



Full wwPDB EM Validation Report ⓘ

Apr 22, 2025 – 02:59 pm BST

PDB ID : 8OGJ / pdb_00008ogj
EMDB ID : EMD-16874
Title : Structure of Candida albicans 80S ribosome in complex with mefloquine
Authors : Kolosova, O.; Zgadzay, Y.; Stetsenko, A.; Guskov, A.; Yusupov, M.
Deposited on : 2023-03-20
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

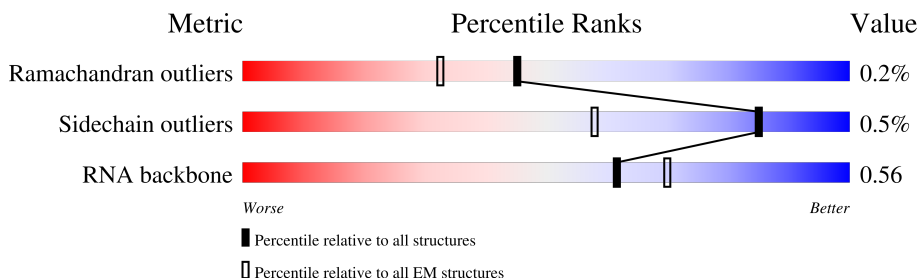
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	1	3359	
2	3	121	
3	4	158	
4	10	76	
5	j	254	
6	k	389	
7	l	363	
8	m	298	

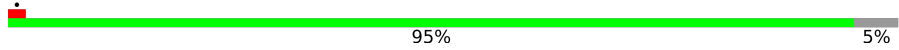
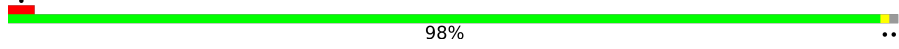
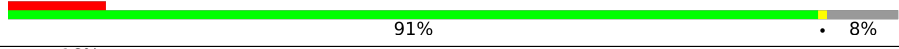
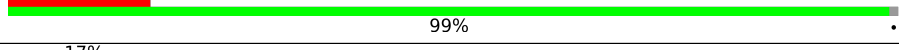
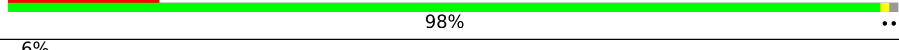
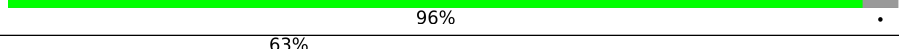
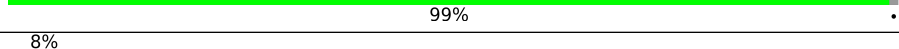
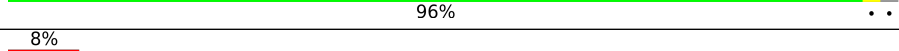
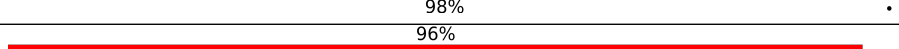
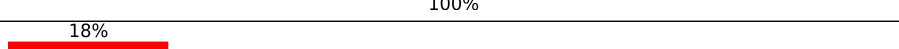
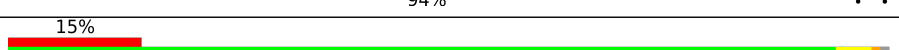
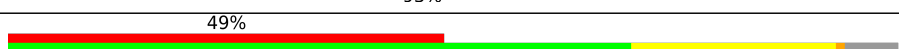




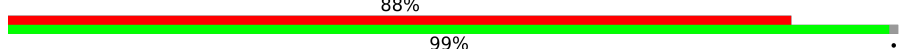

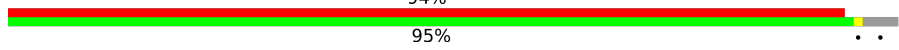
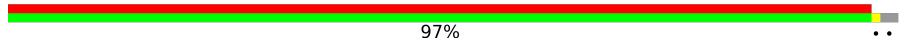

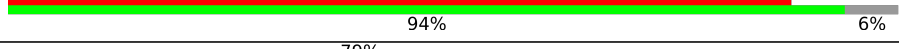



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Mol	Chain	Length	Quality of chain
9	n	176	
10	o	241	
11	p	262	
12	q	191	
13	r	220	
14	s	174	
15	t	202	
16	u	131	
17	v	204	
18	w	200	
19	x	185	
20	y	186	
21	z	190	
22	0	172	
23	2	160	
24	5	124	
25	6	137	
26	7	155	
27	8	142	
28	9	127	
29	AA	136	
30	AB	149	
31	AC	63	
32	AD	106	
33	AE	112	

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Mol	Chain	Length	Quality of chain
34	AF	131	
35	AG	107	
36	AH	122	
37	AI	120	
38	AJ	99	
39	AK	90	
40	AL	78	
41	AM	51	
42	AN	52	
43	AO	25	
44	AP	106	
45	AQ	92	
46	A	1787	
47	B	261	
48	C	256	
49	D	249	
50	E	251	
51	F	262	
52	G	225	
53	H	236	
54	I	186	
55	J	206	
56	K	189	
57	L	118	
58	M	155	

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Mol	Chain	Length	Quality of chain
59	N	143	<div>81%</div> <div>78% 19%</div>
60	O	151	<div>70%</div> <div>99%</div>
61	P	132	<div>64%</div> <div>93%</div>
62	Q	142	<div>83%</div> <div>80% 17%</div>
63	R	142	<div>98%</div> <div>97%</div>
64	S	137	<div>91%</div> <div>91% 9%</div>
65	T	145	<div>98%</div> <div>97%</div>
66	U	145	<div>97%</div> <div>97%</div>
67	V	119	<div>83%</div> <div>83% 16%</div>
68	W	87	<div>90%</div> <div>99%</div>
69	X	130	<div>61%</div> <div>98%</div>
70	Y	145	<div>61%</div> <div>98%</div>
71	Z	135	<div>94%</div> <div>98%</div>
72	a	105	<div>69%</div> <div>69% 31%</div>
73	b	119	<div>43%</div> <div>83% 16%</div>
74	c	82	<div>82%</div> <div>98%</div>
75	d	67	<div>87%</div> <div>85% 13%</div>
76	e	56	<div>95%</div> <div>98%</div>
77	f	63	<div>73%</div> <div>73% 25%</div>
78	g	193	<div>36%</div> <div>35% 64%</div>
79	h	317	<div>98%</div> <div>97%</div>

2 Entry composition

There are 83 unique types of molecules in this entry. The entry contains 196571 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 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	3126	Total	C	N	O	P	0	0
			66827	29854	12018	21829	3126		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	121	Total	C	N	O	P	0	0
			2579	1153	463	842	121		

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	158	Total	C	N	O	P	0	0
			3353	1500	585	1110	158		

- Molecule 4 is a RNA chain called Mixture of endogenous E-tRNAs.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	10	14	Total	C	N	O	P	0	0
			298	133	54	97	14		

- Molecule 5 is a protein called 60S ribosomal protein L2-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	j	249	Total	C	N	O	S	0	0
			1888	1180	376	330	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	k	386	Total	C	N	O	S	1	0
			3084	1955	584	538	7		

- Molecule 7 is a protein called 60S ribosomal protein L4-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	l	361	Total	C	N	O	S	0	0
			2751	1729	529	490	3		

- Molecule 8 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	m	292	Total	C	N	O	S	0	0
			2394	1526	416	450	2		

- Molecule 9 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	n	155	Total	C	N	O		0	0
			1228	788	224	216			

- Molecule 10 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	o	234	Total	C	N	O	S	0	0
			1885	1208	345	331	1		

- Molecule 11 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	p	251	Total	C	N	O	S	0	0
			1929	1235	343	347	4		

- Molecule 12 is a protein called 60S ribosomal protein L9-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	q	190	Total	C	N	O	S	0	0
			1519	958	276	281	4		

- Molecule 13 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	r	208	Total	C	N	O	S	0	0
			1689	1069	322	291	7		

- Molecule 14 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	s	172	Total	C	N	O	S	0	0
			1376	858	260	254	4		

- Molecule 15 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	t	200	Total	C	N	O		0	0
			1610	1009	318	283			

- Molecule 16 is a protein called 60S ribosomal protein L14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	u	130	Total	C	N	O	S	0	0
			1029	660	193	175	1		

- Molecule 17 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	v	203	Total	C	N	O	S	0	0
			1713	1075	356	280	2		

- Molecule 18 is a protein called Ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	w	199	Total	C	N	O	S	0	0
			1590	1025	294	269	2		

- Molecule 19 is a protein called Ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	x	172	Total	C	N	O		0	0
			1375	850	279	246			

- Molecule 20 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	y	185	Total	C	N	O		0	0
			1458	916	297	245			

- Molecule 21 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	z	173	Total	C	N	O	S	1	0
			1411	873	300	235	3		

- Molecule 22 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	171	Total	C	N	O	S	1	0
			1436	929	261	243	3		

- Molecule 23 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	2	159	Total	C	N	O	S	0	0
			1262	798	241	221	2		

- Molecule 24 is a protein called 60S ribosomal protein L22-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	5	103	Total	C	N	O		0	0
			831	539	138	154			

- Molecule 25 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	6	131	Total	C	N	O	S	0	0
			977	615	183	171	8		

- Molecule 26 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	7	63	Total	C	N	O	S	0	0
			524	334	103	86	1		

- Molecule 27 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	8	121	Total	C	N	O	S	0	0
			974	622	175	176	1		

- Molecule 28 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	9	126	Total	C	N	O		
			989	618	190	181	0	0

- Molecule 29 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	AA	135	Total	C	N	O	S	
			1087	705	197	183	2	0

- Molecule 30 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	AB	148	Total	C	N	O	S	
			1170	741	231	197	1	0

- Molecule 31 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	AC	63	Total	C	N	O	S	
			509	317	109	82	1	0

- Molecule 32 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	AD	96	Total	C	N	O	S	
			729	469	121	137	2	0

- Molecule 33 is a protein called 60S ribosomal protein L31-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	AE	109	Total	C	N	O	S	
			889	562	167	158	2	0

- Molecule 34 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	AF	125	Total	C	N	O	S	
			1009	644	196	168	1	0

- Molecule 35 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AG	106	Total	C	N	O	S	1	0
			853	548	162	142	1		

- Molecule 36 is a protein called 60S ribosomal protein L34-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AH	112	Total	C	N	O	S	0	0
			887	547	182	154	4		

- Molecule 37 is a protein called Ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AI	119	Total	C	N	O	S	1	0
			990	629	195	166			

- Molecule 38 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	AJ	98	Total	C	N	O	S	1	0
			772	481	158	131	2		

- Molecule 39 is a protein called 60S ribosomal protein L37-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	AK	86	Total	C	N	O	S	0	0
			677	413	148	110	6		

- Molecule 40 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	AL	77	Total	C	N	O	S	0	0
			617	393	115	109			

- Molecule 41 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AM	50	Total	C	N	O	S	0	0
			438	275	97	66			

- Molecule 42 is a protein called 60S ribosomal protein L40-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AN	52	Total	C	N	O	S	0	0
			419	260	86	67	6		

- Molecule 43 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AO	25	Total	C	N	O	S	0	0
			236	144	63	28	1		

- Molecule 44 is a protein called 60S ribosomal protein L42-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AP	103	Total	C	N	O	S	0	0
			828	521	165	137	5		

- Molecule 45 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AQ	91	Total	C	N	O	S	0	0
			698	430	140	124	4		

- Molecule 46 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	A	1674	Total	C	N	O	P	0	0
			35701	15960	6345	11722	1674		

- Molecule 47 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	B	208	Total	C	N	O	S	0	0
			1627	1041	284	297	5		

- Molecule 48 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	C	201	Total	C	N	O	S	0	0
			1628	1030	297	297	4		

- Molecule 49 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	D	216	Total	C	N	O	S	0	0
			1620	1033	287	295	5		

- Molecule 50 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	E	223	Total	C	N	O	S	0	0
			1707	1087	311	305	4		

- Molecule 51 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	F	260	Total	C	N	O	S	0	0
			2055	1306	386	358	5		

- Molecule 52 is a protein called Ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	G	206	Total	C	N	O	S	0	0
			1614	1008	301	301	4		

- Molecule 53 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	H	226	Total	C	N	O	S	0	0
			1820	1133	351	330	6		

- Molecule 54 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	I	182	Total	C	N	O	S	0	0
			1466	939	264	263			

- Molecule 55 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	J	184	Total	C	N	O	S	0	0
			1448	895	293	259	1		

- Molecule 56 is a protein called Ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	K	178	Total	C	N	O	S	0	0
			1453	918	286	248	1		

- Molecule 57 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	L	93	Total	C	N	O	S	0	0
			783	511	129	142	1		

- Molecule 58 is a protein called 40S ribosomal protein S11A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	M	141	Total	C	N	O	S	0	0
			1129	722	212	192	3		

- Molecule 59 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	N	116	Total	C	N	O	S	0	0
			885	550	158	172	5		

- Molecule 60 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	O	150	Total	C	N	O	S	0	0
			1187	757	219	210	1		

- Molecule 61 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	P	127	Total	C	N	O	S	0	0
			942	579	186	174	3		

- Molecule 62 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Q	118	Total	C	N	O	S	0	0
			935	598	169	162	6		

- Molecule 63 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	R	140	Total	C	N	O	S	0	0
			1091	700	198	192	1		

- Molecule 64 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	S	125	Total	C	N	O	S	0	0
			1002	631	184	186	1		

- Molecule 65 is a protein called 40S ribosomal protein S18-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	T	142	Total	C	N	O	S	0	0
			1169	733	228	205	3		

- Molecule 66 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	U	141	Total	C	N	O	S	0	0
			1100	689	210	200	1		

- Molecule 67 is a protein called Ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	V	100	Total	C	N	O	S	0	0
			790	499	146	143	2		

- Molecule 68 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	W	87	Total	C	N	O	S	0	0
			676	415	126	133	2		

- Molecule 69 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	X	129	Total	C	N	O	S	0	0
			1032	655	191	183	3		

- Molecule 70 is a protein called Ribosomal protein S23 (S12).

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Y	143	Total	C	N	O	S	0	0
			1110	701	219	188	2		

- Molecule 71 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Z	132	Total	C	N	O		0	0
			1072	670	216	186			

- Molecule 72 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	a	72	Total	C	N	O		0	0
			578	369	103	106			

- Molecule 73 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	b	100	Total	C	N	O	S	0	0
			799	494	169	130	6		

- Molecule 74 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	c	81	Total	C	N	O	S	0	0
			614	383	110	114	7		

- Molecule 75 is a protein called 40S ribosomal protein S28-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	d	58	Total	C	N	O	S	0	0
			446	275	85	84	2		

- Molecule 76 is a protein called 40S ribosomal protein S29A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	e	55	Total	C	N	O	S	0	0
			454	281	94	75	4		

- Molecule 77 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	f	47	Total	C	N	O	S	0	0
			375	237	74	62	2		

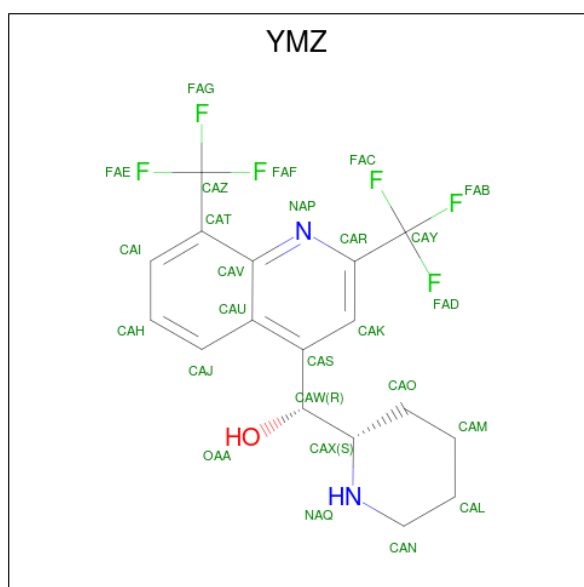
- Molecule 78 is a protein called Ubiquitin-40S ribosomal protein S31 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	g	70	Total	C	N	O	S	0	0
			574	362	113	93	6		

- Molecule 79 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

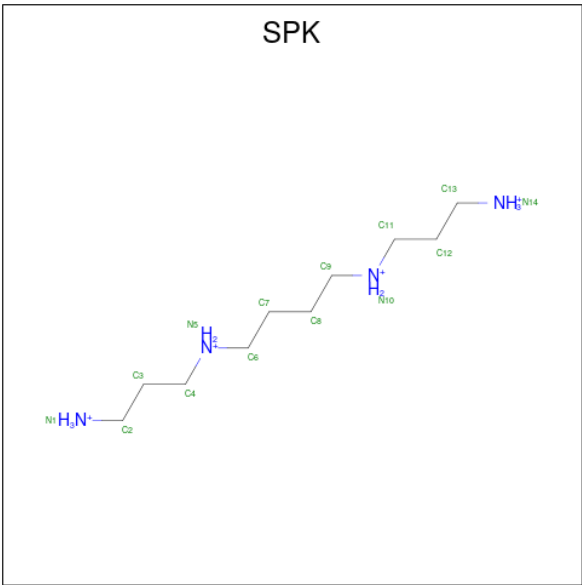
Mol	Chain	Residues	Atoms					AltConf	Trace
79	h	311	Total	C	N	O	S	0	0
			2398	1519	412	462	5		

- Molecule 80 is (11R,12S)- Mefloquine (CCD ID: YMZ) (formula: $C_{17}H_{16}F_6N_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
80	1	1	Total	C	F	N	O	0
			26	17	6	2	1	
80	j	1	Total	C	F	N	O	0
			26	17	6	2	1	

- Molecule 81 is SPERMINE (FULLY PROTONATED FORM) (CCD ID: SPK) (formula: $C_{10}H_{30}N_4$).



Mol	Chain	Residues	Atoms			AltConf
81	1	1	Total	C	N	0
			14	10	4	

- Molecule 82 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
82	1	355	Total	Mg	0
			355	355	
82	3	2	Total	Mg	0
			2	2	
82	4	5	Total	Mg	0
			5	5	
82	j	1	Total	Mg	0
			1	1	
82	k	1	Total	Mg	0
			1	1	
82	v	1	Total	Mg	0
			1	1	
82	x	2	Total	Mg	0
			2	2	
82	z	1	Total	Mg	0
			1	1	
82	6	1	Total	Mg	0
			1	1	
82	AB	1	Total	Mg	0
			1	1	
82	AF	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
82	A	58	Total 58	Mg 58	0
82	Q	1	Total 1	Mg 1	0
82	T	2	Total 2	Mg 2	0

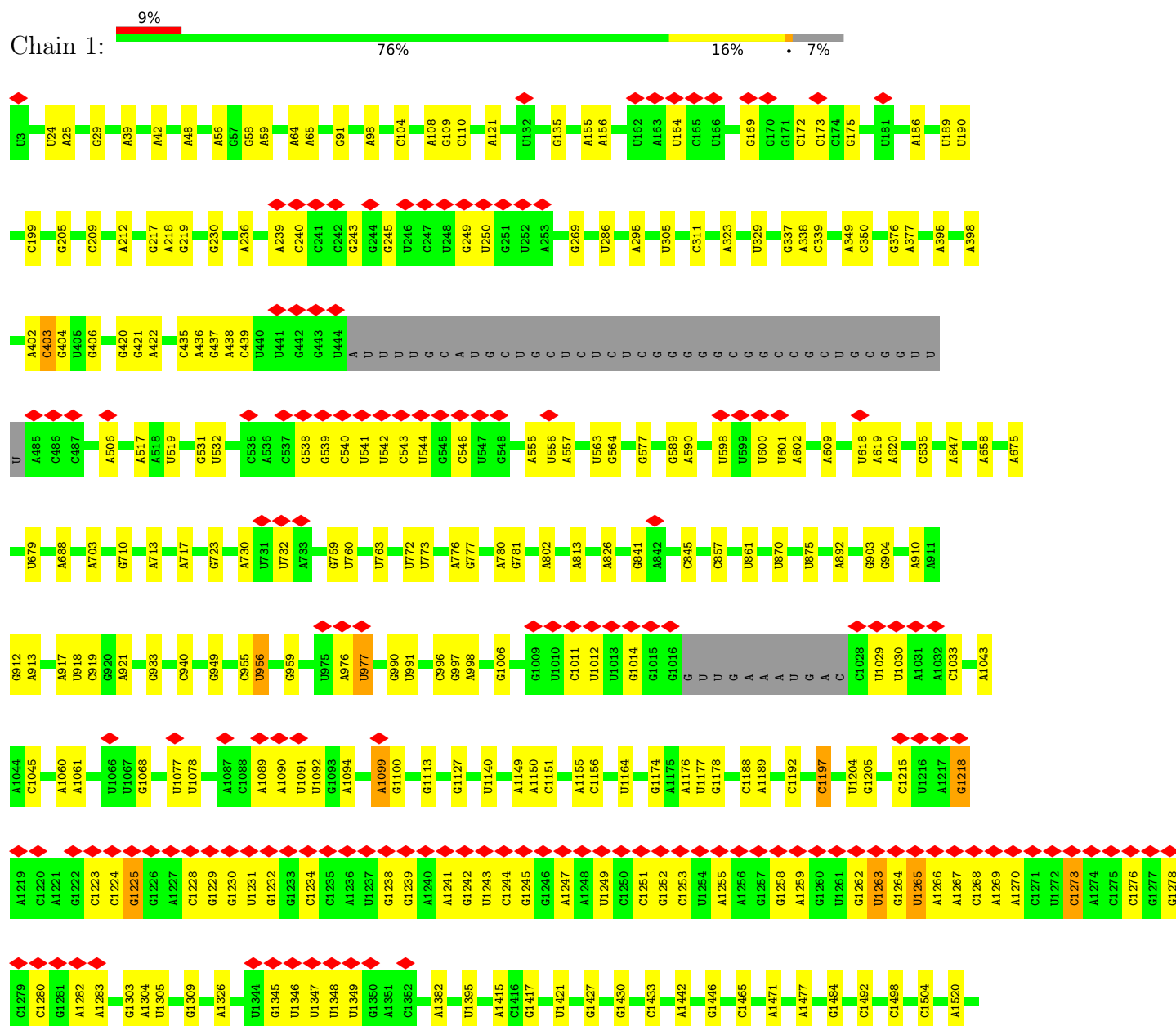
- Molecule 83 is ZINC ION (CCD ID: ZN) (formula: Zn).

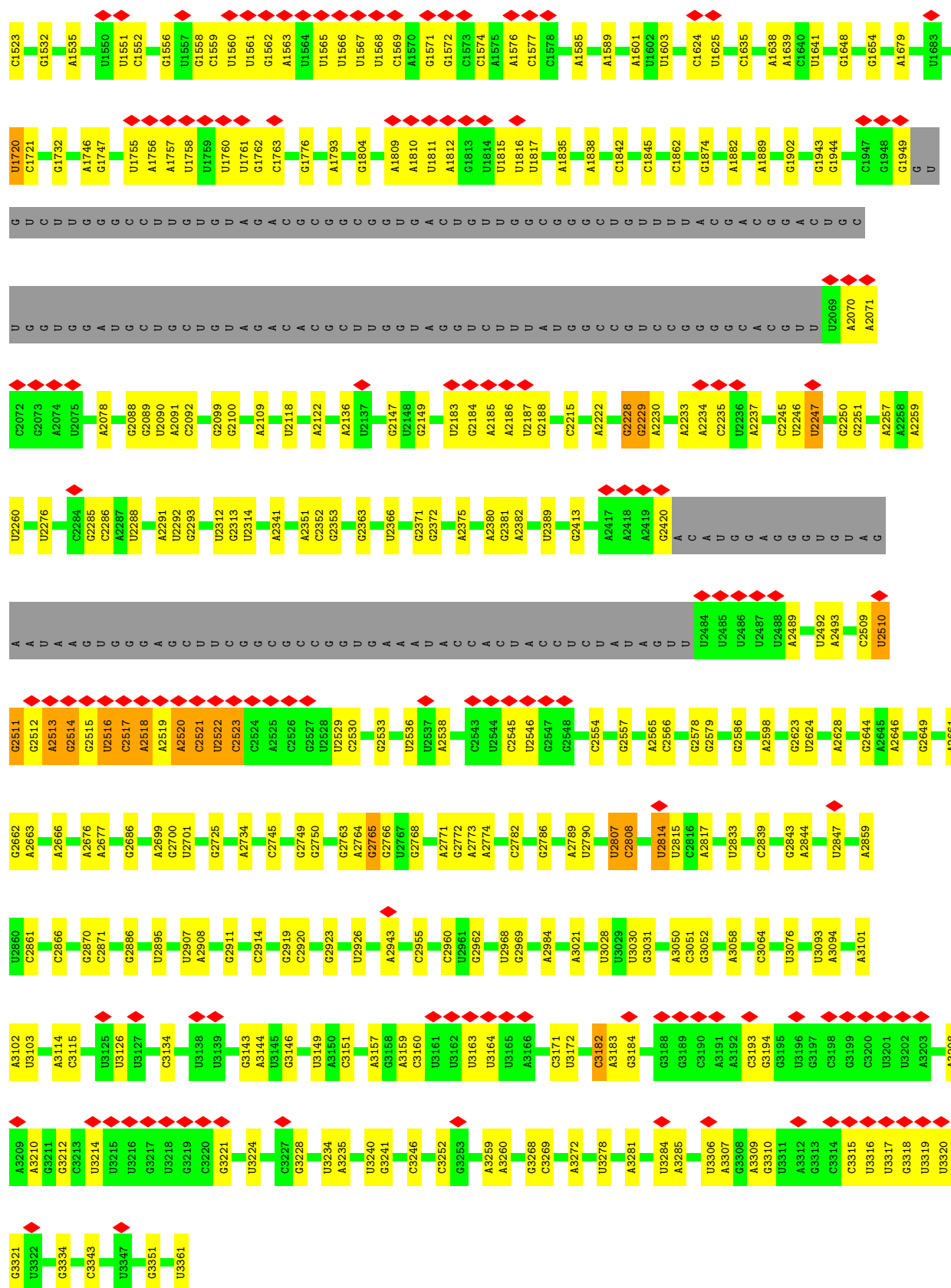
Mol	Chain	Residues	Atoms		AltConf
83	AK	1	Total 1	Zn 1	0
83	AN	1	Total 1	Zn 1	0
83	AP	1	Total 1	Zn 1	0
83	AQ	1	Total 1	Zn 1	0
83	b	1	Total 1	Zn 1	0
83	g	1	Total 1	Zn 1	0

3 Residue-property plots [i](#)

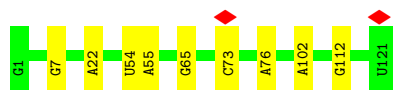
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 25S ribosomal RNA




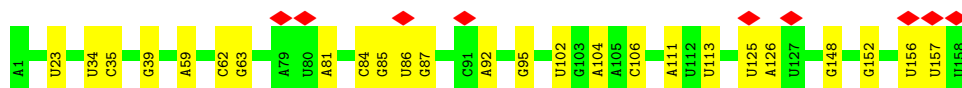


Chain 3:  93% 7%



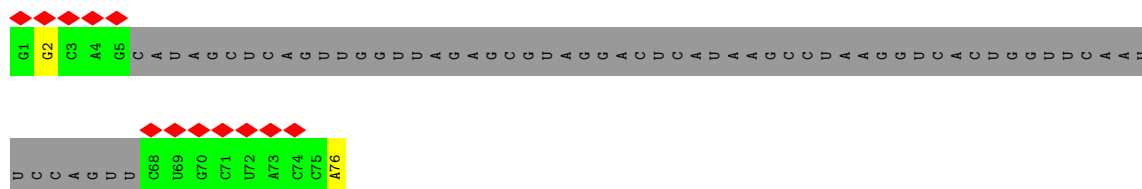
- Molecule 3: 5.8S ribosomal RNA

Chain 4:  6% 84% 16%



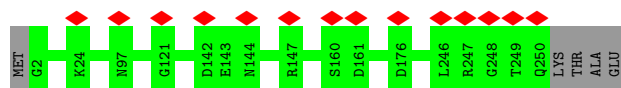
- Molecule 4: Mixture of endogenous E-tRNAs

Chain 10:  16% 16% 82%



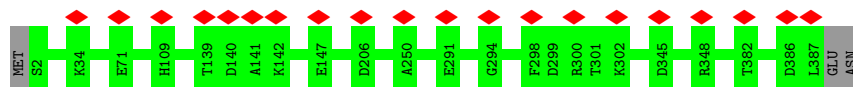
- Molecule 5: 60S ribosomal protein L2-B

Chain j:  6% 98%



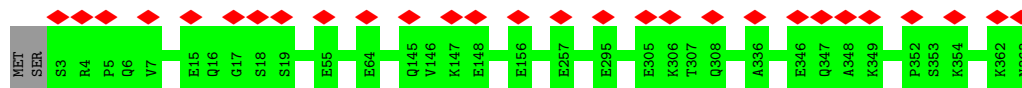
- Molecule 6: 60S ribosomal protein L3

Chain k:  5% 99%



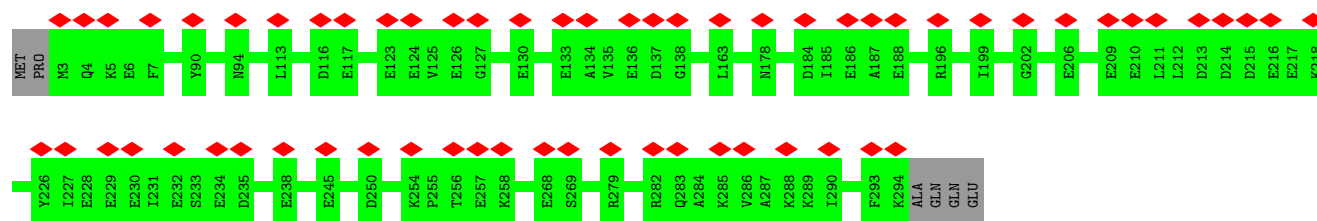
- Molecule 7: 60S ribosomal protein L4-B

Chain l:  8% 99%

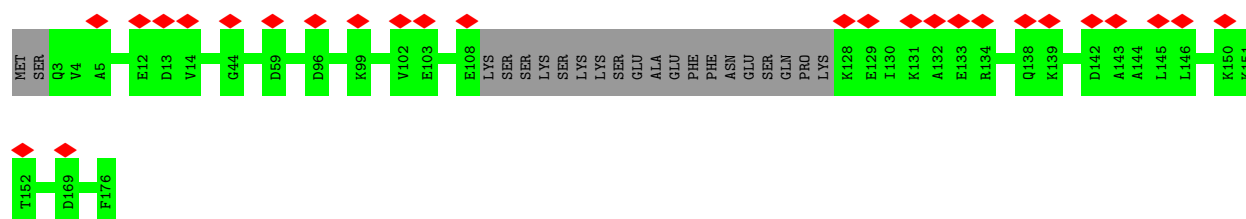
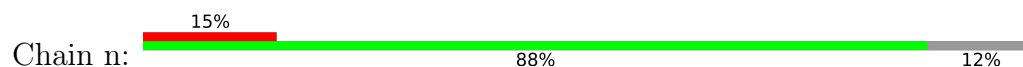


- Molecule 8: 60S ribosomal protein L5

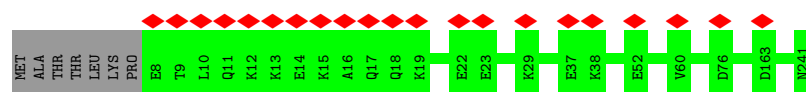
Chain m:  21% 98%



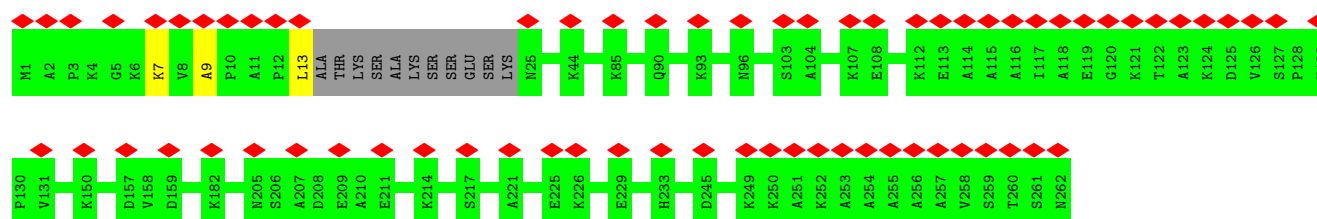
• Molecule 9: 60S ribosomal protein L6



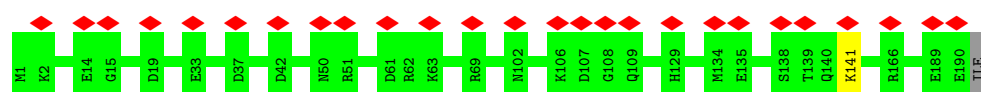
• Molecule 10: 60S ribosomal protein L7-A



• Molecule 11: 60S ribosomal protein L8

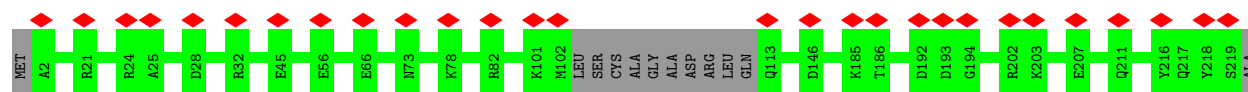


• Molecule 12: 60S ribosomal protein L9-B

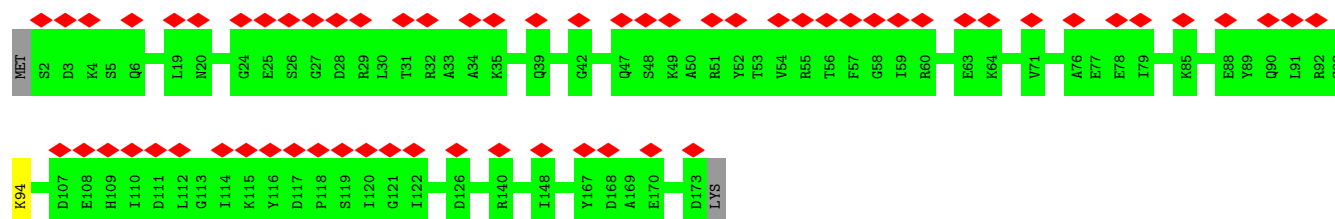


• Molecule 13: 60S ribosomal protein L10

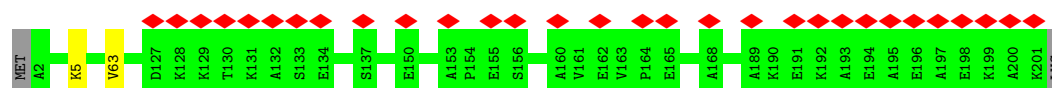




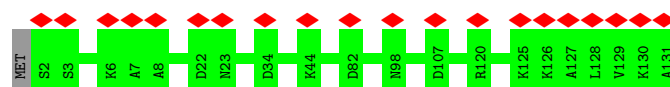
- Molecule 14: 60S ribosomal protein L11-B



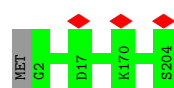
- Molecule 15: 60S ribosomal protein L13



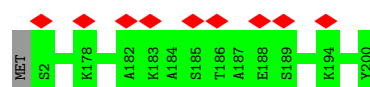
- Molecule 16: 60S ribosomal protein L14-B



- Molecule 17: 60S ribosomal protein L15-A

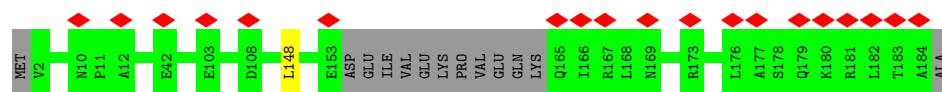


- Molecule 18: Ribosomal protein L13



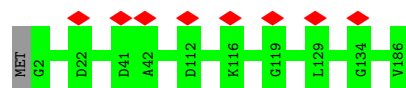
- Molecule 19: Ribosomal protein L22





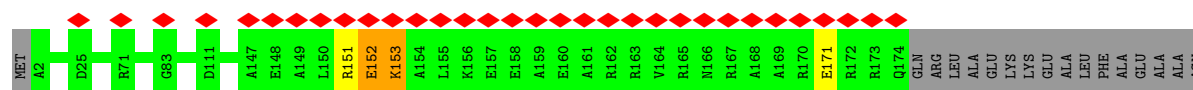
- Molecule 20: 60S ribosomal protein L18-A

Chain y: 99%



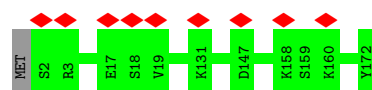
- Molecule 21: 60S ribosomal protein L19-A

Chain z: 17% 89% 9%



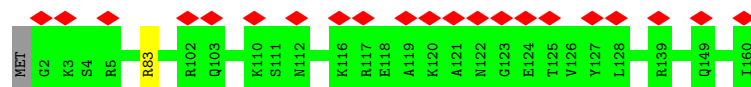
- Molecule 22: 60S ribosomal protein L20

Chain 0: 5% 99%



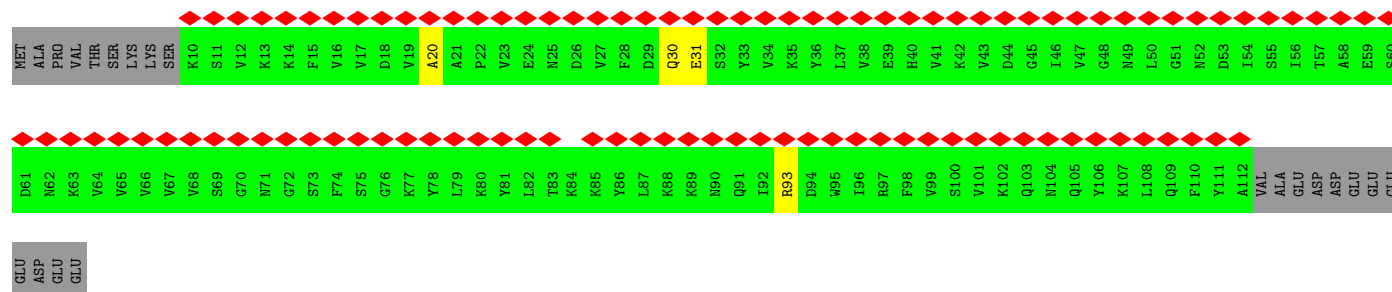
- Molecule 23: 60S ribosomal protein L21-A

Chain 2: 13% 99%

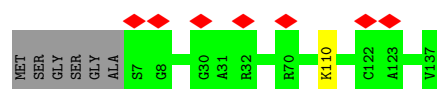


- Molecule 24: 60S ribosomal protein L22-B

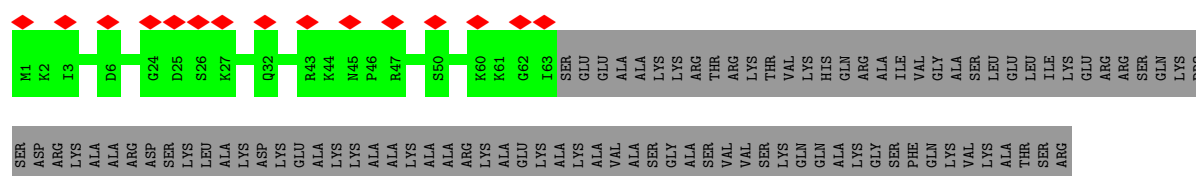
Chain 5: 82% 80% 17%



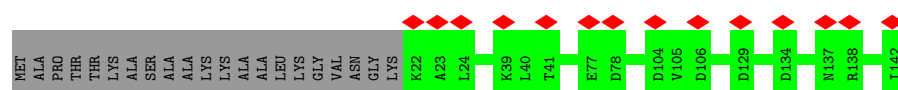
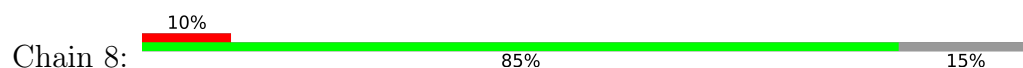
- Molecule 25: 60S ribosomal protein L23-A



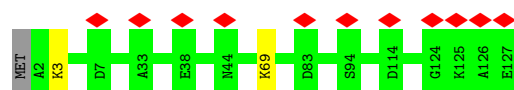
- Molecule 26: 60S ribosomal protein L24-A



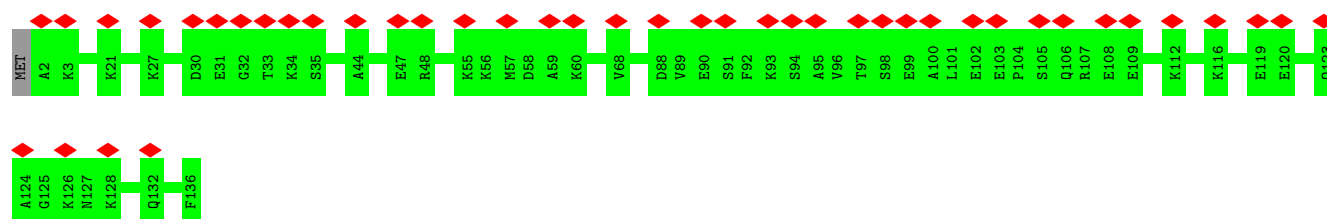
- Molecule 27: 60S ribosomal protein L25



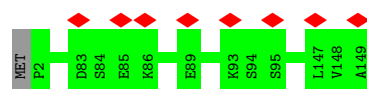
- Molecule 28: Ribosomal protein L24



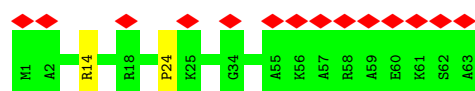
- Molecule 29: 60S ribosomal protein L27



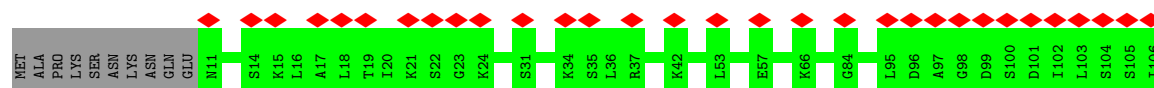
- Molecule 30: 60S ribosomal protein L28



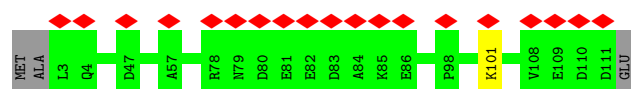
- Molecule 31: 60S ribosomal protein L29



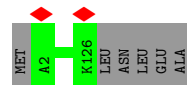
- Molecule 32: 60S ribosomal protein L30



- Molecule 33: 60S ribosomal protein L31-B



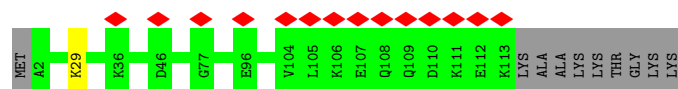
- Molecule 34: 60S ribosomal protein L32



- Molecule 35: 60S ribosomal protein L33-A



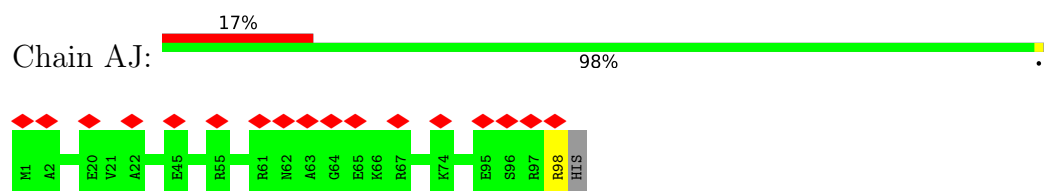
- Molecule 36: 60S ribosomal protein L34-B



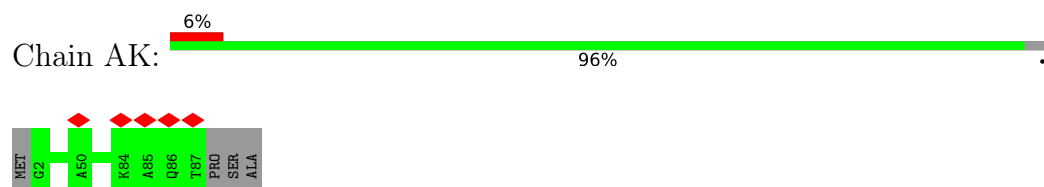
- Molecule 37: Ribosomal protein L29



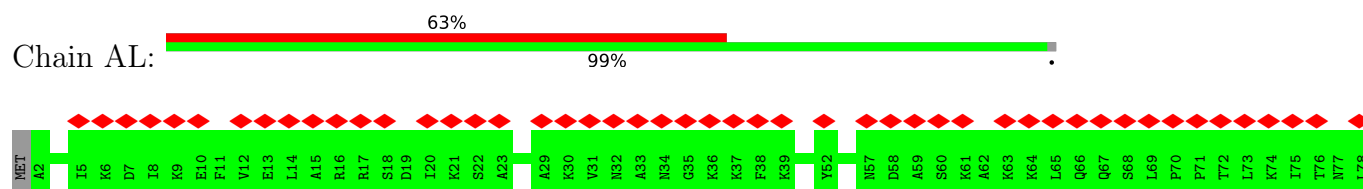
• Molecule 38: 60S ribosomal protein L36



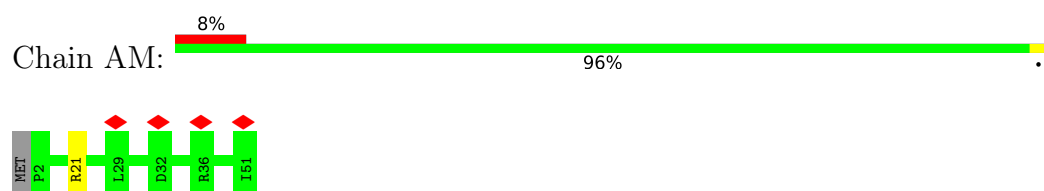
• Molecule 39: 60S ribosomal protein L37-B



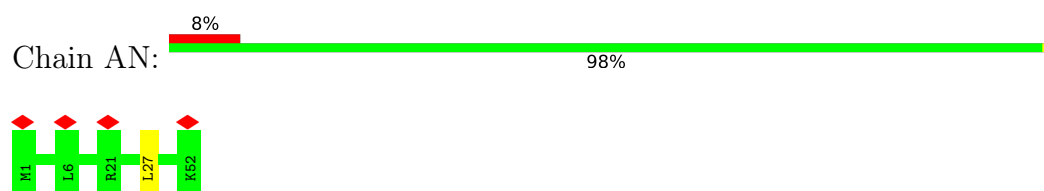
• Molecule 40: 60S ribosomal protein L38



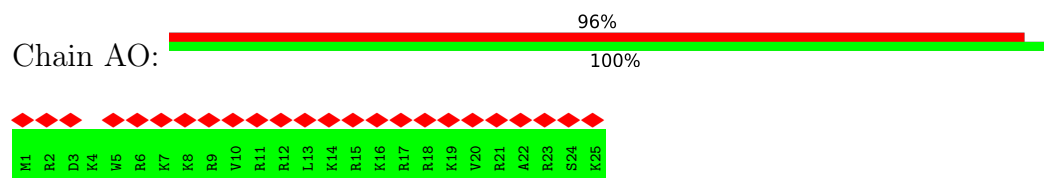
• Molecule 41: 60S ribosomal protein L39



• Molecule 42: 60S ribosomal protein L40-B

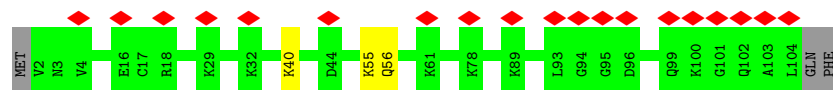


• Molecule 43: 60S ribosomal protein L41

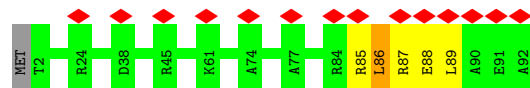


• Molecule 44: 60S ribosomal protein L42-B

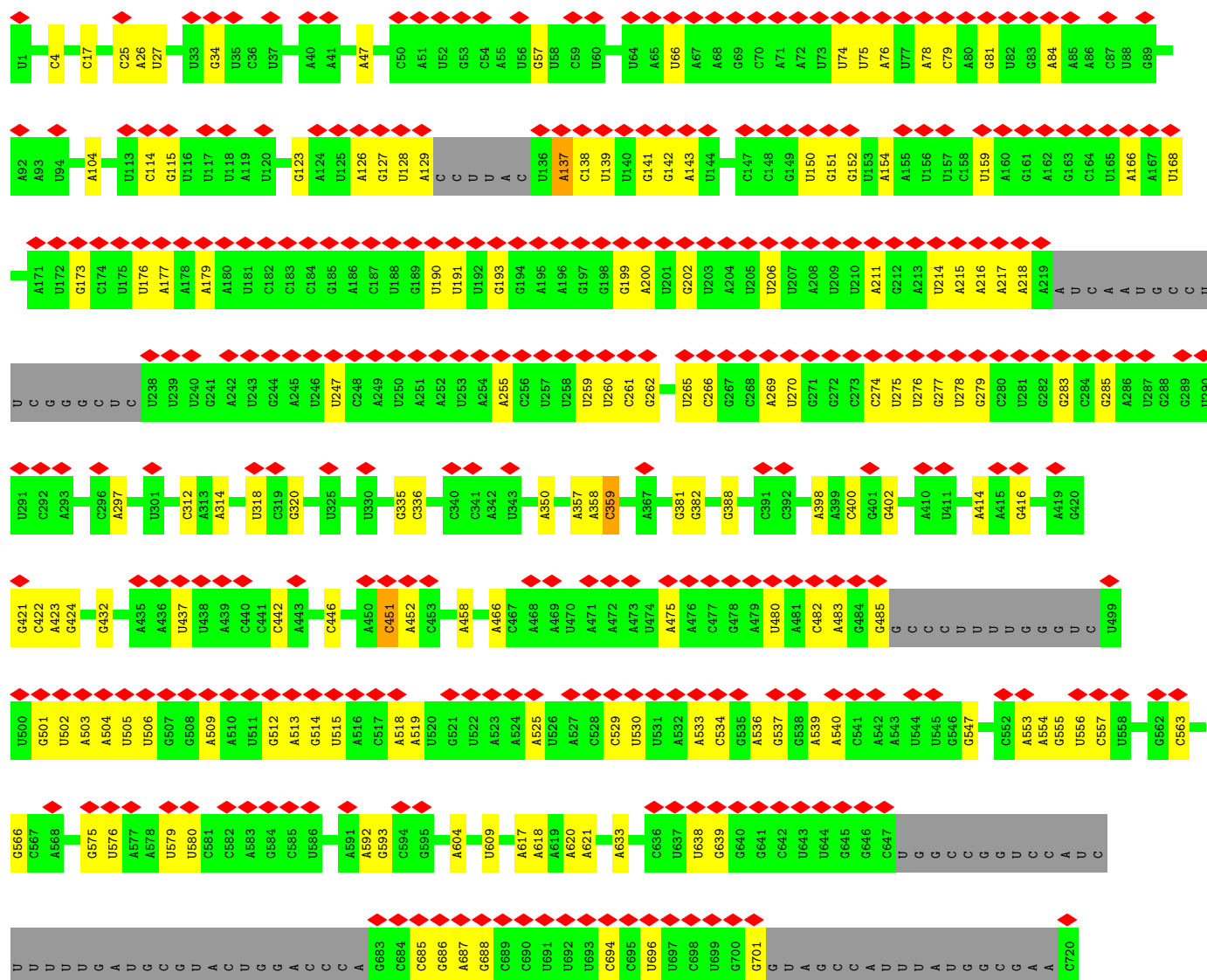




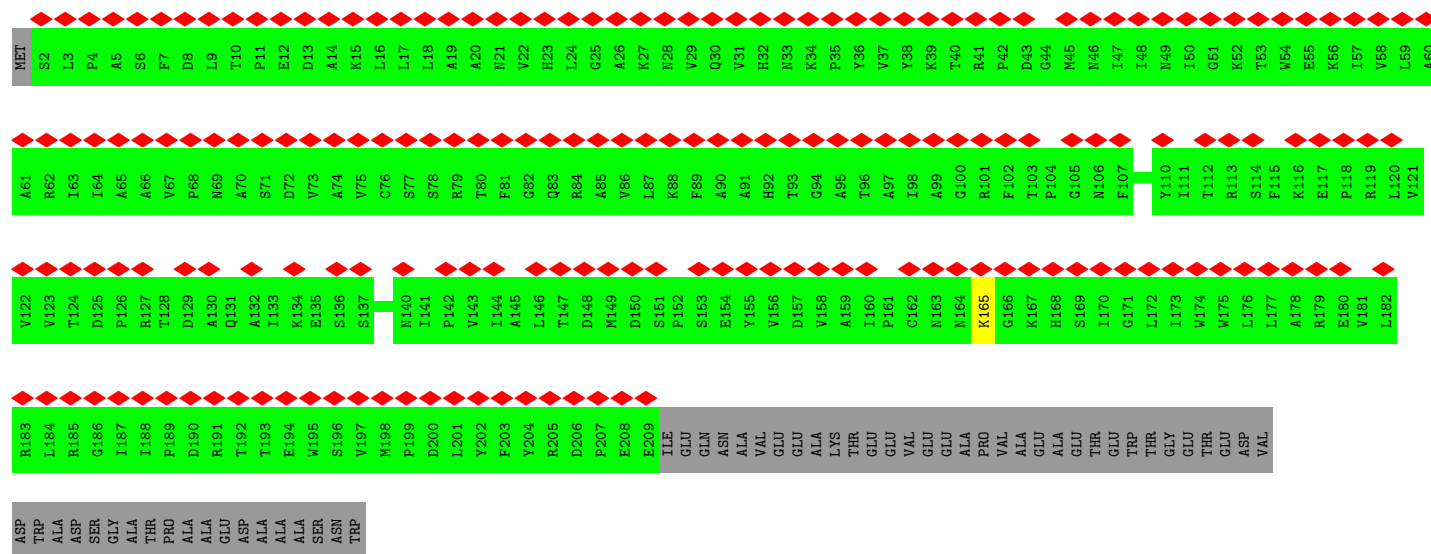
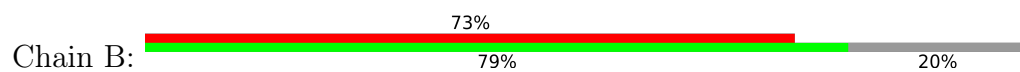
- Molecule 45: 60S ribosomal protein L43-A



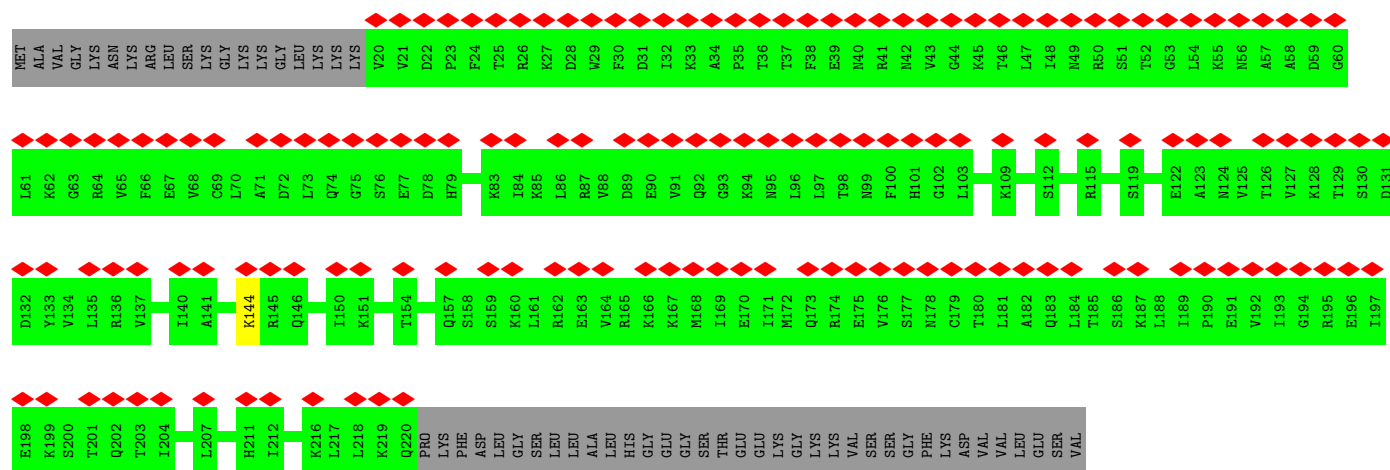
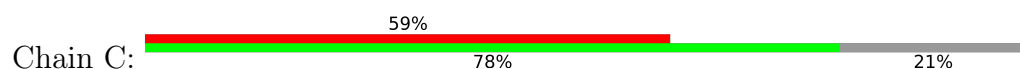
- Molecule 46: 18S ribosomal RNA



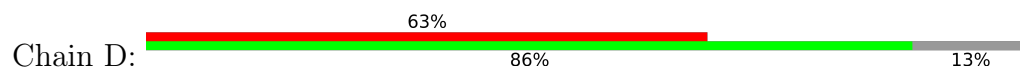


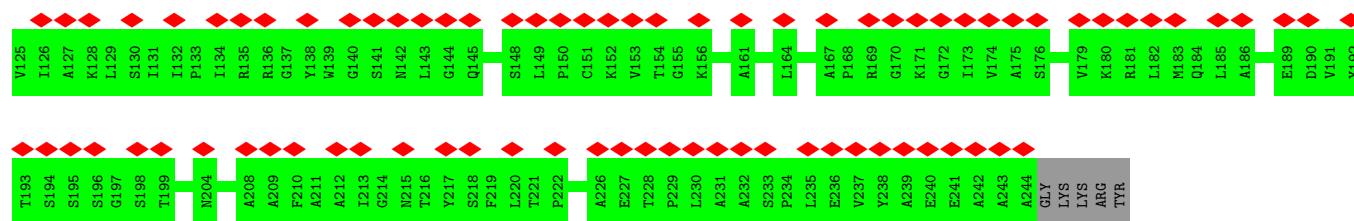


• Molecule 48: 40S ribosomal protein S1

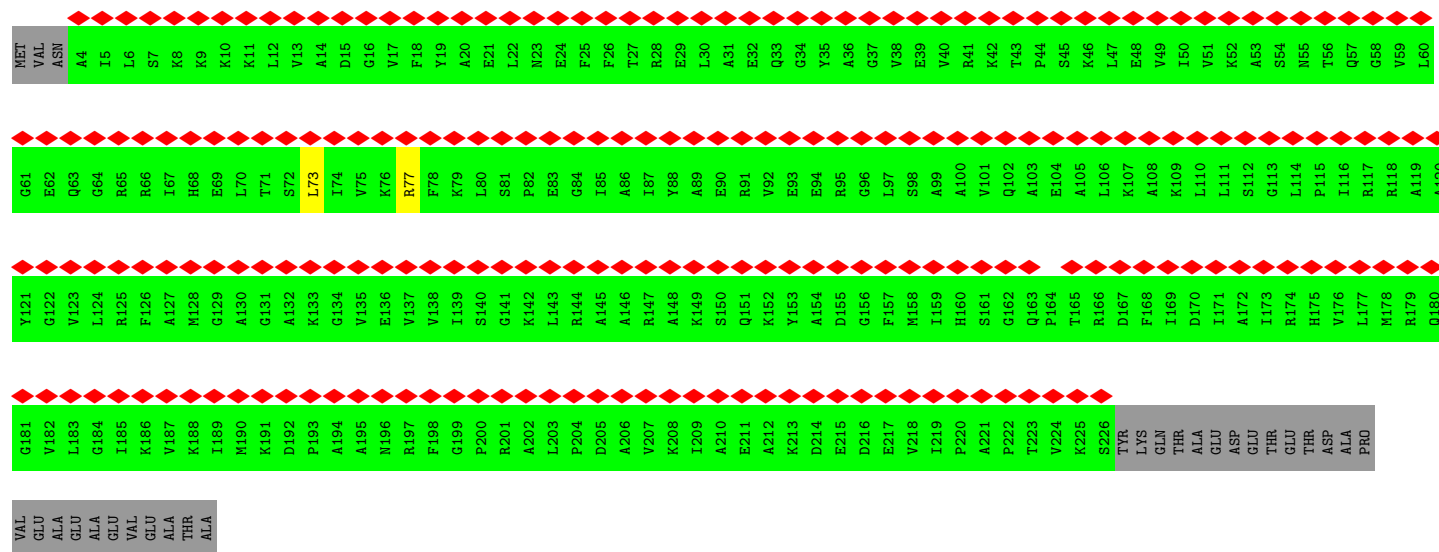
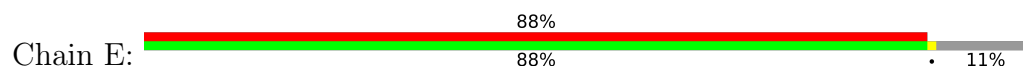


• Molecule 49: Ribosomal protein S5

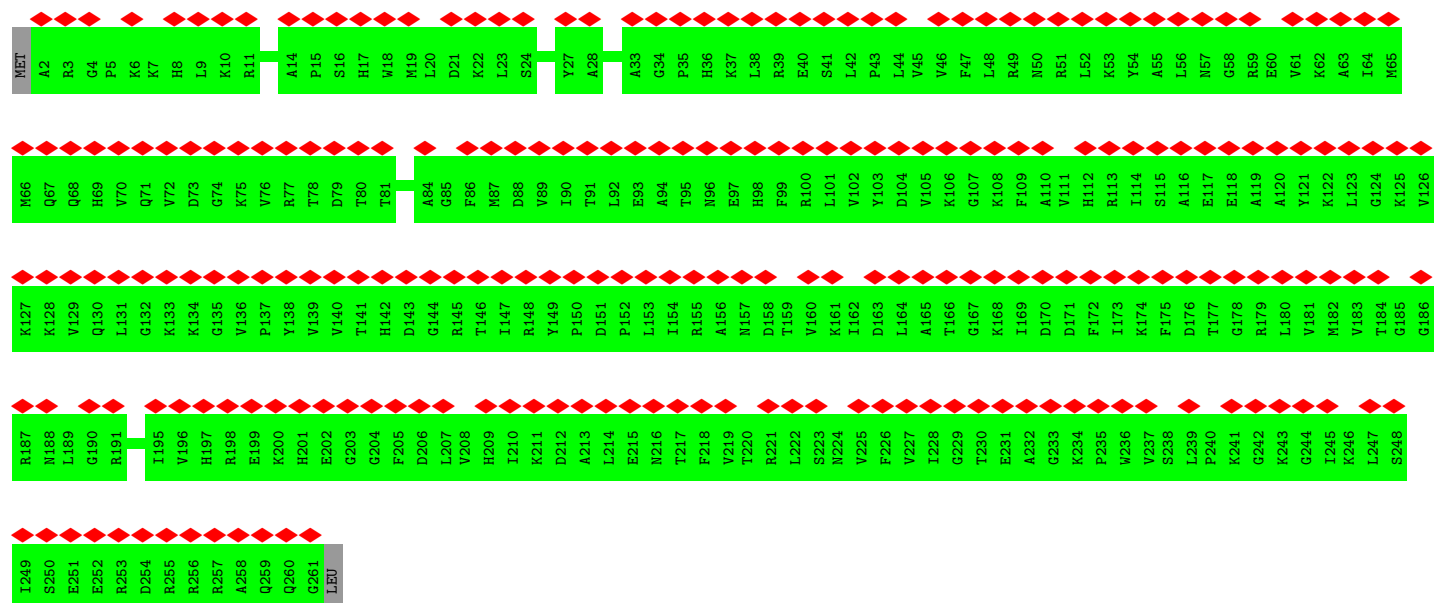
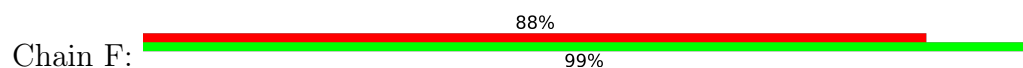




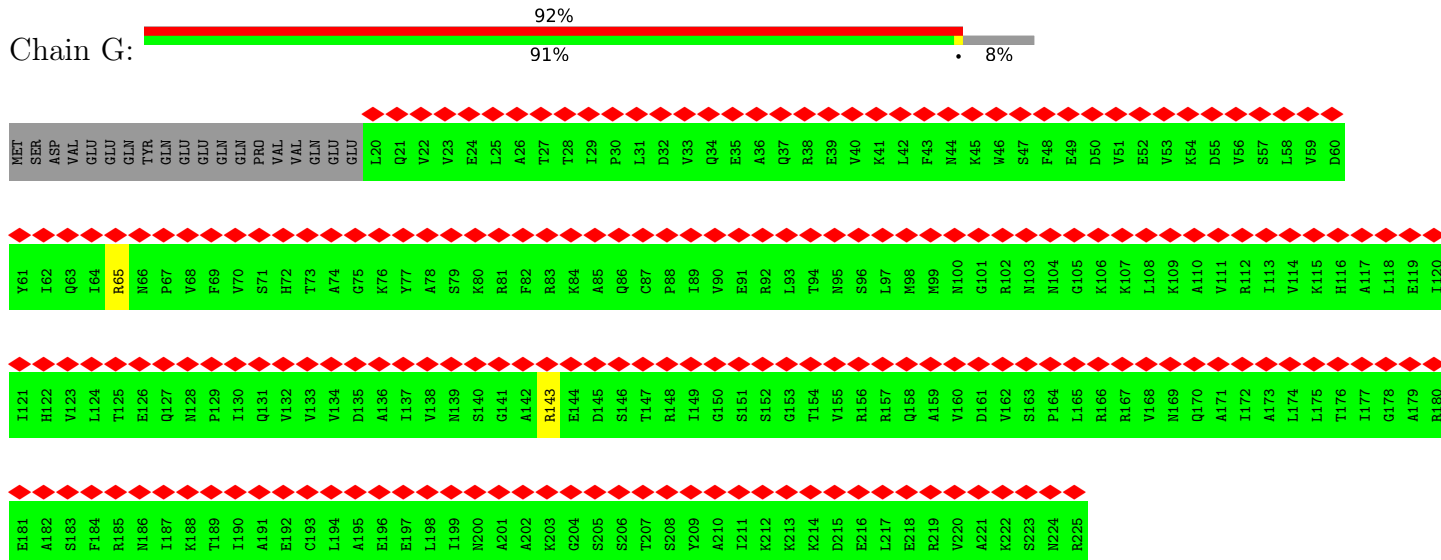
• Molecule 50: Ribosomal protein S3



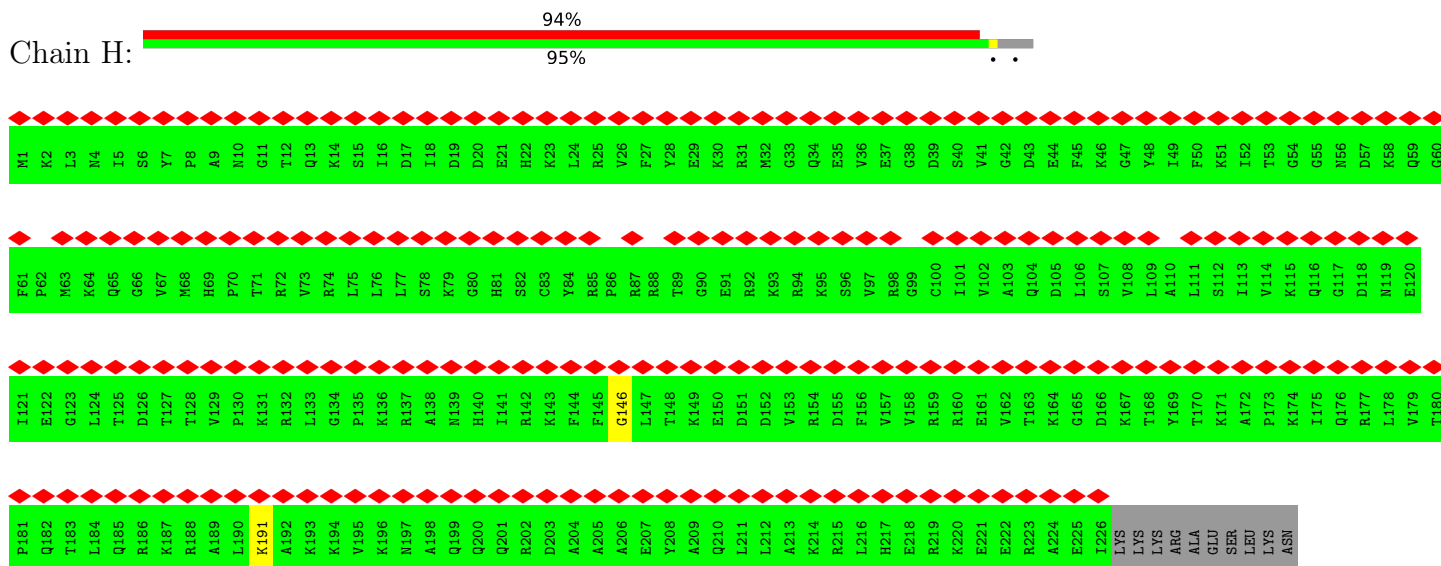
• Molecule 51: 40S ribosomal protein S4



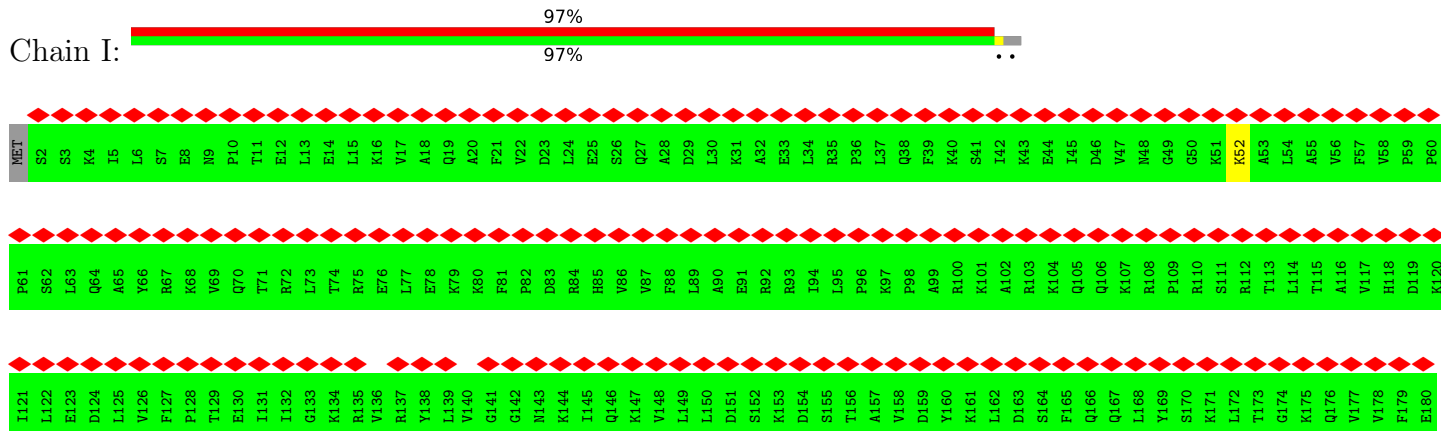
- Molecule 52: Ribosomal protein S7



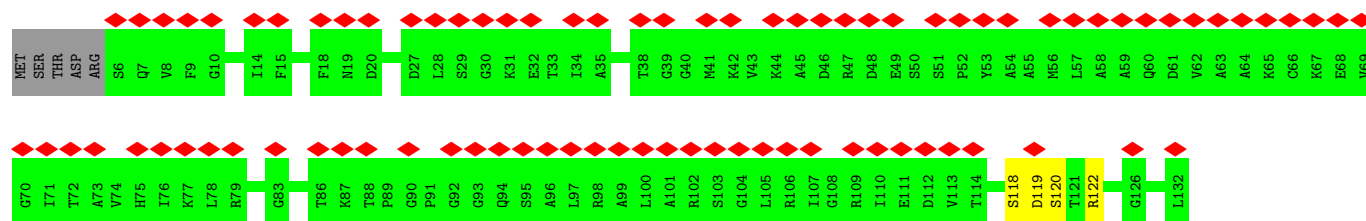
- Molecule 53: 40S ribosomal protein S6



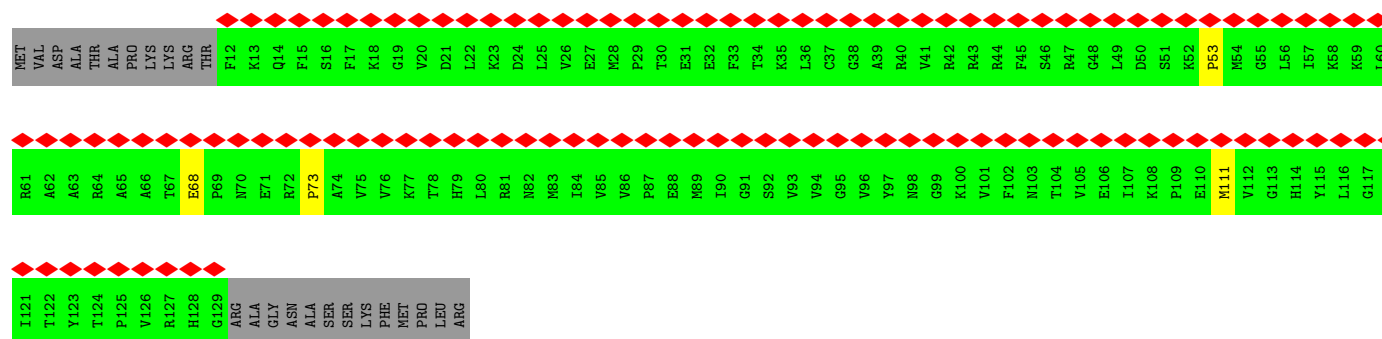
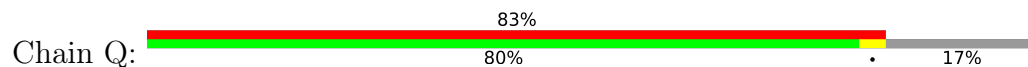
- Molecule 54: 40S ribosomal protein S7



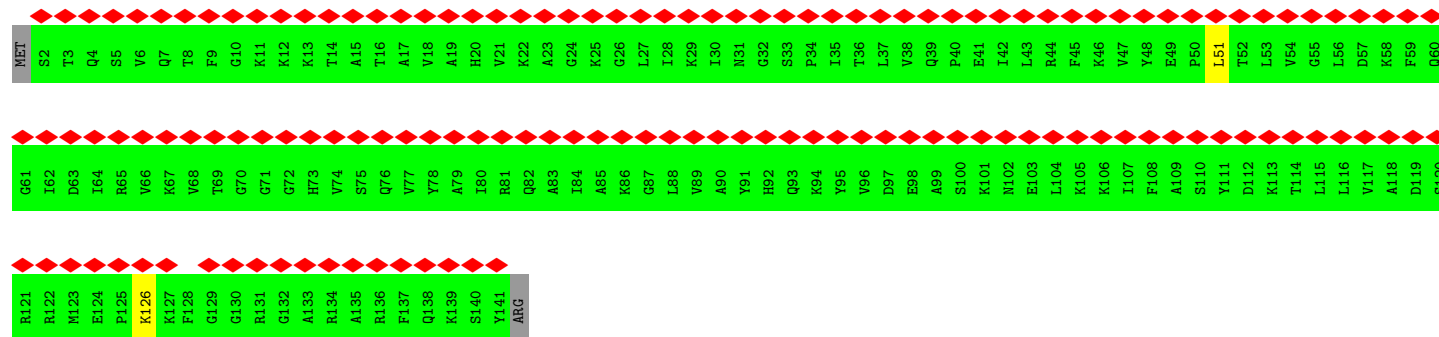




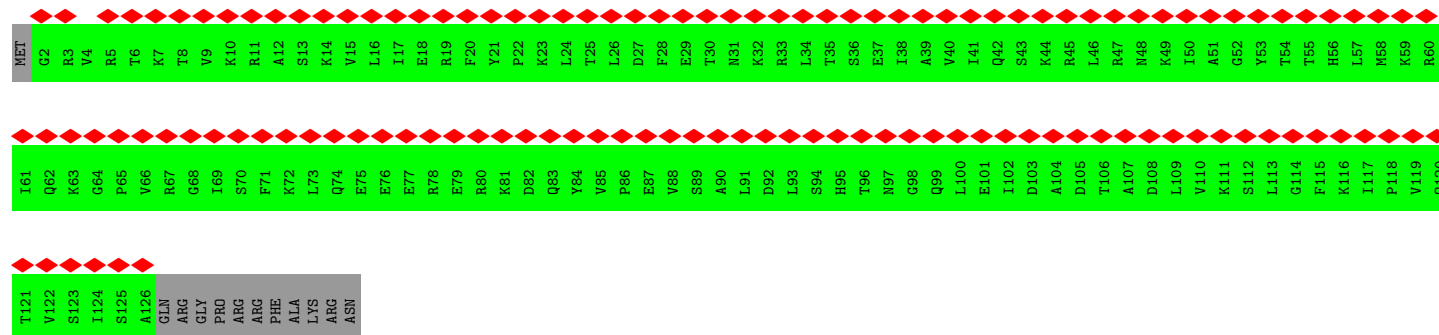
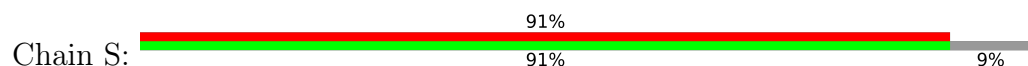
• Molecule 62: 40S ribosomal protein S15



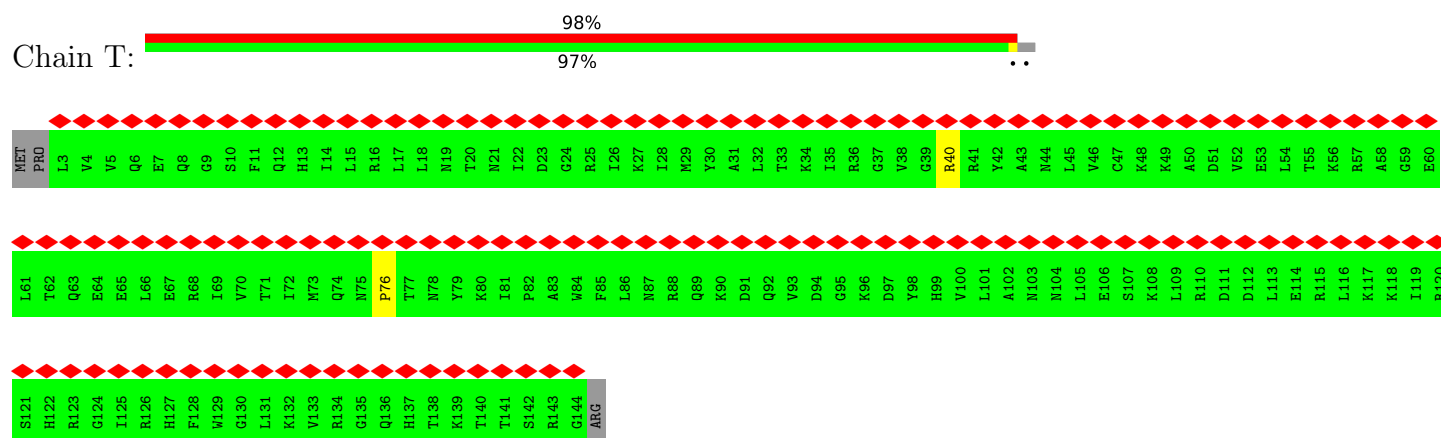
• Molecule 63: 40S ribosomal protein S16



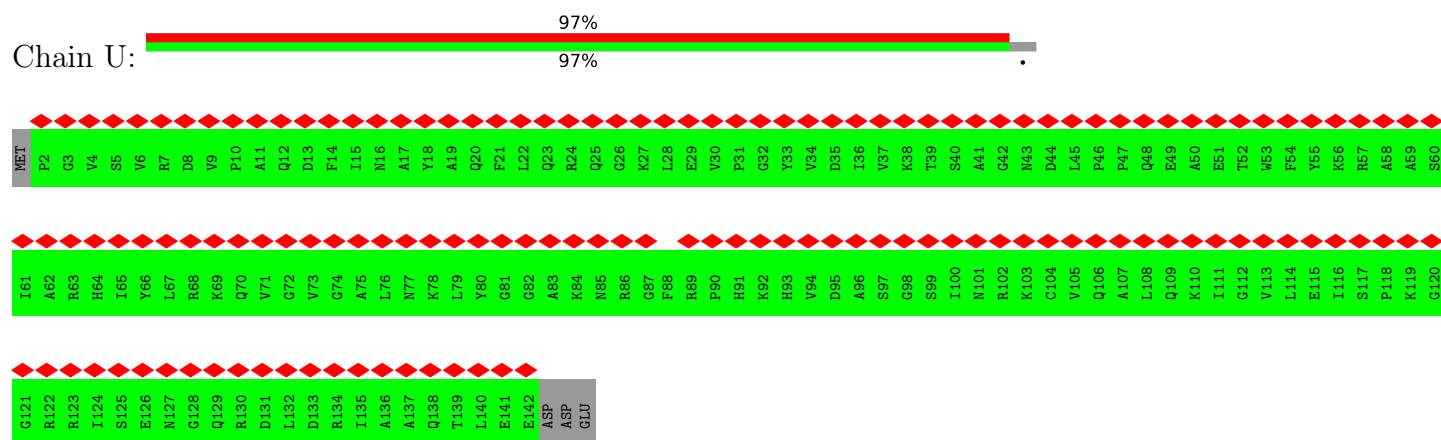
• Molecule 64: 40S ribosomal protein S17-B



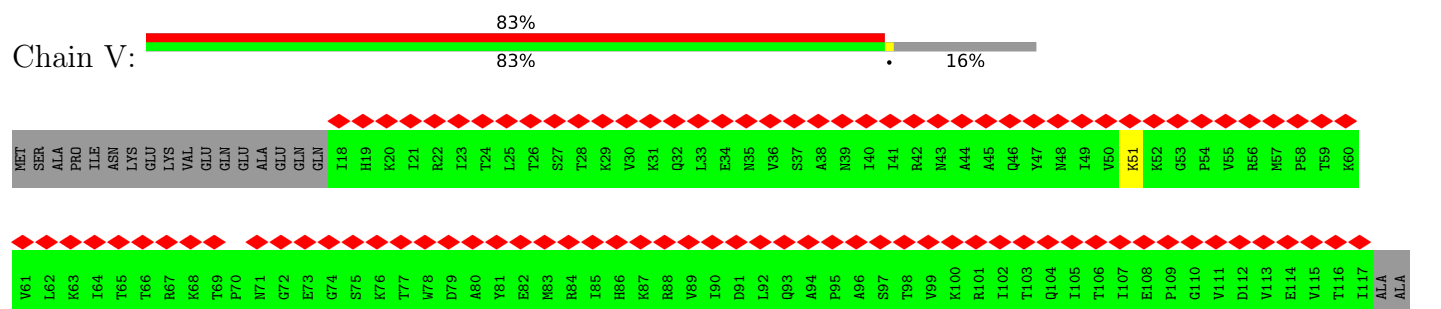
- Molecule 65: 40S ribosomal protein S18-B



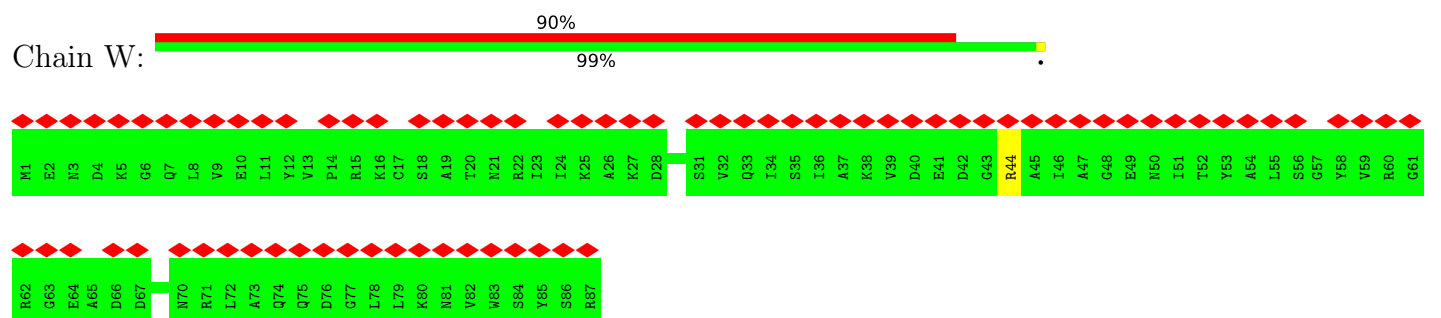
- Molecule 66: 40S ribosomal protein S19-A



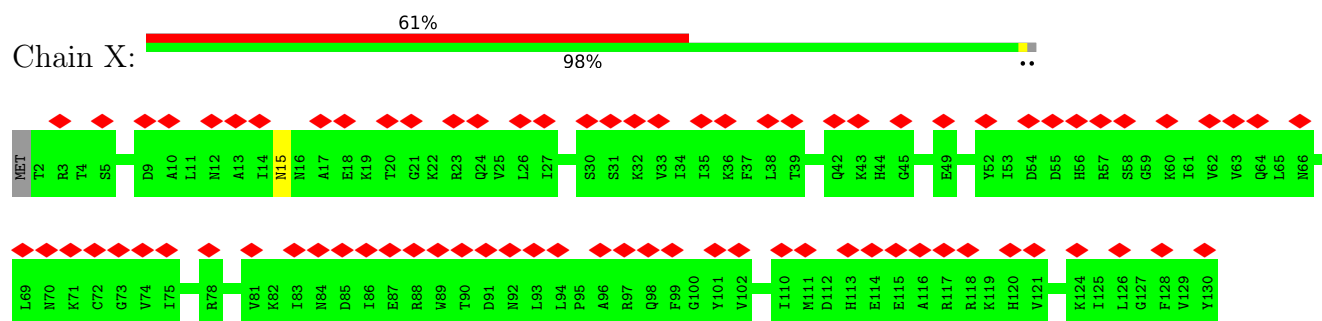
- Molecule 67: Ribosomal protein S10



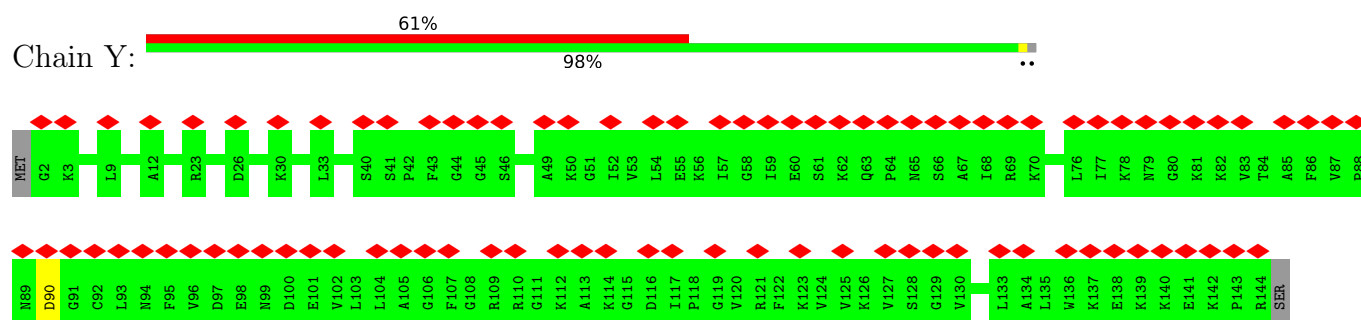
- Molecule 68: 40S ribosomal protein S21



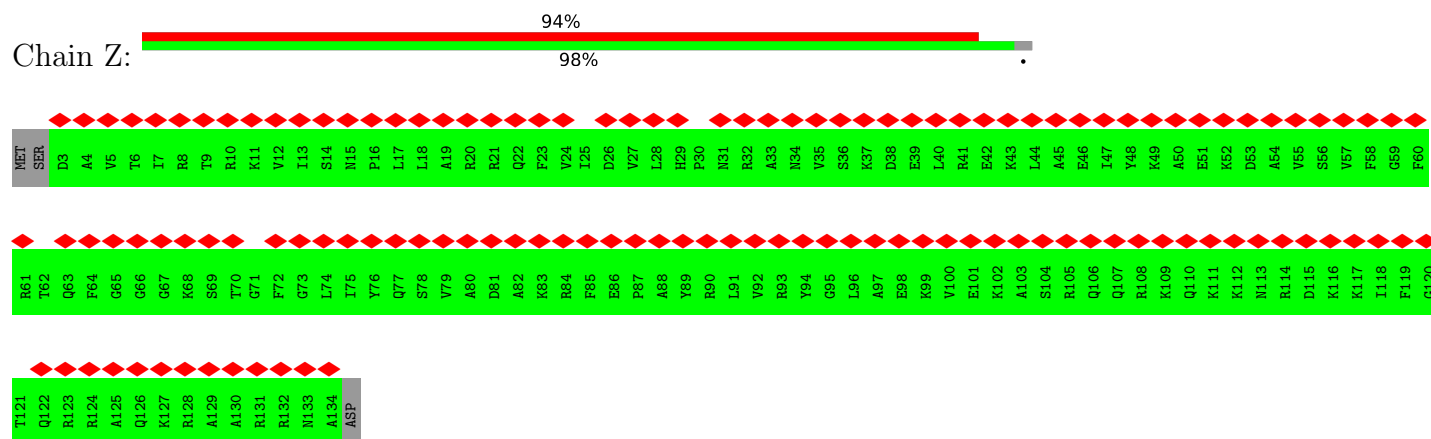
- Molecule 69: 40S ribosomal protein S22-A



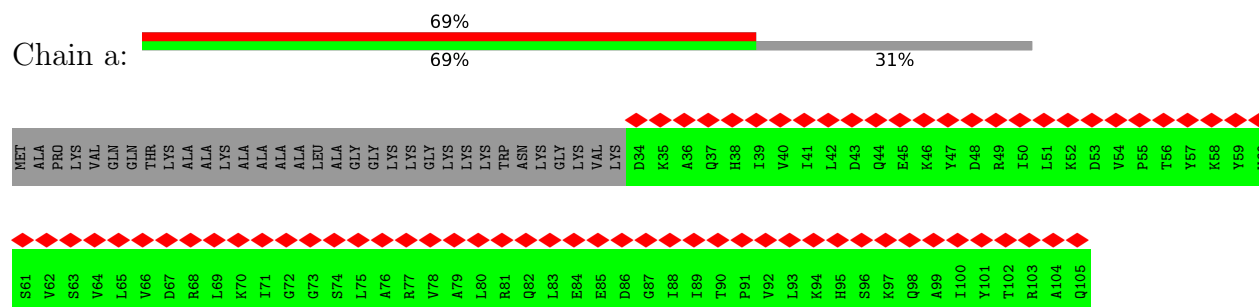
- Molecule 70: Ribosomal protein S23 (S12)



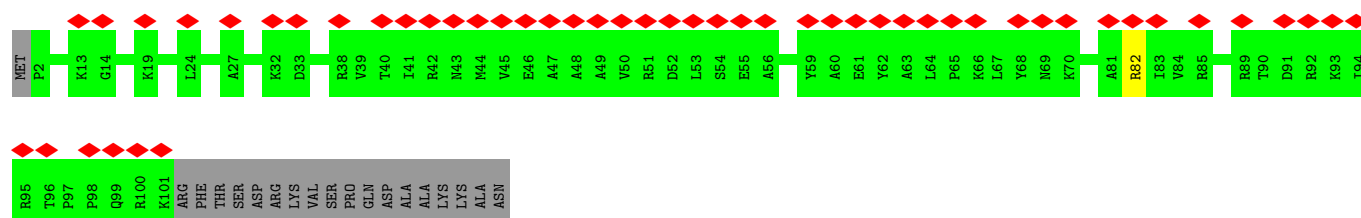
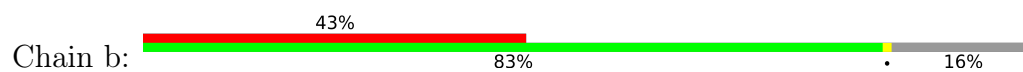
- Molecule 71: 40S ribosomal protein S24



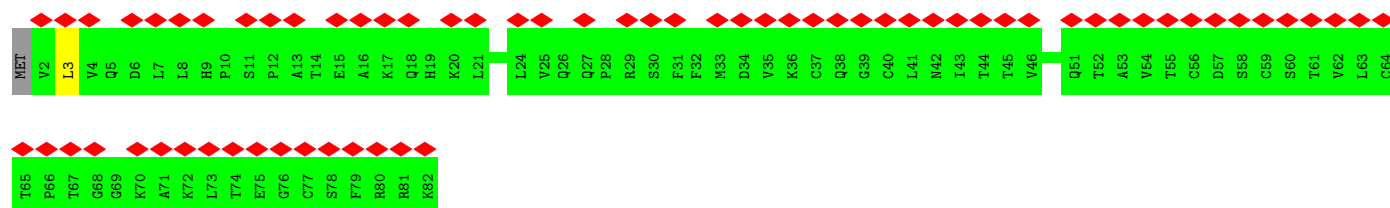
- Molecule 72: 40S ribosomal protein S25



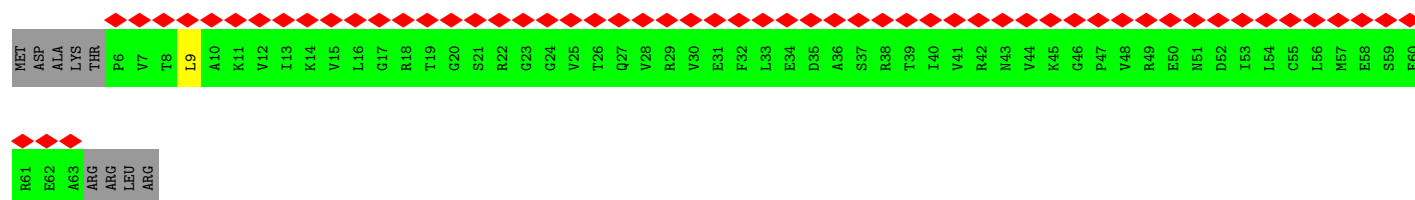
- Molecule 73: 40S ribosomal protein S26



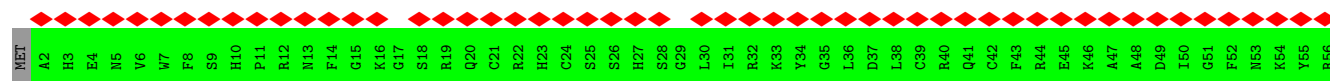
- Molecule 74: 40S ribosomal protein S27



- Molecule 75: 40S ribosomal protein S28-B



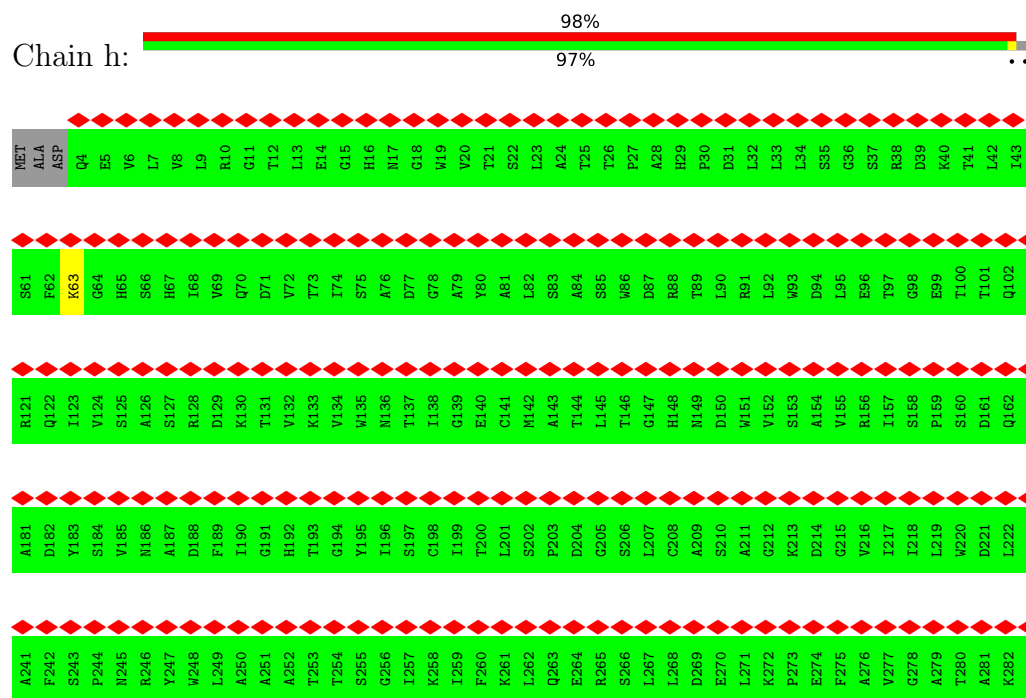
- Molecule 76: 40S ribosomal protein S29A



- Molecule 77: 40S ribosomal protein S30



- Molecule 78: Ubiquitin-40S ribosomal protein S31 fusion protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49801	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.3	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	16000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.644	Depositor
Minimum map value	-0.843	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.31	Depositor
Map size (\AA)	428.4, 428.4, 428.4	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.02, 1.02, 1.02	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: YMZ, SPK, MG, ZN

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	1	0.42	0/74794	0.84	62/116598 (0.1%)
2	3	0.36	0/2884	0.76	0/4492
3	4	0.39	0/3746	0.80	1/5832 (0.0%)
4	10	0.22	0/331	0.79	0/511
5	j	0.32	0/1922	0.59	0/2581
6	k	0.32	0/3156	0.58	0/4246
7	l	0.31	0/2799	0.56	0/3777
8	m	0.30	0/2447	0.56	0/3294
9	n	0.30	0/1249	0.56	0/1685
10	o	0.31	0/1918	0.50	0/2575
11	p	0.31	0/1961	0.54	0/2642
12	q	0.30	0/1537	0.58	0/2067
13	r	0.31	0/1724	0.58	0/2314
14	s	0.32	0/1395	0.67	0/1869
15	t	0.32	0/1637	0.60	0/2195
16	u	0.29	0/1044	0.56	0/1407
17	v	0.34	0/1753	0.60	0/2347
18	w	0.32	0/1620	0.54	0/2167
19	x	0.31	0/1398	0.61	1/1879 (0.1%)
20	y	0.30	0/1482	0.61	0/1985
21	z	0.34	0/1432	0.65	1/1905 (0.1%)
22	0	0.34	0/1474	0.59	0/1985
23	2	0.33	0/1285	0.55	0/1723
24	5	0.32	0/846	0.59	0/1140
25	6	0.33	0/993	0.59	0/1339
26	7	0.33	0/536	0.62	0/712
27	8	0.31	0/990	0.59	0/1337
28	9	0.31	0/999	0.58	0/1334
29	AA	0.30	0/1112	0.55	0/1488
30	AB	0.31	0/1199	0.54	0/1607
31	AC	0.33	0/522	0.66	1/692 (0.1%)
32	AD	0.33	0/738	0.57	0/994

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	AE	0.28	0/902	0.60	0/1212
34	AF	0.32	0/1030	0.56	0/1379
35	AG	0.33	0/875	0.55	0/1176
36	AH	0.32	0/896	0.59	0/1195
37	AI	0.29	0/1004	0.61	0/1337
38	AJ	0.29	0/780	0.61	0/1033
39	AK	0.29	0/690	0.63	0/916
40	AL	0.33	0/623	0.64	0/831
41	AM	0.29	0/447	0.62	0/594
42	AN	0.28	0/425	0.67	1/563 (0.2%)
43	AO	0.26	0/237	0.77	0/304
44	AP	0.32	0/840	0.58	0/1110
45	AQ	0.31	0/705	0.68	1/940 (0.1%)
46	A	0.29	0/39936	0.87	51/62224 (0.1%)
47	B	0.32	0/1666	0.65	0/2273
48	C	0.31	0/1651	0.67	0/2220
49	D	0.30	0/1648	0.63	0/2237
50	E	0.35	0/1731	0.70	1/2324 (0.0%)
51	F	0.32	0/2096	0.63	0/2822
52	G	0.35	0/1631	0.69	0/2199
53	H	0.27	0/1845	0.65	1/2464 (0.0%)
54	I	0.30	0/1490	0.69	0/2004
55	J	0.32	0/1472	0.71	0/1970
56	K	0.33	0/1478	0.66	0/1978
57	L	0.35	0/801	0.75	0/1081
58	M	0.29	0/1154	0.58	0/1553
59	N	0.35	0/892	0.90	4/1203 (0.3%)
60	O	0.31	0/1210	0.63	0/1631
61	P	0.34	0/953	0.72	0/1279
62	Q	0.36	0/954	0.77	2/1282 (0.2%)
63	R	0.31	0/1109	0.66	1/1486 (0.1%)
64	S	0.31	0/1014	0.71	0/1361
65	T	0.34	0/1186	0.73	2/1590 (0.1%)
66	U	0.33	0/1120	0.71	0/1508
67	V	0.35	0/800	0.67	0/1082
68	W	0.32	0/683	0.73	1/918 (0.1%)
69	X	0.31	0/1049	0.63	0/1412
70	Y	0.27	0/1128	0.63	0/1505
71	Z	0.30	0/1086	0.67	0/1447
72	a	0.33	0/585	0.62	0/789
73	b	0.28	0/811	0.65	0/1085
74	c	0.28	0/624	0.65	1/843 (0.1%)
75	d	0.33	0/448	0.77	1/601 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	e	0.34	0/466	0.65	0/620
77	f	0.28	0/381	0.65	1/505 (0.2%)
78	g	0.30	0/585	0.79	1/778 (0.1%)
79	h	0.31	0/2451	0.70	1/3337 (0.0%)
All	All	0.35	0/210511	0.77	136/308920 (0.0%)

There are no bond length outliers.

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2512	G	P-O3'-C3'	-12.24	105.02	119.70
1	1	2522	U	P-O3'-C3'	-11.93	105.38	119.70
1	1	2511	G	P-O3'-C3'	-11.38	106.04	119.70
1	1	2517	C	P-O3'-C3'	-10.88	106.65	119.70
1	1	2807	U	P-O3'-C3'	-9.72	108.04	119.70
1	1	2765	G	P-O3'-C3'	-9.35	108.48	119.70
1	1	2523	C	P-O3'-C3'	-8.89	109.03	119.70
1	1	2230	A	P-O3'-C3'	-8.88	109.04	119.70
46	A	1259	C	N1-C2-O2	8.76	124.16	118.90
1	1	2513	A	P-O3'-C3'	-8.68	109.28	119.70
1	1	2229	G	P-O3'-C3'	-8.57	109.42	119.70
1	1	436	A	P-O3'-C3'	-8.37	109.66	119.70
1	1	2521	C	P-O3'-C3'	-8.15	109.92	119.70
46	A	451	C	N1-C2-O2	8.09	123.75	118.90
46	A	1259	C	C2-N1-C1'	7.99	127.59	118.80
46	A	1468	C	N1-C2-O2	-7.83	114.20	118.90
46	A	451	C	C2-N1-C1'	7.53	127.08	118.80
74	c	3	LEU	CA-CB-CG	7.52	132.60	115.30
1	1	2764	A	P-O3'-C3'	-7.51	110.68	119.70
53	H	146	GLY	N-CA-C	7.51	131.87	113.10
1	1	2518	A	P-O3'-C3'	-7.41	110.81	119.70
46	A	275	U	C2-N1-C1'	7.40	126.58	117.70
1	1	2228	G	P-O3'-C3'	-7.39	110.83	119.70
1	1	2247	U	C2-N1-C1'	7.28	126.43	117.70
1	1	1225	G	N3-C4-N9	7.24	130.34	126.00
1	1	1265	U	N3-C2-O2	-7.16	117.19	122.20
1	1	1218	G	O4'-C1'-N9	7.15	113.92	108.20
46	A	275	U	N1-C2-O2	7.14	127.80	122.80
46	A	1375	C	C2-N1-C1'	7.07	126.57	118.80
46	A	1468	C	N3-C2-O2	7.05	126.83	121.90
45	AQ	89	LEU	CA-CB-CG	7.02	131.45	115.30
1	1	2808	C	P-O3'-C3'	-6.88	111.44	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2814	U	C2-N1-C1'	6.86	125.93	117.70
1	1	977	U	C2-N1-C1'	6.85	125.92	117.70
1	1	1225	G	N3-C4-C5	-6.83	125.18	128.60
46	A	451	C	N3-C2-O2	-6.81	117.13	121.90
46	A	1259	C	N3-C2-O2	-6.80	117.14	121.90
1	1	2247	U	N1-C2-O2	6.79	127.55	122.80
1	1	437	G	P-O3'-C3'	-6.78	111.56	119.70
46	A	824	U	C2-N1-C1'	6.77	125.82	117.70
1	1	918	U	C2-N1-C1'	6.76	125.81	117.70
62	Q	111	MET	CA-CB-CG	6.75	124.78	113.30
46	A	1468	C	O4'-C1'-N1	-6.74	102.81	108.20
1	1	3126	U	C2-N1-C1'	6.68	125.71	117.70
1	1	2247	U	N3-C2-O2	-6.67	117.53	122.20
46	A	1175	C	P-O3'-C3'	6.67	127.70	119.70
1	1	1265	U	C2-N1-C1'	6.67	125.70	117.70
63	R	51	LEU	CA-CB-CG	6.63	130.54	115.30
46	A	824	U	N1-C2-O2	6.62	127.43	122.80
46	A	1468	C	C4-C5-C6	-6.51	114.14	117.40
31	AC	24	PRO	CA-N-CD	-6.49	102.41	111.50
77	f	27	PRO	CA-N-CD	-6.47	102.44	111.50
46	A	1467	C	P-O3'-C3'	6.43	127.42	119.70
1	1	3182	C	N1-C2-O2	6.42	122.75	118.90
46	A	275	U	N3-C2-O2	-6.41	117.71	122.20
46	A	1242	U	C2-N1-C1'	6.40	125.38	117.70
3	4	39	G	O4'-C1'-N9	6.39	113.31	108.20
46	A	846	U	C2-N1-C1'	6.39	125.37	117.70
46	A	824	U	N3-C2-O2	-6.38	117.74	122.20
65	T	76	PRO	CA-N-CD	-6.33	102.63	111.50
1	1	1720	U	O4'-C1'-N1	6.33	113.26	108.20
1	1	1265	U	N1-C2-O2	6.30	127.21	122.80
1	1	2215	C	N3-C2-O2	-6.26	117.52	121.90
1	1	2814	U	N1-C2-O2	6.26	127.18	122.80
1	1	3182	C	C2-N1-C1'	6.20	125.62	118.80
46	A	1462	C	C2-N1-C1'	6.17	125.59	118.80
78	g	142	LEU	CA-CB-CG	6.16	129.46	115.30
1	1	2763	G	P-O3'-C3'	-6.14	112.34	119.70
79	h	120	LEU	CA-CB-CG	6.14	129.41	115.30
1	1	435	C	P-O3'-C3'	-6.12	112.36	119.70
1	1	1276	C	N3-C2-O2	-6.12	117.62	121.90
46	A	579	U	C2-N1-C1'	6.07	124.99	117.70
46	A	1242	U	N3-C2-O2	-5.97	118.02	122.20
1	1	2215	C	N1-C2-O2	5.93	122.46	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3126	U	N1-C2-O2	5.93	126.95	122.80
1	1	403	C	C6-N1-C2	-5.92	117.93	120.30
75	d	9	LEU	CA-CB-CG	5.89	128.86	115.30
46	A	1067	C	C2-N1-C1'	5.80	125.18	118.80
1	1	1225	G	C4-N9-C1'	5.74	133.96	126.50
46	A	1259	C	C6-N1-C1'	-5.71	113.95	120.80
1	1	977	U	N1-C2-O2	5.71	126.80	122.80
59	N	62	LEU	CA-CB-CG	5.67	128.33	115.30
46	A	1067	C	N1-C2-O2	5.66	122.30	118.90
1	1	977	U	N3-C2-O2	-5.62	118.27	122.20
46	A	359	C	C6-N1-C2	-5.60	118.06	120.30
1	1	1099	A	OP2-P-O3'	5.60	117.52	105.20
46	A	4	C	C2-N1-C1'	5.56	124.92	118.80
65	T	76	PRO	N-CD-CG	-5.53	94.90	103.20
46	A	1520	C	N3-C2-O2	-5.53	118.03	121.90
1	1	2814	U	N3-C2-O2	-5.52	118.34	122.20
1	1	1263	U	O4'-C1'-N1	5.52	112.61	108.20
50	E	73	LEU	CA-CB-CG	5.51	127.98	115.30
1	1	1492	C	C2-N1-C1'	5.50	124.85	118.80
1	1	2510	U	P-O3'-C3'	-5.49	113.11	119.70
1	1	3126	U	N3-C2-O2	-5.46	118.38	122.20
46	A	451	C	C6-N1-C2	-5.42	118.13	120.30
46	A	1444	G	C4-N9-C1'	5.41	133.53	126.50
59	N	28	LEU	CA-CB-CG	5.39	127.71	115.30
46	A	827	C	C2-N1-C1'	5.38	124.71	118.80
1	1	2514	G	P-O3'-C3'	-5.38	113.25	119.70
1	1	3030	U	C2-N1-C1'	5.37	124.14	117.70
1	1	918	U	N1-C2-O2	5.36	126.55	122.80
59	N	95	LYS	C-N-CA	5.35	135.08	121.70
1	1	2520	A	P-O3'-C3'	-5.29	113.35	119.70
46	A	382	G	N3-C4-N9	-5.23	122.86	126.00
46	A	1327	C	C2-N1-C1'	5.23	124.55	118.80
46	A	359	C	N3-C2-O2	-5.22	118.25	121.90
46	A	1444	G	N3-C4-N9	5.22	129.13	126.00
46	A	359	C	N1-C2-O2	-5.22	115.77	118.90
46	A	846	U	C6-N1-C1'	-5.20	113.92	121.20
46	A	359	C	C6-N1-C1'	5.19	127.03	120.80
1	1	406	G	O4'-C1'-N9	5.19	112.35	108.20
1	1	2766	G	P-O3'-C3'	-5.19	113.47	119.70
1	1	1197	C	N1-C2-O2	5.18	122.01	118.90
46	A	579	U	N1-C2-O2	5.17	126.42	122.80
46	A	1327	C	N1-C2-O2	5.16	122.00	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2968	U	C2-N1-C1'	5.16	123.89	117.70
62	Q	53	PRO	CA-N-CD	-5.15	104.29	111.50
1	1	956	U	C2-N1-C1'	5.14	123.87	117.70
1	1	2509	C	C2-N1-C1'	5.14	124.46	118.80
46	A	381	G	N3-C4-C5	-5.14	126.03	128.60
46	A	1547	U	N3-C2-O2	-5.14	118.61	122.20
46	A	1375	C	C6-N1-C1'	-5.13	114.64	120.80
59	N	74	LEU	CA-CB-CG	5.12	127.08	115.30
68	W	44	ARG	CB-CG-CD	5.12	124.92	111.60
46	A	1242	U	N1-C2-O2	5.11	126.38	122.80
21	z	171	GLU	N-CA-CB	5.10	119.78	110.60
19	x	148	LEU	CA-CB-CG	5.09	127.00	115.30
1	1	2516	U	P-O3'-C3'	-5.09	113.59	119.70
42	AN	27	LEU	CA-CB-CG	5.09	127.00	115.30
46	A	451	C	C6-N1-C1'	-5.09	114.69	120.80
46	A	1375	C	N1-C2-O2	5.08	121.95	118.90
46	A	137	A	P-O3'-C3'	5.05	125.77	119.70
46	A	1237	C	C2-N1-C1'	5.04	124.35	118.80
46	A	275	U	C6-N1-C1'	-5.02	114.18	121.20
1	1	1273	C	N3-C2-O2	-5.01	118.39	121.90

There are no chirality outliers.

There are no planarity outliers.

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	
5	j	247/254 (97%)	238 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	k	385/389 (99%)	373 (97%)	12 (3%)	0	100	100
7	l	359/363 (99%)	350 (98%)	9 (2%)	0	100	100
8	m	290/298 (97%)	280 (97%)	10 (3%)	0	100	100
9	n	151/176 (86%)	149 (99%)	2 (1%)	0	100	100
10	o	232/241 (96%)	226 (97%)	6 (3%)	0	100	100
11	p	247/262 (94%)	236 (96%)	10 (4%)	1 (0%)	30	63
12	q	188/191 (98%)	184 (98%)	4 (2%)	0	100	100
13	r	204/220 (93%)	202 (99%)	2 (1%)	0	100	100
14	s	170/174 (98%)	166 (98%)	4 (2%)	0	100	100
15	t	198/202 (98%)	194 (98%)	2 (1%)	2 (1%)	13	42
16	u	128/131 (98%)	124 (97%)	4 (3%)	0	100	100
17	v	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
18	w	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
19	x	168/185 (91%)	165 (98%)	3 (2%)	0	100	100
20	y	183/186 (98%)	178 (97%)	5 (3%)	0	100	100
21	z	172/190 (90%)	165 (96%)	4 (2%)	3 (2%)	7	30
22	0	170/172 (99%)	169 (99%)	1 (1%)	0	100	100
23	2	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
24	5	101/124 (82%)	96 (95%)	4 (4%)	1 (1%)	13	42
25	6	129/137 (94%)	124 (96%)	5 (4%)	0	100	100
26	7	61/155 (39%)	61 (100%)	0	0	100	100
27	8	119/142 (84%)	119 (100%)	0	0	100	100
28	9	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
29	AA	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
30	AB	146/149 (98%)	139 (95%)	7 (5%)	0	100	100
31	AC	62/63 (98%)	61 (98%)	1 (2%)	0	100	100
32	AD	94/106 (89%)	93 (99%)	1 (1%)	0	100	100
33	AE	107/112 (96%)	106 (99%)	1 (1%)	0	100	100
34	AF	123/131 (94%)	122 (99%)	1 (1%)	0	100	100
35	AG	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
36	AH	110/122 (90%)	107 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	AI	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
38	AJ	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
39	AK	84/90 (93%)	81 (96%)	3 (4%)	0	100	100
40	AL	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
41	AM	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
42	AN	50/52 (96%)	50 (100%)	0	0	100	100
43	AO	23/25 (92%)	23 (100%)	0	0	100	100
44	AP	101/106 (95%)	99 (98%)	2 (2%)	0	100	100
45	AQ	89/92 (97%)	79 (89%)	6 (7%)	4 (4%)	2	12
47	B	206/261 (79%)	201 (98%)	5 (2%)	0	100	100
48	C	199/256 (78%)	194 (98%)	5 (2%)	0	100	100
49	D	214/249 (86%)	209 (98%)	5 (2%)	0	100	100
50	E	221/251 (88%)	215 (97%)	6 (3%)	0	100	100
51	F	258/262 (98%)	255 (99%)	3 (1%)	0	100	100
52	G	204/225 (91%)	196 (96%)	8 (4%)	0	100	100
53	H	224/236 (95%)	219 (98%)	5 (2%)	0	100	100
54	I	180/186 (97%)	175 (97%)	5 (3%)	0	100	100
55	J	180/206 (87%)	179 (99%)	1 (1%)	0	100	100
56	K	176/189 (93%)	174 (99%)	2 (1%)	0	100	100
57	L	91/118 (77%)	84 (92%)	6 (7%)	1 (1%)	12	39
58	M	139/155 (90%)	136 (98%)	3 (2%)	0	100	100
59	N	114/143 (80%)	98 (86%)	16 (14%)	0	100	100
60	O	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
61	P	125/132 (95%)	118 (94%)	4 (3%)	3 (2%)	5	22
62	Q	116/142 (82%)	106 (91%)	8 (7%)	2 (2%)	7	30
63	R	138/142 (97%)	134 (97%)	4 (3%)	0	100	100
64	S	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
65	T	140/145 (97%)	134 (96%)	6 (4%)	0	100	100
66	U	139/145 (96%)	137 (99%)	2 (1%)	0	100	100
67	V	98/119 (82%)	96 (98%)	2 (2%)	0	100	100
68	W	85/87 (98%)	83 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	X	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
70	Y	141/145 (97%)	139 (99%)	1 (1%)	1 (1%)	19	51
71	Z	130/135 (96%)	130 (100%)	0	0	100	100
72	a	70/105 (67%)	69 (99%)	1 (1%)	0	100	100
73	b	98/119 (82%)	95 (97%)	3 (3%)	0	100	100
74	c	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
75	d	56/67 (84%)	51 (91%)	5 (9%)	0	100	100
76	e	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
77	f	43/63 (68%)	39 (91%)	4 (9%)	0	100	100
78	g	68/193 (35%)	62 (91%)	6 (9%)	0	100	100
79	h	309/317 (98%)	293 (95%)	16 (5%)	0	100	100
All	All	10838/11871 (91%)	10531 (97%)	289 (3%)	18 (0%)	45	74

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	p	9	ALA
15	t	5	LYS
15	t	63	VAL
21	z	152	GLU
21	z	151	ARG
45	AQ	88	GLU
57	L	88	PRO
61	P	118	SER
61	P	120	SER
61	P	122	ARG
21	z	153	LYS
24	5	20	ALA
45	AQ	85	ARG
70	Y	90	ASP
45	AQ	86	LEU
62	Q	73	PRO
45	AQ	87	ARG
62	Q	68	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	j	190/194 (98%)	190 (100%)	0	100	100
6	k	326/328 (99%)	326 (100%)	0	100	100
7	l	290/292 (99%)	290 (100%)	0	100	100
8	m	247/252 (98%)	247 (100%)	0	100	100
9	n	134/154 (87%)	134 (100%)	0	100	100
10	o	198/204 (97%)	198 (100%)	0	100	100
11	p	207/216 (96%)	205 (99%)	2 (1%)	73	86
12	q	169/170 (99%)	168 (99%)	1 (1%)	84	91
13	r	178/186 (96%)	178 (100%)	0	100	100
14	s	147/149 (99%)	146 (99%)	1 (1%)	81	90
15	t	166/168 (99%)	166 (100%)	0	100	100
16	u	108/109 (99%)	108 (100%)	0	100	100
17	v	177/178 (99%)	177 (100%)	0	100	100
18	w	166/167 (99%)	166 (100%)	0	100	100
19	x	142/154 (92%)	142 (100%)	0	100	100
20	y	153/154 (99%)	153 (100%)	0	100	100
21	z	142/153 (93%)	140 (99%)	2 (1%)	62	81
22	0	157/157 (100%)	157 (100%)	0	100	100
23	2	133/134 (99%)	132 (99%)	1 (1%)	79	89
24	5	93/112 (83%)	90 (97%)	3 (3%)	34	63
25	6	101/104 (97%)	100 (99%)	1 (1%)	73	86
26	7	57/127 (45%)	57 (100%)	0	100	100
27	8	108/121 (89%)	108 (100%)	0	100	100
28	9	111/112 (99%)	109 (98%)	2 (2%)	54	76
29	AA	117/118 (99%)	117 (100%)	0	100	100
30	AB	120/121 (99%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	AC	50/49 (102%)	48 (96%)	2 (4%)	27	58
32	AD	81/90 (90%)	81 (100%)	0	100	100
33	AE	98/100 (98%)	97 (99%)	1 (1%)	73	86
34	AF	110/115 (96%)	110 (100%)	0	100	100
35	AG	92/92 (100%)	91 (99%)	1 (1%)	70	84
36	AH	95/102 (93%)	94 (99%)	1 (1%)	70	84
37	AI	106/106 (100%)	106 (100%)	0	100	100
38	AJ	79/79 (100%)	78 (99%)	1 (1%)	65	82
39	AK	70/73 (96%)	70 (100%)	0	100	100
40	AL	68/69 (99%)	68 (100%)	0	100	100
41	AM	46/47 (98%)	45 (98%)	1 (2%)	47	71
42	AN	47/47 (100%)	47 (100%)	0	100	100
43	AO	24/24 (100%)	24 (100%)	0	100	100
44	AP	88/91 (97%)	85 (97%)	3 (3%)	32	62
45	AQ	72/73 (99%)	71 (99%)	1 (1%)	62	81
47	B	176/215 (82%)	175 (99%)	1 (1%)	84	91
48	C	184/229 (80%)	183 (100%)	1 (0%)	86	92
49	D	174/198 (88%)	173 (99%)	1 (1%)	84	91
50	E	174/196 (89%)	173 (99%)	1 (1%)	84	91
51	F	218/220 (99%)	218 (100%)	0	100	100
52	G	178/197 (90%)	176 (99%)	2 (1%)	70	84
53	H	195/204 (96%)	194 (100%)	1 (0%)	86	92
54	I	163/167 (98%)	162 (99%)	1 (1%)	84	91
55	J	147/160 (92%)	146 (99%)	1 (1%)	81	90
56	K	153/160 (96%)	153 (100%)	0	100	100
57	L	87/104 (84%)	87 (100%)	0	100	100
58	M	122/134 (91%)	121 (99%)	1 (1%)	79	89
59	N	98/123 (80%)	98 (100%)	0	100	100
60	O	129/130 (99%)	128 (99%)	1 (1%)	79	89
61	P	97/102 (95%)	96 (99%)	1 (1%)	73	86
62	Q	102/121 (84%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	R	114/116 (98%)	113 (99%)	1 (1%)	75	88
64	S	112/122 (92%)	112 (100%)	0	100	100
65	T	126/129 (98%)	125 (99%)	1 (1%)	79	89
66	U	113/117 (97%)	113 (100%)	0	100	100
67	V	90/105 (86%)	89 (99%)	1 (1%)	70	84
68	W	71/71 (100%)	71 (100%)	0	100	100
69	X	112/113 (99%)	111 (99%)	1 (1%)	75	88
70	Y	116/118 (98%)	116 (100%)	0	100	100
71	Z	109/112 (97%)	109 (100%)	0	100	100
72	a	64/85 (75%)	64 (100%)	0	100	100
73	b	86/102 (84%)	85 (99%)	1 (1%)	67	83
74	c	72/73 (99%)	72 (100%)	0	100	100
75	d	50/58 (86%)	50 (100%)	0	100	100
76	e	47/48 (98%)	47 (100%)	0	100	100
77	f	40/54 (74%)	40 (100%)	0	100	100
78	g	62/175 (35%)	61 (98%)	1 (2%)	58	79
79	h	259/263 (98%)	258 (100%)	1 (0%)	89	94
All	All	9303/10012 (93%)	9260 (100%)	43 (0%)	85	92

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	p	7	LYS
11	p	13	LEU
12	q	141	LYS
14	s	94	LYS
21	z	152	GLU
21	z	153	LYS
23	2	83	ARG
24	5	30	GLN
24	5	31	GLU
24	5	93	ARG
25	6	110	LYS
28	9	3	LYS
28	9	69	LYS
31	AC	14[A]	ARG

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Mol	Chain	Res	Type
31	AC	14[B]	ARG
33	AE	101	LYS
35	AG	48	ARG
36	AH	29	LYS
38	AJ	98	ARG
41	AM	21	ARG
44	AP	40	LYS
44	AP	55	LYS
44	AP	56	GLN
45	AQ	86	LEU
47	B	165	LYS
48	C	144	LYS
49	D	103	ASN
50	E	77	ARG
52	G	65	ARG
52	G	143	ARG
53	H	191	LYS
54	I	52	LYS
55	J	144	LYS
58	M	67	ARG
60	O	106	ARG
61	P	119	ASP
63	R	126	LYS
65	T	40	ARG
67	V	51	LYS
69	X	15	ASN
73	b	82	ARG
78	g	125	LYS
79	h	63	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
5	j	132	ASN
14	s	90	GLN
14	s	95	ASN
15	t	66	ASN
23	2	112	ASN
28	9	41	GLN
40	AL	28	ASN
40	AL	40	GLN
45	AQ	25	GLN

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Mol	Chain	Res	Type
47	B	33	ASN
51	F	197	HIS
52	G	63	GLN
54	I	38	GLN
54	I	106	GLN
64	S	31	ASN
64	S	97	ASN
64	S	120	GLN
65	T	89	GLN
65	T	136	GLN
68	W	75	GLN
79	h	16	HIS
79	h	67	HIS
79	h	102	GLN
79	h	297	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3121/3359 (92%)	543 (17%)	35 (1%)
2	3	120/121 (99%)	9 (7%)	0
3	4	157/158 (99%)	23 (14%)	3 (1%)
4	10	12/76 (15%)	2 (16%)	0
46	A	1667/1787 (93%)	383 (22%)	43 (2%)
All	All	5077/5501 (92%)	960 (18%)	81 (1%)

All (960) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	24	U
1	1	25	A
1	1	29	G
1	1	39	A
1	1	42	A
1	1	48	A
1	1	56	A
1	1	58	G
1	1	59	A
1	1	64	A
1	1	65	A
1	1	91	G

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Mol	Chain	Res	Type
1	1	98	A
1	1	104	C
1	1	108	A
1	1	109	G
1	1	110	C
1	1	121	A
1	1	135	G
1	1	155	A
1	1	156	A
1	1	164	U
1	1	169	G
1	1	172	C
1	1	173	C
1	1	175	G
1	1	186	A
1	1	189	U
1	1	190	U
1	1	199	C
1	1	205	G
1	1	209	C
1	1	212	A
1	1	217	G
1	1	218	A
1	1	219	G
1	1	230	G
1	1	236	A
1	1	239	A
1	1	240	C
1	1	243	G
1	1	245	G
1	1	249	G
1	1	250	U
1	1	269	G
1	1	286	U
1	1	295	A
1	1	305	U
1	1	311	C
1	1	323	A
1	1	329	U
1	1	337	G
1	1	338	A
1	1	339	C

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Mol	Chain	Res	Type
1	1	349	A
1	1	350	C
1	1	376	G
1	1	377	A
1	1	395	A
1	1	398	A
1	1	402	A
1	1	403	C
1	1	404	G
1	1	420	G
1	1	421	G
1	1	422	A
1	1	438	A
1	1	439	C
1	1	506	A
1	1	517	A
1	1	519	U
1	1	531	G
1	1	532	U
1	1	538	G
1	1	539	G
1	1	540	C
1	1	541	U
1	1	542	U
1	1	543	C
1	1	544	U
1	1	546	C
1	1	555	A
1	1	556	U
1	1	557	A
1	1	564	G
1	1	577	G
1	1	589	G
1	1	590	A
1	1	598	U
1	1	600	U
1	1	601	U
1	1	602	A
1	1	609	A
1	1	618	U
1	1	619	A
1	1	620	A

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Mol	Chain	Res	Type
1	1	635	C
1	1	647	A
1	1	658	A
1	1	675	A
1	1	679	U
1	1	688	A
1	1	703	A
1	1	710	G
1	1	713	A
1	1	717	A
1	1	723	G
1	1	730	A
1	1	732	U
1	1	760	U
1	1	763	U
1	1	772	U
1	1	773	U
1	1	776	A
1	1	777	G
1	1	780	A
1	1	781	G
1	1	802	A
1	1	813	A
1	1	826	A
1	1	841	G
1	1	845	C
1	1	857	C
1	1	861	U
1	1	870	U
1	1	875	U
1	1	892	A
1	1	903	G
1	1	904	G
1	1	910	A
1	1	912	G
1	1	913	A
1	1	917	A
1	1	919	C
1	1	921	A
1	1	933	G
1	1	940	C
1	1	949	G

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Mol	Chain	Res	Type
1	1	955	C
1	1	956	U
1	1	959	G
1	1	976	A
1	1	977	U
1	1	990	G
1	1	991	U
1	1	996	C
1	1	997	G
1	1	998	A
1	1	1006	G
1	1	1011	C
1	1	1012	U
1	1	1014	G
1	1	1030	U
1	1	1033	C
1	1	1043	A
1	1	1045	C
1	1	1060	A
1	1	1061	A
1	1	1068	G
1	1	1077	U
1	1	1078	U
1	1	1089	A
1	1	1090	A
1	1	1091	U
1	1	1092	U
1	1	1094	A
1	1	1099	A
1	1	1100	G
1	1	1113	G
1	1	1127	G
1	1	1140	U
1	1	1149	A
1	1	1150	A
1	1	1151	C
1	1	1155	A
1	1	1156	C
1	1	1164	U
1	1	1174	G
1	1	1176	A
1	1	1177	U

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Mol	Chain	Res	Type
1	1	1178	G
1	1	1188	C
1	1	1189	A
1	1	1192	C
1	1	1197	C
1	1	1204	U
1	1	1205	G
1	1	1215	C
1	1	1218	G
1	1	1223	C
1	1	1224	C
1	1	1225	G
1	1	1228	C
1	1	1229	G
1	1	1230	G
1	1	1231	U
1	1	1232	G
1	1	1234	C
1	1	1238	G
1	1	1239	G
1	1	1241	A
1	1	1242	G
1	1	1243	U
1	1	1244	C
1	1	1245	G
1	1	1247	A
1	1	1249	U
1	1	1251	C
1	1	1252	G
1	1	1253	C
1	1	1255	A
1	1	1258	G
1	1	1259	A
1	1	1262	G
1	1	1263	U
1	1	1264	G
1	1	1265	U
1	1	1266	A
1	1	1267	A
1	1	1268	C
1	1	1269	A
1	1	1270	A

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Mol	Chain	Res	Type
1	1	1273	C
1	1	1278	G
1	1	1280	C
1	1	1282	A
1	1	1283	A
1	1	1303	G
1	1	1304	A
1	1	1305	U
1	1	1309	G
1	1	1326	A
1	1	1345	G
1	1	1346	U
1	1	1347	U
1	1	1348	U
1	1	1349	U
1	1	1382	A
1	1	1395	U
1	1	1415	A
1	1	1417	G
1	1	1421	U
1	1	1427	G
1	1	1430	G
1	1	1433	C
1	1	1442	A
1	1	1446	G
1	1	1465	C
1	1	1471	A
1	1	1477	A
1	1	1484	G
1	1	1498	C
1	1	1504	C
1	1	1520	A
1	1	1523	C
1	1	1532	G
1	1	1535	A
1	1	1551	U
1	1	1552	C
1	1	1556	G
1	1	1558	G
1	1	1559	C
1	1	1560	U
1	1	1561	U

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Mol	Chain	Res	Type
1	1	1562	G
1	1	1563	A
1	1	1565	U
1	1	1566	U
1	1	1567	U
1	1	1568	U
1	1	1569	C
1	1	1571	G
1	1	1572	G
1	1	1574	C
1	1	1576	A
1	1	1577	C
1	1	1585	A
1	1	1589	A
1	1	1601	A
1	1	1603	U
1	1	1624	C
1	1	1625	U
1	1	1635	C
1	1	1638	A
1	1	1639	A
1	1	1641	U
1	1	1648	G
1	1	1654	G
1	1	1679	A
1	1	1720	U
1	1	1721	C
1	1	1732	G
1	1	1746	A
1	1	1747	G
1	1	1755	U
1	1	1756	A
1	1	1757	A
1	1	1758	U
1	1	1760	U
1	1	1761	U
1	1	1762	G
1	1	1763	C
1	1	1776	G
1	1	1793	A
1	1	1804	G
1	1	1809	A

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Mol	Chain	Res	Type
1	1	1810	A
1	1	1811	U
1	1	1812	A
1	1	1815	U
1	1	1816	U
1	1	1817	U
1	1	1835	A
1	1	1838	A
1	1	1842	C
1	1	1845	C
1	1	1862	C
1	1	1874	G
1	1	1882	A
1	1	1889	A
1	1	1902	G
1	1	1944	G
1	1	1949	G
1	1	2070	A
1	1	2071	A
1	1	2078	A
1	1	2088	G
1	1	2089	G
1	1	2090	U
1	1	2091	A
1	1	2092	C
1	1	2099	G
1	1	2100	G
1	1	2109	A
1	1	2118	U
1	1	2122	A
1	1	2136	A
1	1	2147	G
1	1	2149	G
1	1	2183	U
1	1	2184	G
1	1	2185	A
1	1	2186	A
1	1	2187	U
1	1	2188	G
1	1	2222	A
1	1	2228	G
1	1	2229	G

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Mol	Chain	Res	Type
1	1	2233	A
1	1	2234	A
1	1	2235	C
1	1	2237	A
1	1	2245	C
1	1	2246	U
1	1	2247	U
1	1	2250	G
1	1	2251	G
1	1	2257	A
1	1	2259	A
1	1	2260	U
1	1	2276	U
1	1	2285	G
1	1	2286	C
1	1	2288	U
1	1	2291	A
1	1	2292	U
1	1	2293	G
1	1	2312	U
1	1	2313	G
1	1	2314	U
1	1	2341	A
1	1	2351	A
1	1	2352	C
1	1	2353	G
1	1	2363	G
1	1	2366	U
1	1	2371	G
1	1	2372	G
1	1	2375	A
1	1	2380	A
1	1	2381	G
1	1	2382	A
1	1	2389	U
1	1	2413	G
1	1	2420	G
1	1	2489	A
1	1	2492	U
1	1	2493	A
1	1	2510	U
1	1	2511	G

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Mol	Chain	Res	Type
1	1	2513	A
1	1	2514	G
1	1	2515	G
1	1	2516	U
1	1	2517	C
1	1	2518	A
1	1	2519	A
1	1	2520	A
1	1	2521	C
1	1	2522	U
1	1	2523	C
1	1	2529	U
1	1	2530	C
1	1	2533	G
1	1	2536	U
1	1	2538	A
1	1	2545	C
1	1	2546	U
1	1	2554	C
1	1	2557	G
1	1	2565	A
1	1	2566	C
1	1	2578	G
1	1	2579	G
1	1	2586	G
1	1	2598	A
1	1	2623	G
1	1	2624	U
1	1	2628	A
1	1	2644	G
1	1	2646	A
1	1	2649	G
1	1	2661	A
1	1	2662	G
1	1	2663	A
1	1	2666	A
1	1	2676	A
1	1	2677	A
1	1	2686	G
1	1	2699	A
1	1	2700	G
1	1	2701	U

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Mol	Chain	Res	Type
1	1	2725	G
1	1	2734	A
1	1	2745	C
1	1	2749	G
1	1	2750	G
1	1	2765	G
1	1	2768	G
1	1	2771	A
1	1	2772	G
1	1	2773	A
1	1	2774	A
1	1	2782	C
1	1	2786	G
1	1	2789	A
1	1	2790	U
1	1	2807	U
1	1	2808	C
1	1	2814	U
1	1	2815	U
1	1	2817	A
1	1	2833	U
1	1	2839	C
1	1	2843	G
1	1	2844	A
1	1	2847	U
1	1	2859	A
1	1	2861	C
1	1	2866	C
1	1	2870	G
1	1	2871	C
1	1	2886	G
1	1	2895	U
1	1	2907	U
1	1	2908	A
1	1	2911	G
1	1	2914	C
1	1	2919	G
1	1	2920	C
1	1	2923	G
1	1	2926	U
1	1	2943	A
1	1	2955	C

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Mol	Chain	Res	Type
1	1	2960	C
1	1	2962	G
1	1	2969	G
1	1	2984	A
1	1	3021	A
1	1	3028	U
1	1	3031	G
1	1	3050	A
1	1	3051	C
1	1	3052	G
1	1	3058	A
1	1	3064	C
1	1	3076	U
1	1	3094	A
1	1	3101	A
1	1	3102	A
1	1	3103	U
1	1	3114	A
1	1	3115	C
1	1	3134	C
1	1	3143	G
1	1	3144	A
1	1	3146	G
1	1	3149	U
1	1	3151	C
1	1	3157	A
1	1	3160	C
1	1	3163	U
1	1	3164	U
1	1	3171	C
1	1	3172	U
1	1	3182	C
1	1	3183	A
1	1	3184	G
1	1	3194	G
1	1	3208	A
1	1	3210	A
1	1	3212	G
1	1	3214	U
1	1	3221	G
1	1	3224	U
1	1	3228	G

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Mol	Chain	Res	Type
1	1	3235	A
1	1	3241	G
1	1	3246	C
1	1	3252	C
1	1	3259	A
1	1	3260	A
1	1	3268	G
1	1	3269	C
1	1	3272	A
1	1	3278	U
1	1	3281	A
1	1	3284	U
1	1	3285	A
1	1	3306	U
1	1	3307	A
1	1	3309	A
1	1	3310	G
1	1	3316	U
1	1	3317	U
1	1	3318	G
1	1	3319	U
1	1	3320	U
1	1	3321	G
1	1	3334	G
1	1	3343	C
1	1	3351	G
1	1	3361	U
2	3	7	G
2	3	22	A
2	3	54	U
2	3	55	A
2	3	65	G
2	3	73	C
2	3	76	A
2	3	102	A
2	3	112	G
3	4	23	U
3	4	34	U
3	4	35	C
3	4	59	A
3	4	62	C
3	4	63	G

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Mol	Chain	Res	Type
3	4	81	A
3	4	84	C
3	4	85	G
3	4	86	U
3	4	87	G
3	4	92	A
3	4	95	G
3	4	102	U
3	4	104	A
3	4	106	C
3	4	111	A
3	4	113	U
3	4	125	U
3	4	126	A
3	4	148	G
3	4	152	G
3	4	157	U
4	10	2	G
4	10	76	A
46	A	17	C
46	A	25	C
46	A	26	A
46	A	27	U
46	A	34	G
46	A	47	A
46	A	57	G
46	A	66	U
46	A	74	U
46	A	75	U
46	A	76	A
46	A	78	A
46	A	79	C
46	A	81	G
46	A	84	A
46	A	104	A
46	A	114	C
46	A	115	G
46	A	123	G
46	A	126	A
46	A	127	G
46	A	128	U
46	A	129	A

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Mol	Chain	Res	Type
46	A	138	C
46	A	139	U
46	A	141	G
46	A	142	G
46	A	143	A
46	A	150	U
46	A	151	G
46	A	152	G
46	A	154	A
46	A	159	U
46	A	166	A
46	A	168	U
46	A	173	G
46	A	176	U
46	A	177	A
46	A	179	A
46	A	190	U
46	A	191	U
46	A	193	G
46	A	199	G
46	A	200	A
46	A	202	G
46	A	206	U
46	A	211	A
46	A	214	U
46	A	215	A
46	A	216	A
46	A	217	A
46	A	218	A
46	A	247	U
46	A	255	A
46	A	259	U
46	A	260	U
46	A	261	C
46	A	262	G
46	A	266	C
46	A	269	A
46	A	270	U
46	A	274	C
46	A	276	U
46	A	277	G
46	A	278	U

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Mol	Chain	Res	Type
46	A	279	G
46	A	283	G
46	A	285	G
46	A	297	A
46	A	312	C
46	A	314	A
46	A	318	U
46	A	320	G
46	A	335	G
46	A	336	C
46	A	350	A
46	A	357	A
46	A	358	A
46	A	359	C
46	A	388	G
46	A	398	A
46	A	400	C
46	A	402	G
46	A	414	A
46	A	416	G
46	A	421	G
46	A	422	C
46	A	423	A
46	A	424	G
46	A	432	G
46	A	437	U
46	A	442	C
46	A	446	C
46	A	452	A
46	A	458	A
46	A	466	A
46	A	475	A
46	A	480	U
46	A	482	C
46	A	483	A
46	A	485	G
46	A	501	G
46	A	502	U
46	A	503	A
46	A	504	A
46	A	505	U
46	A	506	U

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Mol	Chain	Res	Type
46	A	509	A
46	A	512	G
46	A	513	A
46	A	515	U
46	A	518	A
46	A	519	A
46	A	525	A
46	A	530	U
46	A	534	C
46	A	536	A
46	A	537	G
46	A	539	A
46	A	540	A
46	A	547	G
46	A	553	A
46	A	554	A
46	A	555	G
46	A	556	U
46	A	557	C
46	A	563	C
46	A	566	G
46	A	575	G
46	A	576	U
46	A	580	U
46	A	592	A
46	A	593	G
46	A	604	A
46	A	609	U
46	A	617	A
46	A	618	A
46	A	620	A
46	A	621	A
46	A	633	A
46	A	639	G
46	A	686	G
46	A	687	A
46	A	688	G
46	A	694	C
46	A	696	U
46	A	701	G
46	A	721	C
46	A	722	A

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Mol	Chain	Res	Type
46	A	723	G
46	A	729	U
46	A	739	A
46	A	740	A
46	A	741	A
46	A	750	G
46	A	751	U
46	A	756	A
46	A	759	A
46	A	760	G
46	A	762	C
46	A	764	U
46	A	765	U
46	A	766	U
46	A	767	G
46	A	768	C
46	A	770	C
46	A	771	G
46	A	773	A
46	A	775	A
46	A	778	U
46	A	779	U
46	A	796	A
46	A	798	A
46	A	799	G
46	A	802	C
46	A	803	G
46	A	804	U
46	A	805	U
46	A	807	U
46	A	808	G
46	A	814	A
46	A	815	U
46	A	816	U
46	A	818	U
46	A	819	G
46	A	820	U
46	A	821	U
46	A	823	G
46	A	824	U
46	A	825	U
46	A	826	U

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Mol	Chain	Res	Type
46	A	828	U
46	A	831	G
46	A	840	A
46	A	842	U
46	A	848	A
46	A	856	G
46	A	857	G
46	A	869	A
46	A	871	U
46	A	875	C
46	A	877	G
46	A	878	U
46	A	879	U
46	A	881	U
46	A	891	A
46	A	909	A
46	A	910	G
46	A	911	A
46	A	918	A
46	A	920	U
46	A	945	U
46	A	951	A
46	A	973	A
46	A	975	C
46	A	977	A
46	A	988	A
46	A	989	U
46	A	997	U
46	A	998	A
46	A	1004	A
46	A	1005	A
46	A	1011	A
46	A	1013	C
46	A	1017	G
46	A	1024	A
46	A	1025	G
46	A	1039	U
46	A	1042	U
46	A	1043	U
46	A	1044	U
46	A	1047	U
46	A	1055	A

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Mol	Chain	Res	Type
46	A	1056	U
46	A	1057	C
46	A	1058	G
46	A	1059	G
46	A	1060	C
46	A	1061	A
46	A	1067	C
46	A	1077	A
46	A	1081	C
46	A	1085	G
46	A	1123	A
46	A	1135	G
46	A	1143	C
46	A	1145	A
46	A	1152	G
46	A	1168	A
46	A	1169	A
46	A	1170	U
46	A	1176	U
46	A	1179	A
46	A	1181	A
46	A	1184	G
46	A	1185	G
46	A	1186	G
46	A	1187	A
46	A	1193	A
46	A	1202	A
46	A	1203	G
46	A	1206	A
46	A	1207	C
46	A	1212	A
46	A	1215	A
46	A	1219	A
46	A	1220	C
46	A	1221	A
46	A	1229	A
46	A	1230	G
46	A	1231	C
46	A	1236	U
46	A	1243	U
46	A	1250	G
46	A	1270	U

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Mol	Chain	Res	Type
46	A	1284	G
46	A	1299	U
46	A	1300	U
46	A	1301	G
46	A	1306	A
46	A	1325	U
46	A	1330	A
46	A	1336	G
46	A	1339	G
46	A	1342	A
46	A	1343	G
46	A	1345	A
46	A	1346	U
46	A	1348	U
46	A	1349	G
46	A	1352	G
46	A	1355	A
46	A	1356	U
46	A	1357	A
46	A	1359	U
46	A	1360	C
46	A	1364	U
46	A	1365	C
46	A	1369	G
46	A	1370	A
46	A	1376	U
46	A	1380	G
46	A	1381	A
46	A	1382	U
46	A	1384	U
46	A	1385	C
46	A	1392	A
46	A	1397	A
46	A	1398	G
46	A	1399	U
46	A	1400	U
46	A	1401	U
46	A	1410	A
46	A	1413	A
46	A	1414	G
46	A	1415	G
46	A	1422	A

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Mol	Chain	Res	Type
46	A	1431	G
46	A	1433	C
46	A	1445	C
46	A	1446	A
46	A	1455	A
46	A	1457	A
46	A	1461	A
46	A	1462	C
46	A	1463	G
46	A	1468	C
46	A	1476	A
46	A	1477	U
46	A	1483	U
46	A	1491	G
46	A	1503	A
46	A	1508	G
46	A	1510	G
46	A	1511	A
46	A	1523	G
46	A	1524	C
46	A	1529	G
46	A	1530	A
46	A	1541	U
46	A	1544	U
46	A	1546	G
46	A	1547	U
46	A	1548	U
46	A	1556	A
46	A	1560	A
46	A	1561	G
46	A	1569	U
46	A	1571	G
46	A	1574	A
46	A	1575	G
46	A	1577	G
46	A	1580	A
46	A	1582	U
46	A	1584	A
46	A	1588	G
46	A	1621	C
46	A	1644	U
46	A	1645	G

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Mol	Chain	Res	Type
46	A	1665	C
46	A	1667	G
46	A	1670	U
46	A	1671	G
46	A	1672	G
46	A	1673	U
46	A	1674	U
46	A	1677	G
46	A	1700	G
46	A	1704	C
46	A	1737	A
46	A	1743	A
46	A	1747	G
46	A	1749	A
46	A	1753	A
46	A	1756	U
46	A	1767	G
46	A	1769	A
46	A	1770	C
46	A	1779	G
46	A	1780	G
46	A	1781	A
46	A	1782	U
46	A	1783	C

All (81) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	172	C
1	1	403	C
1	1	538	G
1	1	563	U
1	1	601	U
1	1	759	G
1	1	912	G
1	1	1029	U
1	1	1060	A
1	1	1099	A
1	1	1346	U
1	1	1347	U
1	1	1559	C
1	1	1561	U

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Mol	Chain	Res	Type
1	1	1576	A
1	1	1762	G
1	1	1815	U
1	1	1943	G
1	1	2090	U
1	1	2183	U
1	1	2515	G
1	1	2519	A
1	1	2520	A
1	1	2545	C
1	1	2789	A
1	1	2790	U
1	1	3093	U
1	1	3159	A
1	1	3193	C
1	1	3234	U
1	1	3240	U
1	1	3284	U
1	1	3309	A
1	1	3315	C
1	1	3317	U
3	4	85	G
3	4	125	U
3	4	156	U
46	A	25	C
46	A	78	A
46	A	137	A
46	A	151	G
46	A	176	U
46	A	214	U
46	A	259	U
46	A	265	U
46	A	278	U
46	A	451	C
46	A	502	U
46	A	504	A
46	A	505	U
46	A	514	G
46	A	518	A
46	A	529	C
46	A	533	A
46	A	553	A

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Mol	Chain	Res	Type
46	A	556	U
46	A	638	U
46	A	685	C
46	A	740	A
46	A	763	C
46	A	769	U
46	A	817	U
46	A	820	U
46	A	824	U
46	A	855	C
46	A	874	U
46	A	876	A
46	A	1168	A
46	A	1335	U
46	A	1355	A
46	A	1359	U
46	A	1369	G
46	A	1396	A
46	A	1398	G
46	A	1467	C
46	A	1523	G
46	A	1555	C
46	A	1573	A
46	A	1579	A
46	A	1581	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 441 ligands modelled in this entry, 438 are monoatomic - leaving 3 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	SPK	1	3402	-	13,13,13	0.35	0	12,12,12	1.00	0
80	YMZ	j	301	-	28,28,28	0.48	0	41,43,43	0.66	1 (2%)
80	YMZ	1	3401	-	28,28,28	0.47	0	41,43,43	0.64	2 (4%)

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	SPK	1	3402	-	-	6/11/11/11	-
80	YMZ	j	301	-	-	4/20/28/28	1/3/3/3
80	YMZ	1	3401	-	-	12/20/28/28	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	1	3401	YMZ	CAN-NAQ-CAX	2.62	113.25	111.62
80	j	301	YMZ	CAN-NAQ-CAX	2.60	113.24	111.62
80	1	3401	YMZ	CAO-CAX-NAQ	-2.14	108.75	111.90

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
80	1	3401	YMZ	CAV-CAT-CAZ-FAE
80	1	3401	YMZ	CAV-CAT-CAZ-FAF
80	1	3401	YMZ	CAV-CAT-CAZ-FAG
81	1	3402	SPK	N1-C2-C3-C4
81	1	3402	SPK	N5-C6-C7-C8
80	1	3401	YMZ	CAK-CAS-CAW-CAX
80	j	301	YMZ	CAU-CAS-CAW-OAA
80	1	3401	YMZ	CAU-CAS-CAW-CAX
80	1	3401	YMZ	CAI-CAT-CAZ-FAF

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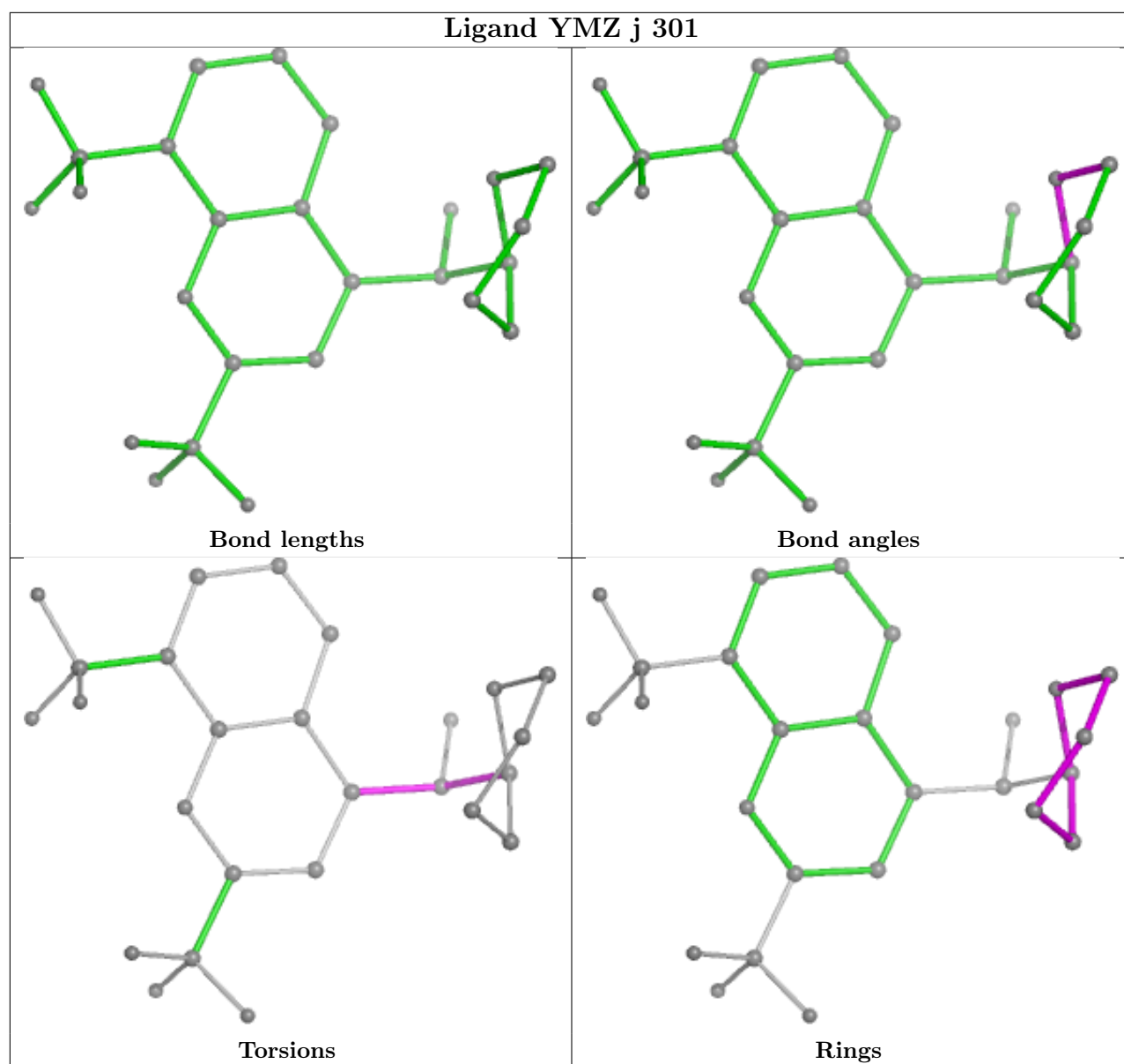
Mol	Chain	Res	Type	Atoms
80	j	301	YMZ	CAK-CAS-CAW-OAA
80	1	3401	YMZ	CAI-CAT-CAZ-FAE
80	1	3401	YMZ	CAS-CAW-CAX-CAO
80	1	3401	YMZ	CAK-CAS-CAW-OAA
80	1	3401	YMZ	CAU-CAS-CAW-OAA
80	1	3401	YMZ	CAI-CAT-CAZ-FAG
81	1	3402	SPK	C12-C11-N10-C9
80	1	3401	YMZ	CAS-CAW-CAX-NAQ
80	j	301	YMZ	OAA-CAW-CAX-CAO
81	1	3402	SPK	C7-C8-C9-N10
81	1	3402	SPK	C6-C7-C8-C9
80	j	301	YMZ	CAS-CAW-CAX-NAQ
81	1	3402	SPK	C3-C4-N5-C6

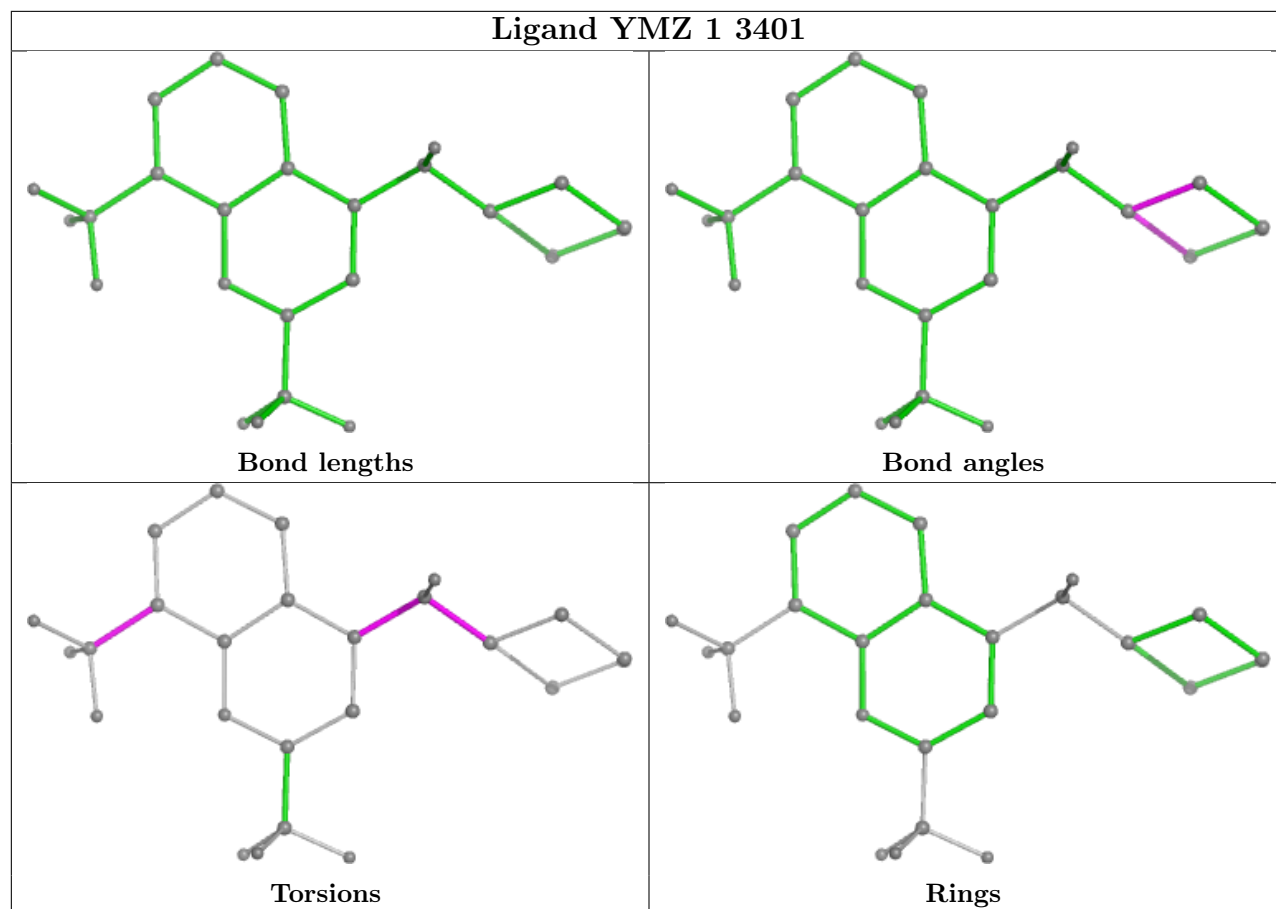
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
80	j	301	YMZ	CAL-CAM-CAN-CAO-CAX-NAQ

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.

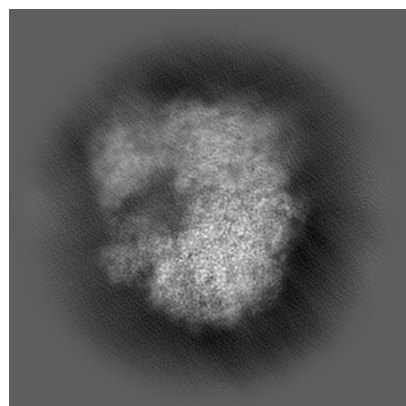
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16874. These allow visual inspection of the internal detail of the map and identification of artifacts.

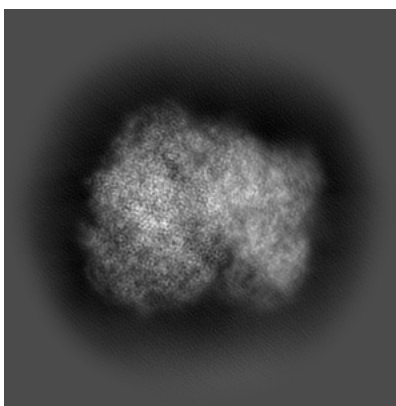
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

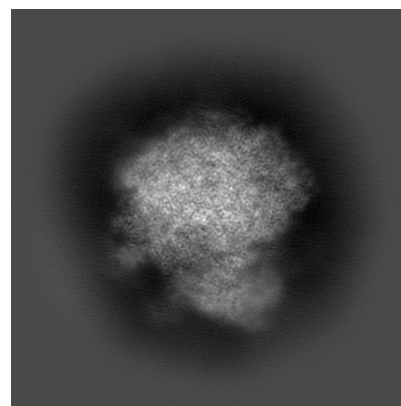
6.1.1 Primary map



X

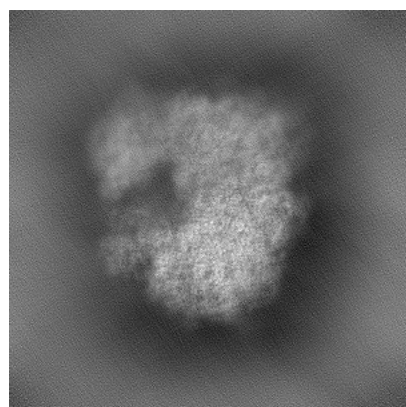


Y

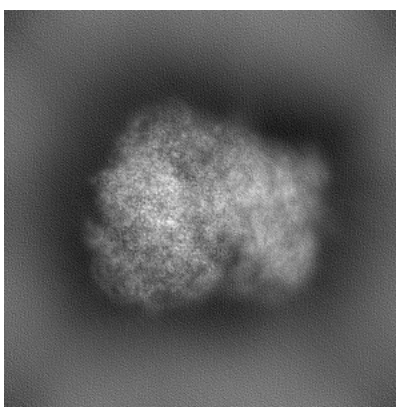


Z

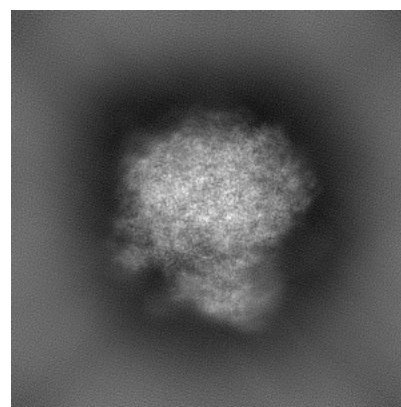
6.1.2 Raw map



X



Y

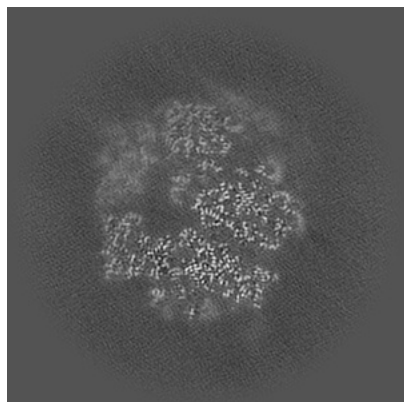


Z

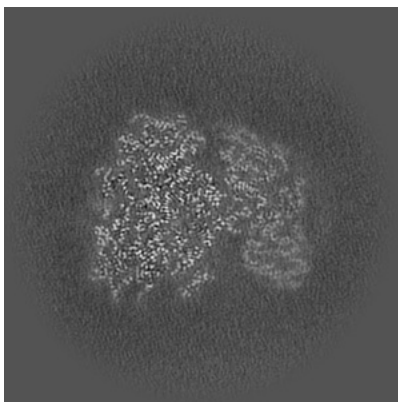
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

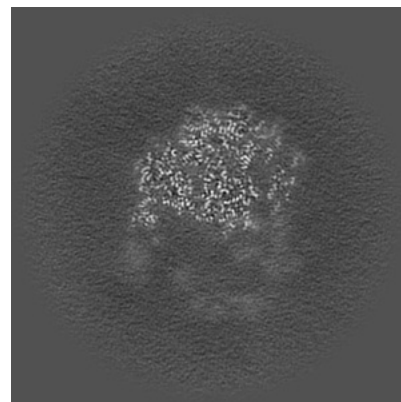
6.2.1 Primary map



X Index: 210

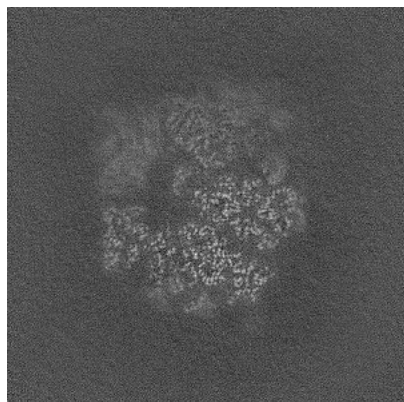


Y Index: 210

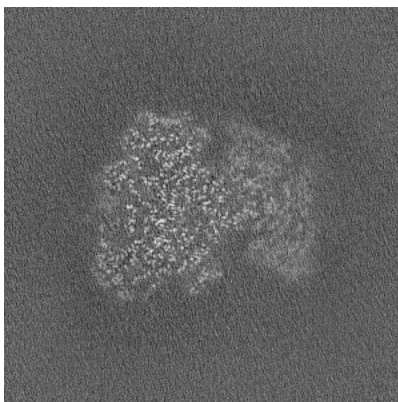


Z Index: 210

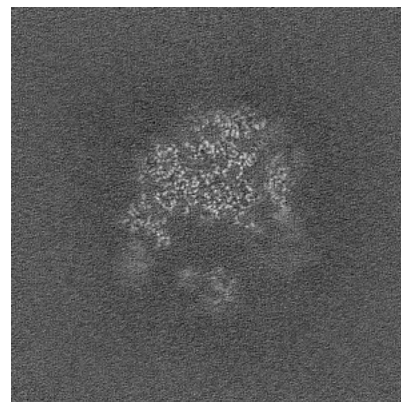
6.2.2 Raw map



X Index: 210



Y Index: 210

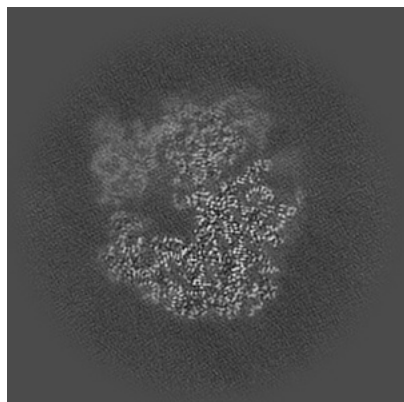


Z Index: 210

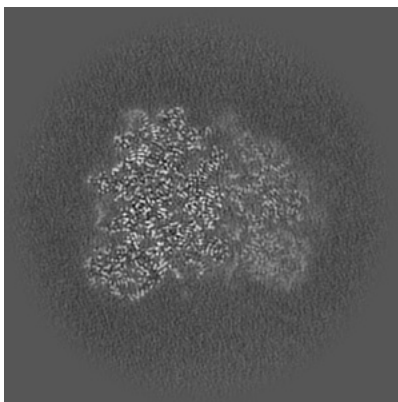
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

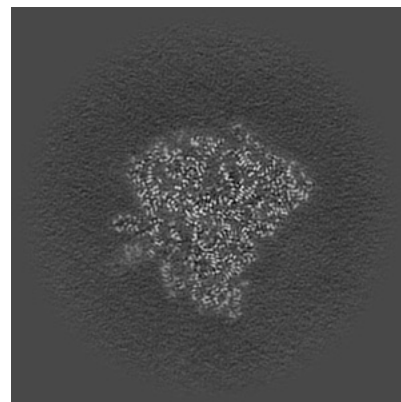
6.3.1 Primary map



X Index: 225

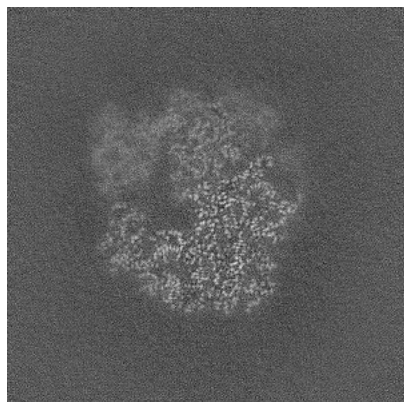


Y Index: 220

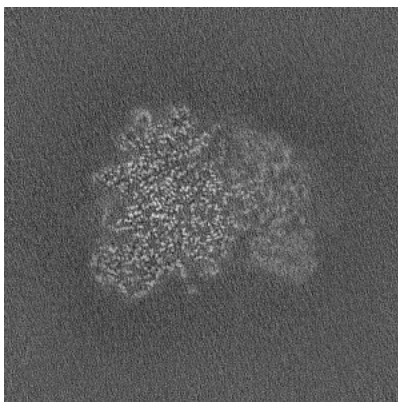


Z Index: 166

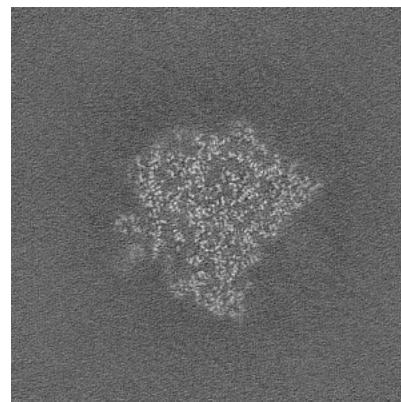
6.3.2 Raw map



X Index: 227



Y Index: 216

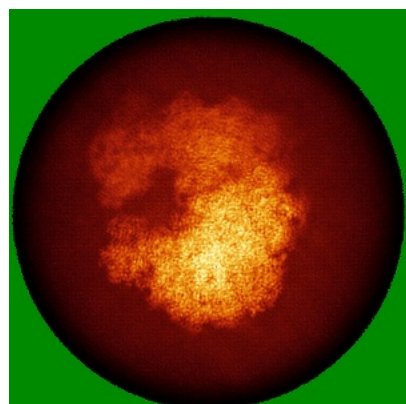


Z Index: 173

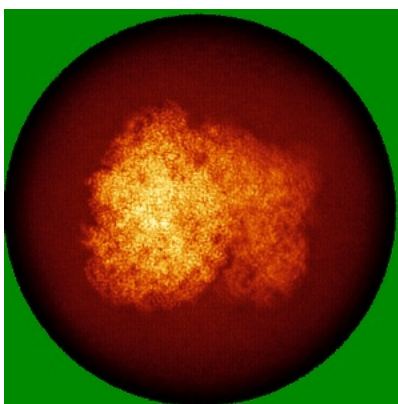
The images above show the largest variance slices of the map in three orthogonal directions.

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

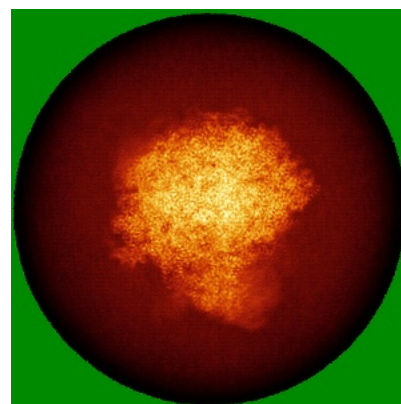
6.4.1 Primary map



X

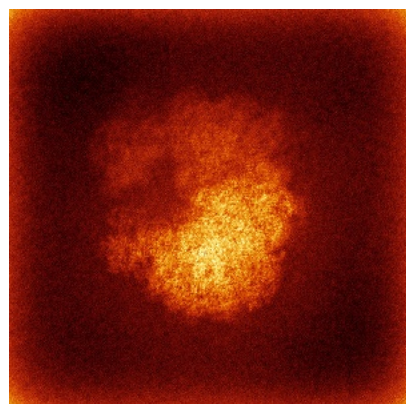


Y

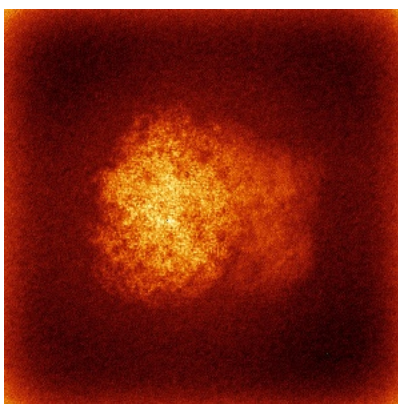


Z

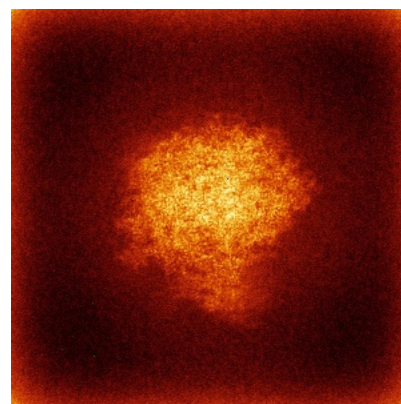
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



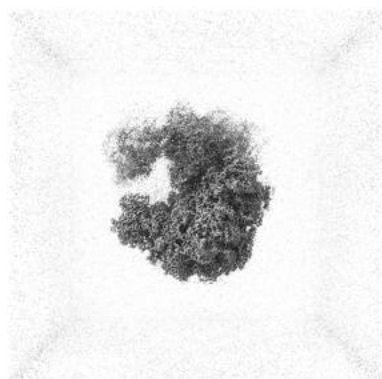
Y



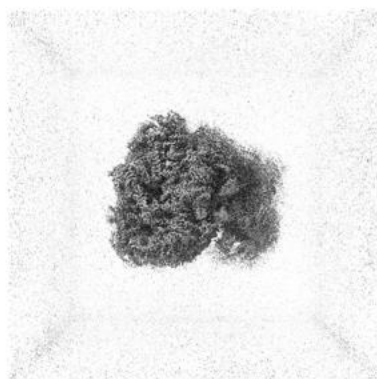
Z

The images above show the 3D surface view of the map at the recommended contour level 0.31. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

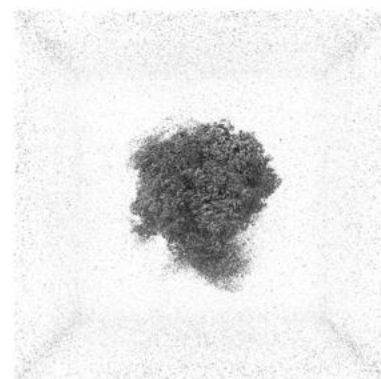
6.5.2 Raw map



X



Y



Z

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

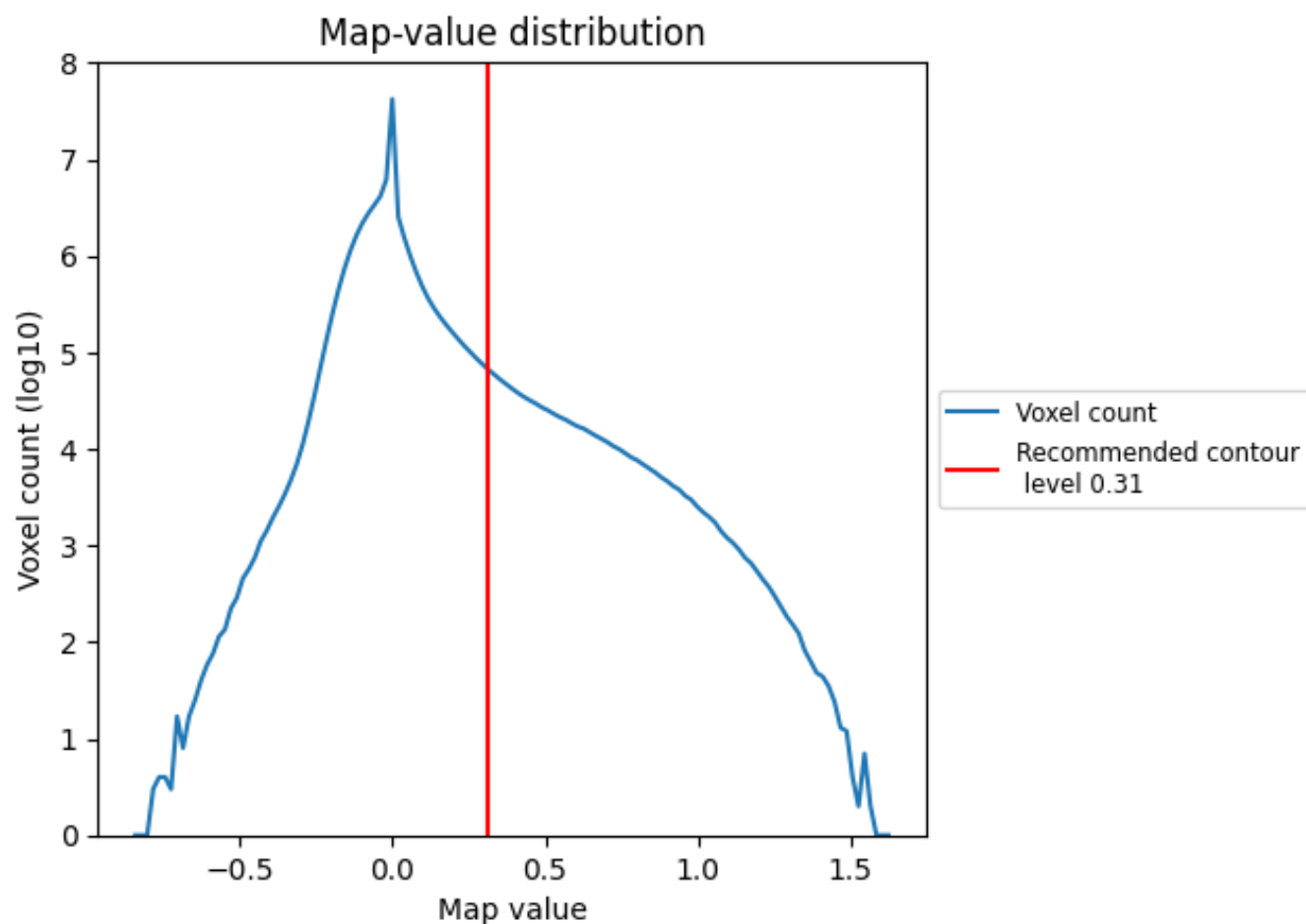
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

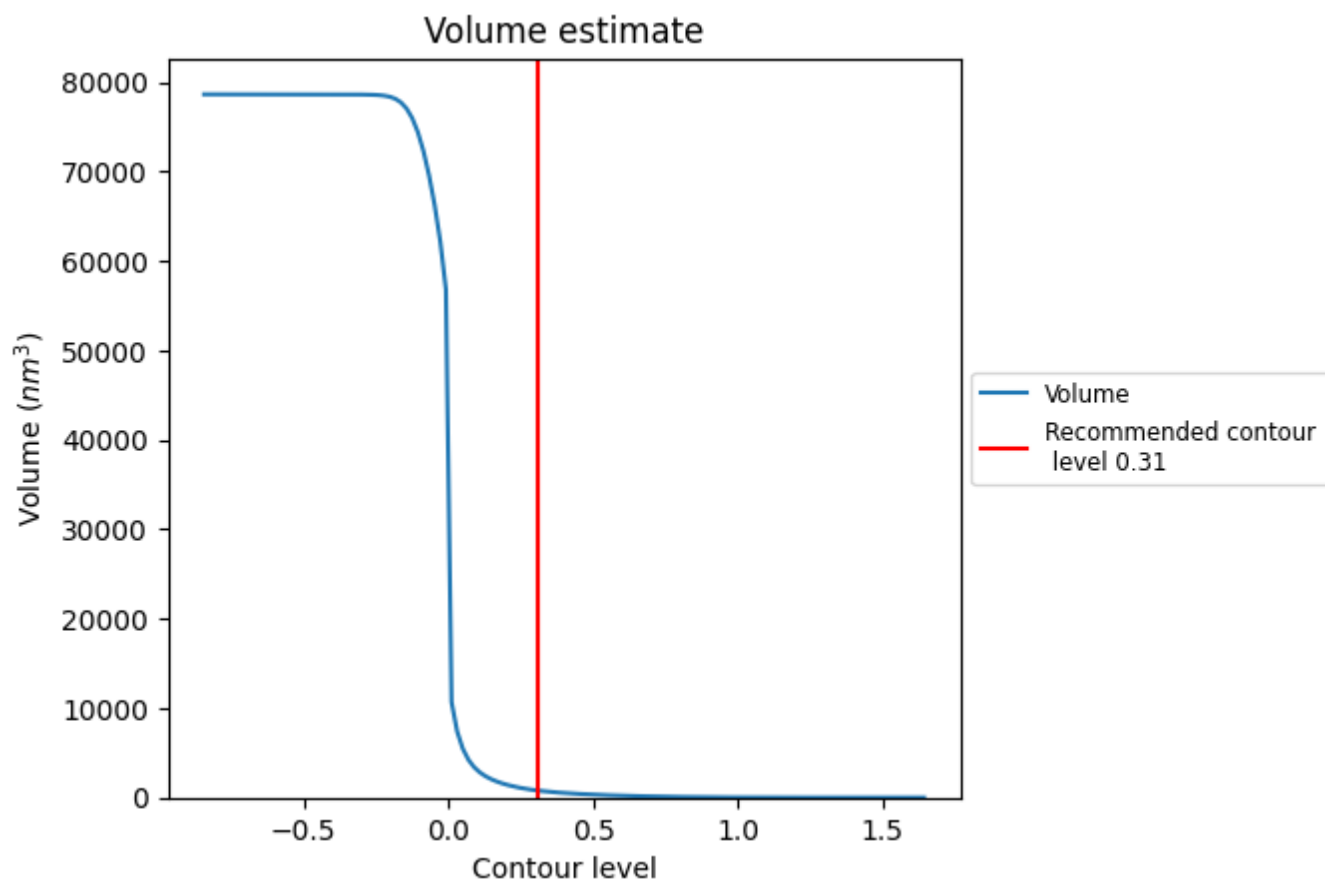
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

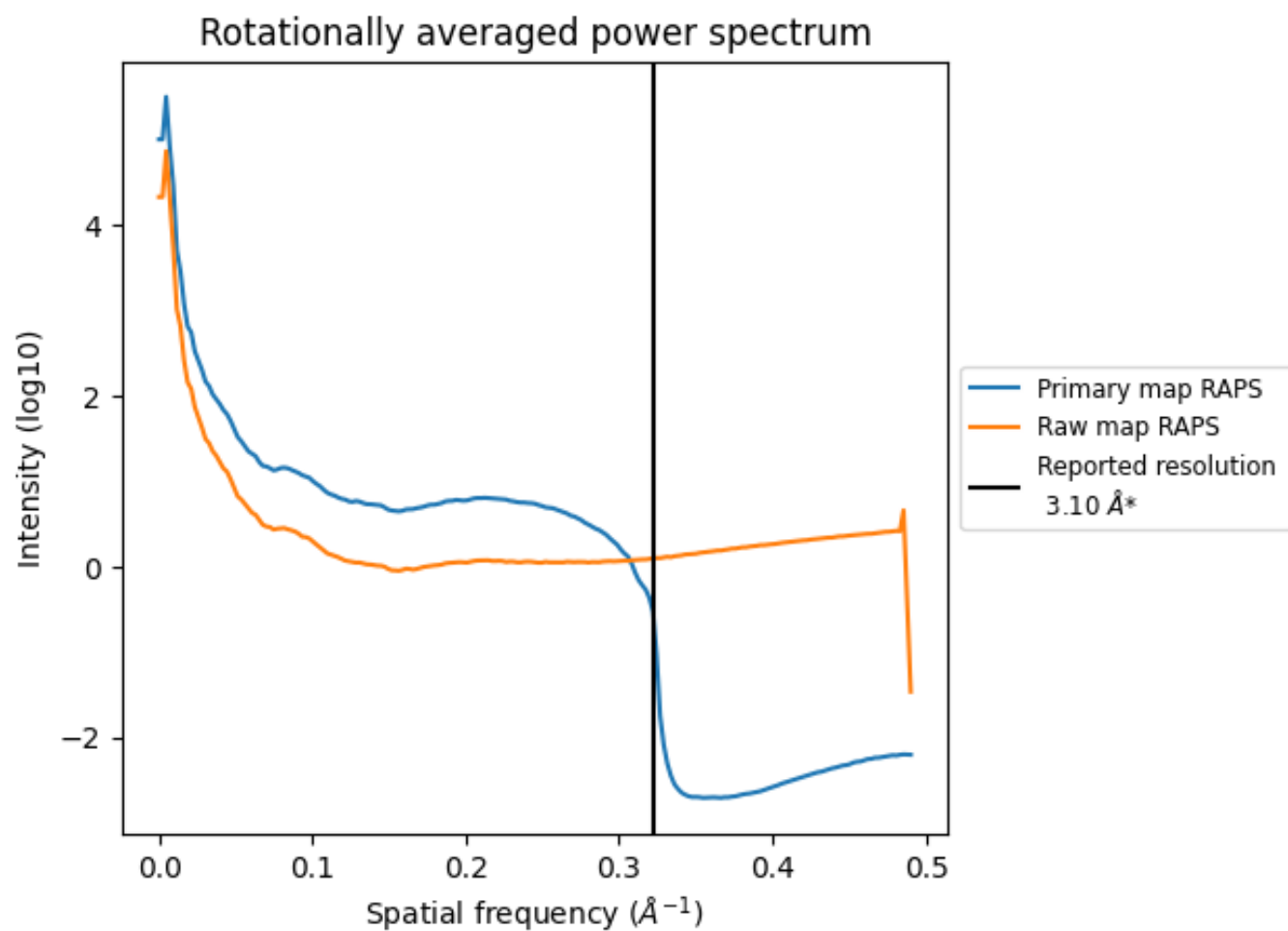
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 787 nm³; this corresponds to an approximate mass of 711 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](#)

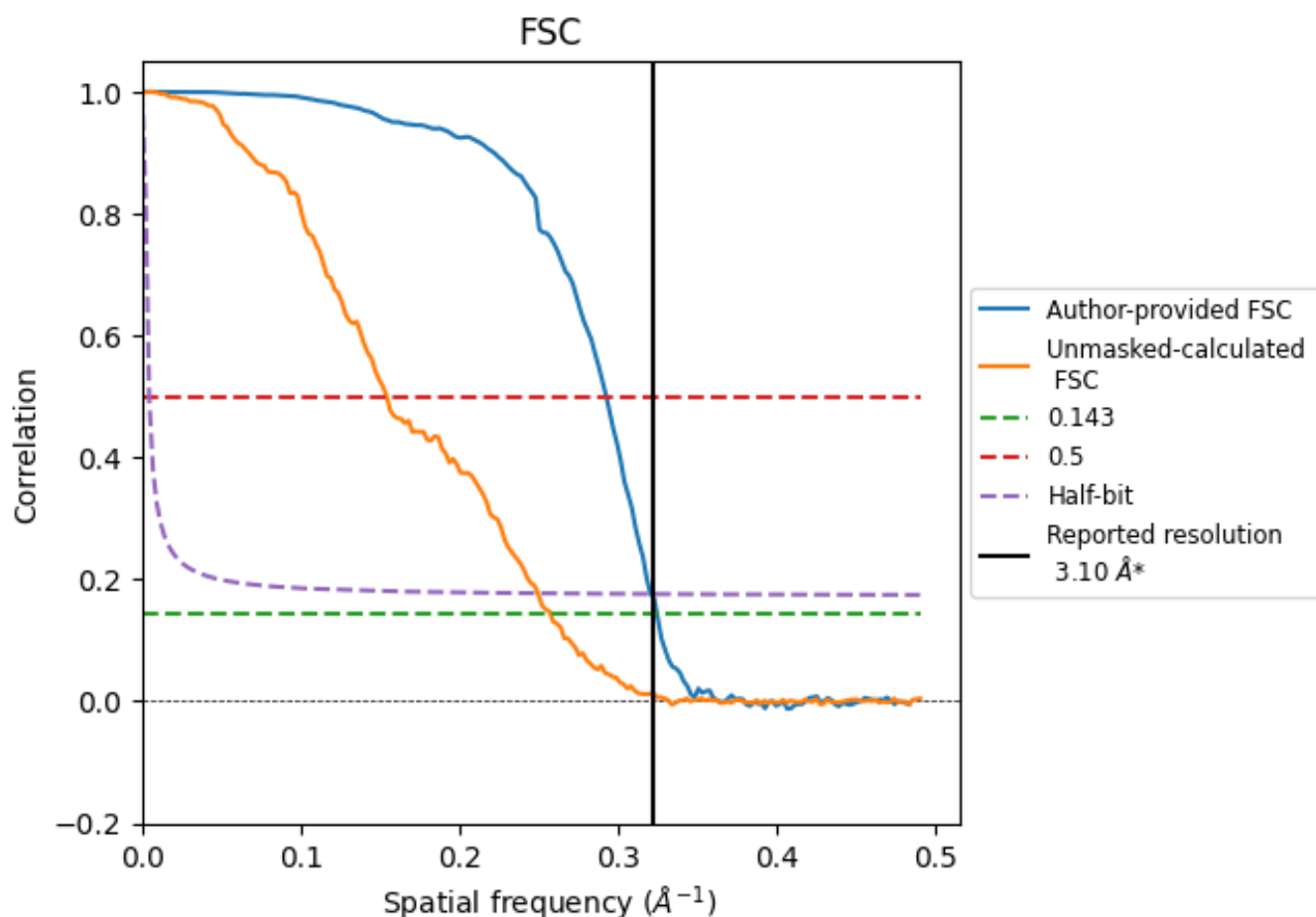


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

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 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

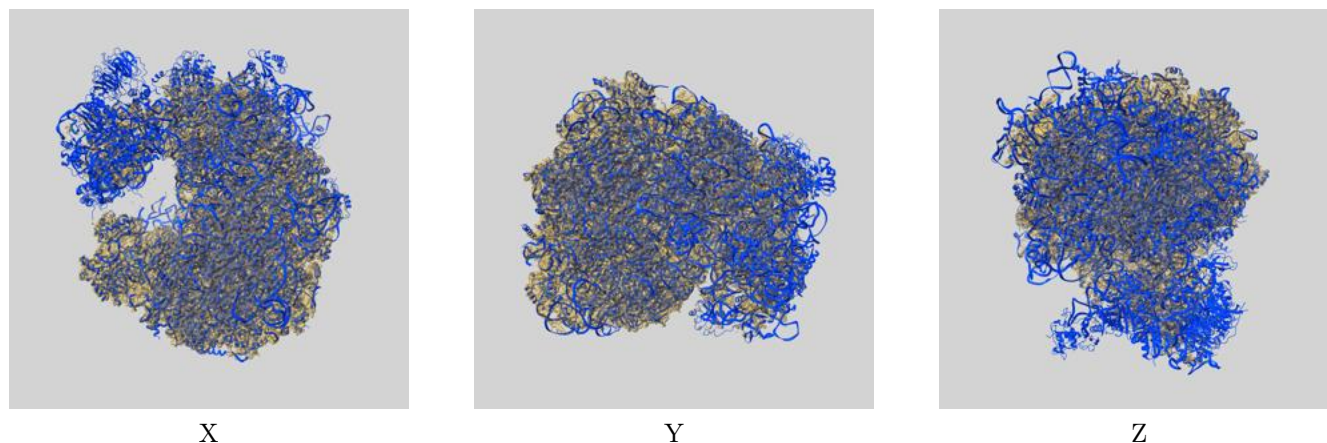
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	3.42	3.12
Unmasked-calculated*	3.89	6.49	4.01

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

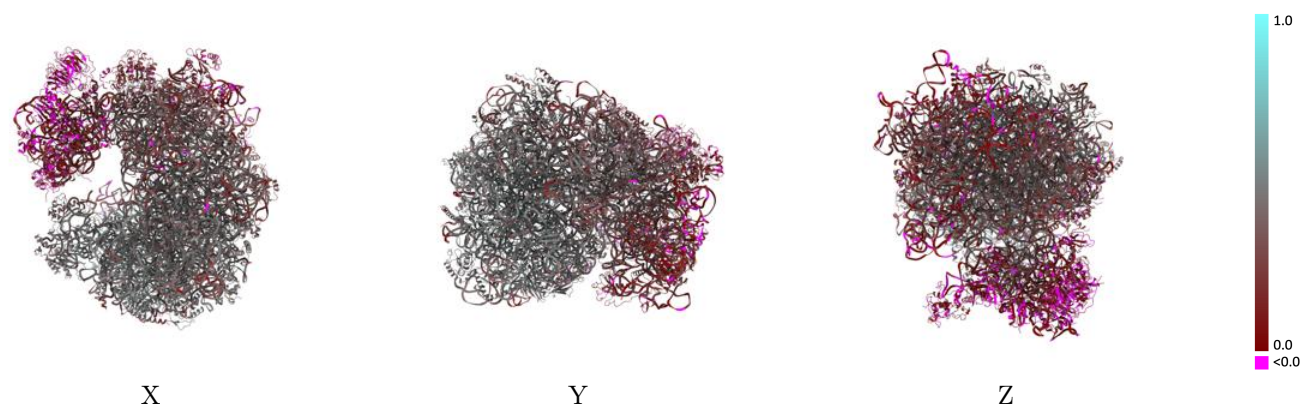
This section contains information regarding the fit between EMDB map EMD-16874 and PDB model 8OGJ. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



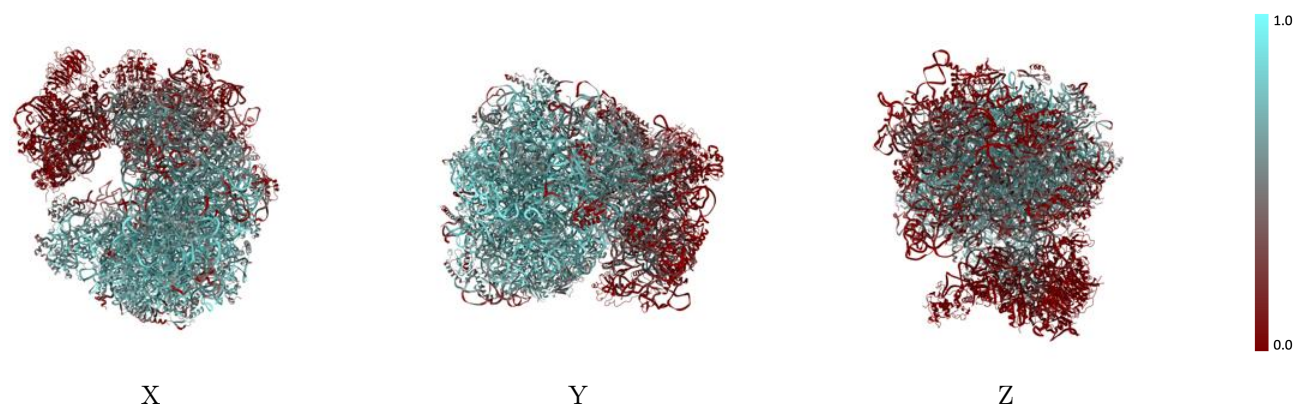
The images above show the 3D surface view of the map at the recommended contour level 0.31 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



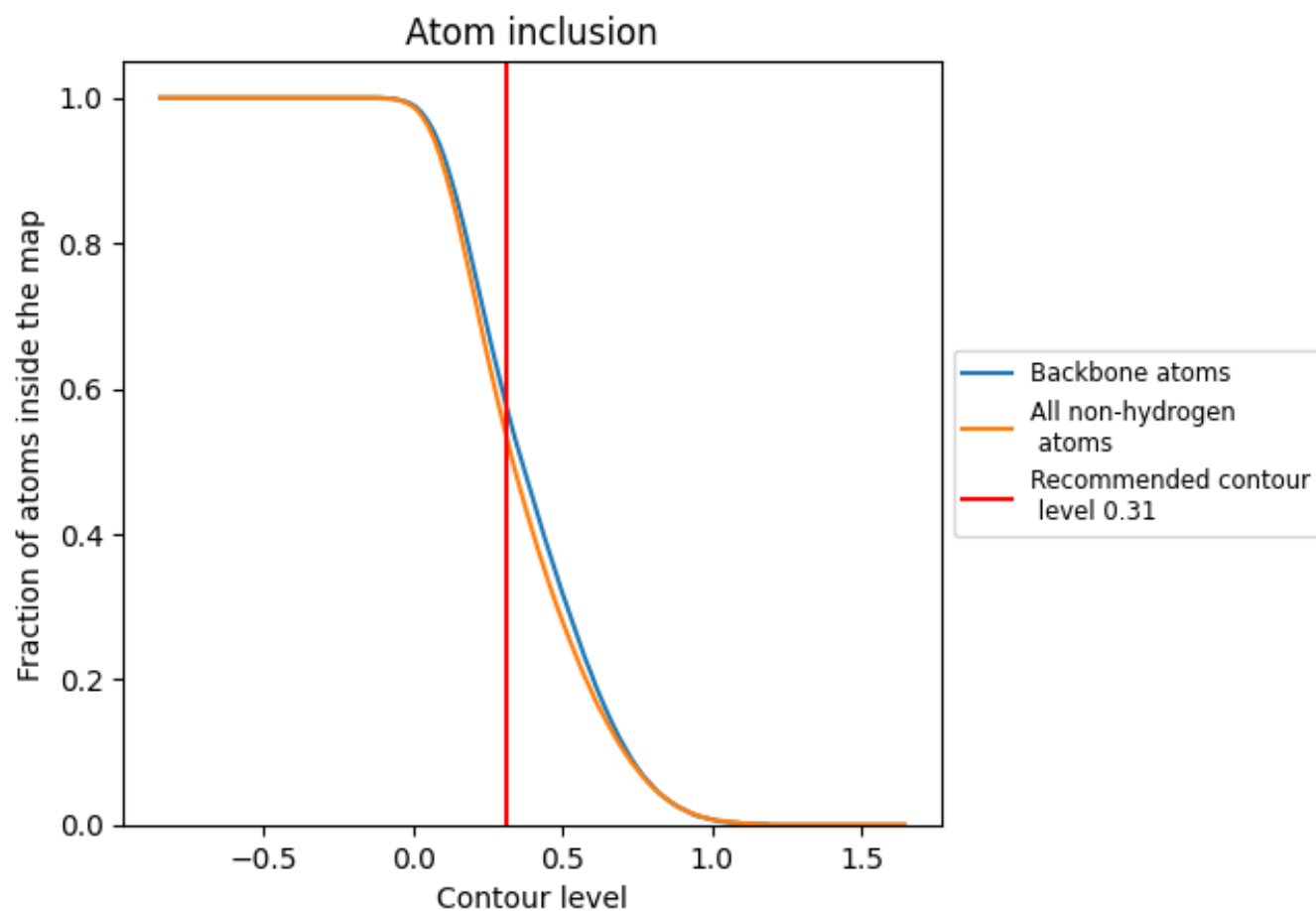
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.31).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 54% 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 (0.31) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5390	 0.3660
0	 0.7140	 0.5020
1	 0.7560	 0.4400
10	 0.0810	 0.3260
2	 0.6700	 0.4750
3	 0.8080	 0.4710
4	 0.7770	 0.4380
5	 0.0510	 0.2850
6	 0.6940	 0.4690
7	 0.5740	 0.4440
8	 0.6480	 0.4380
9	 0.6520	 0.4480
A	 0.3900	 0.2690
AA	 0.4930	 0.3910
AB	 0.7350	 0.4880
AC	 0.6070	 0.4290
AD	 0.4920	 0.3870
AE	 0.5990	 0.4320
AF	 0.7350	 0.4800
AG	 0.7400	 0.4970
AH	 0.6250	 0.4190
AI	 0.6180	 0.4320
AJ	 0.6000	 0.4280
AK	 0.7310	 0.4630
AL	 0.3220	 0.3590
AM	 0.7050	 0.4440
AN	 0.6650	 0.4820
AO	 0.1440	 0.3270
AP	 0.6120	 0.4670
AQ	 0.6370	 0.4200
B	 0.1370	 0.2610
C	 0.2570	 0.2960
D	 0.2760	 0.3010
E	 0.0300	 0.1080
F	 0.1690	 0.2530









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Chain	Atom inclusion	Q-score
G	 0.0070	 0.0840
H	 0.0710	 0.2370
I	 0.0320	 0.1830
J	 0.1390	 0.2240
K	 0.1280	 0.1830
L	 0.0060	 0.1040
M	 0.2070	 0.3030
N	 0.0000	 0.0920
O	 0.3250	 0.3190
P	 0.3210	 0.3540
Q	 0.0050	 0.0870
R	 0.0380	 0.1050
S	 0.0170	 0.1390
T	 0.0130	 0.1040
U	 0.0170	 0.0760
V	 0.0290	 0.0820
W	 0.1660	 0.2880
X	 0.3650	 0.3510
Y	 0.3380	 0.3570
Z	 0.1070	 0.2380
a	 0.0050	 0.0710
b	 0.3970	 0.3660
c	 0.1730	 0.2710
d	 0.0000	 0.0930
e	 0.0570	 0.1800
f	 0.0770	 0.2130
g	 0.0000	 0.1540
h	 0.0000	 0.0690
j	 0.6830	 0.4400
k	 0.7190	 0.4760
l	 0.6990	 0.4710
m	 0.5930	 0.4500
n	 0.6090	 0.4620
o	 0.6720	 0.4830
p	 0.5440	 0.4070
q	 0.6100	 0.4700
r	 0.6220	 0.4780
s	 0.4830	 0.4220
t	 0.6420	 0.4380
u	 0.6070	 0.4850
v	 0.7620	 0.4570
w	 0.7190	 0.4910

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Chain	Atom inclusion	Q-score
x	 0.6950	 0.4590
y	 0.7410	 0.4830
z	 0.5800	 0.3950