Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 08:23 PM EDT

PDB ID : 9CAI
EMDB ID : EMD-45392
Title : High-resolution C. elegans 80S ribosome structure - class 1
Authors : Sehgal, E.; Serrao, V.H.B.; Arribere, J.
Deposited on : 2024-06-17
Resolution : 2.59 Å(reported)
Based on initial model : .

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

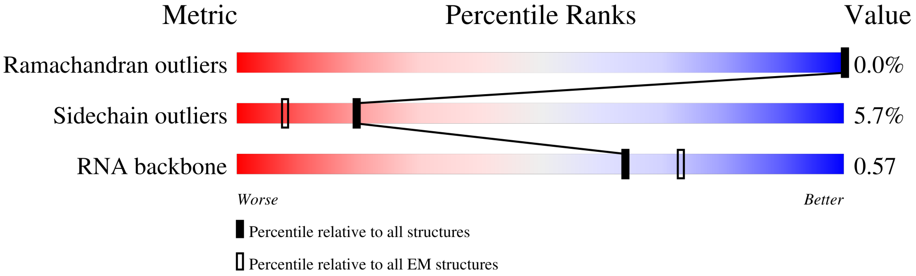
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance ⓘ

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

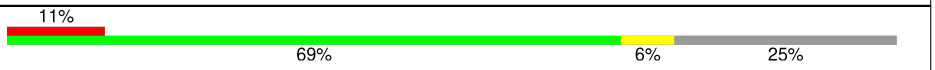
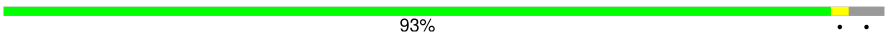
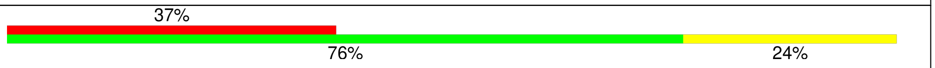
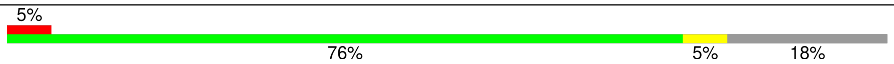
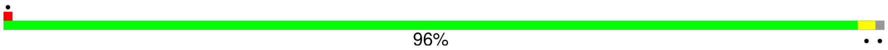
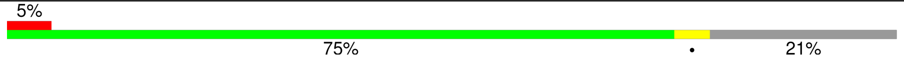
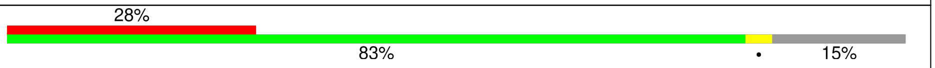
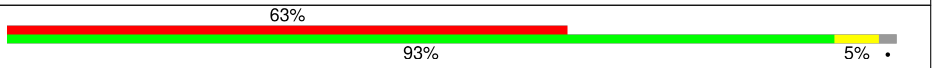
The reported resolution of this entry is 2.59 Å.

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 <=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	AA	276	
2	CA	260	
3	DA	76	
4	AB	257	
5	CB	401	
6	AC	272	
7	AD	247	
8	AE	259	

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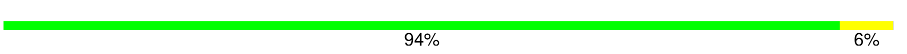
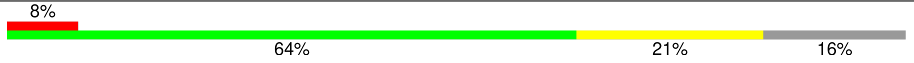
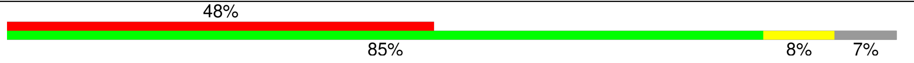
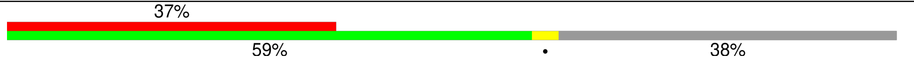
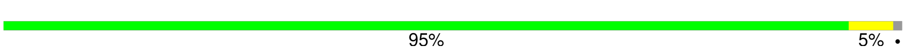
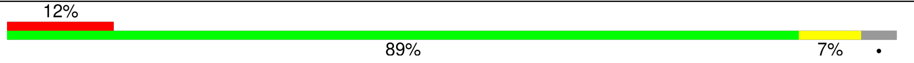
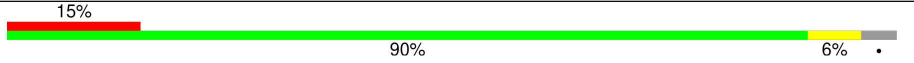
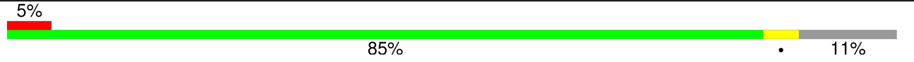
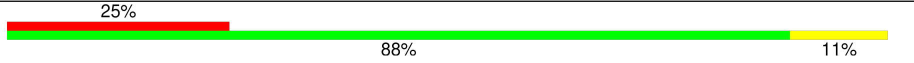
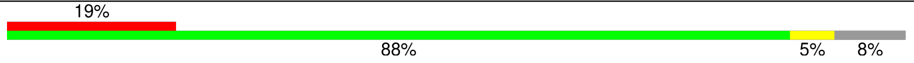
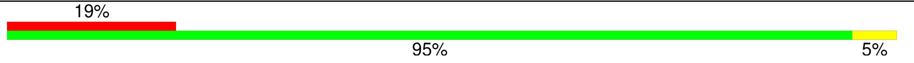
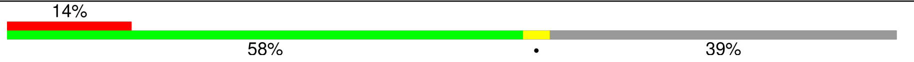
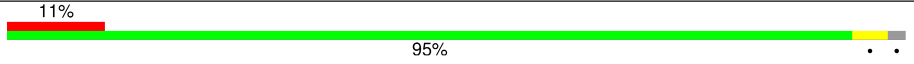
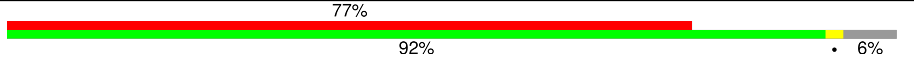
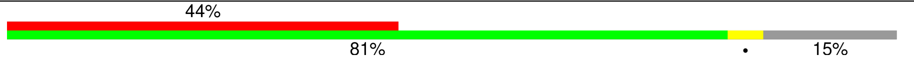
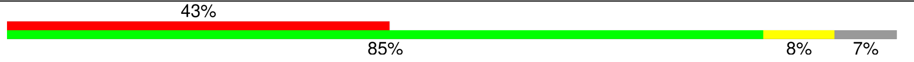
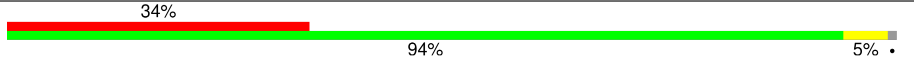
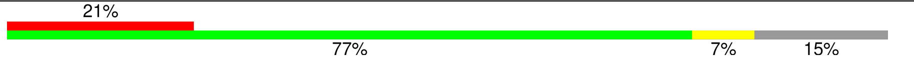
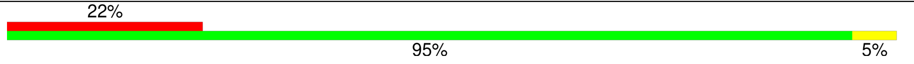
Mol	Chain	Length	Quality of chain
9	A7	119	
10	A8	153	
11	B2	1754	
12	A5	3510	
13	AR	130	
14	AK	149	
15	AW	130	
16	AS	154	
17	AT	146	
18	Aa	117	
19	Af	163	
20	AO	152	
21	AI	208	
22	AF	210	
23	AM	140	
24	AV	88	
25	AN	151	
26	AZ	117	
27	Ad	56	
28	AY	131	
29	AU	117	
30	AG	246	
31	Ab	83	
32	AP	151	
33	Ac	65	

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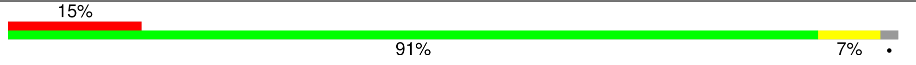
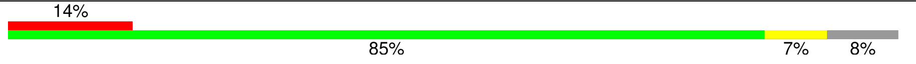
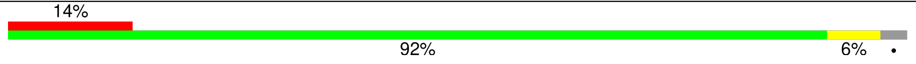
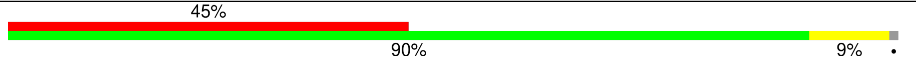
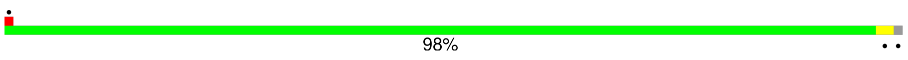
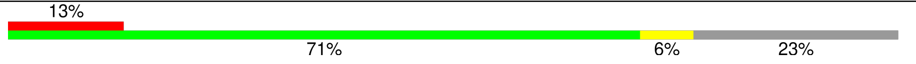
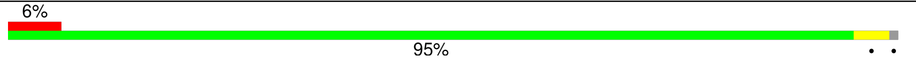
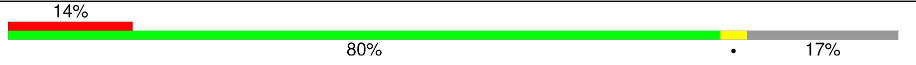
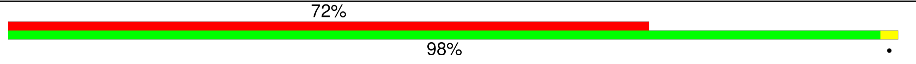
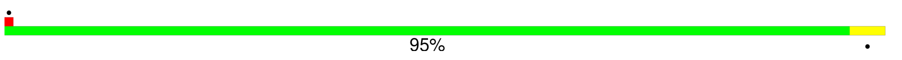
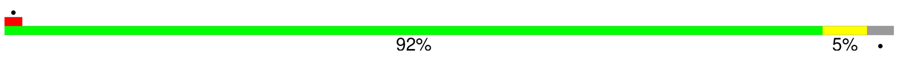
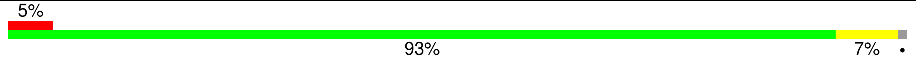
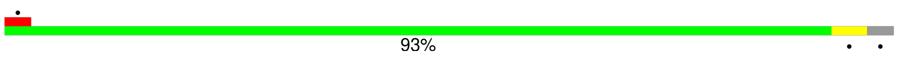
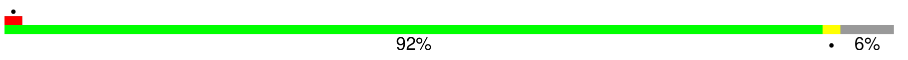
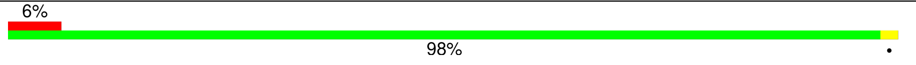
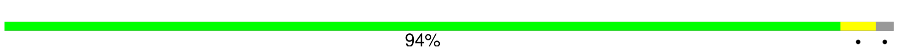
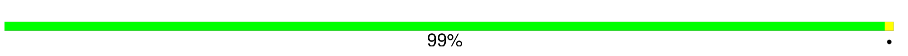
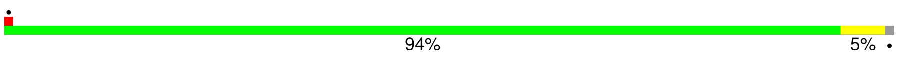
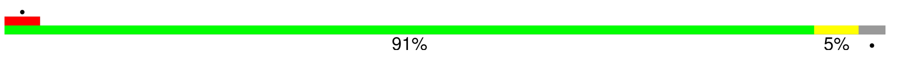
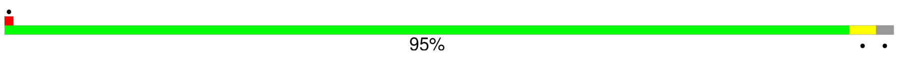
Mol	Chain	Length	Quality of chain
34	Ae	130	
35	AX	143	
36	AL	155	
37	AJ	189	
38	AQ	144	
39	AH	194	
40	CF	244	
41	CS	180	
42	CV	140	
43	CU	130	
44	CL	207	
45	CG	265	
46	CI	214	
47	CO	202	
48	CC	345	
49	Ch	123	
50	CE	217	
51	Co	105	
52	Cf	124	
53	Ci	104	
54	Cl	51	
55	CN	204	
56	Ca	145	
57	Cp	91	
58	CM	135	

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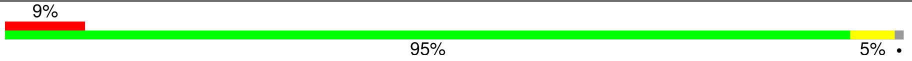
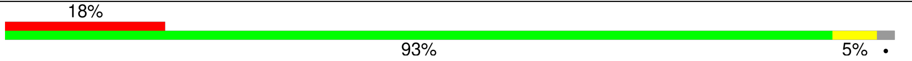
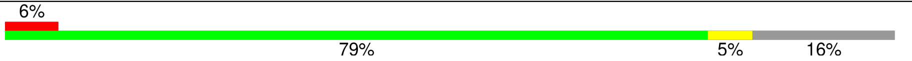
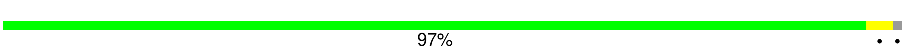
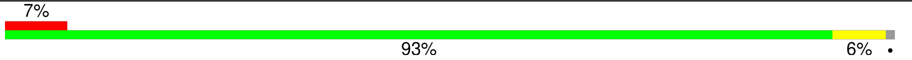
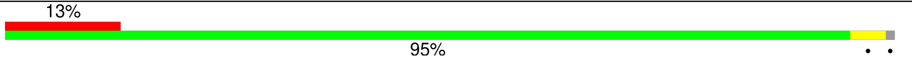
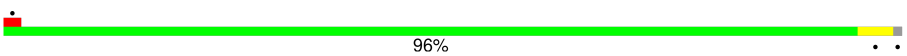
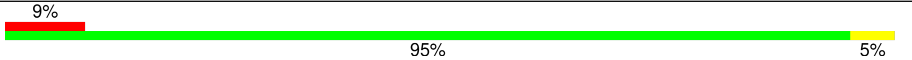
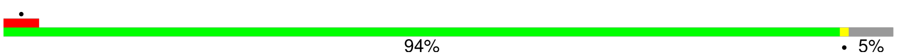
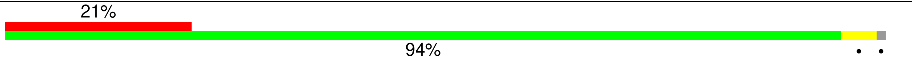
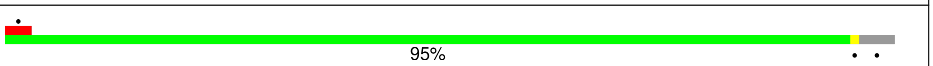
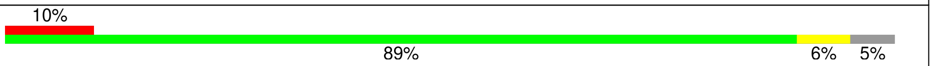
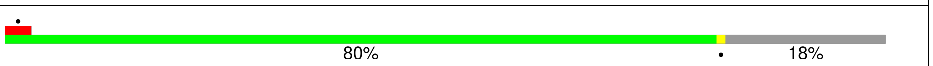
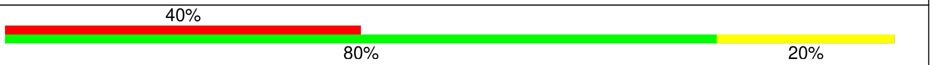
Mol	Chain	Length	Quality of chain
59	Cc	115	
60	CH	189	
61	CY	142	
62	CR	198	
63	Cb	62	
64	CQ	188	
65	CT	161	
66	CD	293	
67	CZ	136	
68	CP	187	
69	Cn	22	
70	Cg	110	
71	Ck	70	
72	Cm	128	
73	Cd	122	
74	Ce	134	
75	CW	159	
76	Cj	92	
77	CJ	196	
78	CX	146	
79	DC	10	

2 Entry composition ⓘ

There are 81 unique types of molecules in this entry. The entry contains 330203 atoms, of which 141530 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 Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	AA	207	3264	1035	1652	281	289	7	0	0

- Molecule 2 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	CA	249	3875	1178	1980	391	321	5	0	0

- Molecule 3 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
3	DA	76	2448	725	821	294	532	76	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DA	74	C	U	conflict	GB 351064414
DA	75	C	G	conflict	GB 351064414
DA	76	A	U	conflict	GB 351064414

- Molecule 4 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	AB	210	3453	1071	1769	298	307	8	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	CB	395	6478	2016	3300	605	547	10	0	0

- Molecule 6 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	AC	215	3389	1062	1735	293	292	7	0	0

- Molecule 7 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	AD	211	3343	1029	1706	308	291	9	0	0

- Molecule 8 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	AE	255	4120	1277	2107	382	347	7	0	0

- Molecule 9 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
9	A7	119	3810	1131	1281	447	833	118	0	0

- Molecule 10 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
10	A8	146	4679	1390	1568	551	1025	145	0	0

- Molecule 11 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
11	B2	1476	47369	14078	15858	5637	10320	1476	0	0

- Molecule 12 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
12	A5	3022	96979	28814	32467	11522	21154	3022	0	0

- Molecule 13 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	AR	121	1985	604	1009	183	184	5	0	0

- Molecule 14 is a protein called Plectin/S10 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	AK	93	1555	509	786	124	135	1	0	0

- Molecule 15 is a protein called Ribosomal Protein, Small subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	AW	129	2110	654	1082	193	177	4	0	0

- Molecule 16 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	AS	148	2453	754	1248	237	209	5	0	0

- Molecule 17 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
17	AT	140	2260	704	1149	213	193	1	0	0

- Molecule 18 is a protein called Small ribosomal subunit protein eS26.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
18	Aa	99	1631	496	828	172	129	6	0	0

- Molecule 19 is a protein called Ubiquitin-like protein 1-ribosomal protein eS31 fusion protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
19	Af	50	789	246	392	77	69	5	0	0

- Molecule 20 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
20	AO	135	2063	624	1049	200	185	5	0	0

- Molecule 21 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
21	AI	207	3391	1044	1723	326	296	2	0	0

- Molecule 22 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
22	AF	185	2969	914	1515	275	259	6	0	0

- Molecule 23 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
23	AM	117	1808	565	904	162	170	7	0	0

- Molecule 24 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
24	AV	81	1239	378	622	114	120	5	0	0

- Molecule 25 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
25	AN	151	2514	769	1297	236	206	6	0	0

- Molecule 26 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	AZ	71	1165	363	601	100	99	2	0	0

- Molecule 27 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	Ad	55	895	284	443	93	71	4	0	0

- Molecule 28 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	AY	123	2085	637	1093	188	165	2	0	0

- Molecule 29 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	AU	100	1650	500	854	154	138	4	0	0

- Molecule 30 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
30	AG	228	3791	1159	1954	350	321	7	0	0

- Molecule 31 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
31	Ab	82	1305	404	663	119	111	8	0	0

- Molecule 32 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
32	AP	128	2112	658	1090	189	169	6	0	0

- Molecule 33 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
33	Ac	65	1069	314	549	106	98	2	0	0

- Molecule 34 is a protein called Ubiquitin-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
34	Ae	45	752	219	388	84	61	0	0

- Molecule 35 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
35	AX	140	2242	691	1150	212	186	3	0	0

- Molecule 36 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
36	AL	143	2380	736	1222	223	194	5	0	0

- Molecule 37 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
37	AJ	177	3060	936	1592	288	243	1	0	0

- Molecule 38 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
38	AQ	140	2305	715	1181	215	193	1	0	0

- Molecule 39 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
39	AH	192	3187	993	1643	280	271	0	0

- Molecule 40 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
40	CF	213	3534	1119	1791	320	302	2	0	0

- Molecule 41 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
41	CS	179	2976	936	1506	278	250	6	0	0

- Molecule 42 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
42	CV	128	1991	614	1020	182	169	6	0	0

- Molecule 43 is a protein called Large ribosomal subunit protein eL22.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
43	CU	100	1692	532	868	147	144	1	0	0

- Molecule 44 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
44	CL	204	3388	1025	1740	338	283	2	0	0

- Molecule 45 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
45	CG	221	3680	1123	1892	354	309	2	0	0

- Molecule 46 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
46	CI	213	3485	1083	1756	343	290	13	0	0

- Molecule 47 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
47	CO	201	3328	1031	1714	314	264	5	0	0

- Molecule 48 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
48	CC	335	5420	1675	2769	521	449	6	0	0

- Molecule 49 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
49	Ch	122	2094	618	1105	201	169	1	0	0

- Molecule 50 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
50	CE	139	2311	727	1195	203	185	1	0	0

- Molecule 51 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
51	Co	102	1739	522	902	174	135	6	0	0

- Molecule 52 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
52	Cf	117	1901	594	971	183	153	0	0

- Molecule 53 is a protein called Large ribosomal subunit protein eL36.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
53	Ci	104	1754	521	918	176	137	2	0	0

- Molecule 54 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
54	Cl	50	922	276	487	93	63	3	0	0

- Molecule 55 is a protein called Large ribosomal subunit protein eL15.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	CN	203	Total 3463	C 1068	H 1763	N 358	O 272	S 2	0	0

- Molecule 56 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	Ca	144	Total 2299	C 717	H 1163	N 232	O 183	S 4	0	0

- Molecule 57 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	Cp	88	Total 1404	C 425	H 726	N 134	O 113	S 6	0	0

- Molecule 58 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	CM	132	Total 2204	C 668	H 1151	N 205	O 178	S 2	0	0

- Molecule 59 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	Cc	96	Total 1497	C 464	H 762	N 129	O 137	S 5	0	0

- Molecule 60 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	CH	188	Total 3081	C 954	H 1577	N 278	O 266	S 6	0	0

- Molecule 61 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	CY	132	Total 2181	C 651	H 1131	N 219	O 176	S 4	0	0

- Molecule 62 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
62	CR	194	3384	1012	1746	349	274	3	0	0

- Molecule 63 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
63	Cb	52	892	268	460	94	69	1	0	0

- Molecule 64 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
64	CQ	187	3023	918	1550	299	255	1	0	0

- Molecule 65 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
65	CT	160	2621	806	1338	256	218	3	0	0

- Molecule 66 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
66	CD	289	4701	1468	2373	430	428	2	0	0

- Molecule 67 is a protein called Large ribosomal subunit protein eL27.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
67	CZ	135	2301	716	1199	200	184	2	0	0

- Molecule 68 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
68	CP	154	2506	780	1257	249	215	5	0	0

- Molecule 69 is a protein called eL41.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
69	Cn	22	461	128	252	54	25	2	0	0

- Molecule 70 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
70	Cg	104	1759	526	922	170	139	2	0	0

- Molecule 71 is a protein called Large ribosomal subunit protein eL38.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
71	Ck	69	1181	359	622	100	99	1	0	0

- Molecule 72 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
72	Cm	51	874	258	456	86	69	5	0	0

- Molecule 73 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
73	Cd	105	1770	544	903	169	151	3	0	0

- Molecule 74 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
74	Ce	128	2160	652	1119	216	169	4	0	0

- Molecule 75 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
75	CW	88	1447	442	745	140	118	2	0	0

- Molecule 76 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
76	Cj	88	1433	431	727	154	117	4	0	0

- Molecule 77 is a protein called Large ribosomal subunit protein uL5B.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
77	CJ	186	3062	952	1555	281	269	5	0	0

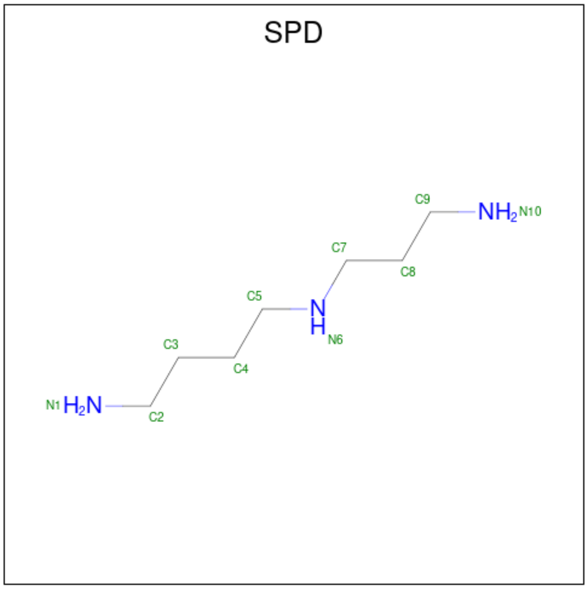
- Molecule 78 is a protein called Large ribosomal subunit protein uL23B.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
78	CX	119	1958	606	1004	181	166	1	0	0

- Molecule 79 is a RNA chain called mRNA.

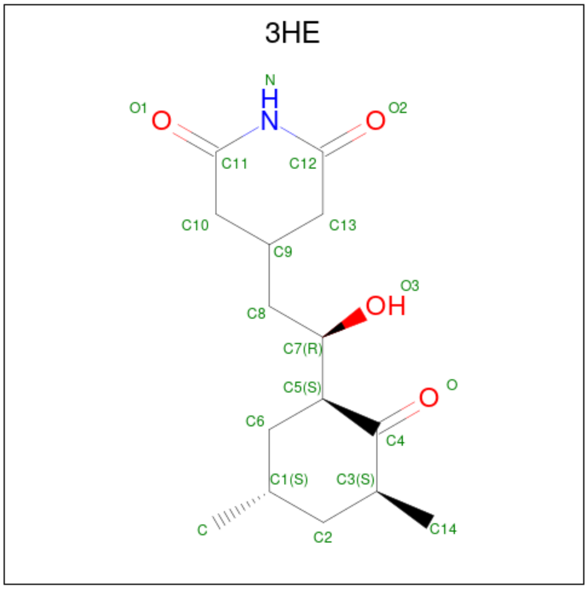
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
79	DC	10	301	90	101	20	80	10	0	0

- Molecule 80 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
80	A5	1	10	7	3	0

- Molecule 81 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (three-letter code: 3HE) (formula: $C_{15}H_{23}NO_4$).

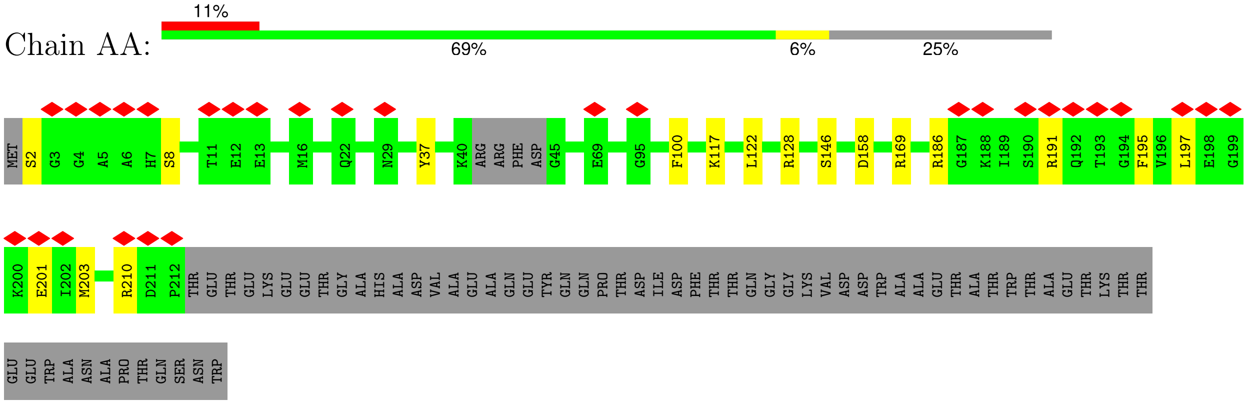


Mol	Chain	Residues	Atoms	AltConf
81	A5	1	Total C H N O 43 15 23 1 4	0

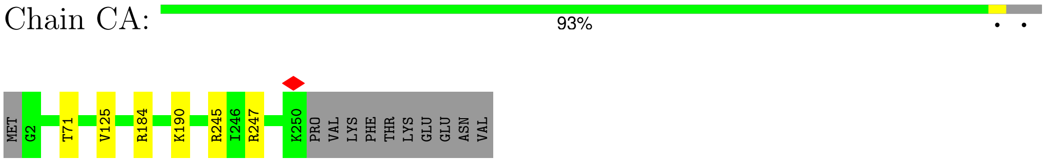
3 Residue-property plots ⓘ

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.

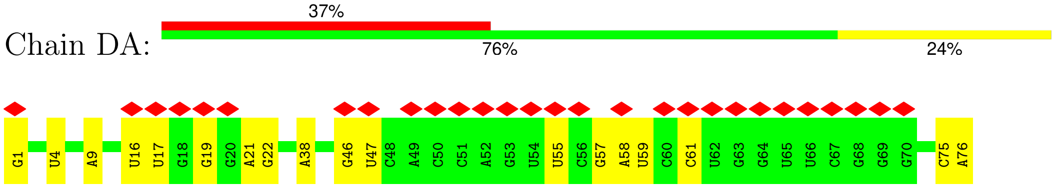
- Molecule 1: Small ribosomal subunit protein uS2



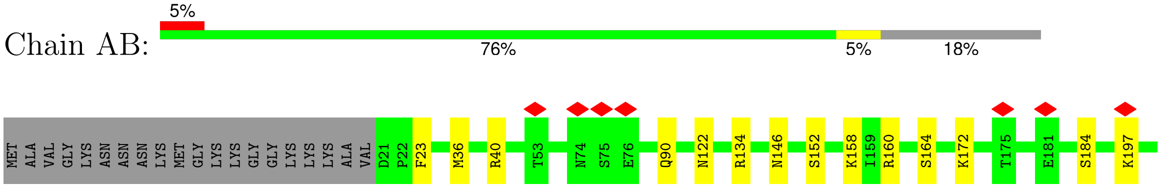
- Molecule 2: Large ribosomal subunit protein uL2

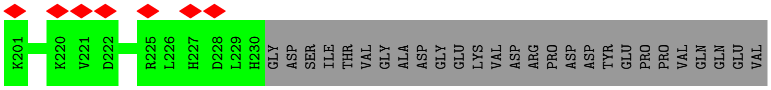


- Molecule 3: tRNA



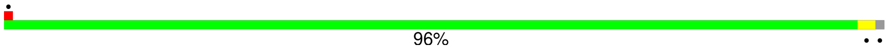
- Molecule 4: Small ribosomal subunit protein eS1





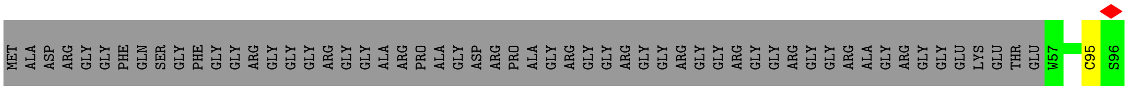
- Molecule 5: Large ribosomal subunit protein uL3

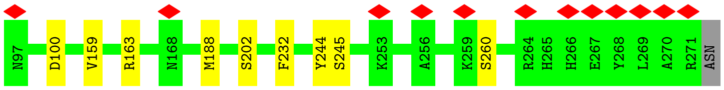
Chain CB:



- Molecule 6: Small ribosomal subunit protein uS5

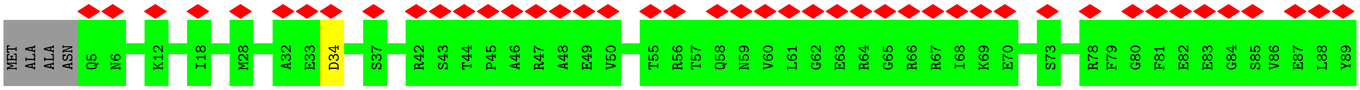
Chain AC:

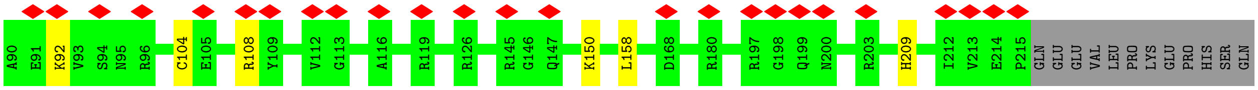




- Molecule 7: Small ribosomal subunit protein uS3

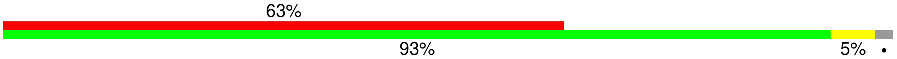
Chain AD:

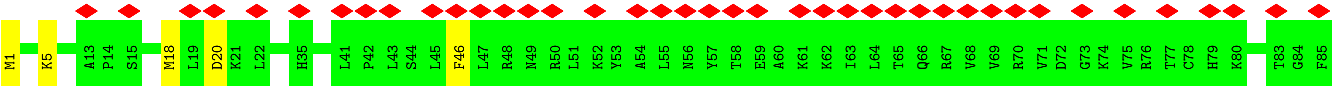


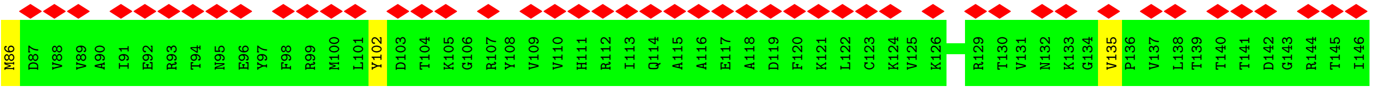


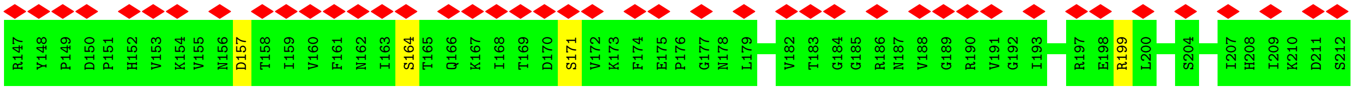
- Molecule 8: Small ribosomal subunit protein eS4

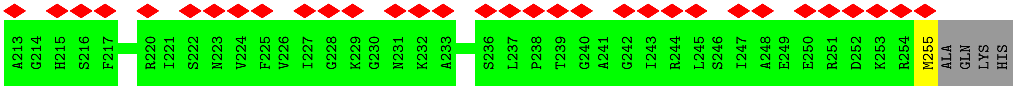
Chain AE:





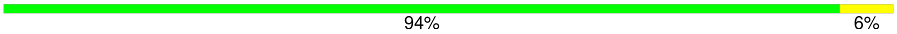


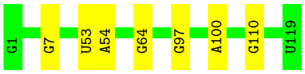




- Molecule 9: 5S rRNA

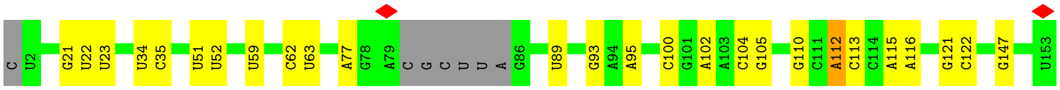
Chain A7:





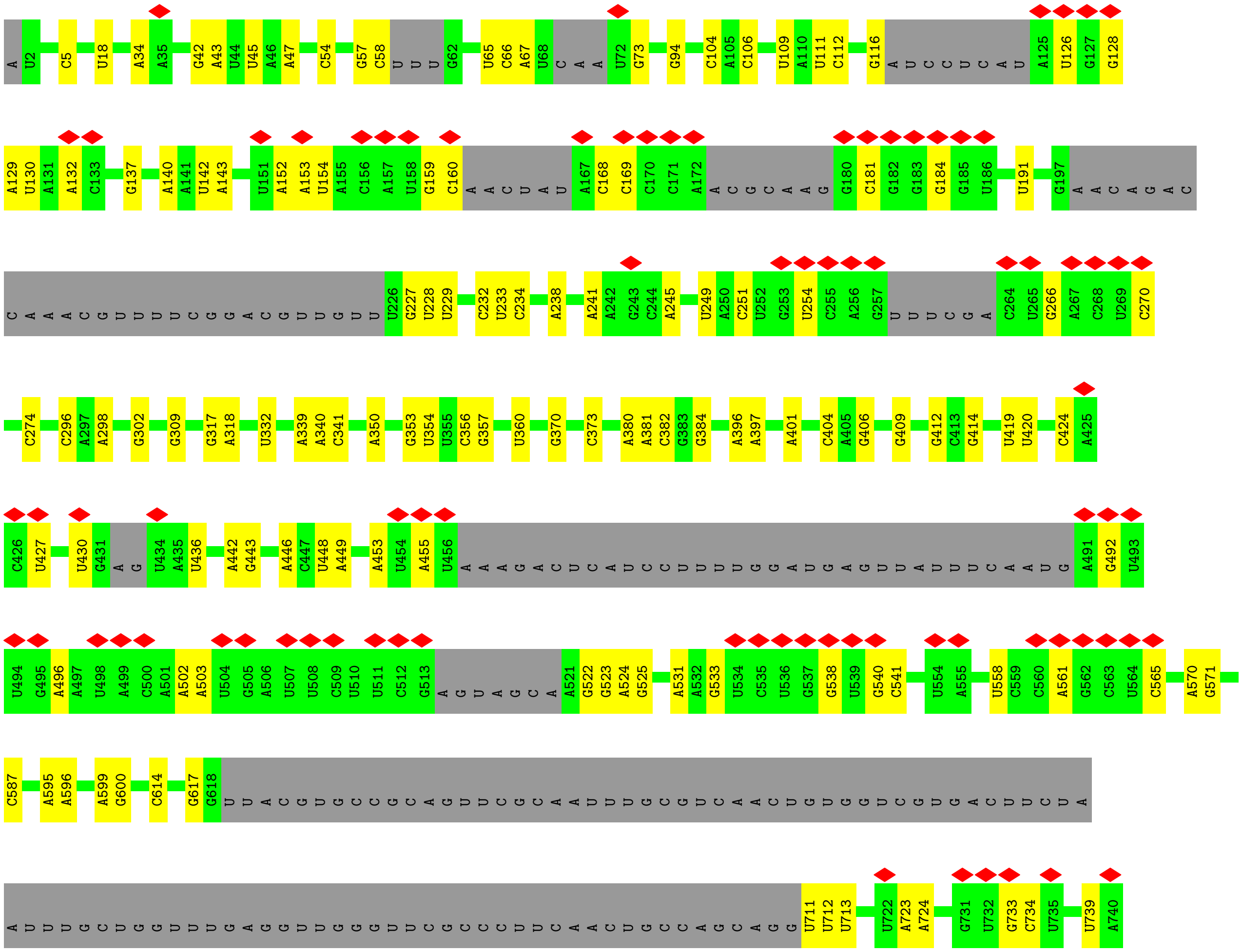
- Molecule 10: 5.8S rRNA

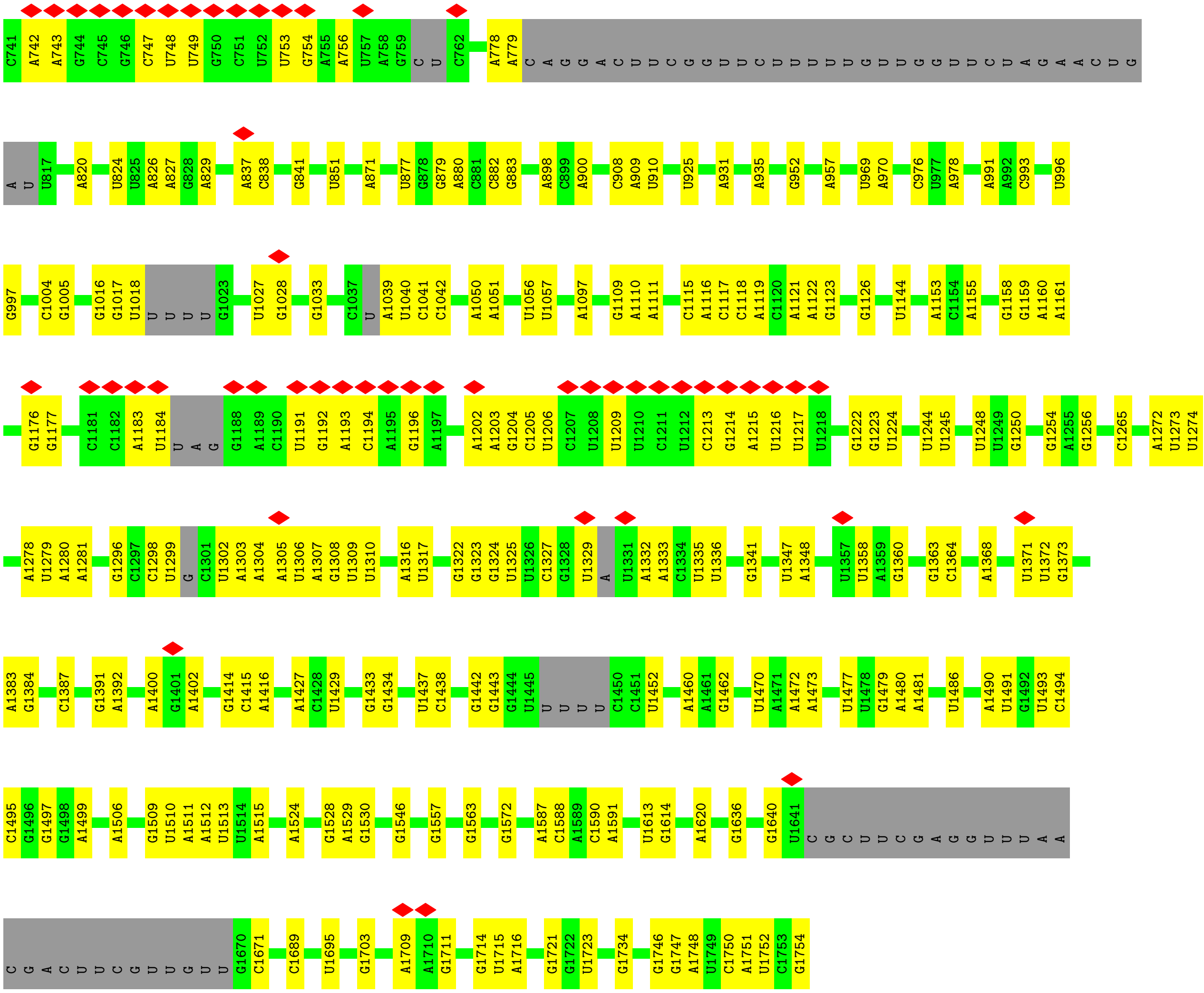
Chain A8:



- Molecule 11: 18S rRNA

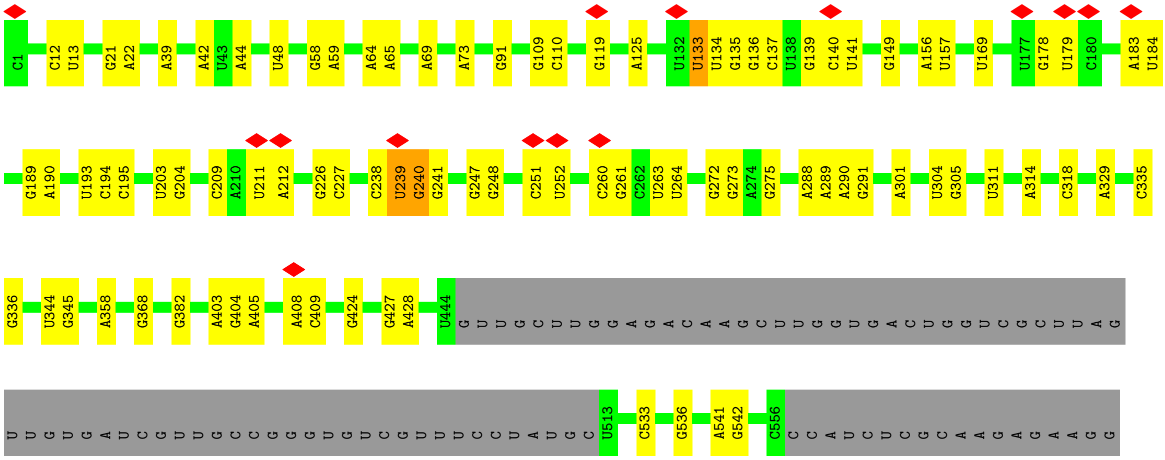
Chain B2:

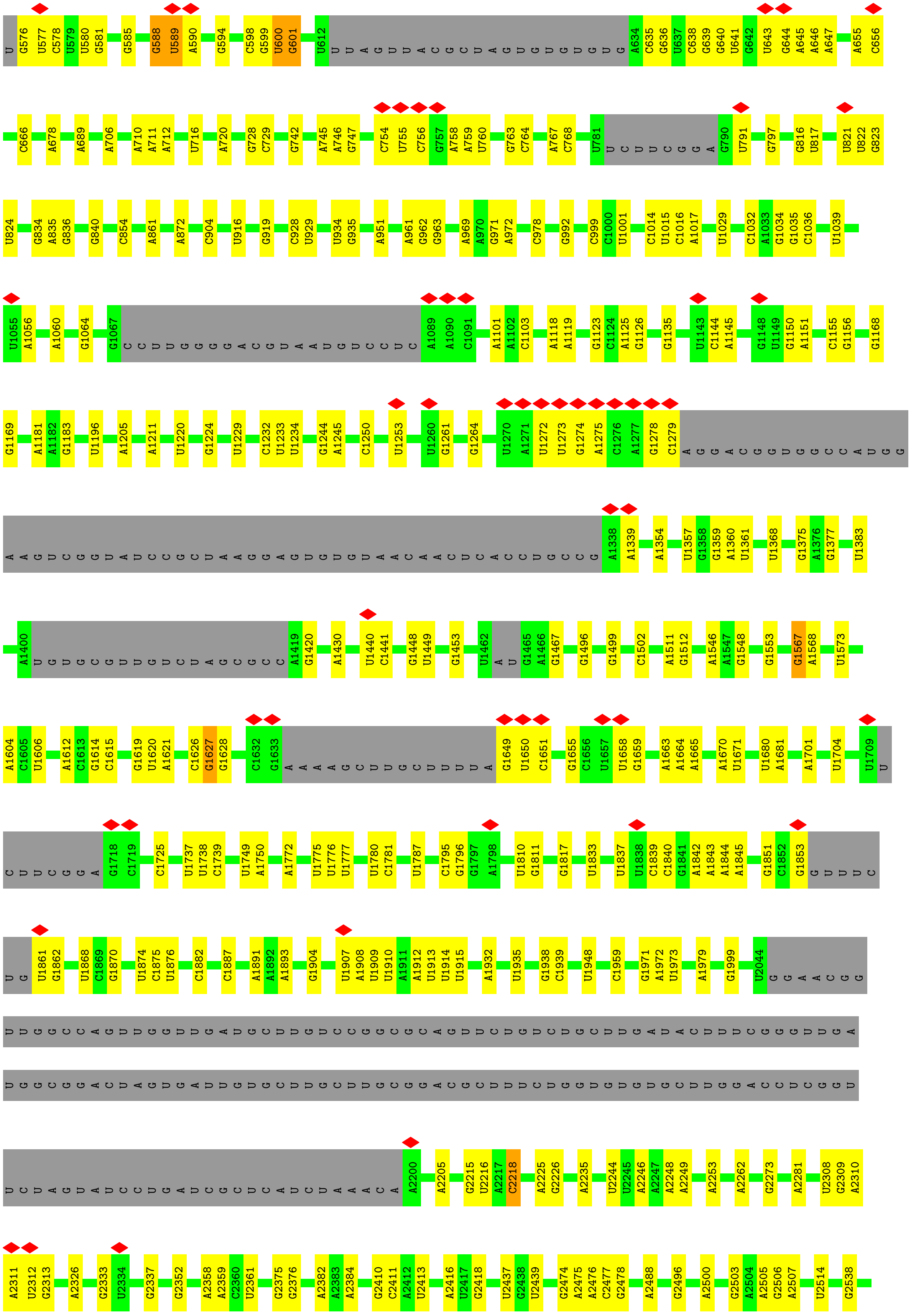




- Molecule 12: 28S rRNA

Chain A5:

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C U U C G G A G1718 C1719 C1725 U1737 U1738 C1739 U1749 A1750 A1772 U1775 U1776 U1777 U1780 C1781 U1787 C1795 G1796 G1797 A1798 U1810 G1811 G1817 U1833 U1837 U1838 C1839 C1840 G1841 A1842 A1843 A1844 A1845 G1851 C1852 G1853 G U U U C
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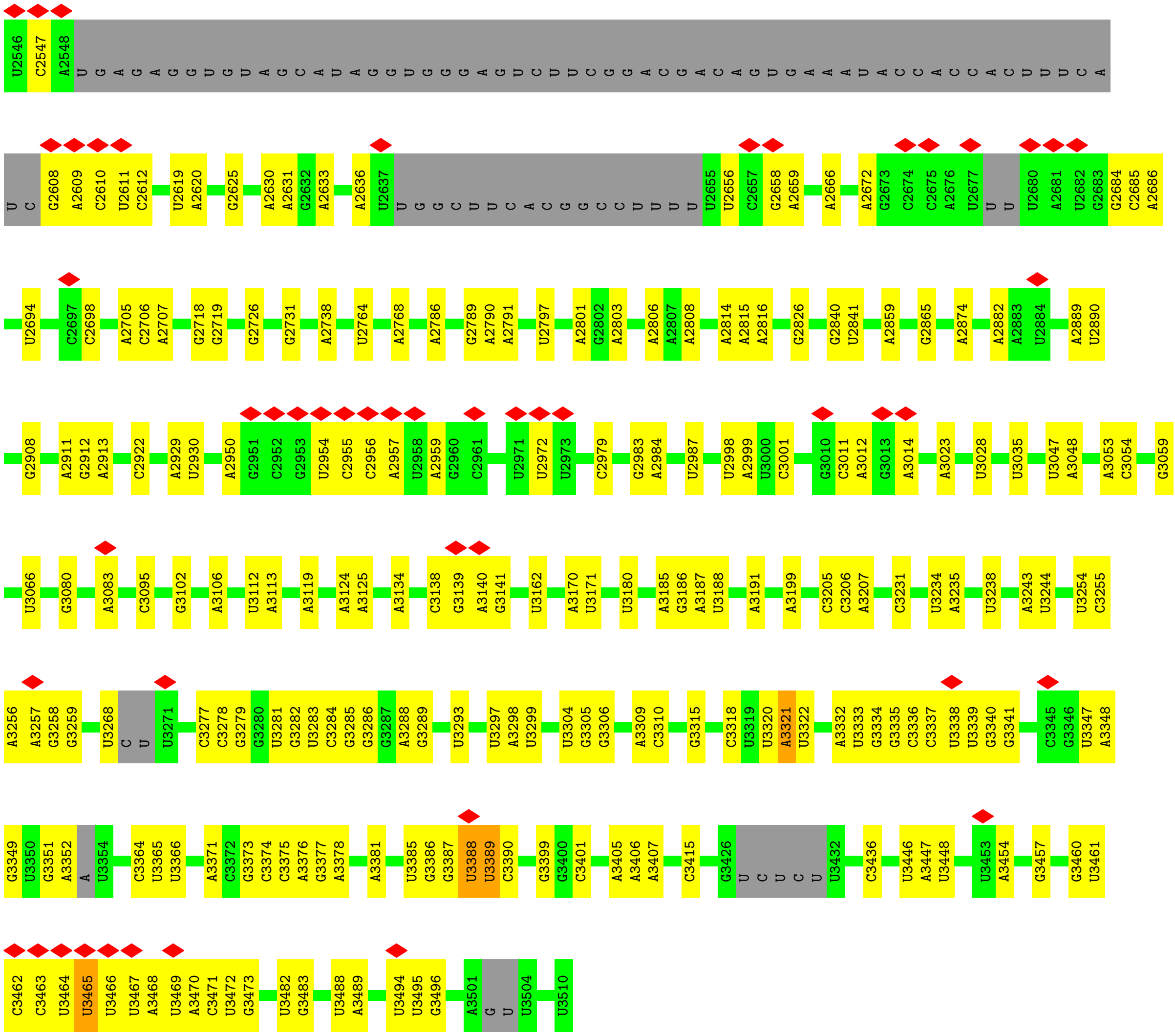
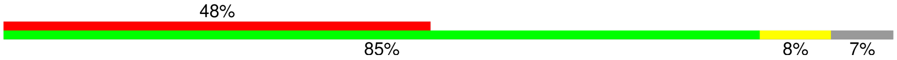
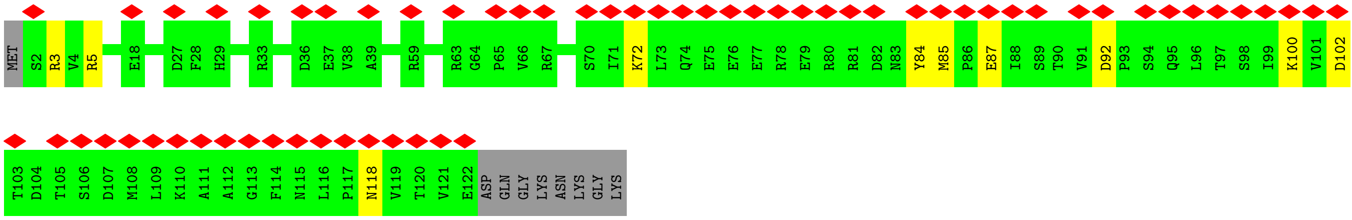


- Molecule 13: Small ribosomal subunit protein eS17

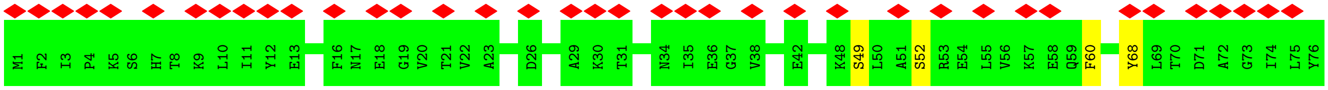
Chain AR:



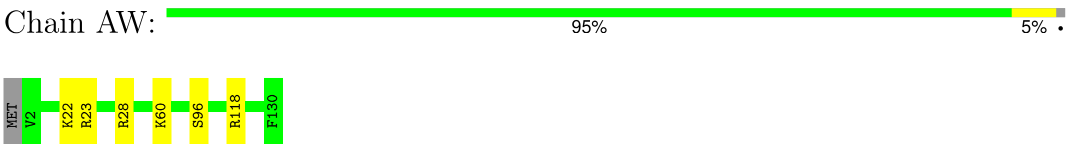


- Molecule 14: Plectin/S10 N-terminal domain-containing protein

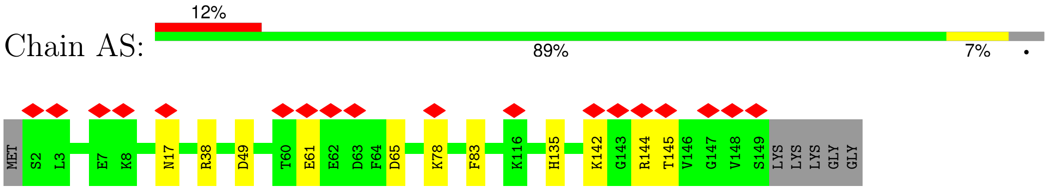
Chain AK:



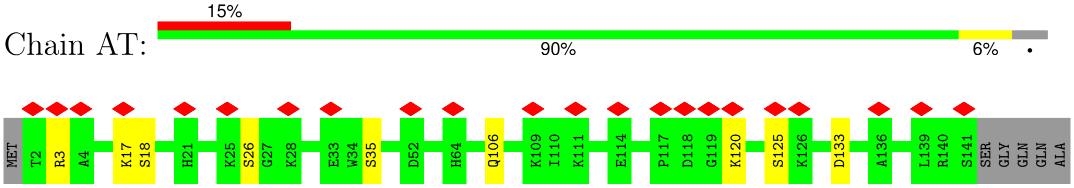
- Molecule 15: Ribosomal Protein, Small subunit



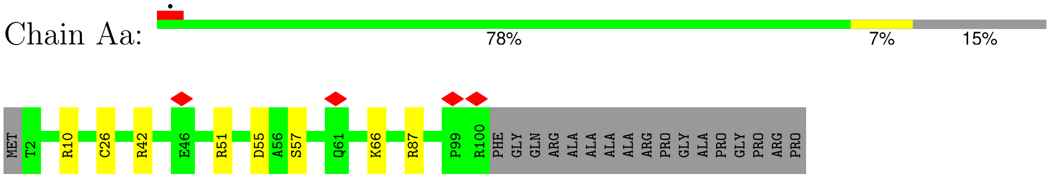
- Molecule 16: Small ribosomal subunit protein uS13



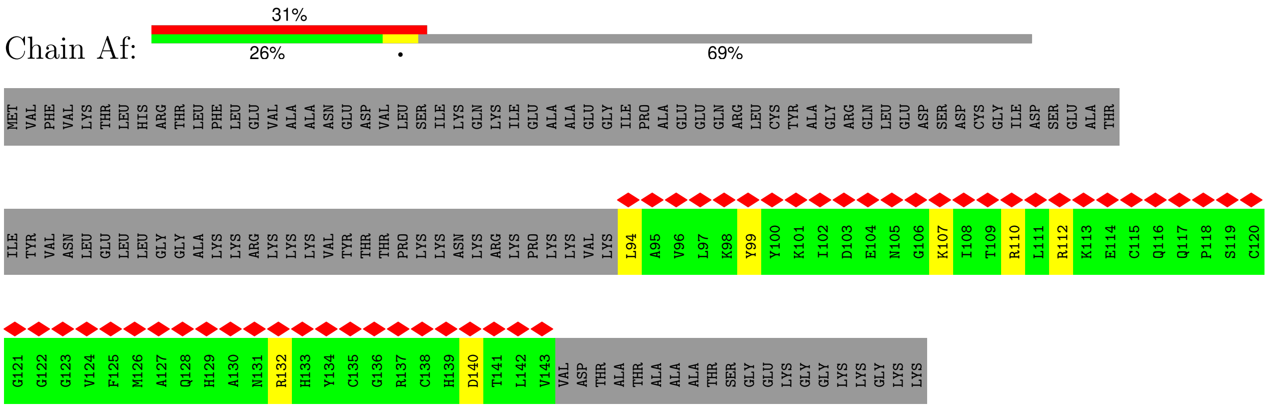
- Molecule 17: Small ribosomal subunit protein eS19



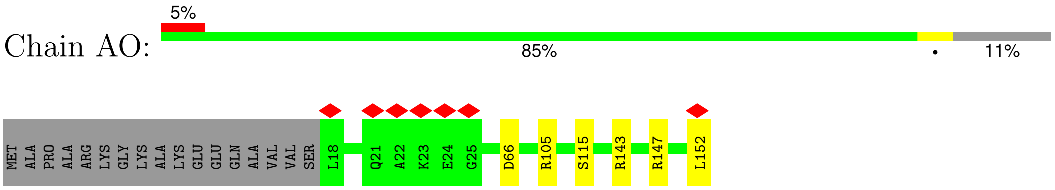
- Molecule 18: Small ribosomal subunit protein eS26



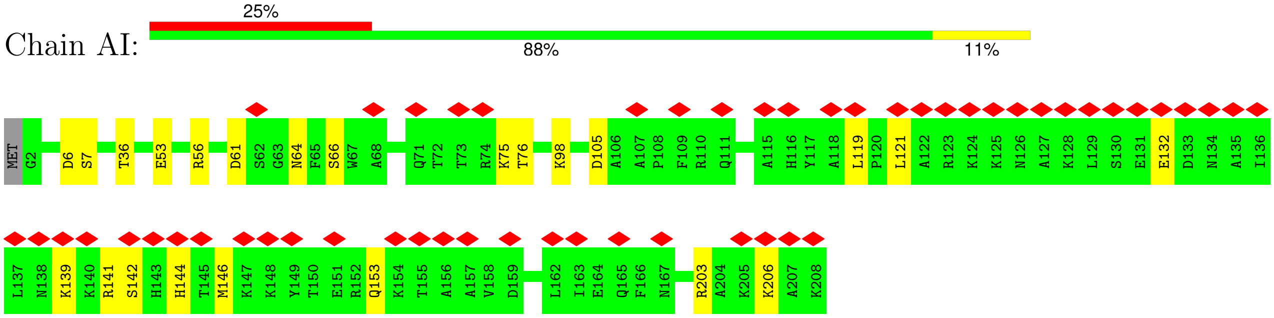
- Molecule 19: Ubiquitin-like protein 1-ribosomal protein eS31 fusion protein



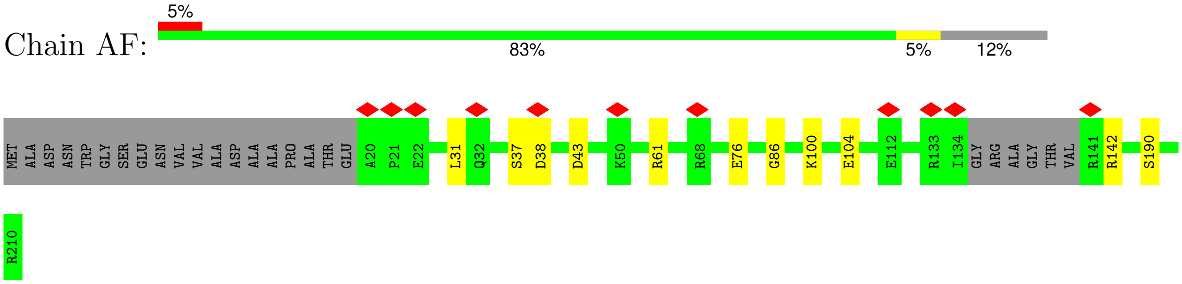
- Molecule 20: Small ribosomal subunit protein uS11



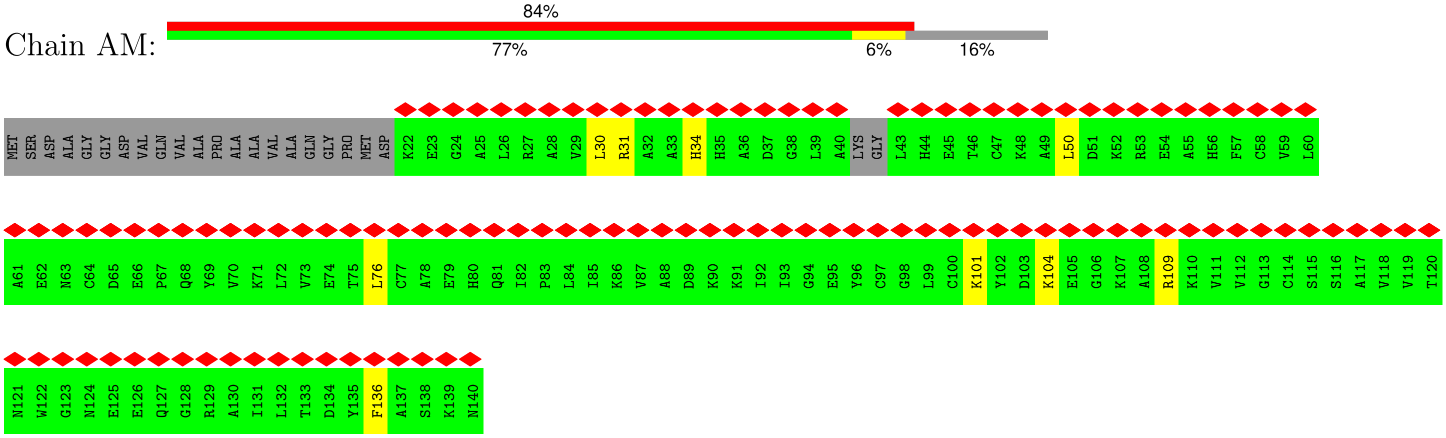
• Molecule 21: Small ribosomal subunit protein eS8



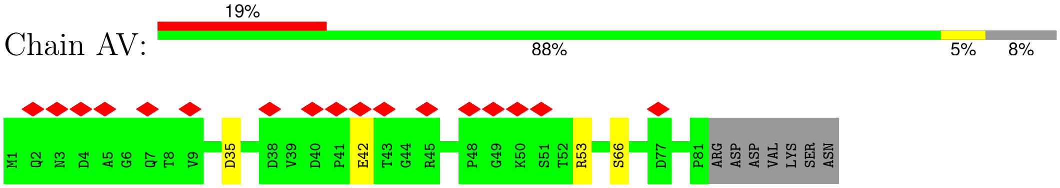
• Molecule 22: Small ribosomal subunit protein uS7



• Molecule 23: Small ribosomal subunit protein eS12

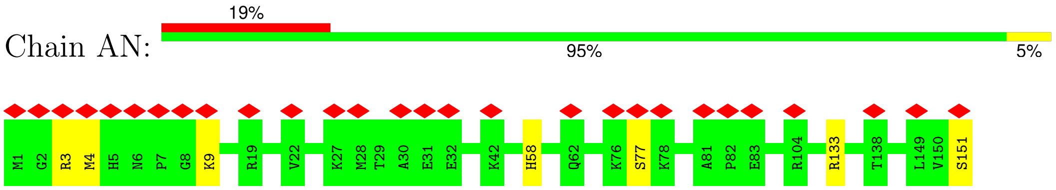


• Molecule 24: Small ribosomal subunit protein eS21



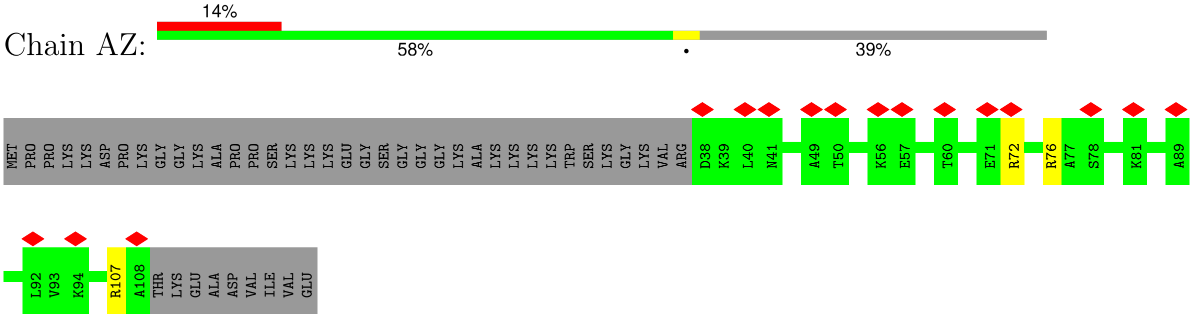
• Molecule 25: Small ribosomal subunit protein uS15

Chain AN:



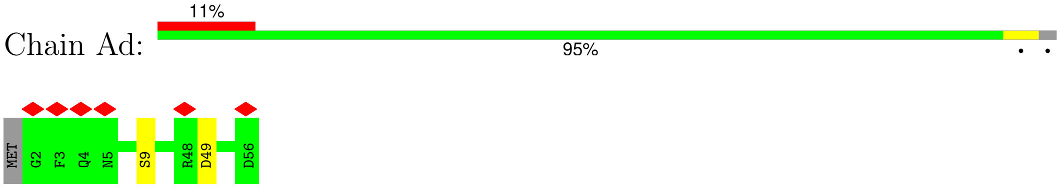
- Molecule 26: Small ribosomal subunit protein eS25

Chain AZ:



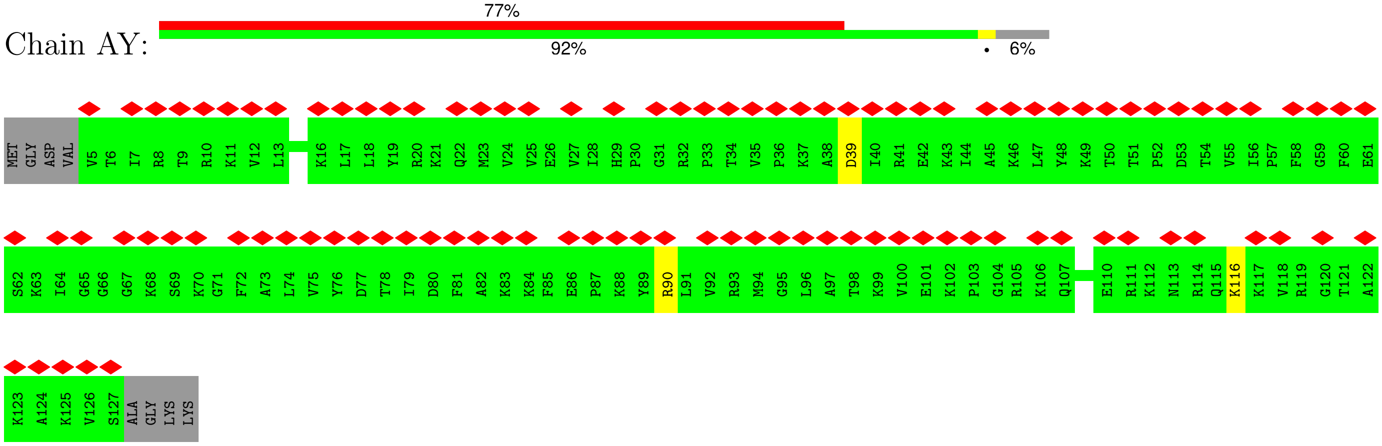
- Molecule 27: Small ribosomal subunit protein uS14

Chain Ad:



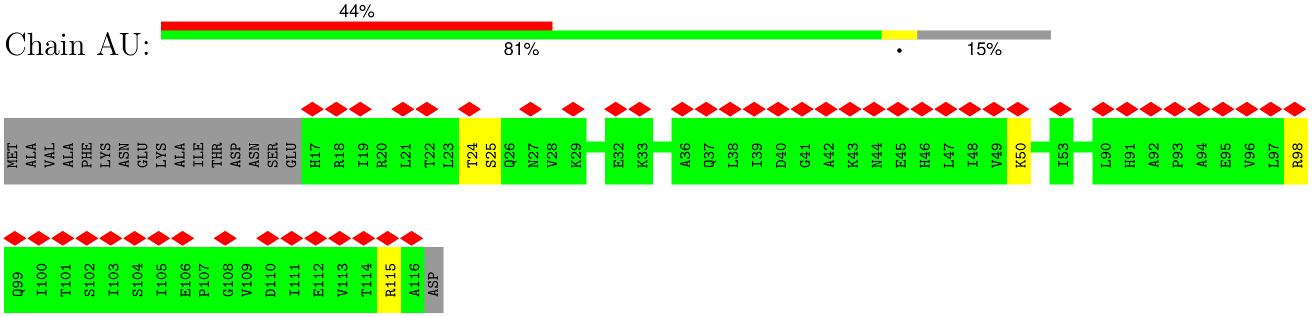
- Molecule 28: Small ribosomal subunit protein eS24

Chain AY:

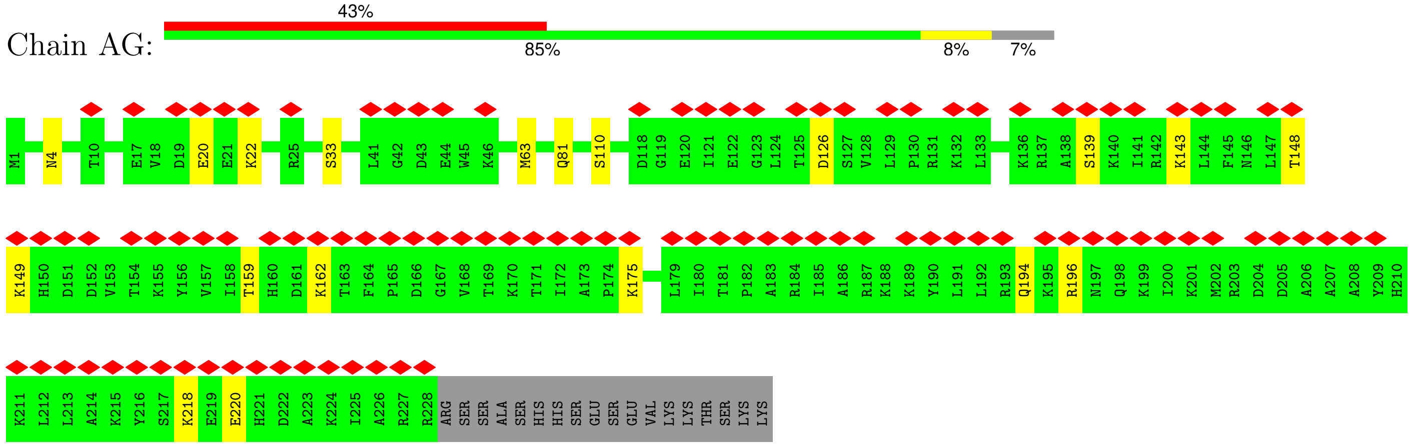


- Molecule 29: Small ribosomal subunit protein uS10

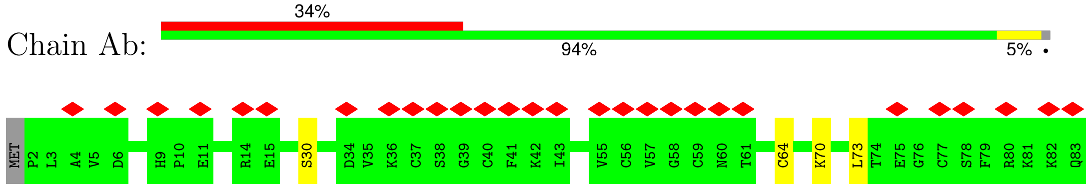
Chain AU:



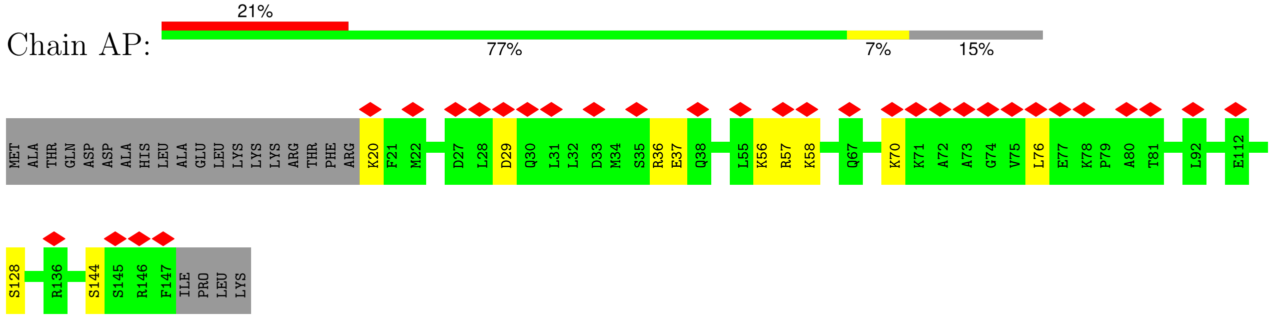
- Molecule 30: Small ribosomal subunit protein eS6



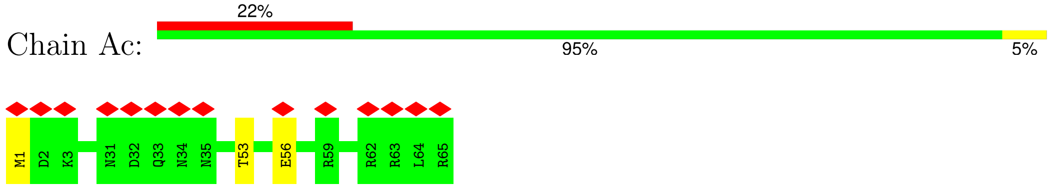
- Molecule 31: Small ribosomal subunit protein eS27



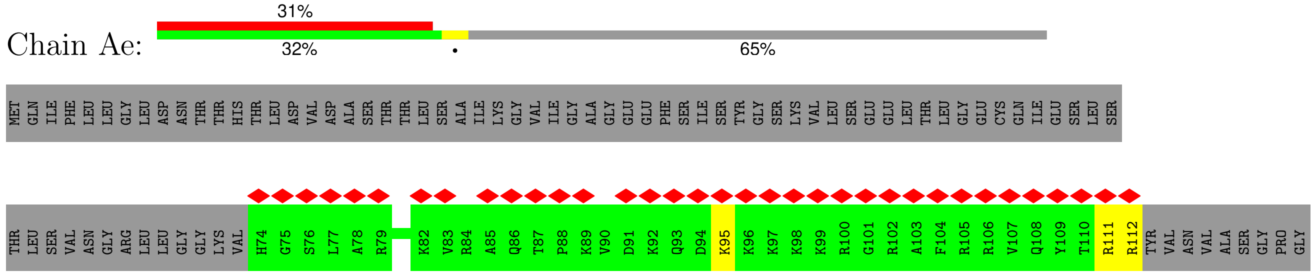
- Molecule 32: Small ribosomal subunit protein uS19

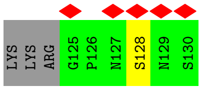


- Molecule 33: Small ribosomal subunit protein eS28



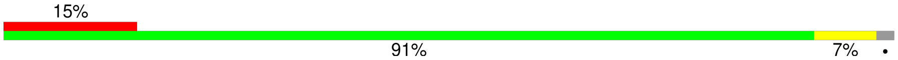
- Molecule 34: Ubiquitin-like domain-containing protein

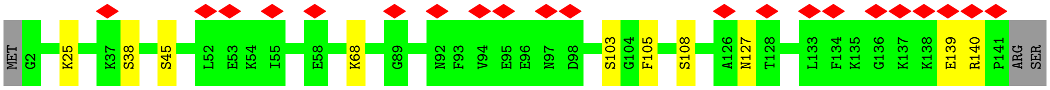




- Molecule 35: Small ribosomal subunit protein uS12

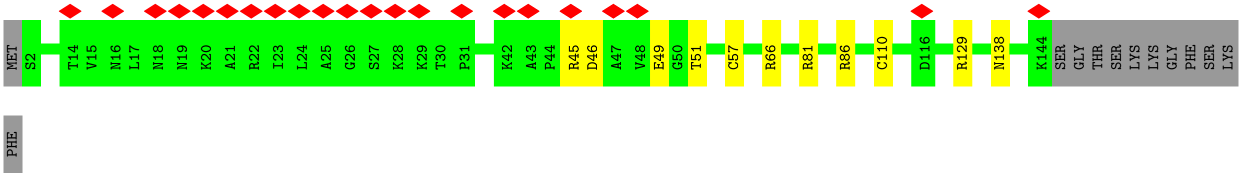
Chain AX:





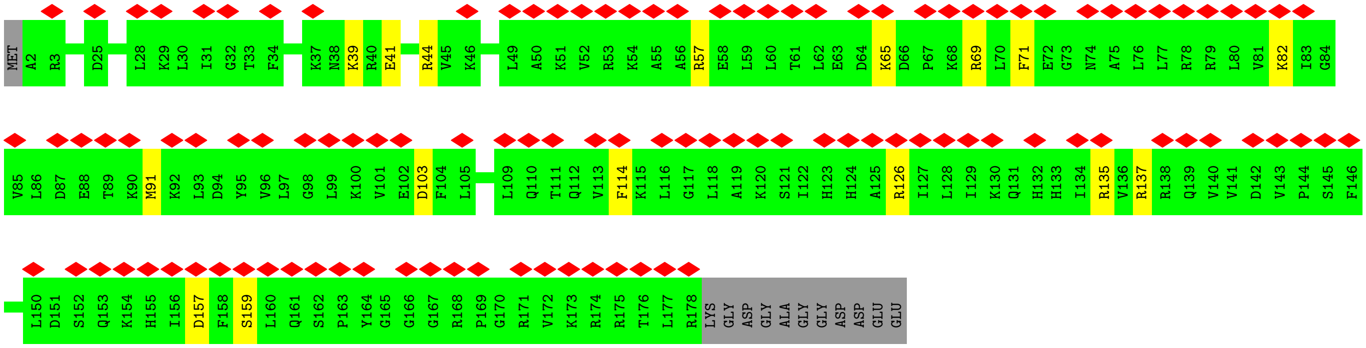
- Molecule 36: Small ribosomal subunit protein uS17

Chain AL:



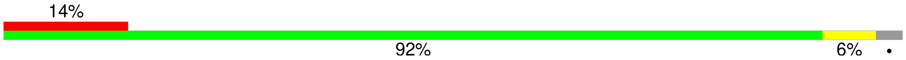
- Molecule 37: Small ribosomal subunit protein uS4

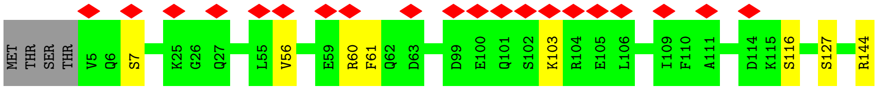
Chain AJ:



- Molecule 38: Small ribosomal subunit protein uS9

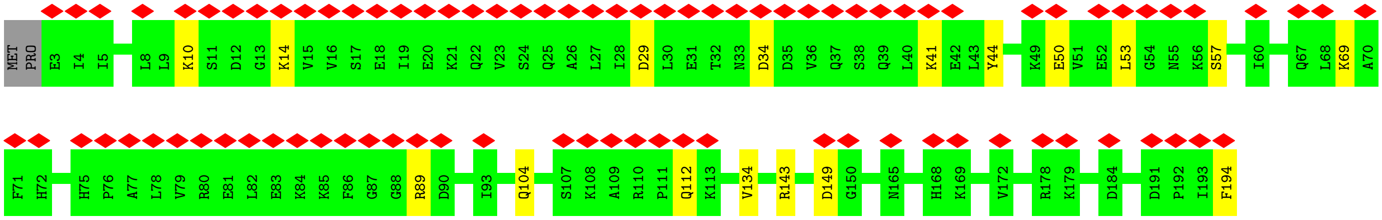
Chain AQ:





- Molecule 39: Small ribosomal subunit protein eS7

Chain AH:

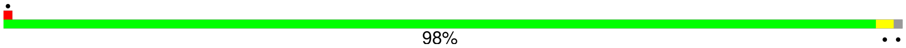


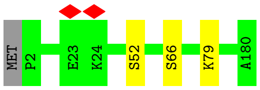
- Molecule 40: Large ribosomal subunit protein uL30

Chain CF:

- Molecule 41: Large ribosomal subunit protein eL20

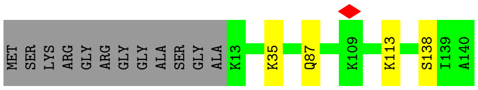
Chain CS:





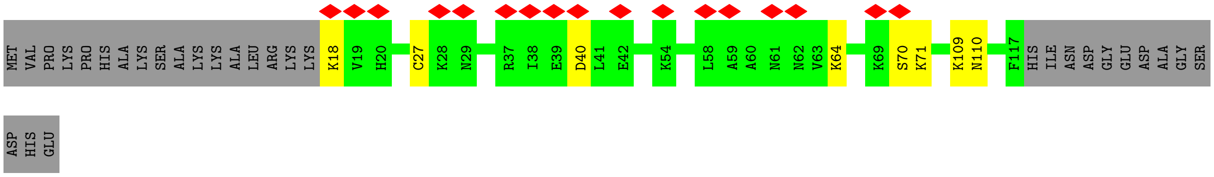
- Molecule 42: Large ribosomal subunit protein uL14

Chain CV:



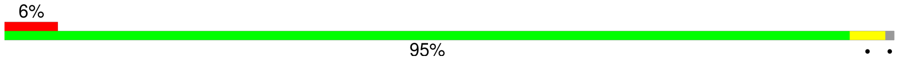
- Molecule 43: Large ribosomal subunit protein eL22

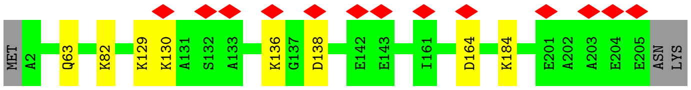
Chain CU:



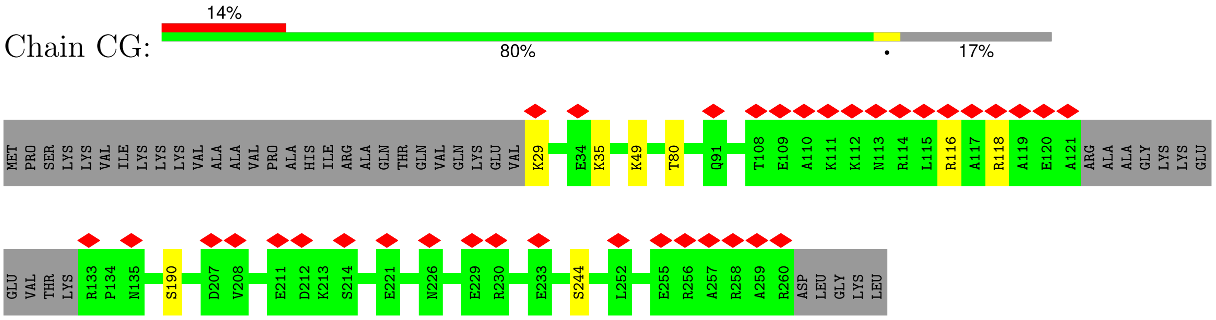
- Molecule 44: Large ribosomal subunit protein eL13

Chain CL:

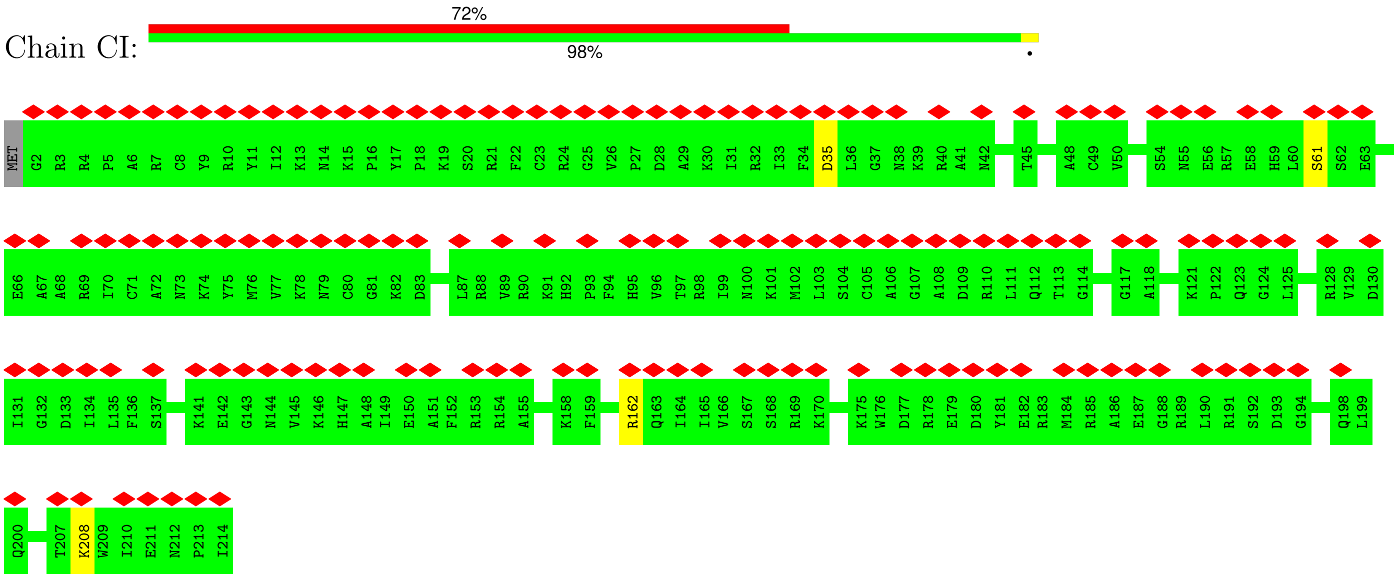




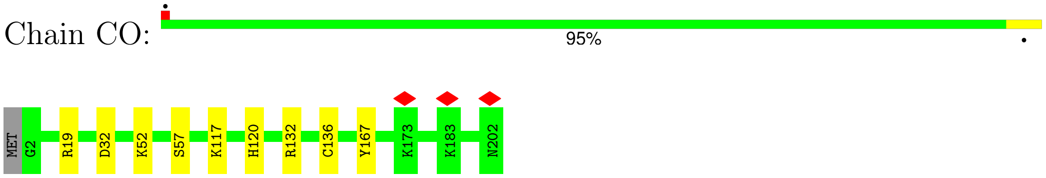
- Molecule 45: Large ribosomal subunit protein eL8



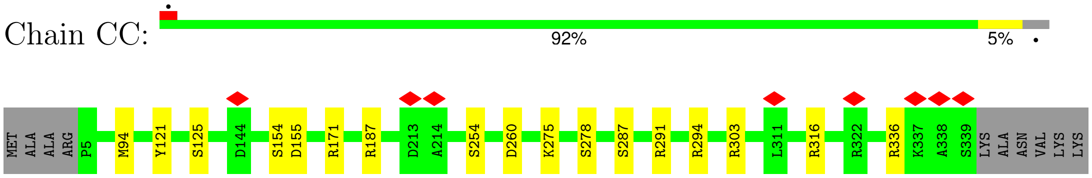
- Molecule 46: Large ribosomal subunit protein uL16



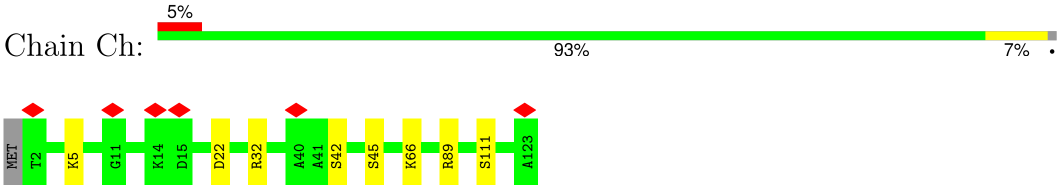
- Molecule 47: Large ribosomal subunit protein uL13



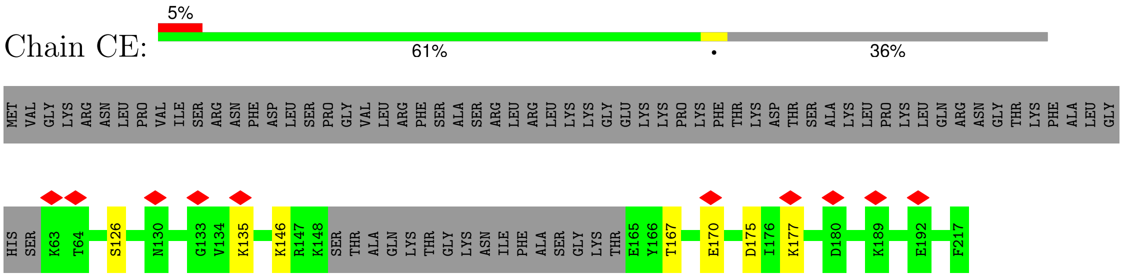
- Molecule 48: Large ribosomal subunit protein uL4



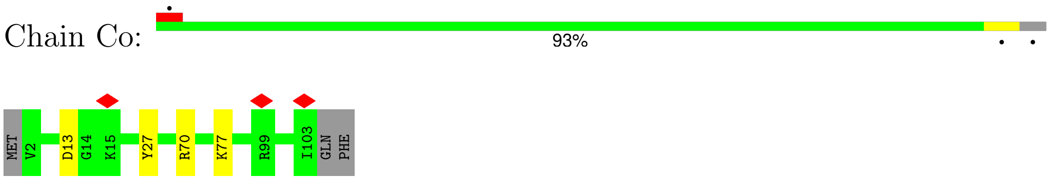
- Molecule 49: Large ribosomal subunit protein uL29



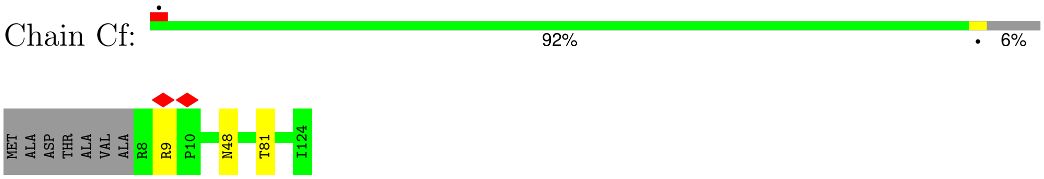
- Molecule 50: Large ribosomal subunit protein eL6



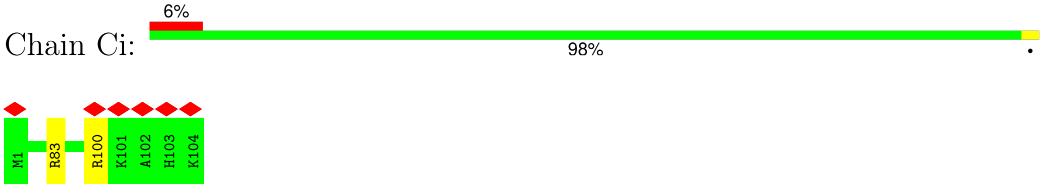
- Molecule 51: Large ribosomal subunit protein eL42



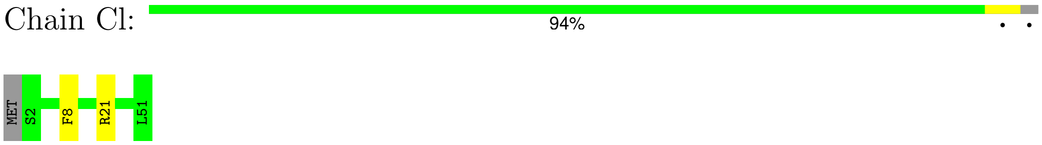
- Molecule 52: Large ribosomal subunit protein eL33



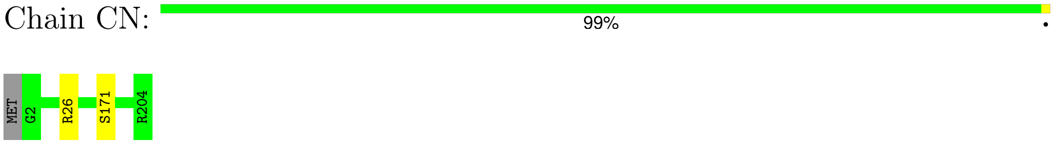
- Molecule 53: Large ribosomal subunit protein eL36



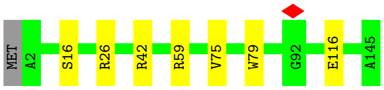
- Molecule 54: Large ribosomal subunit protein eL39



- Molecule 55: Large ribosomal subunit protein eL15

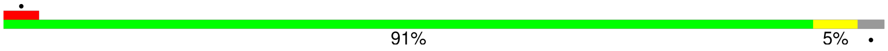


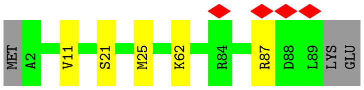
- Molecule 56: Large ribosomal subunit protein uL15



- Molecule 57: Large ribosomal subunit protein eL43

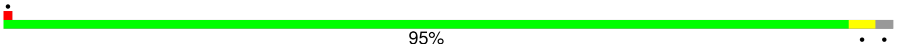
Chain Cp:

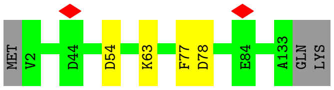




- Molecule 58: Large ribosomal subunit protein eL14

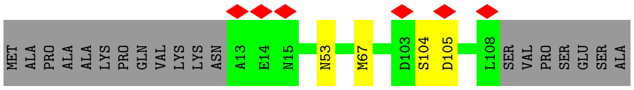
Chain CM:





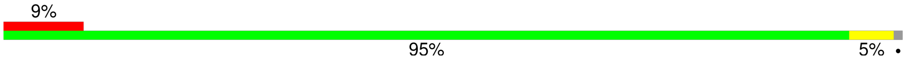
- Molecule 59: Large ribosomal subunit protein eL30

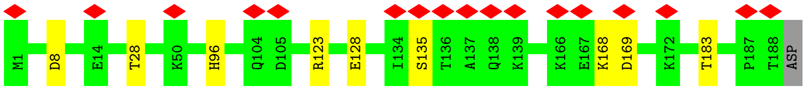
Chain Cc:



- Molecule 60: Large ribosomal subunit protein uL6

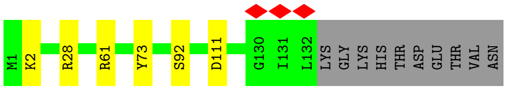
Chain CH:





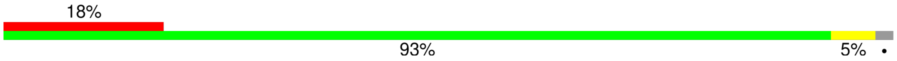
- Molecule 61: Large ribosomal subunit protein uL24

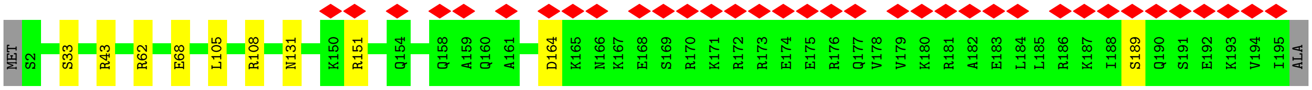
Chain CY:



- Molecule 62: Large ribosomal subunit protein eL19

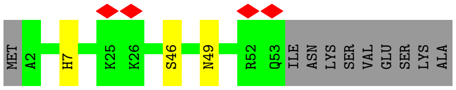
Chain CR:





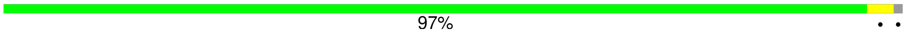
- Molecule 63: 60S ribosomal protein L29

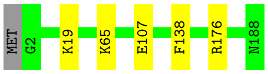
Chain Cb:



- Molecule 64: Large ribosomal subunit protein eL18

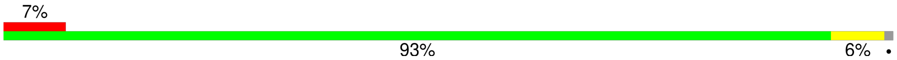
Chain CQ:

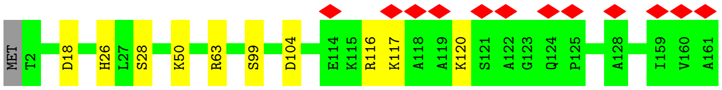




- Molecule 65: Large ribosomal subunit protein eL21

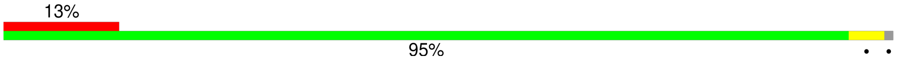
Chain CT:

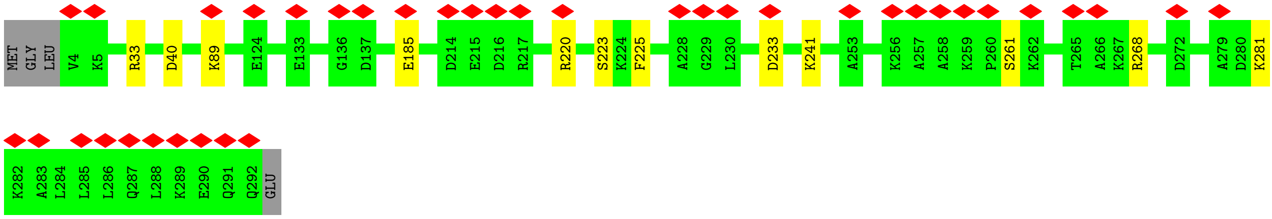




- Molecule 66: Large ribosomal subunit protein uL18

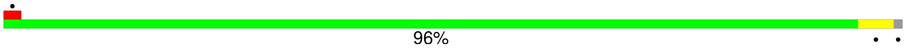
Chain CD:

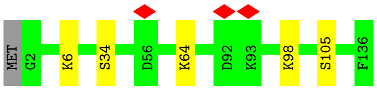




- Molecule 67: Large ribosomal subunit protein eL27

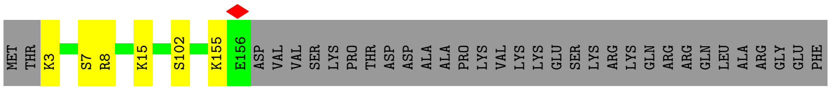
Chain CZ:





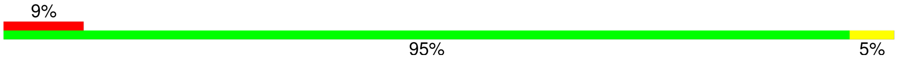
- Molecule 68: Large ribosomal subunit protein uL22

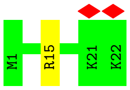
Chain CP:



- Molecule 69: eL41

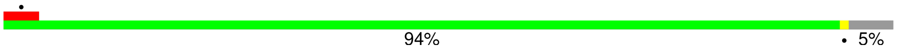
Chain Cn:

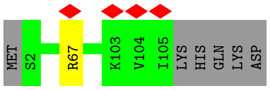




- Molecule 70: Large ribosomal subunit protein eL34

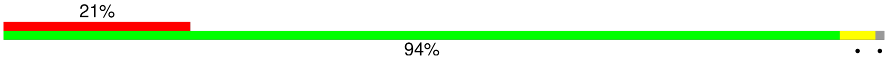
Chain Cg:

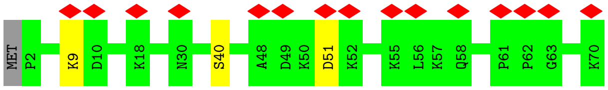




- Molecule 71: Large ribosomal subunit protein eL38

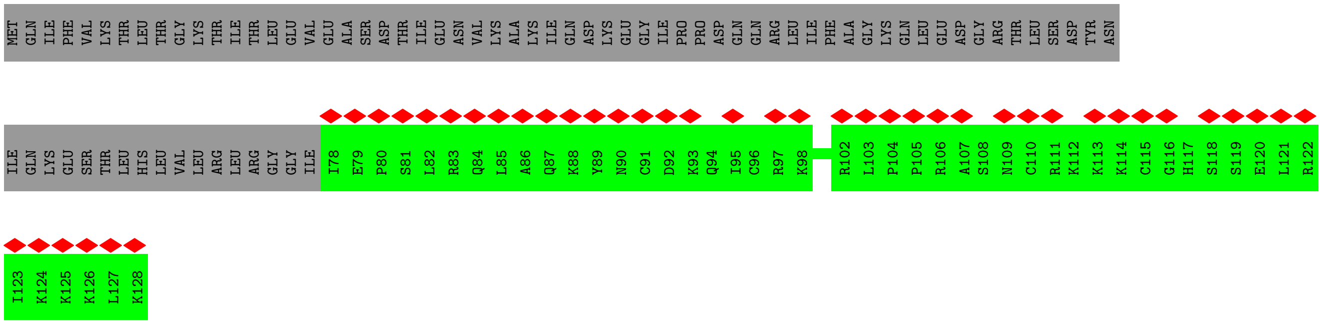
Chain Ck:





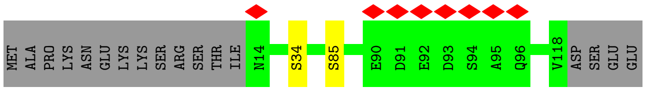
- Molecule 72: Ubiquitin-ribosomal protein eL40 fusion protein

Chain Cm:



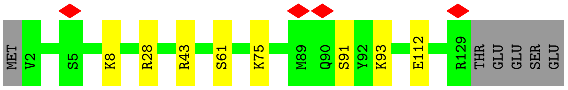
- Molecule 73: Large ribosomal subunit protein eL31

Chain Cd:



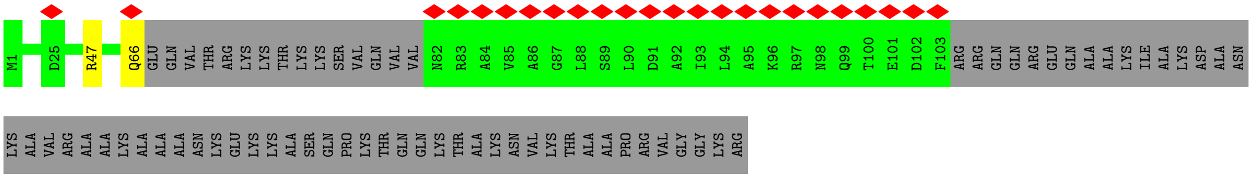
- Molecule 74: Large ribosomal subunit protein eL32

Chain Ce:



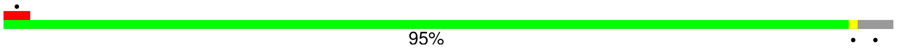
- Molecule 75: Large ribosomal subunit protein eL24

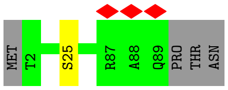
Chain CW:



- Molecule 76: Ribosomal protein L37

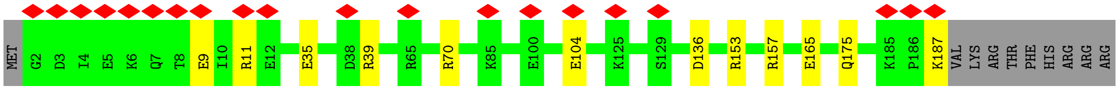
Chain Cj:





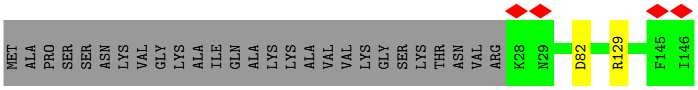
- Molecule 77: Large ribosomal subunit protein uL5B

Chain CJ:



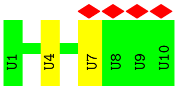
- Molecule 78: Large ribosomal subunit protein uL23B

Chain CX:



- Molecule 79: mRNA

Chain DC:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	145659	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	40.94	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	2.035	Depositor
Minimum map value	-1.231	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.199	Depositor
Map size (Å)	441.99997, 441.99997, 441.99997	wwPDB
Map dimensions	680, 680, 680	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.65, 0.65, 0.65	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: SPD, 3HE

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	AA	0.26	0/1645	0.51	0/2230
2	CA	0.25	0/1932	0.58	0/2593
3	DA	0.32	1/1819 (0.1%)	0.73	0/2833
4	AB	0.25	0/1710	0.52	0/2294
5	CB	0.26	0/3247	0.54	0/4355
6	AC	0.26	0/1689	0.49	0/2289
7	AD	0.26	0/1659	0.54	0/2226
8	AE	0.27	0/2053	0.58	0/2767
9	A7	0.24	0/2826	0.73	0/4402
10	A8	0.27	0/3477	0.78	1/5416 (0.0%)
11	B2	0.26	0/35236	0.77	1/54876 (0.0%)
12	A5	0.52	12/72151 (0.0%)	0.85	38/112424 (0.0%)
13	AR	0.26	0/988	0.56	0/1328
14	AK	0.28	0/790	0.53	0/1072
15	AW	0.26	0/1043	0.57	0/1399
16	AS	0.25	0/1225	0.56	0/1641
17	AT	0.25	0/1135	0.51	0/1524
18	Aa	0.25	0/819	0.59	0/1097
19	Af	0.25	0/404	0.54	0/540
20	AO	0.26	0/1027	0.60	0/1377
21	AI	0.27	0/1698	0.59	0/2277
22	AF	0.24	0/1475	0.54	0/1986
23	AM	0.25	0/917	0.55	0/1231
24	AV	0.29	0/625	0.57	0/842
25	AN	0.26	0/1240	0.55	0/1658
26	AZ	0.25	0/572	0.51	0/770
27	Ad	0.26	0/464	0.59	0/615
28	AY	0.26	0/1008	0.56	0/1344
29	AU	0.27	0/808	0.64	0/1090
30	AG	0.27	0/1863	0.58	0/2483
31	Ab	0.28	0/655	0.54	0/880
32	AP	0.26	0/1041	0.53	0/1391

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Ac	0.26	0/521	0.63	0/695
34	Ae	0.25	0/367	0.63	0/480
35	AX	0.26	0/1112	0.54	0/1487
36	AL	0.27	0/1182	0.58	0/1591
37	AJ	0.26	0/1490	0.60	0/1991
38	AQ	0.27	0/1143	0.57	0/1529
39	AH	0.27	0/1572	0.57	0/2114
40	CF	0.26	0/1782	0.51	0/2402
41	CS	0.26	0/1505	0.55	0/2026
42	CV	0.27	0/985	0.55	0/1319
43	CU	0.28	0/838	0.53	0/1126
44	CL	0.25	0/1673	0.57	0/2235
45	CG	0.26	0/1816	0.56	0/2443
46	CI	0.25	0/1767	0.59	0/2362
47	CO	0.26	0/1645	0.53	0/2198
48	CC	0.25	0/2706	0.55	0/3649
49	Ch	0.24	0/995	0.55	0/1318
50	CE	0.27	0/1140	0.51	0/1530
51	Co	0.26	0/850	0.56	0/1118
52	Cf	0.26	0/953	0.58	0/1283
53	Ci	0.26	0/845	0.55	0/1119
54	Cl	0.24	0/443	0.59	0/582
55	CN	0.25	0/1741	0.59	0/2328
56	Ca	0.25	0/1166	0.53	0/1561
57	Cp	0.26	0/687	0.57	0/915
58	CM	0.26	0/1062	0.56	0/1418
59	Cc	0.26	0/744	0.50	0/1004
60	CH	0.26	0/1528	0.57	0/2058
61	CY	0.25	0/1065	0.60	0/1421
62	CR	0.25	0/1658	0.58	0/2201
63	Cb	0.24	0/439	0.50	0/578
64	CQ	0.25	0/1498	0.58	0/2012
65	CT	0.26	0/1308	0.58	0/1755
66	CD	0.26	0/2368	0.53	0/3179
67	CZ	0.27	0/1123	0.52	0/1497
68	CP	0.25	0/1277	0.54	0/1717
69	Cn	0.26	0/210	0.78	0/266
70	Cg	0.26	0/847	0.60	0/1136
71	Ck	0.30	0/565	0.54	0/748
72	Cm	0.24	0/423	0.55	0/557
73	Cd	0.25	0/881	0.55	0/1184
74	Ce	0.25	0/1057	0.59	0/1407
75	CW	0.26	0/712	0.56	0/949

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
76	Cj	0.25	0/720	0.60	0/956
77	CJ	0.26	0/1533	0.57	0/2052
78	CX	0.25	0/972	0.51	0/1310
79	DC	0.16	0/219	0.77	0/336
All	All	0.37	13/202374 (0.0%)	0.73	40/296392 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
15	AW	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A5	3465	U	C2-N3	56.56	1.77	1.37
12	A5	3465	U	N3-C4	49.44	1.82	1.38
12	A5	3465	U	N1-C2	42.53	1.76	1.38
12	A5	3465	U	N1-C6	38.47	1.72	1.38
12	A5	3462	C	C1'-N1	36.83	2.04	1.48
12	A5	3462	C	N1-C6	35.40	1.58	1.37
12	A5	3465	U	C4-C5	30.14	1.70	1.43
12	A5	3465	U	C5-C6	29.66	1.60	1.34
12	A5	3462	C	N1-C2	23.70	1.63	1.40
3	DA	1	G	OP3-P	-10.63	1.48	1.61
12	A5	3462	C	N3-C4	-7.57	1.28	1.33
12	A5	3462	C	C4-C5	-6.54	1.37	1.43
12	A5	3462	C	C2'-C1'	6.21	1.60	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A5	3462	C	C6-N1-C2	-95.10	82.26	120.30
12	A5	3462	C	C5-C6-N1	42.23	142.11	121.00
12	A5	3462	C	N1-C2-N3	29.06	139.54	119.20
12	A5	3462	C	N3-C4-C5	-23.73	112.41	121.90
12	A5	3462	C	N3-C2-O2	-22.96	105.83	121.90
12	A5	3462	C	C2-N1-C1'	16.84	137.33	118.80
12	A5	3462	C	C6-N1-C1'	16.30	140.36	120.80
12	A5	3462	C	O4'-C1'-N1	11.75	117.60	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A5	600	U	OP1-P-O3’	-11.56	79.77	105.20
12	A5	588	G	OP1-P-O3’	-10.87	81.29	105.20
12	A5	3388	U	OP1-P-O3’	-10.84	81.34	105.20
12	A5	239	U	OP2-P-O3’	-10.82	81.40	105.20
12	A5	588	G	OP2-P-O3’	-9.95	83.31	105.20
12	A5	3388	U	OP2-P-O3’	-9.84	83.55	105.20
12	A5	3462	C	N1-C1’-C2’	9.75	126.67	114.00
12	A5	239	U	OP1-P-O3’	-9.40	84.51	105.20
12	A5	3465	U	N1-C2-N3	-9.12	109.43	114.90
12	A5	600	U	OP2-P-O3’	-8.24	87.08	105.20
12	A5	240	G	OP1-P-OP2	7.97	131.56	119.60
12	A5	601	G	OP1-P-OP2	7.83	131.34	119.60
12	A5	3465	U	C6-N1-C2	7.63	125.58	121.00
12	A5	3462	C	N1-C2-O2	-7.12	114.63	118.90
12	A5	133	U	C2-N1-C1’	6.95	126.04	117.70
12	A5	3389	U	OP1-P-OP2	6.93	130.00	119.60
12	A5	589	U	OP1-P-OP2	6.85	129.87	119.60
12	A5	3462	C	C5-C4-N4	6.73	124.91	120.20
12	A5	3462	C	N3-C4-N4	6.69	122.68	118.00
12	A5	1567	G	O4’-C1’-N9	6.66	113.53	108.20
12	A5	3462	C	C4-C5-C6	6.36	120.58	117.40
12	A5	3462	C	C2-N3-C4	6.35	123.07	119.90
12	A5	1680	U	C2-N1-C1’	5.91	124.79	117.70
12	A5	2218	C	N3-C2-O2	-5.77	117.86	121.90
10	A8	112	A	O4’-C1’-N9	5.52	112.61	108.20
12	A5	600	U	C2-N1-C1’	5.44	124.23	117.70
12	A5	639	G	C4-N9-C1’	5.32	133.42	126.50
11	B2	1429	U	C2-N1-C1’	5.31	124.07	117.70
12	A5	3465	U	C6-N1-C1’	-5.22	113.89	121.20
12	A5	3321	A	P-O3’-C3’	5.04	125.75	119.70
12	A5	639	G	C8-N9-C1’	-5.02	120.48	127.00
12	A5	1627	G	O4’-C1’-N9	5.00	112.20	108.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	AW	28	ARG	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	203/276 (74%)	195 (96%)	8 (4%)	0	100	100
2	CA	247/260 (95%)	238 (96%)	9 (4%)	0	100	100
4	AB	208/257 (81%)	205 (99%)	3 (1%)	0	100	100
5	CB	393/401 (98%)	389 (99%)	4 (1%)	0	100	100
6	AC	213/272 (78%)	211 (99%)	2 (1%)	0	100	100
7	AD	209/247 (85%)	206 (99%)	3 (1%)	0	100	100
8	AE	253/259 (98%)	244 (96%)	9 (4%)	0	100	100
13	AR	119/130 (92%)	116 (98%)	3 (2%)	0	100	100
14	AK	91/149 (61%)	88 (97%)	3 (3%)	0	100	100
15	AW	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
16	AS	146/154 (95%)	140 (96%)	6 (4%)	0	100	100
17	AT	138/146 (94%)	132 (96%)	6 (4%)	0	100	100
18	Aa	97/117 (83%)	95 (98%)	2 (2%)	0	100	100
19	Af	48/163 (29%)	43 (90%)	5 (10%)	0	100	100
20	AO	133/152 (88%)	127 (96%)	6 (4%)	0	100	100
21	AI	205/208 (99%)	196 (96%)	9 (4%)	0	100	100
22	AF	181/210 (86%)	174 (96%)	6 (3%)	1 (1%)	22	43
23	AM	113/140 (81%)	100 (88%)	13 (12%)	0	100	100
24	AV	79/88 (90%)	75 (95%)	4 (5%)	0	100	100
25	AN	149/151 (99%)	148 (99%)	1 (1%)	0	100	100
26	AZ	69/117 (59%)	68 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	Ad	53/56 (95%)	53 (100%)	0	0	100	100
28	AY	121/131 (92%)	115 (95%)	6 (5%)	0	100	100
29	AU	98/117 (84%)	96 (98%)	2 (2%)	0	100	100
30	AG	226/246 (92%)	221 (98%)	5 (2%)	0	100	100
31	Ab	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
32	AP	126/151 (83%)	120 (95%)	6 (5%)	0	100	100
33	Ac	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
34	Ae	41/130 (32%)	40 (98%)	1 (2%)	0	100	100
35	AX	138/143 (96%)	137 (99%)	1 (1%)	0	100	100
36	AL	141/155 (91%)	137 (97%)	4 (3%)	0	100	100
37	AJ	175/189 (93%)	165 (94%)	10 (6%)	0	100	100
38	AQ	138/144 (96%)	136 (99%)	2 (1%)	0	100	100
39	AH	190/194 (98%)	176 (93%)	14 (7%)	0	100	100
40	CF	211/244 (86%)	202 (96%)	9 (4%)	0	100	100
41	CS	177/180 (98%)	170 (96%)	7 (4%)	0	100	100
42	CV	126/140 (90%)	126 (100%)	0	0	100	100
43	CU	98/130 (75%)	95 (97%)	3 (3%)	0	100	100
44	CL	202/207 (98%)	200 (99%)	2 (1%)	0	100	100
45	CG	217/265 (82%)	212 (98%)	5 (2%)	0	100	100
46	CI	211/214 (99%)	209 (99%)	2 (1%)	0	100	100
47	CO	199/202 (98%)	197 (99%)	2 (1%)	0	100	100
48	CC	333/345 (96%)	327 (98%)	6 (2%)	0	100	100
49	Ch	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
50	CE	135/217 (62%)	127 (94%)	8 (6%)	0	100	100
51	Co	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
52	Cf	115/124 (93%)	112 (97%)	3 (3%)	0	100	100
53	Ci	102/104 (98%)	97 (95%)	5 (5%)	0	100	100
54	Cl	48/51 (94%)	48 (100%)	0	0	100	100
55	CN	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
56	Ca	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
57	Cp	86/91 (94%)	82 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	CM	130/135 (96%)	126 (97%)	4 (3%)	0	100	100
59	Cc	94/115 (82%)	94 (100%)	0	0	100	100
60	CH	186/189 (98%)	180 (97%)	6 (3%)	0	100	100
61	CY	130/142 (92%)	125 (96%)	5 (4%)	0	100	100
62	CR	192/198 (97%)	190 (99%)	2 (1%)	0	100	100
63	Cb	50/62 (81%)	45 (90%)	5 (10%)	0	100	100
64	CQ	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
65	CT	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
66	CD	287/293 (98%)	278 (97%)	9 (3%)	0	100	100
67	CZ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
68	CP	152/187 (81%)	149 (98%)	3 (2%)	0	100	100
69	Cn	20/22 (91%)	20 (100%)	0	0	100	100
70	Cg	102/110 (93%)	101 (99%)	1 (1%)	0	100	100
71	Ck	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
72	Cm	49/128 (38%)	49 (100%)	0	0	100	100
73	Cd	103/122 (84%)	99 (96%)	4 (4%)	0	100	100
74	Ce	126/134 (94%)	122 (97%)	4 (3%)	0	100	100
75	CW	84/159 (53%)	83 (99%)	1 (1%)	0	100	100
76	Cj	86/92 (94%)	84 (98%)	2 (2%)	0	100	100
77	CJ	184/196 (94%)	182 (99%)	2 (1%)	0	100	100
78	CX	117/146 (80%)	116 (99%)	1 (1%)	0	100	100
All	All	10469/11907 (88%)	10172 (97%)	296 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	AF	86	GLY

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	AA	172/228 (75%)	155 (90%)	17 (10%)	6	13
2	CA	191/202 (95%)	185 (97%)	6 (3%)	35	62
4	AB	191/228 (84%)	177 (93%)	14 (7%)	11	25
5	CB	335/338 (99%)	326 (97%)	9 (3%)	40	66
6	AC	175/202 (87%)	165 (94%)	10 (6%)	17	37
7	AD	173/204 (85%)	166 (96%)	7 (4%)	27	52
8	AE	218/221 (99%)	205 (94%)	13 (6%)	16	35
13	AR	111/118 (94%)	101 (91%)	10 (9%)	8	16
14	AK	82/122 (67%)	77 (94%)	5 (6%)	15	34
15	AW	110/111 (99%)	105 (96%)	5 (4%)	23	47
16	AS	130/134 (97%)	119 (92%)	11 (8%)	8	18
17	AT	116/120 (97%)	107 (92%)	9 (8%)	10	22
18	Aa	84/94 (89%)	76 (90%)	8 (10%)	7	14
19	Af	42/134 (31%)	35 (83%)	7 (17%)	2	3
20	AO	103/115 (90%)	97 (94%)	6 (6%)	17	36
21	AI	172/173 (99%)	149 (87%)	23 (13%)	3	6
22	AF	156/172 (91%)	146 (94%)	10 (6%)	14	32
23	AM	94/108 (87%)	85 (90%)	9 (10%)	7	14
24	AV	68/75 (91%)	64 (94%)	4 (6%)	16	35
25	AN	130/130 (100%)	123 (95%)	7 (5%)	18	39
26	AZ	62/98 (63%)	59 (95%)	3 (5%)	21	44
27	Ad	46/47 (98%)	44 (96%)	2 (4%)	25	49
28	AY	107/112 (96%)	104 (97%)	3 (3%)	38	65
29	AU	90/104 (86%)	85 (94%)	5 (6%)	17	38
30	AG	195/212 (92%)	176 (90%)	19 (10%)	6	14
31	Ab	75/76 (99%)	71 (95%)	4 (5%)	19	40
32	AP	108/128 (84%)	97 (90%)	11 (10%)	6	12
33	Ac	58/58 (100%)	55 (95%)	3 (5%)	19	41
34	Ae	37/107 (35%)	33 (89%)	4 (11%)	5	10
35	AX	115/118 (98%)	105 (91%)	10 (9%)	8	17
36	AL	126/136 (93%)	115 (91%)	11 (9%)	8	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	AJ	160/167 (96%)	144 (90%)	16 (10%)	6	13
38	AQ	115/119 (97%)	107 (93%)	8 (7%)	12	27
39	AH	170/172 (99%)	153 (90%)	17 (10%)	6	13
40	CF	184/210 (88%)	182 (99%)	2 (1%)	70	86
41	CS	156/157 (99%)	153 (98%)	3 (2%)	52	75
42	CV	101/107 (94%)	97 (96%)	4 (4%)	27	52
43	CU	92/116 (79%)	84 (91%)	8 (9%)	8	17
44	CL	167/170 (98%)	159 (95%)	8 (5%)	21	44
45	CG	192/228 (84%)	184 (96%)	8 (4%)	25	50
46	CI	179/180 (99%)	175 (98%)	4 (2%)	47	72
47	CO	165/166 (99%)	156 (94%)	9 (6%)	18	38
48	CC	279/286 (98%)	262 (94%)	17 (6%)	15	34
49	Ch	106/107 (99%)	98 (92%)	8 (8%)	11	24
50	CE	122/188 (65%)	115 (94%)	7 (6%)	17	37
51	Co	90/93 (97%)	86 (96%)	4 (4%)	24	48
52	Cf	95/99 (96%)	92 (97%)	3 (3%)	34	60
53	Ci	86/86 (100%)	84 (98%)	2 (2%)	45	71
54	Cl	46/47 (98%)	44 (96%)	2 (4%)	25	49
55	CN	172/173 (99%)	170 (99%)	2 (1%)	67	85
56	Ca	116/117 (99%)	109 (94%)	7 (6%)	16	35
57	Cp	68/71 (96%)	63 (93%)	5 (7%)	11	24
58	CM	111/114 (97%)	107 (96%)	4 (4%)	30	56
59	Cc	80/95 (84%)	76 (95%)	4 (5%)	20	43
60	CH	167/168 (99%)	158 (95%)	9 (5%)	18	39
61	CY	114/123 (93%)	108 (95%)	6 (5%)	19	40
62	CR	172/174 (99%)	162 (94%)	10 (6%)	17	36
63	Cb	47/56 (84%)	44 (94%)	3 (6%)	14	32
64	CQ	152/153 (99%)	147 (97%)	5 (3%)	33	59
65	CT	135/136 (99%)	125 (93%)	10 (7%)	11	24
66	CD	239/242 (99%)	227 (95%)	12 (5%)	20	43
67	CZ	119/120 (99%)	114 (96%)	5 (4%)	25	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	CP	130/159 (82%)	124 (95%)	6 (5%)	23	46
69	Cn	20/20 (100%)	19 (95%)	1 (5%)	20	43
70	Cg	92/98 (94%)	91 (99%)	1 (1%)	70	86
71	Ck	63/64 (98%)	60 (95%)	3 (5%)	21	44
72	Cm	47/115 (41%)	47 (100%)	0	100	100
73	Cd	96/112 (86%)	94 (98%)	2 (2%)	48	73
74	Ce	111/117 (95%)	103 (93%)	8 (7%)	12	26
75	CW	73/128 (57%)	71 (97%)	2 (3%)	40	66
76	Cj	73/77 (95%)	72 (99%)	1 (1%)	62	82
77	CJ	160/170 (94%)	148 (92%)	12 (8%)	11	24
78	CX	103/124 (83%)	101 (98%)	2 (2%)	52	75
All	All	9037/10049 (90%)	8522 (94%)	515 (6%)	20	37

All (515) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	2	SER
1	AA	8	SER
1	AA	37	TYR
1	AA	100	PHE
1	AA	117	LYS
1	AA	122	LEU
1	AA	128	ARG
1	AA	146	SER
1	AA	158	ASP
1	AA	169	ARG
1	AA	186	ARG
1	AA	191	ARG
1	AA	195	PHE
1	AA	197	LEU
1	AA	201	GLU
1	AA	203	MET
1	AA	210	ARG
2	CA	71	THR
2	CA	125	VAL
2	CA	184	ARG
2	CA	190	LYS
2	CA	245	ARG

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Mol	Chain	Res	Type
2	CA	247	ARG
4	AB	23	PHE
4	AB	36	MET
4	AB	40	ARG
4	AB	90	GLN
4	AB	122	ASN
4	AB	134	ARG
4	AB	146	ASN
4	AB	152	SER
4	AB	158	LYS
4	AB	160	ARG
4	AB	164	SER
4	AB	172	LYS
4	AB	184	SER
4	AB	197	LYS
5	CB	38	SER
5	CB	66	LYS
5	CB	143	LYS
5	CB	298	ASN
5	CB	304	PHE
5	CB	326	ASP
5	CB	331	ARG
5	CB	338	LYS
5	CB	388	LYS
6	AC	95	CYS
6	AC	100	ASP
6	AC	159	VAL
6	AC	163	ARG
6	AC	188	MET
6	AC	202	SER
6	AC	232	PHE
6	AC	244	TYR
6	AC	245	SER
6	AC	260	SER
7	AD	34	ASP
7	AD	92	LYS
7	AD	104	CYS
7	AD	108	ARG
7	AD	150	LYS
7	AD	158	LEU
7	AD	209	HIS
8	AE	1	MET

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Mol	Chain	Res	Type
8	AE	5	LYS
8	AE	18	MET
8	AE	20	ASP
8	AE	46	PHE
8	AE	86	MET
8	AE	102	TYR
8	AE	135	VAL
8	AE	157	ASP
8	AE	164	SER
8	AE	171	SER
8	AE	199	ARG
8	AE	255	MET
13	AR	3	ARG
13	AR	5	ARG
13	AR	72	LYS
13	AR	84	TYR
13	AR	85	MET
13	AR	87	GLU
13	AR	92	ASP
13	AR	100	LYS
13	AR	102	ASP
13	AR	118	ASN
14	AK	49	SER
14	AK	52	SER
14	AK	60	PHE
14	AK	68	TYR
14	AK	88	VAL
15	AW	22	LYS
15	AW	23	ARG
15	AW	60	LYS
15	AW	96	SER
15	AW	118	ARG
16	AS	17	ASN
16	AS	38	ARG
16	AS	49	ASP
16	AS	61	GLU
16	AS	65	ASP
16	AS	78	LYS
16	AS	83	PHE
16	AS	135	HIS
16	AS	142	LYS
16	AS	144	ARG

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Mol	Chain	Res	Type
16	AS	145	THR
17	AT	3	ARG
17	AT	17	LYS
17	AT	18	SER
17	AT	26	SER
17	AT	35	SER
17	AT	106	GLN
17	AT	120	LYS
17	AT	125	SER
17	AT	133	ASP
18	Aa	10	ARG
18	Aa	26	CYS
18	Aa	42	ARG
18	Aa	51	ARG
18	Aa	55	ASP
18	Aa	57	SER
18	Aa	66	LYS
18	Aa	87	ARG
19	Af	94	LEU
19	Af	99	TYR
19	Af	107	LYS
19	Af	110	ARG
19	Af	112	ARG
19	Af	132	ARG
19	Af	140	ASP
20	AO	66	ASP
20	AO	105	ARG
20	AO	115	SER
20	AO	143	ARG
20	AO	147	ARG
20	AO	152	LEU
21	AI	6	ASP
21	AI	7	SER
21	AI	36	THR
21	AI	53	GLU
21	AI	56	ARG
21	AI	61	ASP
21	AI	64	ASN
21	AI	66	SER
21	AI	75	LYS
21	AI	76	THR
21	AI	98	LYS

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Mol	Chain	Res	Type
21	AI	105	ASP
21	AI	119	LEU
21	AI	121	LEU
21	AI	132	GLU
21	AI	139	LYS
21	AI	141	ARG
21	AI	142	SER
21	AI	144	HIS
21	AI	146	MET
21	AI	153	GLN
21	AI	203	ARG
21	AI	206	LYS
22	AF	31	LEU
22	AF	37	SER
22	AF	38	ASP
22	AF	43	ASP
22	AF	61	ARG
22	AF	76	GLU
22	AF	100	LYS
22	AF	104	GLU
22	AF	142	ARG
22	AF	190	SER
23	AM	30	LEU
23	AM	31	ARG
23	AM	34	HIS
23	AM	50	LEU
23	AM	76	LEU
23	AM	101	LYS
23	AM	104	LYS
23	AM	109	ARG
23	AM	136	PHE
24	AV	35	ASP
24	AV	42	GLU
24	AV	53	ARG
24	AV	66	SER
25	AN	3	ARG
25	AN	4	MET
25	AN	9	LYS
25	AN	58	HIS
25	AN	77	SER
25	AN	133	ARG
25	AN	151	SER

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Mol	Chain	Res	Type
26	AZ	72	ARG
26	AZ	76	ARG
26	AZ	107	ARG
27	Ad	9	SER
27	Ad	49	ASP
28	AY	39	ASP
28	AY	90	ARG
28	AY	116	LYS
29	AU	24	THR
29	AU	25	SER
29	AU	50	LYS
29	AU	98	ARG
29	AU	115	ARG
30	AG	4	ASN
30	AG	20	GLU
30	AG	22	LYS
30	AG	33	SER
30	AG	63	MET
30	AG	81	GLN
30	AG	110	SER
30	AG	126	ASP
30	AG	139	SER
30	AG	143	LYS
30	AG	148	THR
30	AG	149	LYS
30	AG	159	THR
30	AG	162	LYS
30	AG	175	LYS
30	AG	194	GLN
30	AG	196	ARG
30	AG	218	LYS
30	AG	220	GLU
31	Ab	30	SER
31	Ab	64	CYS
31	Ab	70	LYS
31	Ab	73	LEU
32	AP	20	LYS
32	AP	29	ASP
32	AP	36	ARG
32	AP	37	GLU
32	AP	56	LYS
32	AP	57	ARG

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Mol	Chain	Res	Type
32	AP	58	LYS
32	AP	70	LYS
32	AP	76	LEU
32	AP	128	SER
32	AP	144	SER
33	Ac	1	MET
33	Ac	53	THR
33	Ac	56	GLU
34	Ae	95	LYS
34	Ae	111	ARG
34	Ae	112	ARG
34	Ae	128	SER
35	AX	25	LYS
35	AX	38	SER
35	AX	45	SER
35	AX	68	LYS
35	AX	103	SER
35	AX	105	PHE
35	AX	108	SER
35	AX	127	ASN
35	AX	139	GLU
35	AX	140	ARG
36	AL	45	ARG
36	AL	46	ASP
36	AL	49	GLU
36	AL	51	THR
36	AL	57	CYS
36	AL	66	ARG
36	AL	81	ARG
36	AL	86	ARG
36	AL	110	CYS
36	AL	129	ARG
36	AL	138	ASN
37	AJ	39	LYS
37	AJ	41	GLU
37	AJ	44	ARG
37	AJ	57	ARG
37	AJ	65	LYS
37	AJ	69	ARG
37	AJ	71	PHE
37	AJ	82	LYS
37	AJ	91	MET

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Mol	Chain	Res	Type
37	AJ	103	ASP
37	AJ	114	PHE
37	AJ	126	ARG
37	AJ	135	ARG
37	AJ	137	ARG
37	AJ	157	ASP
37	AJ	159	SER
38	AQ	7	SER
38	AQ	56	VAL
38	AQ	60	ARG
38	AQ	61	PHE
38	AQ	103	LYS
38	AQ	116	SER
38	AQ	127	SER
38	AQ	144	ARG
39	AH	10	LYS
39	AH	14	LYS
39	AH	29	ASP
39	AH	34	ASP
39	AH	41	LYS
39	AH	44	TYR
39	AH	50	GLU
39	AH	53	LEU
39	AH	57	SER
39	AH	69	LYS
39	AH	89	ARG
39	AH	104	GLN
39	AH	112	GLN
39	AH	134	VAL
39	AH	143	ARG
39	AH	149	ASP
39	AH	194	PHE
40	CF	40	LYS
40	CF	152	LYS
41	CS	52	SER
41	CS	66	SER
41	CS	79	LYS
42	CV	35	LYS
42	CV	87	GLN
42	CV	113	LYS
42	CV	138	SER
43	CU	18	LYS

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Mol	Chain	Res	Type
43	CU	27	CYS
43	CU	40	ASP
43	CU	64	LYS
43	CU	70	SER
43	CU	71	LYS
43	CU	109	LYS
43	CU	110	ASN
44	CL	63	GLN
44	CL	82	LYS
44	CL	129	LYS
44	CL	130	LYS
44	CL	136	LYS
44	CL	138	ASP
44	CL	164	ASP
44	CL	184	LYS
45	CG	29	LYS
45	CG	35	LYS
45	CG	49	LYS
45	CG	80	THR
45	CG	116	ARG
45	CG	118	ARG
45	CG	190	SER
45	CG	244	SER
46	CI	35	ASP
46	CI	61	SER
46	CI	162	ARG
46	CI	208	LYS
47	CO	19	ARG
47	CO	32	ASP
47	CO	52	LYS
47	CO	57	SER
47	CO	117	LYS
47	CO	120	HIS
47	CO	132	ARG
47	CO	136	CYS
47	CO	167	TYR
48	CC	94	MET
48	CC	121	TYR
48	CC	125	SER
48	CC	154	SER
48	CC	155	ASP
48	CC	171	ARG

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Mol	Chain	Res	Type
48	CC	187	ARG
48	CC	254	SER
48	CC	260	ASP
48	CC	275	LYS
48	CC	278	SER
48	CC	287	SER
48	CC	291	ARG
48	CC	294	ARG
48	CC	303	ARG
48	CC	316	ARG
48	CC	336	ARG
49	Ch	5	LYS
49	Ch	22	ASP
49	Ch	32	ARG
49	Ch	42	SER
49	Ch	45	SER
49	Ch	66	LYS
49	Ch	89	ARG
49	Ch	111	SER
50	CE	126	SER
50	CE	135	LYS
50	CE	146	LYS
50	CE	167	THR
50	CE	170	GLU
50	CE	175	ASP
50	CE	177	LYS
51	Co	13	ASP
51	Co	27	TYR
51	Co	70	ARG
51	Co	77	LYS
52	Cf	9	ARG
52	Cf	48	ASN
52	Cf	81	THR
53	Ci	83	ARG
53	Ci	100	ARG
54	Cl	8	PHE
54	Cl	21	ARG
55	CN	26	ARG
55	CN	171	SER
56	Ca	16	SER
56	Ca	26	ARG
56	Ca	42	ARG

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Mol	Chain	Res	Type
56	Ca	59	ARG
56	Ca	75	VAL
56	Ca	79	TRP
56	Ca	116	GLU
57	Cp	11	VAL
57	Cp	21	SER
57	Cp	25	MET
57	Cp	62	LYS
57	Cp	87	ARG
58	CM	54	ASP
58	CM	63	LYS
58	CM	77	PHE
58	CM	78	ASP
59	Cc	53	ASN
59	Cc	67	MET
59	Cc	104	SER
59	Cc	105	ASP
60	CH	8	ASP
60	CH	28	THR
60	CH	96	HIS
60	CH	123	ARG
60	CH	128	GLU
60	CH	135	SER
60	CH	168	LYS
60	CH	169	ASP
60	CH	183	THR
61	CY	2	LYS
61	CY	28	ARG
61	CY	61	ARG
61	CY	73	TYR
61	CY	92	SER
61	CY	111	ASP
62	CR	33	SER
62	CR	43	ARG
62	CR	62	ARG
62	CR	68	GLU
62	CR	105	LEU
62	CR	108	ARG
62	CR	131	ASN
62	CR	151	ARG
62	CR	164	ASP
62	CR	189	SER

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Mol	Chain	Res	Type
63	Cb	7	HIS
63	Cb	46	SER
63	Cb	49	ASN
64	CQ	19	LYS
64	CQ	65	LYS
64	CQ	107	GLU
64	CQ	138	PHE
64	CQ	176	ARG
65	CT	18	ASP
65	CT	26	HIS
65	CT	28	SER
65	CT	50	LYS
65	CT	63	ARG
65	CT	99	SER
65	CT	104	ASP
65	CT	116	ARG
65	CT	117	LYS
65	CT	120	LYS
66	CD	33	ARG
66	CD	40	ASP
66	CD	89	LYS
66	CD	185	GLU
66	CD	220	ARG
66	CD	223	SER
66	CD	225	PHE
66	CD	233	ASP
66	CD	241	LYS
66	CD	261	SER
66	CD	268	ARG
66	CD	281	LYS
67	CZ	6	LYS
67	CZ	34	SER
67	CZ	64	LYS
67	CZ	98	LYS
67	CZ	105	SER
68	CP	3	LYS
68	CP	7	SER
68	CP	8	ARG
68	CP	15	LYS
68	CP	102	SER
68	CP	155	LYS
69	Cn	15	ARG

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Mol	Chain	Res	Type
70	Cg	67	ARG
71	Ck	9	LYS
71	Ck	40	SER
71	Ck	51	ASP
73	Cd	34	SER
73	Cd	85	SER
74	Ce	8	LYS
74	Ce	28	ARG
74	Ce	43	ARG
74	Ce	61	SER
74	Ce	75	LYS
74	Ce	91	SER
74	Ce	93	LYS
74	Ce	112	GLU
75	CW	47	ARG
75	CW	66	GLN
76	Cj	25	SER
77	CJ	9	GLU
77	CJ	11	ARG
77	CJ	35	GLU
77	CJ	39	ARG
77	CJ	70	ARG
77	CJ	104	GLU
77	CJ	136	ASP
77	CJ	153	ARG
77	CJ	157	ARG
77	CJ	165	GLU
77	CJ	175	GLN
77	CJ	187	LYS
78	CX	82	ASP
78	CX	129	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
5	CB	213	GLN
5	CB	298	ASN
7	AD	5	GLN
7	AD	25	ASN
14	AK	28	ASN
14	AK	34	ASN
15	AW	56	HIS

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Mol	Chain	Res	Type
23	AM	124	ASN
23	AM	140	ASN
25	AN	36	GLN
30	AG	194	GLN
37	AJ	155	HIS
47	CO	180	GLN
47	CO	184	ASN
52	Cf	48	ASN
56	Ca	68	HIS
58	CM	97	GLN
60	CH	114	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A8	144/153 (94%)	26 (18%)	0
11	B2	1457/1754 (83%)	338 (23%)	31 (2%)
12	A5	3005/3510 (85%)	572 (19%)	75 (2%)
3	DA	75/76 (98%)	17 (22%)	0
79	DC	9/10 (90%)	2 (22%)	0
9	A7	118/119 (99%)	7 (5%)	0
All	All	4808/5622 (85%)	962 (20%)	106 (2%)

All (962) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	DA	4	U
3	DA	9	A
3	DA	16	U
3	DA	17	U
3	DA	19	G
3	DA	21	A
3	DA	22	G
3	DA	38	A
3	DA	46	G
3	DA	47	U
3	DA	55	U
3	DA	57	G
3	DA	58	A
3	DA	59	U
3	DA	61	C

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Mol	Chain	Res	Type
3	DA	75	C
3	DA	76	A
9	A7	7	G
9	A7	53	U
9	A7	54	A
9	A7	64	G
9	A7	97	G
9	A7	100	A
9	A7	110	G
10	A8	21	G
10	A8	22	U
10	A8	23	U
10	A8	34	U
10	A8	35	C
10	A8	51	U
10	A8	52	U
10	A8	59	U
10	A8	62	C
10	A8	63	U
10	A8	77	A
10	A8	89	U
10	A8	93	G
10	A8	95	A
10	A8	100	C
10	A8	102	A
10	A8	104	C
10	A8	105	G
10	A8	110	G
10	A8	112	A
10	A8	113	C
10	A8	115	A
10	A8	116	A
10	A8	121	G
10	A8	122	C
10	A8	147	G
11	B2	5	C
11	B2	18	U
11	B2	34	A
11	B2	42	G
11	B2	43	A
11	B2	45	U
11	B2	47	A

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Mol	Chain	Res	Type
11	B2	54	C
11	B2	57	G
11	B2	58	C
11	B2	65	U
11	B2	66	C
11	B2	67	A
11	B2	73	G
11	B2	94	G
11	B2	104	C
11	B2	106	C
11	B2	109	U
11	B2	111	U
11	B2	112	C
11	B2	116	G
11	B2	126	U
11	B2	128	G
11	B2	129	A
11	B2	130	U
11	B2	132	A
11	B2	137	G
11	B2	140	A
11	B2	142	U
11	B2	143	A
11	B2	152	A
11	B2	153	A
11	B2	154	U
11	B2	159	G
11	B2	160	C
11	B2	168	C
11	B2	169	C
11	B2	181	C
11	B2	184	G
11	B2	191	U
11	B2	227	G
11	B2	229	U
11	B2	232	C
11	B2	233	U
11	B2	234	C
11	B2	238	A
11	B2	241	A
11	B2	245	A
11	B2	249	U

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Mol	Chain	Res	Type
11	B2	251	C
11	B2	254	U
11	B2	266	G
11	B2	270	C
11	B2	274	C
11	B2	296	C
11	B2	298	A
11	B2	302	G
11	B2	309	G
11	B2	317	G
11	B2	318	A
11	B2	332	U
11	B2	339	A
11	B2	340	A
11	B2	341	C
11	B2	350	A
11	B2	354	U
11	B2	357	G
11	B2	360	U
11	B2	370	G
11	B2	373	C
11	B2	380	A
11	B2	381	A
11	B2	382	C
11	B2	384	G
11	B2	396	A
11	B2	397	A
11	B2	401	A
11	B2	404	C
11	B2	406	G
11	B2	409	G
11	B2	412	G
11	B2	414	G
11	B2	419	U
11	B2	420	U
11	B2	424	C
11	B2	427	U
11	B2	430	U
11	B2	436	U
11	B2	442	A
11	B2	443	G
11	B2	446	A

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Mol	Chain	Res	Type
11	B2	449	A
11	B2	453	A
11	B2	455	A
11	B2	492	G
11	B2	496	A
11	B2	502	A
11	B2	503	A
11	B2	522	G
11	B2	523	G
11	B2	524	A
11	B2	525	G
11	B2	531	A
11	B2	533	G
11	B2	538	G
11	B2	540	G
11	B2	541	C
11	B2	558	U
11	B2	561	A
11	B2	565	C
11	B2	570	A
11	B2	571	G
11	B2	587	C
11	B2	595	A
11	B2	596	A
11	B2	599	A
11	B2	600	G
11	B2	614	C
11	B2	617	G
11	B2	712	U
11	B2	713	U
11	B2	723	A
11	B2	724	A
11	B2	733	G
11	B2	734	C
11	B2	739	U
11	B2	742	A
11	B2	743	A
11	B2	747	C
11	B2	748	U
11	B2	749	U
11	B2	753	U
11	B2	754	G

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Mol	Chain	Res	Type
11	B2	756	A
11	B2	778	A
11	B2	779	A
11	B2	820	A
11	B2	824	U
11	B2	826	A
11	B2	827	A
11	B2	829	A
11	B2	837	A
11	B2	838	C
11	B2	841	G
11	B2	851	U
11	B2	871	A
11	B2	877	U
11	B2	879	G
11	B2	880	A
11	B2	882	C
11	B2	883	G
11	B2	898	A
11	B2	900	A
11	B2	909	A
11	B2	910	U
11	B2	925	U
11	B2	931	A
11	B2	935	A
11	B2	952	G
11	B2	957	A
11	B2	969	U
11	B2	970	A
11	B2	976	C
11	B2	978	A
11	B2	991	A
11	B2	993	C
11	B2	996	U
11	B2	997	G
11	B2	1004	C
11	B2	1005	G
11	B2	1016	G
11	B2	1017	G
11	B2	1018	U
11	B2	1028	G
11	B2	1033	G

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Mol	Chain	Res	Type
11	B2	1040	U
11	B2	1042	C
11	B2	1050	A
11	B2	1051	A
11	B2	1056	U
11	B2	1057	U
11	B2	1097	A
11	B2	1109	G
11	B2	1110	A
11	B2	1111	A
11	B2	1115	C
11	B2	1116	A
11	B2	1117	C
11	B2	1118	C
11	B2	1119	A
11	B2	1122	A
11	B2	1123	G
11	B2	1126	G
11	B2	1144	U
11	B2	1153	A
11	B2	1155	A
11	B2	1158	G
11	B2	1159	G
11	B2	1160	A
11	B2	1161	A
11	B2	1176	G
11	B2	1177	G
11	B2	1184	U
11	B2	1191	U
11	B2	1193	A
11	B2	1194	C
11	B2	1196	G
11	B2	1202	A
11	B2	1203	A
11	B2	1204	G
11	B2	1205	C
11	B2	1206	U
11	B2	1209	U
11	B2	1214	G
11	B2	1215	A
11	B2	1216	U
11	B2	1217	U

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Mol	Chain	Res	Type
11	B2	1222	G
11	B2	1223	G
11	B2	1224	U
11	B2	1244	U
11	B2	1245	U
11	B2	1248	U
11	B2	1250	G
11	B2	1254	G
11	B2	1256	G
11	B2	1265	C
11	B2	1272	A
11	B2	1273	U
11	B2	1274	U
11	B2	1279	U
11	B2	1280	A
11	B2	1281	A
11	B2	1296	G
11	B2	1298	C
11	B2	1299	U
11	B2	1302	U
11	B2	1303	A
11	B2	1304	A
11	B2	1305	A
11	B2	1306	U
11	B2	1307	A
11	B2	1308	G
11	B2	1310	U
11	B2	1316	A
11	B2	1317	U
11	B2	1322	G
11	B2	1323	G
11	B2	1324	G
11	B2	1325	U
11	B2	1327	C
11	B2	1329	U
11	B2	1332	A
11	B2	1333	A
11	B2	1335	U
11	B2	1336	U
11	B2	1341	G
11	B2	1347	U
11	B2	1348	A

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Mol	Chain	Res	Type
11	B2	1358	U
11	B2	1360	G
11	B2	1364	C
11	B2	1368	A
11	B2	1371	U
11	B2	1372	U
11	B2	1373	G
11	B2	1383	A
11	B2	1384	G
11	B2	1387	C
11	B2	1391	G
11	B2	1392	A
11	B2	1400	A
11	B2	1402	A
11	B2	1414	G
11	B2	1415	C
11	B2	1416	A
11	B2	1427	A
11	B2	1433	G
11	B2	1434	G
11	B2	1438	C
11	B2	1442	G
11	B2	1443	G
11	B2	1452	U
11	B2	1460	A
11	B2	1462	G
11	B2	1470	U
11	B2	1472	A
11	B2	1473	A
11	B2	1477	U
11	B2	1479	G
11	B2	1480	A
11	B2	1481	A
11	B2	1486	U
11	B2	1491	U
11	B2	1493	U
11	B2	1494	C
11	B2	1495	C
11	B2	1497	G
11	B2	1499	A
11	B2	1506	A
11	B2	1510	U

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Mol	Chain	Res	Type
11	B2	1512	A
11	B2	1513	U
11	B2	1515	A
11	B2	1524	A
11	B2	1528	G
11	B2	1529	A
11	B2	1530	G
11	B2	1546	G
11	B2	1557	G
11	B2	1563	G
11	B2	1572	G
11	B2	1587	A
11	B2	1588	C
11	B2	1590	C
11	B2	1591	A
11	B2	1613	U
11	B2	1614	G
11	B2	1620	A
11	B2	1636	G
11	B2	1640	G
11	B2	1671	C
11	B2	1689	C
11	B2	1695	U
11	B2	1703	G
11	B2	1709	A
11	B2	1711	G
11	B2	1714	G
11	B2	1716	A
11	B2	1721	G
11	B2	1723	U
11	B2	1734	G
11	B2	1746	G
11	B2	1747	G
11	B2	1748	A
11	B2	1750	C
11	B2	1752	U
11	B2	1754	G
12	A5	12	C
12	A5	13	U
12	A5	22	A
12	A5	39	A
12	A5	42	A

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Mol	Chain	Res	Type
12	A5	44	A
12	A5	48	U
12	A5	58	G
12	A5	59	A
12	A5	64	A
12	A5	65	A
12	A5	69	A
12	A5	73	A
12	A5	91	G
12	A5	109	G
12	A5	110	C
12	A5	119	G
12	A5	125	A
12	A5	133	U
12	A5	134	U
12	A5	135	G
12	A5	136	G
12	A5	137	C
12	A5	139	G
12	A5	140	C
12	A5	141	U
12	A5	149	G
12	A5	156	A
12	A5	157	U
12	A5	169	U
12	A5	178	G
12	A5	179	U
12	A5	183	A
12	A5	184	U
12	A5	189	G
12	A5	190	A
12	A5	193	U
12	A5	194	C
12	A5	195	C
12	A5	203	U
12	A5	204	G
12	A5	209	C
12	A5	211	U
12	A5	212	A
12	A5	226	G
12	A5	227	C
12	A5	238	C

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Mol	Chain	Res	Type
12	A5	239	U
12	A5	240	G
12	A5	241	G
12	A5	247	G
12	A5	248	G
12	A5	252	U
12	A5	260	C
12	A5	261	G
12	A5	264	U
12	A5	272	G
12	A5	273	G
12	A5	275	G
12	A5	289	A
12	A5	290	A
12	A5	291	G
12	A5	301	A
12	A5	304	U
12	A5	305	G
12	A5	311	U
12	A5	314	A
12	A5	318	C
12	A5	329	A
12	A5	335	C
12	A5	336	G
12	A5	344	U
12	A5	345	G
12	A5	358	A
12	A5	368	G
12	A5	382	G
12	A5	404	G
12	A5	405	A
12	A5	408	A
12	A5	409	C
12	A5	424	G
12	A5	427	G
12	A5	428	A
12	A5	533	C
12	A5	536	G
12	A5	541	A
12	A5	542	G
12	A5	577	U
12	A5	578	C

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Mol	Chain	Res	Type
12	A5	581	G
12	A5	585	G
12	A5	588	G
12	A5	590	A
12	A5	594	G
12	A5	598	C
12	A5	599	G
12	A5	600	U
12	A5	601	G
12	A5	635	C
12	A5	636	G
12	A5	638	C
12	A5	640	G
12	A5	641	U
12	A5	643	U
12	A5	644	G
12	A5	645	A
12	A5	647	A
12	A5	655	A
12	A5	656	C
12	A5	666	C
12	A5	678	A
12	A5	689	A
12	A5	706	A
12	A5	710	A
12	A5	712	A
12	A5	716	U
12	A5	720	A
12	A5	728	G
12	A5	729	C
12	A5	742	G
12	A5	745	A
12	A5	746	A
12	A5	747	G
12	A5	755	U
12	A5	756	C
12	A5	758	A
12	A5	759	A
12	A5	760	U
12	A5	763	G
12	A5	764	C
12	A5	767	A

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Mol	Chain	Res	Type
12	A5	768	C
12	A5	791	U
12	A5	797	G
12	A5	816	G
12	A5	817	U
12	A5	821	U
12	A5	822	U
12	A5	823	G
12	A5	824	U
12	A5	834	G
12	A5	835	A
12	A5	836	G
12	A5	840	G
12	A5	854	C
12	A5	861	A
12	A5	872	A
12	A5	904	C
12	A5	916	U
12	A5	919	G
12	A5	929	U
12	A5	934	U
12	A5	935	G
12	A5	951	A
12	A5	961	A
12	A5	962	G
12	A5	963	G
12	A5	969	A
12	A5	971	G
12	A5	972	A
12	A5	978	C
12	A5	992	G
12	A5	999	C
12	A5	1001	U
12	A5	1014	C
12	A5	1015	U
12	A5	1016	C
12	A5	1017	A
12	A5	1029	U
12	A5	1032	C
12	A5	1034	G
12	A5	1036	C
12	A5	1039	U

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Mol	Chain	Res	Type
12	A5	1056	A
12	A5	1060	A
12	A5	1064	G
12	A5	1101	A
12	A5	1103	C
12	A5	1118	A
12	A5	1119	A
12	A5	1123	G
12	A5	1125	A
12	A5	1126	G
12	A5	1135	G
12	A5	1144	C
12	A5	1145	A
12	A5	1150	G
12	A5	1151	A
12	A5	1156	G
12	A5	1168	G
12	A5	1169	G
12	A5	1181	A
12	A5	1183	G
12	A5	1196	U
12	A5	1205	A
12	A5	1211	A
12	A5	1220	U
12	A5	1224	G
12	A5	1229	U
12	A5	1232	C
12	A5	1233	U
12	A5	1234	U
12	A5	1244	G
12	A5	1245	A
12	A5	1250	C
12	A5	1253	U
12	A5	1261	G
12	A5	1264	G
12	A5	1272	U
12	A5	1273	U
12	A5	1274	G
12	A5	1275	A
12	A5	1278	G
12	A5	1279	C
12	A5	1339	A

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Mol	Chain	Res	Type
12	A5	1354	A
12	A5	1357	U
12	A5	1359	G
12	A5	1360	A
12	A5	1361	U
12	A5	1368	U
12	A5	1375	G
12	A5	1377	G
12	A5	1383	U
12	A5	1420	G
12	A5	1430	A
12	A5	1440	U
12	A5	1441	C
12	A5	1448	G
12	A5	1449	U
12	A5	1453	G
12	A5	1467	G
12	A5	1496	G
12	A5	1499	G
12	A5	1502	C
12	A5	1511	A
12	A5	1512	G
12	A5	1546	A
12	A5	1548	G
12	A5	1553	G
12	A5	1567	G
12	A5	1568	A
12	A5	1573	U
12	A5	1604	A
12	A5	1606	U
12	A5	1612	A
12	A5	1614	G
12	A5	1615	C
12	A5	1619	G
12	A5	1620	U
12	A5	1621	A
12	A5	1626	C
12	A5	1627	G
12	A5	1628	G
12	A5	1650	U
12	A5	1651	C
12	A5	1655	G

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Mol	Chain	Res	Type
12	A5	1658	U
12	A5	1659	G
12	A5	1663	A
12	A5	1664	A
12	A5	1665	A
12	A5	1670	A
12	A5	1671	U
12	A5	1681	A
12	A5	1701	A
12	A5	1704	U
12	A5	1725	C
12	A5	1738	U
12	A5	1739	C
12	A5	1749	U
12	A5	1750	A
12	A5	1772	A
12	A5	1775	U
12	A5	1776	U
12	A5	1777	U
12	A5	1780	U
12	A5	1781	C
12	A5	1787	U
12	A5	1795	C
12	A5	1796	G
12	A5	1810	U
12	A5	1811	G
12	A5	1817	G
12	A5	1833	U
12	A5	1837	U
12	A5	1839	C
12	A5	1840	C
12	A5	1842	A
12	A5	1843	A
12	A5	1845	A
12	A5	1851	G
12	A5	1853	G
12	A5	1862	G
12	A5	1868	U
12	A5	1870	G
12	A5	1874	U
12	A5	1875	C
12	A5	1876	U

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Mol	Chain	Res	Type
12	A5	1882	C
12	A5	1887	C
12	A5	1891	A
12	A5	1893	A
12	A5	1904	G
12	A5	1908	A
12	A5	1910	U
12	A5	1913	U
12	A5	1914	U
12	A5	1915	U
12	A5	1932	A
12	A5	1935	U
12	A5	1938	G
12	A5	1939	C
12	A5	1948	U
12	A5	1959	C
12	A5	1971	G
12	A5	1972	A
12	A5	1973	U
12	A5	1979	A
12	A5	1999	G
12	A5	2205	A
12	A5	2215	G
12	A5	2216	U
12	A5	2218	C
12	A5	2225	A
12	A5	2226	G
12	A5	2235	A
12	A5	2244	U
12	A5	2246	A
12	A5	2248	A
12	A5	2249	A
12	A5	2253	A
12	A5	2262	A
12	A5	2273	G
12	A5	2281	A
12	A5	2308	U
12	A5	2309	G
12	A5	2310	A
12	A5	2311	A
12	A5	2312	U
12	A5	2313	G

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Mol	Chain	Res	Type
12	A5	2326	A
12	A5	2333	G
12	A5	2337	G
12	A5	2352	G
12	A5	2358	A
12	A5	2359	A
12	A5	2361	U
12	A5	2375	G
12	A5	2376	G
12	A5	2382	A
12	A5	2384	A
12	A5	2410	G
12	A5	2411	C
12	A5	2413	U
12	A5	2416	A
12	A5	2418	G
12	A5	2437	U
12	A5	2439	U
12	A5	2474	G
12	A5	2475	A
12	A5	2476	A
12	A5	2477	C
12	A5	2478	G
12	A5	2488	A
12	A5	2496	G
12	A5	2500	A
12	A5	2503	G
12	A5	2505	A
12	A5	2506	G
12	A5	2507	A
12	A5	2514	U
12	A5	2538	G
12	A5	2547	C
12	A5	2609	A
12	A5	2610	C
12	A5	2611	U
12	A5	2612	C
12	A5	2619	U
12	A5	2620	A
12	A5	2625	G
12	A5	2631	A
12	A5	2633	A

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Mol	Chain	Res	Type
12	A5	2636	A
12	A5	2656	U
12	A5	2658	G
12	A5	2659	A
12	A5	2666	A
12	A5	2672	A
12	A5	2684	G
12	A5	2685	C
12	A5	2686	A
12	A5	2694	U
12	A5	2698	C
12	A5	2705	A
12	A5	2706	C
12	A5	2707	A
12	A5	2718	G
12	A5	2719	G
12	A5	2726	G
12	A5	2731	G
12	A5	2738	A
12	A5	2764	U
12	A5	2768	A
12	A5	2786	A
12	A5	2789	G
12	A5	2791	A
12	A5	2797	U
12	A5	2801	A
12	A5	2803	A
12	A5	2806	A
12	A5	2808	A
12	A5	2814	A
12	A5	2815	A
12	A5	2816	A
12	A5	2826	G
12	A5	2840	G
12	A5	2841	U
12	A5	2859	A
12	A5	2865	G
12	A5	2874	A
12	A5	2882	A
12	A5	2889	A
12	A5	2890	U
12	A5	2908	G

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Mol	Chain	Res	Type
12	A5	2911	A
12	A5	2912	G
12	A5	2913	A
12	A5	2922	C
12	A5	2929	A
12	A5	2930	U
12	A5	2950	A
12	A5	2954	U
12	A5	2956	C
12	A5	2957	A
12	A5	2959	A
12	A5	2972	U
12	A5	2979	C
12	A5	2983	G
12	A5	2984	A
12	A5	2987	U
12	A5	2998	U
12	A5	2999	A
12	A5	3001	C
12	A5	3011	C
12	A5	3012	A
12	A5	3014	A
12	A5	3023	A
12	A5	3028	U
12	A5	3035	U
12	A5	3047	U
12	A5	3048	A
12	A5	3053	A
12	A5	3054	C
12	A5	3059	G
12	A5	3066	U
12	A5	3080	G
12	A5	3083	A
12	A5	3095	C
12	A5	3102	G
12	A5	3106	A
12	A5	3112	U
12	A5	3113	A
12	A5	3119	A
12	A5	3124	A
12	A5	3125	A
12	A5	3134	A

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Mol	Chain	Res	Type
12	A5	3138	C
12	A5	3140	A
12	A5	3141	G
12	A5	3162	U
12	A5	3170	A
12	A5	3171	U
12	A5	3180	U
12	A5	3185	A
12	A5	3186	G
12	A5	3187	A
12	A5	3188	U
12	A5	3191	A
12	A5	3199	A
12	A5	3205	C
12	A5	3206	C
12	A5	3207	A
12	A5	3231	C
12	A5	3235	A
12	A5	3238	U
12	A5	3243	A
12	A5	3244	U
12	A5	3254	U
12	A5	3255	C
12	A5	3257	A
12	A5	3258	G
12	A5	3259	G
12	A5	3268	U
12	A5	3278	C
12	A5	3279	G
12	A5	3282	G
12	A5	3284	C
12	A5	3285	G
12	A5	3286	G
12	A5	3288	A
12	A5	3289	G
12	A5	3293	U
12	A5	3298	A
12	A5	3299	U
12	A5	3305	G
12	A5	3306	G
12	A5	3310	C
12	A5	3315	G

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Mol	Chain	Res	Type
12	A5	3318	C
12	A5	3320	U
12	A5	3321	A
12	A5	3322	U
12	A5	3332	A
12	A5	3333	U
12	A5	3334	G
12	A5	3335	G
12	A5	3336	C
12	A5	3337	C
12	A5	3338	U
12	A5	3339	U
12	A5	3341	G
12	A5	3347	U
12	A5	3349	G
12	A5	3351	G
12	A5	3352	A
12	A5	3364	C
12	A5	3366	U
12	A5	3371	A
12	A5	3373	G
12	A5	3375	C
12	A5	3376	A
12	A5	3377	G
12	A5	3378	A
12	A5	3381	A
12	A5	3385	U
12	A5	3386	G
12	A5	3387	G
12	A5	3388	U
12	A5	3389	U
12	A5	3390	C
12	A5	3399	G
12	A5	3401	C
12	A5	3405	A
12	A5	3406	A
12	A5	3407	A
12	A5	3415	C
12	A5	3436	C
12	A5	3446	U
12	A5	3447	A
12	A5	3448	U

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Mol	Chain	Res	Type
12	A5	3454	A
12	A5	3457	G
12	A5	3461	U
12	A5	3463	C
12	A5	3464	U
12	A5	3465	U
12	A5	3466	U
12	A5	3467	U
12	A5	3468	A
12	A5	3469	U
12	A5	3470	A
12	A5	3471	C
12	A5	3472	U
12	A5	3473	G
12	A5	3482	U
12	A5	3483	G
12	A5	3488	U
12	A5	3489	A
12	A5	3494	U
12	A5	3495	U
12	A5	3496	G
79	DC	4	U
79	DC	7	U

All (106) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	B2	128	G
11	B2	159	G
11	B2	228	U
11	B2	353	G
11	B2	356	C
11	B2	448	U
11	B2	711	U
11	B2	753	U
11	B2	879	G
11	B2	908	C
11	B2	1027	U
11	B2	1039	A
11	B2	1041	C
11	B2	1110	A
11	B2	1121	A

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Mol	Chain	Res	Type
11	B2	1183	A
11	B2	1192	G
11	B2	1213	C
11	B2	1278	A
11	B2	1280	A
11	B2	1305	A
11	B2	1309	U
11	B2	1363	G
11	B2	1371	U
11	B2	1437	U
11	B2	1490	A
11	B2	1509	G
11	B2	1511	A
11	B2	1529	A
11	B2	1715	U
11	B2	1751	A
12	A5	12	C
12	A5	21	G
12	A5	133	U
12	A5	189	G
12	A5	194	C
12	A5	238	C
12	A5	251	C
12	A5	263	U
12	A5	288	A
12	A5	403	A
12	A5	576	G
12	A5	580	U
12	A5	589	U
12	A5	598	C
12	A5	635	C
12	A5	646	A
12	A5	711	A
12	A5	754	C
12	A5	759	A
12	A5	763	G
12	A5	816	G
12	A5	823	G
12	A5	834	G
12	A5	928	C
12	A5	971	G
12	A5	1035	G

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Mol	Chain	Res	Type
12	A5	1118	A
12	A5	1144	C
12	A5	1150	G
12	A5	1155	C
12	A5	1649	G
12	A5	1650	U
12	A5	1658	U
12	A5	1737	U
12	A5	1844	A
12	A5	1861	U
12	A5	1875	C
12	A5	1907	U
12	A5	1909	U
12	A5	1912	A
12	A5	2608	G
12	A5	2609	A
12	A5	2610	C
12	A5	2630	A
12	A5	2658	G
12	A5	2790	A
12	A5	2955	C
12	A5	3047	U
12	A5	3139	G
12	A5	3234	U
12	A5	3256	A
12	A5	3257	A
12	A5	3258	G
12	A5	3277	C
12	A5	3281	U
12	A5	3283	U
12	A5	3285	G
12	A5	3297	U
12	A5	3304	U
12	A5	3309	A
12	A5	3320	U
12	A5	3321	A
12	A5	3333	U
12	A5	3334	G
12	A5	3337	C
12	A5	3338	U
12	A5	3340	G
12	A5	3348	A

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Mol	Chain	Res	Type
12	A5	3365	U
12	A5	3374	C
12	A5	3375	C
12	A5	3376	A
12	A5	3377	G
12	A5	3389	U
12	A5	3460	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
80	SPD	A5	3601	-	9,9,9	0.33	0	8,8,8	0.82	0
81	3HE	A5	3602	-	21,21,21	0.42	0	23,30,30	0.99	1 (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
80	SPD	A5	3601	-	-	1/7/7/7	-
81	3HE	A5	3602	-	-	2/8/36/36	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	A5	3602	3HE	C6-C5-C4	2.13	111.81	108.29

There are no chirality outliers.

All (3) torsion outliers are listed below:

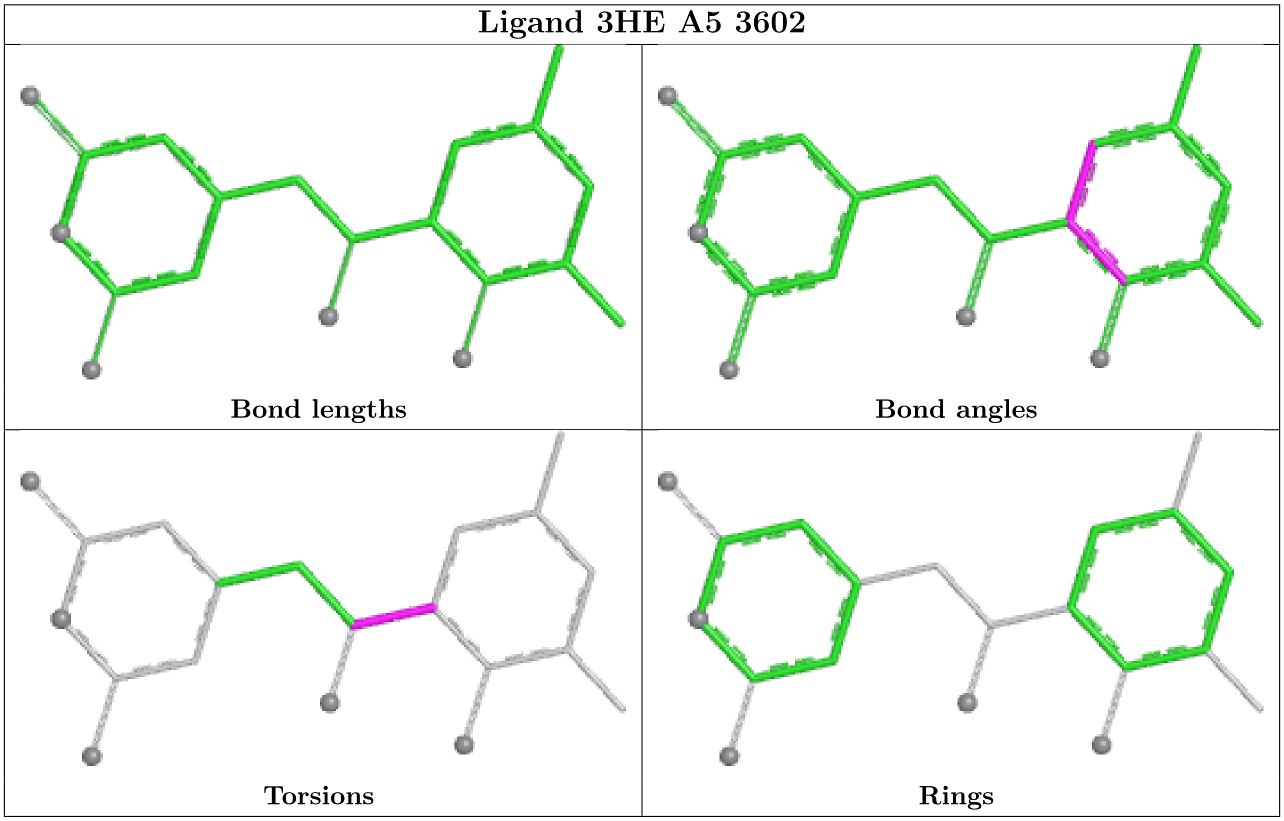
Mol	Chain	Res	Type	Atoms
81	A5	3602	3HE	C6-C5-C7-C8
81	A5	3602	3HE	C6-C5-C7-O3
80	A5	3601	SPD	C4-C5-N6-C7

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 then 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.

Ligand 3HE A5 3602



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
12	A5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A5	3461:U	O3’	3462:C	P	8.47

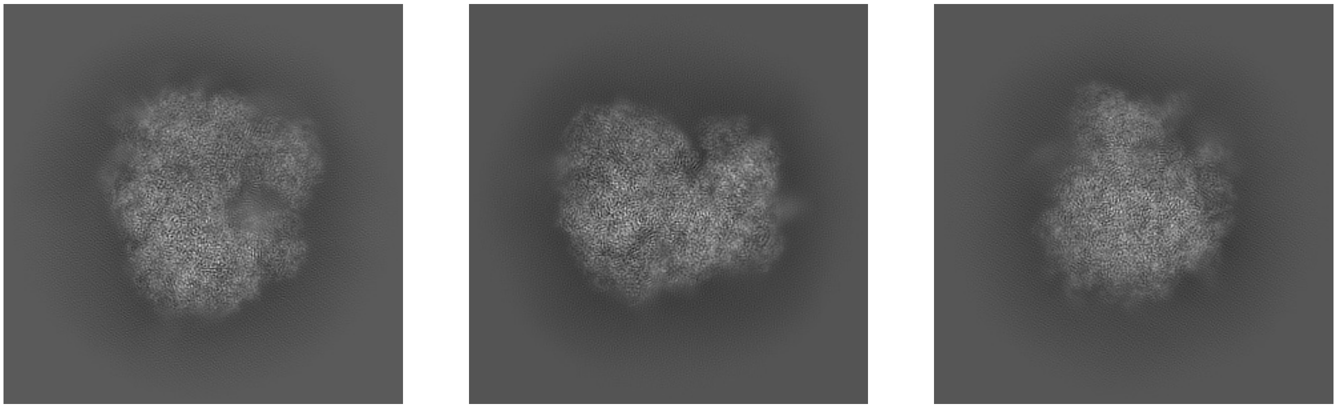
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45392. 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.

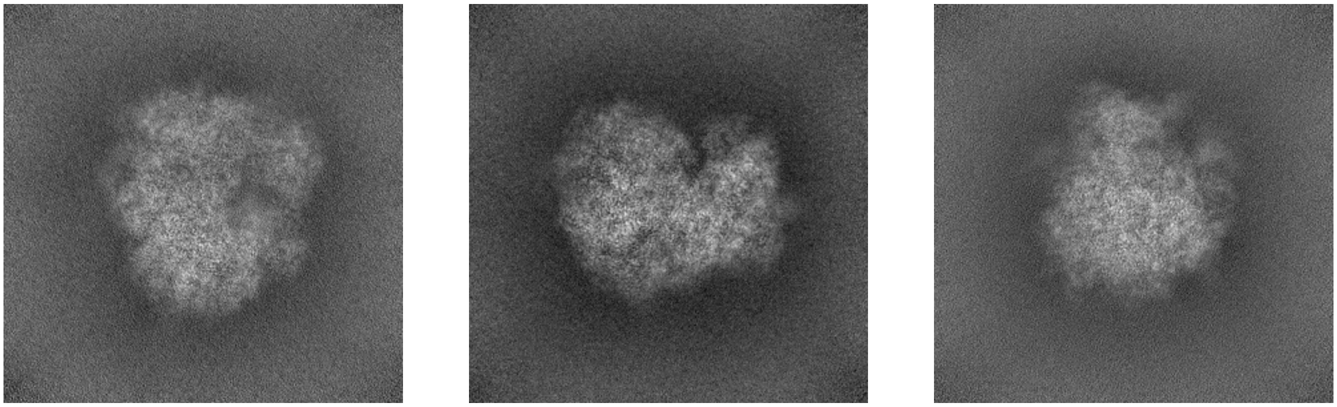
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

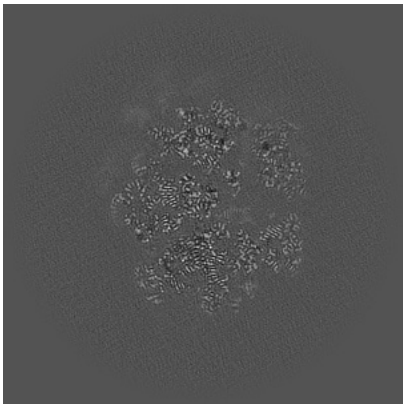


X Y Z

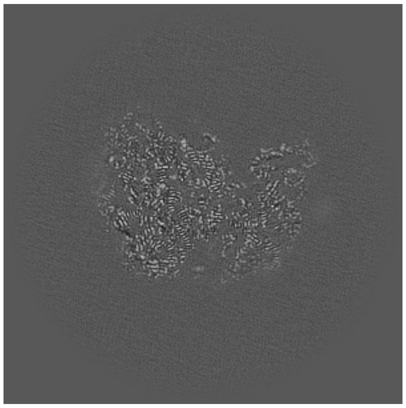
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

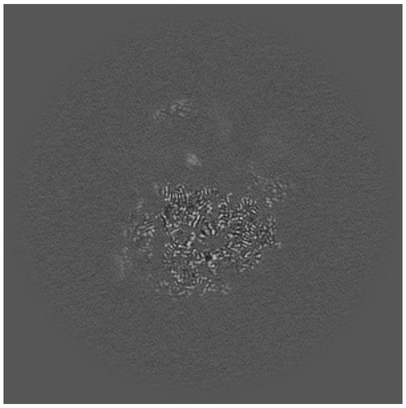
6.2.1 Primary map



X Index: 340

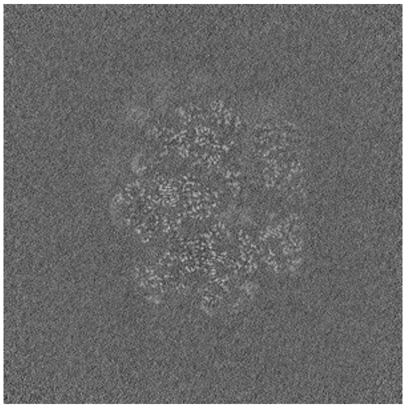


Y Index: 340

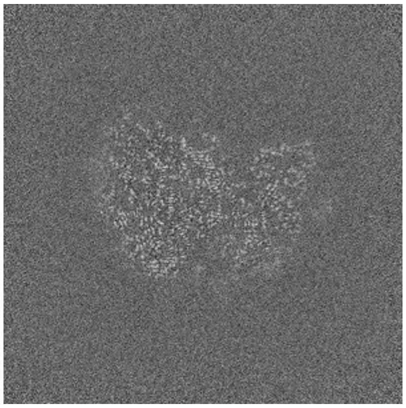


Z Index: 340

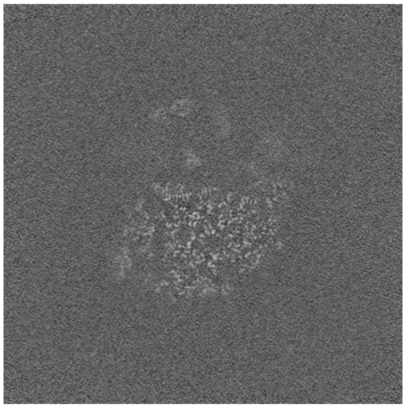
6.2.2 Raw map



X Index: 340



Y Index: 340

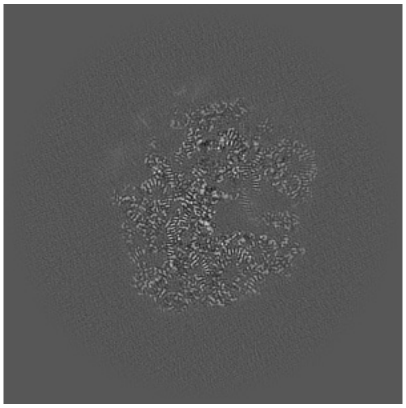


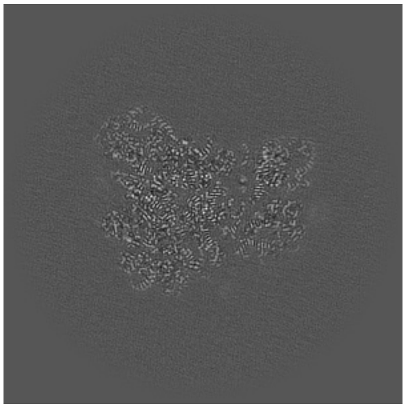
Z Index: 340

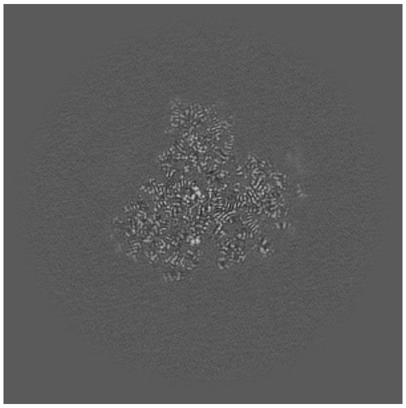
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

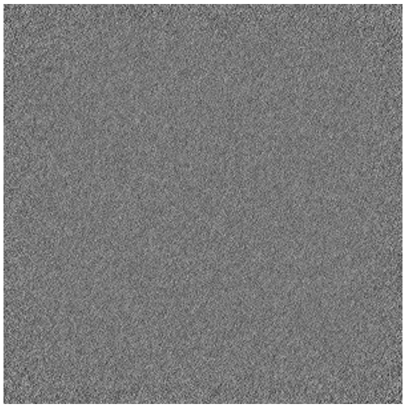
6.3.1 Primary map

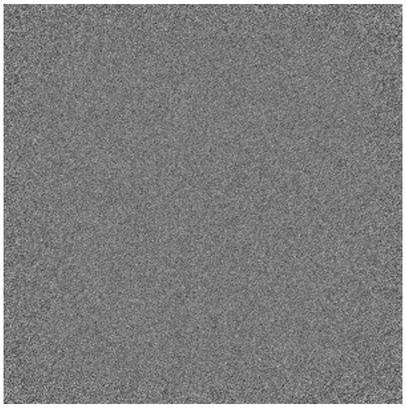

X Index: 317

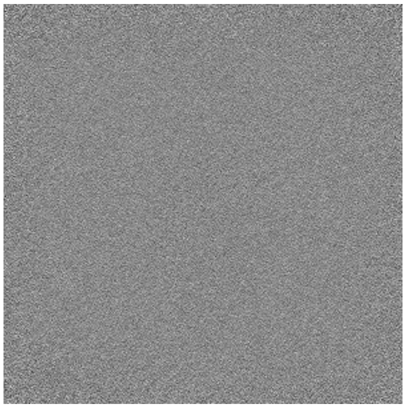

Y Index: 324


Z Index: 266

6.3.2 Raw map


X Index: 0

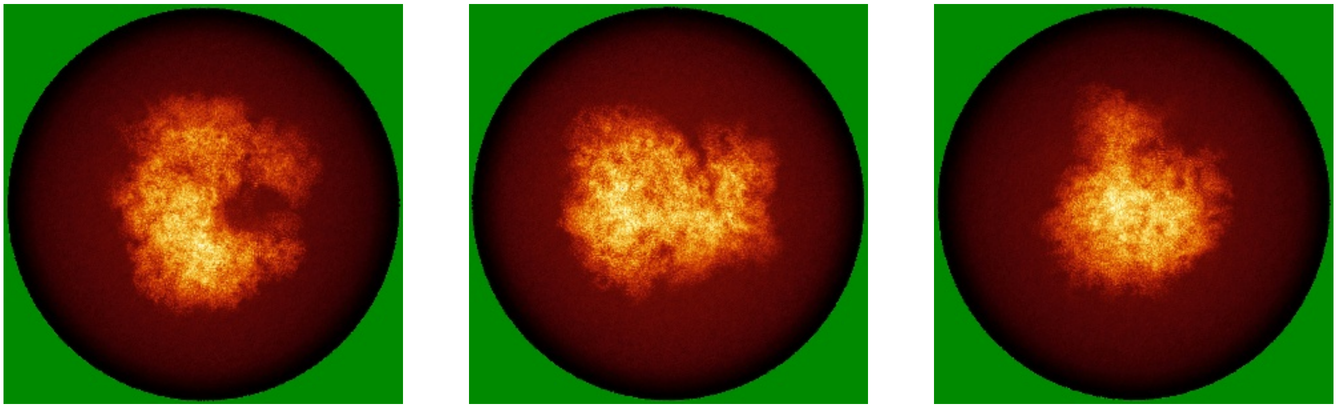

Y Index: 0


Z Index: 679

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

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map

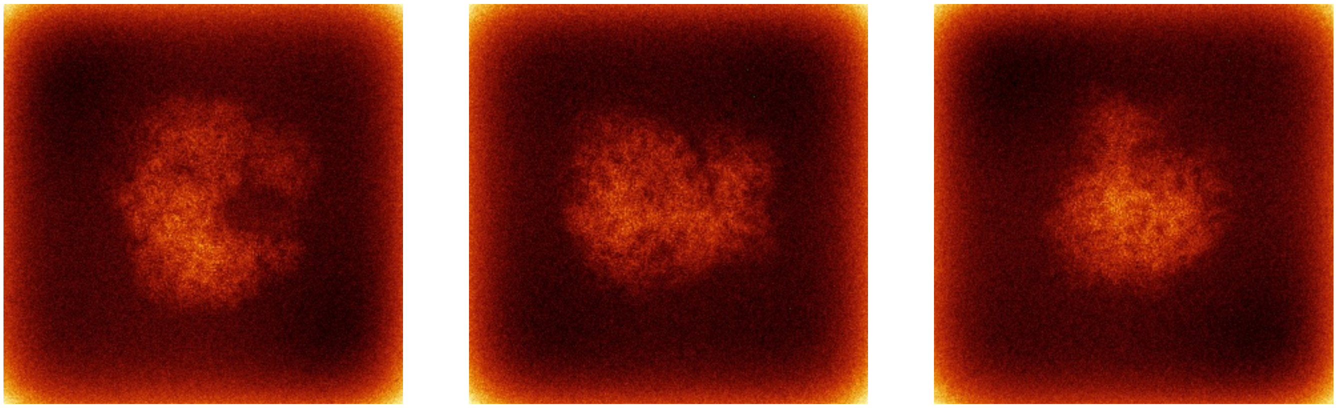


X

Y

Z

6.4.2 Raw map



X

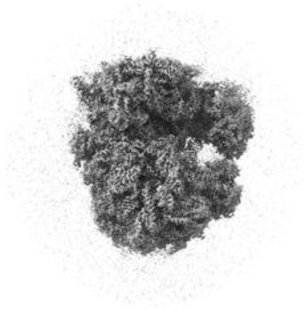
Y

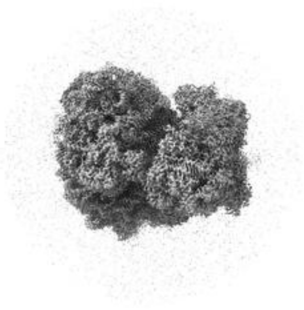
Z

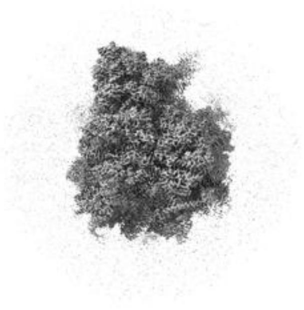
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

6.5.1 Primary map

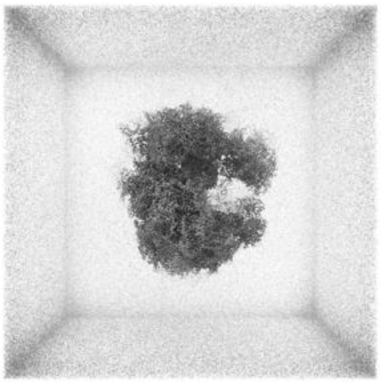

X

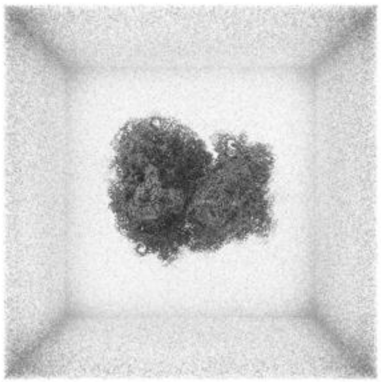

Y

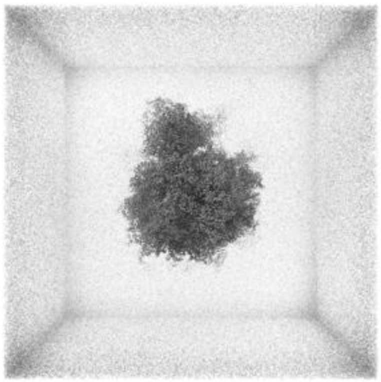

Z

The images above show the 3D surface view of the map at the recommended contour level 0.199. 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.

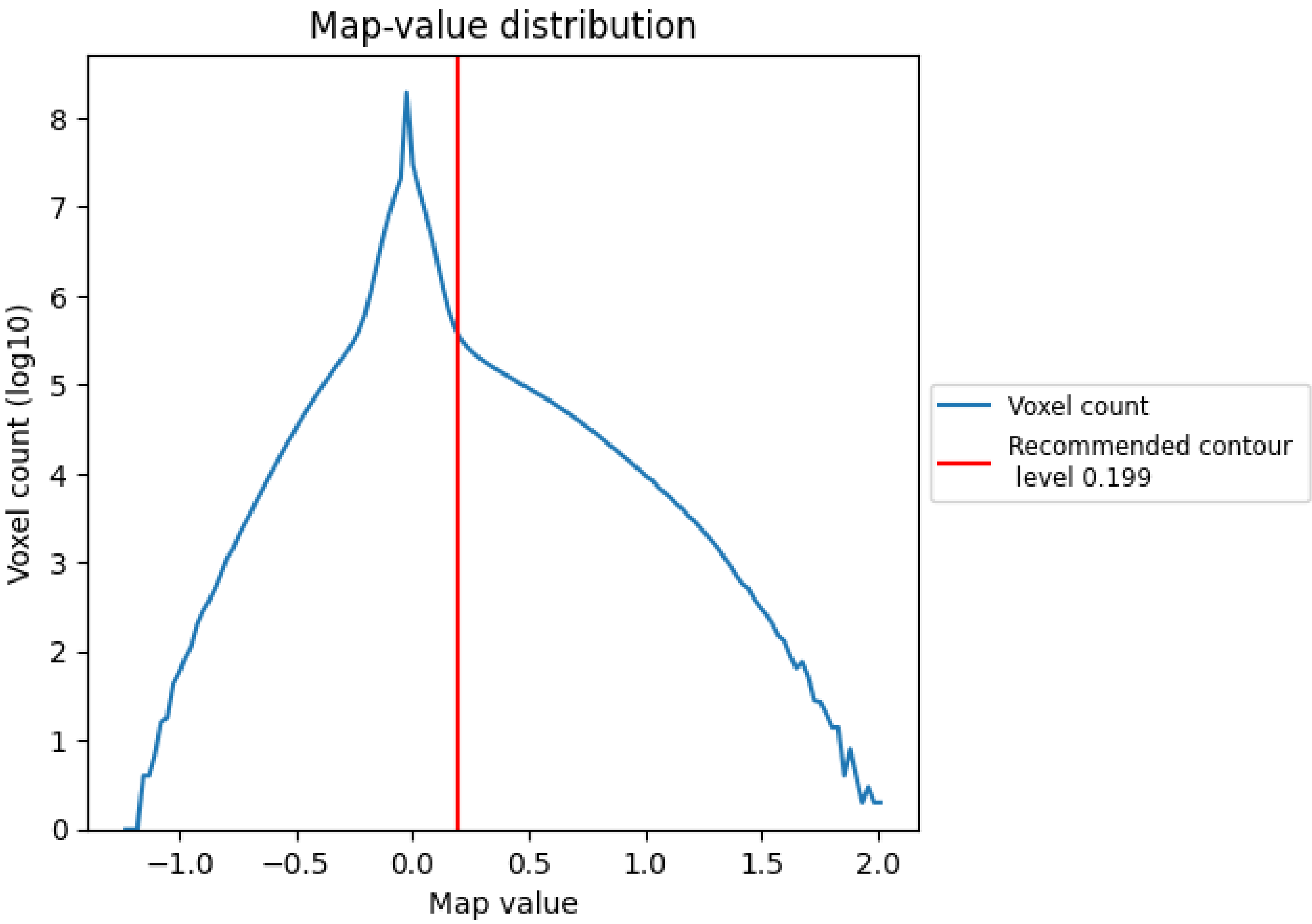
6.6 Mask visualisation

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

7 Map analysis ⓘ

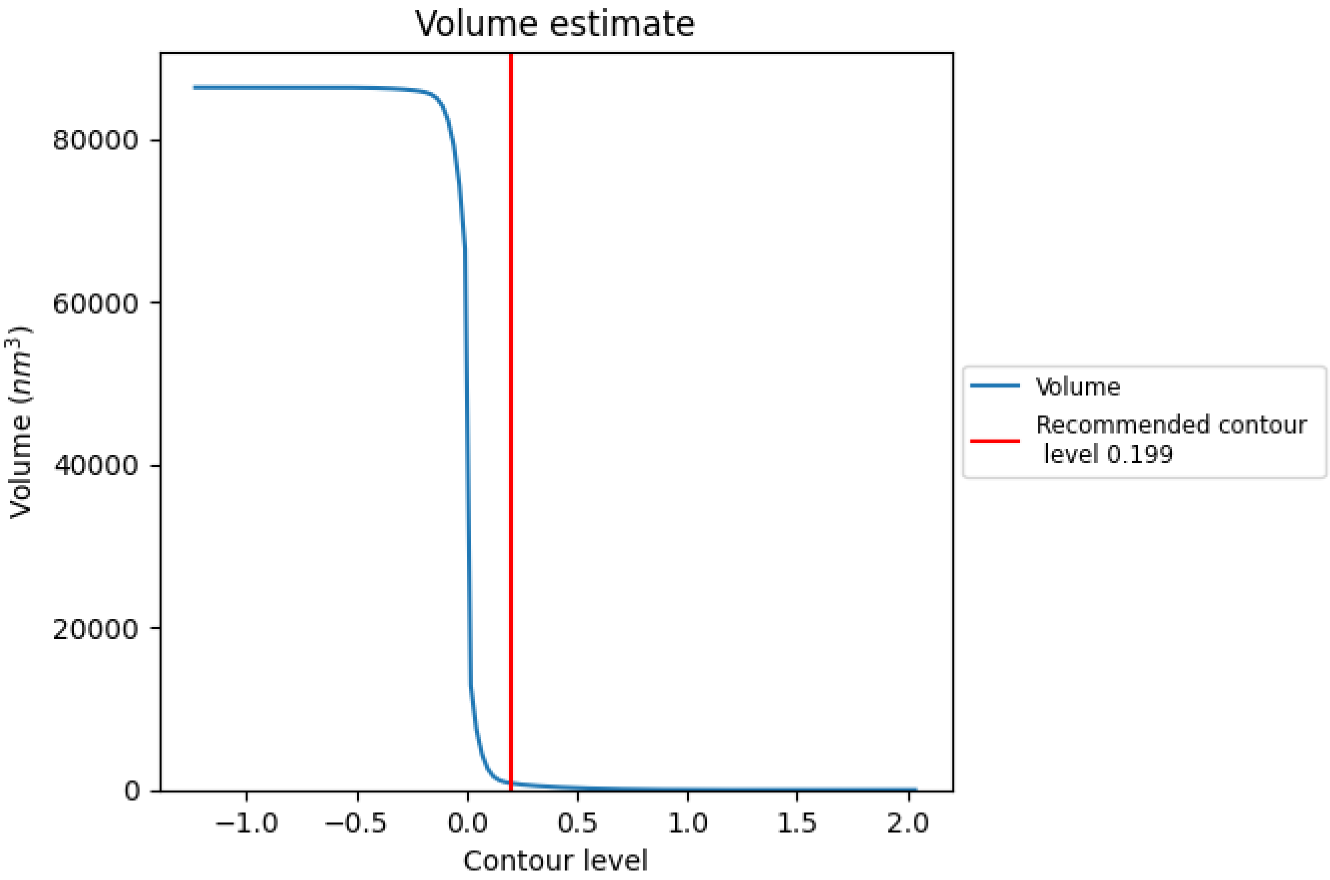
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

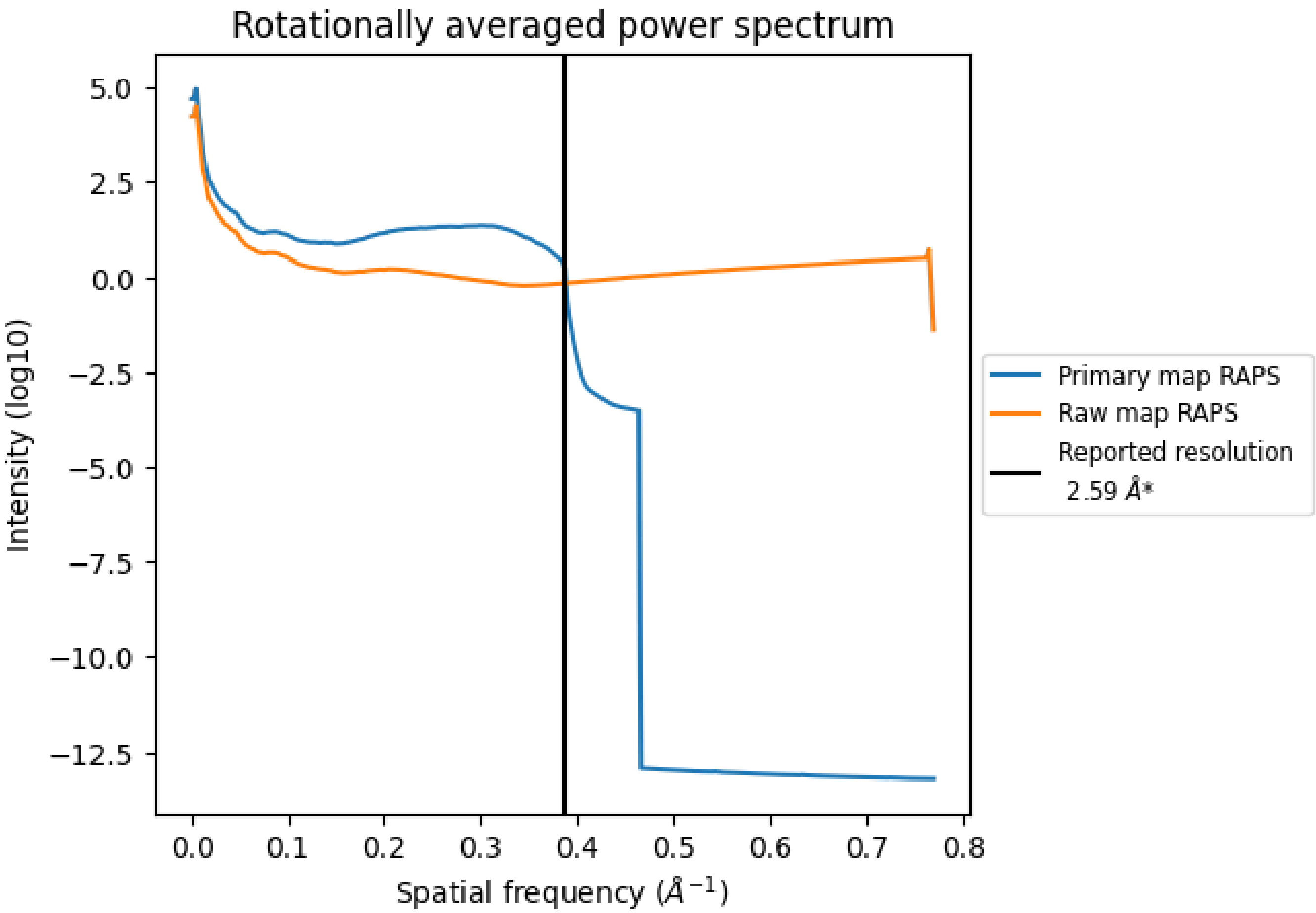
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 836 nm^3; this corresponds to an approximate mass of 755 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 ⓘ

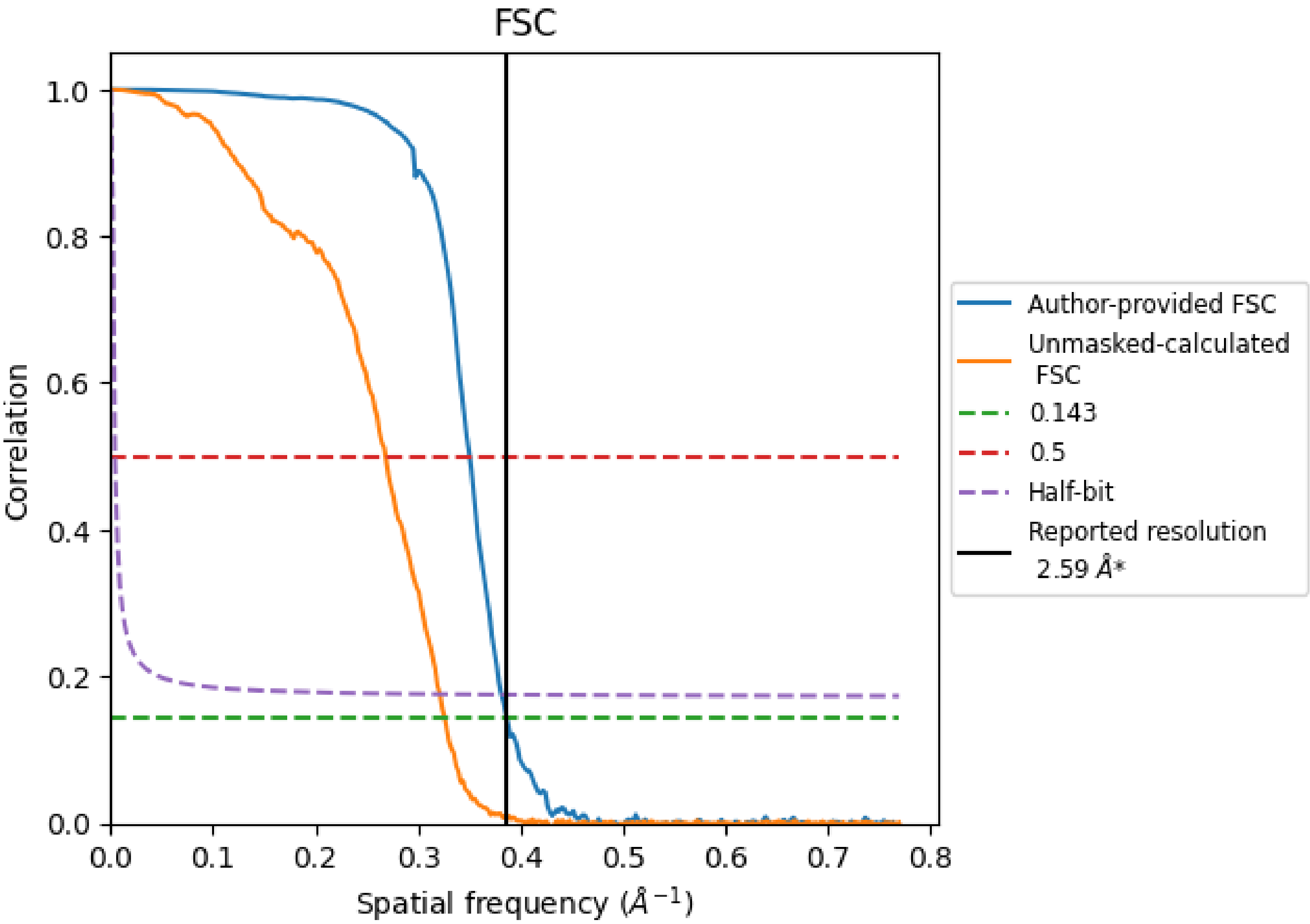


*Reported resolution corresponds to spatial frequency of 0.386 $Å^{-1}$

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.386 Å^{-1}

8.2 Resolution estimates ⓘ

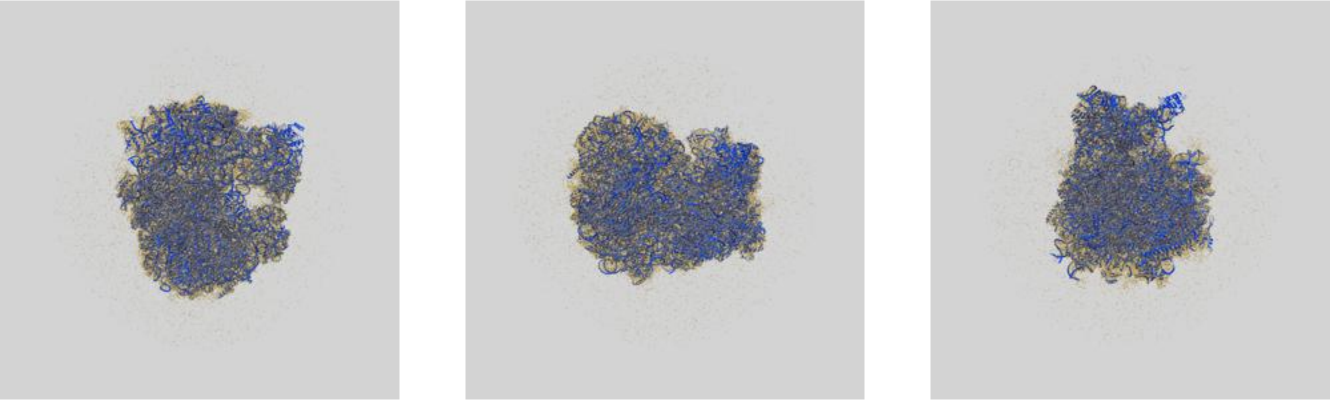
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.59	-	-
Author-provided FSC curve	2.59	2.85	2.62
Unmasked-calculated*	3.07	3.73	3.11

*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 3.07 differs from the reported value 2.59 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-45392 and PDB model 9CAI. Per-residue inclusion information can be found in section 3 on page 19.

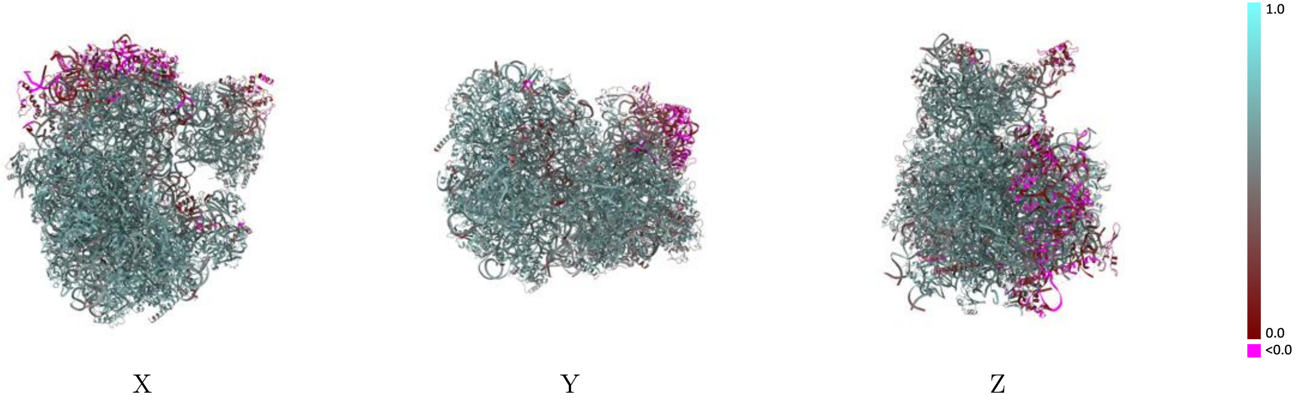
9.1 Map-model overlay ⓘ



X Y Z

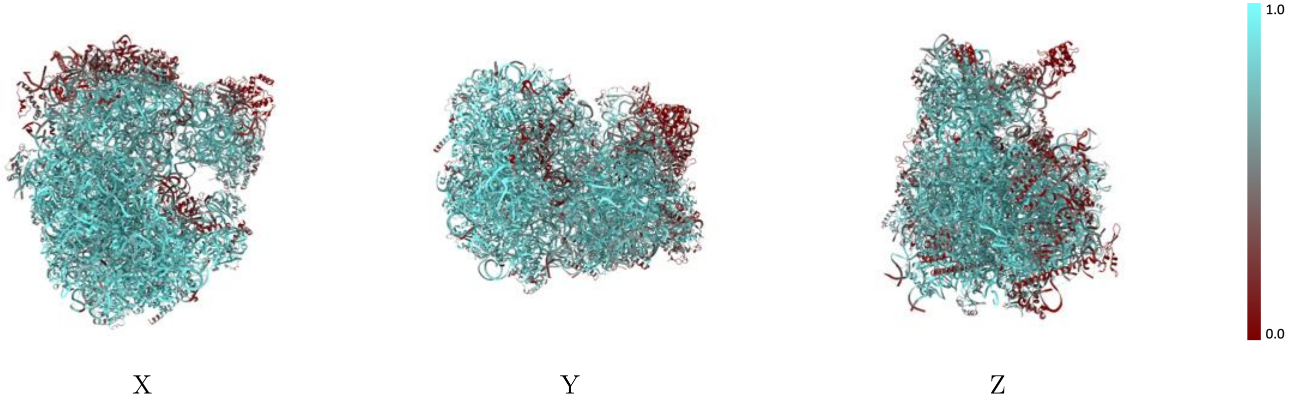
The images above show the 3D surface view of the map at the recommended contour level 0.199 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



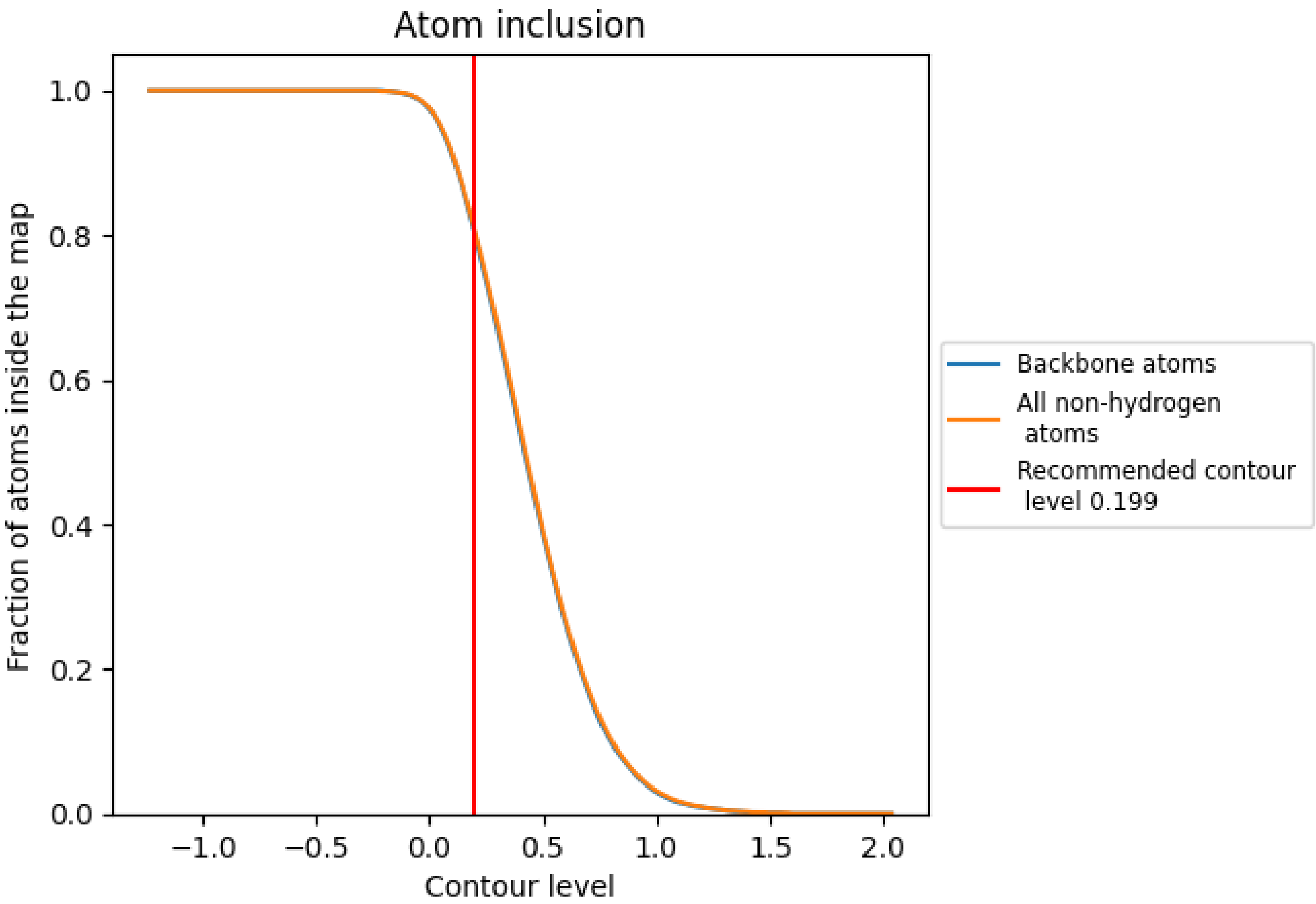
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.199).

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 81% 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 (0.199) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8070	0.5750
A5	0.8980	0.6140
A7	0.9460	0.6350
A8	0.9330	0.6220
AA	0.7030	0.5720
AB	0.7470	0.5860
AC	0.8250	0.6280
AD	0.5490	0.5360
AE	0.3460	0.1420
AF	0.7570	0.5840
AG	0.4570	0.3320
AH	0.4720	0.4430
AI	0.6510	0.4300
AJ	0.3230	0.1320
AK	0.3770	0.4860
AL	0.7690	0.5170
AM	0.0190	0.1640
AN	0.6800	0.5620
AO	0.8470	0.6110
AP	0.5890	0.5350
AQ	0.6900	0.5650
AR	0.4810	0.4810
AS	0.7000	0.5830
AT	0.6680	0.5650
AU	0.4830	0.4660
AV	0.6740	0.5490
AW	0.8980	0.6380
AX	0.7420	0.5140
AY	0.2280	0.0580
AZ	0.5700	0.5240
Aa	0.8450	0.6240
Ab	0.5510	0.4950
Ac	0.6520	0.5320
Ad	0.7560	0.5920
Ae	0.1700	0.1380

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Chain	Atom inclusion	Q-score
Af	0.0600	0.1980
B2	0.8230	0.5530
CA	0.9500	0.6630
CB	0.9250	0.6580
CC	0.8810	0.6380
CD	0.7670	0.5860
CE	0.7810	0.5980
CF	0.8980	0.6440
CG	0.7280	0.5740
CH	0.7560	0.5900
CI	0.2900	0.4140
CJ	0.7130	0.5740
CL	0.8320	0.6220
CM	0.8570	0.6300
CN	0.9640	0.6610
CO	0.9150	0.6520
CP	0.9310	0.6580
CQ	0.9420	0.6590
CR	0.7550	0.5630
CS	0.9010	0.6410
CT	0.8480	0.6250
CU	0.6660	0.5570
CV	0.9300	0.6580
CW	0.6780	0.5110
CX	0.8380	0.6190
CY	0.8690	0.6330
CZ	0.8320	0.6180
Ca	0.9290	0.6530
Cb	0.8260	0.6070
Cc	0.8390	0.6220
Cd	0.8590	0.6260
Ce	0.8890	0.6420
Cf	0.9300	0.6560
Cg	0.8840	0.6380
Ch	0.8260	0.6170
Ci	0.8140	0.6110
Cj	0.9230	0.6460
Ck	0.6640	0.5690
Cl	0.8950	0.6460
Cm	0.2350	0.4620
Cn	0.7340	0.5880
Co	0.8760	0.6500

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Chain	Atom inclusion	Q-score
Cp	▬ 0.9020	▬ 0.6480
DA	▬ 0.5330	▬ 0.4730
DC	▬ 0.5200	▬ 0.4420