



wwPDB EM Validation Summary Report ⓘ

Dec 19, 2022 – 06:19 am GMT

PDB ID : 7NWH
EMDB ID : EMD-12632
Title : Mammalian pre-termination 80S ribosome with eRF1 and eRF3 bound by Blasticidin S.
Authors : Powers, K.T.; Yadav, S.K.N.; Bufton, J.C.; Schaffitzel, C.
Deposited on : 2021-03-16
Resolution : 4.10 Å(reported)
Based on initial model : 5LZT

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

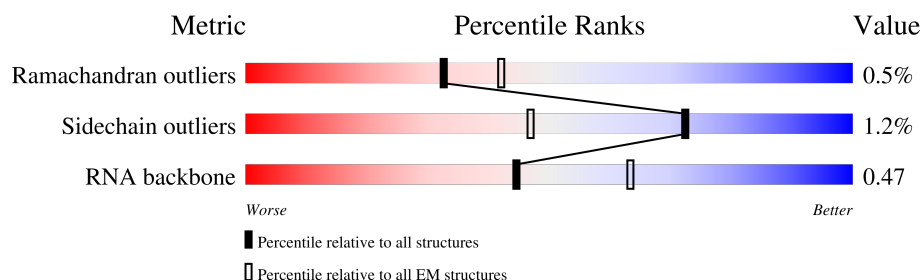
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 4.10 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.





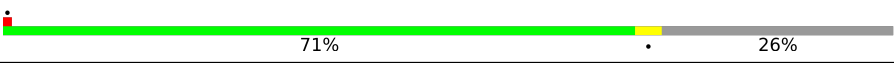
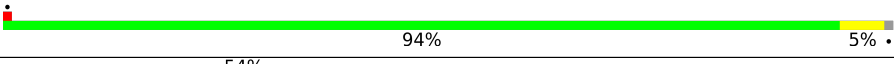

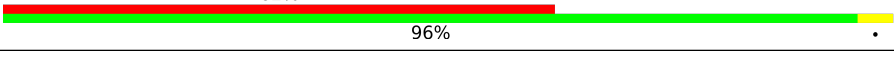
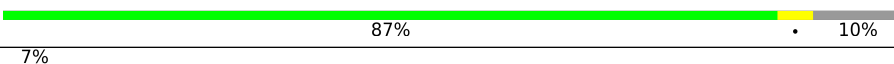

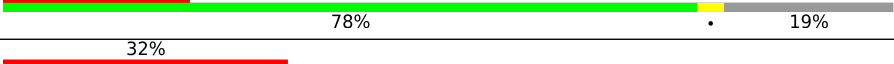
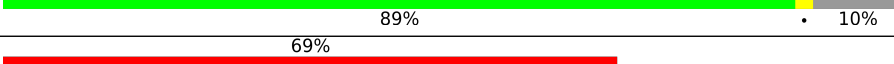
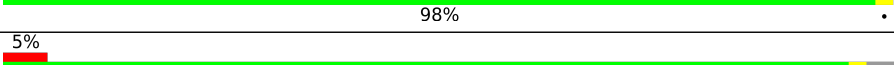
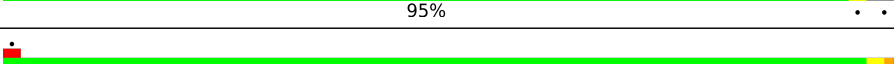
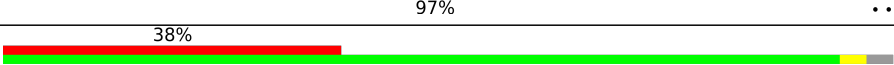
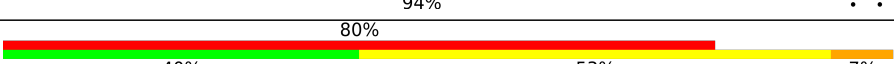
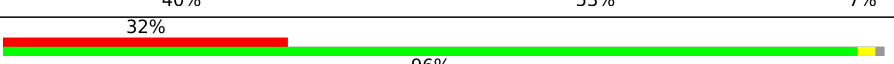
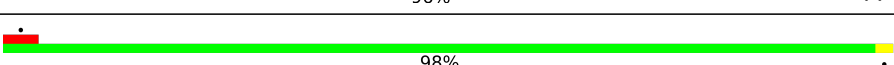
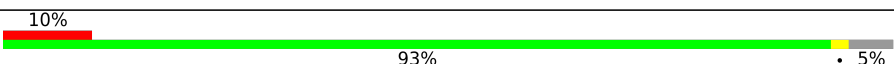
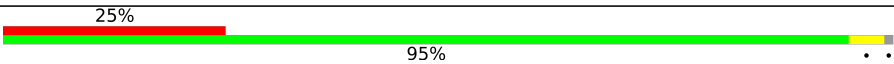
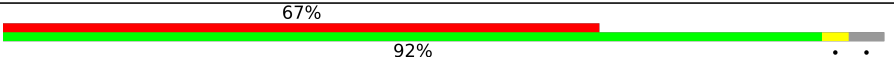
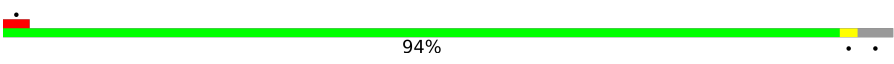

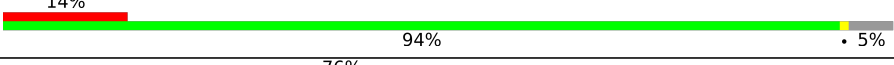
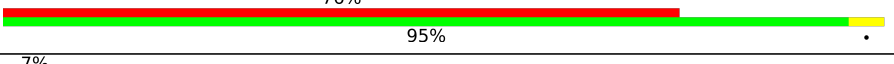
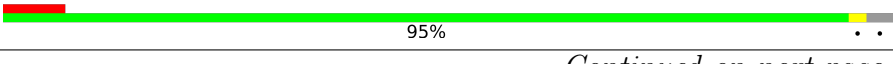

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	249	 95%
2	C	378	 92%
3	d	108	 93% 6% ..
4	DD	281	 47% 78% .. 19%
5	dd	56	 98%
6	D	296	 98%
7	e	129	 96% ..
8	EE	263	 20% 98%

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Mol	Chain	Length	Quality of chain
9	ee	133	
10	b	226	
11	E	291	
12	f	110	
13	FF	204	
14	ff	68	
15	F	249	
16	g	126	
17	BB	264	
18	GG	263	
19	gg	314	
20	G	242	
21	h	123	
22	HH	191	
23	hh	15	
24	bb	84	
25	H	190	
26	i	107	
27	II	208	
28	ii	437	
29	I	214	
30	j	97	
31	JJ	194	
32	jj	428	
33	J	176	

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Mol	Chain	Length	Quality of chain
34	k	70	
35	KK	151	
36	L	211	
37	l	51	
38	LL	158	
39	M	218	
40	m	128	
41	MM	123	
42	N	204	
43	n	25	
44	NN	150	
45	O	203	
46	o	142	
47	OO	156	
48	P	199	
49	p	109	
50	PP	145	
51	Q	188	
52	r	137	
53	QQ	158	
54	R	196	
55	s	318	
56	RR	145	
57	S	176	
58	t	196	

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Mol	Chain	Length	Quality of chain
59	SS	152	
60	T	160	
61	TT	145	
62	U	128	
63	UU	118	
64	V	132	
65	VV	83	
66	W	134	
67	5	3705	
68	WW	139	
69	X	156	
70	7	120	
71	XX	142	
72	Y	134	
73	8	151	
74	YY	146	
75	Z	136	
76	9	1779	
77	ZZ	122	
78	a	147	
79	AA	295	
80	aa	117	
81	B	402	
82	c	115	
83	CC	259	

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Mol	Chain	Length	Quality of chain
84	cc	69	<div><div></div><div>67%</div><div></div><div>84%</div><div></div><div>6%</div><div>10%</div></div>

2 Entry composition [i](#)

There are 88 unique types of molecules in this entry. The entry contains 385116 atoms, of which 165738 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	248	Total	C	H	N	O	S	0	0
			3891	1189	1993	389	314	6		

- Molecule 2 is a protein called uL4.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	362	Total	C	H	N	O	S	0	0
			5936	1812	3053	577	480	14		

- Molecule 3 is a protein called eL31.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	d	107	Total	C	H	N	O	S	0	0
			1818	560	930	171	155	2		

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	DD	228	Total	C	H	N	O	S	0	0
			3632	1126	1864	318	316	8		

- Molecule 5 is a protein called S29.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	dd	55	Total	C	H	N	O	S	0	0
			908	286	449	94	74	5		

- Molecule 6 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	D	293	Total	C	H	N	O	S	0	0
			4815	1512	2424	438	427	14		

- Molecule 7 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	e	128	Total	C	H	N	O	S	0	0
			2200	667	1147	216	165	5		

- Molecule 8 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	EE	262	Total	C	H	N	O	S	0	0
			4253	1324	2177	386	358	8		

- Molecule 9 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	ee	55	Total	C	H	N	O	S	0	0
			935	274	492	97	71	1		

- Molecule 10 is a protein called eL29.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	b	104	Total	C	H	N	O	S	0	0
			1768	527	920	189	129	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	E	216	Total	C	H	N	O	S	0	0
			3617	1115	1888	329	282	3		

- Molecule 12 is a protein called eL33.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	f	109	Total	C	H	N	O	S	0	0
			1788	555	912	174	143	4		

- Molecule 13 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	FF	185	Total	C	H	N	O	S	0	0
			2993	921	1522	277	266	7		

- Molecule 14 is a protein called 40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	ff	68	Total	C	H	N	O	S	0	0
			1120	351	565	103	94	7		

- Molecule 15 is a protein called uL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	F	225	Total	C	H	N	O	S	0	0
			3870	1205	1995	358	303	9		

- Molecule 16 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	g	114	Total	C	H	N	O	S	0	0
			1905	566	999	187	147	6		

- Molecule 17 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	BB	213	Total	C	H	N	O	S	0	0
			3532	1098	1803	309	308	14		

- Molecule 18 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	GG	237	Total	C	H	N	O	S	0	0
			4005	1200	2082	387	329	7		

- Molecule 19 is a protein called Epididymis tissue sperm binding protein Li 3a.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	gg	313	Total	C	H	N	O	S	0	0
			4830	1535	2394	424	465	12		

- Molecule 20 is a protein called L7a.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	G	233	Total	C	H	N	O	S	0	0
			3906	1199	2027	361	315	4		

- Molecule 21 is a protein called uL29.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	h	122	Total	C	H	N	O	S	0	0
			2160	640	1147	204	168	1		

- Molecule 22 is a protein called S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	HH	185	Total	C	H	N	O	S	0	0
			3070	952	1582	271	264	1		

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	hh	15	Total	C	H	N	O	P	0	0
			478	142	161	54	106	15		

- Molecule 24 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	bb	83	Total	C	H	N	O	S	0	0
			1323	408	672	121	115	7		

- Molecule 25 is a protein called L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	H	190	Total	C	H	N	O	S	0	0
			3113	954	1597	284	272	6		

- Molecule 26 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	i	102	Total	C	H	N	O	S	0	0
			1746	520	916	176	129	5		

- Molecule 27 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	II	206	Total	C	H	N	O	S	0	0
			3459	1058	1773	332	291	5		

- Molecule 28 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	ii	419	Total	C	H	N	O	S	0	0
			6638	2104	3331	562	629	12		

- Molecule 29 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	I	205	Total	C	H	N	O	S	0	0
			3376	1056	1712	321	274	13		

- Molecule 30 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	j	86	Total	C	H	N	O	S	0	0
			1442	434	737	155	111	5		

- Molecule 31 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	JJ	185	Total	C	H	N	O	S	0	0
			3165	969	1640	306	248	2		

- Molecule 32 is a protein called eRF3a.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	jj	428	Total	C	H	N	O	S	0	0
			6787	2144	3419	580	623	21		

- Molecule 33 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	J	170	Total	C	H	N	O	S	0	0
			2761	861	1399	254	241	6		

- Molecule 34 is a protein called L38.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	k	69	Total	C	H	N	O	S	0	0
			1206	366	637	103	99	1		

- Molecule 35 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	KK	96	Total	C	H	N	O	S	0	0
			1646	530	836	143	131	6		

- Molecule 36 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	L	210	Total	C	H	N	O	S	0	0
			3522	1065	1820	354	279	4		

- Molecule 37 is a protein called eL39.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	1	50	Total	C	H	N	O	S	0	0
			927	286	480	96	64	1		

- Molecule 38 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	LL	143	Total	C	H	N	O	S	0	0
			2425	749	1250	222	198	6		

- Molecule 39 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	M	138	Total	C	H	N	O	S	0	0
			2348	727	1211	221	182	7		

- Molecule 40 is a protein called 60S RIBOSOMAL PROTEIN EL40.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	m	52	Total	C	H	N	O	S	0	0
			894	266	465	90	67	6		

- Molecule 41 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	MM	117	Total	C	H	N	O	S	0	0
			1847	570	939	161	169	8		

- Molecule 42 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	N	203	Total	C	H	N	O	S	0	0
			3451	1072	1750	359	266	4		

- Molecule 43 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	n	25	Total	C	H	N	O	S	0	0
			525	145	286	64	27	3		

- Molecule 44 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	NN	149	Total	C	H	N	O	S	0	0
			2491	770	1289	228	203	1		

- Molecule 45 is a protein called 60S RIBOSOMAL PROTEIN UL13.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	O	199	Total	C	H	N	O	S	0	0
			3408	1051	1778	319	255	5		

- Molecule 46 is a protein called eL42.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	o	104	Total	C	H	N	O	S	0	0
			1771	533	920	174	138	6		

- Molecule 47 is a protein called uS11.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	OO	136	Total	C	H	N	O	S	0	0
			2055	621	1039	199	190	6		

- Molecule 48 is a protein called uL22.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	P	153	Total	C	H	N	O	S	0	0
			2516	777	1274	241	215	9		

- Molecule 49 is a protein called ribosomal protein eL43.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	p	91	Total	C	H	N	O	S	0	0
			1466	445	758	136	120	7		

- Molecule 50 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	PP	120	Total	C	H	N	O	S	0	0
			2042	635	1045	187	168	7		

- Molecule 51 is a protein called eL18.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	Q	187	Total	C	H	N	O	S	0	0
			3149	946	1634	315	250	4		

- Molecule 52 is a protein called eL28.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	r	124	Total	C	H	N	O	S	0	0
			2045	616	1051	205	167	6		

- Molecule 53 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	QQ	142	Total	C	H	N	O	S	0	0
			2323	717	1195	213	195	3		

- Molecule 54 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	R	180	Total	C	H	N	O	S	0	0
			3172	933	1664	328	238	9		

- Molecule 55 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	s	196	Total	C	H	N	O	S	0	0
			3071	959	1564	263	276	9		

- Molecule 56 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	RR	132	Total	C	H	N	O	S	0	0
			2189	670	1121	199	195	4		

- Molecule 57 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	S	176	Total	C	H	N	O	S	0	0
			2970	930	1508	285	236	11		

- Molecule 58 is a protein called uL12.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	t	153	Total	C	H	N	O	S	0	0
			2375	722	1215	218	217	3		

- Molecule 59 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	SS	144	Total	C	H	N	O	S	0	0
			2437	746	1247	241	202	1		

- Molecule 60 is a protein called eL21.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	T	159	Total	C	H	N	O	S	0	0
			2665	823	1367	252	217	6		

- Molecule 61 is a protein called eS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	TT	141	Total	C	H	N	O	S	0	0
			2229	688	1132	211	195	3		

- Molecule 62 is a protein called L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	U	99	Total	C	H	N	O	S	0	0
			1642	519	833	141	147	2		

- Molecule 63 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	UU	100	Total	C	H	N	O	S	0	0
			1657	498	862	152	141	4		

- Molecule 64 is a protein called eL14.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	V	131	Total	C	H	N	O	S	0	0
			2018	618	1039	184	172	5		

- Molecule 65 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	VV	83	Total	C	H	N	O	S	0	0
			1273	393	637	117	121	5		

- Molecule 66 is a protein called 60S ribosomal protein L24-like protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	W	106	Total	C	H	N	O	S	0	0
			1752	538	892	174	144	4		

- Molecule 67 is a RNA chain called 28S Ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	5	3543	Total	C	H	N	O	P	0	0
			114361	33833	38389	13910	24686	3543		

- Molecule 68 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	WW	129	Total	C	H	N	O	S	0	0
			2114	659	1080	193	176	6		

- Molecule 69 is a protein called uL23.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	X	118	Total	C	H	N	O	S	0	0
			2007	618	1040	181	167	1		

- Molecule 70 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	7	120	Total	C	H	N	O	P	0	0
			3854	1141	1296	456	842	119		

- Molecule 71 is a protein called 40S ribosomal protein uS12.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	XX	141	Total	C	H	N	O	S	0	0
			2263	693	1165	219	183	3		

- Molecule 72 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	Y	134	Total	C	H	N	O	S	0	0
			2320	700	1205	226	186	3		

- Molecule 73 is a RNA chain called 5.8S Ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	8	151	Total	C	H	N	O	P	0	0
			4837	1432	1629	564	1062	150		

- Molecule 74 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	YY	124	Total	C	H	N	O	S	0	0
			2094	640	1083	198	168	5		

- Molecule 75 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	Z	135	Total	C	H	N	O	S	0	0
			2289	714	1182	208	182	3		

- Molecule 76 is a RNA chain called 18S Ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	9	1698	Total	C	H	N	O	P	0	0
			54557	16180	18308	6508	11864	1697		

- Molecule 77 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	ZZ	75	Total	C	H	N	O	S	0	0
			1254	382	656	111	104	1		

- Molecule 78 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	a	147	Total	C	H	N	O	S	0	0
			2372	734	1210	239	185	4		

- Molecule 79 is a protein called 40S_SA_C domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	AA	217	Total	C	H	N	O	S	0	0
			3418	1086	1708	300	316	8		

- Molecule 80 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	aa	101	Total	C	H	N	O	S	0	0
			1678	507	864	170	132	5		

- Molecule 81 is a protein called uL3.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	B	394	Total	C	H	N	O	S	0	0
			6482	2020	3310	597	542	13		

- Molecule 82 is a protein called eL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	c	98	Total	C	H	N	O	S	0	0
			1555	481	794	134	140	6		

- Molecule 83 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	CC	221	Total	C	H	N	O	S	0	0
			3522	1111	1806	295	301	9		

- Molecule 84 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	cc	62	Total	C	H	N	O	S	0	0
			1002	297	514	97	92	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
cc	5	HIS	ARG	conflict	UNP G1TIB4

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	dd	1	Total	Zn	0
			1	1	
85	ff	1	Total	Zn	0
			1	1	
85	g	1	Total	Zn	0
			1	1	
85	j	1	Total	Zn	0
			1	1	
85	m	1	Total	Zn	0
			1	1	
85	o	1	Total	Zn	0
			1	1	
85	p	1	Total	Zn	0
			1	1	
85	aa	1	Total	Zn	0
			1	1	

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

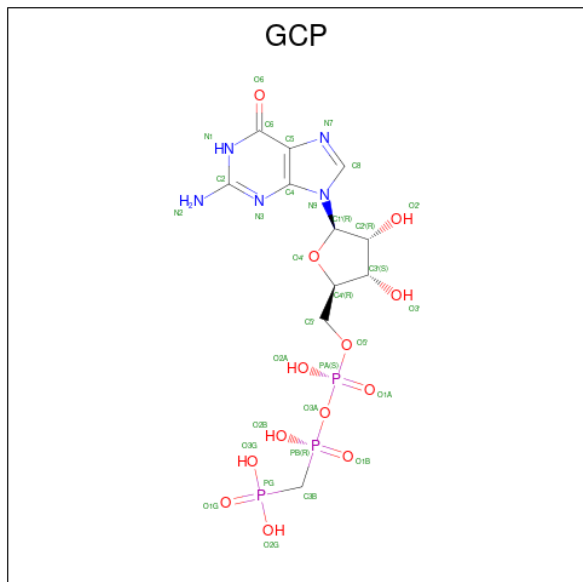
Mol	Chain	Residues	Atoms		AltConf
86	hh	2	Total	Mg	0
			2	2	
86	j	1	Total	Mg	0
			1	1	
86	jj	1	Total	Mg	0
			1	1	
86	o	1	Total	Mg	0
			1	1	
86	P	1	Total	Mg	0
			1	1	
86	V	1	Total	Mg	0
			1	1	

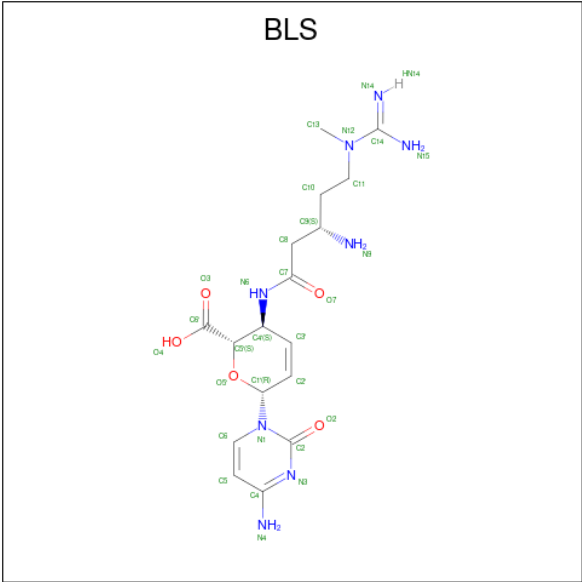
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Mol	Chain	Residues	Atoms		AltConf
86	5	189	Total	Mg	0
			189	189	
86	7	4	Total	Mg	0
			4	4	
86	8	10	Total	Mg	0
			10	10	
86	9	70	Total	Mg	0
			70	70	
86	a	1	Total	Mg	0
			1	1	

- Molecule 87 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



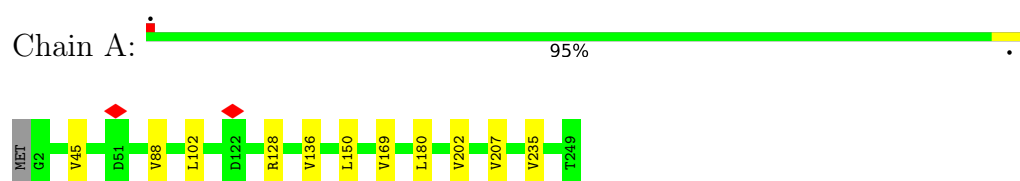


Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
88	5	1	55	17	25	8	5	0

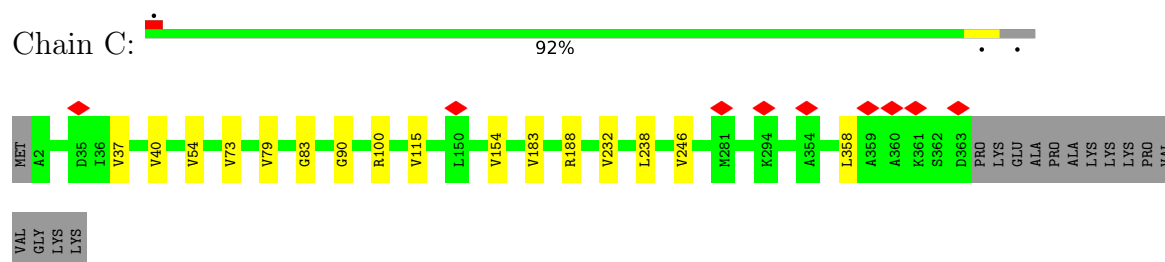
3 Residue-property plots [i](#)

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.

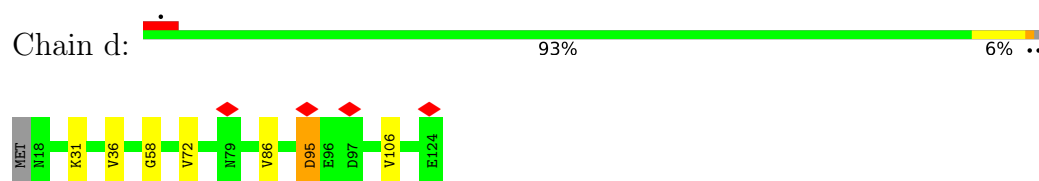
- Molecule 1: 60S ribosomal protein L8



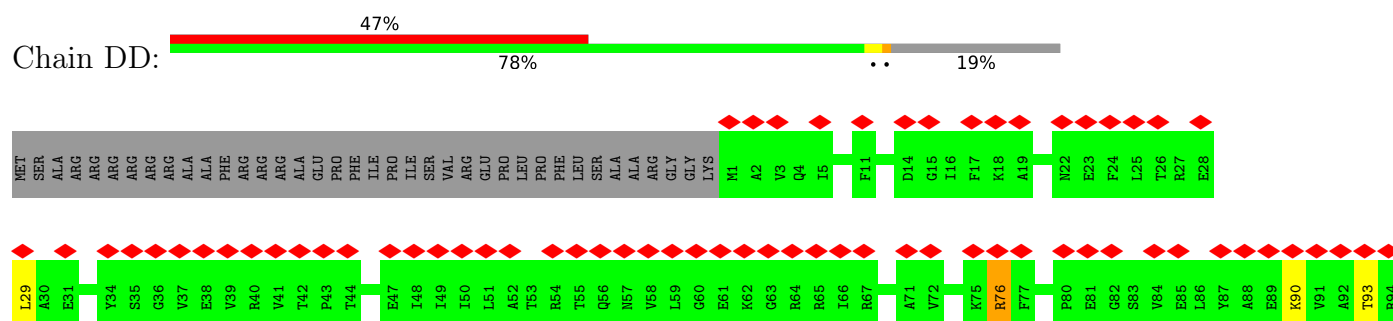
- Molecule 2: uL4

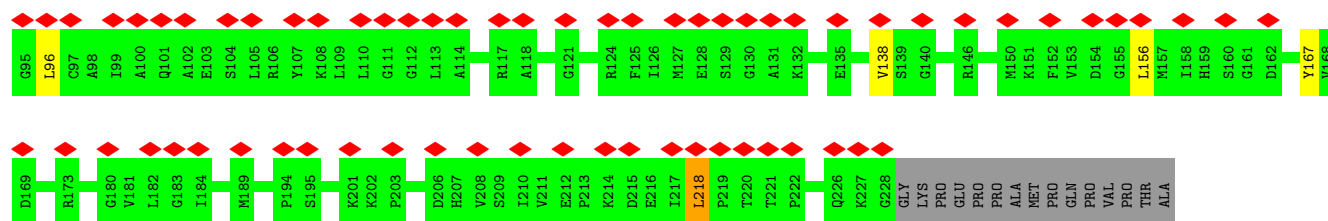


- Molecule 3: eL31

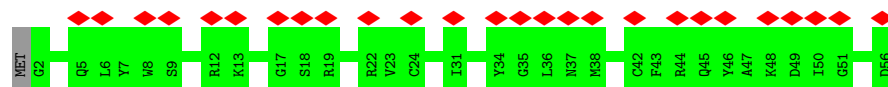


- Molecule 4: 40S ribosomal protein S3

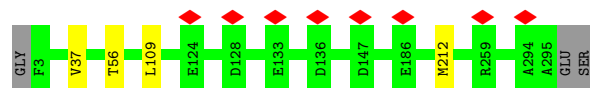




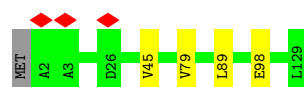
• Molecule 5: S29



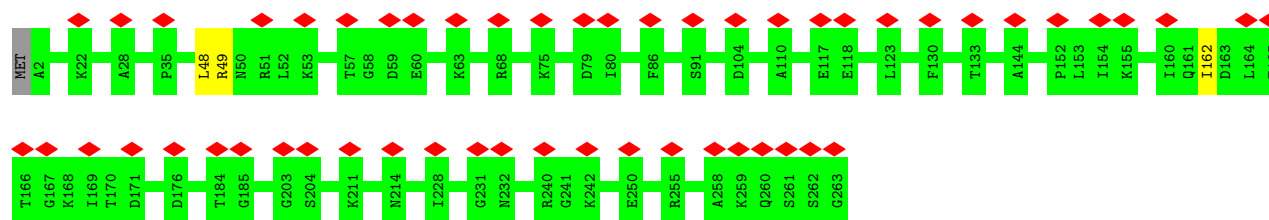
• Molecule 6: 60S ribosomal protein L5



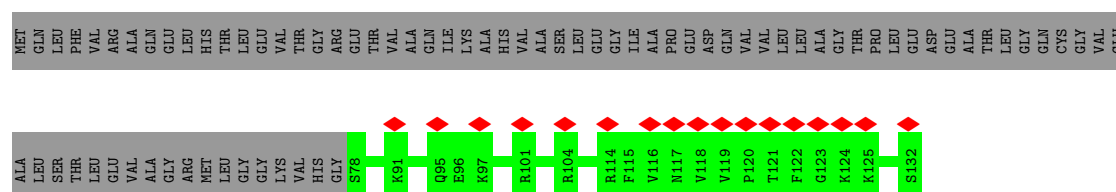
• Molecule 7: Ribosomal protein L32



• Molecule 8: 40S ribosomal protein S4

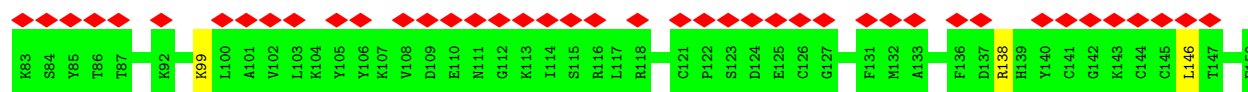


• Molecule 9: 40S ribosomal protein S30



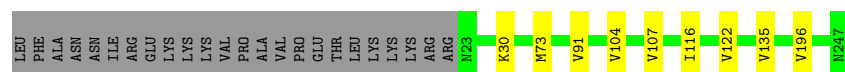
Chain b: 

Chain ff:  62% 96%



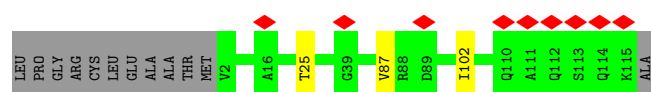
• Molecule 15: uL30

Chain F: 87% 10%



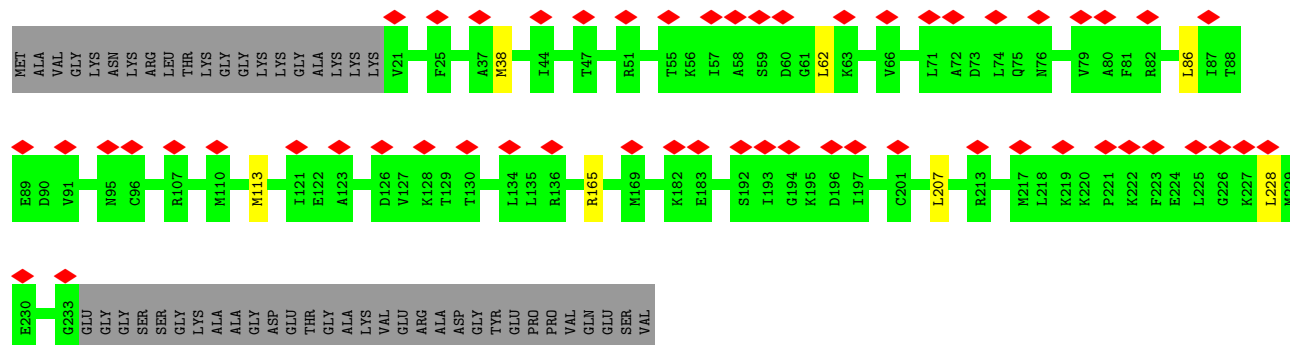
• Molecule 16: 60S ribosomal protein L34

Chain g: 7% 88% 10%



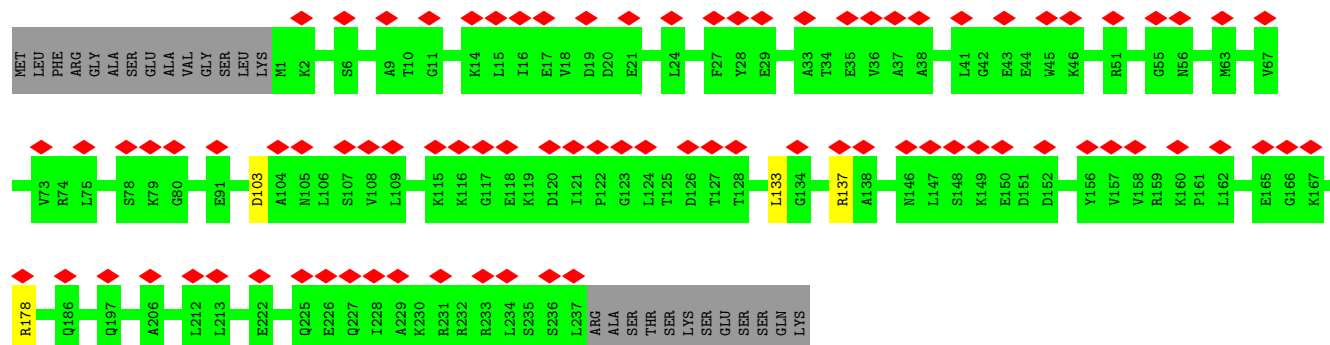
• Molecule 17: 40S ribosomal protein S3a

Chain BB: 21% 78% 19%

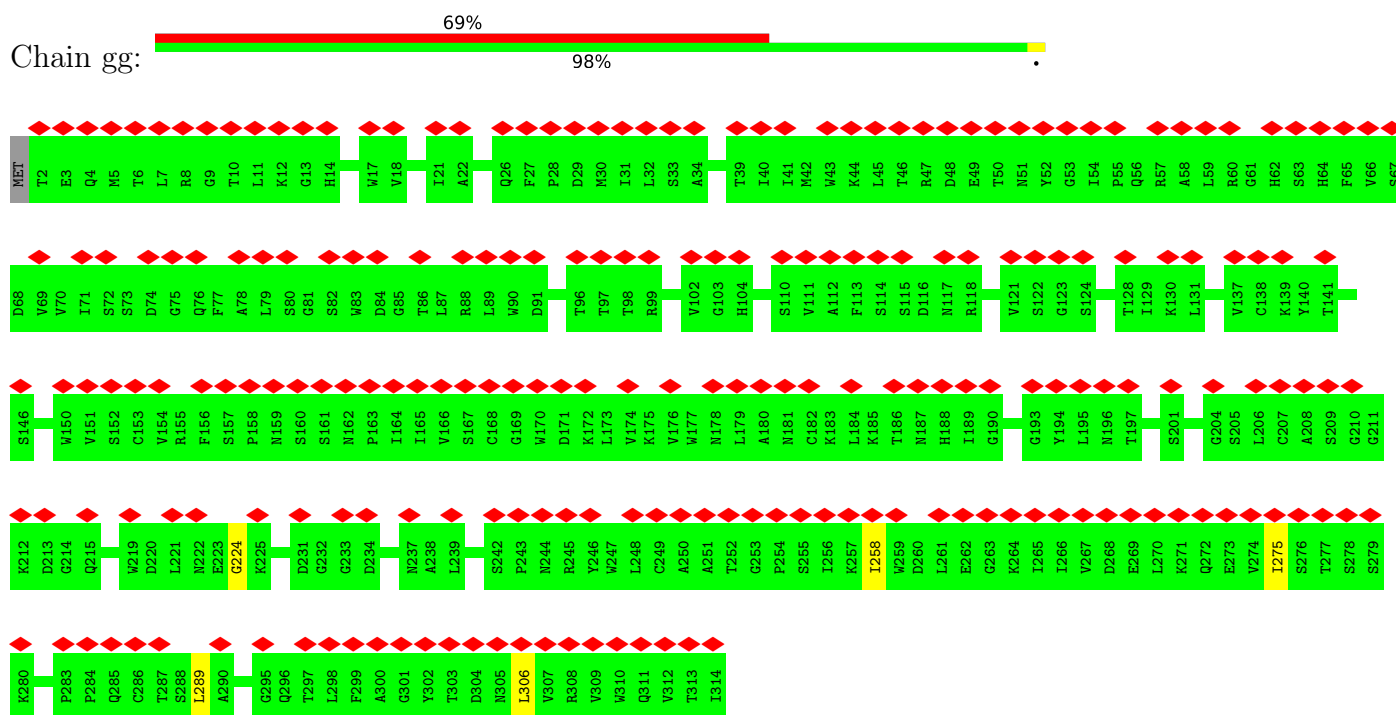


• Molecule 18: 40S ribosomal protein S6

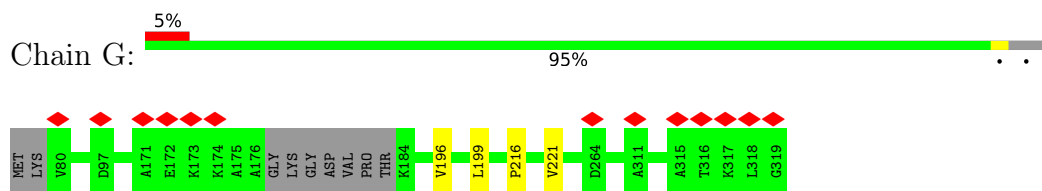
Chain GG: 32% 89% 10%



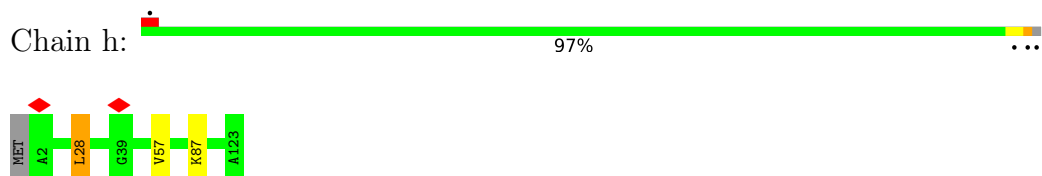
• Molecule 19: Epididymis tissue sperm binding protein Li 3a



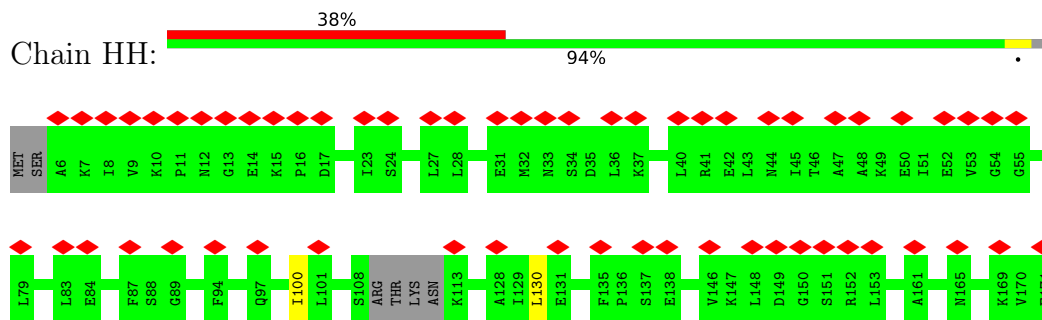
- Molecule 20: L7a



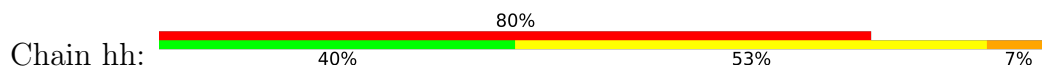
- Molecule 21: uL29

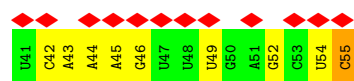


- Molecule 22: S7

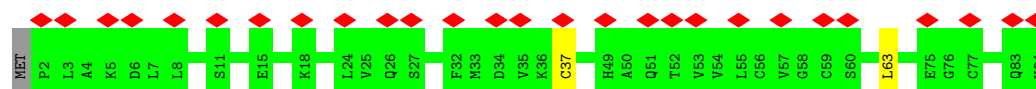


- Molecule 23: mRNA

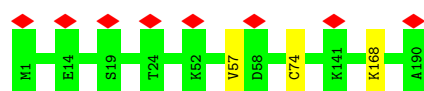




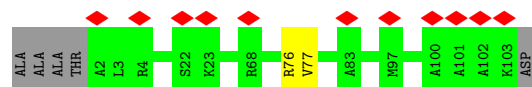
- Molecule 24: 40S ribosomal protein S27



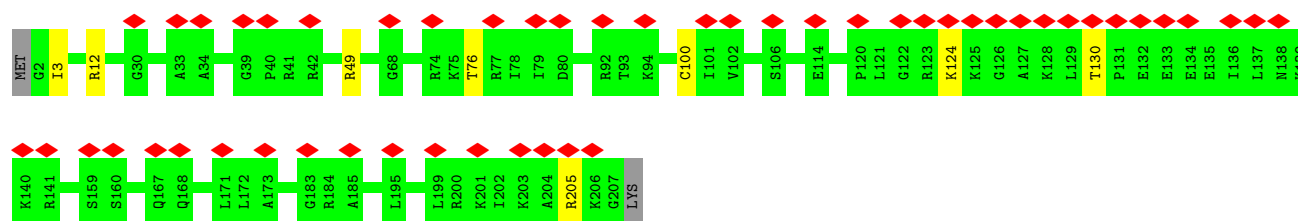
- Molecule 25: L9



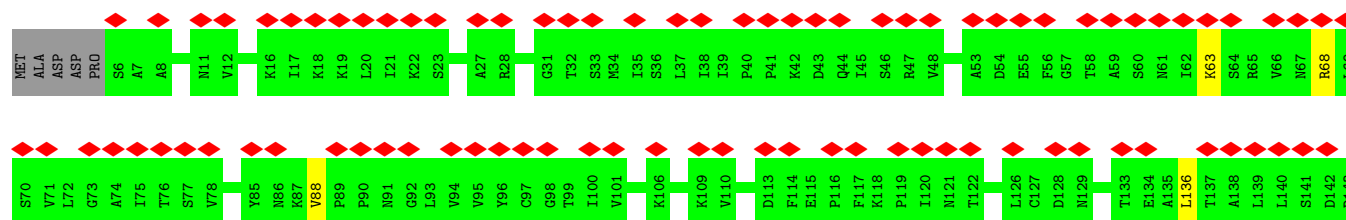
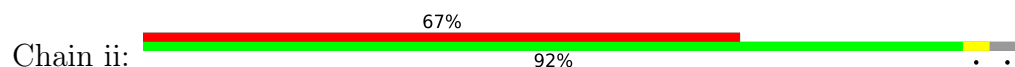
- Molecule 26: 60S ribosomal protein L36

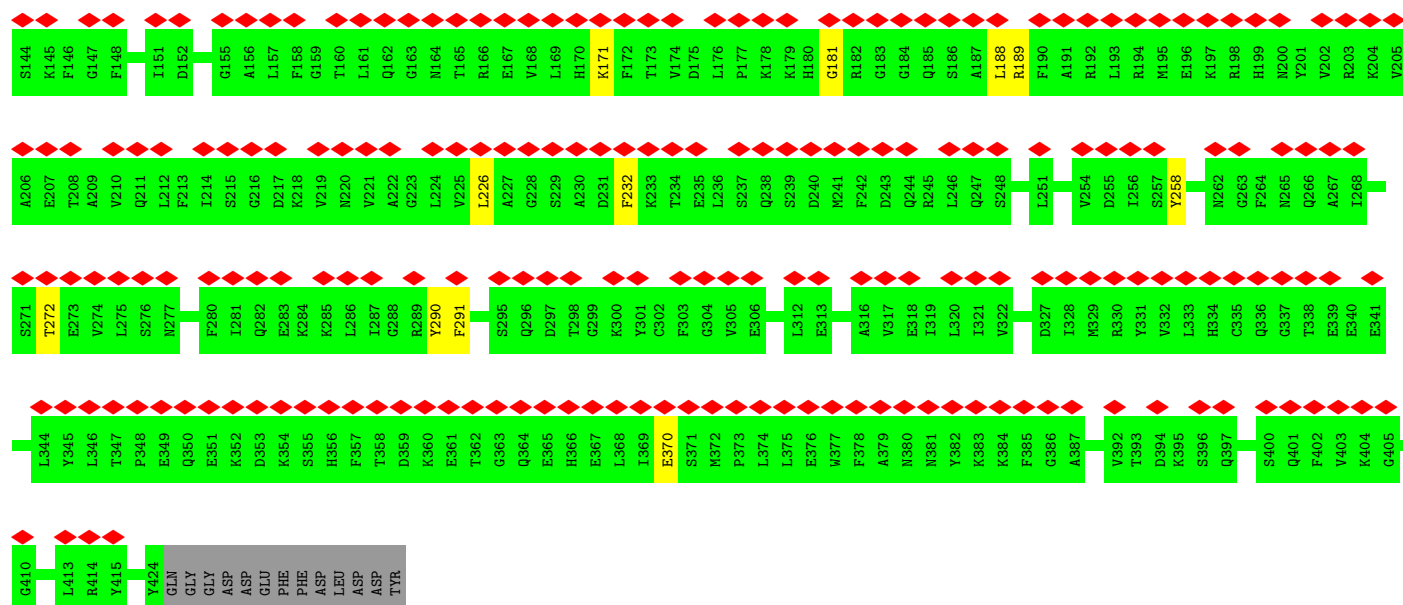


- Molecule 27: 40S ribosomal protein S8



- Molecule 28: Eukaryotic peptide chain release factor subunit 1

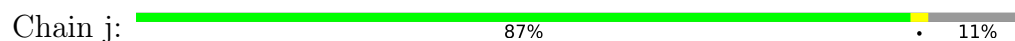




- Molecule 29: 60S ribosomal protein L10



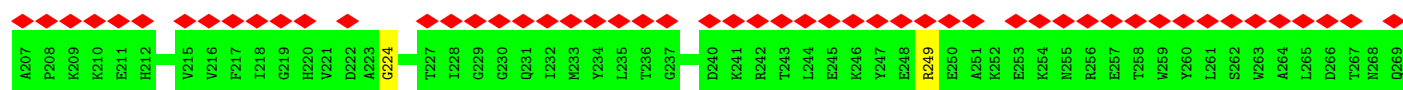
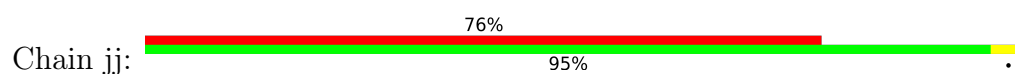
- Molecule 30: Ribosomal protein L37

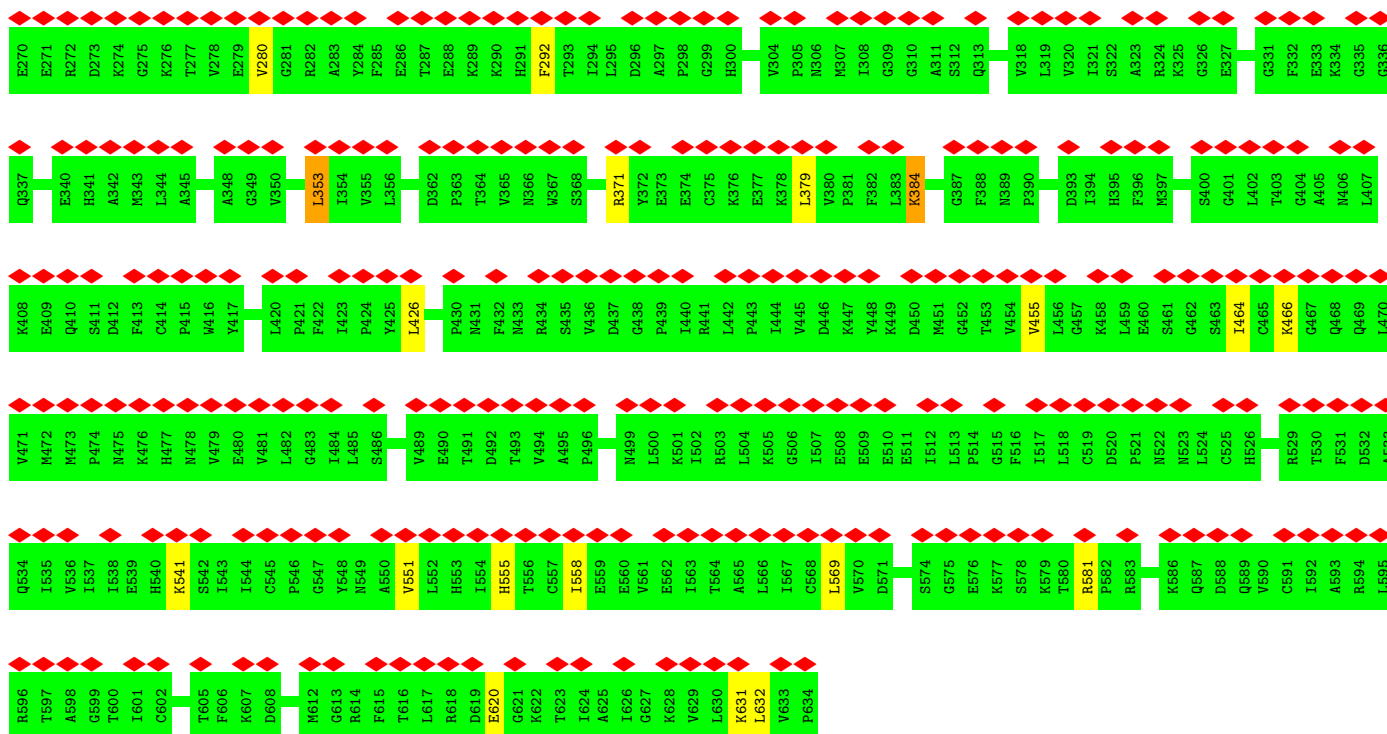


- Molecule 31: 40S ribosomal protein S9

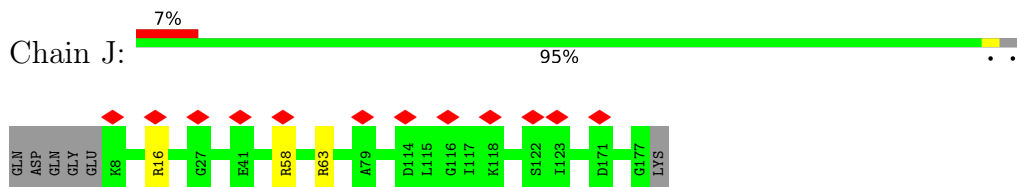


- Molecule 32: eRF3a

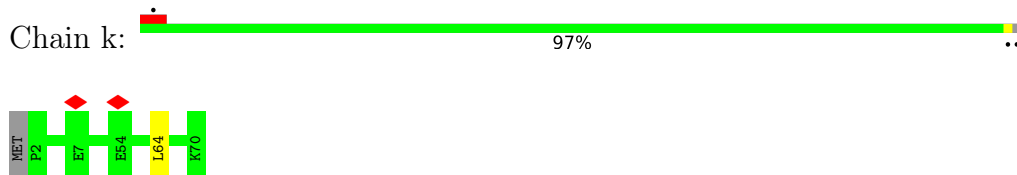




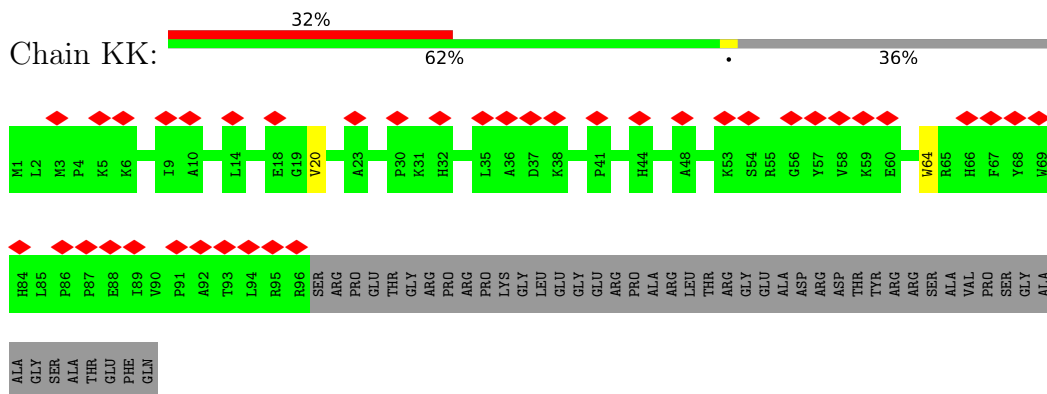
• Molecule 33: 60S ribosomal protein L11



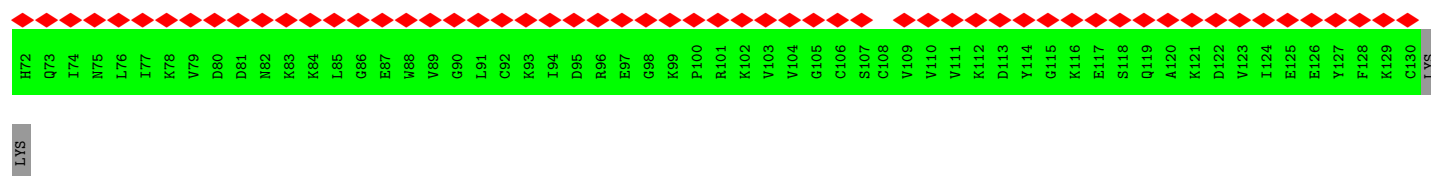
• Molecule 34: L38



• Molecule 35: 40S ribosomal protein S10



- [illegible]



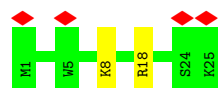
- Molecule 42: Ribosomal protein L15

Chain N: 93% 6%



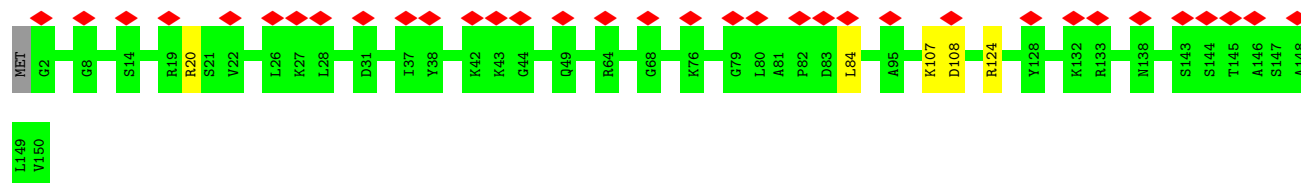
- Molecule 43: 60s ribosomal protein l41

Chain n: 16% 92% 8%



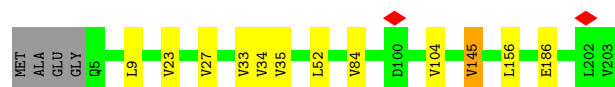
- Molecule 44: ribosomal protein uS15

Chain NN: 23% 96% . .



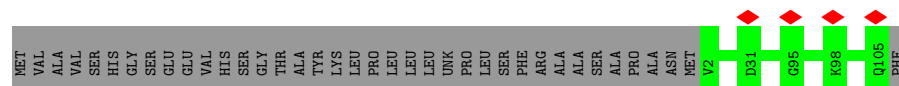
- Molecule 45: 60S RIBOSOMAL PROTEIN UL13

Chain O: 92% 5% .



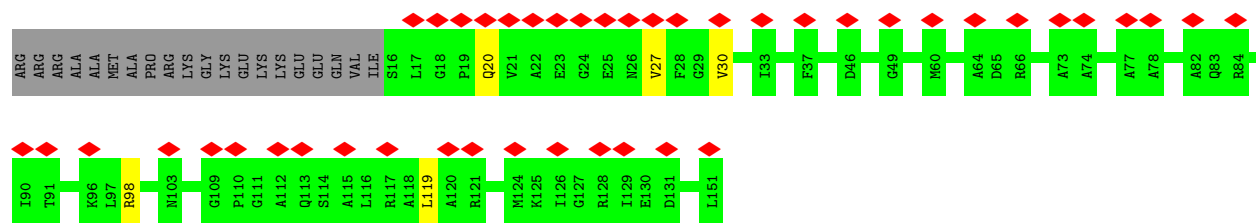
- Molecule 46: eL42

Chain o: 73% 27%

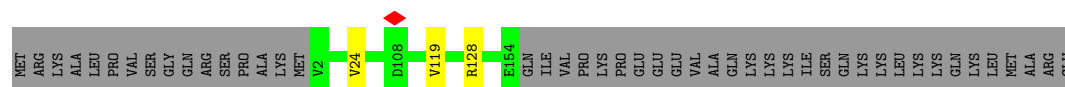


- Molecule 47: uS11

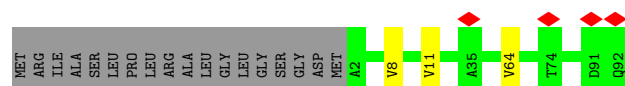
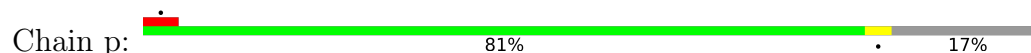
Chain OO: 28% 84% . 13%



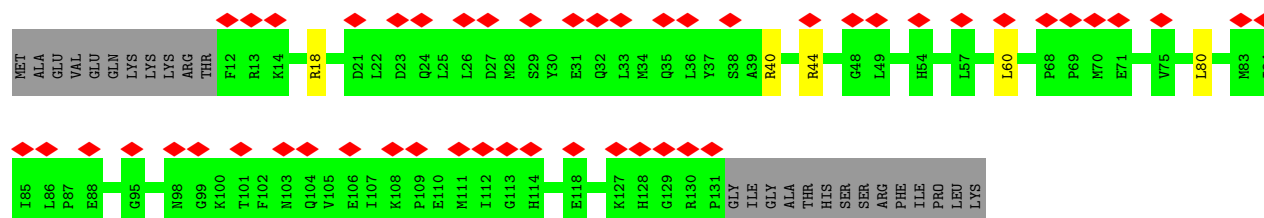
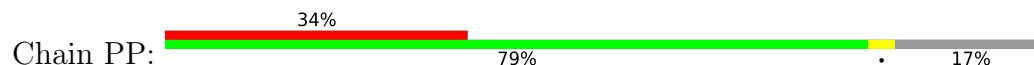
• Molecule 48: uL22



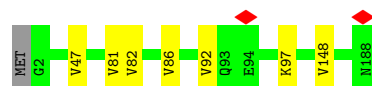
• Molecule 49: ribosomal protein eL43



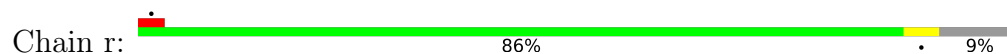
• Molecule 50: 40S ribosomal protein uS19




• Molecule 51: eL18

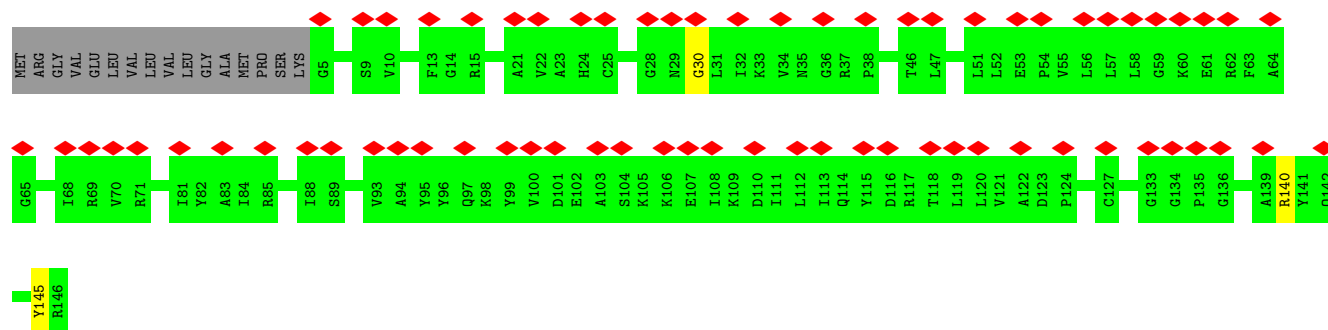


• Molecule 52: eL28




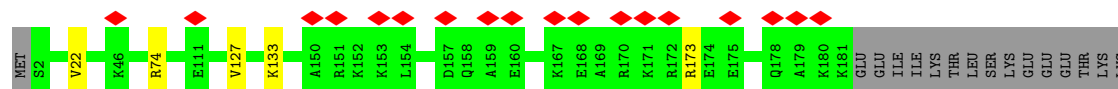
• Molecule 53: Ribosomal protein S16

Chain QQ: 



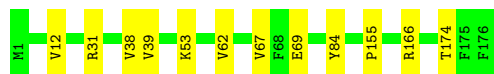
- Molecule 54: 60S ribosomal protein L19

Chain R: 




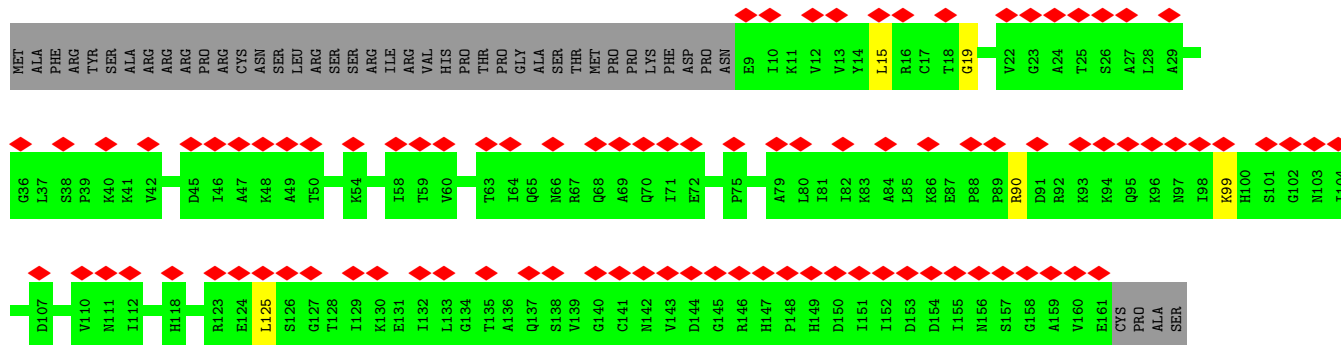
- Molecule 57: 60S ribosomal protein L18a

Chain S:  93% 7%



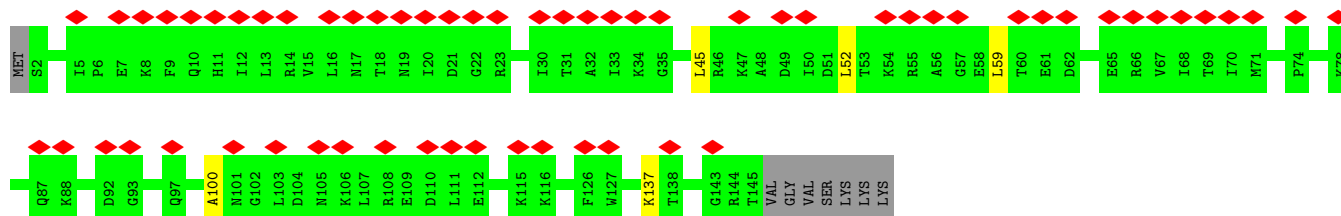
- Molecule 58: uL12

Chain t:  48% 76% 22%



- Molecule 59: 40S ribosomal protein uS13

Chain SS:  40% 91% 5%



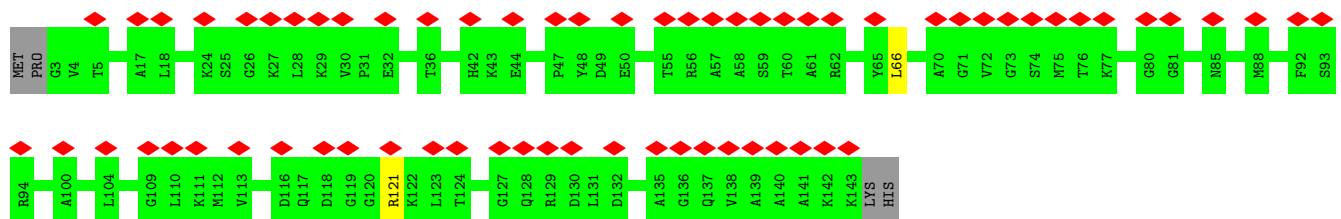
- Molecule 60: eL21

Chain T:  97% 2% 1%




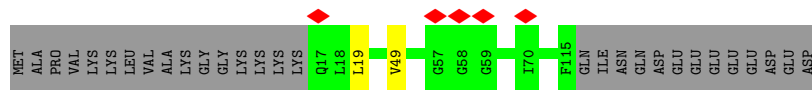
- Molecule 61: eS19

Chain TT:  46% 96% 2% 1%




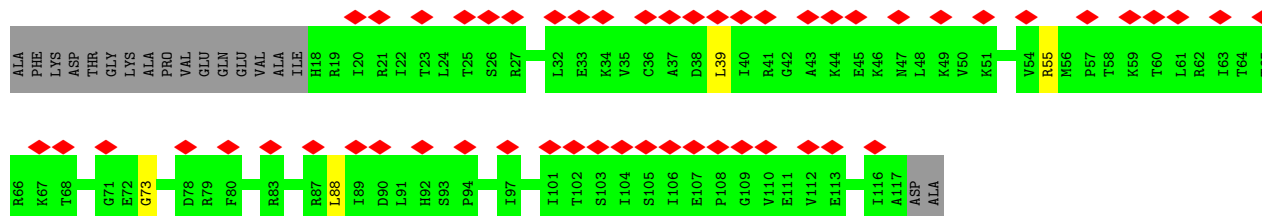
- Molecule 62: L22

Chain U:  76% 23%



- Molecule 63: 40S ribosomal protein S20

Chain UU:  45% 81% 15%



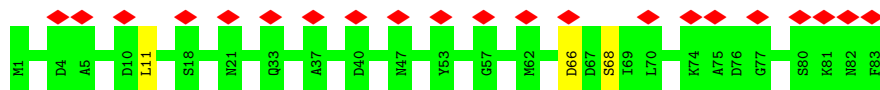
- Molecule 64: eL14

Chain V:  5% 95%




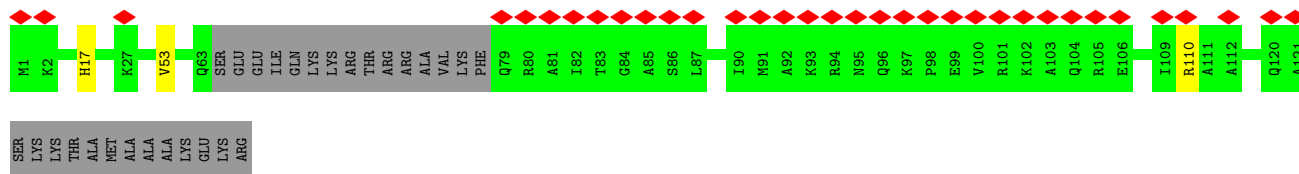
- Molecule 65: 40S ribosomal protein S21

Chain VV:  25% 96%



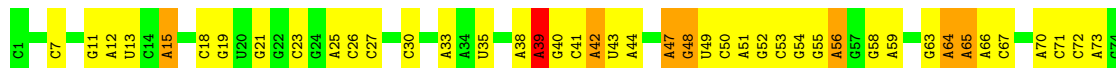
- Molecule 66: 60S ribosomal protein L24-like protein

Chain W:  25% 77% 21%



- Molecule 67: 28S Ribosomal RNA

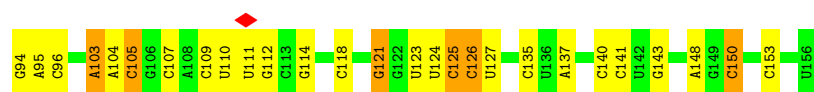
Chain 5:  50% 39% 7%



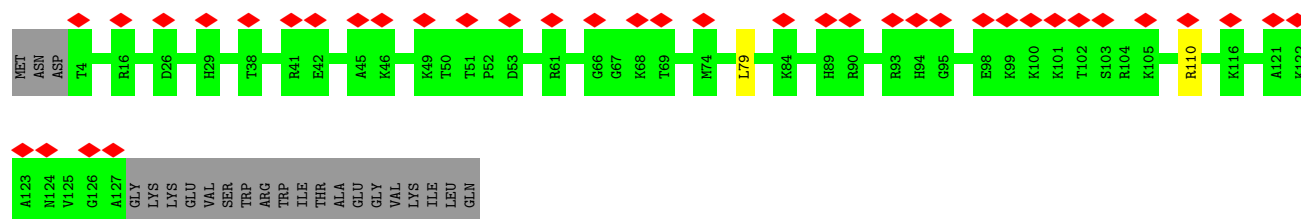
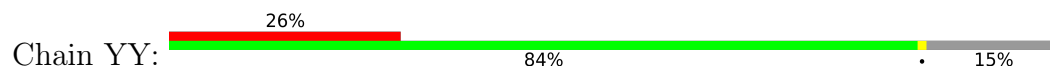
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A1553	A1554	U1556	G1561	G1562	A1563	A1564	A1565	C1566	G1573	A1574	A1575	U1576	U1577	U1578	U1579	C1580	G1581	G1584	G1585	G1586	G1587	U1588	C1589	C1590	U1591	C1594	G1595	U1596	U1599	A1600	A1601	U1602	C1603	C1607	G1608	U1609	C1610	C1611	G1612	A1613	G1619	G1623	G1625	G1626	G1627	C1628	C1629	A1630	A1631	A1632	G1633																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
C1384	A1387	G1390	G1394	U1395	G1396	A1397	A1398	C1401	C1402	G1403	G1404	G1411C	G1415	G1416	C1417	C	A	G1418	G1419	A1420	G1421	A1427	U1428	C1429	G1435	C1436	C1437	U1438	U1440	C1441	C1442	U1445	U1446	A1451	A1452	G1453	G1454	G1455	C1456	G1457	C1458	U1459	C1460	G1465	C1469	G1475																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
C1313	C1314	C1315	G1316	U1317	C1318	G1321	A1322	A1323	A1326	C1327	G1328	G1329	A1330	C1331	C1332	A1333	A1337	G1338	U1339	C1340	U1341	A1342	A1343	C1346	C1350	G1351	C1352	G1353	A1354	C1357	G1358	G1359	G1360	C1363	U1364	A	C	A	A1368	C1369	G1370	A1371	A1372	A1373	G1377	C1378	C1379	G1380	U1381	G1382	G1383																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
C1237	A1238	C1239	A	C	C	G1244	C1252	A	C	C	C	C	C	C	C	C	A	G1271	C1272	G1273	A1274	G1275	C1276	C1277	C1278	C1280	G1281	G1282	G1283	G1284	G1287	G1288	G1291	C1292	G1293	A1294	U1295	G1296	U1297	C1298	G1299	G1300	C1301	U1302	A1303	C1304	C1305	C1306	A1307	C1308	C1309	C1310																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
U1100	A	C	A	C	A	A	A	A	G1168	G1169	G1170	G1171	G1174	U1177	G1178	U1179	C1180	A	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
U945	G951	G955	A956	G957	G958	G959	A960	G961	C962	G965	A966	C967	C968	C969	G970	U971	G971A	C972	C973	C977	G978	C979	C983	C990	G1064	G1065	C1071	C1072	A	C	A	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
C738A	G739	C740	C741	A747	G748	G749	U750	G756	G757	G758	G759	G760	A	C	A	C	A	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
C	A	C	A	G638	C643	A649	C650	C651	C654	G655	C656	C657	C658	G666	A667	C668	C671	C672	C676	C683	G684	C685	A686	U687	C696	G697	C704	G705	C706	C707	G708	A711	C712	C713	C719	G722	C727	U728	G729	G730	G731	A732	A733	G734	C738																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
G437	C446	C449	G450	C451	A452	U454	G457	U467	U468	C469	C480	G481	C481A	G482	G483	U484	C485	C486	C489	U492	G493	C494	C495	G496	G497	C498	G499	G500	A	C	C	G504	G505	U510	C511	U512	A	C	C	C515	C521	C522	C523	A	C	A	C	C	C	C	A																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
C339	C340	G342	C343	A344	C350	C351	G352	A353	U354	A355	G356	U357	C358	A359	A360	C361	A362	A363	G364	G375	G382	A383	A384	A385	A386	G387	G399	A400	G401	C406	A407	A408	G409	A410	U313	G314	G315	U316	C320	U321	C322	G223	G224	U225	G226	A227	G229	U233	G234	C238	C239	G240	G241	C245	G246	G253																																																																																																																																																																																																																																																																																																																																																																																																																																																														
G262	G263	C264	C265	C266	G267	C275	C276	G277	G278	A279	G280	U281	A	C	C	A	G182	A	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C

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G2855	U2819	U2554	C2470	G2394	U2298	G2098	C2022	G1945	G1877	G1798	A
G2856	C2820	G2555	G2471	A2395	G2299	C2099	C2023	G1948	G1879	U1800	
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G2859	U2826	G2566	G2474	U2398	G2302	G2102	A2026	U1957	U1882	A1804	
U2661	G2827	G2567	G2475	G2399	A2313	A2103	A2026	U1958	U1883	U1726	
G2862	G2828	G2568	G2476	G2400	G2314	A2104	A2026	A1959	G1884	U1727	
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G2864	G2751	C2572	G2478	A2402	C2317	G2106	A2026	U1961	U1886	U1728	
	G2752	C2573	G2479	A2403	G2318	A2107	A2026	U1962	U1887	A1729	
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		G2602	G2507	G2431	G2346	G2135	A2026		G1762		
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		G2606	G2511	G2435	G2350	G2139	A2026		U1847		
		G2607	G2512	G2436	G2351	G2140	A2026		G1851		
		G2608	G2513	G2437	G2352	G2141	A2026		U1852		
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		G2693	G2598	G2522	G2437	G2226	A2026				
		G2694	G2599	G2523	G2438	G2227	A2026				
		G2695	G2600	G2524	G2439	G2228	A2026				
		G2696	G2601	G2525	G2440	G2229	A2026				
		G2697	G2602	G2526	G2441	G2230	A2026				
		G2698	G2603	G2527	G2442	G2231	A2026				
		G2699	G2604	G2528	G2443	G2232	A2026				
		G2700	G2605	G2529	G2444	G2233	A2026				
		G2701	G2606	G2530	G2445	G2234	A2026				
		G2702	G2607	G2531	G2446	G2235	A2026				
		G2703	G2608	G2532	G2447	G2236	A2026				
		G2704	G2609	G2533	G2448	G2237	A2026				
		G2705	G2610	G2534	G2449	G2238	A2026				
		G2706	G26								

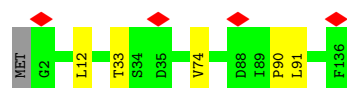




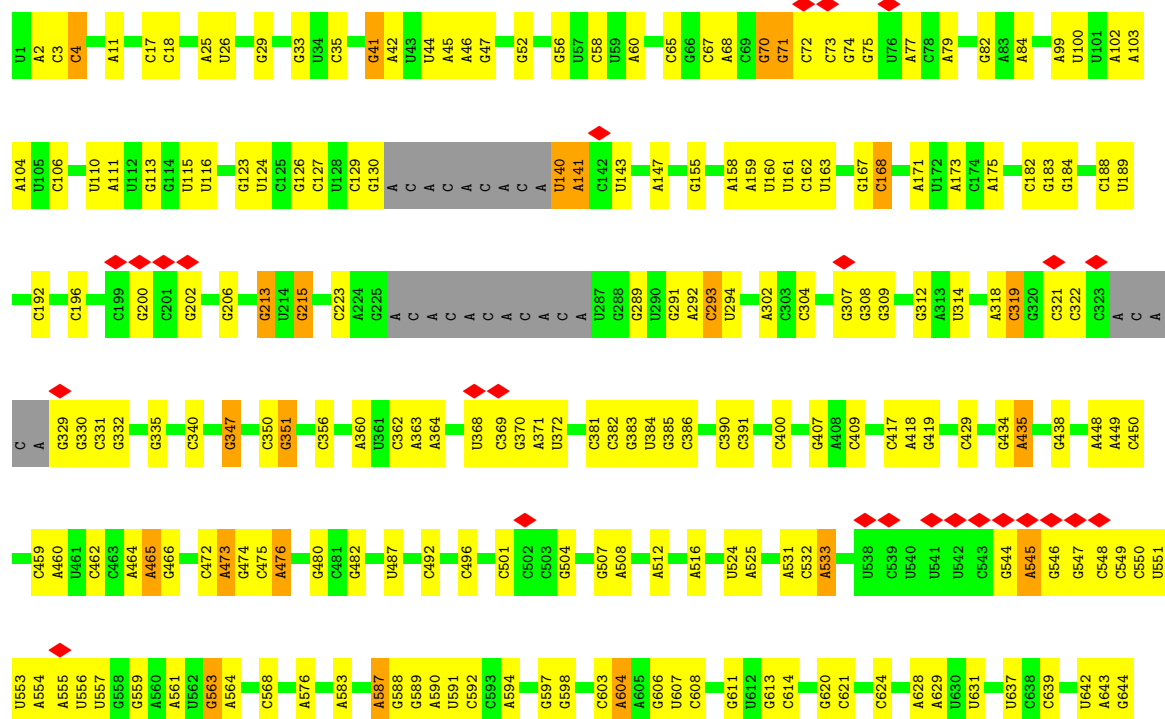
- Molecule 74: 40S ribosomal protein S24

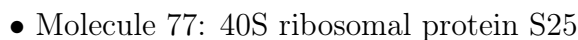


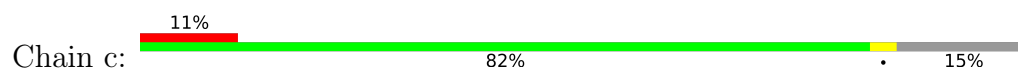
- Molecule 75: 60S ribosomal protein L27

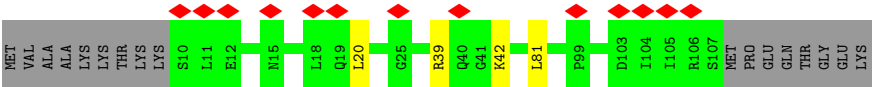


- Molecule 76: 18S Ribosomal RNA

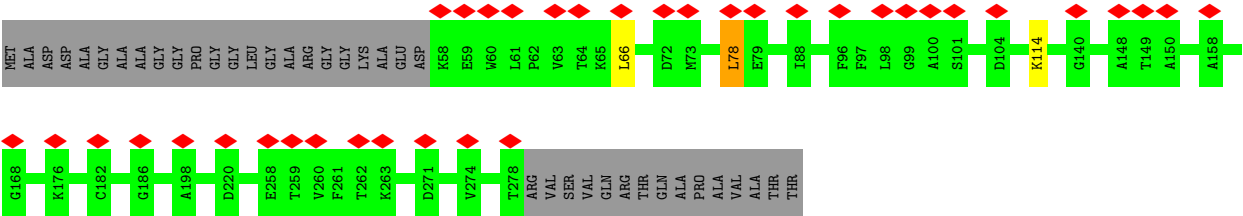
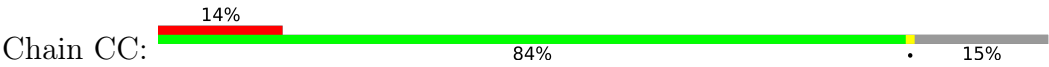




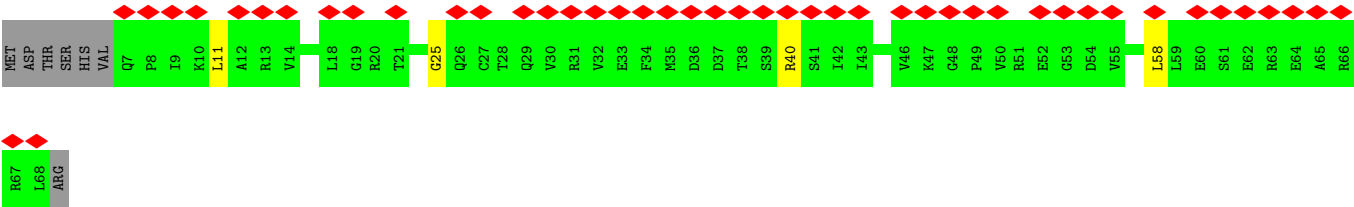
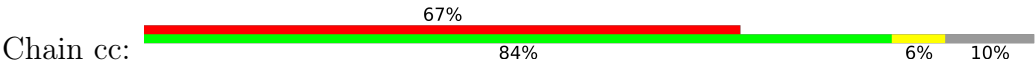




• Molecule 83: 40S ribosomal protein S2



• Molecule 84: 40S ribosomal protein S28



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18937	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 ($e^-/\text{\AA}^2$)	41.92	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	79000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	405.0, 405.0, 405.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BLS, GCP, 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	A	1.11	10/1936 (0.5%)	0.97	2/2596 (0.1%)
2	C	1.10	13/2937 (0.4%)	0.98	4/3946 (0.1%)
3	d	1.02	4/903 (0.4%)	0.95	0/1216
4	DD	0.59	0/1796	1.01	5/2417 (0.2%)
5	dd	0.64	0/470	0.96	0/623
6	D	0.83	0/2437	0.87	2/3264 (0.1%)
7	e	1.18	5/1071 (0.5%)	0.97	0/1429
8	EE	0.59	0/2118	0.90	3/2849 (0.1%)
9	ee	0.67	0/447	0.91	0/587
10	b	0.82	0/861	0.91	0/1138
11	E	0.88	3/1762 (0.2%)	0.93	2/2362 (0.1%)
12	f	1.14	3/895 (0.3%)	0.96	1/1198 (0.1%)
13	FF	0.55	0/1492	0.92	1/2005 (0.0%)
14	ff	0.57	0/567	1.04	1/753 (0.1%)
15	F	1.17	7/1911 (0.4%)	0.96	1/2549 (0.0%)
16	g	0.93	1/916 (0.1%)	0.96	1/1220 (0.1%)
17	BB	0.58	0/1756	0.90	5/2350 (0.2%)
18	GG	0.54	0/1946	0.89	1/2590 (0.0%)
19	gg	0.46	0/2493	0.83	1/3394 (0.0%)
20	G	0.88	1/1910 (0.1%)	0.92	1/2569 (0.0%)
21	h	0.91	1/1021 (0.1%)	0.97	2/1348 (0.1%)
22	HH	0.61	1/1510 (0.1%)	0.88	4/2022 (0.2%)
23	hh	0.67	0/353	1.37	3/547 (0.5%)
24	bb	0.56	0/665	0.84	2/891 (0.2%)
25	H	0.94	1/1535 (0.1%)	0.88	1/2063 (0.0%)
26	i	0.90	2/841 (0.2%)	0.94	0/1112
27	II	0.62	0/1715	0.88	1/2287 (0.0%)
28	ii	0.56	0/3361	0.98	10/4519 (0.2%)
29	I	1.01	3/1702 (0.2%)	0.89	0/2272
30	j	1.05	1/720 (0.1%)	1.00	0/952
31	JJ	0.68	0/1550	0.86	0/2069
32	jj	0.57	0/3435	0.95	8/4633 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	J	0.77	0/1385	0.92	1/1852 (0.1%)
34	k	0.85	0/575	0.88	1/761 (0.1%)
35	KK	0.55	0/834	0.90	1/1125 (0.1%)
36	L	0.91	3/1733 (0.2%)	0.96	0/2316
37	l	0.93	0/459	0.92	1/608 (0.2%)
38	LL	0.68	0/1195	0.85	0/1597
39	M	0.94	0/1158	0.92	0/1547
40	m	0.85	0/435	0.85	0/575
41	MM	0.43	0/918	0.75	1/1233 (0.1%)
42	N	1.14	6/1746 (0.3%)	0.97	2/2338 (0.1%)
43	n	0.71	0/240	1.29	2/305 (0.7%)
44	NN	0.63	0/1226	0.88	1/1649 (0.1%)
45	O	1.16	12/1662 (0.7%)	1.01	1/2222 (0.0%)
46	o	0.85	0/864	0.93	0/1140
47	OO	0.61	0/1029	0.94	1/1380 (0.1%)
48	P	1.07	3/1268 (0.2%)	0.91	0/1700
49	p	1.03	2/718 (0.3%)	0.89	0/953
50	PP	0.62	0/1017	1.03	2/1358 (0.1%)
51	Q	1.13	5/1539 (0.3%)	1.00	0/2054
52	r	0.99	0/1010	0.94	1/1354 (0.1%)
53	QQ	0.56	0/1146	0.92	1/1534 (0.1%)
54	R	0.87	3/1524 (0.2%)	1.01	1/2013 (0.0%)
55	s	0.55	0/1530	0.92	3/2064 (0.1%)
56	RR	0.58	0/1082	0.87	1/1452 (0.1%)
57	S	1.08	7/1501 (0.5%)	0.93	2/2012 (0.1%)
58	t	0.52	1/1174 (0.1%)	0.90	2/1582 (0.1%)
59	SS	0.56	0/1208	1.03	2/1618 (0.1%)
60	T	1.03	3/1326 (0.2%)	0.97	1/1770 (0.1%)
61	TT	0.55	0/1115	0.87	1/1493 (0.1%)
62	U	0.80	1/823 (0.1%)	0.91	1/1104 (0.1%)
63	UU	0.62	0/805	0.98	2/1081 (0.2%)
64	V	1.12	1/993 (0.1%)	0.96	0/1332
65	VV	0.60	0/643	0.81	0/860
66	W	0.87	1/873 (0.1%)	0.89	0/1158
67	5	1.40	348/84975 (0.4%)	1.67	1993/132516 (1.5%)
68	WW	0.73	0/1051	0.87	0/1406
69	X	0.95	1/984 (0.1%)	0.95	1/1323 (0.1%)
70	7	1.29	6/2858 (0.2%)	1.49	26/4455 (0.6%)
71	XX	0.73	0/1116	0.88	0/1490
72	Y	1.01	1/1132 (0.1%)	0.98	3/1504 (0.2%)
73	8	1.37	9/3581 (0.3%)	1.65	76/5577 (1.4%)
74	YY	0.53	0/1028	0.82	0/1366
75	Z	0.92	1/1130 (0.1%)	0.93	1/1507 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	9	0.91	11/40524 (0.0%)	1.44	428/63134 (0.7%)
77	ZZ	0.50	0/604	0.93	0/810
78	a	1.18	6/1191 (0.5%)	0.94	0/1590
79	AA	0.61	0/1747	0.80	0/2374
80	aa	0.69	0/828	0.86	0/1109
81	B	1.05	11/3240 (0.3%)	0.95	2/4339 (0.0%)
82	c	0.85	0/771	1.09	4/1034 (0.4%)
83	CC	0.73	0/1753	0.92	2/2369 (0.1%)
84	cc	0.61	0/490	1.07	3/656 (0.5%)
All	All	1.10	498/234789 (0.2%)	1.37	2633/343469 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	d	0	1
53	QQ	0	1
67	5	0	7
71	XX	0	1
76	9	0	1
79	AA	0	1
All	All	0	12

The worst 5 of 498 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	5	2836	A	N9-C4	-8.41	1.32	1.37
67	5	1637	A	N9-C4	-8.35	1.32	1.37
67	5	1907	A	N9-C4	-8.30	1.32	1.37
48	P	119	VAL	CB-CG1	-7.97	1.36	1.52
67	5	2849	A	N9-C4	-7.93	1.33	1.37

The worst 5 of 2633 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	5	3911	C	C6-N1-C2	-12.96	115.12	120.30
67	5	1535	C	C5-C4-N4	-12.52	111.44	120.20
67	5	1081	C	C6-N1-C2	-12.39	115.34	120.30
67	5	4723	A	C6-N1-C2	-12.38	111.17	118.60
67	5	143	C	O4'-C1'-N1	12.29	118.03	108.20

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
67	5	1081	C	Sidechain
67	5	39	A	Sidechain
67	5	914	U	Sidechain
53	QQ	140	ARG	Peptide
3	d	95	ASP	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/249 (99%)	219 (89%)	27 (11%)	0	100	100
2	C	360/378 (95%)	335 (93%)	24 (7%)	1 (0%)	41	75
3	d	105/108 (97%)	90 (86%)	13 (12%)	2 (2%)	8	39
4	DD	226/281 (80%)	212 (94%)	13 (6%)	1 (0%)	34	71
5	dd	53/56 (95%)	46 (87%)	7 (13%)	0	100	100
6	D	291/296 (98%)	273 (94%)	18 (6%)	0	100	100
7	e	126/129 (98%)	121 (96%)	5 (4%)	0	100	100
8	EE	260/263 (99%)	244 (94%)	16 (6%)	0	100	100
9	ee	53/133 (40%)	51 (96%)	2 (4%)	0	100	100
10	b	100/226 (44%)	94 (94%)	5 (5%)	1 (1%)	15	52
11	E	208/291 (72%)	189 (91%)	19 (9%)	0	100	100
12	f	107/110 (97%)	98 (92%)	7 (6%)	2 (2%)	8	39
13	FF	181/204 (89%)	164 (91%)	14 (8%)	3 (2%)	9	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	ff	66/68 (97%)	62 (94%)	4 (6%)	0	100	100
15	F	223/249 (90%)	213 (96%)	9 (4%)	1 (0%)	34	71
16	g	112/126 (89%)	106 (95%)	6 (5%)	0	100	100
17	BB	211/264 (80%)	193 (92%)	18 (8%)	0	100	100
18	GG	235/263 (89%)	223 (95%)	12 (5%)	0	100	100
19	gg	311/314 (99%)	282 (91%)	27 (9%)	2 (1%)	25	63
20	G	229/242 (95%)	218 (95%)	9 (4%)	2 (1%)	17	54
21	h	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
22	HH	181/191 (95%)	173 (96%)	8 (4%)	0	100	100
24	bb	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
25	H	188/190 (99%)	178 (95%)	10 (5%)	0	100	100
26	i	100/107 (94%)	94 (94%)	6 (6%)	0	100	100
27	II	204/208 (98%)	188 (92%)	14 (7%)	2 (1%)	15	52
28	ii	417/437 (95%)	389 (93%)	24 (6%)	4 (1%)	15	52
29	I	201/214 (94%)	182 (90%)	19 (10%)	0	100	100
30	j	84/97 (87%)	78 (93%)	6 (7%)	0	100	100
31	JJ	183/194 (94%)	177 (97%)	6 (3%)	0	100	100
32	jj	426/428 (100%)	373 (88%)	46 (11%)	7 (2%)	9	43
33	J	168/176 (96%)	160 (95%)	8 (5%)	0	100	100
34	k	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
35	KK	94/151 (62%)	88 (94%)	5 (5%)	1 (1%)	14	50
36	L	208/211 (99%)	192 (92%)	15 (7%)	1 (0%)	29	67
37	l	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
38	LL	139/158 (88%)	133 (96%)	6 (4%)	0	100	100
39	M	136/218 (62%)	123 (90%)	13 (10%)	0	100	100
40	m	50/128 (39%)	46 (92%)	4 (8%)	0	100	100
41	MM	115/123 (94%)	103 (90%)	12 (10%)	0	100	100
42	N	201/204 (98%)	186 (92%)	11 (6%)	4 (2%)	7	39
43	n	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
44	NN	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	22	60
45	O	197/203 (97%)	189 (96%)	7 (4%)	1 (0%)	29	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	o	102/142 (72%)	98 (96%)	4 (4%)	0	100	100
47	OO	134/156 (86%)	124 (92%)	8 (6%)	2 (2%)	10	44
48	P	151/199 (76%)	143 (95%)	8 (5%)	0	100	100
49	p	89/109 (82%)	82 (92%)	7 (8%)	0	100	100
50	PP	118/145 (81%)	104 (88%)	12 (10%)	2 (2%)	9	42
51	Q	185/188 (98%)	173 (94%)	11 (6%)	1 (0%)	29	67
52	r	122/137 (89%)	112 (92%)	9 (7%)	1 (1%)	19	58
53	QQ	140/158 (89%)	133 (95%)	6 (4%)	1 (1%)	22	60
54	R	178/196 (91%)	173 (97%)	5 (3%)	0	100	100
55	s	194/318 (61%)	175 (90%)	17 (9%)	2 (1%)	15	52
56	RR	130/145 (90%)	121 (93%)	9 (7%)	0	100	100
57	S	174/176 (99%)	159 (91%)	12 (7%)	3 (2%)	9	42
58	t	151/196 (77%)	134 (89%)	16 (11%)	1 (1%)	22	60
59	SS	142/152 (93%)	137 (96%)	4 (3%)	1 (1%)	22	60
60	T	157/160 (98%)	146 (93%)	11 (7%)	0	100	100
61	TT	139/145 (96%)	131 (94%)	8 (6%)	0	100	100
62	U	97/128 (76%)	89 (92%)	8 (8%)	0	100	100
63	UU	98/118 (83%)	91 (93%)	7 (7%)	0	100	100
64	V	129/132 (98%)	119 (92%)	10 (8%)	0	100	100
65	VV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
66	W	102/134 (76%)	98 (96%)	4 (4%)	0	100	100
68	WW	127/139 (91%)	118 (93%)	7 (6%)	2 (2%)	9	43
69	X	116/156 (74%)	107 (92%)	9 (8%)	0	100	100
71	XX	139/142 (98%)	125 (90%)	11 (8%)	3 (2%)	6	37
72	Y	132/134 (98%)	121 (92%)	11 (8%)	0	100	100
74	YY	122/146 (84%)	115 (94%)	7 (6%)	0	100	100
75	Z	133/136 (98%)	125 (94%)	6 (4%)	2 (2%)	10	44
77	ZZ	73/122 (60%)	69 (94%)	4 (6%)	0	100	100
78	a	145/147 (99%)	129 (89%)	16 (11%)	0	100	100
79	AA	215/295 (73%)	201 (94%)	13 (6%)	1 (0%)	29	67
80	aa	99/117 (85%)	89 (90%)	9 (9%)	1 (1%)	15	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
81	B	392/402 (98%)	355 (91%)	35 (9%)	2 (0%)	29	67
82	c	96/115 (84%)	94 (98%)	2 (2%)	0	100	100
83	CC	219/259 (85%)	205 (94%)	14 (6%)	0	100	100
84	cc	60/69 (87%)	58 (97%)	2 (3%)	0	100	100
All	All	12362/14087 (88%)	11478 (93%)	823 (7%)	61 (0%)	32	67

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	d	95	ASP
28	ii	272	THR
32	jj	466	LYS
32	jj	620	GLU
42	N	76	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/191 (100%)	188 (99%)	2 (1%)	73	84
2	C	302/315 (96%)	301 (100%)	1 (0%)	92	95
3	d	98/99 (99%)	97 (99%)	1 (1%)	76	85
4	DD	190/232 (82%)	185 (97%)	5 (3%)	46	67
5	dd	48/49 (98%)	48 (100%)	0	100	100
6	D	247/249 (99%)	245 (99%)	2 (1%)	81	88
7	e	114/115 (99%)	113 (99%)	1 (1%)	78	87
8	EE	224/225 (100%)	223 (100%)	1 (0%)	91	94
9	ee	46/106 (43%)	46 (100%)	0	100	100
10	b	84/172 (49%)	84 (100%)	0	100	100
11	E	190/251 (76%)	186 (98%)	4 (2%)	53	72
12	f	88/89 (99%)	87 (99%)	1 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	FF	158/170 (93%)	157 (99%)	1 (1%)	86	92
14	ff	61/61 (100%)	59 (97%)	2 (3%)	38	62
15	F	196/218 (90%)	195 (100%)	1 (0%)	88	93
16	g	98/106 (92%)	97 (99%)	1 (1%)	76	85
17	BB	194/229 (85%)	192 (99%)	2 (1%)	76	85
18	GG	207/228 (91%)	204 (99%)	3 (1%)	67	80
19	gg	272/273 (100%)	270 (99%)	2 (1%)	84	90
20	G	200/207 (97%)	200 (100%)	0	100	100
21	h	109/110 (99%)	108 (99%)	1 (1%)	78	87
22	HH	165/171 (96%)	164 (99%)	1 (1%)	86	92
24	bb	75/76 (99%)	74 (99%)	1 (1%)	69	81
25	H	169/169 (100%)	168 (99%)	1 (1%)	86	92
26	i	86/88 (98%)	86 (100%)	0	100	100
27	II	178/180 (99%)	173 (97%)	5 (3%)	43	65
28	ii	361/376 (96%)	358 (99%)	3 (1%)	81	88
29	I	175/181 (97%)	174 (99%)	1 (1%)	86	92
30	j	73/80 (91%)	72 (99%)	1 (1%)	67	80
31	JJ	161/168 (96%)	159 (99%)	2 (1%)	71	83
32	jj	372/372 (100%)	363 (98%)	9 (2%)	49	69
33	J	143/148 (97%)	141 (99%)	2 (1%)	67	80
34	k	64/65 (98%)	64 (100%)	0	100	100
35	KK	87/127 (68%)	86 (99%)	1 (1%)	73	84
36	L	175/176 (99%)	174 (99%)	1 (1%)	86	92
37	l	47/48 (98%)	46 (98%)	1 (2%)	53	72
38	LL	130/143 (91%)	128 (98%)	2 (2%)	65	79
39	M	117/161 (73%)	112 (96%)	5 (4%)	29	56
40	m	48/116 (41%)	48 (100%)	0	100	100
41	MM	99/104 (95%)	98 (99%)	1 (1%)	76	85
42	N	171/172 (99%)	168 (98%)	3 (2%)	59	77
43	n	24/24 (100%)	24 (100%)	0	100	100
44	NN	130/131 (99%)	127 (98%)	3 (2%)	50	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	O	171/173 (99%)	168 (98%)	3 (2%)	59	77
46	o	92/121 (76%)	92 (100%)	0	100	100
47	OO	106/122 (87%)	104 (98%)	2 (2%)	57	75
48	P	134/175 (77%)	133 (99%)	1 (1%)	84	90
49	p	74/87 (85%)	73 (99%)	1 (1%)	67	80
50	PP	109/130 (84%)	108 (99%)	1 (1%)	78	87
51	Q	164/165 (99%)	163 (99%)	1 (1%)	86	92
52	r	108/121 (89%)	104 (96%)	4 (4%)	34	59
53	QQ	117/130 (90%)	117 (100%)	0	100	100
54	R	159/175 (91%)	157 (99%)	2 (1%)	69	81
55	s	164/258 (64%)	162 (99%)	2 (1%)	71	83
56	RR	119/131 (91%)	117 (98%)	2 (2%)	60	78
57	S	157/157 (100%)	155 (99%)	2 (1%)	69	81
58	t	126/164 (77%)	124 (98%)	2 (2%)	62	78
59	SS	125/132 (95%)	123 (98%)	2 (2%)	62	78
60	T	139/140 (99%)	138 (99%)	1 (1%)	84	90
61	TT	111/115 (96%)	110 (99%)	1 (1%)	78	87
62	U	89/114 (78%)	89 (100%)	0	100	100
63	UU	92/105 (88%)	90 (98%)	2 (2%)	52	71
64	V	101/102 (99%)	97 (96%)	4 (4%)	31	57
65	VV	67/67 (100%)	64 (96%)	3 (4%)	27	54
66	W	86/109 (79%)	84 (98%)	2 (2%)	50	70
68	WW	112/119 (94%)	110 (98%)	2 (2%)	59	77
69	X	106/134 (79%)	106 (100%)	0	100	100
71	XX	113/114 (99%)	112 (99%)	1 (1%)	78	87
72	Y	124/124 (100%)	124 (100%)	0	100	100
74	YY	107/126 (85%)	105 (98%)	2 (2%)	57	75
75	Z	117/118 (99%)	116 (99%)	1 (1%)	78	87
77	ZZ	66/100 (66%)	65 (98%)	1 (2%)	65	79
78	a	119/119 (100%)	119 (100%)	0	100	100
79	AA	180/245 (74%)	177 (98%)	3 (2%)	60	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
80	aa	88/99 (89%)	87 (99%)	1 (1%)	73	84
81	B	342/347 (99%)	340 (99%)	2 (1%)	86	92
82	c	84/98 (86%)	84 (100%)	0	100	100
83	CC	187/208 (90%)	185 (99%)	2 (1%)	73	84
84	cc	55/62 (89%)	54 (98%)	1 (2%)	59	77
All	All	10776/11977 (90%)	10648 (99%)	128 (1%)	72	83

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
74	YY	79	LEU
79	AA	58	LEU
32	jj	371	ARG
32	jj	353	LEU
79	AA	163	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 157 such sidechains are listed below:

Mol	Chain	Res	Type
55	s	200	ASN
77	ZZ	45	ASN
58	t	100	HIS
61	TT	126	GLN
81	B	3	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	hh	14/15 (93%)	8 (57%)	0
67	5	3516/3705 (94%)	857 (24%)	155 (4%)
70	7	119/120 (99%)	14 (11%)	0
73	8	149/151 (98%)	34 (22%)	5 (3%)
76	9	1679/1779 (94%)	420 (25%)	66 (3%)
All	All	5477/5770 (94%)	1333 (24%)	226 (4%)

5 of 1333 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
23	hh	42	C
23	hh	43	A
23	hh	45	A
23	hh	46	G
23	hh	49	U

5 of 226 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
67	5	3625	G
76	9	1744	G
67	5	4699	U
76	9	1679	A
76	9	1253	A

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 291 ligands modelled in this entry, 289 are monoatomic - leaving 2 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
87	GCP	jj	700	-	27,34,34	4.66	10 (37%)	34,54,54	1.74	8 (23%)
88	BLS	5	5122	67	28,31,31	3.73	14 (50%)	28,43,43	2.06	10 (35%)

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
87	GCP	jj	700	-	-	5/15/38/38	0/3/3/3
88	BLS	5	5122	67	-	8/21/38/38	0/2/2/2

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	jj	700	GCP	O4'-C1'	15.21	1.62	1.41
87	jj	700	GCP	C2'-C1'	-14.43	1.31	1.53
88	5	5122	BLS	O5'-C5'	-11.48	1.24	1.43
88	5	5122	BLS	C3'-C2'	7.36	1.55	1.33
88	5	5122	BLS	C4'-C5'	7.17	1.69	1.53

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	5	5122	BLS	C8-C7-N6	4.97	122.84	116.33
87	jj	700	GCP	N3-C2-N1	-4.76	120.88	127.22
87	jj	700	GCP	C2-N3-C4	4.62	120.63	115.36
88	5	5122	BLS	C4-N3-C2	3.71	120.10	116.34
87	jj	700	GCP	PB-O3A-PA	-3.32	122.04	132.56

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

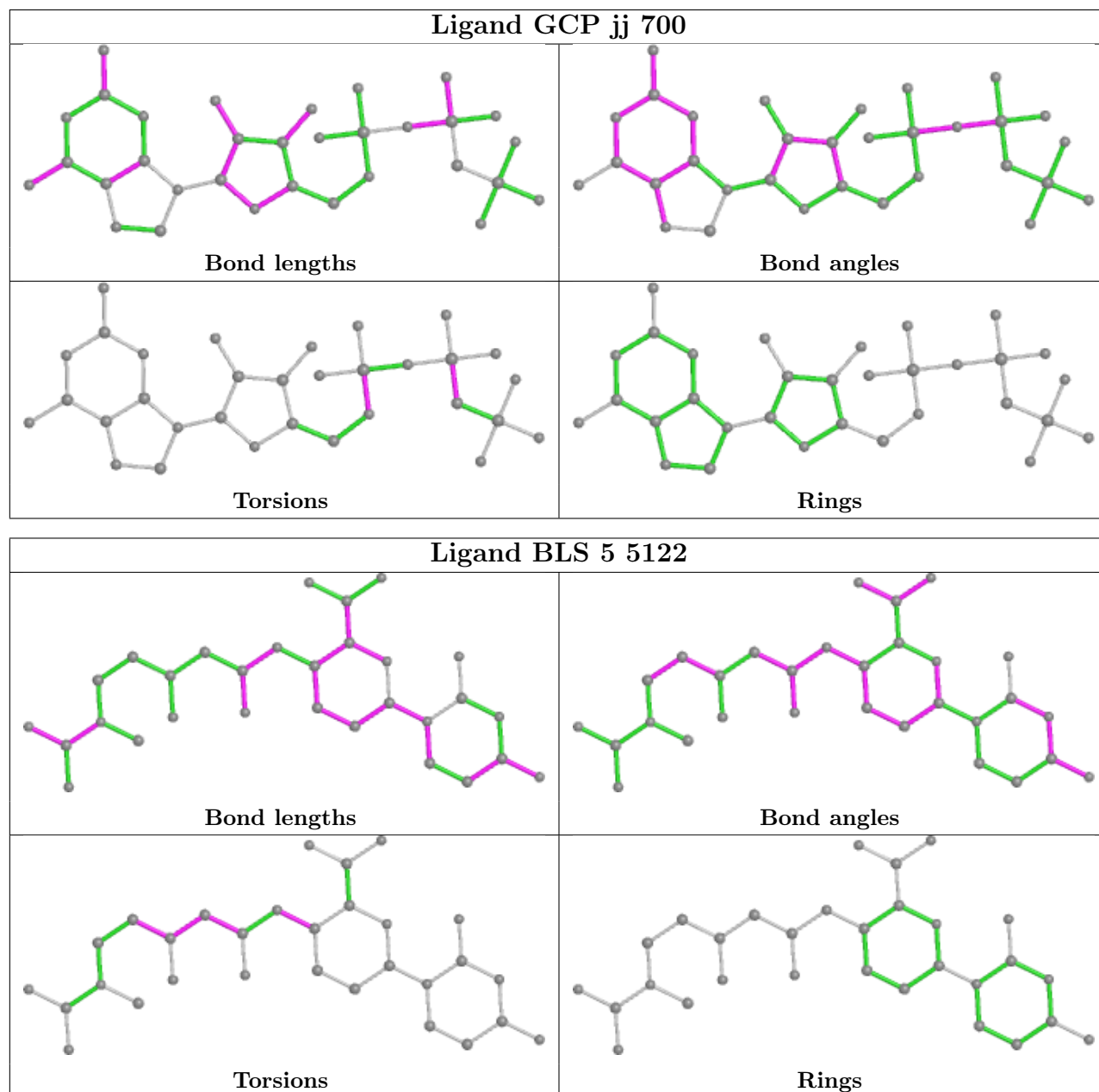
Mol	Chain	Res	Type	Atoms
87	jj	700	GCP	PG-C3B-PB-O1B
87	jj	700	GCP	PG-C3B-PB-O2B
87	jj	700	GCP	PG-C3B-PB-O3A
87	jj	700	GCP	C5'-O5'-PA-O3A
88	5	5122	BLS	C3'-C4'-N6-C7

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
67	5	7
76	9	7
73	8	1

The worst 5 of 15 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	990:C	O3'	1064:G	P	17.61
1	5	1406(C):G	O3'	1411:C	P	17.48
1	8	79:G	O3'	85:U	P	15.70
1	5	4138:C	O3'	4146:G	P	15.08
1	9	322:C	O3'	323:C	P	9.57

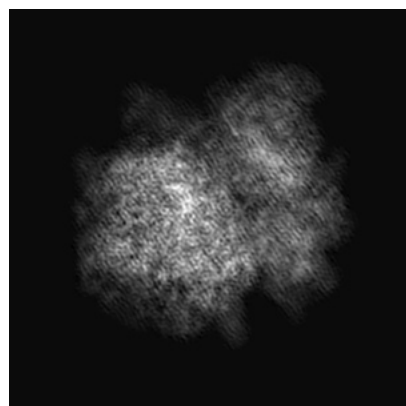
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12632. These allow visual inspection of the internal detail of the map and identification of artifacts.

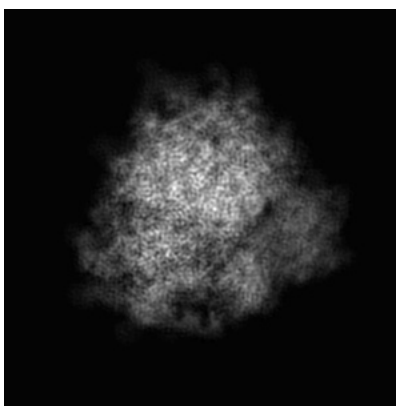
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

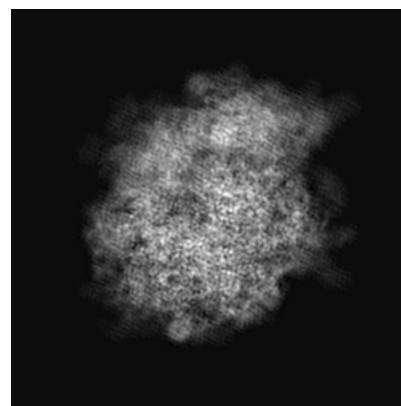
6.1.1 Primary map



X

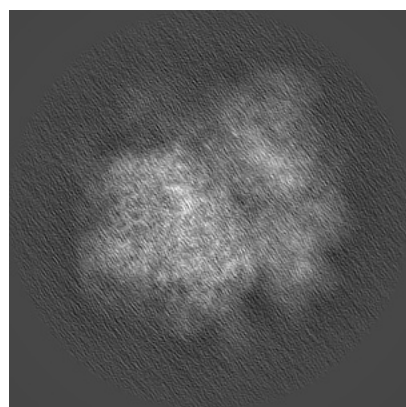


Y

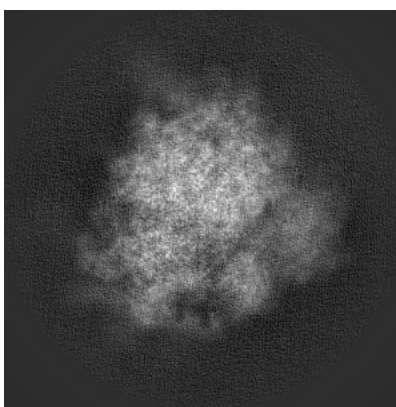


Z

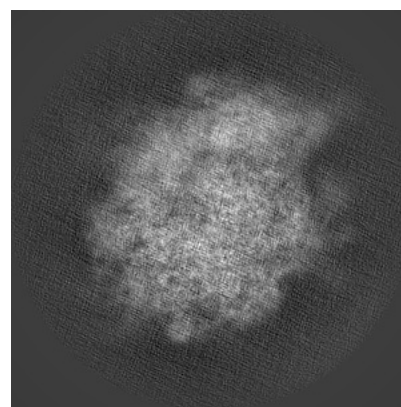
6.1.2 Raw map



X



Y

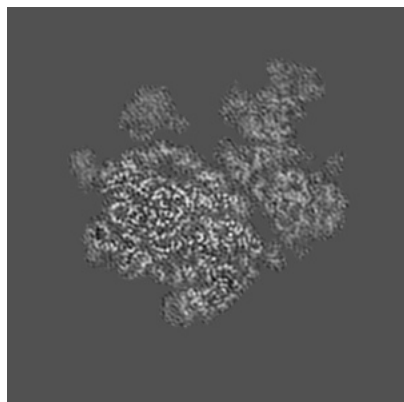


Z

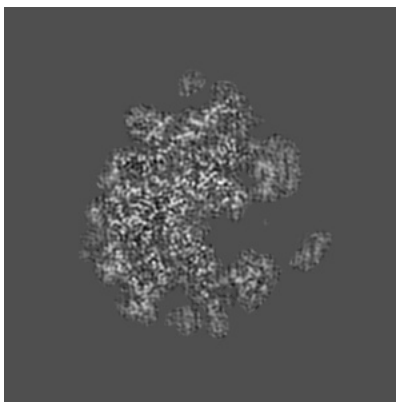
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

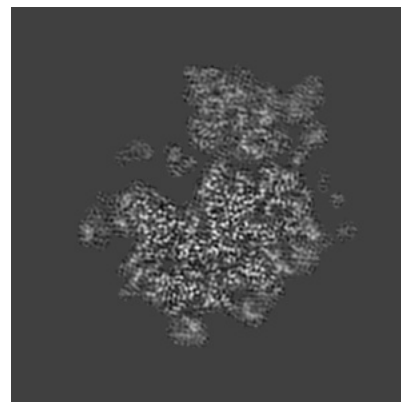
6.2.1 Primary map



X Index: 150

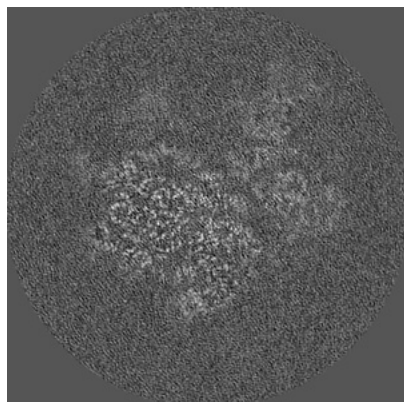


Y Index: 150

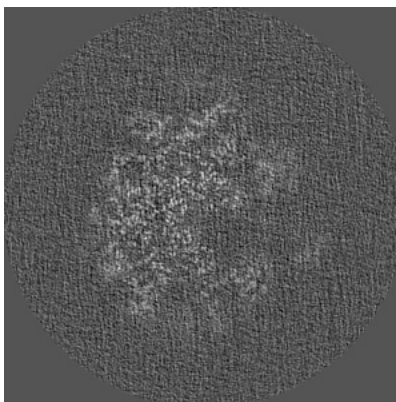


Z Index: 150

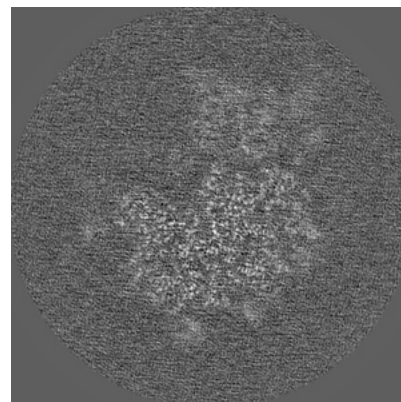
6.2.2 Raw map



X Index: 150



Y Index: 150

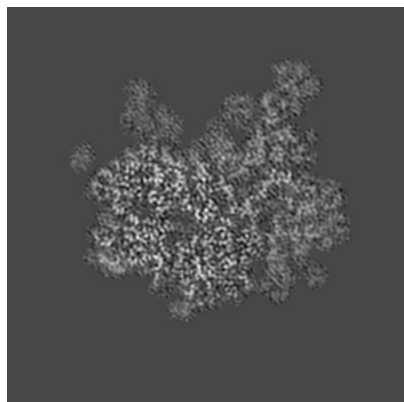


Z Index: 150

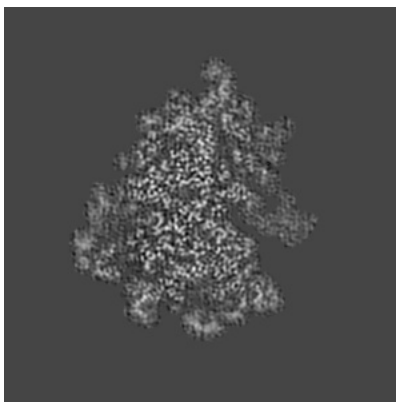
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

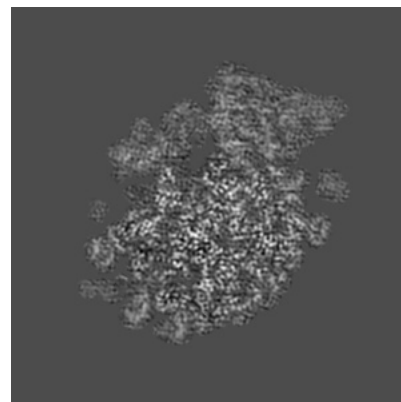
6.3.1 Primary map



X Index: 158

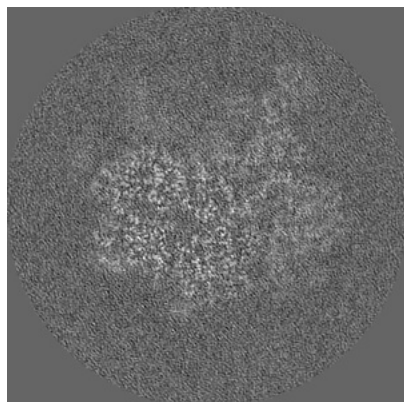


Y Index: 130

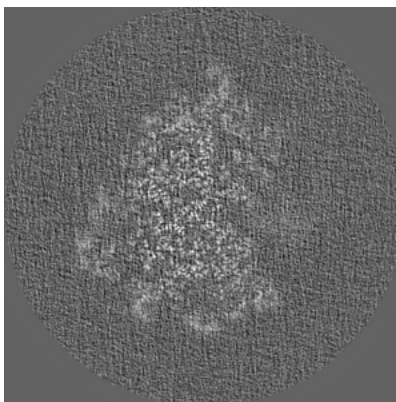


Z Index: 128

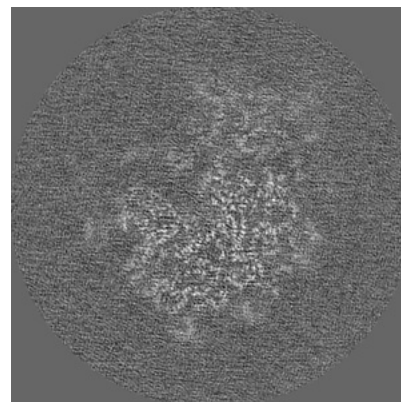
6.3.2 Raw map



X Index: 158



Y Index: 130

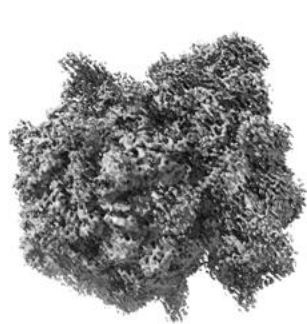


Z Index: 148

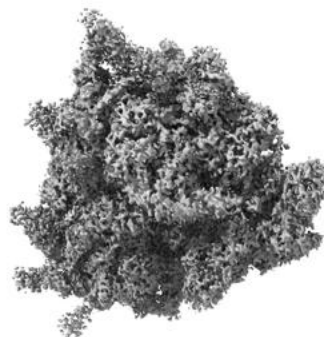
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

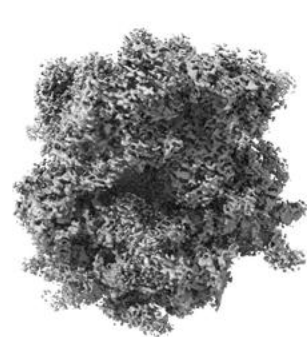
6.4.1 Primary map



X



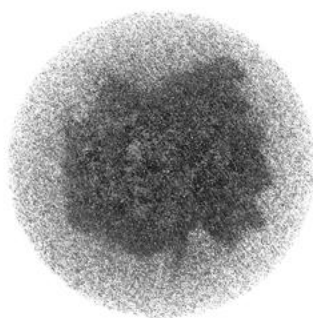
Y



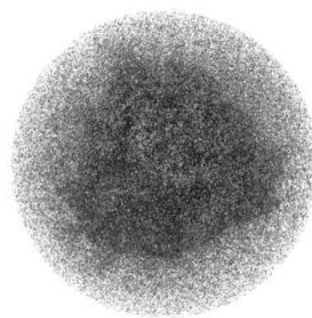
Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

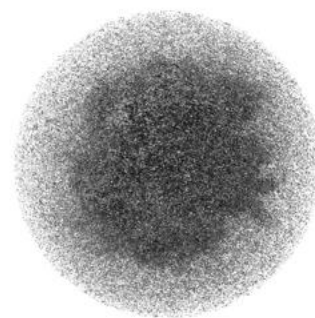
6.4.2 Raw map



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.

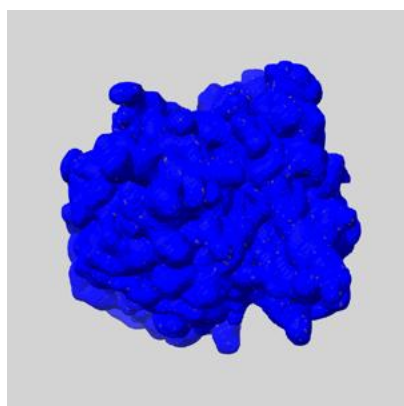
6.5 Mask visualisation [i](#)

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

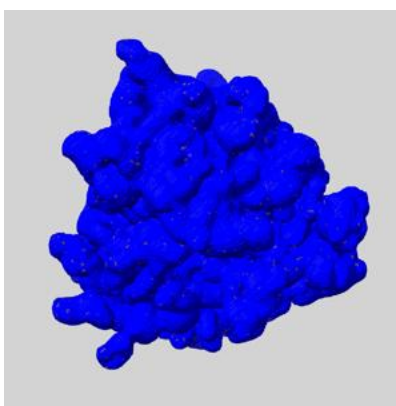
A mask typically either:

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

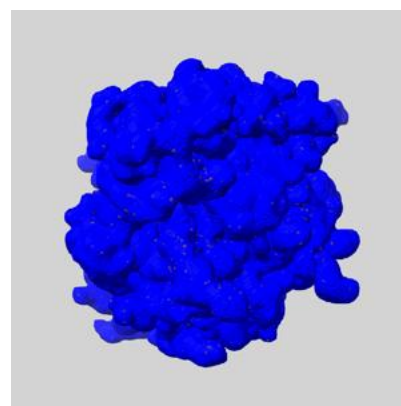
6.5.1 emd_12632_msk_1.map [i](#)



X



Y

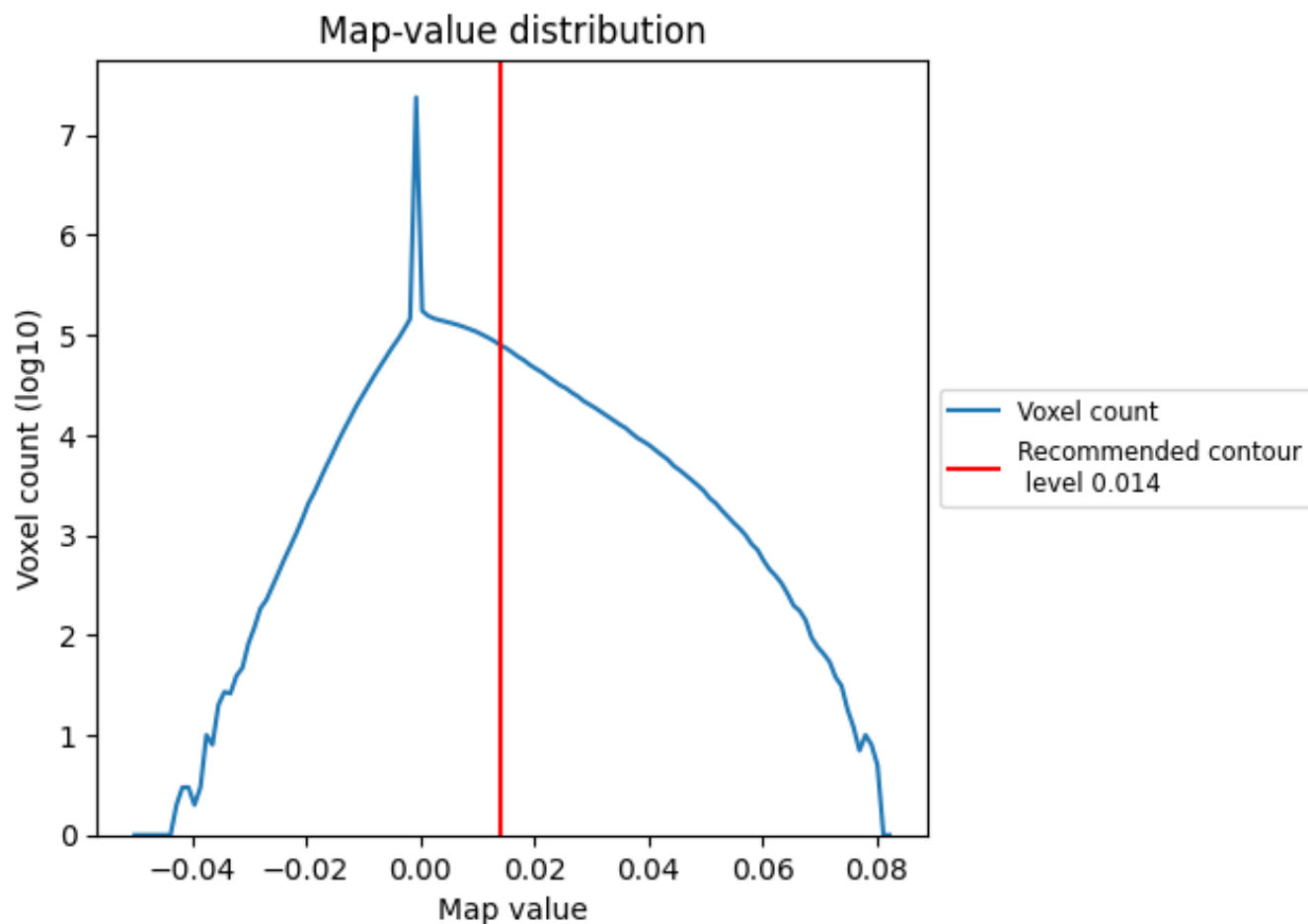


Z

7 Map analysis [i](#)

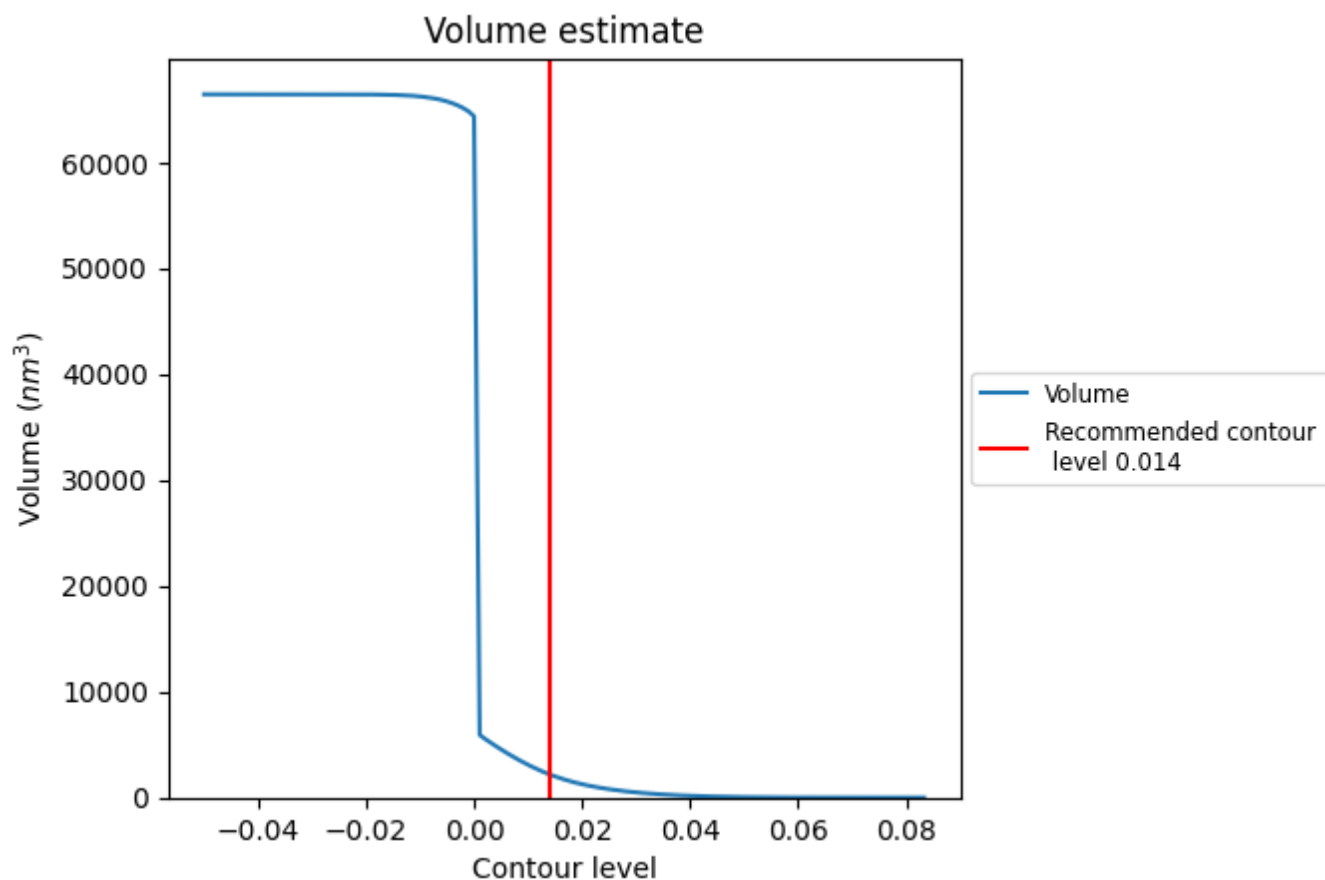
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

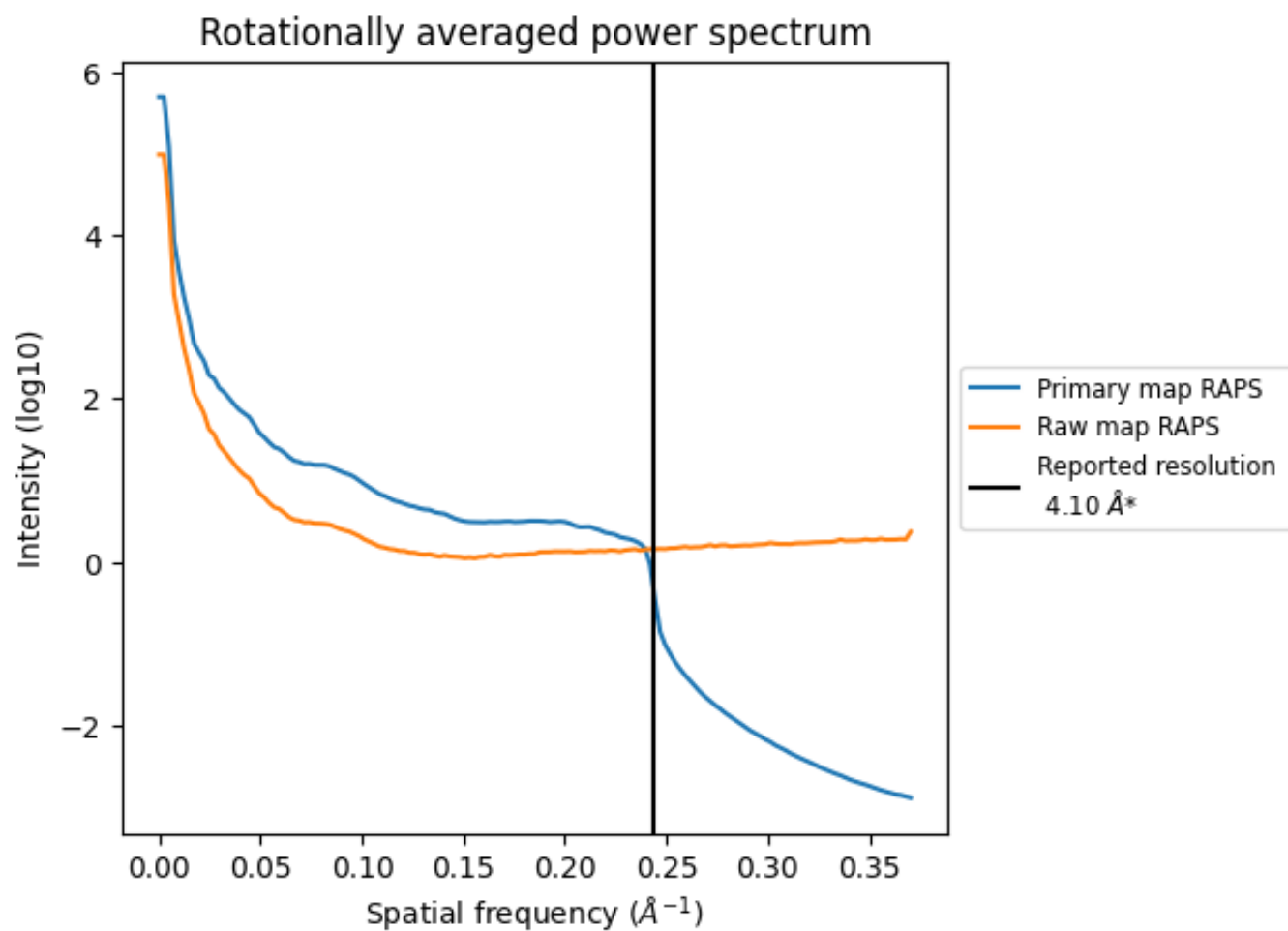
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2180 nm^3 ; this corresponds to an approximate mass of 1970 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

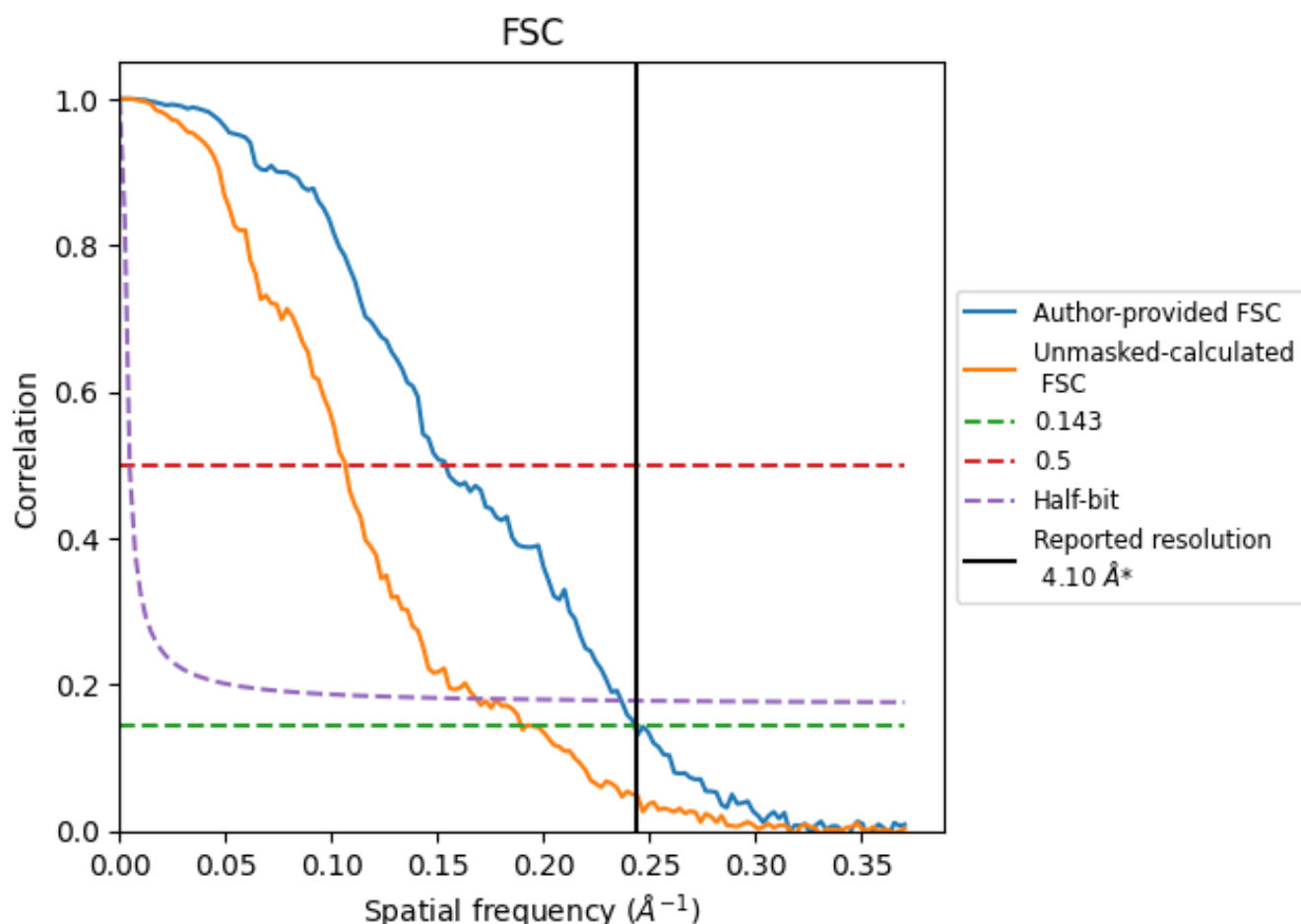


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.244 \AA^{-1}

8.2 Resolution estimates [i](#)

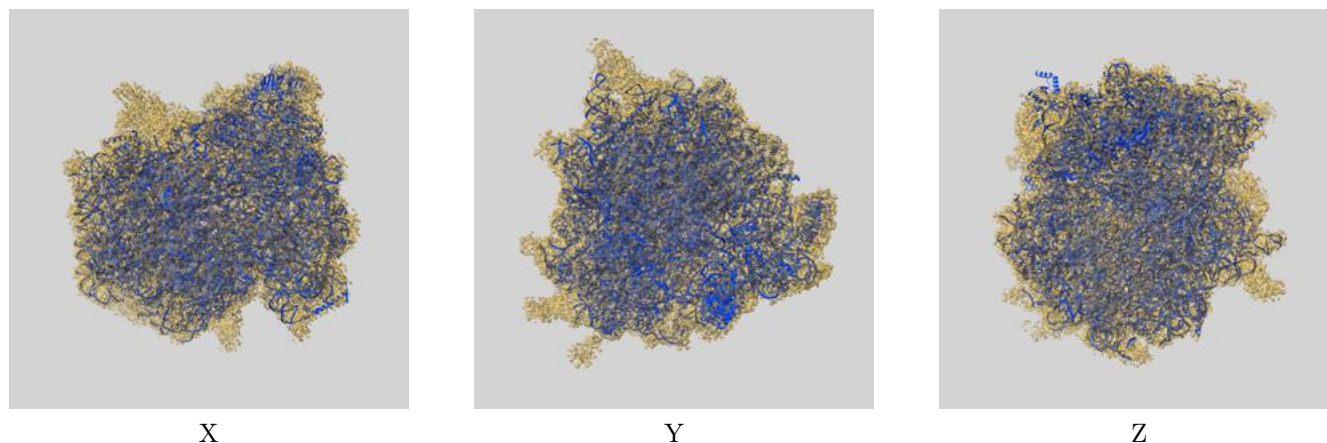
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.12	6.51	4.22
Unmasked-calculated*	5.28	9.40	5.94

*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 5.28 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

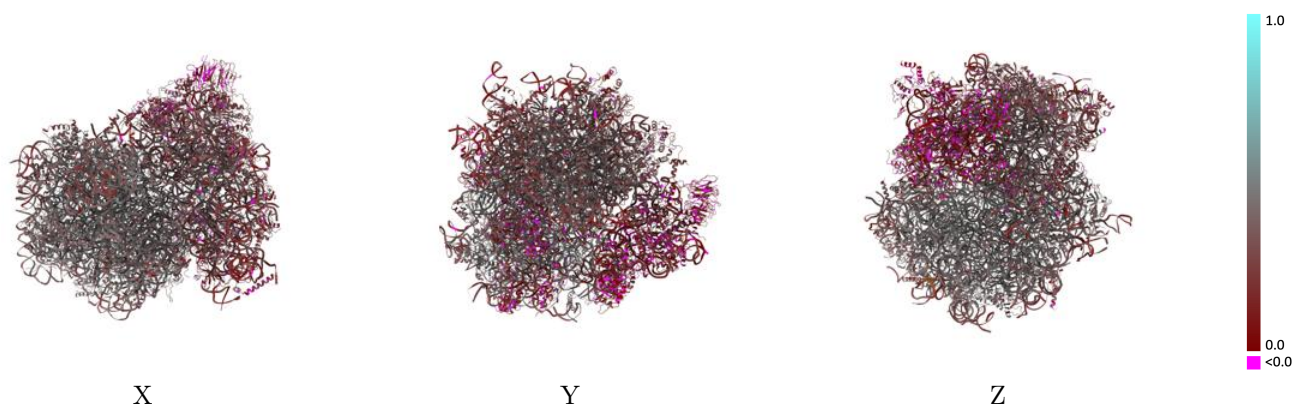
This section contains information regarding the fit between EMDB map EMD-12632 and PDB model 7NWH. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

9.1 Map-model overlay [i](#)



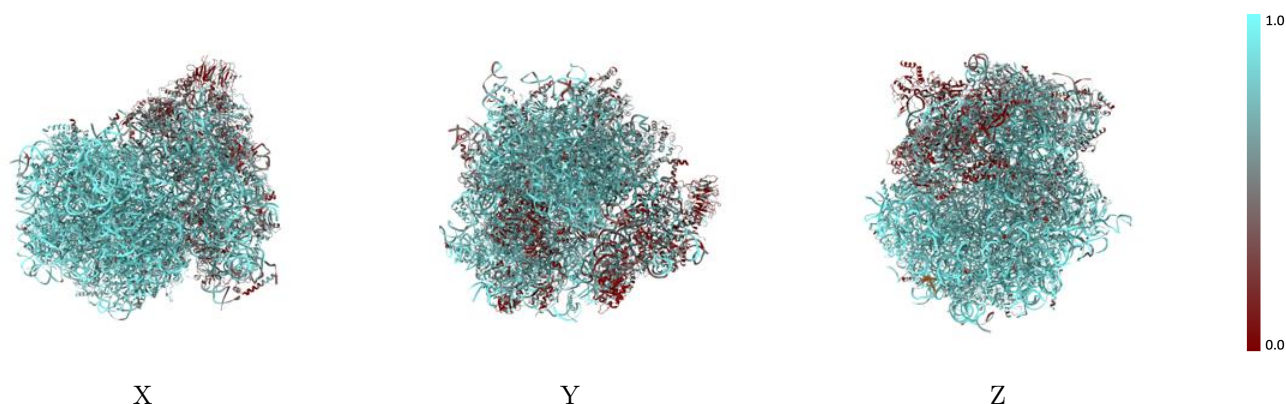
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



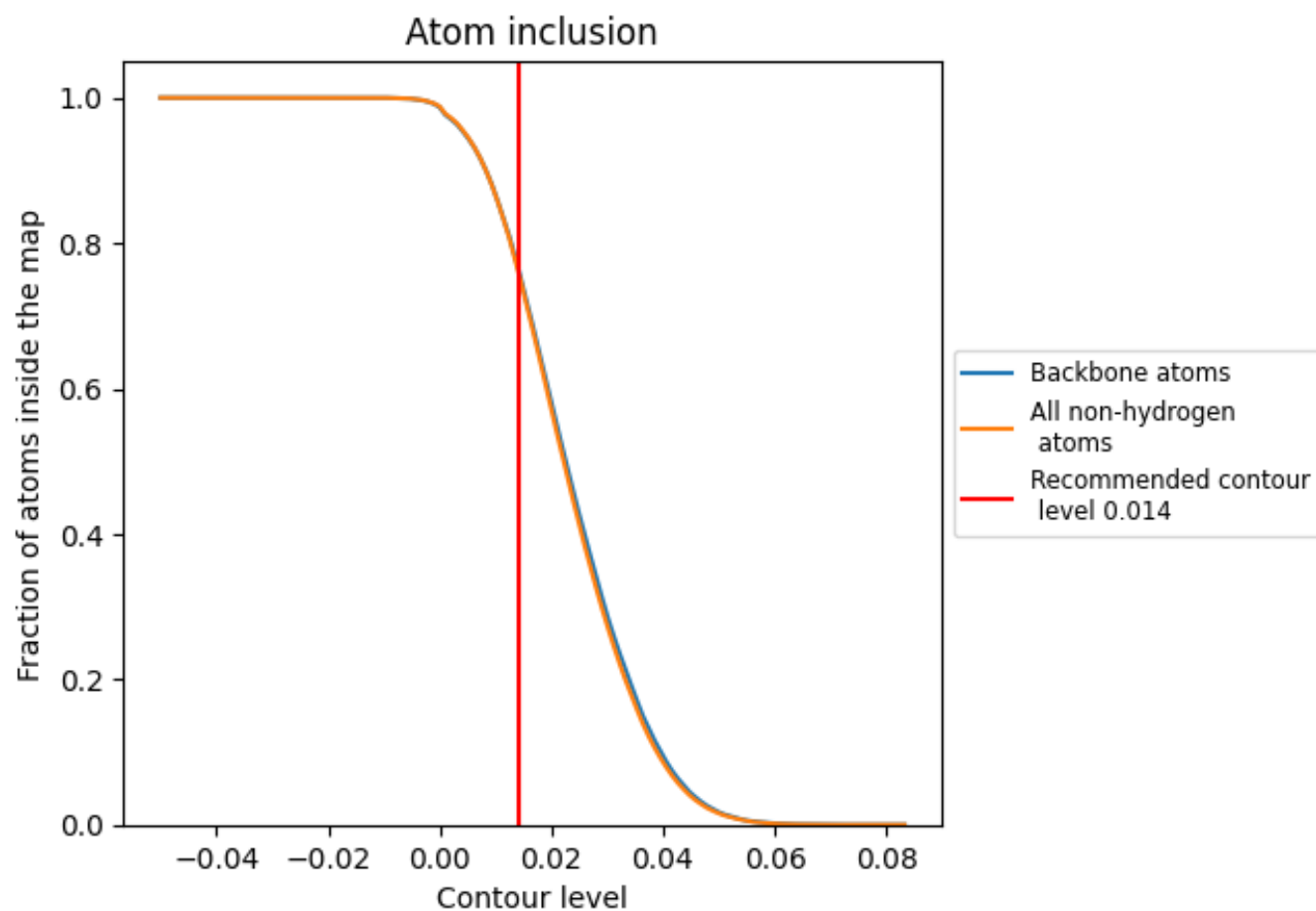
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 76% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7638	 0.3480
5	 0.9284	 0.3970
7	 0.9629	 0.4130
8	 0.9481	 0.4100
9	 0.7792	 0.2790
A	 0.8125	 0.4540
AA	 0.6058	 0.3260
B	 0.8007	 0.4370
BB	 0.5574	 0.2980
C	 0.8136	 0.4440
CC	 0.6568	 0.3580
D	 0.7991	 0.3880
DD	 0.3699	 0.2000
E	 0.8023	 0.4100
EE	 0.6000	 0.3260
F	 0.8010	 0.4240
FF	 0.3401	 0.1590
G	 0.7540	 0.3880
GG	 0.5024	 0.2420
H	 0.7740	 0.4150
HH	 0.4887	 0.2780
I	 0.8055	 0.4320
II	 0.5821	 0.3030
J	 0.7540	 0.3480
JJ	 0.6526	 0.3220
KK	 0.3987	 0.1850
L	 0.7748	 0.4060
LL	 0.6596	 0.3600
M	 0.8089	 0.4130
MM	 0.0805	 0.0870
N	 0.8451	 0.4470
NN	 0.6132	 0.3210
O	 0.8186	 0.4320
OO	 0.5512	 0.2680
P	 0.8260	 0.4440



















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Chain	Atom inclusion	Q-score
PP	 0.4933	 0.1590
Q	 0.8021	 0.4370
QQ	 0.4359	 0.1810
R	 0.7495	 0.3910
RR	 0.3998	 0.2170
S	 0.8210	 0.4420
SS	 0.4812	 0.1830
T	 0.7981	 0.4440
TT	 0.4499	 0.1640
U	 0.7383	 0.3510
UU	 0.4083	 0.1710
V	 0.7724	 0.4530
VV	 0.5997	 0.3340
W	 0.5704	 0.3100
WW	 0.6485	 0.3580
X	 0.8064	 0.4180
XX	 0.7283	 0.3910
Y	 0.8089	 0.4200
YY	 0.5403	 0.2790
Z	 0.7931	 0.3830
ZZ	 0.3688	 0.1690
a	 0.8220	 0.4490
aa	 0.6624	 0.3430
b	 0.7215	 0.3870
bb	 0.5540	 0.3160
c	 0.6935	 0.3420
cc	 0.2745	 0.1690
d	 0.7783	 0.4200
dd	 0.4502	 0.1990
e	 0.8269	 0.4580
ee	 0.5915	 0.3220
f	 0.8468	 0.4600
ff	 0.3457	 0.2120
g	 0.7805	 0.4170
gg	 0.2727	 0.1370
h	 0.8018	 0.3970
hh	 0.2132	 0.1730
i	 0.7714	 0.3880
ii	 0.2776	 0.1660
j	 0.8739	 0.4480
jj	 0.2419	 0.1590
k	 0.7397	 0.3890

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Chain	Atom inclusion	Q-score
l	 0.8361	 0.4370
m	 0.8149	 0.4180
n	 0.6284	 0.3300
o	 0.7787	 0.4390
p	 0.7939	 0.4420
r	 0.8025	 0.4280
s	 0.3246	 0.1490
t	 0.3155	 0.1860