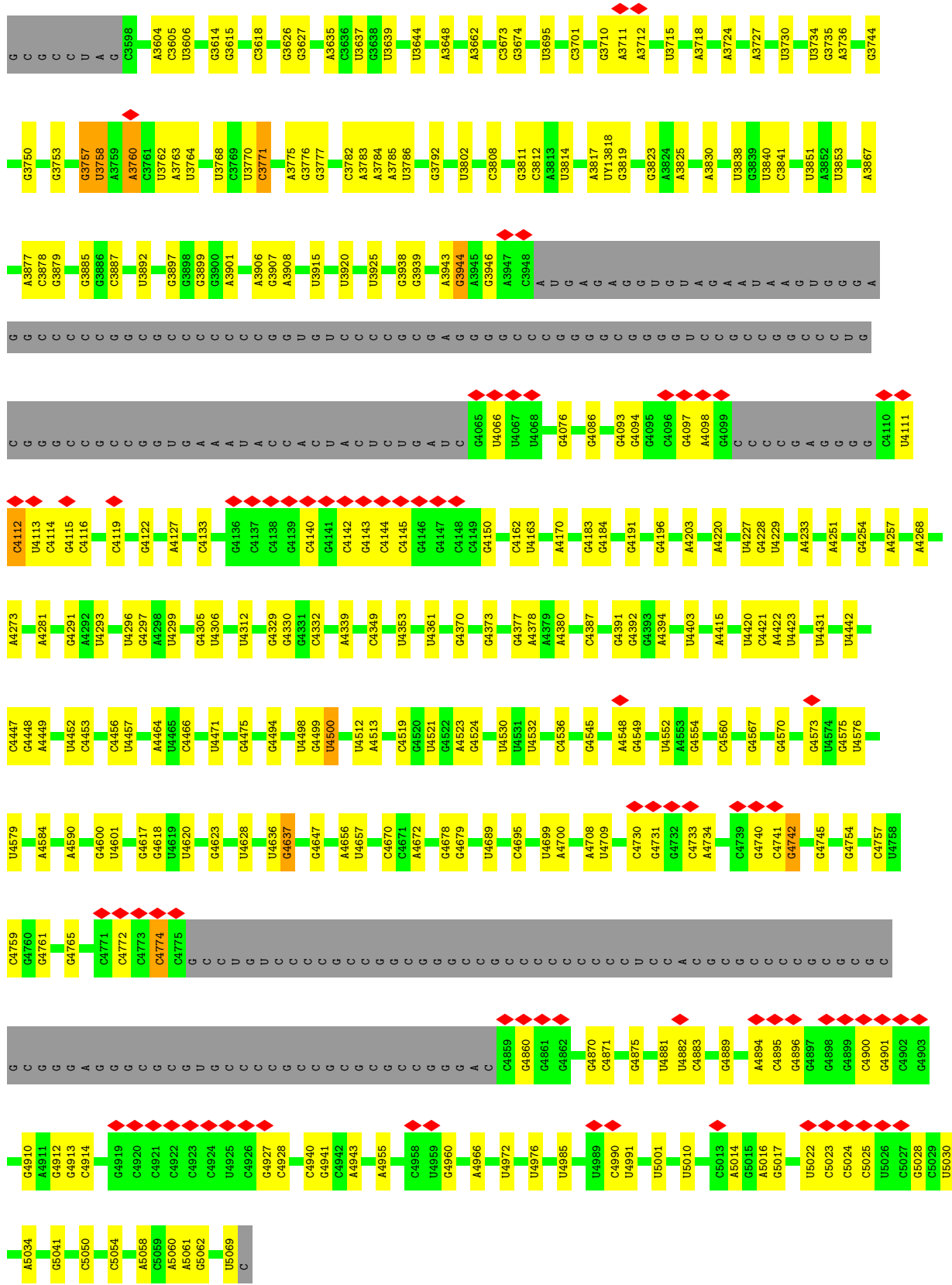


- Molecule 3: 28S ribosomal RNA

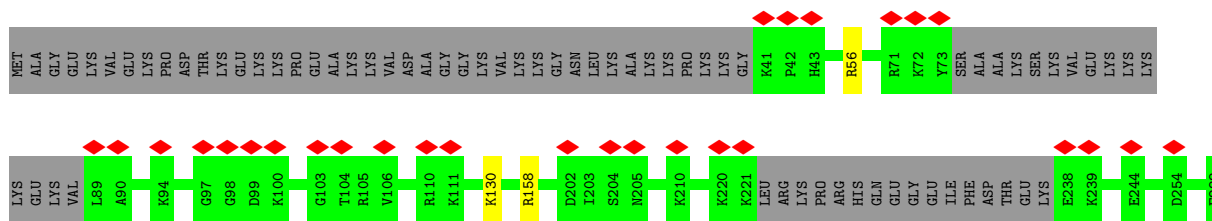






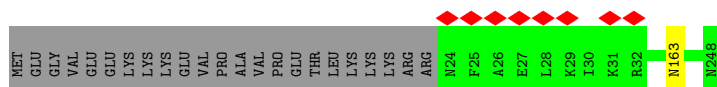


• Molecule 4: 5S ribosomal RNA



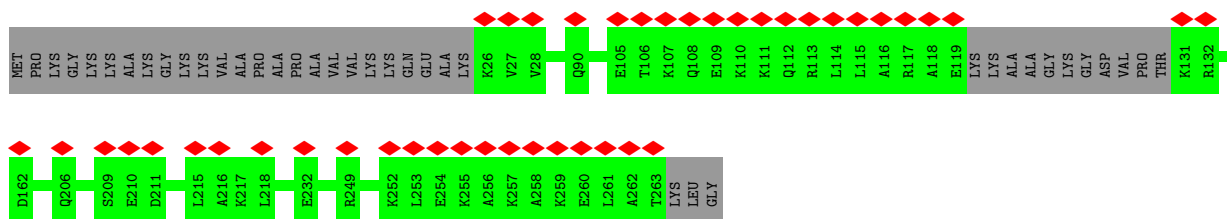
- Molecule 11: 60S ribosomal protein L7

Chain L: 90% 9%



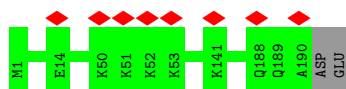
- Molecule 12: 60S ribosomal protein L7a

Chain M: 16% 85% 15%



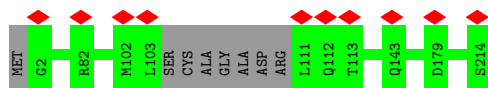
- Molecule 13: 60S ribosomal protein L9

Chain N: 99%



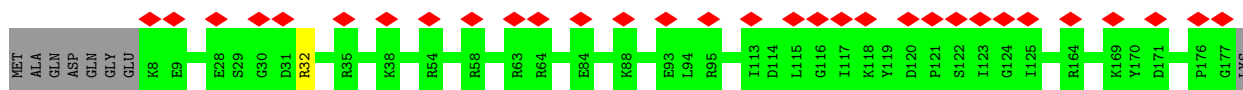
- Molecule 14: 60S ribosomal protein L10-like

Chain O: 5% 96%

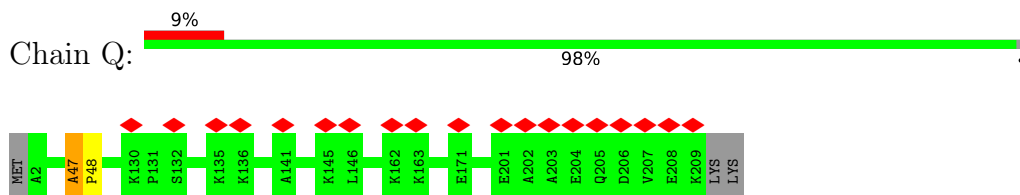


- Molecule 15: 60S ribosomal protein L11

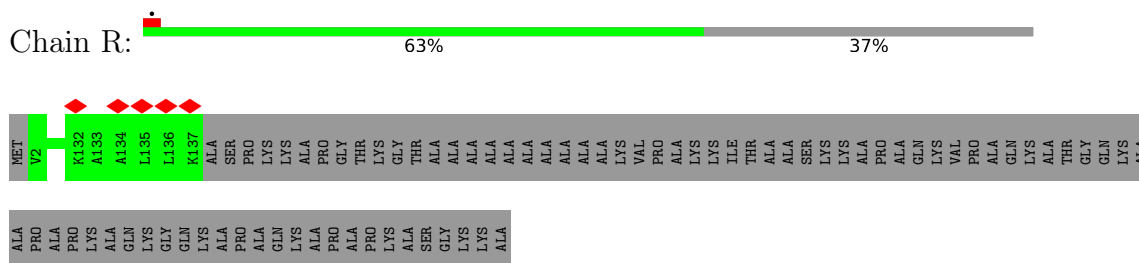
Chain P: 17% 95%



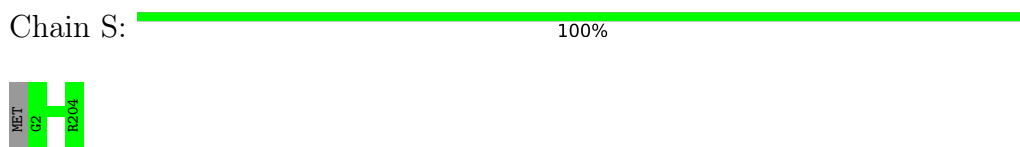
- Molecule 16: 60S ribosomal protein L13



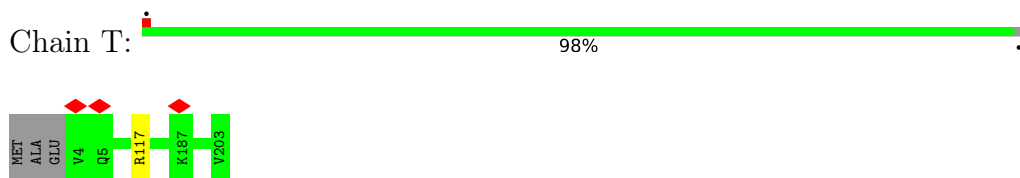
• Molecule 17: 60S ribosomal protein L14



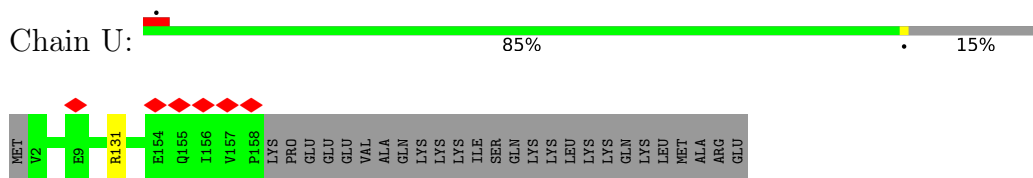
• Molecule 18: 60S ribosomal protein L15



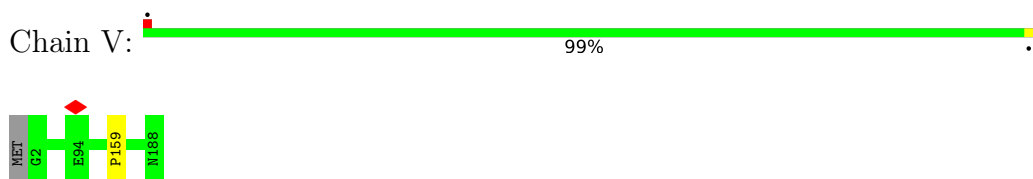
• Molecule 19: 60S ribosomal protein L13a



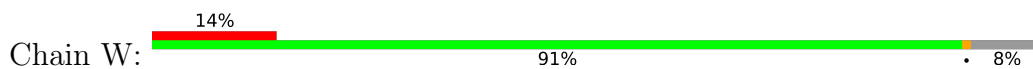
• Molecule 20: 60S ribosomal protein L17

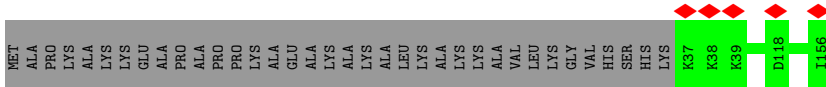


• Molecule 21: 60S ribosomal protein L18

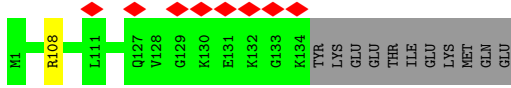
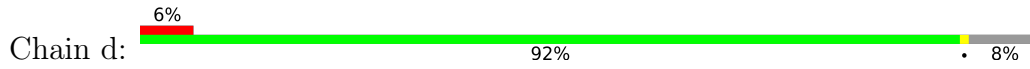


• Molecule 22: 60S ribosomal protein L19

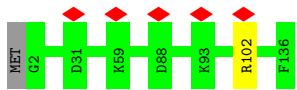




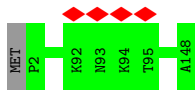
- Molecule 29: 60S ribosomal protein L26



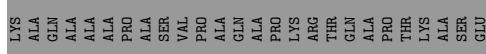
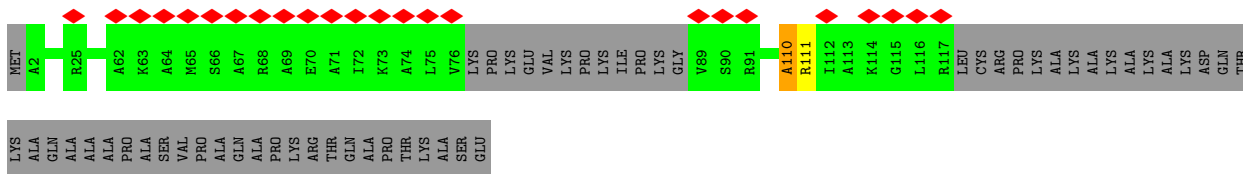
- Molecule 30: 60S ribosomal protein L27



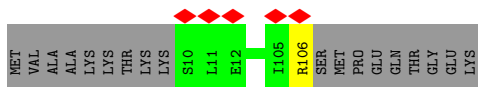
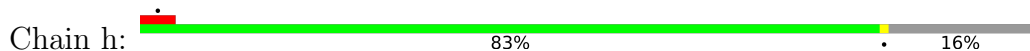
- Molecule 31: 60S ribosomal protein L27a



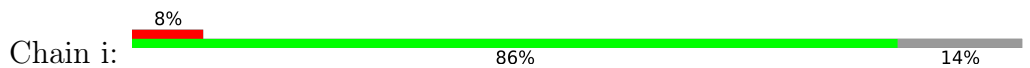
- Molecule 32: 60S ribosomal protein L29

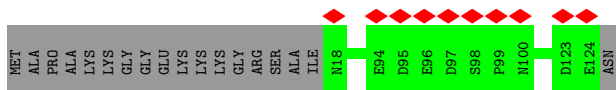


- Molecule 33: 60S ribosomal protein L30

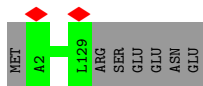


- Molecule 34: 60S ribosomal protein L31





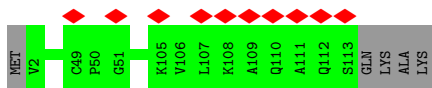
• Molecule 35: 60S ribosomal protein L32



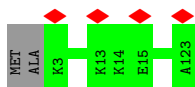
• Molecule 36: 60S ribosomal protein L35a



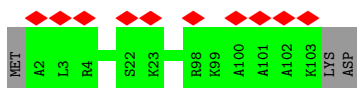
• Molecule 37: 60S ribosomal protein L34



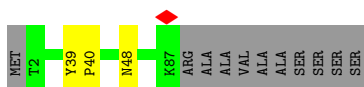
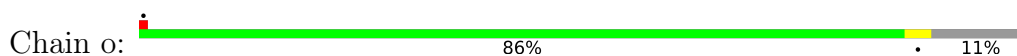
• Molecule 38: 60S ribosomal protein L35



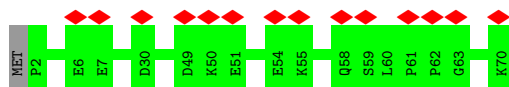
• Molecule 39: 60S ribosomal protein L36



• Molecule 40: 60S ribosomal protein L37



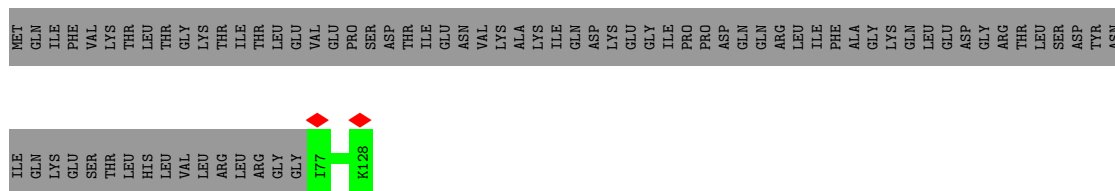
• Molecule 41: 60S ribosomal protein L38



- Molecule 42: 60S ribosomal protein L39



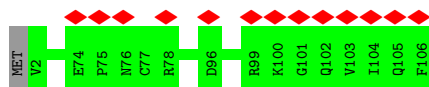
- Molecule 43: Ubiquitin-60S ribosomal protein L40



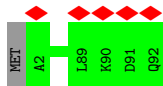
- Molecule 44: 60S ribosomal protein L41



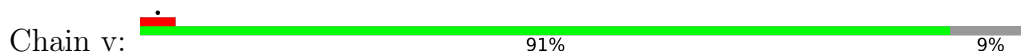
- Molecule 45: 60S ribosomal protein L36a

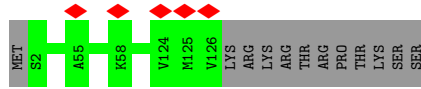


- Molecule 46: 60S ribosomal protein L37a

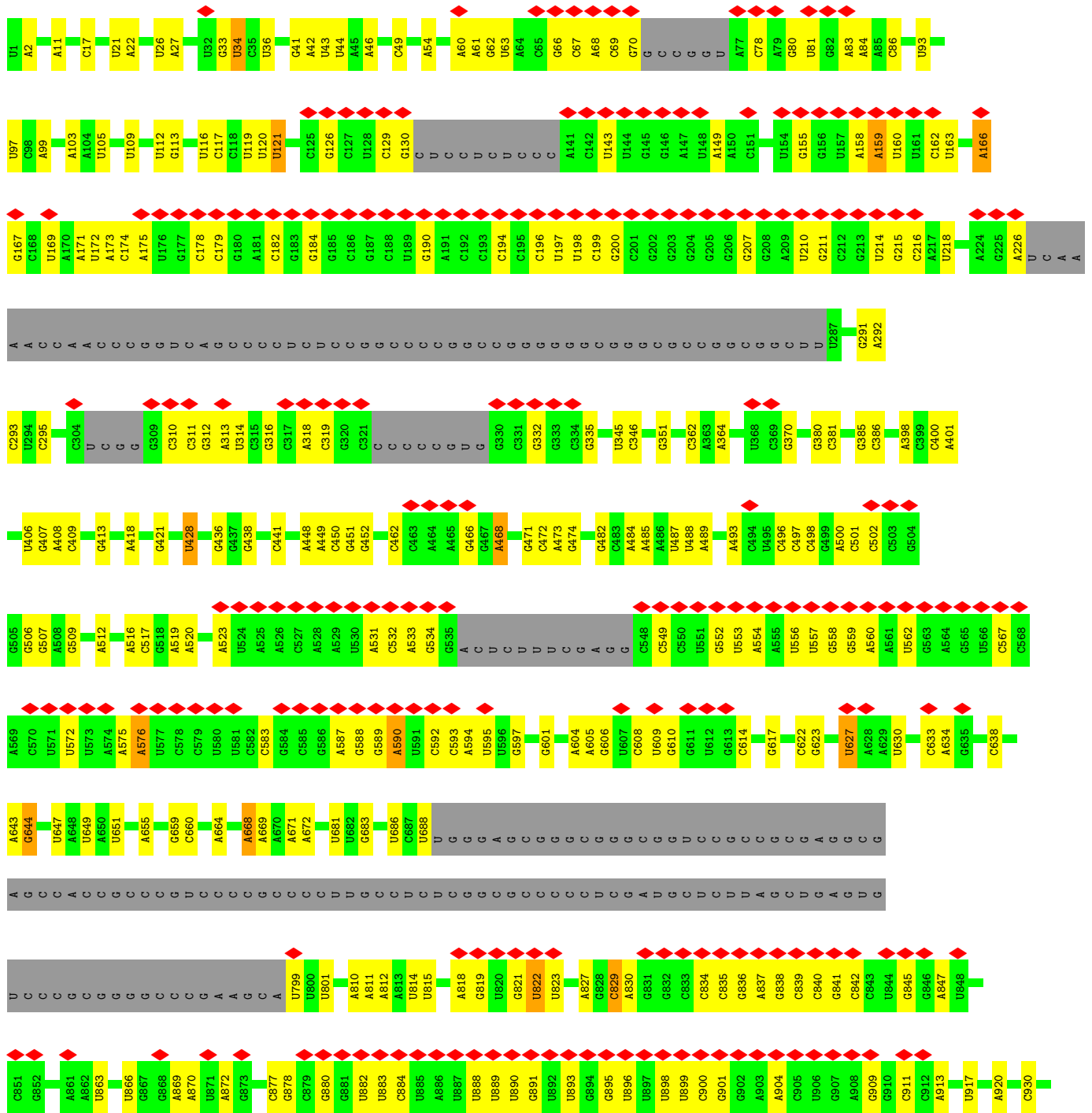


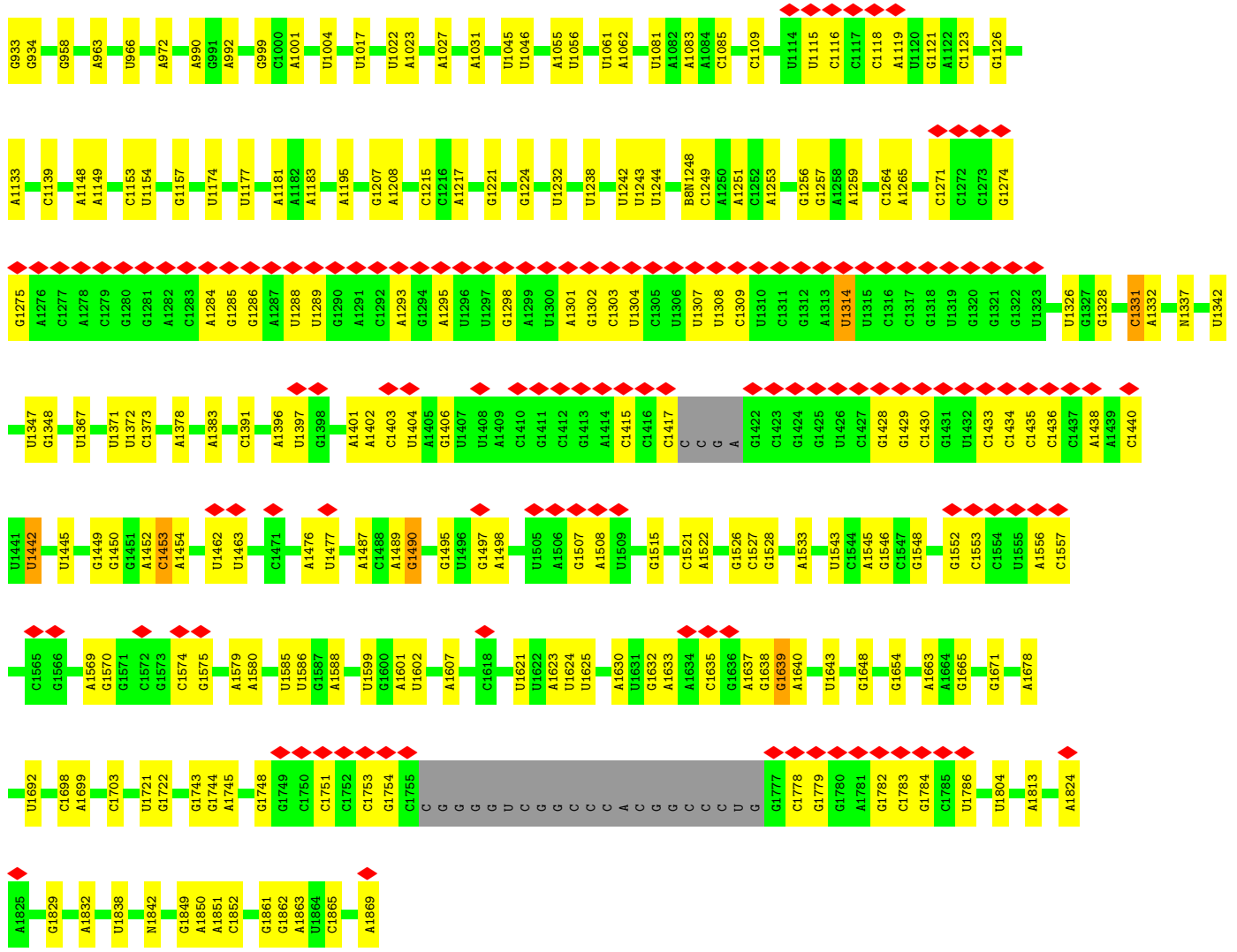
- Molecule 47: 60S ribosomal protein L28



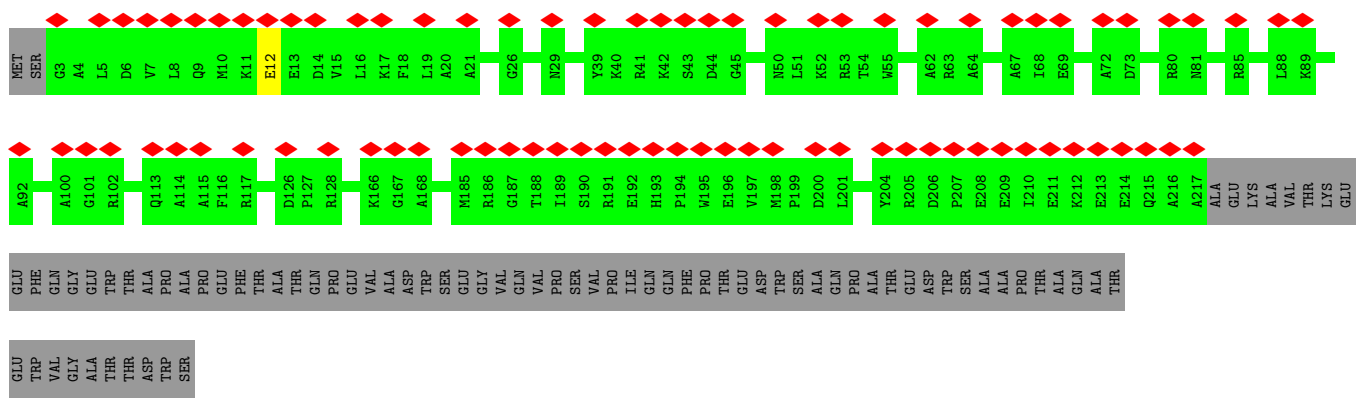
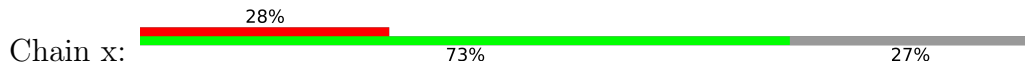


• Molecule 48: 18S ribosomal RNA

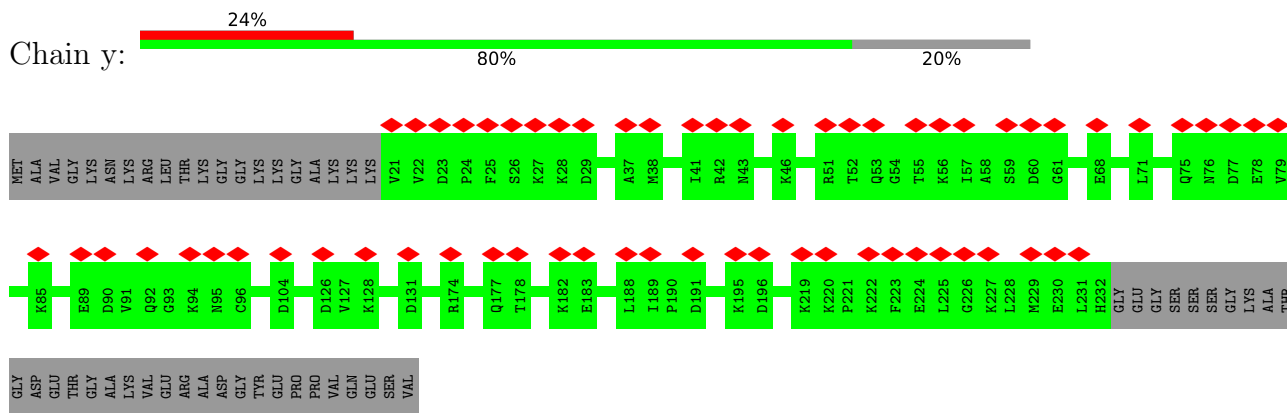




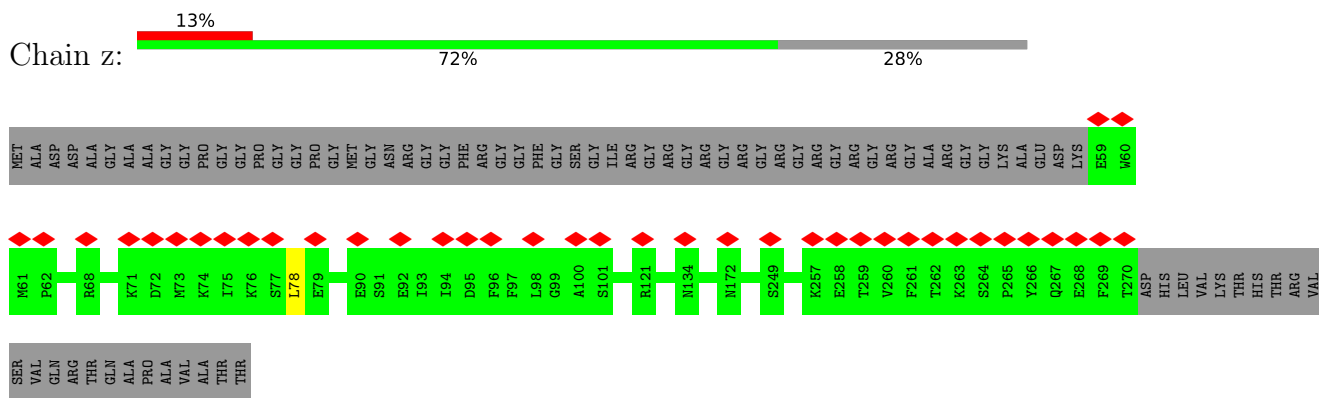
• Molecule 49: 40S ribosomal protein SA



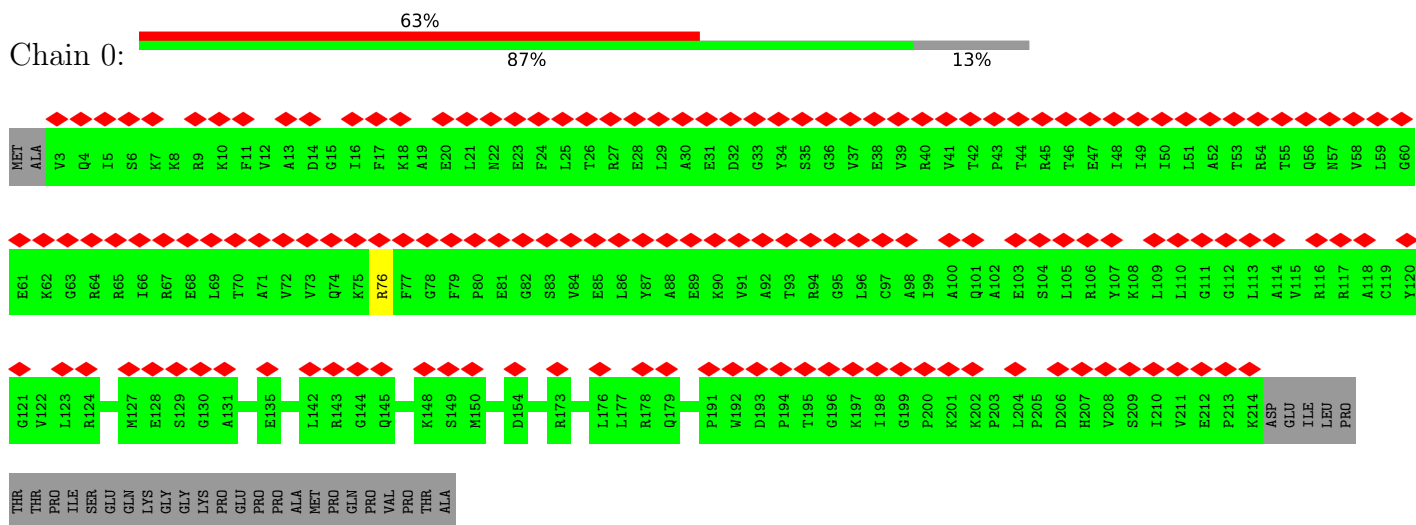
• Molecule 50: 40S ribosomal protein S3a



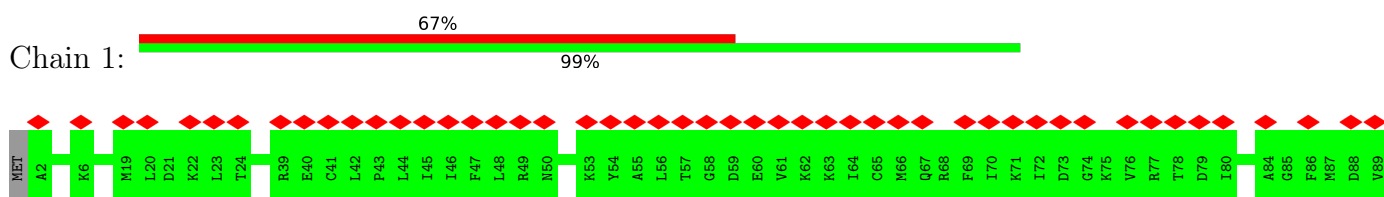
• Molecule 51: 40S ribosomal protein S2

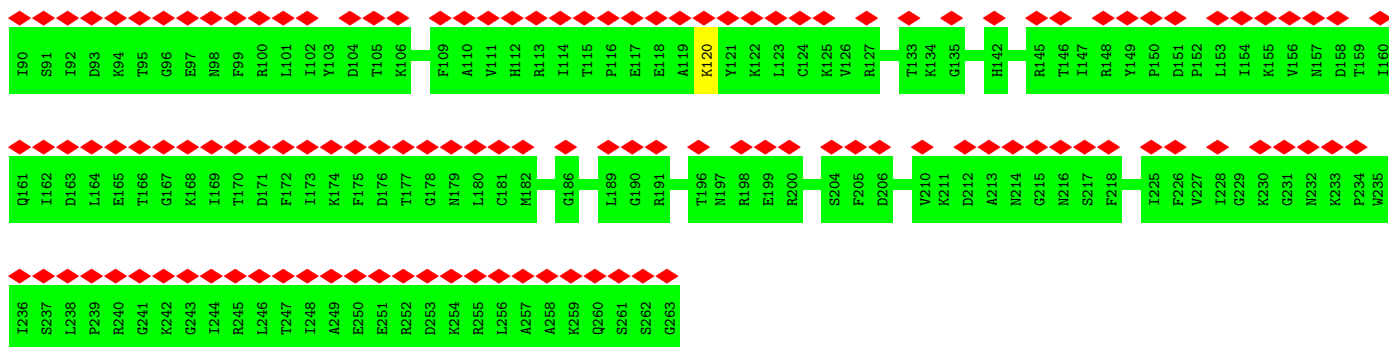


• Molecule 52: 40S ribosomal protein S3

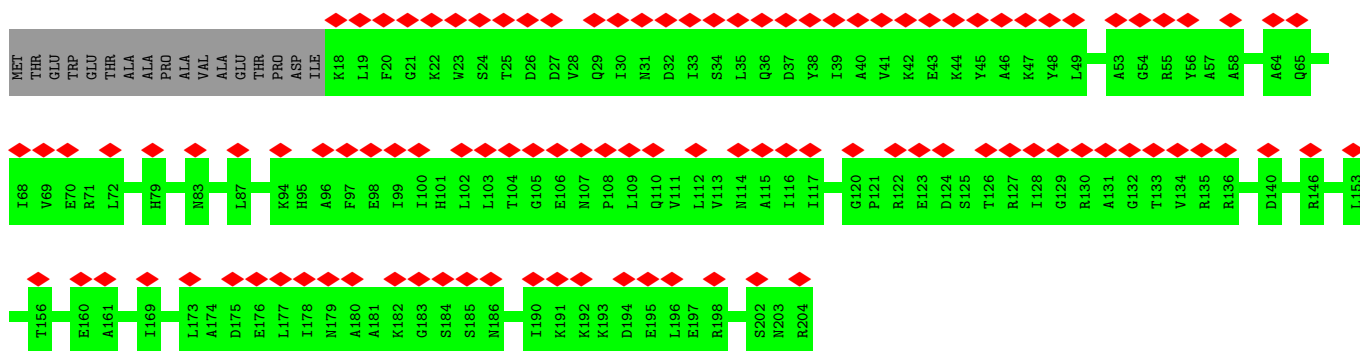
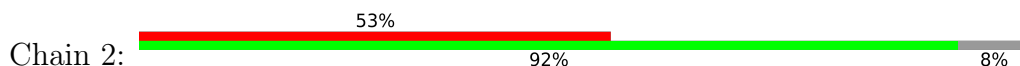


• Molecule 53: 40S ribosomal protein S4, X isoform

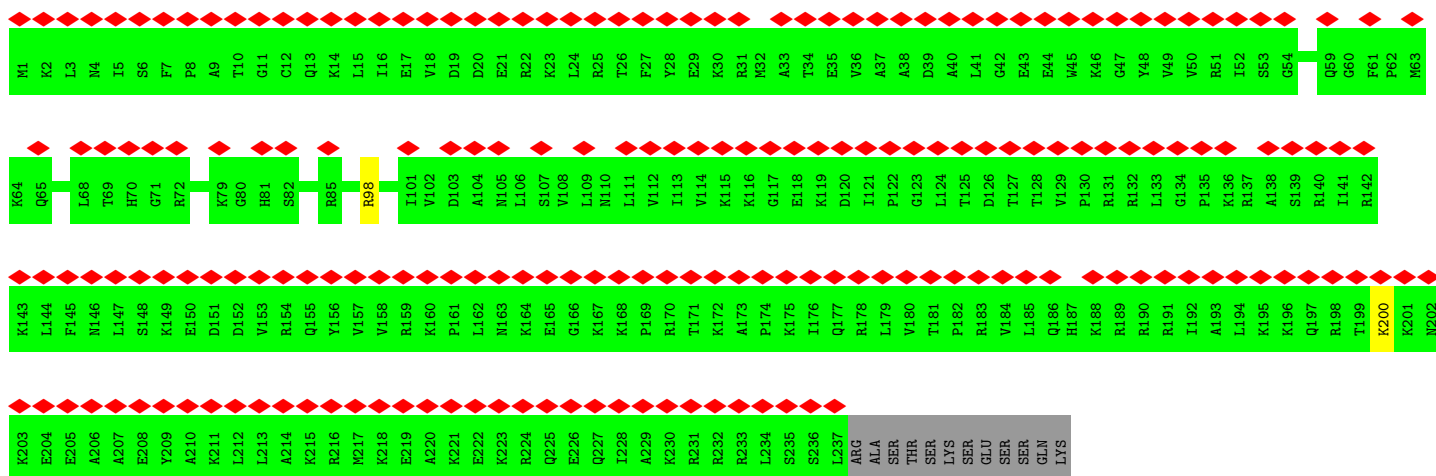
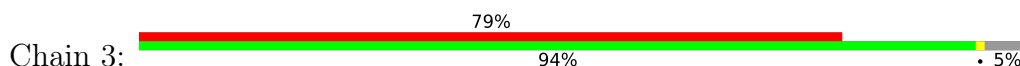




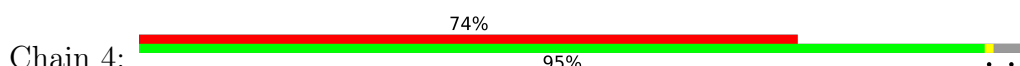
• Molecule 54: 40S ribosomal protein S5

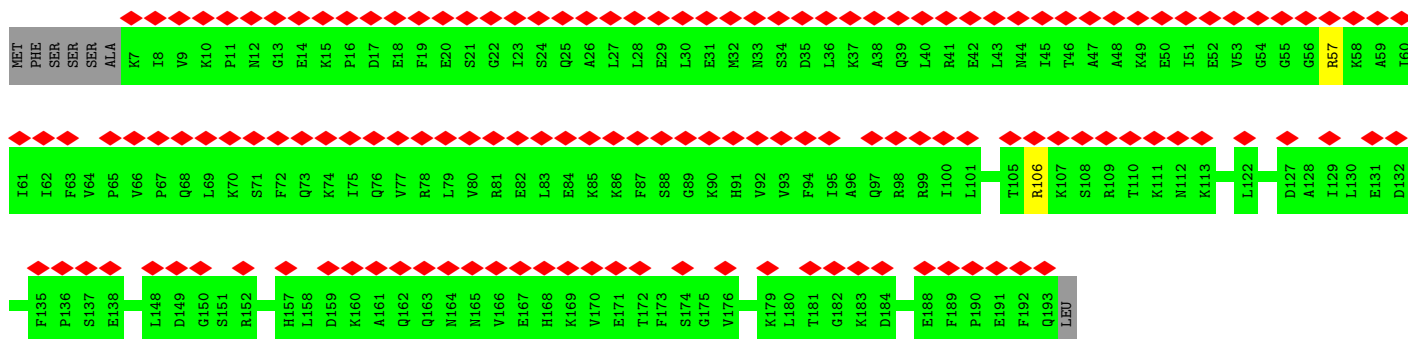


• Molecule 55: 40S ribosomal protein S6

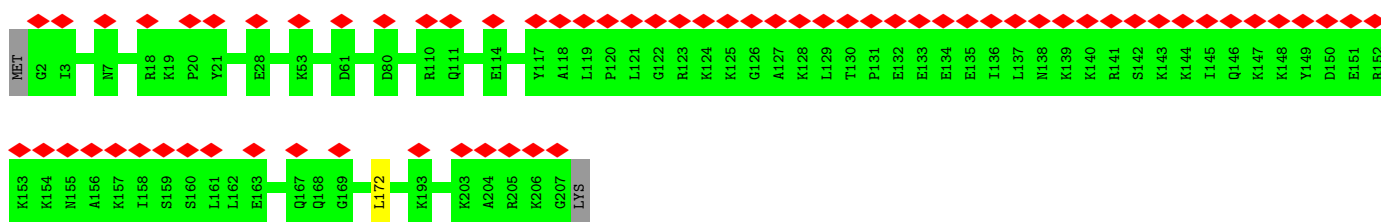


• Molecule 56: 40S ribosomal protein S7

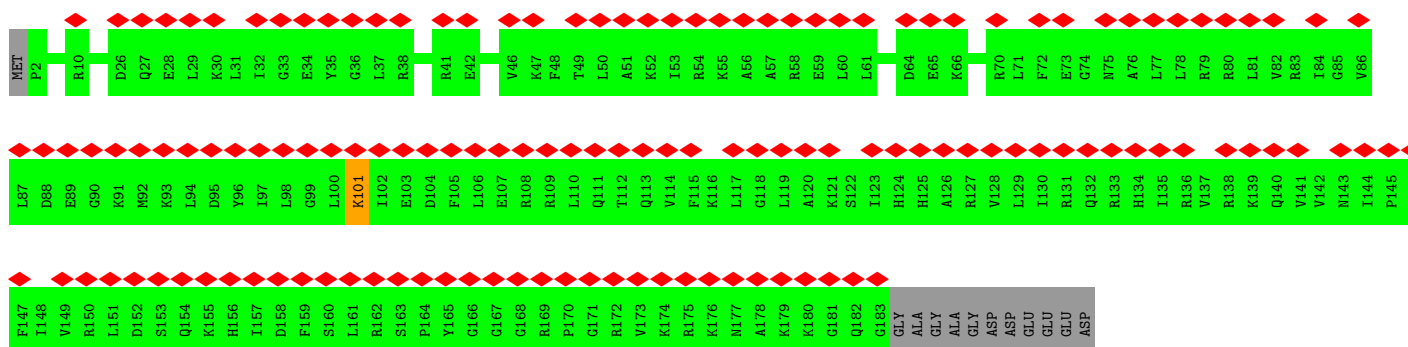




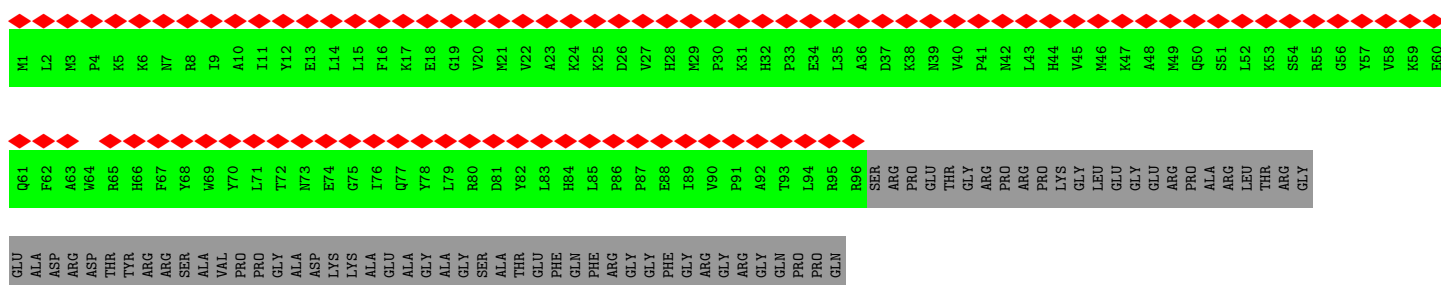
• Molecule 57: 40S ribosomal protein S8



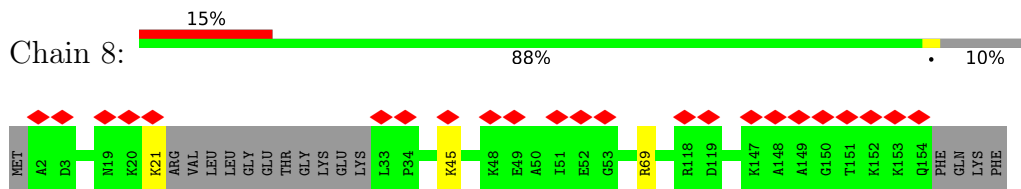
• Molecule 58: 40S ribosomal protein S9



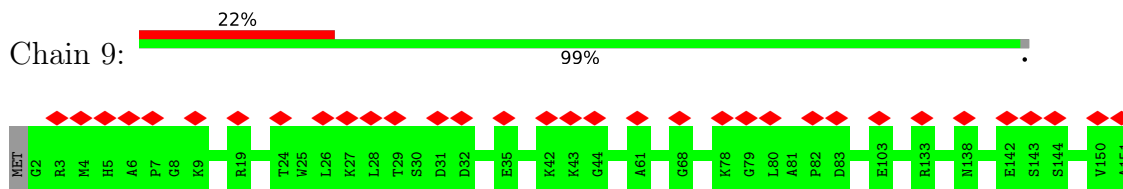
• Molecule 59: 40S ribosomal protein S10



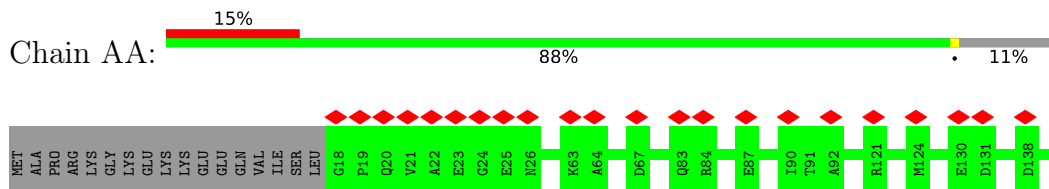
• Molecule 60: 40S ribosomal protein S11



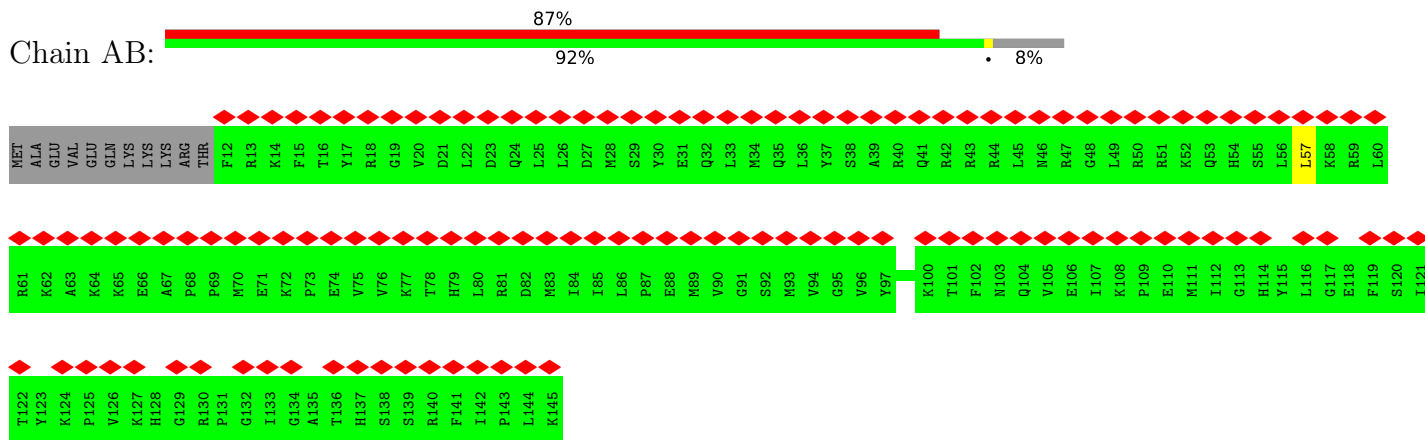
• Molecule 61: 40S ribosomal protein S13



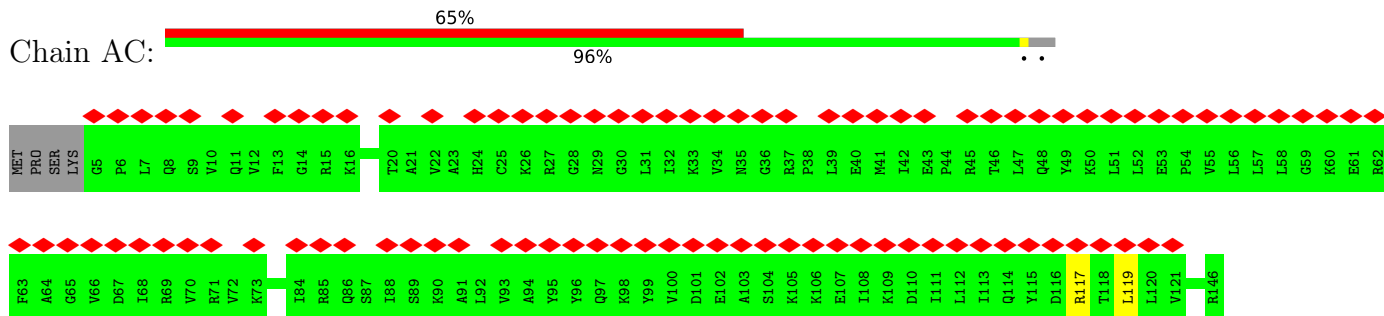
• Molecule 62: 40S ribosomal protein S14



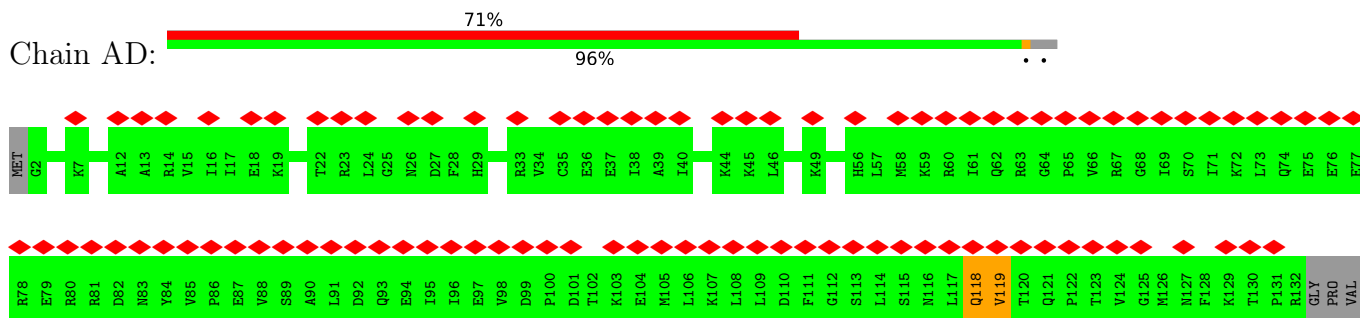
• Molecule 63: 40S ribosomal protein S15



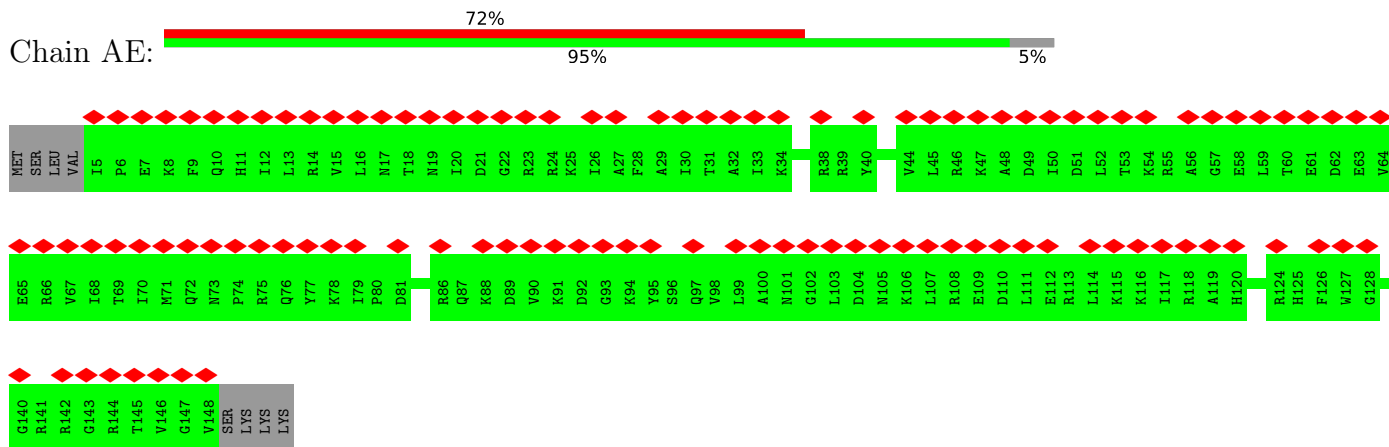
• Molecule 64: 40S ribosomal protein S16



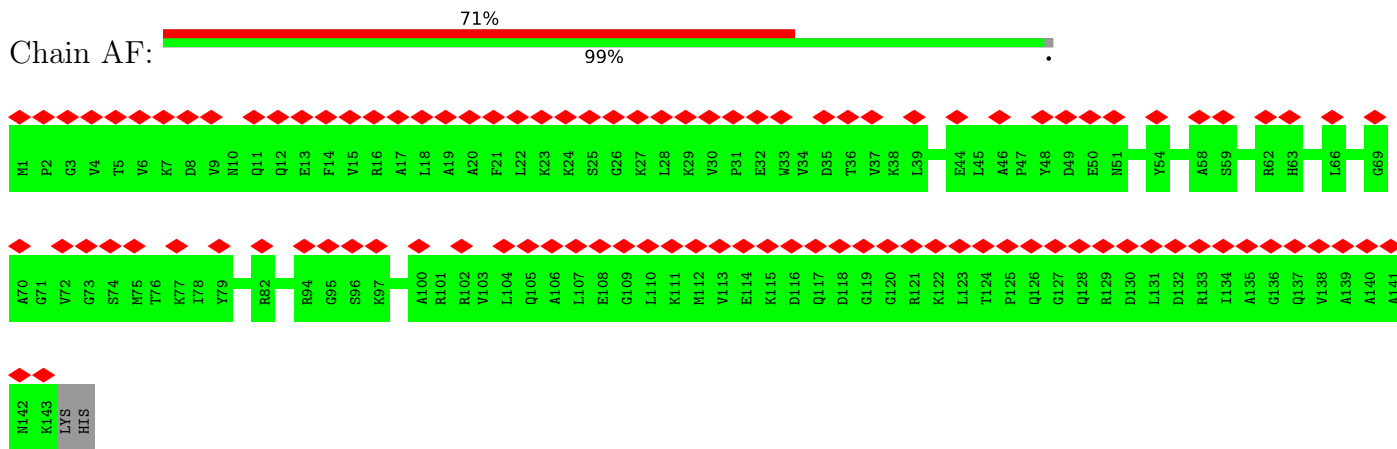
• Molecule 65: 40S ribosomal protein S17



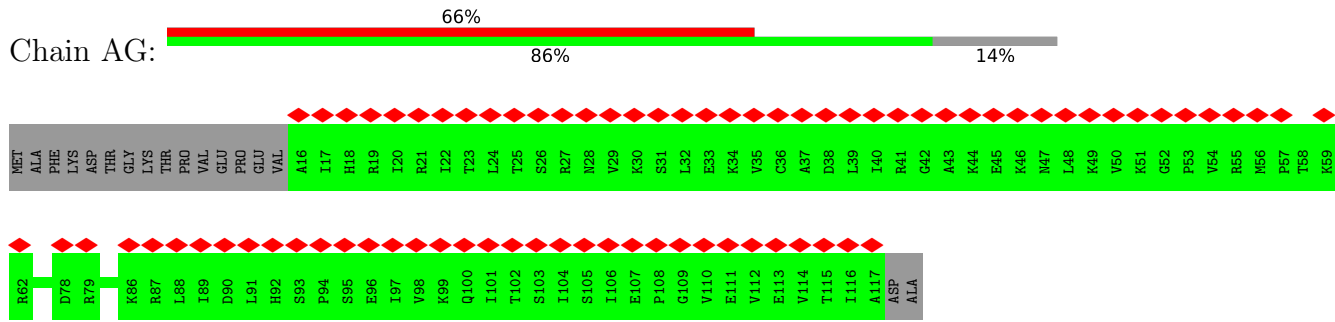
• Molecule 66: 40S ribosomal protein S18



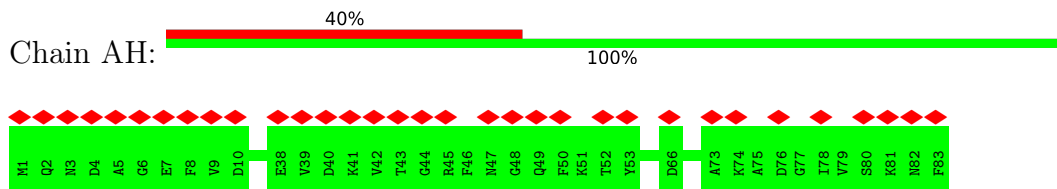
• Molecule 67: 40S ribosomal protein S19



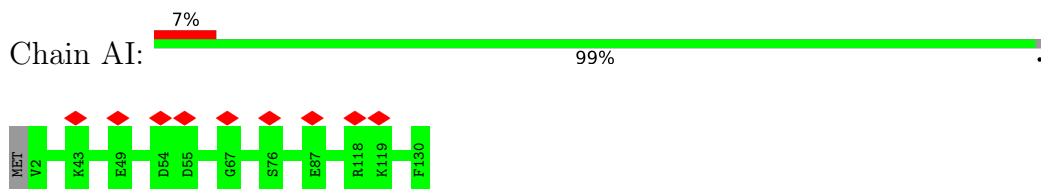
• Molecule 68: 40S ribosomal protein S20



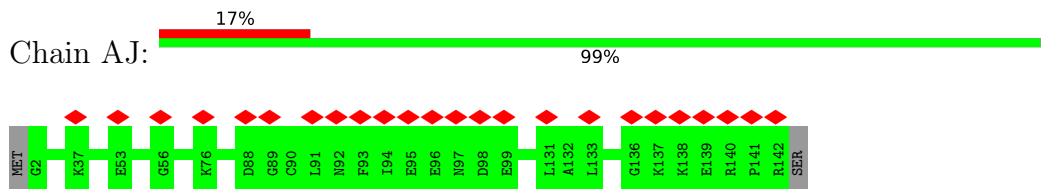
• Molecule 69: 40S ribosomal protein S21



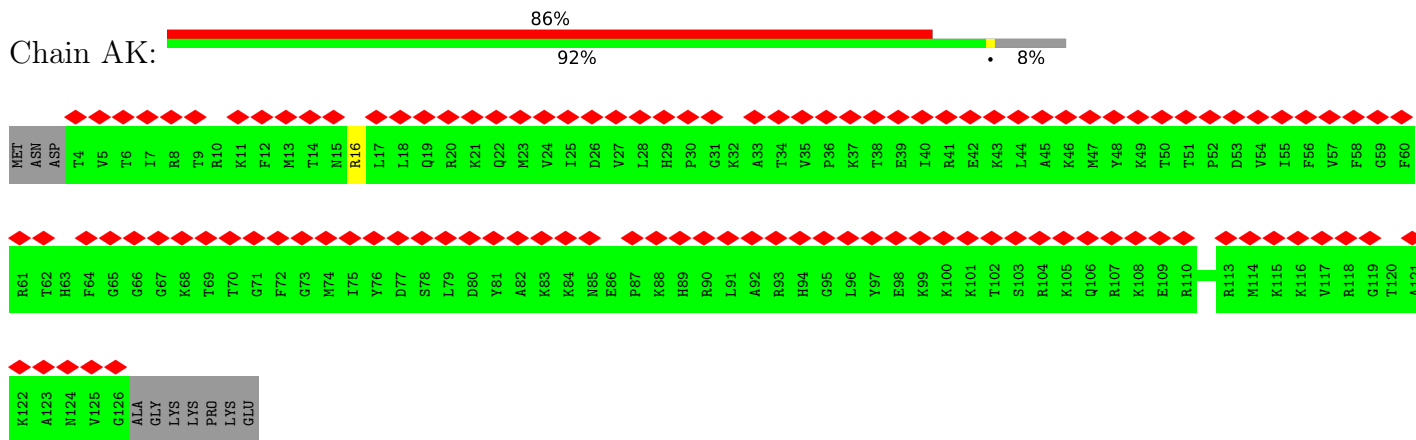
• Molecule 70: 40S ribosomal protein S15a



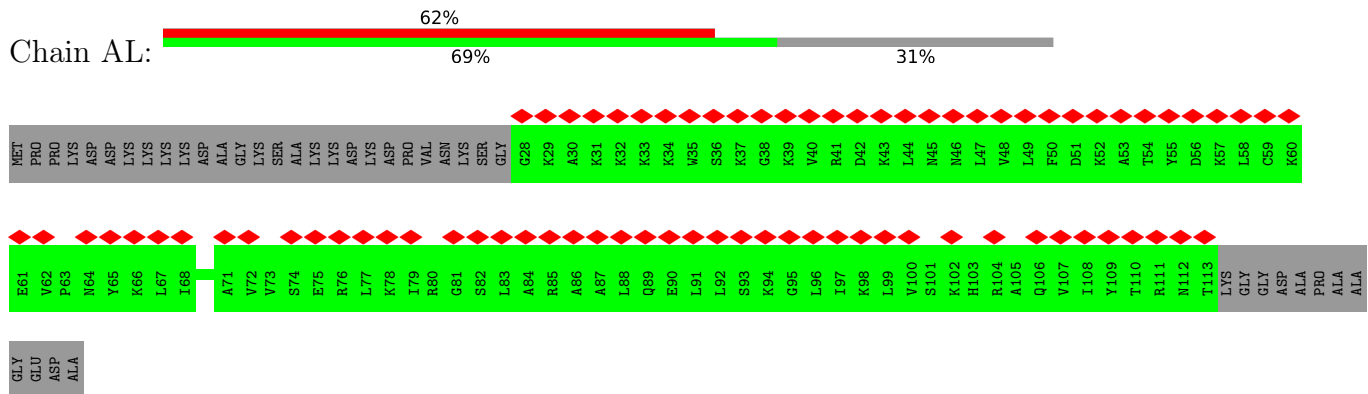
• Molecule 71: 40S ribosomal protein S23



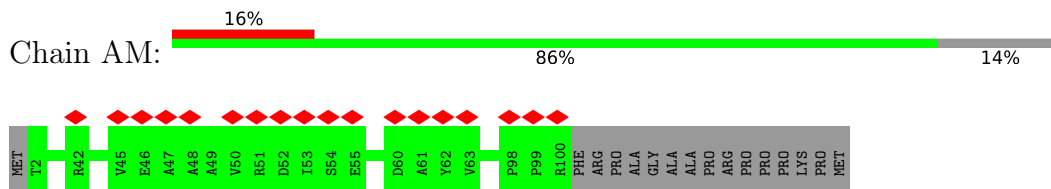
• Molecule 72: 40S ribosomal protein S24



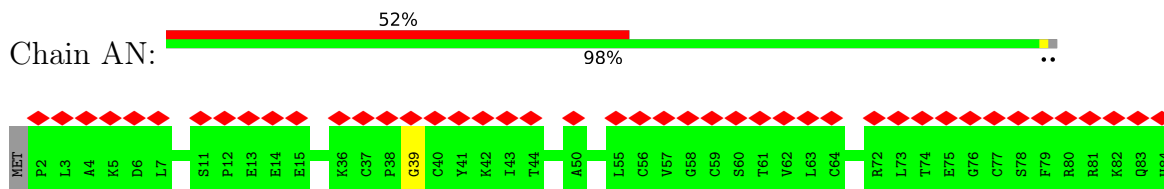
• Molecule 73: 40S ribosomal protein S25



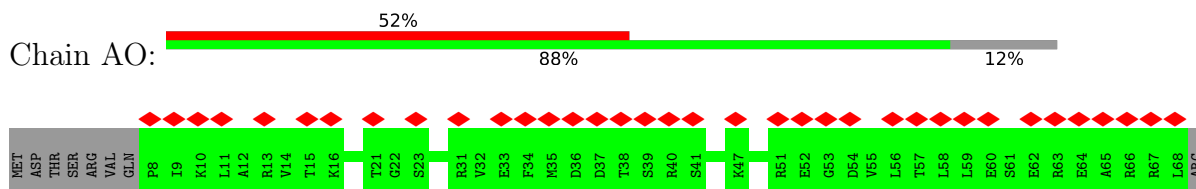
- Molecule 74: 40S ribosomal protein S26



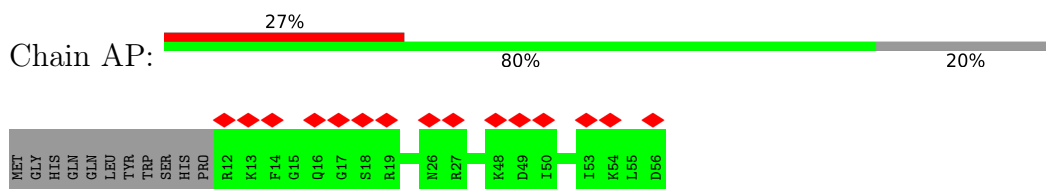
- Molecule 75: 40S ribosomal protein S27



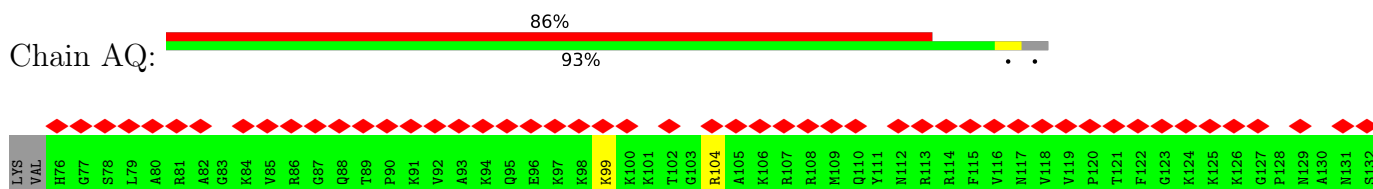
- Molecule 76: 40S ribosomal protein S28



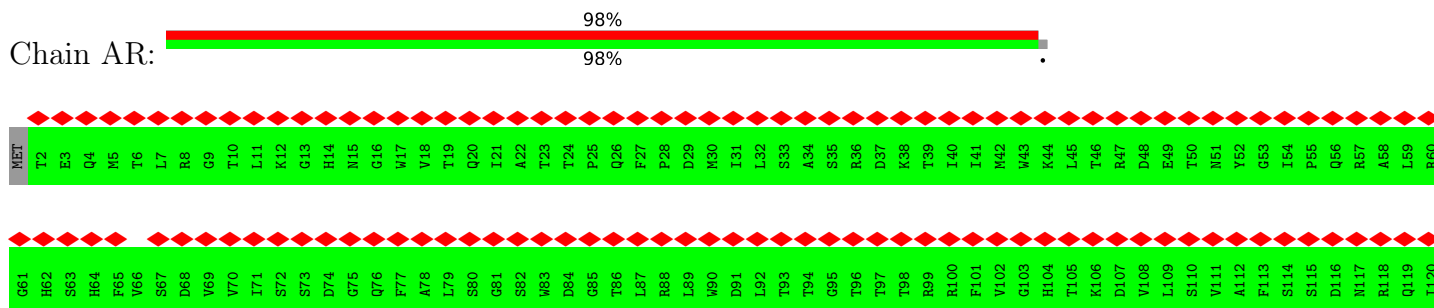
- Molecule 77: 40S ribosomal protein S29



- Molecule 78: 40S ribosomal protein S30



- Molecule 79: Receptor of activated protein C kinase 1



V121
S122
G123
S124
R125
D126
K127
T128
I129
K130
L131
W132
N133
T134
L135
G136
V137
C138
K139
Y140
T141
V142
Q143
D144
E145
S146
H147
S148
E149
W150
V151
S152
C153
V154
R155
F156
S157
P158
N159
S160
S161
N162
P163
I164
I165
V166
S167
C168
G169
W170
D171
K172
L173
V174
K175
V176
W177
N178
L179
A180
M181
C182
K183
L184
K185
T186
M187
H188
I189
G190
H191
T192
G193
Y194
L195
M196
T197
V198
T199
V200
S201
P202
D203
G204
S205
L206
C207
A208
S209
G210
G211
K212
D213
G214
Q215
A216
M217
L218
W219
D220
L221
N222
E223
G224
K225
H226
L227
Y228
T229
L230
D231
G232
G233
D234
I235
I236
N237
A238
L239
C240
F241
S242
P243
N244
R245
Y246
W247
L248
C249
A250
A251
T252
G253
P254
S255
I256
K257
I258
W259
D260
L261
E262
G263
K264
I265
I266
V267
D268
E269
L270
K271
Q272
E273
V274
I275
S276
T277
S278
S279
K280
A281
E282
P283
P284
Q285
C286
T287
S288
L289
A290
W291
S292
A293
D294
G295
Q296
T297
L298
F299
A300
G301
Y302
T303
D304
N305
L306
V307
R308
V309
W310
Q311
V312
T313
I314
GLY
THR
ARG

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	148464	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)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.176	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0191	Depositor
Map size (Å)	439.9, 439.9, 439.9	wwPDB
Map dimensions	530, 530, 530	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: 56B, H2U, 2MG, OMG, GAL, UR3, 5MC, PSU, M2G, 6MZ, OMC, 1MG, G7M, 4AC, 5MU, ZN, UY1, A2M, OMU, MA6, 1MA, B8N, MG, 3AU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/250	0.69	0/385
2	B	0.25	0/1402	0.82	1/2179 (0.0%)
3	D	0.55	0/81567	0.83	35/127232 (0.0%)
4	E	0.54	0/2858	0.78	0/4455
5	F	0.52	0/3675	0.81	1/5725 (0.0%)
6	G	0.35	0/1929	0.52	0/2586
7	H	0.34	0/3279	0.53	1/4388 (0.0%)
8	I	0.33	0/2938	0.48	1/3946 (0.0%)
9	J	0.33	0/2425	0.47	0/3248
10	K	0.30	0/1785	0.50	0/2394
11	L	0.35	0/1905	0.49	0/2539
12	M	0.30	0/1863	0.49	0/2510
13	N	0.31	0/1537	0.51	0/2066
14	O	0.32	0/1699	0.48	0/2270
15	P	0.30	0/1385	0.49	0/1852
16	Q	0.31	0/1713	0.46	0/2293
17	R	0.33	0/1142	0.47	0/1527
18	S	0.36	0/1746	0.47	0/2338
19	T	0.35	0/1673	0.48	0/2238
20	U	0.34	0/1300	0.50	0/1746
21	V	0.34	0/1537	0.51	0/2052
22	W	0.30	0/1524	0.47	1/2013 (0.0%)
23	X	0.35	0/1493	0.46	0/2003
24	Y	0.34	0/1326	0.46	0/1770
25	Z	0.29	0/835	0.48	0/1122
26	a	0.33	0/993	0.48	0/1332
27	b	0.33	0/541	0.43	0/720
28	c	0.30	0/998	0.46	0/1340
29	d	0.33	0/1132	0.48	0/1504
30	e	0.34	0/1130	0.48	0/1507
31	f	0.34	0/1191	0.48	0/1591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.29	0/844	0.47	0/1115
33	h	0.33	0/765	0.48	0/1027
34	i	0.32	0/903	0.49	0/1216
35	j	0.34	0/1071	0.44	0/1429
36	k	0.37	0/895	0.55	0/1198
37	l	0.34	0/898	0.49	0/1197
38	m	0.30	0/1018	0.43	0/1344
39	n	0.28	0/843	0.40	0/1115
40	o	0.34	0/720	0.48	0/952
41	p	0.30	0/575	0.46	0/761
42	q	0.30	0/454	0.41	0/599
43	r	0.30	0/435	0.46	0/575
44	s	0.29	0/240	0.41	0/305
45	t	0.33	0/876	0.51	0/1156
46	u	0.35	0/718	0.48	0/953
47	v	0.34	0/1017	0.50	0/1364
48	w	0.35	0/37158	0.83	15/57908 (0.0%)
49	x	0.27	0/1732	0.48	0/2355
50	y	0.26	0/1752	0.46	0/2345
51	z	0.29	0/1668	0.47	0/2254
52	0	0.28	0/1672	0.48	0/2250
53	1	0.26	0/2112	0.49	0/2842
54	2	0.25	0/1485	0.47	0/1998
55	3	0.27	0/1940	0.50	0/2583
56	4	0.26	0/1533	0.51	0/2053
57	5	0.27	0/1703	0.47	1/2275 (0.0%)
58	6	0.28	0/1531	0.51	0/2045
59	7	0.27	0/834	0.46	0/1125
60	8	0.29	0/1170	0.47	0/1568
61	9	0.27	0/1232	0.46	0/1656
62	AA	0.28	0/1015	0.54	0/1361
63	AB	0.27	0/1126	0.49	1/1505 (0.1%)
64	AC	0.27	0/1146	0.47	0/1534
65	AD	0.26	0/1071	0.51	1/1438 (0.1%)
66	AE	0.26	0/1187	0.50	0/1593
67	AF	0.26	0/1130	0.45	0/1515
68	AG	0.24	0/809	0.50	0/1087
69	AH	0.27	0/643	0.46	0/860
70	AI	0.28	0/1051	0.48	0/1406
71	AJ	0.27	0/1116	0.46	0/1490
72	AK	0.27	0/1019	0.53	0/1355
73	AL	0.25	0/688	0.49	0/921
74	AM	0.29	0/805	0.46	0/1079

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	AN	0.27	0/657	0.51	0/883
76	AO	0.25	0/481	0.54	0/643
77	AP	0.31	0/375	0.52	0/492
78	AQ	0.27	0/458	0.51	0/602
79	AR	0.24	0/2493	0.52	0/3394
All	All	0.42	0/217835	0.72	58/319592 (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
6	G	0	2
7	H	0	1
8	I	0	2
10	K	0	1
11	L	0	1
16	Q	0	1
20	U	0	1
21	V	0	1
22	W	0	1
24	Y	0	1
29	d	0	1
32	g	0	1
40	o	0	1
58	6	0	1
65	AD	0	1
All	All	0	17

There are no bond length outliers.

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2101	C	OP1-P-OP2	-26.59	79.71	119.60
3	D	2101	C	O5'-P-OP1	-26.43	78.98	110.70
3	D	2100	A	OP2-P-O3'	-15.77	70.50	105.20
3	D	2101	C	O5'-P-OP2	15.65	129.49	110.70
3	D	2100	A	OP1-P-O3'	14.25	136.56	105.20

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	G	123	ARG	Peptide
6	G	239	ALA	Peptide
7	H	258	HIS	Peptide
8	I	110	ARG	Peptide
8	I	91	ALA	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	G	245/257 (95%)	228 (93%)	17 (7%)	0	100	100
7	H	396/403 (98%)	375 (95%)	21 (5%)	0	100	100
8	I	361/427 (84%)	338 (94%)	23 (6%)	0	100	100
9	J	291/297 (98%)	271 (93%)	20 (7%)	0	100	100
10	K	211/288 (73%)	189 (90%)	22 (10%)	0	100	100
11	L	223/248 (90%)	213 (96%)	10 (4%)	0	100	100
12	M	223/266 (84%)	208 (93%)	15 (7%)	0	100	100
13	N	188/192 (98%)	176 (94%)	12 (6%)	0	100	100
14	O	202/214 (94%)	187 (93%)	15 (7%)	0	100	100
15	P	168/178 (94%)	158 (94%)	10 (6%)	0	100	100
16	Q	206/211 (98%)	189 (92%)	15 (7%)	2 (1%)	15	22
17	R	134/215 (62%)	122 (91%)	12 (9%)	0	100	100
18	S	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
19	T	198/203 (98%)	191 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	U	155/184 (84%)	143 (92%)	12 (8%)	0	100	100
21	V	185/188 (98%)	174 (94%)	11 (6%)	0	100	100
22	W	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
23	X	173/176 (98%)	160 (92%)	13 (8%)	0	100	100
24	Y	157/160 (98%)	147 (94%)	10 (6%)	0	100	100
25	Z	99/128 (77%)	92 (93%)	6 (6%)	1 (1%)	15	22
26	a	129/140 (92%)	119 (92%)	10 (8%)	0	100	100
27	b	61/157 (39%)	59 (97%)	2 (3%)	0	100	100
28	c	118/156 (76%)	110 (93%)	8 (7%)	0	100	100
29	d	132/145 (91%)	123 (93%)	9 (7%)	0	100	100
30	e	133/136 (98%)	126 (95%)	7 (5%)	0	100	100
31	f	145/148 (98%)	132 (91%)	13 (9%)	0	100	100
32	g	100/159 (63%)	92 (92%)	6 (6%)	2 (2%)	7	8
33	h	95/115 (83%)	94 (99%)	1 (1%)	0	100	100
34	i	105/125 (84%)	100 (95%)	5 (5%)	0	100	100
35	j	126/135 (93%)	122 (97%)	4 (3%)	0	100	100
36	k	107/110 (97%)	101 (94%)	6 (6%)	0	100	100
37	l	110/117 (94%)	104 (94%)	6 (6%)	0	100	100
38	m	119/123 (97%)	116 (98%)	3 (2%)	0	100	100
39	n	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
40	o	84/97 (87%)	79 (94%)	4 (5%)	1 (1%)	13	17
41	p	67/70 (96%)	60 (90%)	7 (10%)	0	100	100
42	q	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
43	r	50/128 (39%)	48 (96%)	2 (4%)	0	100	100
44	s	23/25 (92%)	23 (100%)	0	0	100	100
45	t	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
46	u	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
47	v	123/137 (90%)	114 (93%)	9 (7%)	0	100	100
49	x	213/295 (72%)	205 (96%)	7 (3%)	1 (0%)	29	40
50	y	210/264 (80%)	196 (93%)	14 (7%)	0	100	100
51	z	210/293 (72%)	198 (94%)	11 (5%)	1 (0%)	29	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	0	210/243 (86%)	190 (90%)	20 (10%)	0	100	100
53	1	260/263 (99%)	242 (93%)	18 (7%)	0	100	100
54	2	185/204 (91%)	169 (91%)	16 (9%)	0	100	100
55	3	235/249 (94%)	227 (97%)	8 (3%)	0	100	100
56	4	185/194 (95%)	168 (91%)	17 (9%)	0	100	100
57	5	204/208 (98%)	196 (96%)	8 (4%)	0	100	100
58	6	180/194 (93%)	166 (92%)	14 (8%)	0	100	100
59	7	94/165 (57%)	89 (95%)	5 (5%)	0	100	100
60	8	138/158 (87%)	128 (93%)	10 (7%)	0	100	100
61	9	148/151 (98%)	140 (95%)	8 (5%)	0	100	100
62	AA	132/151 (87%)	120 (91%)	12 (9%)	0	100	100
63	AB	132/145 (91%)	125 (95%)	7 (5%)	0	100	100
64	AC	140/146 (96%)	124 (89%)	15 (11%)	1 (1%)	22	31
65	AD	129/135 (96%)	108 (84%)	19 (15%)	2 (2%)	9	12
66	AE	142/152 (93%)	128 (90%)	14 (10%)	0	100	100
67	AF	141/145 (97%)	131 (93%)	10 (7%)	0	100	100
68	AG	100/119 (84%)	92 (92%)	8 (8%)	0	100	100
69	AH	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
70	AI	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
71	AJ	139/143 (97%)	135 (97%)	4 (3%)	0	100	100
72	AK	121/133 (91%)	115 (95%)	6 (5%)	0	100	100
73	AL	84/125 (67%)	76 (90%)	8 (10%)	0	100	100
74	AM	97/115 (84%)	93 (96%)	4 (4%)	0	100	100
75	AN	81/84 (96%)	69 (85%)	11 (14%)	1 (1%)	13	17
76	AO	59/69 (86%)	53 (90%)	6 (10%)	0	100	100
77	AP	43/56 (77%)	43 (100%)	0	0	100	100
78	AQ	55/59 (93%)	48 (87%)	7 (13%)	0	100	100
79	AR	311/317 (98%)	268 (86%)	43 (14%)	0	100	100
All	All	10947/12400 (88%)	10216 (93%)	719 (7%)	12 (0%)	54	67

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Q	48	PRO
32	g	111	ARG
64	AC	119	LEU
65	AD	119	VAL
32	g	110	ALA

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	
6	G	189/199 (95%)	189 (100%)	0	100	100
7	H	346/349 (99%)	343 (99%)	3 (1%)	78	89
8	I	301/348 (86%)	299 (99%)	2 (1%)	84	92
9	J	245/250 (98%)	245 (100%)	0	100	100
10	K	193/252 (77%)	191 (99%)	2 (1%)	76	87
11	L	194/215 (90%)	194 (100%)	0	100	100
12	M	195/223 (87%)	195 (100%)	0	100	100
13	N	169/171 (99%)	169 (100%)	0	100	100
14	O	174/181 (96%)	174 (100%)	0	100	100
15	P	143/149 (96%)	142 (99%)	1 (1%)	84	92
16	Q	174/177 (98%)	174 (100%)	0	100	100
17	R	116/161 (72%)	116 (100%)	0	100	100
18	S	171/172 (99%)	171 (100%)	0	100	100
19	T	172/174 (99%)	171 (99%)	1 (1%)	86	93
20	U	138/163 (85%)	138 (100%)	0	100	100
21	V	164/165 (99%)	164 (100%)	0	100	100
22	W	159/175 (91%)	159 (100%)	0	100	100
23	X	156/157 (99%)	156 (100%)	0	100	100
24	Y	139/140 (99%)	139 (100%)	0	100	100
25	Z	90/115 (78%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	a	101/107 (94%)	101 (100%)	0	100	100
27	b	55/126 (44%)	55 (100%)	0	100	100
28	c	107/133 (80%)	107 (100%)	0	100	100
29	d	124/135 (92%)	124 (100%)	0	100	100
30	e	117/118 (99%)	116 (99%)	1 (1%)	78	89
31	f	120/121 (99%)	120 (100%)	0	100	100
32	g	81/126 (64%)	81 (100%)	0	100	100
33	h	82/97 (84%)	81 (99%)	1 (1%)	71	84
34	i	98/110 (89%)	98 (100%)	0	100	100
35	j	114/121 (94%)	114 (100%)	0	100	100
36	k	88/89 (99%)	88 (100%)	0	100	100
37	l	96/100 (96%)	96 (100%)	0	100	100
38	m	109/110 (99%)	109 (100%)	0	100	100
39	n	86/89 (97%)	86 (100%)	0	100	100
40	o	73/80 (91%)	72 (99%)	1 (1%)	67	81
41	p	64/65 (98%)	64 (100%)	0	100	100
42	q	47/48 (98%)	47 (100%)	0	100	100
43	r	48/116 (41%)	48 (100%)	0	100	100
44	s	24/24 (100%)	24 (100%)	0	100	100
45	t	93/94 (99%)	93 (100%)	0	100	100
46	u	74/75 (99%)	74 (100%)	0	100	100
47	v	109/121 (90%)	109 (100%)	0	100	100
49	x	178/243 (73%)	178 (100%)	0	100	100
50	y	194/231 (84%)	194 (100%)	0	100	100
51	z	176/225 (78%)	176 (100%)	0	100	100
52	0	175/202 (87%)	174 (99%)	1 (1%)	86	93
53	1	223/225 (99%)	222 (100%)	1 (0%)	91	96
54	2	154/170 (91%)	154 (100%)	0	100	100
55	3	206/218 (94%)	204 (99%)	2 (1%)	76	87
56	4	168/174 (97%)	166 (99%)	2 (1%)	71	84
57	5	175/180 (97%)	175 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	6	160/168 (95%)	159 (99%)	1 (1%)	86	93
59	7	87/136 (64%)	87 (100%)	0	100	100
60	8	125/142 (88%)	122 (98%)	3 (2%)	49	67
61	9	130/131 (99%)	130 (100%)	0	100	100
62	AA	104/119 (87%)	103 (99%)	1 (1%)	76	87
63	AB	120/130 (92%)	120 (100%)	0	100	100
64	AC	117/121 (97%)	116 (99%)	1 (1%)	78	89
65	AD	117/122 (96%)	117 (100%)	0	100	100
66	AE	119/132 (90%)	119 (100%)	0	100	100
67	AF	113/115 (98%)	113 (100%)	0	100	100
68	AG	89/107 (83%)	89 (100%)	0	100	100
69	AH	67/67 (100%)	67 (100%)	0	100	100
70	AI	112/113 (99%)	112 (100%)	0	100	100
71	AJ	113/115 (98%)	113 (100%)	0	100	100
72	AK	106/115 (92%)	105 (99%)	1 (1%)	78	89
73	AL	73/103 (71%)	73 (100%)	0	100	100
74	AM	86/98 (88%)	86 (100%)	0	100	100
75	AN	73/76 (96%)	73 (100%)	0	100	100
76	AO	54/62 (87%)	54 (100%)	0	100	100
77	AP	39/49 (80%)	39 (100%)	0	100	100
78	AQ	46/48 (96%)	44 (96%)	2 (4%)	29	44
79	AR	272/275 (99%)	271 (100%)	1 (0%)	91	96
All	All	9509/10553 (90%)	9481 (100%)	28 (0%)	92	97

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
55	3	98	ARG
79	AR	245	ARG
56	4	106	ARG
72	AK	16	ARG
56	4	57	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
62	AA	103	ASN
66	AE	87	GLN
79	AR	143	GLN
79	AR	14	HIS
25	Z	38	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	10/14 (71%)	1 (10%)	0
2	B	72/76 (94%)	18 (25%)	3 (4%)
3	D	3494/5070 (68%)	614 (17%)	24 (0%)
4	E	119/120 (99%)	14 (11%)	0
48	w	1618/1869 (86%)	417 (25%)	0
5	F	155/156 (99%)	28 (18%)	2 (1%)
All	All	5468/7305 (74%)	1092 (19%)	29 (0%)

5 of 1092 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	21	U
2	B	4	U
2	B	5	C
2	B	6	2MG
2	B	11	C

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	D	2101	C
5	F	16	G
3	D	2763	U
3	D	4699	U
3	D	2675	G

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

211 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
3	PSU	D	2508	3	18,21,22	1.02	1 (5%)	22,30,33	1.79	4 (18%)
3	PSU	D	5001	80,3	18,21,22	1.05	1 (5%)	22,30,33	1.77	4 (18%)
48	PSU	w	1004	48	18,21,22	1.03	1 (5%)	22,30,33	1.77	4 (18%)
48	OMG	w	509	48	18,26,27	2.82	8 (44%)	19,38,41	1.53	4 (21%)
3	OMC	D	2422	80,3	19,22,23	2.90	8 (42%)	26,31,34	0.72	0
3	OMC	D	4536	3	19,22,23	2.86	8 (42%)	26,31,34	0.75	0
2	H2U	B	16	2	18,21,22	1.00	2 (11%)	21,30,33	1.27	2 (9%)
48	A2M	w	1678	48	18,25,26	1.52	2 (11%)	18,36,39	1.01	1 (5%)
3	6MZ	D	4220	3	18,25,26	2.02	2 (11%)	16,36,39	2.06	3 (18%)
3	OMC	D	3887	3	19,22,23	2.87	8 (42%)	26,31,34	0.76	0
48	PSU	w	1367	48	18,21,22	1.06	1 (5%)	22,30,33	1.80	5 (22%)
3	PSU	D	1683	80,3	18,21,22	1.08	1 (5%)	22,30,33	1.87	4 (18%)
3	PSU	D	3768	3	18,21,22	1.07	1 (5%)	22,30,33	1.79	4 (18%)
48	OMC	w	1391	48	19,22,23	2.99	8 (42%)	26,31,34	0.68	0
3	OMG	D	1316	3	18,26,27	2.73	8 (44%)	19,38,41	1.52	4 (21%)
3	PSU	D	3851	3	18,21,22	1.02	1 (5%)	22,30,33	1.79	4 (18%)
48	PSU	w	572	48	18,21,22	1.12	1 (5%)	22,30,33	1.78	4 (18%)
3	PSU	D	1792	3	18,21,22	1.01	1 (5%)	22,30,33	1.73	4 (18%)
3	OMG	D	4392	3	18,26,27	2.72	8 (44%)	19,38,41	1.51	4 (21%)
3	PSU	D	1744	80,3	18,21,22	1.01	1 (5%)	22,30,33	1.85	4 (18%)
48	OMC	w	1703	80,48	19,22,23	2.94	8 (42%)	26,31,34	0.70	0
48	A2M	w	590	48	18,25,26	1.46	1 (5%)	18,36,39	1.07	1 (5%)
48	MA6	w	1850	48	19,26,27	0.98	1 (5%)	18,38,41	1.58	3 (16%)
3	A2M	D	1326	3	18,25,26	1.48	1 (5%)	18,36,39	1.03	1 (5%)
2	1MA	B	58	2	16,25,26	1.00	1 (6%)	18,37,40	0.83	0
3	OMC	D	2351	80,3	19,22,23	2.85	8 (42%)	26,31,34	0.92	2 (7%)
48	PSU	w	1177	48	18,21,22	1.03	1 (5%)	22,30,33	1.79	4 (18%)
3	OMC	D	1340	3	19,22,23	2.84	8 (42%)	26,31,34	0.75	0
48	OMU	w	116	48	19,22,23	2.90	7 (36%)	26,31,34	1.67	4 (15%)
3	PSU	D	3853	80,3	18,21,22	0.99	1 (5%)	22,30,33	1.66	4 (18%)
3	PSU	D	4403	80,3	18,21,22	1.07	1 (5%)	22,30,33	1.80	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	D	4689	3	18,21,22	1.07	1 (5%)	22,30,33	1.81	4 (18%)
48	A2M	w	1383	48	18,25,26	1.44	1 (5%)	18,36,39	1.15	2 (11%)
3	OMG	D	1625	80,3	18,26,27	2.77	8 (44%)	19,38,41	1.49	4 (21%)
48	PSU	w	1643	80,48	18,21,22	1.08	1 (5%)	22,30,33	1.76	4 (18%)
2	M2G	B	26	2	20,27,28	1.49	4 (20%)	22,40,43	1.35	2 (9%)
3	5MC	D	4447	80,3	18,22,23	3.66	7 (38%)	26,32,35	1.14	1 (3%)
3	PSU	D	1860	3	18,21,22	1.04	1 (5%)	22,30,33	1.83	5 (22%)
48	PSU	w	1445	48	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)
3	A2M	D	2787	3	18,25,26	1.45	1 (5%)	18,36,39	1.05	1 (5%)
48	PSU	w	36	48	18,21,22	1.06	1 (5%)	22,30,33	1.78	5 (22%)
48	PSU	w	1045	48	18,21,22	1.02	1 (5%)	22,30,33	1.77	4 (18%)
48	PSU	w	1347	48	18,21,22	1.02	1 (5%)	22,30,33	1.78	4 (18%)
48	OMU	w	1288	48	19,22,23	2.97	8 (42%)	26,31,34	1.66	4 (15%)
2	PSU	B	55	2	18,21,22	1.11	1 (5%)	22,30,33	1.74	4 (18%)
3	A2M	D	1871	80,3	18,25,26	1.54	2 (11%)	18,36,39	1.12	1 (5%)
48	PSU	w	34	48	18,21,22	1.08	1 (5%)	22,30,33	1.74	4 (18%)
48	PSU	w	1625	48	18,21,22	1.06	1 (5%)	22,30,33	1.70	4 (18%)
3	UR3	D	4530	80,3	19,22,23	2.66	7 (36%)	26,32,35	1.30	2 (7%)
3	A2M	D	1534	80,3	18,25,26	1.42	1 (5%)	18,36,39	1.40	3 (16%)
3	PSU	D	3637	80,3	18,21,22	1.01	1 (5%)	22,30,33	1.81	4 (18%)
3	OMG	D	4196	2,80,3	18,26,27	2.73	8 (44%)	19,38,41	1.48	4 (21%)
3	PSU	D	3730	3	18,21,22	1.03	1 (5%)	22,30,33	1.77	4 (18%)
3	A2M	D	3718	3	18,25,26	1.45	1 (5%)	18,36,39	1.02	1 (5%)
3	PSU	D	4431	3	18,21,22	1.03	1 (5%)	22,30,33	1.82	4 (18%)
48	A2M	w	668	80,48	18,25,26	1.53	2 (11%)	18,36,39	0.95	0
3	PSU	D	4296	3	18,21,22	1.06	1 (5%)	22,30,33	1.76	4 (18%)
3	OMU	D	4498	80,3	19,22,23	2.79	6 (31%)	26,31,34	1.73	5 (19%)
2	5MU	B	54	2	19,22,23	4.74	5 (26%)	28,32,35	3.60	9 (32%)
48	OMG	w	1328	48	18,26,27	2.83	8 (44%)	19,38,41	1.49	4 (21%)
3	PSU	D	4457	3	18,21,22	1.02	1 (5%)	22,30,33	1.75	5 (22%)
3	PSU	D	4521	80,3	18,21,22	1.05	1 (5%)	22,30,33	1.86	4 (18%)
48	PSU	w	406	48	18,21,22	1.03	1 (5%)	22,30,33	1.82	4 (18%)
3	PSU	D	3764	3	18,21,22	1.02	1 (5%)	22,30,33	1.73	4 (18%)
3	A2M	D	3724	3	18,25,26	1.47	1 (5%)	18,36,39	1.00	1 (5%)
3	A2M	D	1524	3	18,25,26	1.53	2 (11%)	18,36,39	0.97	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	D	1862	3	18,21,22	1.02	1 (5%)	22,30,33	1.83	4 (18%)
3	PSU	D	4423	3	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)
3	OMU	D	3925	3	19,22,23	2.80	6 (31%)	26,31,34	1.74	4 (15%)
3	PSU	D	4312	3	18,21,22	1.02	1 (5%)	22,30,33	1.82	4 (18%)
2	M2G	B	27	2	20,27,28	1.56	4 (20%)	22,40,43	1.34	2 (9%)
48	OMU	w	1442	80,48	19,22,23	2.93	8 (42%)	26,31,34	1.68	4 (15%)
3	OMC	D	2804	3	19,22,23	2.86	8 (42%)	26,31,34	0.86	1 (3%)
3	OMG	D	3744	3	18,26,27	2.76	8 (44%)	19,38,41	1.50	4 (21%)
48	A2M	w	27	48	18,25,26	1.47	1 (5%)	18,36,39	0.98	0
48	OMC	w	517	80,48	19,22,23	3.00	8 (42%)	26,31,34	0.76	0
48	OMG	w	601	48	18,26,27	2.81	8 (44%)	19,38,41	1.48	4 (21%)
3	OMC	D	3701	80,3	19,22,23	2.87	8 (42%)	26,31,34	0.73	0
3	PSU	D	3770	3	18,21,22	1.07	1 (5%)	22,30,33	1.82	4 (18%)
3	OMG	D	4618	3	18,26,27	2.76	8 (44%)	19,38,41	1.51	4 (21%)
3	1MA	D	1322	3	16,25,26	0.84	1 (6%)	18,37,40	0.88	0
2	5MC	B	48	2	18,22,23	3.82	8 (44%)	26,32,35	1.02	2 (7%)
2	G7M	B	46	2	20,26,27	2.76	8 (40%)	17,39,42	1.02	1 (5%)
2	UY1	B	39	2	19,22,23	1.24	2 (10%)	22,31,34	0.97	1 (4%)
48	OMU	w	1804	48	19,22,23	2.89	8 (42%)	26,31,34	1.76	5 (19%)
48	PSU	w	651	48	18,21,22	1.05	1 (5%)	22,30,33	1.78	4 (18%)
48	PSU	w	119	48	18,21,22	1.06	1 (5%)	22,30,33	1.73	4 (18%)
48	PSU	w	109	48	18,21,22	1.08	1 (5%)	22,30,33	1.84	5 (22%)
3	A2M	D	3760	3	18,25,26	1.51	1 (5%)	18,36,39	1.17	2 (11%)
3	A2M	D	2363	80,3	18,25,26	1.46	2 (11%)	18,36,39	1.02	1 (5%)
5	OMG	F	75	5	18,26,27	2.78	8 (44%)	19,38,41	1.47	4 (21%)
3	OMG	D	1522	3	18,26,27	2.75	8 (44%)	19,38,41	1.51	4 (21%)
48	OMU	w	172	48	19,22,23	2.91	7 (36%)	26,31,34	1.72	5 (19%)
48	PSU	w	1046	48	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)
48	PSU	w	863	48	18,21,22	1.07	1 (5%)	22,30,33	1.80	4 (18%)
48	PSU	w	866	48	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
48	PSU	w	815	48	18,21,22	1.05	1 (5%)	22,30,33	1.84	5 (22%)
48	OMU	w	1326	48	19,22,23	2.91	8 (42%)	26,31,34	1.70	4 (15%)
3	A2M	D	400	3	18,25,26	1.49	1 (5%)	18,36,39	1.02	1 (5%)
3	OMG	D	2364	3	18,26,27	2.71	8 (44%)	19,38,41	1.50	4 (21%)
48	OMU	w	799	48	19,22,23	2.93	8 (42%)	26,31,34	1.69	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	D	3715	3	18,21,22	1.03	1 (5%)	22,30,33	1.73	4 (18%)
3	PSU	D	1782	3	18,21,22	1.04	1 (5%)	22,30,33	1.78	4 (18%)
48	B8N	w	1248	48	24,29,30	0.91	1 (4%)	29,42,45	1.05	1 (3%)
3	PSU	D	5010	3	18,21,22	1.03	1 (5%)	22,30,33	1.80	4 (18%)
3	OMG	D	4494	3	18,26,27	2.75	8 (44%)	19,38,41	1.48	4 (21%)
3	PSU	D	3695	3	18,21,22	1.04	1 (5%)	22,30,33	1.81	4 (18%)
48	PSU	w	1174	80,48	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
48	OMU	w	627	48	19,22,23	2.96	8 (42%)	26,31,34	1.67	4 (15%)
3	PSU	D	4471	3	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
3	OMC	D	2365	80,3	19,22,23	2.85	8 (42%)	26,31,34	0.69	0
3	OMG	D	4637	3	18,26,27	2.74	8 (44%)	19,38,41	1.49	4 (21%)
3	PSU	D	3734	3	18,21,22	1.06	1 (5%)	22,30,33	1.85	5 (22%)
3	A2M	D	3825	3	18,25,26	1.47	1 (5%)	18,36,39	1.05	1 (5%)
48	PSU	w	609	48	18,21,22	1.03	1 (5%)	22,30,33	1.89	5 (22%)
3	A2M	D	2815	3	18,25,26	1.59	1 (5%)	18,36,39	1.00	1 (5%)
48	PSU	w	966	48	18,21,22	1.05	1 (5%)	22,30,33	1.81	4 (18%)
3	PSU	D	4552	3	18,21,22	1.06	1 (5%)	22,30,33	1.83	4 (18%)
3	OMU	D	2837	3	19,22,23	2.77	6 (31%)	26,31,34	1.83	5 (19%)
3	PSU	D	4628	3	18,21,22	1.01	1 (5%)	22,30,33	1.77	4 (18%)
48	A2M	w	159	48	18,25,26	1.59	2 (11%)	18,36,39	0.97	1 (5%)
3	A2M	D	398	3	18,25,26	1.48	1 (5%)	18,36,39	1.06	1 (5%)
3	OMC	D	3808	3	19,22,23	2.86	8 (42%)	26,31,34	0.80	0
48	OMU	w	428	48	19,22,23	2.89	7 (36%)	26,31,34	1.72	4 (15%)
3	A2M	D	3830	3	18,25,26	1.45	1 (5%)	18,36,39	1.09	1 (5%)
48	OMG	w	1490	80,48	18,26,27	2.81	8 (44%)	19,38,41	1.45	4 (21%)
2	H2U	B	47	2	18,21,22	1.03	2 (11%)	21,30,33	0.77	0
48	A2M	w	468	48	18,25,26	1.58	1 (5%)	18,36,39	1.01	1 (5%)
48	MA6	w	1851	48	19,26,27	0.97	1 (5%)	18,38,41	1.71	3 (16%)
2	3AU	B	20	2	24,28,29	2.78	9 (37%)	33,40,43	1.40	5 (15%)
3	OMU	D	4306	3	19,22,23	2.75	6 (31%)	26,31,34	1.72	5 (19%)
48	A2M	w	512	48	18,25,26	1.52	1 (5%)	18,36,39	1.00	0
48	OMC	w	462	48	19,22,23	3.02	8 (42%)	26,31,34	0.78	0
3	5MC	D	3782	80,3	18,22,23	3.64	8 (44%)	26,32,35	1.06	2 (7%)
3	PSU	D	4576	3	18,21,22	1.02	1 (5%)	22,30,33	1.79	4 (18%)
3	UY1	D	3818	80,3	19,22,23	1.14	1 (5%)	22,31,34	0.94	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	OMG	w	436	48	18,26,27	2.82	8 (44%)	19,38,41	1.51	4 (21%)
3	A2M	D	3785	80,3	18,25,26	1.54	2 (11%)	18,36,39	1.20	1 (5%)
3	PSU	D	1781	3	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
48	PSU	w	105	48	18,21,22	1.04	1 (5%)	22,30,33	1.79	4 (18%)
48	A2M	w	99	80,48	18,25,26	1.48	1 (5%)	18,36,39	1.04	1 (5%)
3	PSU	D	3639	3	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
3	OMG	D	3792	3	18,26,27	2.73	8 (44%)	19,38,41	1.43	4 (21%)
2	2MG	B	10	2	18,26,27	2.24	5 (27%)	16,38,41	1.50	4 (25%)
48	OMC	w	174	48	19,22,23	3.03	8 (42%)	26,31,34	0.69	0
48	A2M	w	1031	48	18,25,26	1.43	1 (5%)	18,36,39	1.01	0
48	PSU	w	649	48	18,21,22	1.07	1 (5%)	22,30,33	1.81	5 (22%)
48	PSU	w	1232	48	18,21,22	1.06	1 (5%)	22,30,33	1.76	4 (18%)
3	PSU	D	3762	3	18,21,22	1.07	1 (5%)	22,30,33	1.78	4 (18%)
3	PSU	D	1536	3	18,21,22	1.03	1 (5%)	22,30,33	1.86	4 (18%)
3	A2M	D	4523	80,3	18,25,26	1.54	1 (5%)	18,36,39	1.06	1 (5%)
2	H2U	B	17	2	18,21,22	1.01	2 (11%)	21,30,33	0.89	2 (9%)
48	PSU	w	681	80,48	18,21,22	1.05	1 (5%)	22,30,33	1.79	4 (18%)
48	PSU	w	1081	48	18,21,22	1.02	1 (5%)	22,30,33	1.82	5 (22%)
3	OMG	D	2424	3	18,26,27	2.78	8 (44%)	19,38,41	1.51	4 (21%)
3	PSU	D	4972	3	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
48	PSU	w	218	48	18,21,22	1.05	1 (5%)	22,30,33	1.78	4 (18%)
48	PSU	w	814	48	18,21,22	1.02	1 (5%)	22,30,33	1.70	4 (18%)
3	OMU	D	2415	3	19,22,23	2.83	6 (31%)	26,31,34	1.88	5 (19%)
3	PSU	D	4420	3	18,21,22	1.05	1 (5%)	22,30,33	1.67	4 (18%)
48	A2M	w	576	48	18,25,26	1.45	1 (5%)	18,36,39	1.15	2 (11%)
3	OMG	D	3627	3	18,26,27	2.73	8 (44%)	19,38,41	1.54	4 (21%)
48	PSU	w	822	48	18,21,22	1.10	1 (5%)	22,30,33	1.74	4 (18%)
3	PSU	D	4353	3	18,21,22	1.05	1 (5%)	22,30,33	1.85	4 (18%)
3	OMU	D	4620	3	19,22,23	2.79	6 (31%)	26,31,34	1.73	5 (19%)
3	PSU	D	4442	3	18,21,22	1.04	2 (11%)	22,30,33	1.86	5 (22%)
48	PSU	w	686	48	18,21,22	1.06	1 (5%)	22,30,33	1.82	4 (18%)
48	PSU	w	801	48	18,21,22	1.09	1 (5%)	22,30,33	1.71	4 (18%)
3	OMU	D	1773	3	19,22,23	2.95	8 (42%)	26,31,34	1.64	4 (15%)
2	56B	B	34	2,81	27,35,36	2.85	11 (40%)	28,52,55	4.77	4 (14%)
3	OMG	D	4228	3	18,26,27	2.74	8 (44%)	19,38,41	1.50	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	OMU	w	121	48	19,22,23	2.87	6 (31%)	26,31,34	1.60	5 (19%)
3	PSU	D	4299	3	18,21,22	1.02	1 (5%)	22,30,33	1.74	4 (18%)
3	PSU	D	3920	80,3	18,21,22	1.08	1 (5%)	22,30,33	1.78	4 (18%)
48	A2M	w	166	48	18,25,26	1.50	1 (5%)	18,36,39	1.12	2 (11%)
3	OMC	D	2861	3	19,22,23	2.89	8 (42%)	26,31,34	0.68	0
2	PSU	B	35	2,1	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	4500	3	18,21,22	1.04	1 (5%)	22,30,33	1.89	5 (22%)
3	PSU	D	3758	3	18,21,22	0.97	1 (5%)	22,30,33	1.80	4 (18%)
3	OMU	D	4227	3	19,22,23	2.82	6 (31%)	26,31,34	1.79	4 (15%)
3	OMG	D	1760	3	18,26,27	2.89	8 (44%)	19,38,41	1.50	4 (21%)
48	A2M	w	484	48	18,25,26	1.46	1 (5%)	18,36,39	1.02	1 (5%)
3	PSU	D	4293	3	18,21,22	0.99	1 (5%)	22,30,33	1.65	4 (18%)
3	OMC	D	3841	3	19,22,23	2.86	8 (42%)	26,31,34	0.70	0
3	OMC	D	4456	3	19,22,23	2.86	8 (42%)	26,31,34	0.77	0
48	OMG	w	683	48	18,26,27	2.81	8 (44%)	19,38,41	1.49	4 (21%)
3	OMC	D	2824	3	19,22,23	2.89	8 (42%)	26,31,34	0.76	0
48	PSU	w	210	48	18,21,22	1.09	1 (5%)	22,30,33	1.76	4 (18%)
48	G7M	w	1639	2,48	20,26,27	2.76	7 (35%)	17,39,42	1.17	1 (5%)
3	A2M	D	2401	80,3	18,25,26	1.44	1 (5%)	18,36,39	1.02	1 (5%)
2	1MG	B	37	2	18,26,27	2.65	7 (38%)	19,39,42	1.43	3 (15%)
3	OMG	D	4499	3	18,26,27	2.76	8 (44%)	19,38,41	1.49	4 (21%)
2	2MG	B	6	2	18,26,27	2.22	5 (27%)	16,38,41	1.43	3 (18%)
3	PSU	D	4532	3	18,21,22	1.01	1 (5%)	22,30,33	1.72	4 (18%)
3	PSU	D	4579	3	18,21,22	1.02	1 (5%)	22,30,33	1.81	4 (18%)
48	PSU	w	1056	48	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
3	OMG	D	3944	3	18,26,27	2.83	8 (44%)	19,38,41	1.50	4 (21%)
3	PSU	D	1677	80,3	18,21,22	1.04	1 (5%)	22,30,33	1.76	3 (13%)
3	OMG	D	3899	3	18,26,27	2.73	8 (44%)	19,38,41	1.50	3 (15%)
48	PSU	w	1244	48	18,21,22	1.07	1 (5%)	22,30,33	1.79	5 (22%)
48	4AC	w	1842	48	21,24,25	0.57	0	29,34,37	1.19	4 (13%)
48	PSU	w	1692	48	18,21,22	1.02	1 (5%)	22,30,33	1.77	4 (18%)
48	OMG	w	644	48	18,26,27	2.82	8 (44%)	19,38,41	1.50	4 (21%)
3	PSU	D	4361	3	18,21,22	1.06	1 (5%)	22,30,33	1.79	4 (18%)
48	6MZ	w	1832	80,48	18,25,26	2.01	3 (16%)	16,36,39	1.89	2 (12%)
48	PSU	w	1238	48	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	D	4623	3	18,26,27	2.72	8 (44%)	19,38,41	1.52	4 (21%)
48	4AC	w	1337	48	21,24,25	0.63	0	29,34,37	1.17	5 (17%)
3	OMG	D	4370	3	18,26,27	2.76	8 (44%)	19,38,41	1.49	4 (21%)
3	PSU	D	2632	3	18,21,22	1.02	1 (5%)	22,30,33	1.71	4 (18%)
48	PSU	w	93	48	18,21,22	1.04	1 (5%)	22,30,33	1.67	4 (18%)

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
3	PSU	D	2508	3	-	0/7/25/26	0/2/2/2
3	PSU	D	5001	80,3	-	0/7/25/26	0/2/2/2
48	PSU	w	1004	48	-	0/7/25/26	0/2/2/2
48	OMG	w	509	48	-	0/5/27/28	0/3/3/3
3	OMC	D	2422	80,3	-	1/9/27/28	0/2/2/2
3	OMC	D	4536	3	-	0/9/27/28	0/2/2/2
2	H2U	B	16	2	-	6/7/38/39	0/2/2/2
48	A2M	w	1678	48	-	1/5/27/28	0/3/3/3
3	6MZ	D	4220	3	-	0/5/27/28	0/3/3/3
3	OMC	D	3887	3	-	0/9/27/28	0/2/2/2
48	PSU	w	1367	48	-	0/7/25/26	0/2/2/2
3	PSU	D	1683	80,3	-	0/7/25/26	0/2/2/2
3	PSU	D	3768	3	-	0/7/25/26	0/2/2/2
48	OMC	w	1391	48	-	0/9/27/28	0/2/2/2
3	OMG	D	1316	3	-	0/5/27/28	0/3/3/3
3	PSU	D	3851	3	-	0/7/25/26	0/2/2/2
48	PSU	w	572	48	-	2/7/25/26	0/2/2/2
3	PSU	D	1792	3	-	0/7/25/26	0/2/2/2
3	OMG	D	4392	3	-	0/5/27/28	0/3/3/3
3	PSU	D	1744	80,3	-	0/7/25/26	0/2/2/2
48	OMC	w	1703	80,48	-	2/9/27/28	0/2/2/2
48	A2M	w	590	48	-	2/5/27/28	0/3/3/3
48	MA6	w	1850	48	-	0/7/29/30	0/3/3/3
3	A2M	D	1326	3	-	1/5/27/28	0/3/3/3
2	1MA	B	58	2	-	0/3/25/26	0/3/3/3
3	OMC	D	2351	80,3	-	4/9/27/28	0/2/2/2
48	PSU	w	1177	48	-	0/7/25/26	0/2/2/2
3	OMC	D	1340	3	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	OMU	w	116	48	-	1/9/27/28	0/2/2/2
3	PSU	D	3853	80,3	-	0/7/25/26	0/2/2/2
3	PSU	D	4403	80,3	-	0/7/25/26	0/2/2/2
3	PSU	D	4689	3	-	0/7/25/26	0/2/2/2
48	A2M	w	1383	48	-	1/5/27/28	0/3/3/3
3	OMG	D	1625	80,3	-	0/5/27/28	0/3/3/3
48	PSU	w	1643	80,48	-	0/7/25/26	0/2/2/2
2	M2G	B	26	2	-	0/7/29/30	0/3/3/3
3	5MC	D	4447	80,3	-	4/7/25/26	0/2/2/2
3	PSU	D	1860	3	-	0/7/25/26	0/2/2/2
48	PSU	w	1445	48	-	0/7/25/26	0/2/2/2
3	A2M	D	2787	3	-	0/5/27/28	0/3/3/3
48	PSU	w	36	48	-	0/7/25/26	0/2/2/2
48	PSU	w	1045	48	-	0/7/25/26	0/2/2/2
48	PSU	w	1347	48	-	0/7/25/26	0/2/2/2
48	OMU	w	1288	48	-	1/9/27/28	0/2/2/2
2	PSU	B	55	2	-	1/7/25/26	0/2/2/2
3	A2M	D	1871	80,3	-	0/5/27/28	0/3/3/3
48	PSU	w	34	48	-	3/7/25/26	0/2/2/2
48	PSU	w	1625	48	-	0/7/25/26	0/2/2/2
3	UR3	D	4530	80,3	-	0/7/25/26	0/2/2/2
3	A2M	D	1534	80,3	-	3/5/27/28	0/3/3/3
3	PSU	D	3637	80,3	-	0/7/25/26	0/2/2/2
3	OMG	D	4196	2,80,3	-	1/5/27/28	0/3/3/3
3	PSU	D	3730	3	-	0/7/25/26	0/2/2/2
3	A2M	D	3718	3	-	0/5/27/28	0/3/3/3
3	PSU	D	4431	3	-	0/7/25/26	0/2/2/2
48	A2M	w	668	80,48	-	2/5/27/28	0/3/3/3
3	PSU	D	4296	3	-	0/7/25/26	0/2/2/2
3	OMU	D	4498	80,3	-	0/9/27/28	0/2/2/2
2	5MU	B	54	2	-	0/7/25/26	0/2/2/2
48	OMG	w	1328	48	-	1/5/27/28	0/3/3/3
3	PSU	D	4457	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4521	80,3	-	0/7/25/26	0/2/2/2
48	PSU	w	406	48	-	0/7/25/26	0/2/2/2
3	PSU	D	3764	3	-	0/7/25/26	0/2/2/2
3	A2M	D	3724	3	-	1/5/27/28	0/3/3/3
3	A2M	D	1524	3	-	2/5/27/28	0/3/3/3
3	PSU	D	1862	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4423	3	-	0/7/25/26	0/2/2/2
3	OMU	D	3925	3	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	D	4312	3	-	0/7/25/26	0/2/2/2
2	M2G	B	27	2	-	0/7/29/30	0/3/3/3
48	OMU	w	1442	80,48	-	1/9/27/28	0/2/2/2
3	OMC	D	2804	3	-	0/9/27/28	0/2/2/2
3	OMG	D	3744	3	-	1/5/27/28	0/3/3/3
48	A2M	w	27	48	-	0/5/27/28	0/3/3/3
48	OMC	w	517	80,48	-	0/9/27/28	0/2/2/2
48	OMG	w	601	48	-	1/5/27/28	0/3/3/3
3	OMC	D	3701	80,3	-	4/9/27/28	0/2/2/2
3	PSU	D	3770	3	-	0/7/25/26	0/2/2/2
3	OMG	D	4618	3	-	0/5/27/28	0/3/3/3
3	1MA	D	1322	3	-	0/3/25/26	0/3/3/3
2	5MC	B	48	2	-	0/7/25/26	0/2/2/2
2	G7M	B	46	2	-	3/3/25/26	0/3/3/3
2	UY1	B	39	2	-	1/9/27/28	0/2/2/2
48	OMU	w	1804	48	-	1/9/27/28	0/2/2/2
48	PSU	w	651	48	-	0/7/25/26	0/2/2/2
48	PSU	w	119	48	-	0/7/25/26	0/2/2/2
48	PSU	w	109	48	-	0/7/25/26	0/2/2/2
3	A2M	D	3760	3	-	2/5/27/28	0/3/3/3
3	A2M	D	2363	80,3	-	0/5/27/28	0/3/3/3
5	OMG	F	75	5	-	0/5/27/28	0/3/3/3
3	OMG	D	1522	3	-	0/5/27/28	0/3/3/3
48	OMU	w	172	48	-	0/9/27/28	0/2/2/2
48	PSU	w	1046	48	-	0/7/25/26	0/2/2/2
48	PSU	w	863	48	-	0/7/25/26	0/2/2/2
48	PSU	w	866	48	-	0/7/25/26	0/2/2/2
48	PSU	w	815	48	-	0/7/25/26	0/2/2/2
48	OMU	w	1326	48	-	4/9/27/28	0/2/2/2
3	A2M	D	400	3	-	0/5/27/28	0/3/3/3
3	OMG	D	2364	3	-	2/5/27/28	0/3/3/3
48	OMU	w	799	48	-	3/9/27/28	0/2/2/2
3	PSU	D	3715	3	-	0/7/25/26	0/2/2/2
3	PSU	D	1782	3	-	0/7/25/26	0/2/2/2
48	B8N	w	1248	48	-	2/16/34/35	0/2/2/2
3	PSU	D	5010	3	-	0/7/25/26	0/2/2/2
3	OMG	D	4494	3	-	1/5/27/28	0/3/3/3
3	PSU	D	3695	3	-	0/7/25/26	0/2/2/2
48	PSU	w	1174	80,48	-	0/7/25/26	0/2/2/2
48	OMU	w	627	48	-	0/9/27/28	0/2/2/2
3	PSU	D	4471	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	D	2365	80,3	-	0/9/27/28	0/2/2/2
3	OMG	D	4637	3	-	1/5/27/28	0/3/3/3
3	PSU	D	3734	3	-	0/7/25/26	0/2/2/2
3	A2M	D	3825	3	-	0/5/27/28	0/3/3/3
48	PSU	w	609	48	-	0/7/25/26	0/2/2/2
3	A2M	D	2815	3	-	3/5/27/28	0/3/3/3
48	PSU	w	966	48	-	0/7/25/26	0/2/2/2
3	PSU	D	4552	3	-	0/7/25/26	0/2/2/2
3	OMU	D	2837	3	-	0/9/27/28	0/2/2/2
3	PSU	D	4628	3	-	0/7/25/26	0/2/2/2
48	A2M	w	159	48	-	4/5/27/28	0/3/3/3
3	A2M	D	398	3	-	1/5/27/28	0/3/3/3
3	OMC	D	3808	3	-	0/9/27/28	0/2/2/2
48	OMU	w	428	48	-	7/9/27/28	0/2/2/2
3	A2M	D	3830	3	-	0/5/27/28	0/3/3/3
48	OMG	w	1490	80,48	-	3/5/27/28	0/3/3/3
2	H2U	B	47	2	-	2/7/38/39	0/2/2/2
48	A2M	w	468	48	-	3/5/27/28	0/3/3/3
48	MA6	w	1851	48	-	3/7/29/30	0/3/3/3
2	3AU	B	20	2	-	8/16/34/35	0/2/2/2
3	OMU	D	4306	3	-	0/9/27/28	0/2/2/2
48	A2M	w	512	48	-	0/5/27/28	0/3/3/3
48	OMC	w	462	48	-	1/9/27/28	0/2/2/2
3	5MC	D	3782	80,3	-	0/7/25/26	0/2/2/2
3	PSU	D	4576	3	-	0/7/25/26	0/2/2/2
3	UY1	D	3818	80,3	-	4/9/27/28	0/2/2/2
48	OMG	w	436	48	-	0/5/27/28	0/3/3/3
3	A2M	D	3785	80,3	-	3/5/27/28	0/3/3/3
3	PSU	D	1781	3	-	0/7/25/26	0/2/2/2
48	PSU	w	105	48	-	0/7/25/26	0/2/2/2
48	A2M	w	99	80,48	-	1/5/27/28	0/3/3/3
3	PSU	D	3639	3	-	0/7/25/26	0/2/2/2
3	OMG	D	3792	3	-	0/5/27/28	0/3/3/3
2	2MG	B	10	2	-	0/5/27/28	0/3/3/3
48	OMC	w	174	48	-	0/9/27/28	0/2/2/2
48	A2M	w	1031	48	-	0/5/27/28	0/3/3/3
48	PSU	w	649	48	-	0/7/25/26	0/2/2/2
48	PSU	w	1232	48	-	0/7/25/26	0/2/2/2
3	PSU	D	3762	3	-	0/7/25/26	0/2/2/2
3	PSU	D	1536	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	D	4523	80,3	-	0/5/27/28	0/3/3/3
2	H2U	B	17	2	-	1/7/38/39	0/2/2/2
48	PSU	w	681	80,48	-	0/7/25/26	0/2/2/2
48	PSU	w	1081	48	-	0/7/25/26	0/2/2/2
3	OMG	D	2424	3	-	2/5/27/28	0/3/3/3
3	PSU	D	4972	3	-	0/7/25/26	0/2/2/2
48	PSU	w	218	48	-	0/7/25/26	0/2/2/2
48	PSU	w	814	48	-	0/7/25/26	0/2/2/2
3	OMU	D	2415	3	-	1/9/27/28	0/2/2/2
3	PSU	D	4420	3	-	0/7/25/26	0/2/2/2
48	A2M	w	576	48	-	2/5/27/28	0/3/3/3
3	OMG	D	3627	3	-	0/5/27/28	0/3/3/3
48	PSU	w	822	48	-	0/7/25/26	0/2/2/2
3	PSU	D	4353	3	-	0/7/25/26	0/2/2/2
3	OMU	D	4620	3	-	0/9/27/28	0/2/2/2
3	PSU	D	4442	3	-	0/7/25/26	0/2/2/2
48	PSU	w	686	48	-	0/7/25/26	0/2/2/2
48	PSU	w	801	48	-	0/7/25/26	0/2/2/2
3	OMU	D	1773	3	-	0/9/27/28	0/2/2/2
2	56B	B	34	2,81	-	1/6/43/44	0/4/4/4
3	OMG	D	4228	3	-	0/5/27/28	0/3/3/3
48	OMU	w	121	48	-	0/9/27/28	0/2/2/2
3	PSU	D	4299	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3920	80,3	-	0/7/25/26	0/2/2/2
48	A2M	w	166	48	-	3/5/27/28	0/3/3/3
3	OMC	D	2861	3	-	0/9/27/28	0/2/2/2
2	PSU	B	35	2,1	-	0/7/25/26	0/2/2/2
3	PSU	D	4500	3	-	4/7/25/26	0/2/2/2
3	PSU	D	3758	3	-	0/7/25/26	0/2/2/2
3	OMU	D	4227	3	-	0/9/27/28	0/2/2/2
3	OMG	D	1760	3	-	2/5/27/28	0/3/3/3
48	A2M	w	484	48	-	0/5/27/28	0/3/3/3
3	PSU	D	4293	3	-	0/7/25/26	0/2/2/2
3	OMC	D	3841	3	-	0/9/27/28	0/2/2/2
3	OMC	D	4456	3	-	0/9/27/28	0/2/2/2
48	OMG	w	683	48	-	0/5/27/28	0/3/3/3
3	OMC	D	2824	3	-	1/9/27/28	0/2/2/2
48	PSU	w	210	48	-	0/7/25/26	0/2/2/2
48	G7M	w	1639	2,48	-	2/3/25/26	0/3/3/3
3	A2M	D	2401	80,3	-	1/5/27/28	0/3/3/3
2	1MG	B	37	2	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	D	4499	3	-	0/5/27/28	0/3/3/3
2	2MG	B	6	2	-	2/5/27/28	0/3/3/3
3	PSU	D	4532	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4579	3	-	0/7/25/26	0/2/2/2
48	PSU	w	1056	48	-	0/7/25/26	0/2/2/2
3	OMG	D	3944	3	-	3/5/27/28	0/3/3/3
3	PSU	D	1677	80,3	-	4/7/25/26	0/2/2/2
3	OMG	D	3899	3	-	0/5/27/28	0/3/3/3
48	PSU	w	1244	48	-	0/7/25/26	0/2/2/2
48	4AC	w	1842	48	-	0/11/29/30	0/2/2/2
48	PSU	w	1692	48	-	0/7/25/26	0/2/2/2
48	OMG	w	644	48	-	3/5/27/28	0/3/3/3
3	PSU	D	4361	3	-	0/7/25/26	0/2/2/2
48	6MZ	w	1832	80,48	-	2/5/27/28	0/3/3/3
48	PSU	w	1238	48	-	2/7/25/26	0/2/2/2
3	OMG	D	4623	3	-	0/5/27/28	0/3/3/3
48	4AC	w	1337	48	-	0/11/29/30	0/2/2/2
3	OMG	D	4370	3	-	2/5/27/28	0/3/3/3
3	PSU	D	2632	3	-	0/7/25/26	0/2/2/2
48	PSU	w	93	48	-	0/7/25/26	0/2/2/2

The worst 5 of 734 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	54	5MU	C2-N1	10.87	1.55	1.38
2	B	54	5MU	C6-N1	10.82	1.56	1.38
3	D	4447	5MC	C6-C5	9.48	1.50	1.34
2	B	48	5MC	C6-C5	9.47	1.50	1.34
2	B	54	5MU	C4-C5	9.33	1.60	1.44

The worst 5 of 664 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	34	56B	C8-N9-C1'	23.85	146.61	125.48
2	B	54	5MU	C5-C4-N3	12.08	125.63	115.31
2	B	54	5MU	C5-C6-N1	-9.63	113.43	123.34
48	w	1851	MA6	N3-C2-N1	-5.76	119.67	128.68
3	D	4220	6MZ	N3-C2-N1	-5.75	119.69	128.68

There are no chirality outliers.

5 of 149 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	6	2MG	O4'-C4'-C5'-O5'
2	B	6	2MG	C3'-C4'-C5'-O5'
2	B	16	H2U	O4'-C1'-N1-C2
2	B	16	H2U	O4'-C1'-N1-C6
2	B	20	3AU	O4'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 546 ligands modelled in this entry, 545 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	GAL	B	101	2	11,11,12	2.07	4 (36%)	15,15,17	1.69	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	GAL	B	101	2	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	B	101	GAL	O5-C1	-3.53	1.38	1.43
81	B	101	GAL	C2-C3	3.31	1.57	1.52
81	B	101	GAL	C4-C5	2.61	1.58	1.53
81	B	101	GAL	C1-C2	2.14	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	B	101	GAL	O2-C2-C3	-3.29	103.56	110.14
81	B	101	GAL	O4-C4-C5	-2.55	102.97	109.30
81	B	101	GAL	C2-C3-C4	-2.40	106.75	110.89
81	B	101	GAL	C6-C5-C4	-2.14	108.00	113.00

There are no chirality outliers.

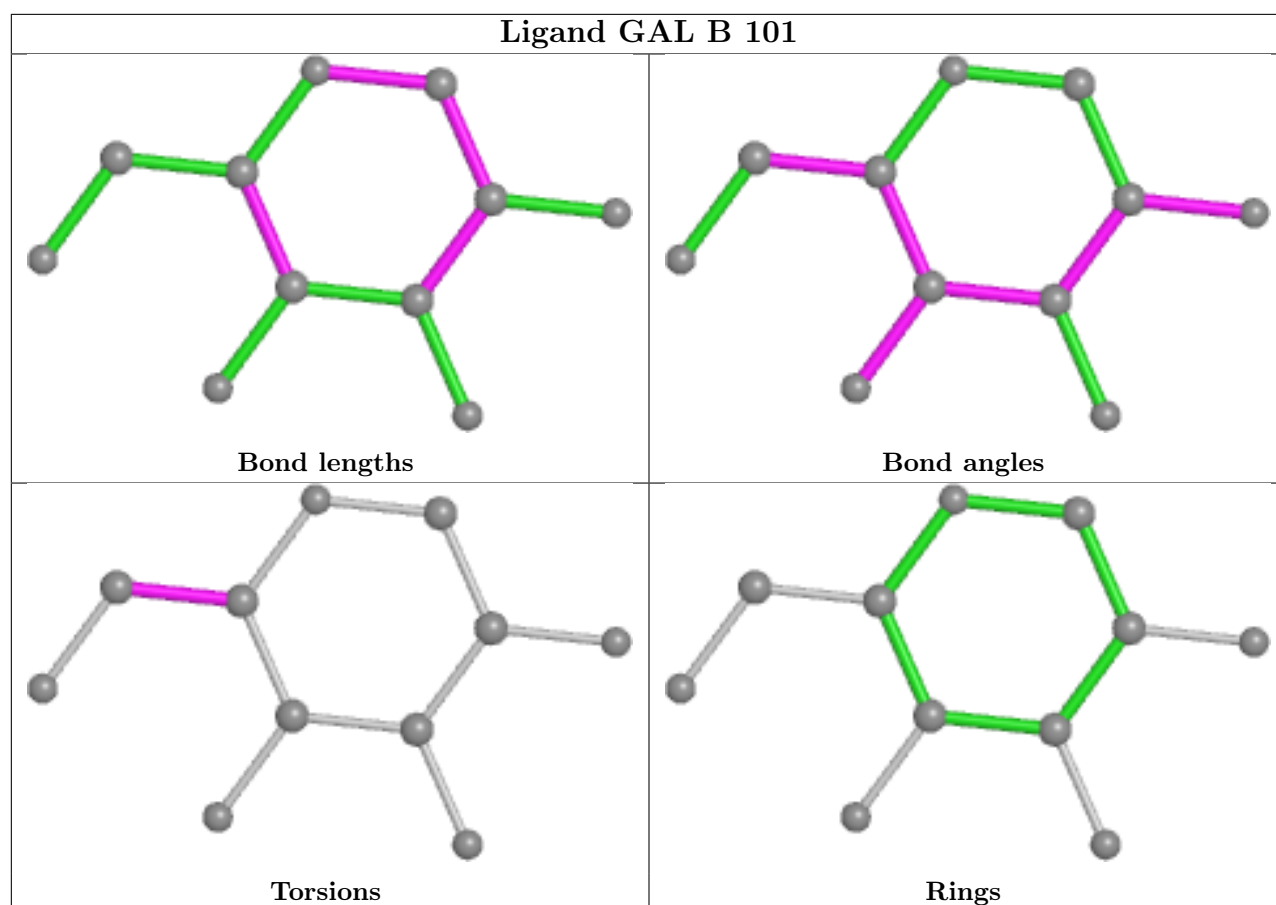
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	B	101	GAL	O5-C5-C6-O6
81	B	101	GAL	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

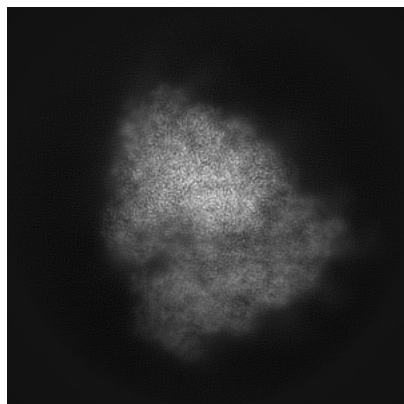
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36180. These allow visual inspection of the internal detail of the map and identification of artifacts.

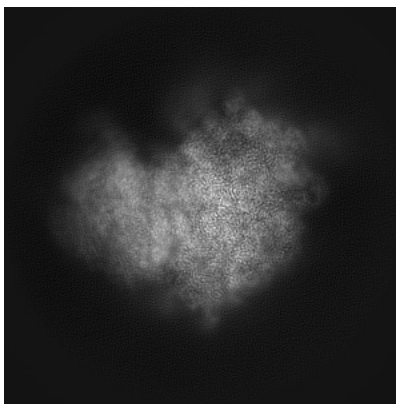
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

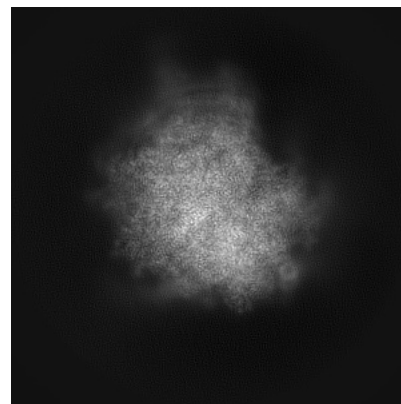
6.1.1 Primary map



X

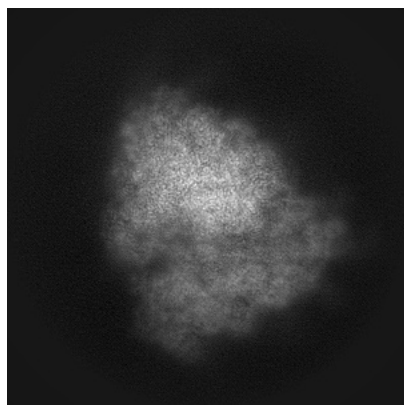


Y

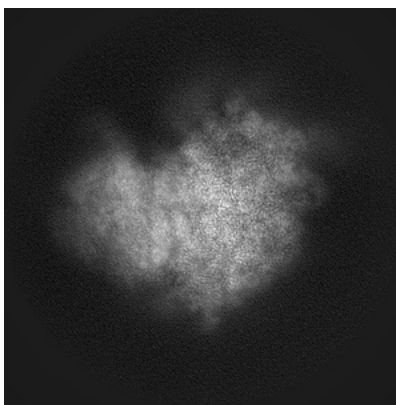


Z

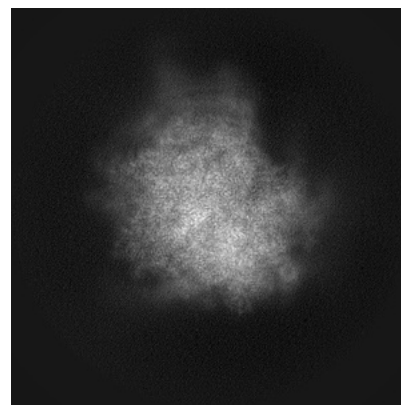
6.1.2 Raw map



X



Y

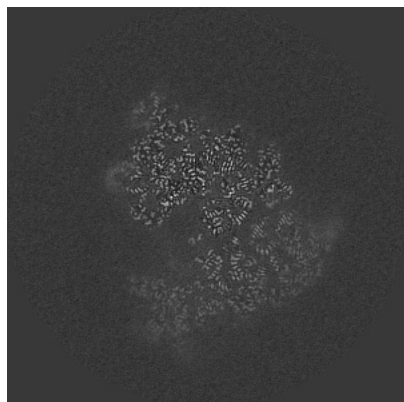


Z

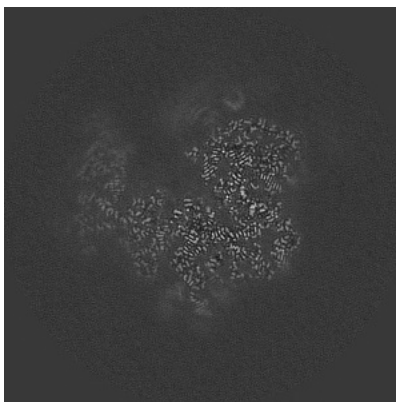
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

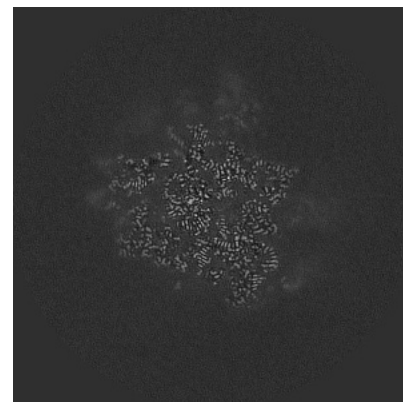
6.2.1 Primary map



X Index: 265

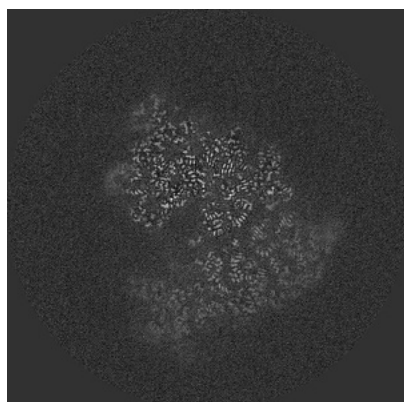


Y Index: 265

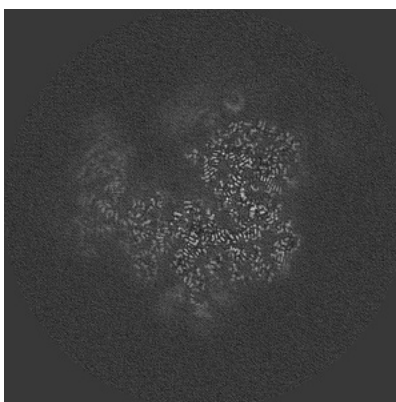


Z Index: 265

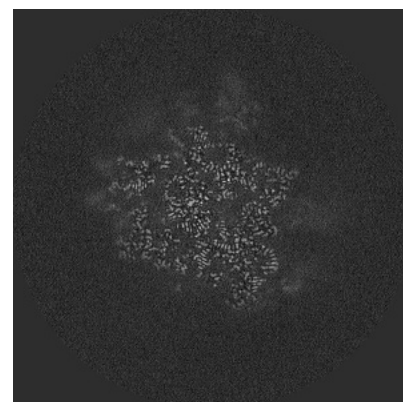
6.2.2 Raw map



X Index: 265



Y Index: 265

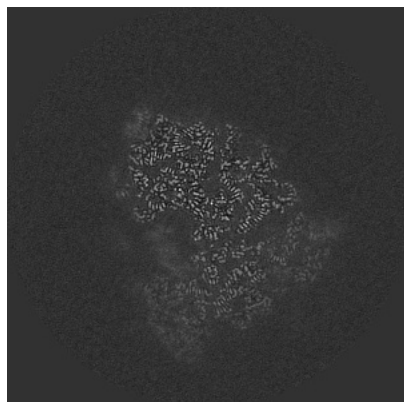


Z Index: 265

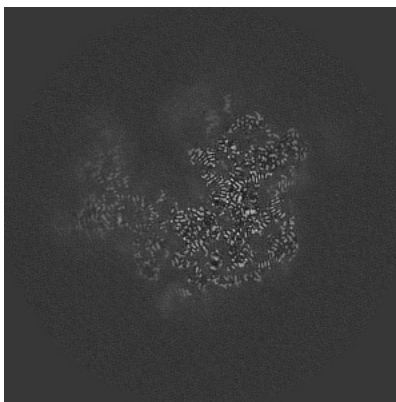
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

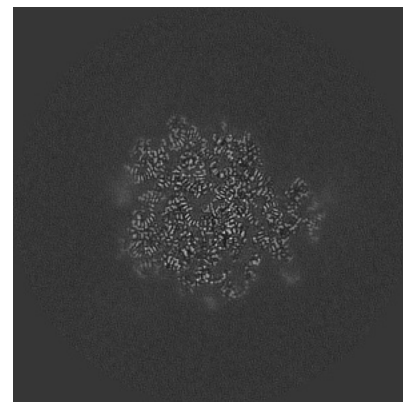
6.3.1 Primary map



X Index: 253

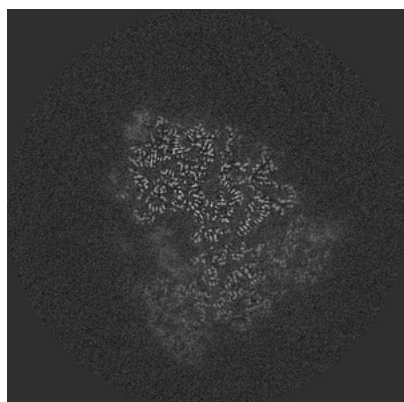


Y Index: 258

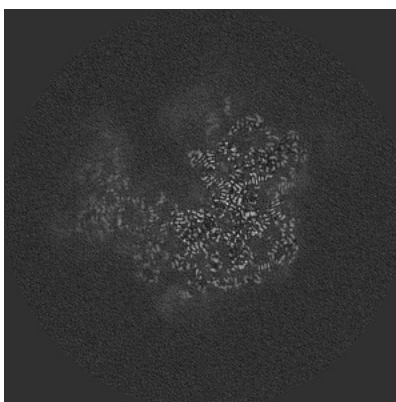


Z Index: 300

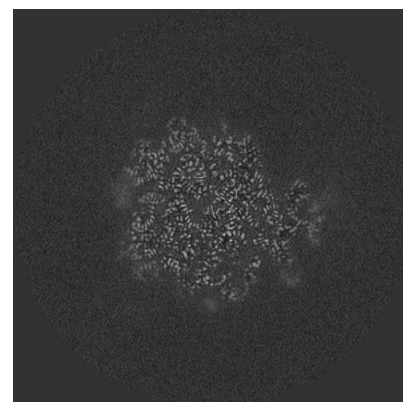
6.3.2 Raw map



X Index: 253



Y Index: 258

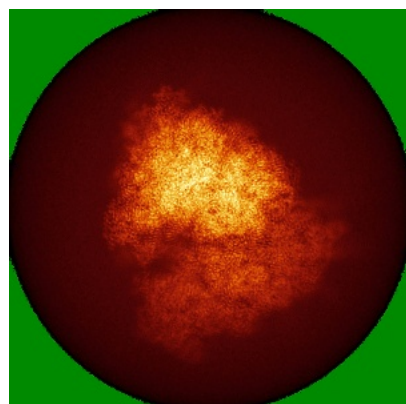


Z Index: 300

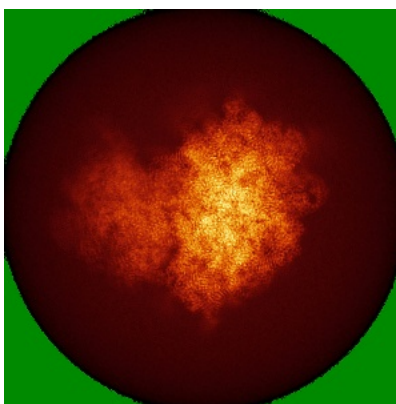
The images above show the largest variance slices of the map in three orthogonal directions.

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

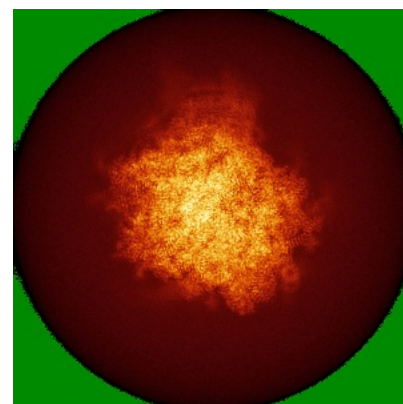
6.4.1 Primary map



X

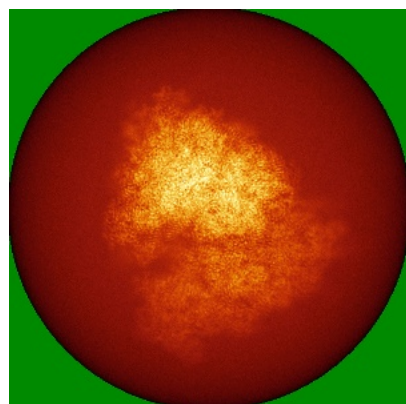


Y

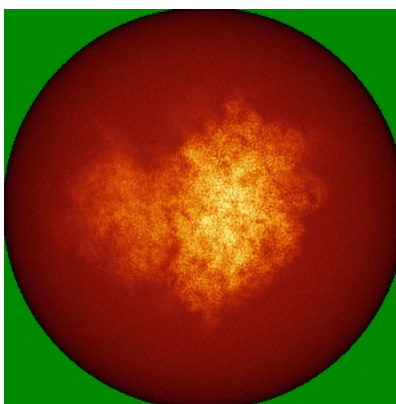


Z

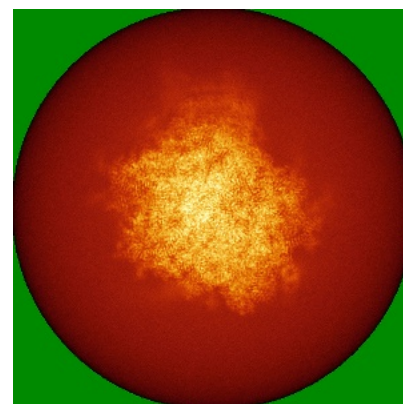
6.4.2 Raw map



X



Y

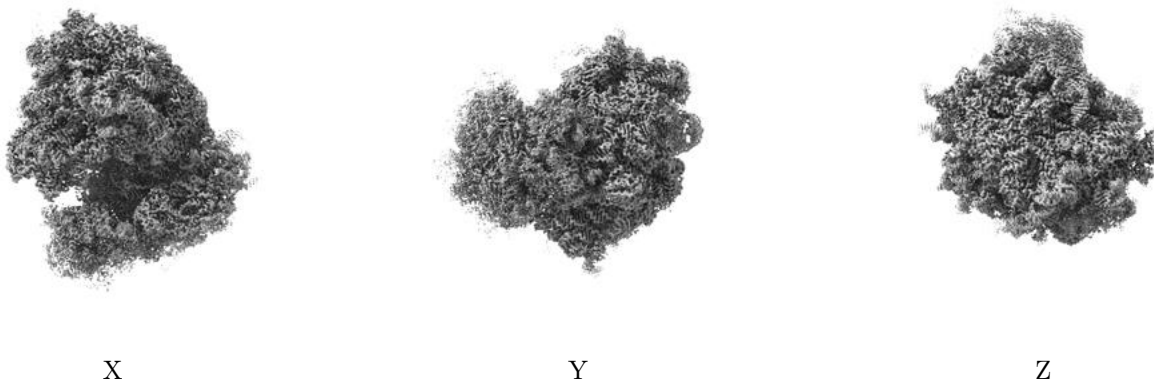


Z

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

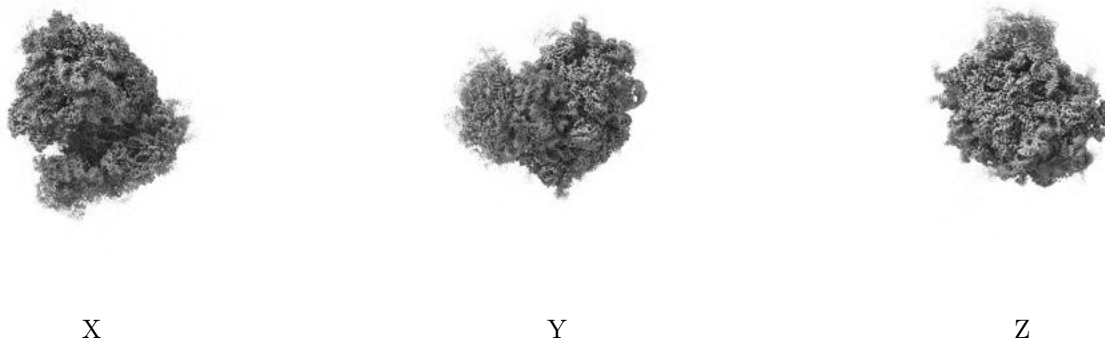
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0191. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

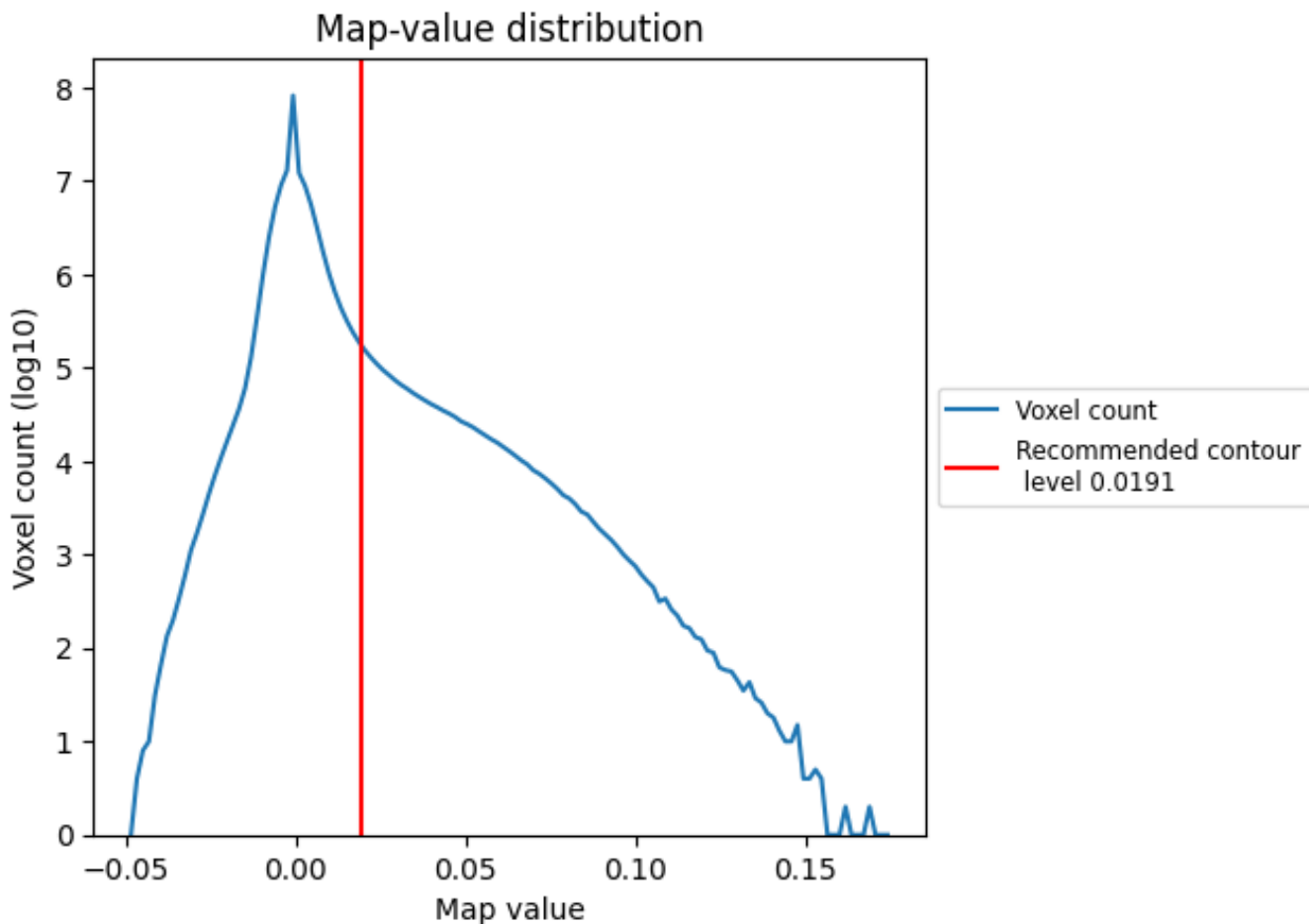
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

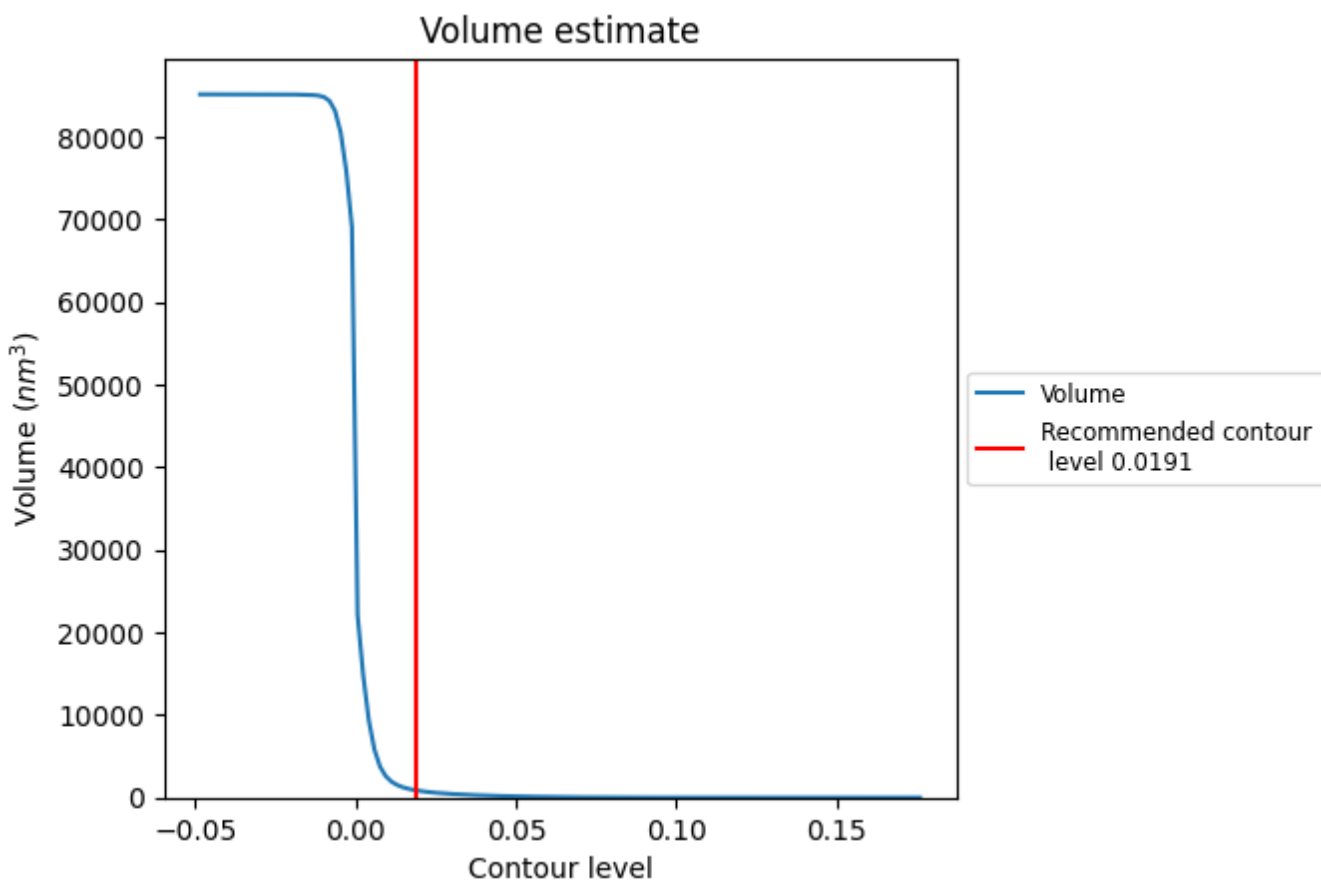
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

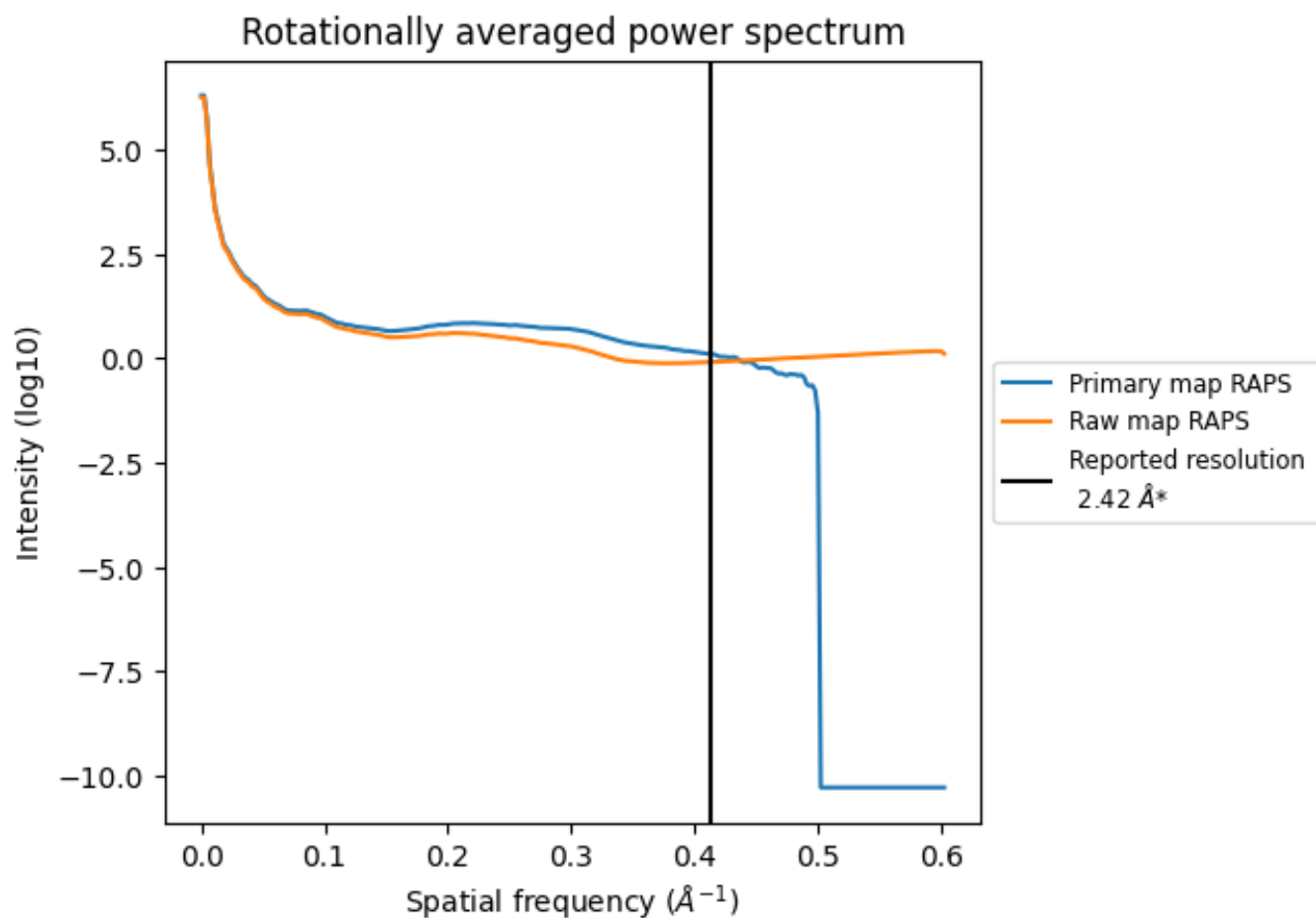
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 860 nm³; this corresponds to an approximate mass of 777 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](#)

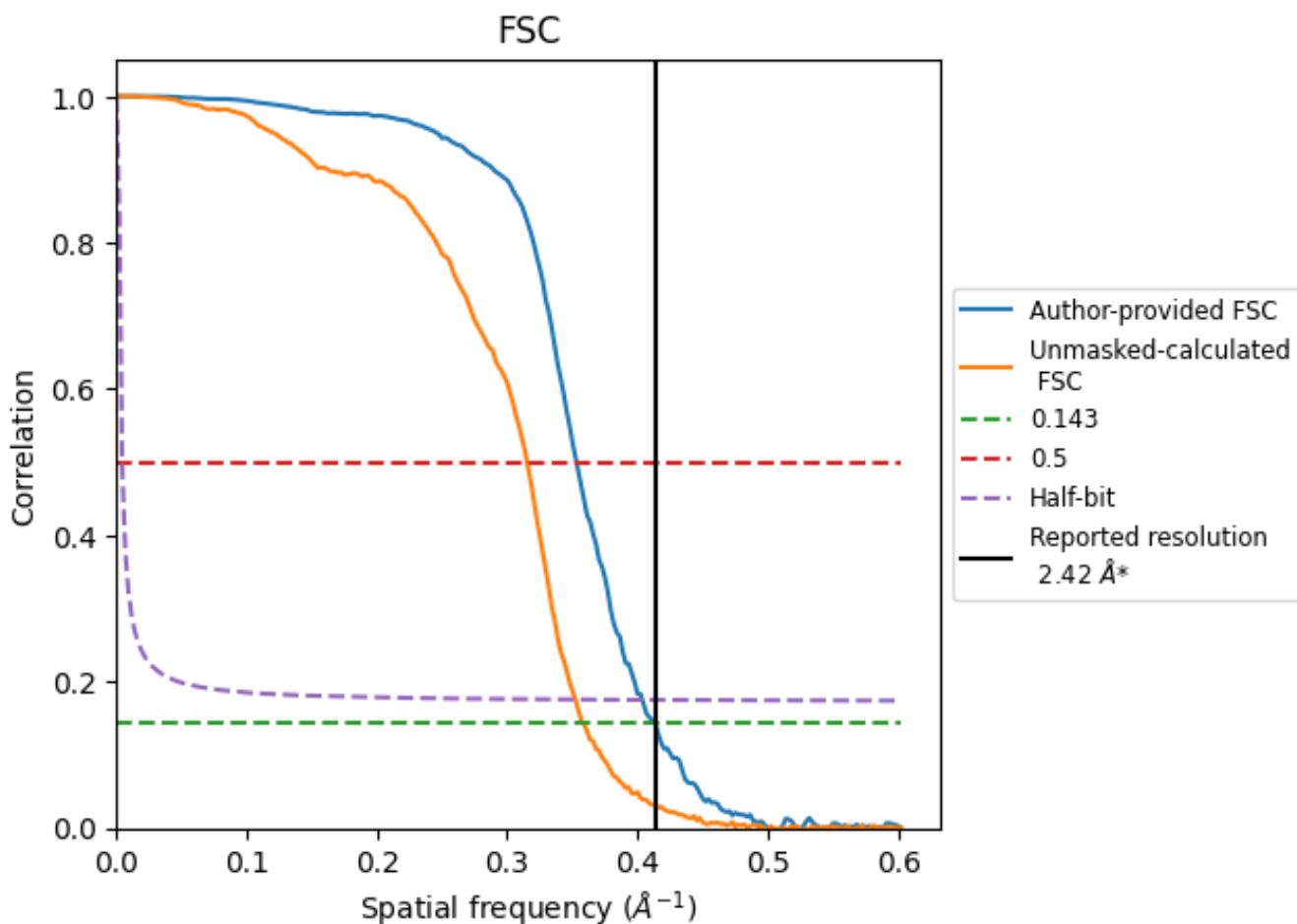


*Reported resolution corresponds to spatial frequency of 0.413 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.413 Å⁻¹

8.2 Resolution estimates [i](#)

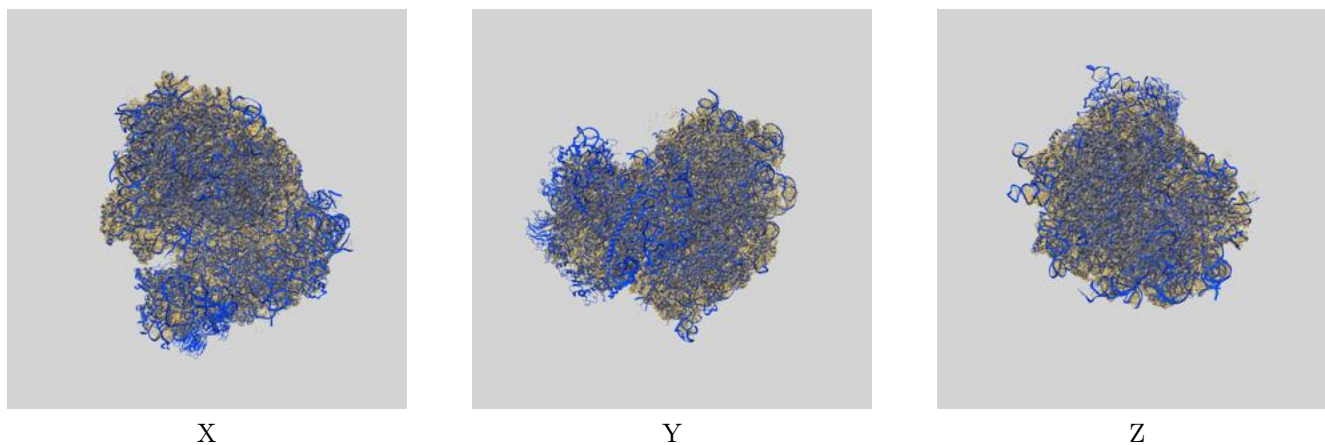
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.42	-	-
Author-provided FSC curve	2.42	2.83	2.48
Unmasked-calculated*	2.79	3.17	2.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.79 differs from the reported value 2.42 by more than 10 %

9 Map-model fit [i](#)

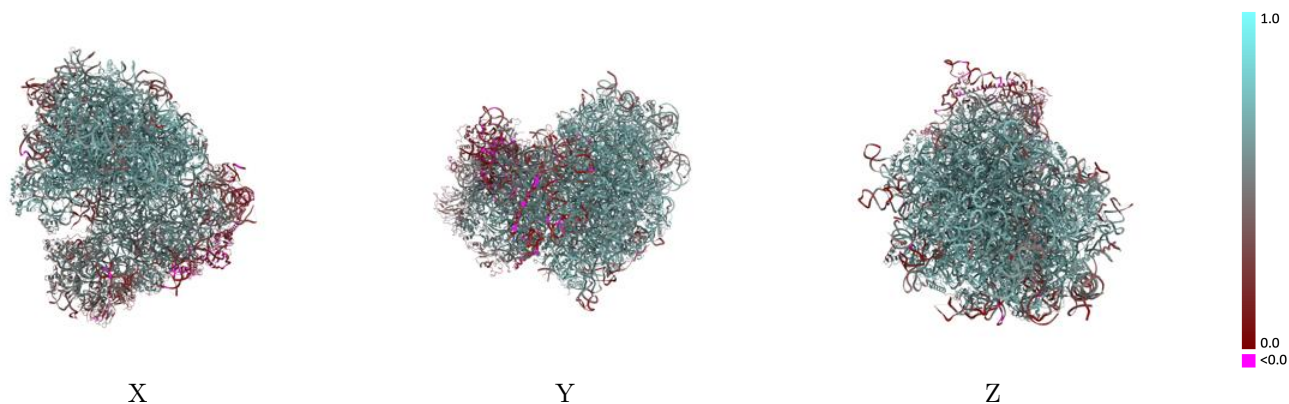
This section contains information regarding the fit between EMDB map EMD-36180 and PDB model 8JDL. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



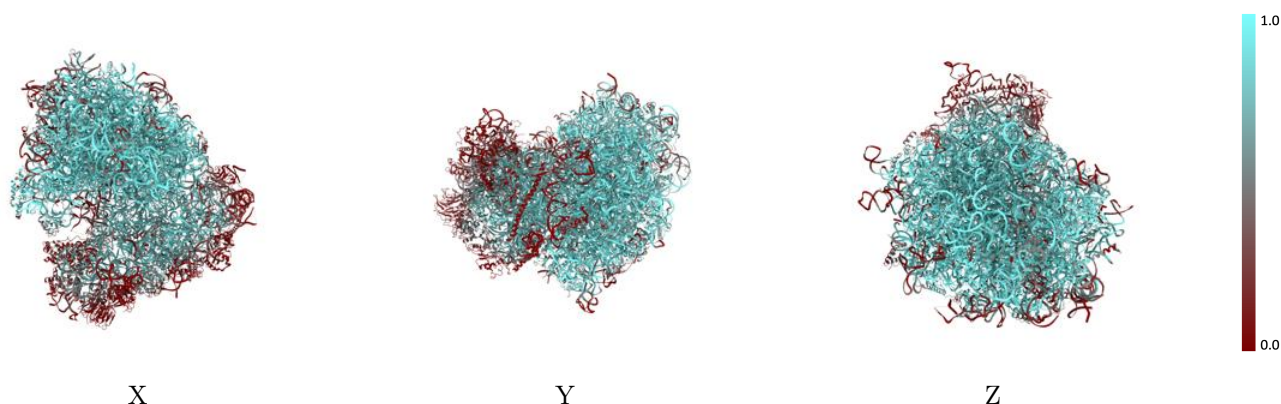
The images above show the 3D surface view of the map at the recommended contour level 0.0191 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



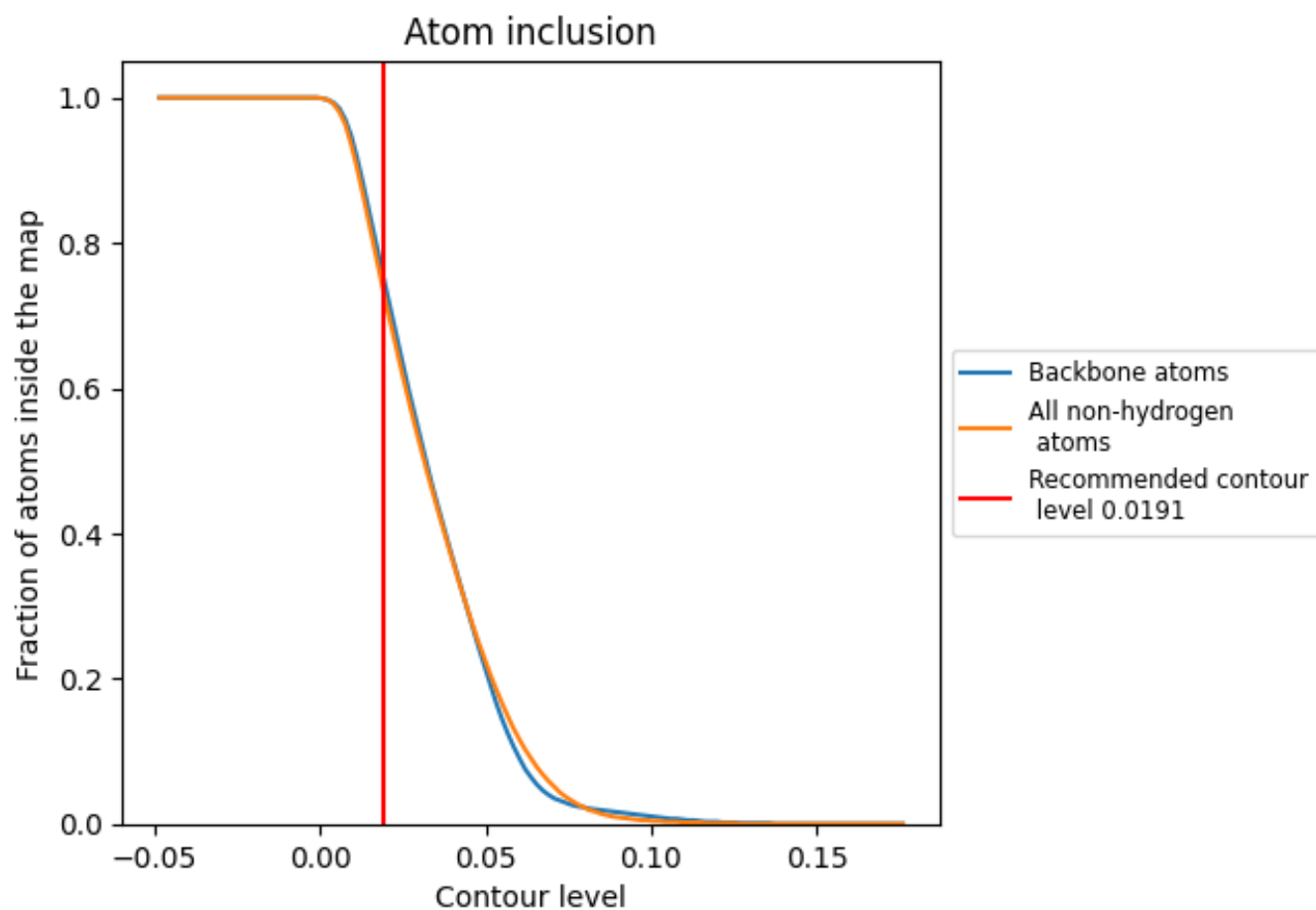
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0191).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 74% 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 (0.0191) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7350	 0.5730
0	 0.2460	 0.4230
1	 0.3220	 0.3450
2	 0.3830	 0.4840
3	 0.1560	 0.2800
4	 0.2200	 0.4010
5	 0.5270	 0.5120
6	 0.2500	 0.2290
7	 0.0520	 0.3010
8	 0.6910	 0.5920
9	 0.6360	 0.5790
A	 0.4890	 0.4710
AA	 0.6660	 0.5800
AB	 0.1410	 0.3950
AC	 0.3210	 0.4620
AD	 0.2250	 0.4190
AE	 0.2540	 0.4570
AF	 0.2730	 0.4540
AG	 0.2290	 0.3700
AH	 0.4820	 0.5530
AI	 0.7290	 0.6070
AJ	 0.6450	 0.5500
AK	 0.1130	 0.1930
AL	 0.1580	 0.3970
AM	 0.7120	 0.5870
AN	 0.4150	 0.4820
AO	 0.3510	 0.4680
AP	 0.5180	 0.5330
AQ	 0.1330	 0.2160
AR	 0.0240	 0.2980
B	 0.2670	 0.3860
D	 0.8520	 0.6160
E	 0.9700	 0.6660
F	 0.9050	 0.6340
G	 0.9540	 0.6890









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Chain	Atom inclusion	Q-score
H	 0.8850	 0.6660
I	 0.9040	 0.6550
J	 0.7840	 0.6120
K	 0.7610	 0.6050
L	 0.9050	 0.6690
M	 0.7080	 0.5780
N	 0.8240	 0.6330
O	 0.8550	 0.6460
P	 0.6500	 0.5430
Q	 0.8040	 0.6190
R	 0.8570	 0.6290
S	 0.9640	 0.6900
T	 0.9120	 0.6760
U	 0.8900	 0.6710
V	 0.9410	 0.6790
W	 0.7820	 0.6030
X	 0.9260	 0.6730
Y	 0.8550	 0.6440
Z	 0.5890	 0.5300
a	 0.9130	 0.6770
b	 0.8660	 0.6640
c	 0.8430	 0.6310
d	 0.8170	 0.6280
e	 0.8170	 0.6280
f	 0.9070	 0.6730
g	 0.7150	 0.5750
h	 0.8350	 0.6270
i	 0.8310	 0.6390
j	 0.9450	 0.6880
k	 0.9410	 0.6780
l	 0.8570	 0.6390
m	 0.8290	 0.6290
n	 0.7720	 0.6160
o	 0.9500	 0.6850
p	 0.6460	 0.5650
q	 0.9010	 0.6590
r	 0.8750	 0.6560
s	 0.8810	 0.6610
t	 0.8060	 0.6260
u	 0.8790	 0.6670
v	 0.9020	 0.6410
w	 0.6880	 0.5150

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Chain	Atom inclusion	Q-score
x	 0.4640	 0.5430
y	 0.5690	 0.5650
z	 0.6350	 0.5760