wwPDB EM Validation Summary Report

Sep 11, 2026 – 02:57 am BST

PDB ID	:	7O80 / pdb_00007o80
EMDB ID	:	EMD-12758
Title	:	Rabbit 80S ribosome in complex with eRF1 and ABCE1 stalled at the STOP codon in the mutated SARS-CoV-2 slippery site
Authors	:	Bhatt, P.R.; Scaiola, A.; Leibundgut, M.A.; Atkins, J.F.; Ban, N.
Deposited on	:	2021-04-14
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

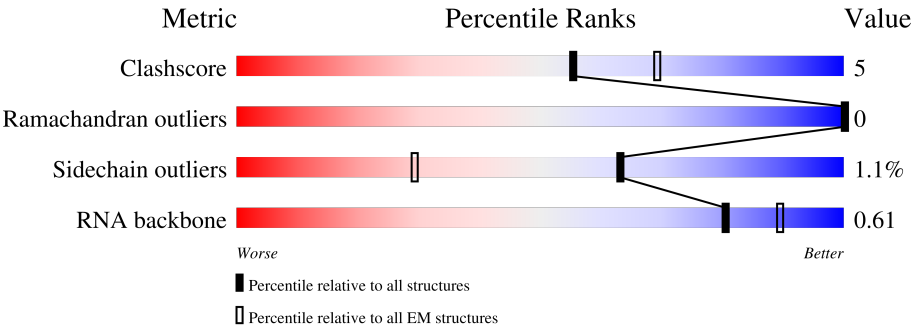
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

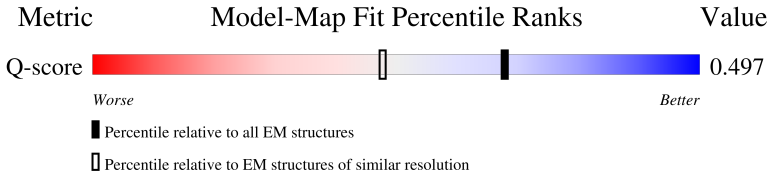
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

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





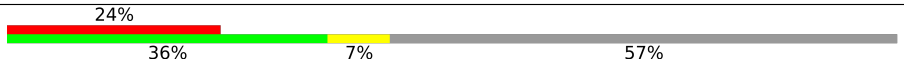
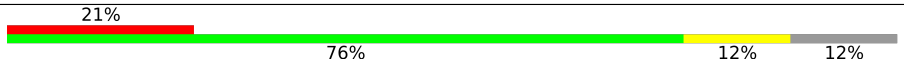
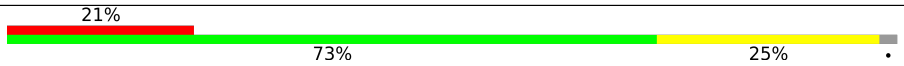
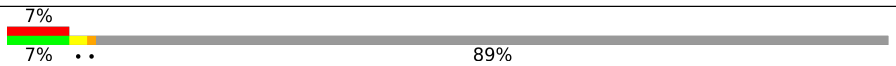
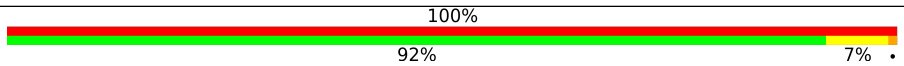
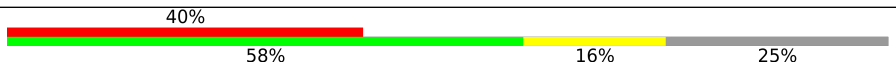
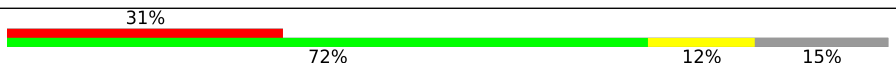
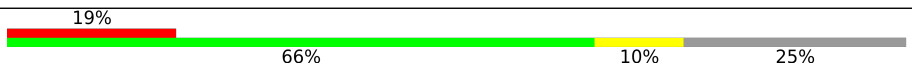
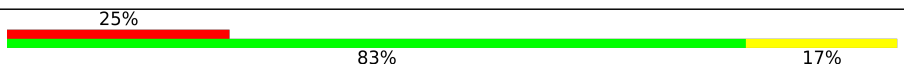
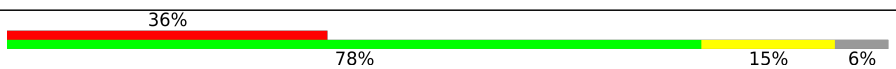
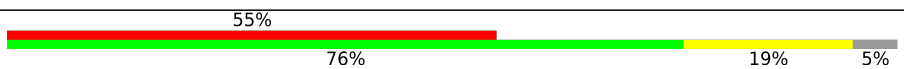
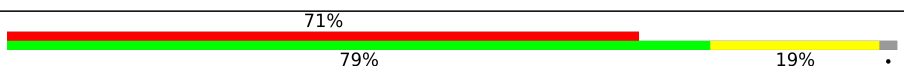
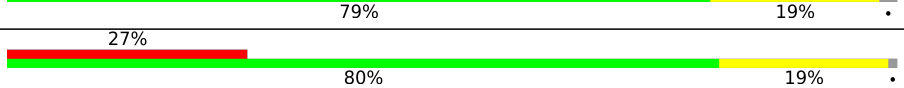
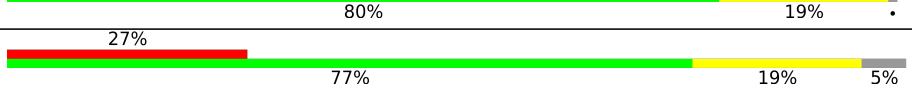
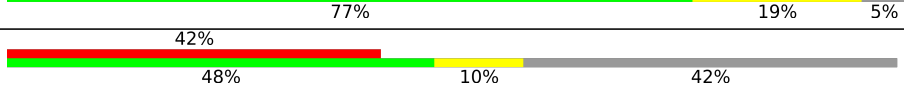
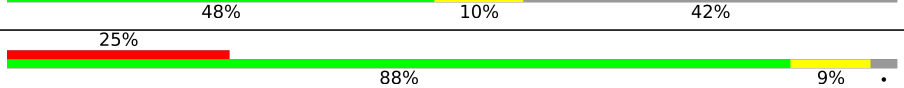
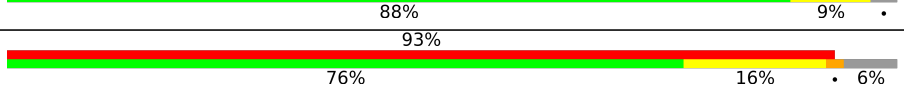
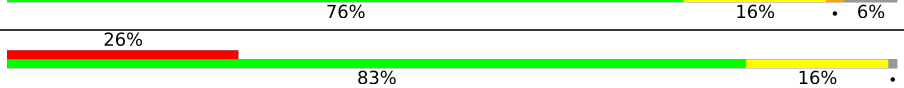
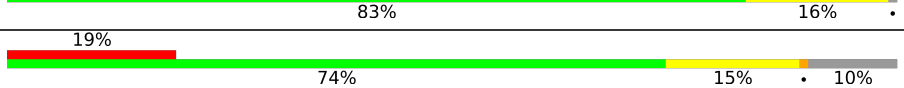
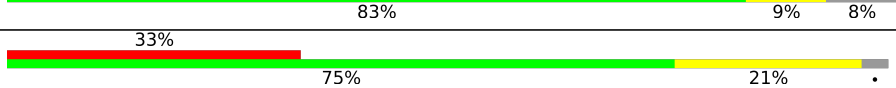
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	A2	1870	16% 61% 28% 5% 5%
2	AA	84	49% 83% 15% .
3	AB	69	49% 81% 10% 9%

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Mol	Chain	Length	Quality of chain
4	AC	156	
5	AD	133	
6	AE	115	
7	AF	317	
8	AG	56	
9	AH	217	
10	AI	76	
11	AT	86	
12	AZ	295	
13	Aa	264	
14	Ab	293	
15	Ac	281	
16	Ad	263	
17	Ae	204	
18	Af	249	
19	Ag	194	
20	Ah	208	
21	Ai	194	
22	Aj	165	
23	Ak	158	
24	Al	132	
25	Am	151	
26	An	151	
27	Ao	145	
28	Ap	146	

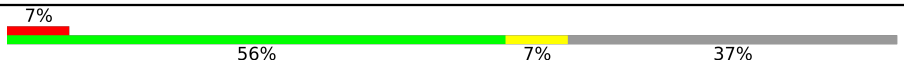
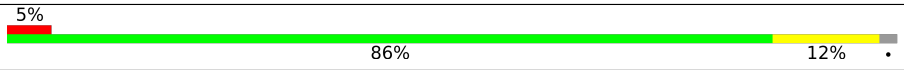
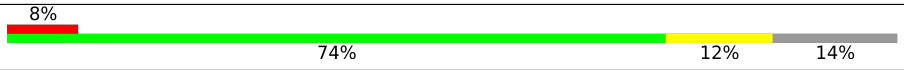
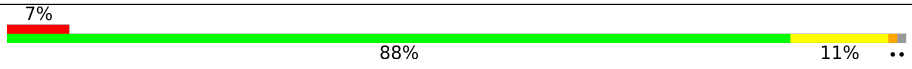
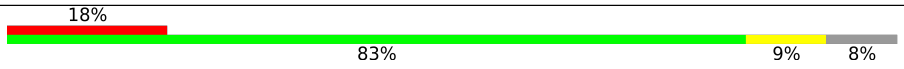
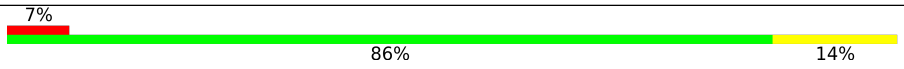
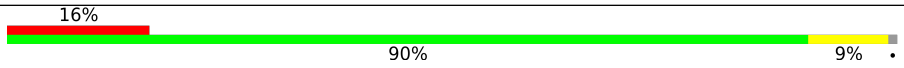
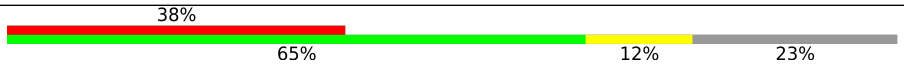
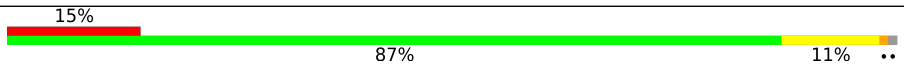
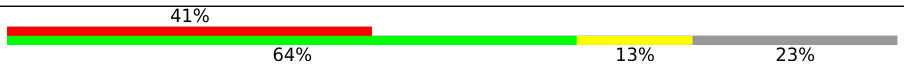
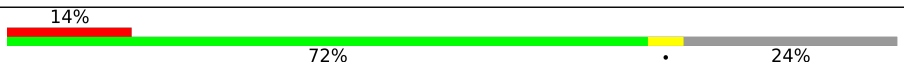
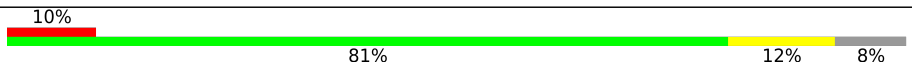
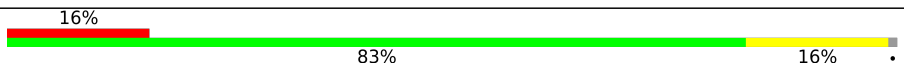
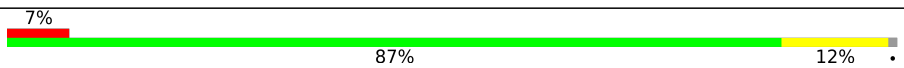
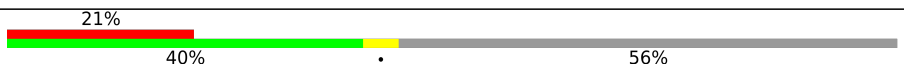
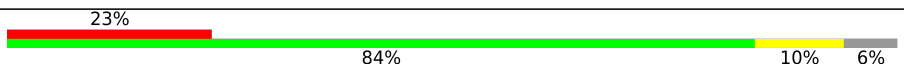
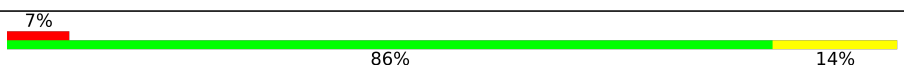
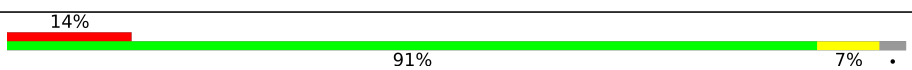
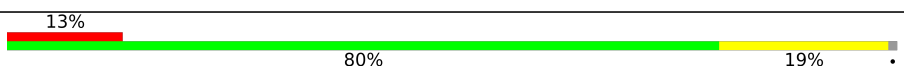
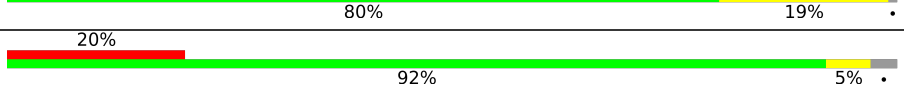
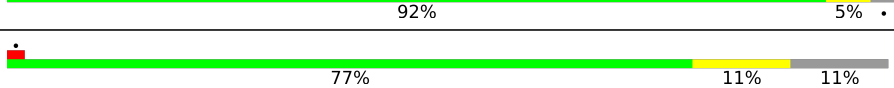
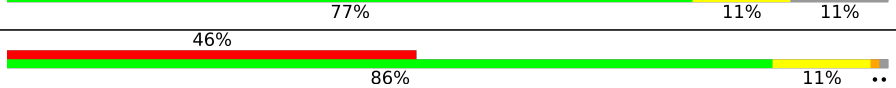
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Mol	Chain	Length	Quality of chain
29	Aq	135	69% 82% 17%
30	Ar	152	48% 70% 26% 5%
31	As	145	38% 86% 13%
32	At	119	59% 77% 10% 13%
33	Au	83	54% 86% 13%
34	Av	130	6% 90% 9%
35	Aw	143	19% 85% 14%
36	Ax	130	35% 78% 18%
37	Ay	124	45% 57% 11% 31%
38	Az	25	92% 8%
39	B5	4808	14% 55% 20% 22%
40	B7	119	82% 17%
41	B8	158	9% 69% 28%
42	BA	257	6% 82% 17%
43	BB	403	9% 85% 14%
44	BC	413	7% 78% 9% 12%
45	BD	297	19% 85% 14%
46	BE	291	26% 66% 17% 16%
47	BF	247	6% 81% 11% 9%
48	BG	266	24% 79% 9% 12%
49	BH	192	19% 85% 14%
50	BI	214	21% 84% 15%
51	BJ	178	31% 78% 17%
52	BK	1071	97%
53	BL	211	18% 85% 13%

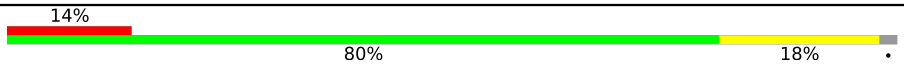
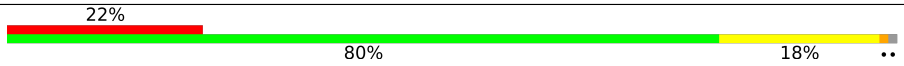
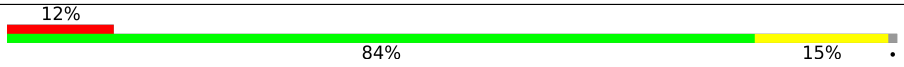
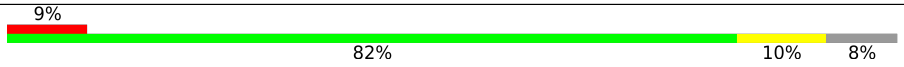
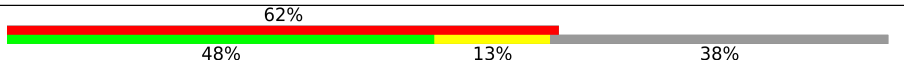
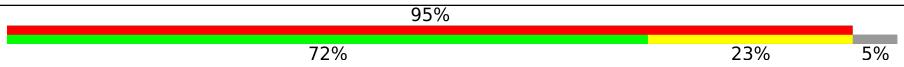
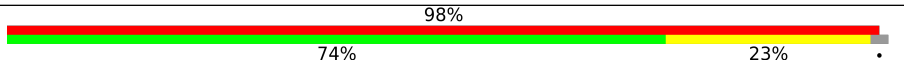
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Mol	Chain	Length	Quality of chain
54	BM	218	
55	BN	204	
56	BO	203	
57	BP	184	
58	BQ	188	
59	BR	196	
60	BS	176	
61	BT	160	
62	BU	128	
63	BV	140	
64	BW	157	
65	BX	156	
66	BY	145	
67	BZ	136	
68	Ba	148	
69	Bb	245	
70	Bc	115	
71	Bd	125	
72	Be	135	
73	Bf	110	
74	Bg	117	
75	Bh	123	
76	Bi	105	
77	Bj	97	
78	Bk	70	

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Mol	Chain	Length	Quality of chain
79	Bl	51	
80	Bm	128	
81	Bo	106	
82	Bp	92	
83	Br	137	
84	Bs	318	
85	Bt	165	
86	Bv	217	
87	By	437	
88	Bz	599	

2 Entry composition (i)

There are 95 unique types of molecules in this entry. The entry contains 235677 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A2	1770	37833	16911	6781	12371	1770	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	1249	B8N	C	conflict	GB GBCT01000564.1
A2	1338	4AC	C	conflict	GB GBCT01000564.1
A2	1843	4AC	C	conflict	GB GBCT01000564.1

- Molecule 2 is a protein called 40S ribosomal protein S27.

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

- Molecule 3 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AB	63	495	302	98	93	2	0	0

- Molecule 4 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AC	73	601	379	115	100	7	0	0

- Molecule 5 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AD	57	457	282	101	73	1	0	0

- Molecule 6 is a protein called Ribosomal protein eS26.

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

- Molecule 7 is a protein called RACK1.

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

- Molecule 8 is a protein called uS14.

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

- Molecule 9 is a RNA chain called mRNA containing SARS-CoV-2 sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AH	24	Total	C	N	O	P	0	0
			508	227	84	173	24		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AH	3466	U	A	conflict	GB NC_045512.2
AH	3468	A	C	conflict	GB NC_045512.2

- Molecule 10 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AI	76	Total	C	N	O	P	0	0
			939	393	11	459	76		

- Molecule 11 is a RNA chain called P-site Leu-tRNA(Leu).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AT	86	Total	C	N	O	P	0	0
			1840	820	330	604	86		

- Molecule 12 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AZ	221	Total	C	N	O	S	0	0
			1743	1107	305	323	8		

- Molecule 13 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Aa	224	Total	C	N	O	S	0	0
			1815	1152	328	321	14		

- Molecule 14 is a protein called Ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Ab	220	Total	C	N	O	S	0	0
			1706	1105	292	300	9		

- Molecule 15 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ac	225	Total	C	N	O	S	0	0
			1751	1116	315	313	7		

- Molecule 16 is a protein called Ribosomal protein eS4.

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

- Molecule 17 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Ae	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

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

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

- Molecule 19 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Ag	190	Total	C	N	O	S	0	0
			1529	975	281	272	1		

- Molecule 20 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Ah	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 21 is a protein called Ribosomal protein S9 (Predicted).

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

- Molecule 22 is a protein called Ribosomal protein eS10.

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

- Molecule 23 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Ak	154	Total	C	N	O	S	0	0
			1262	804	236	216	6		

- Molecule 24 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Al	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 25 is a protein called uS15.

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

- Molecule 26 is a protein called 40S ribosomal protein uS11.

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

- Molecule 27 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Ao	133	Total	C	N	O	S	0	0
			1091	694	205	185	7		

- Molecule 28 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Ap	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 29 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Aq	134	Total	C	N	O	S	0	0
			1080	678	201	197	4		

- Molecule 30 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ar	145	Total	C	N	O	S	0	0
			1200	753	242	204	1		

- Molecule 31 is a protein called Ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	As	143	Total	C	N	O	S	0	0
			1113	698	214	198	3		

- Molecule 32 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	At	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 33 is a protein called Ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Au	83	Total	C	N	O	S	0	0
			640	394	117	124	5		

- Molecule 34 is a protein called Ribosomal protein S15a.

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

- Molecule 35 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Aw	141	Total	C	N	O	S	0	0
			1099	693	219	184	3		

- Molecule 36 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ax	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 37 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ay	85	Total	C	N	O	S	0	0
			683	439	128	115	1		

- Molecule 38 is a protein called 60s ribosomal protein l41.

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

- Molecule 39 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	B5	3764	Total	C	N	O	P	0	0
			80772	36003	14762	26243	3764		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	3550	UY1	U	conflict	GB GBCN01009604.1

- Molecule 40 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	B7	119	Total	C	N	O	P	0	0
			2538	1131	451	837	119		

- Molecule 41 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	B8	156	Total	C	N	O	P	0	0
			3319	1481	585	1097	156		

- Molecule 42 is a protein called Ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BA	253	Total	C	N	O	S	0	0
			1940	1214	396	324	6		

- Molecule 43 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BB	398	Total	C	N	O	S	0	0
			3206	2042	605	546	13		

- Molecule 44 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BC	362	Total	C	N	O	S	0	0
			2886	1814	577	481	14		

- Molecule 45 is a protein called Ribosomal_L18_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BD	294	Total	C	N	O	S	0	0
			2398	1516	439	429	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BD	2	AAC	GLY	conflict	UNP G1SYJ6

- Molecule 46 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BE	243	Total	C	N	O	S	0	0
			1960	1258	378	321	3		

- Molecule 47 is a protein called Ribosomal Protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BF	226	Total	C	N	O	S	0	0
			1886	1211	362	304	9		

- Molecule 48 is a protein called Ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BG	233	Total	C	N	O	S	0	0
			1877	1197	361	315	4		

- Molecule 49 is a protein called 60S ribosomal protein L9.

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

- Molecule 50 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BI	213	Total	C	N	O	S	0	0
			1717	1086	332	285	14		

- Molecule 51 is a protein called Ribosomal protein L11.

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

- Molecule 52 is a protein called Replicase polyprotein 1ab.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BK	36	Total	C	N	O	S	0	0
			273	169	46	52	6		

- Molecule 53 is a protein called Ribosomal protein eL13.

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

- Molecule 54 is a protein called Ribosomal protein L14.

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

- Molecule 55 is a protein called Ribosomal protein L15.

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

- Molecule 56 is a protein called Ribosomal protein L13a.

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

- Molecule 57 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BP	159	Total	C	N	O	S	0	0
			1289	809	249	222	9		

- Molecule 58 is a protein called Ribosomal protein L18.

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

- Molecule 59 is a protein called 60S ribosomal protein L19.

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

- Molecule 60 is a protein called Ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BS	176	Total	C	N	O	S	0	0
			1457	924	288	234	11		

- Molecule 61 is a protein called eL21.

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

- Molecule 62 is a protein called Ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	BU	99	Total	C	N	O	S	0	0
			806	516	141	147	2		

- Molecule 63 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BV	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 64 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	BW	121	Total	C	N	O	S	0	0
			991	619	202	166	4		

- Molecule 65 is a protein called uL23.

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

- Molecule 66 is a protein called Ribosomal protein L26.

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

- Molecule 67 is a protein called 60S ribosomal protein L27.

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

- Molecule 68 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Ba	147	Total	C	N	O	S	0	0
			1163	734	239	186	4		

- Molecule 69 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Bb	108	Total	C	N	O	S	0	0
			881	548	196	134	3		

- Molecule 70 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Bc	108	Total	C	N	O	S	0	0
			836	530	148	151	7		

- Molecule 71 is a protein called eL31.

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

- Molecule 72 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Be	130	Total	C	N	O	S	0	0
			1070	676	221	168	5		

- Molecule 73 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Bf	110	Total	C	N	O	S	0	0
			884	560	175	144	5		

- Molecule 74 is a protein called 60S ribosomal protein L34.

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

- Molecule 75 is a protein called uL29.

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

- Molecule 76 is a protein called 60S ribosomal protein L36.

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

- Molecule 77 is a protein called Ribosomal protein L37.

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

- Molecule 78 is a protein called eL38.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bk	24	LYS	ASN	conflict	UNP G1U001

- Molecule 79 is a protein called eL39.

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

- Molecule 80 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Bm	52	Total	C	N	O	S	0	0
			432	269	90	67	6		

- Molecule 81 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Bo	105	Total	C	N	O	S	0	0
			863	543	175	139	6		

- Molecule 82 is a protein called eL43.

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

- Molecule 83 is a protein called Ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Br	126	Total	C	N	O	S	0	0
			1014	629	209	170	6		

- Molecule 84 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Bs	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 85 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Bt	156	Total	C	N	O	S	0	0
			1178	733	221	220	4		

- Molecule 86 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Bv	212	Total	C	N	O	S	0	0
			1707	1092	308	299	8		

- Molecule 87 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	By	416	Total	C	N	O	S	0	0
			3280	2087	559	623	11		

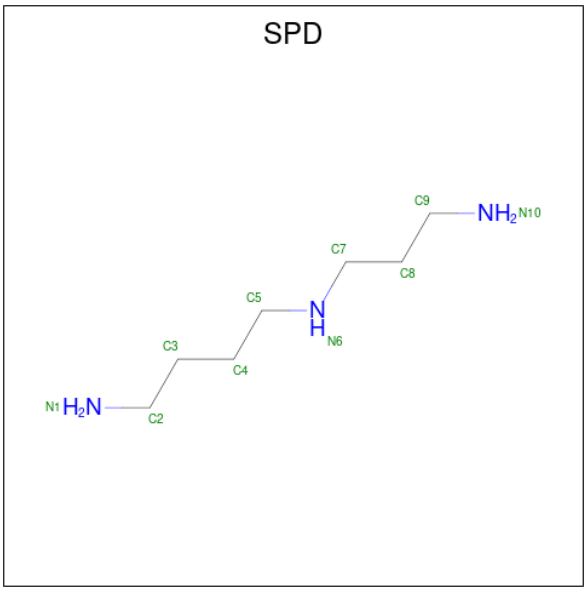
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
By	183	ALA	GLY	engineered mutation	UNP P62497
By	184	ALA	GLY	engineered mutation	UNP P62497

- Molecule 88 is a protein called ATP binding cassette subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	Bz	595	Total	C	N	O	S	0	0
			4668	2982	801	854	31		

- Molecule 89 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	AltConf
89	A2	1	Total C N 10 7 3	0

- Molecule 90 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
90	A2	102	Total Mg 102 102	0
90	AH	1	Total Mg 1 1	0
90	AT	2	Total Mg 2 2	0
90	B5	235	Total Mg 235 235	0
90	B7	4	Total Mg 4 4	0
90	B8	6	Total Mg 6 6	0
90	BI	1	Total Mg 1 1	0
90	BP	1	Total Mg 1 1	0
90	BR	1	Total Mg 1 1	0
90	BV	1	Total Mg 1 1	0
90	Ba	1	Total Mg 1 1	0

- Molecule 91 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms	AltConf
91	A2	76	Total X 76 76	0
91	AT	4	Total X 4 4	0
91	Ab	1	Total X 1 1	0
91	Ak	1	Total X 1 1	0
91	Ar	1	Total X 1 1	0
91	B5	244	Total X 244 244	0
91	B7	10	Total X 10 10	0
91	B8	16	Total X 16 16	0
91	BA	2	Total X 2 2	0
91	BB	3	Total X 3 3	0
91	BC	1	Total X 1 1	0
91	BH	1	Total X 1 1	0
91	BI	1	Total X 1 1	0
91	BL	1	Total X 1 1	0
91	BN	2	Total X 2 2	0
91	BP	1	Total X 1 1	0
91	BQ	2	Total X 2 2	0
91	BT	1	Total X 1 1	0
91	Bb	1	Total X 1 1	0
91	Be	2	Total X 2 2	0
91	Bf	1	Total X 1 1	0

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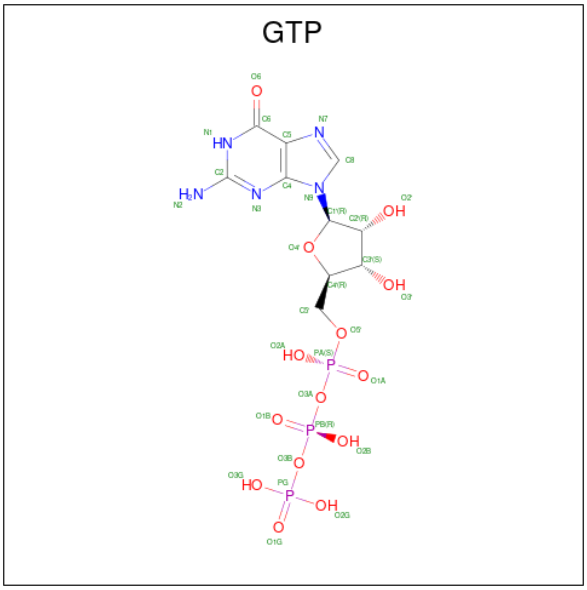
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Mol	Chain	Residues	Atoms	AltConf
91	Bg	1	Total X 1 1	0
91	Bo	1	Total X 1 1	0

- Molecule 92 is ZINC ION (CCD ID: ZN) (formula: Zn).

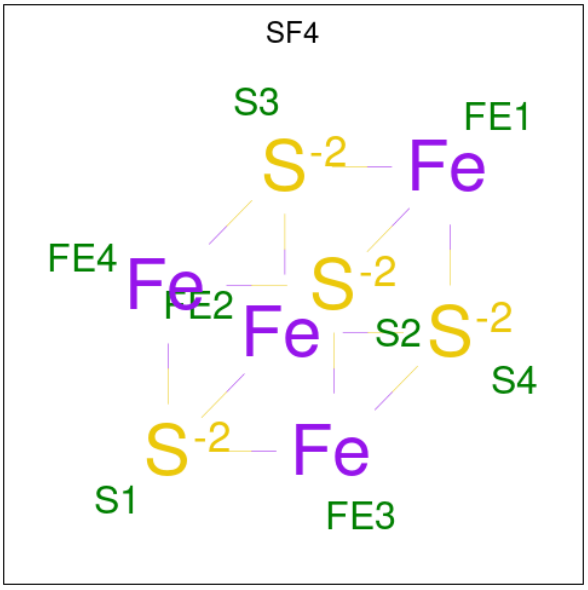
Mol	Chain	Residues	Atoms	AltConf
92	AC	1	Total Zn 1 1	0
92	AE	1	Total Zn 1 1	0
92	AG	1	Total Zn 1 1	0
92	Bg	1	Total Zn 1 1	0
92	Bj	1	Total Zn 1 1	0
92	Bm	1	Total Zn 1 1	0
92	Bo	1	Total Zn 1 1	0
92	Bp	1	Total Zn 1 1	0

- Molecule 93 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
93	B7	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 94 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
94	Bz	1	Total	Fe	S	0
			8	4	4	
94	Bz	1	Total	Fe	S	0
			8	4	4	

- Molecule 95 is water.

Mol	Chain	Residues	Atoms		AltConf
95	A2	473	Total	O	0
			473	473	
95	AH	10	Total	O	0
			10	10	
95	AT	12	Total	O	0
			12	12	
95	Aa	2	Total	O	0
			2	2	
95	Ab	1	Total	O	0
			1	1	
95	Ad	1	Total	O	0
			1	1	
95	Af	2	Total	O	0
			2	2	

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Mol	Chain	Residues	Atoms	AltConf
95	Ak	1	Total O 1 1	0
95	Am	1	Total O 1 1	0
95	An	2	Total O 2 2	0
95	Ap	4	Total O 4 4	0
95	Ar	1	Total O 1 1	0
95	As	4	Total O 4 4	0
95	Aw	4	Total O 4 4	0
95	B5	1117	Total O 1117 1117	0
95	B7	17	Total O 17 17	0
95	B8	31	Total O 31 31	0
95	BA	5	Total O 5 5	0
95	BB	7	Total O 7 7	0
95	BC	3	Total O 3 3	0
95	BD	1	Total O 1 1	0
95	BF	1	Total O 1 1	0
95	BH	1	Total O 1 1	0
95	BI	1	Total O 1 1	0
95	BL	1	Total O 1 1	0
95	BN	2	Total O 2 2	0
95	BO	3	Total O 3 3	0
95	BP	3	Total O 3 3	0

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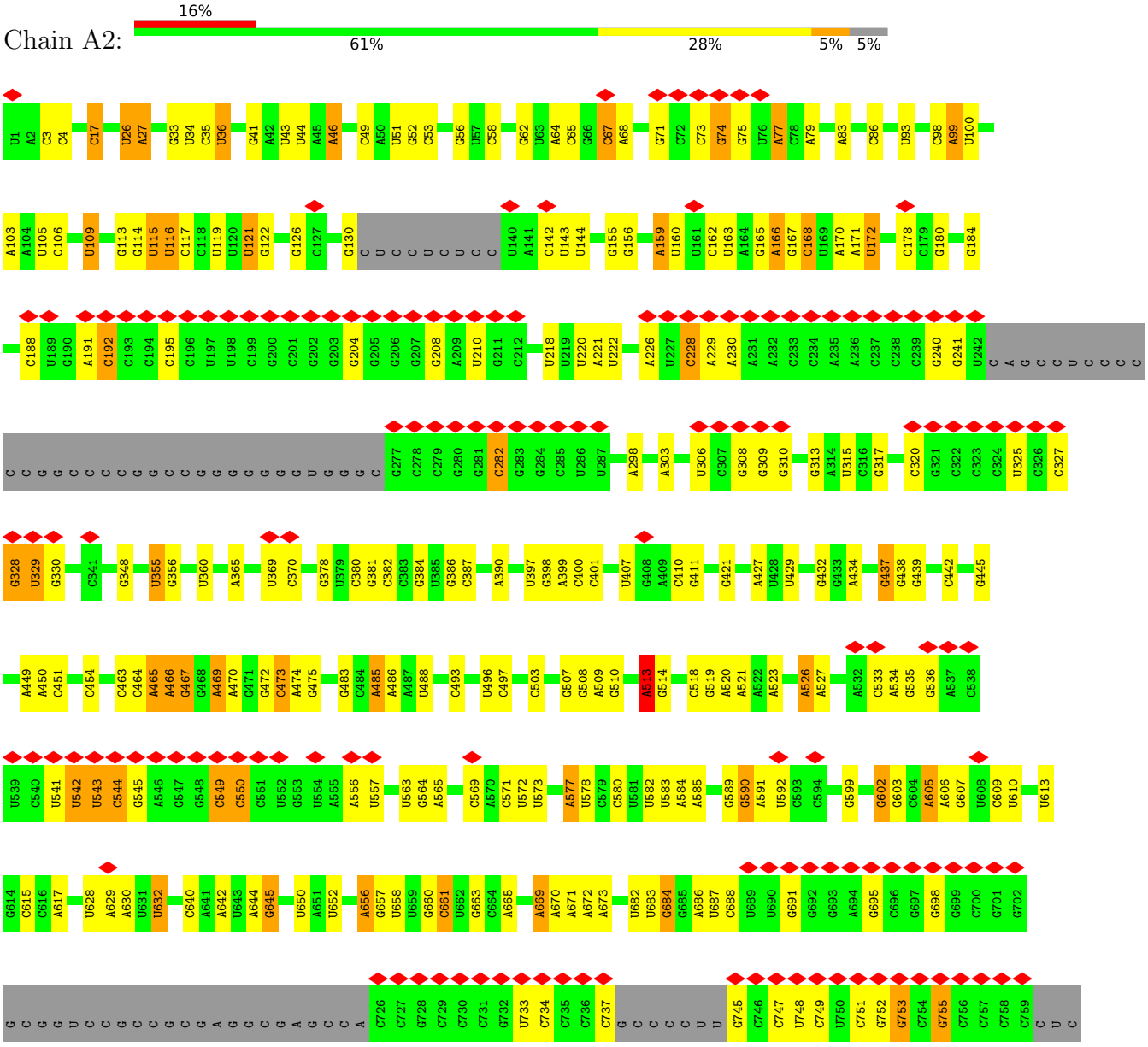
Mol	Chain	Residues	Atoms	AltConf
95	BR	5	Total O 5 5	0
95	BV	4	Total O 4 4	0
95	BX	1	Total O 1 1	0
95	BY	1	Total O 1 1	0
95	Ba	7	Total O 7 7	0
95	Bb	1	Total O 1 1	0
95	Bd	1	Total O 1 1	0
95	Be	4	Total O 4 4	0
95	Bf	1	Total O 1 1	0
95	By	1	Total O 1 1	0

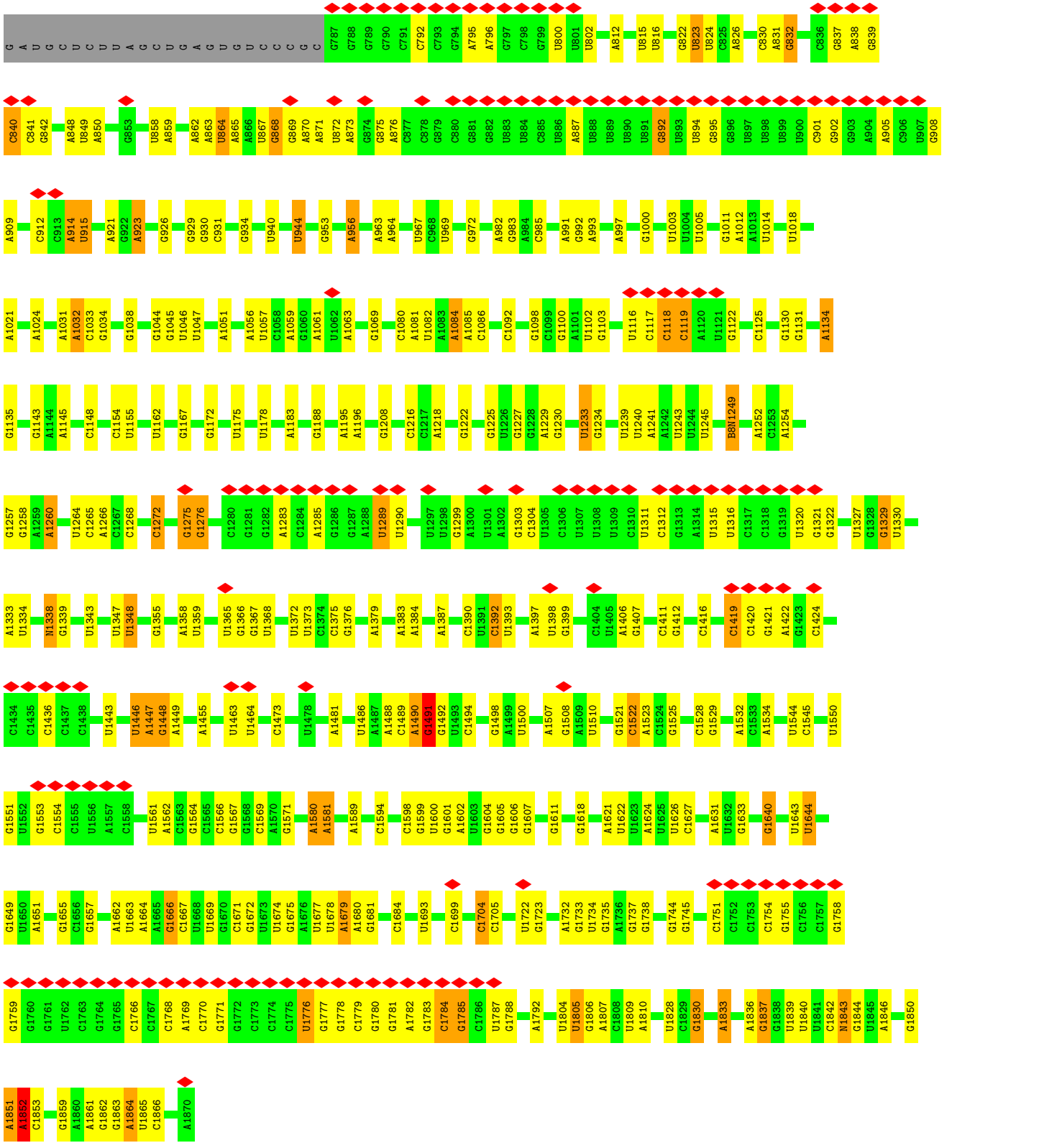
3 Residue-property plots (i)

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

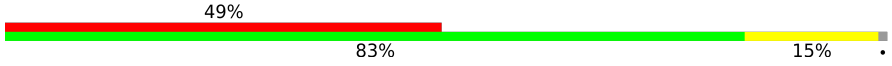
- Molecule 1: 18S rRNA

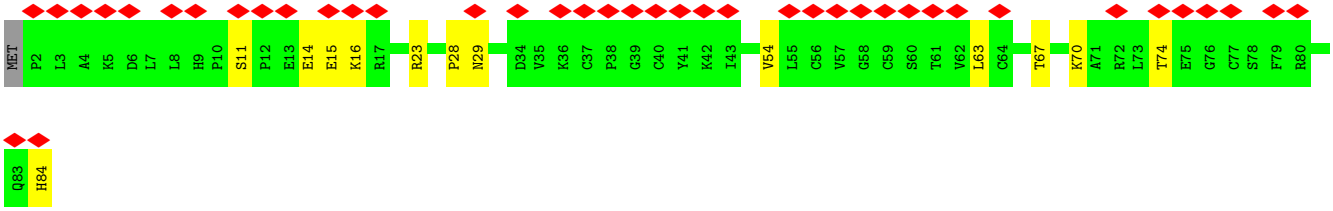
Chain A2:





• Molecule 2: 40S ribosomal protein S27

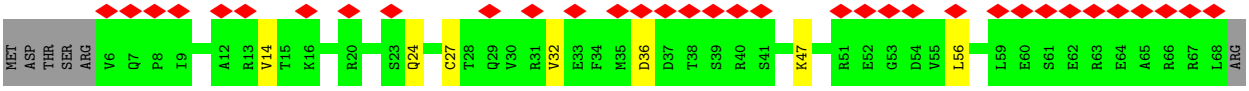




• Molecule 3: Ribosomal protein S28

Chain AB:

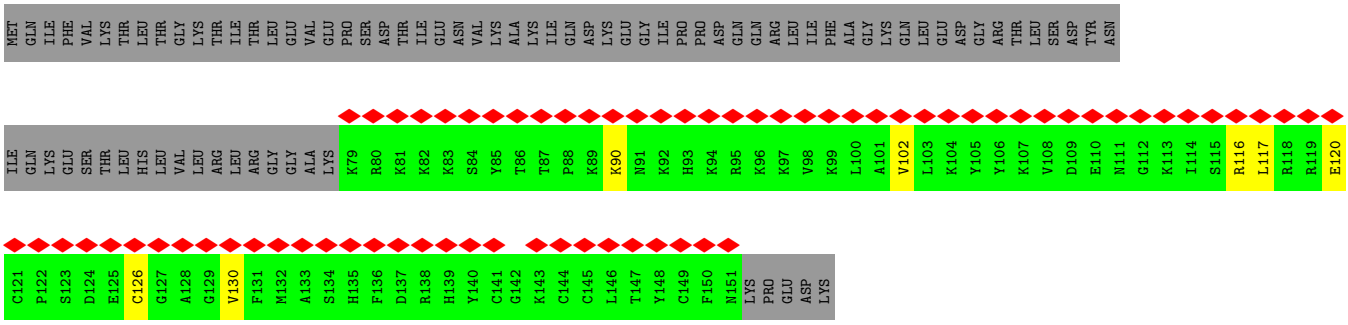




• Molecule 4: Ribosomal protein S27a

Chain AC:

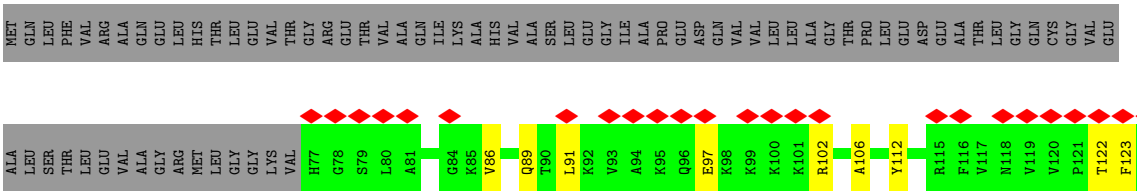




• Molecule 5: 40S ribosomal protein S30

Chain AD:

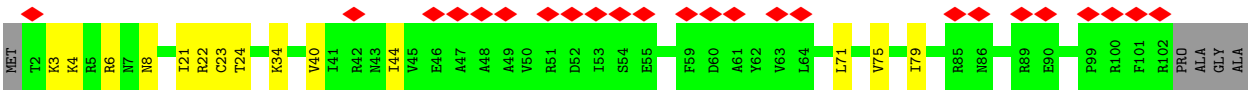




• Molecule 6: Ribosomal protein eS26

Chain AE:



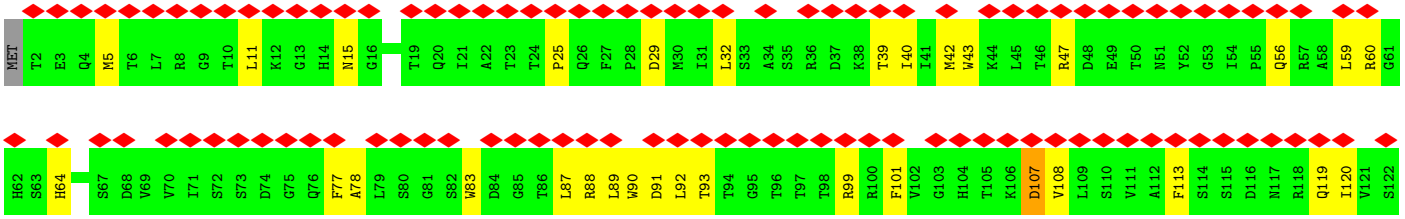




• Molecule 7: RACK1

Chain AF:

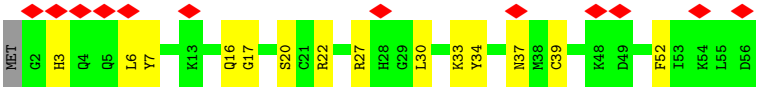




• Molecule 8: uS14

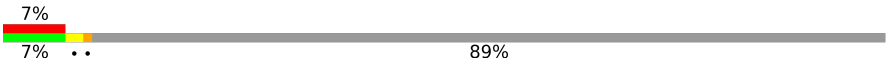
Chain AG:

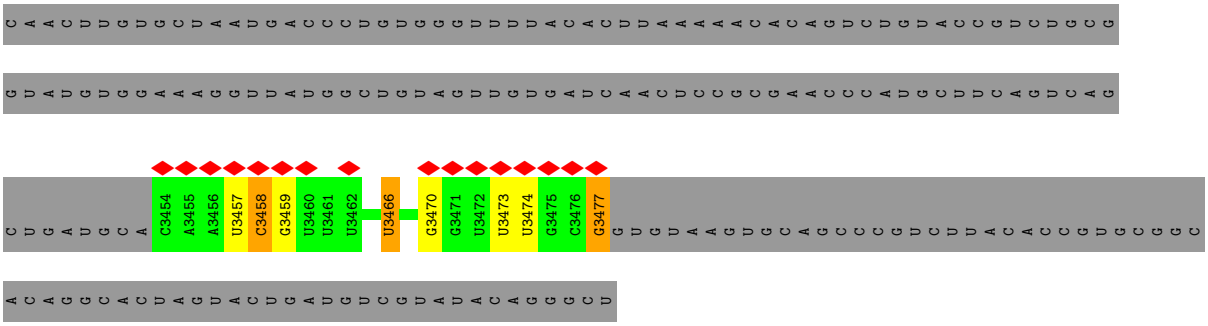




• Molecule 9: mRNA containing SARS-CoV-2 sequence

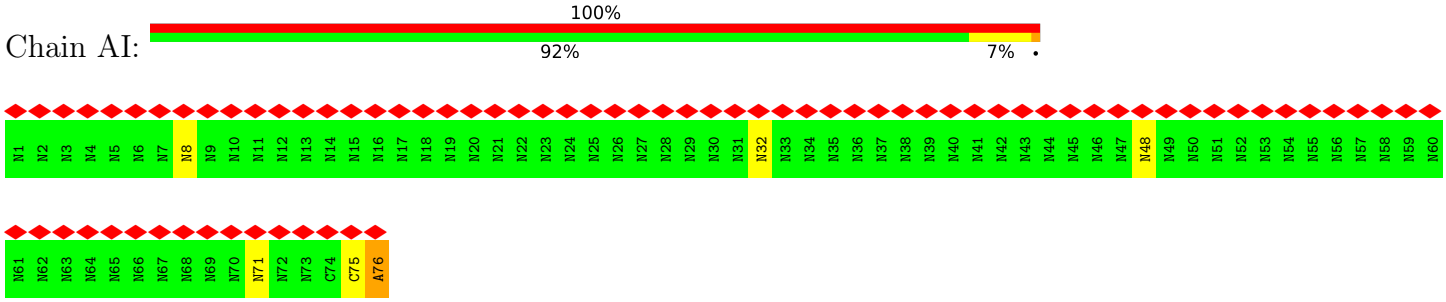
Chain AH:





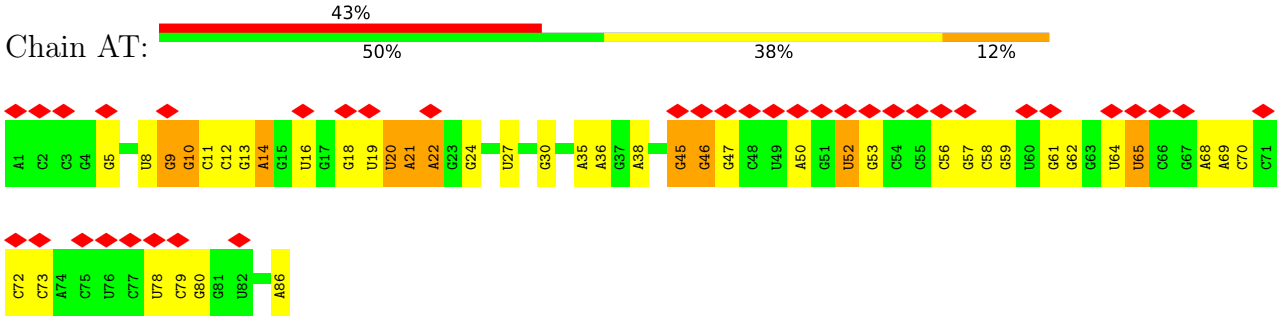
• Molecule 10: E-site tRNA

Chain AI:



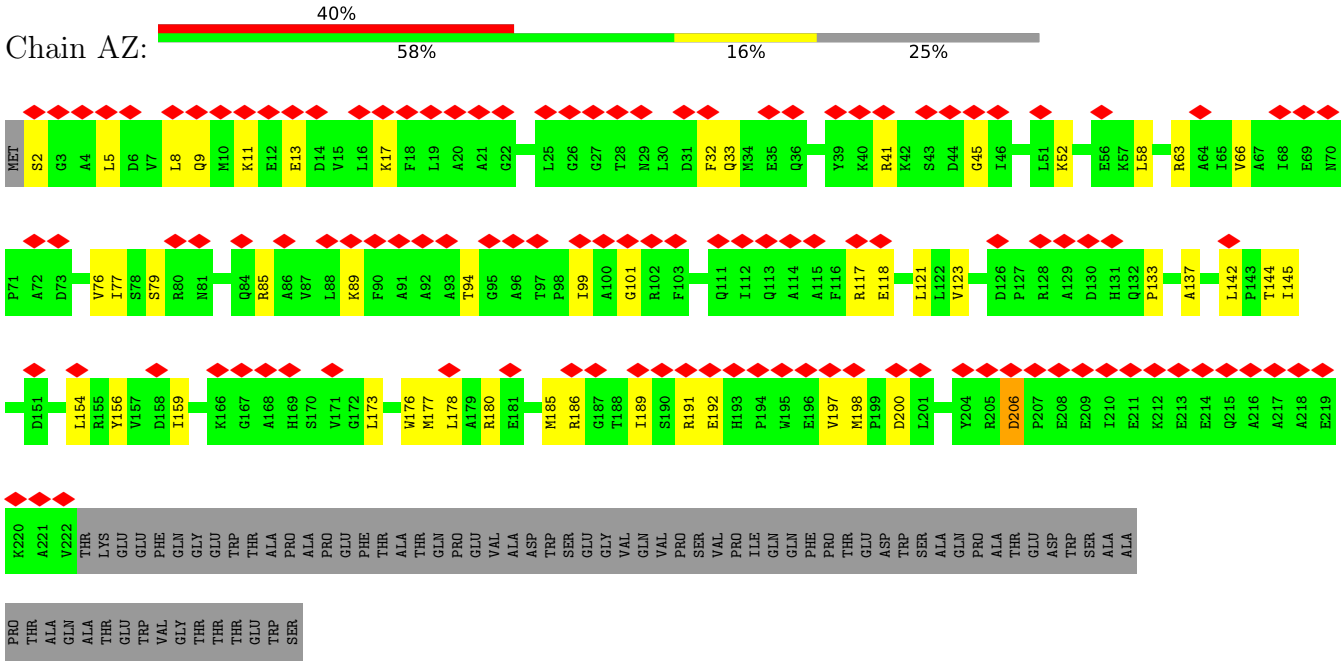
• Molecule 11: P-site Leu-tRNA(Leu)

Chain AT:



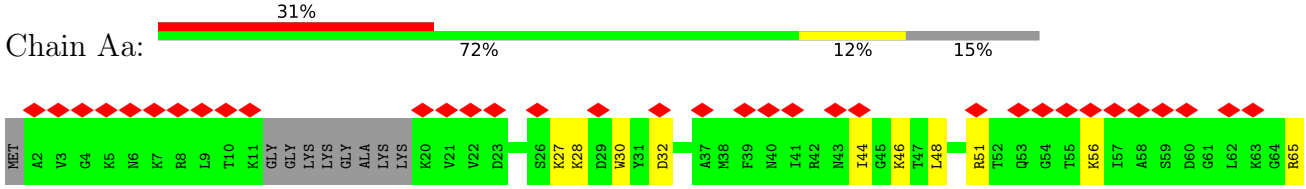
• Molecule 12: 40S ribosomal protein SA

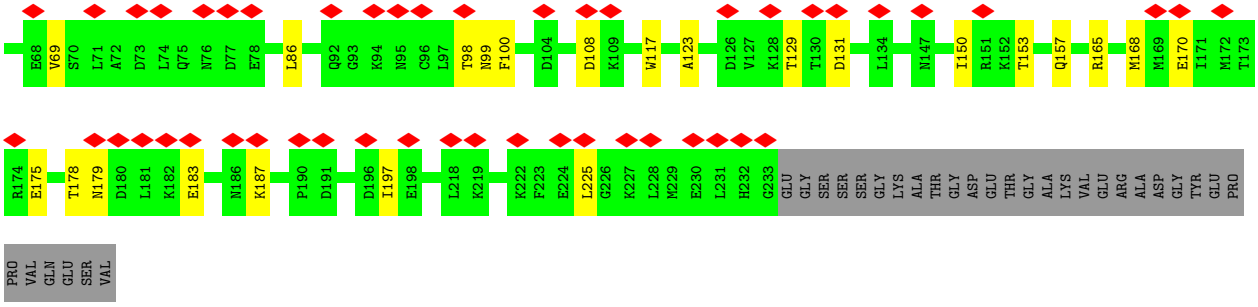
Chain AZ:



• Molecule 13: 40S ribosomal protein S3a

Chain Aa:

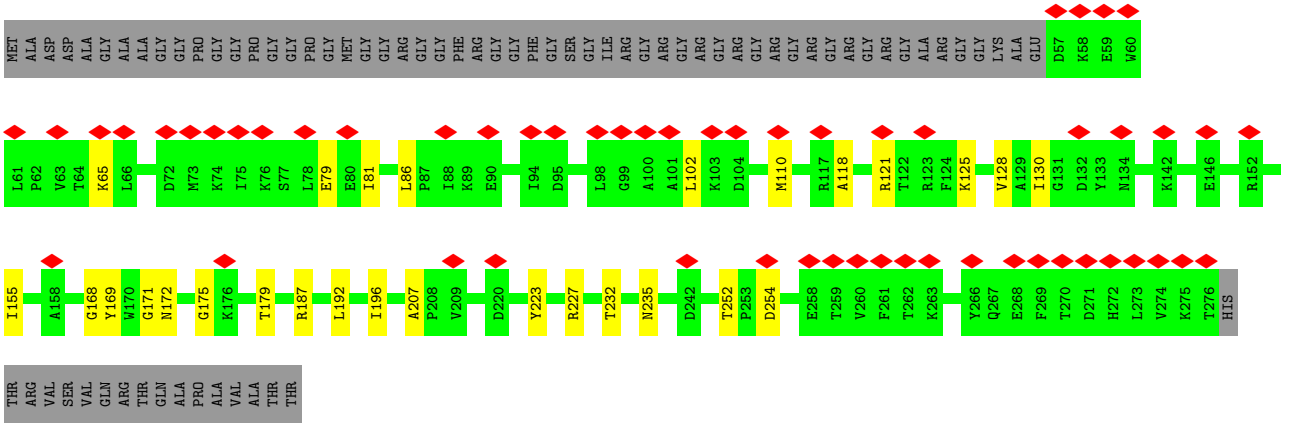




• Molecule 14: Ribosomal protein uS5

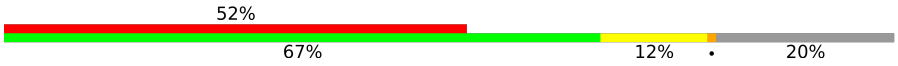
Chain Ab:

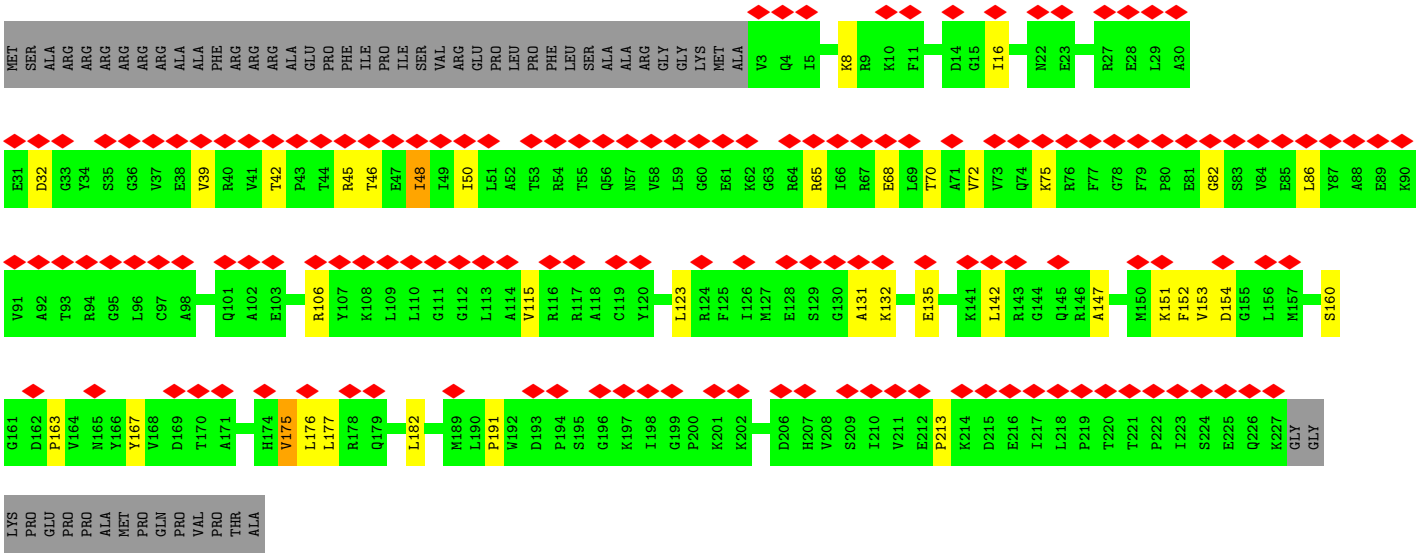




• Molecule 15: 40S ribosomal protein S3

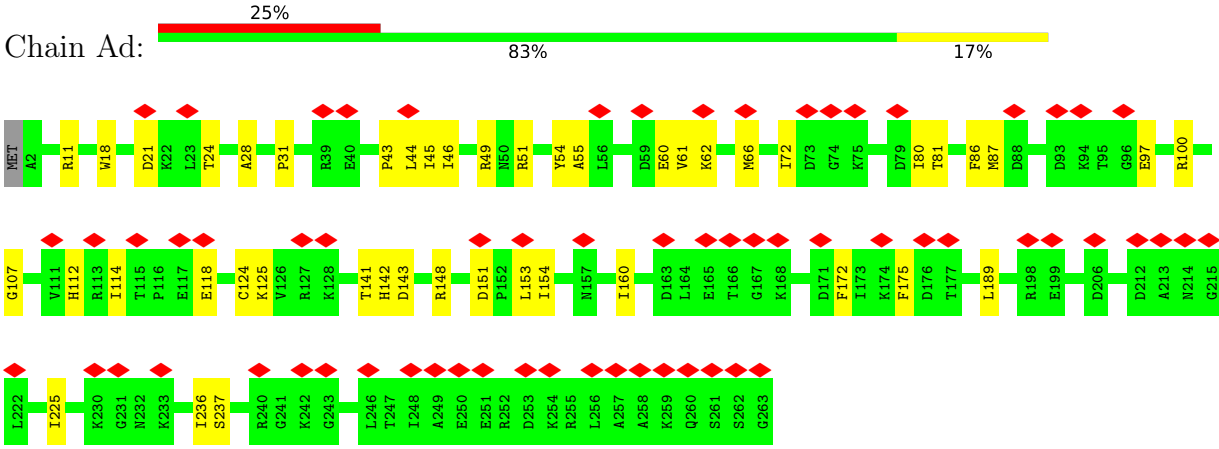
Chain Ac:





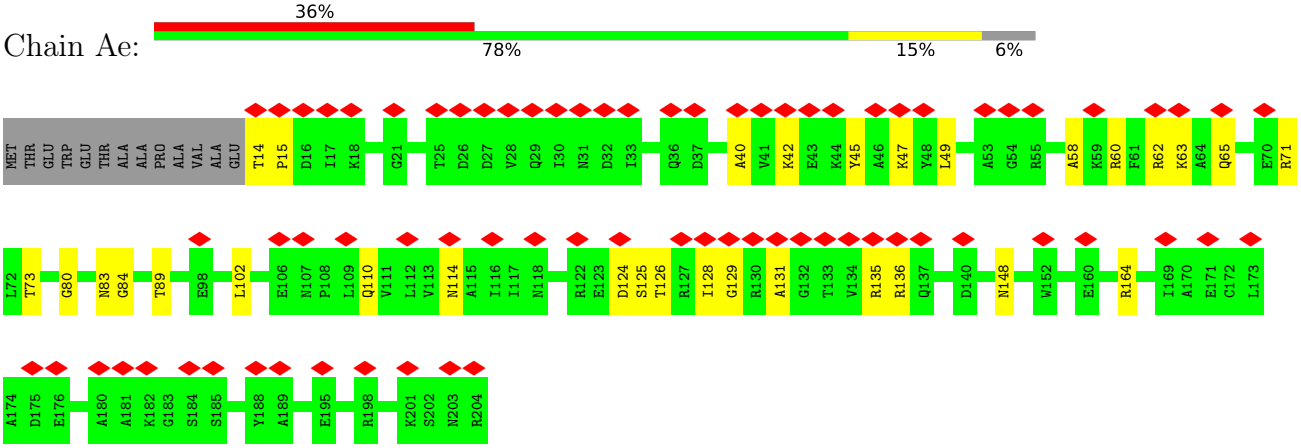
• Molecule 16: Ribosomal protein eS4

Chain Ad:



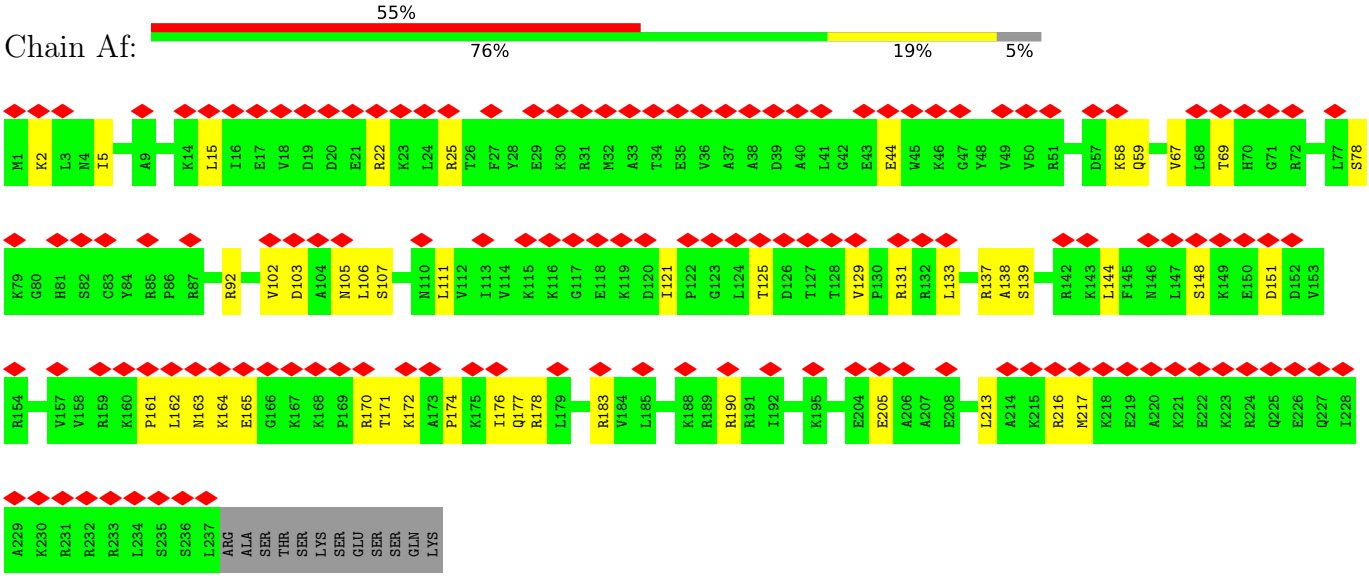
• Molecule 17: Ribosomal protein S5

Chain Ae:



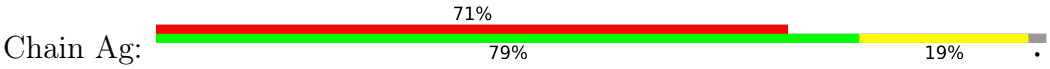
• Molecule 18: 40S ribosomal protein S6

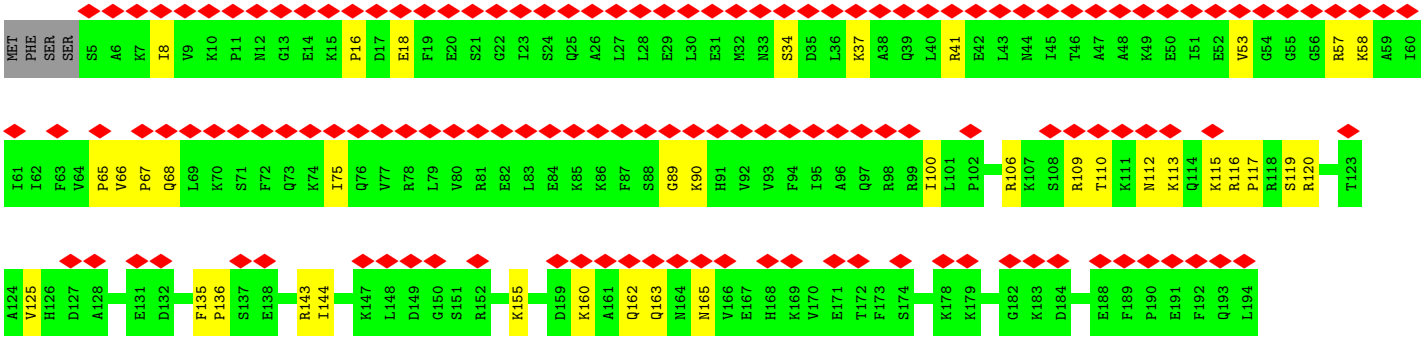
Chain Af:



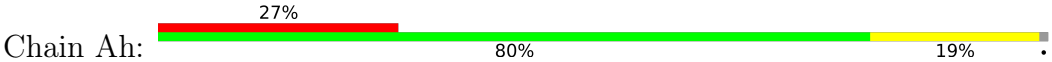
• Molecule 19: 40S ribosomal protein S7

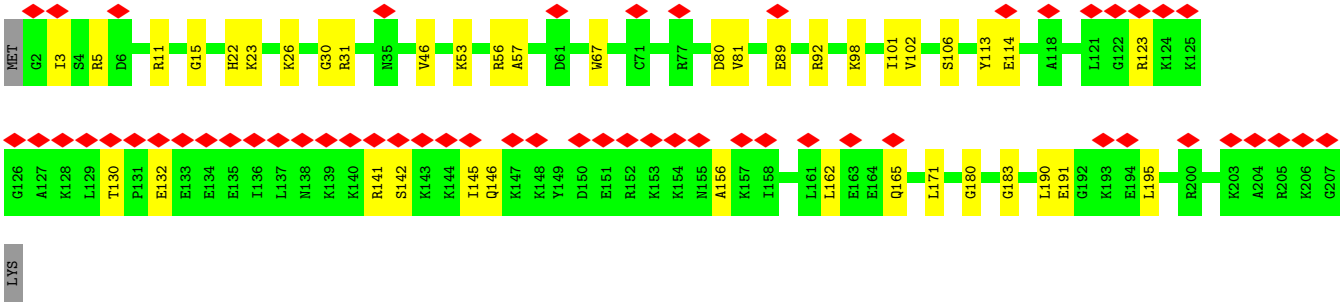
Chain Ag:



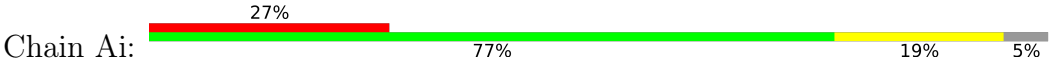


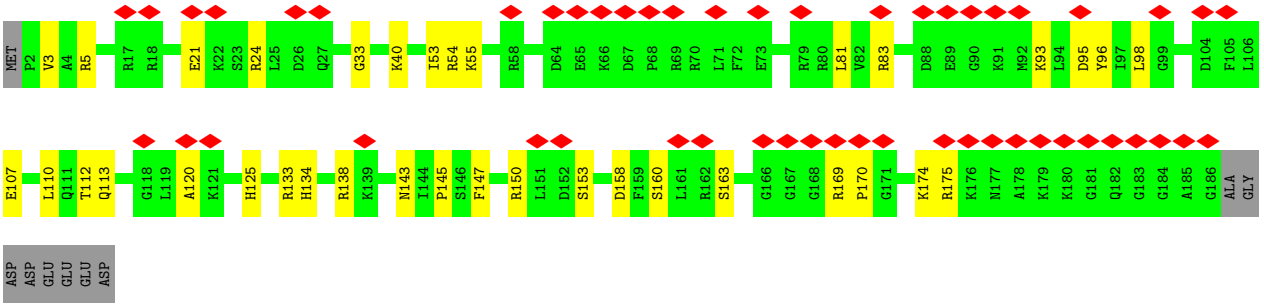
• Molecule 20: 40S ribosomal protein S8



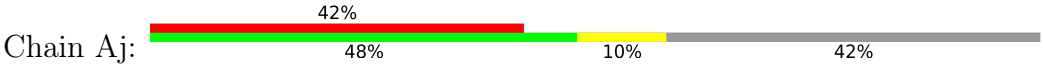


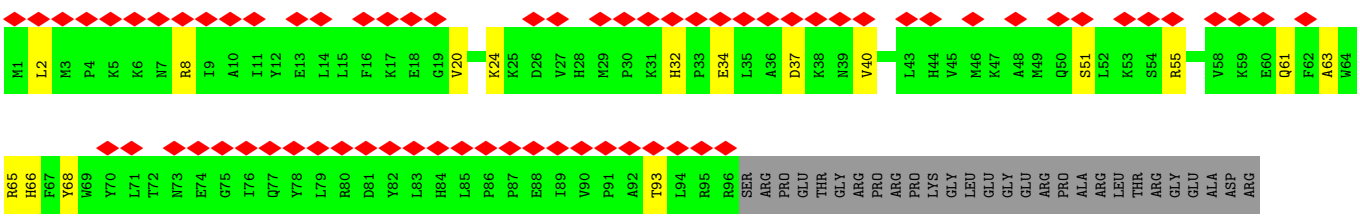
• Molecule 21: Ribosomal protein S9 (Predicted)





• Molecule 22: Ribosomal protein eS10

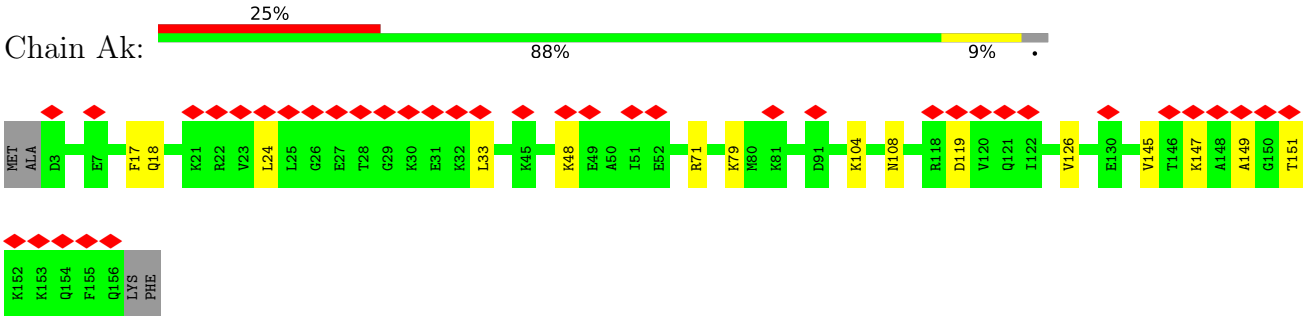






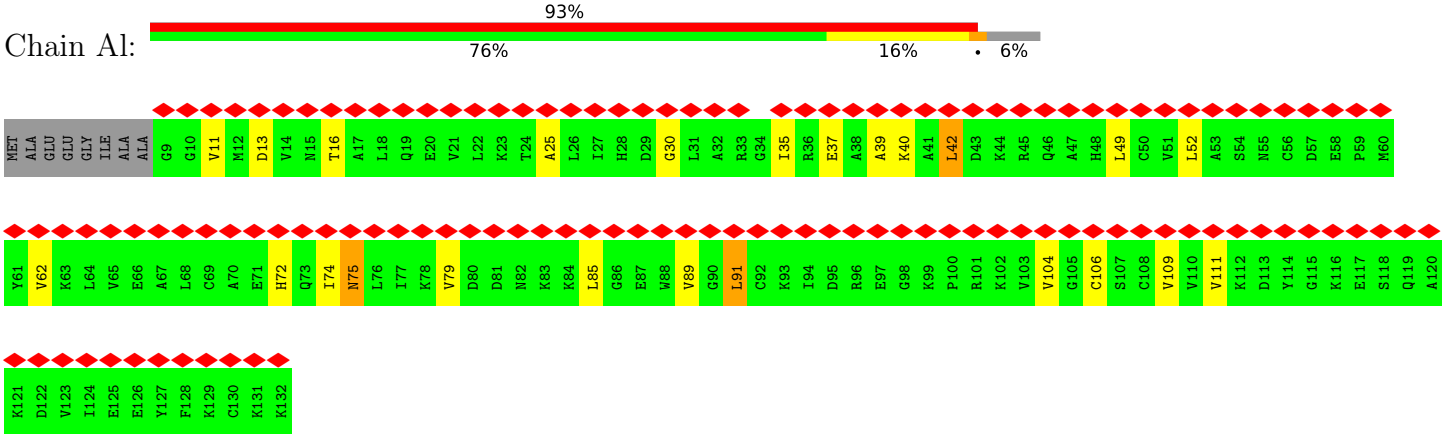
• Molecule 23: 40S ribosomal protein S11

Chain Ak:



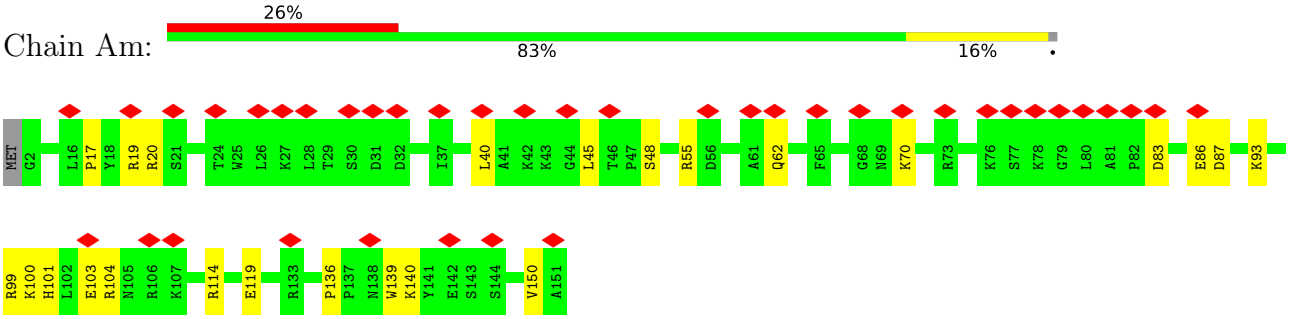
• Molecule 24: 40S ribosomal protein S12

Chain Al:



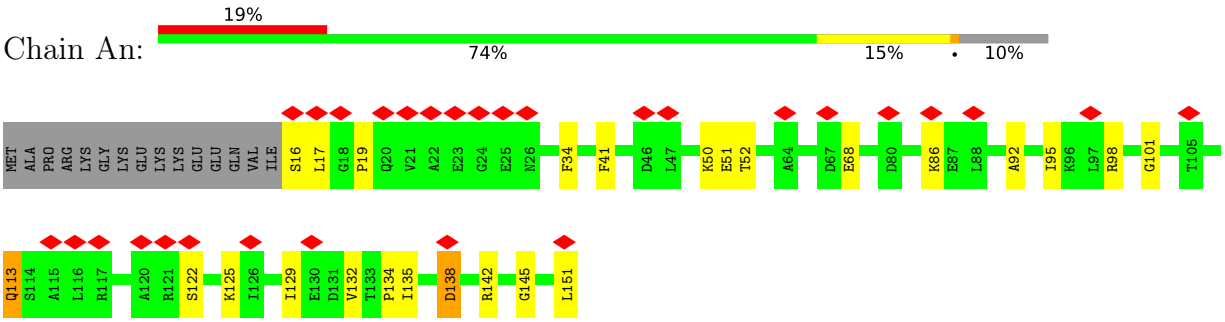
• Molecule 25: uS15

Chain Am:



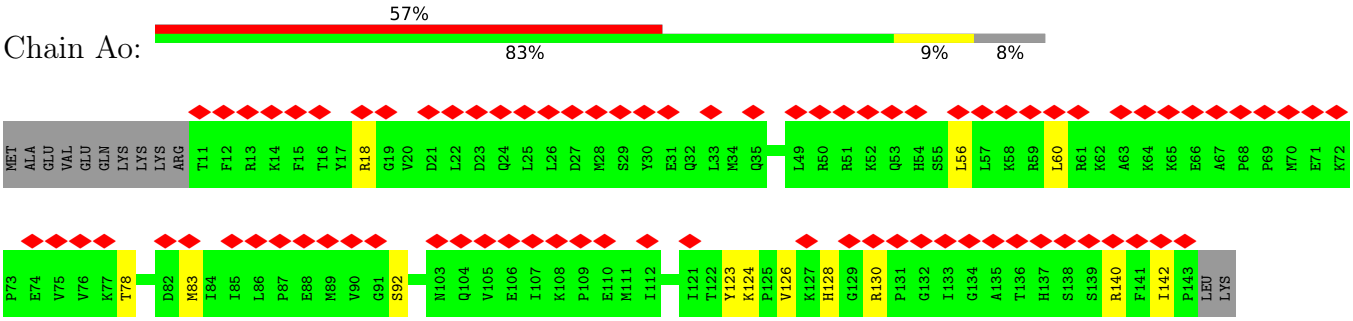
• Molecule 26: 40S ribosomal protein uS11

Chain An:



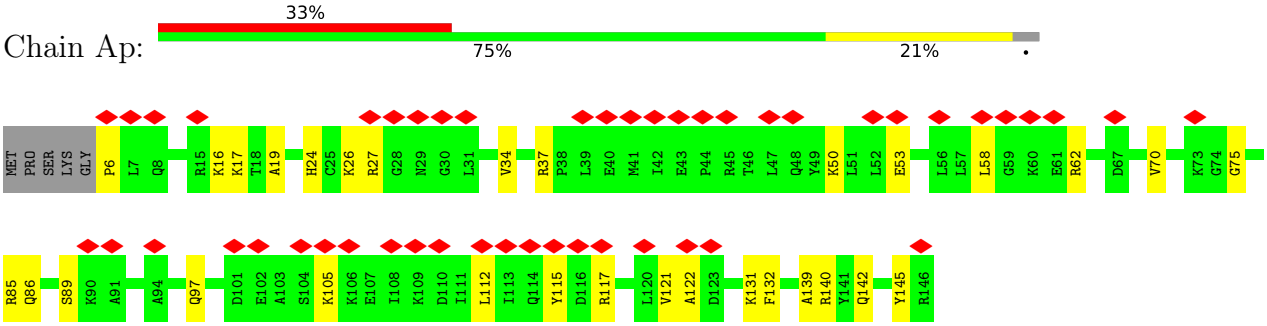
• Molecule 27: 40S ribosomal protein uS19

Chain Ao:



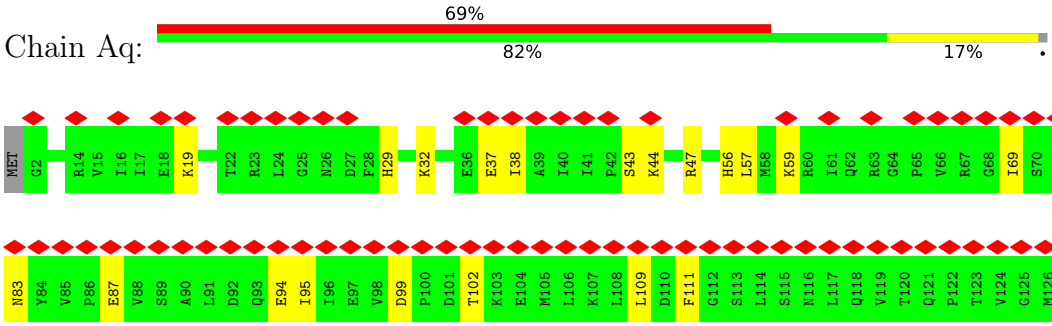
• Molecule 28: Ribosomal protein S16

Chain Ap:



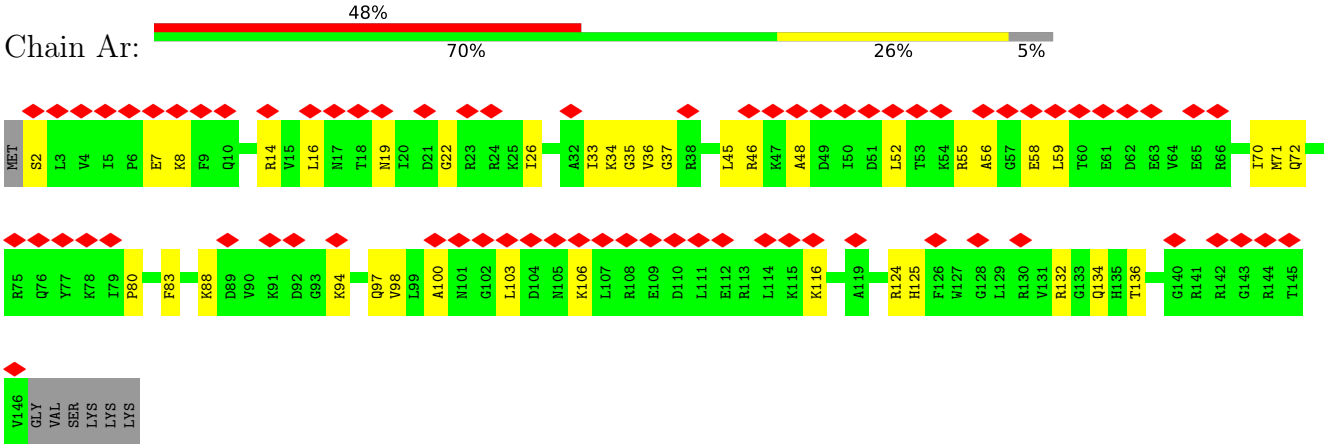
• Molecule 29: 40S ribosomal protein eS17

Chain Aq:



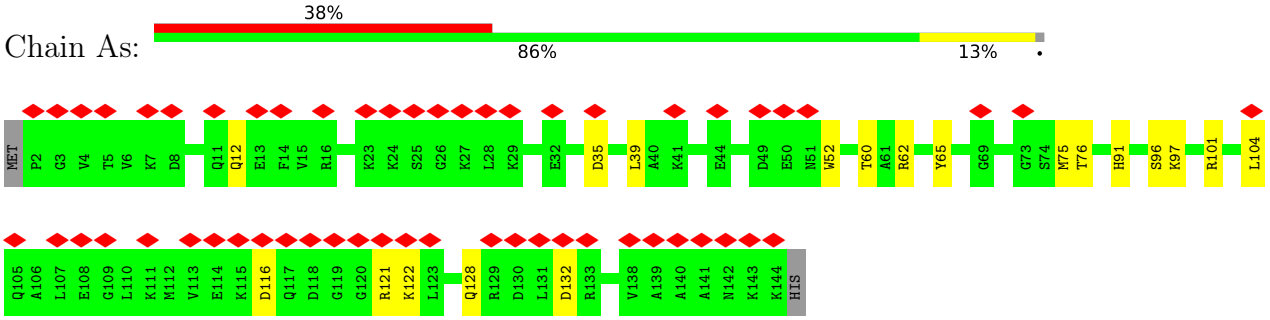
• Molecule 30: 40S ribosomal protein S18

Chain Ar:



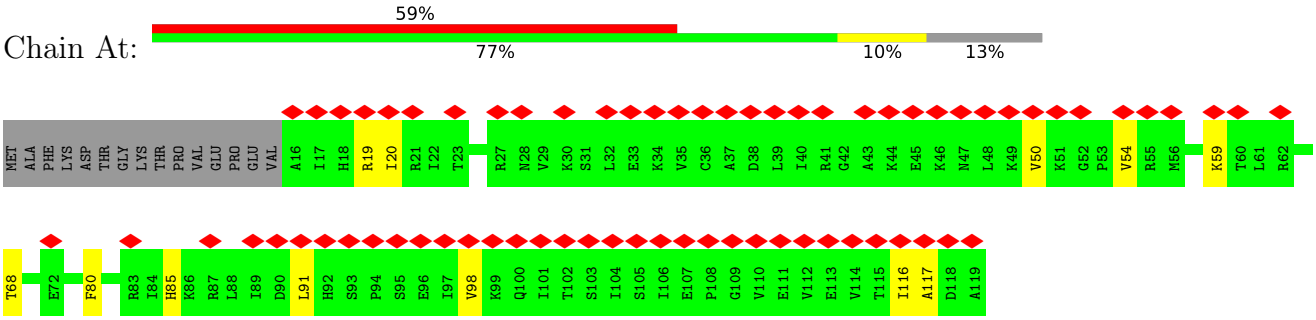
• Molecule 31: Ribosomal protein eS19

Chain As:



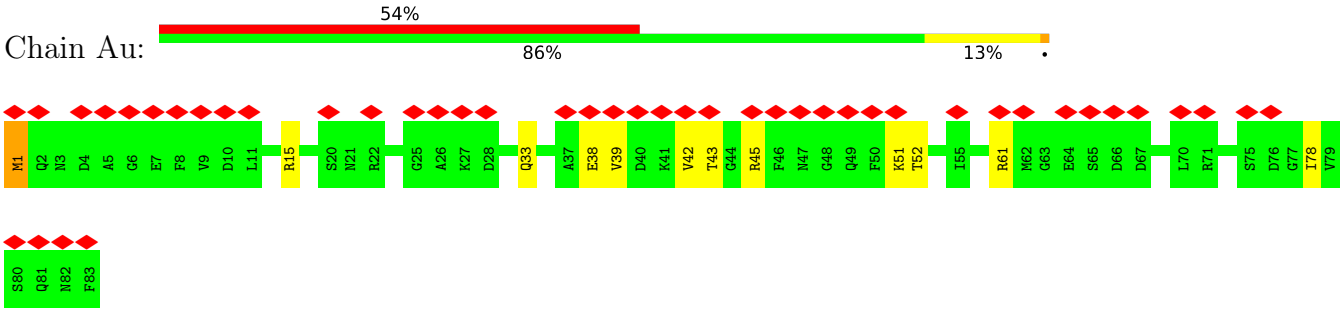
• Molecule 32: 40S ribosomal protein uS10

Chain At:



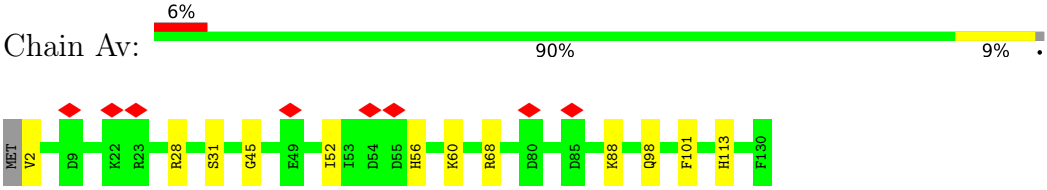
• Molecule 33: Ribosomal protein eS21

Chain Au:



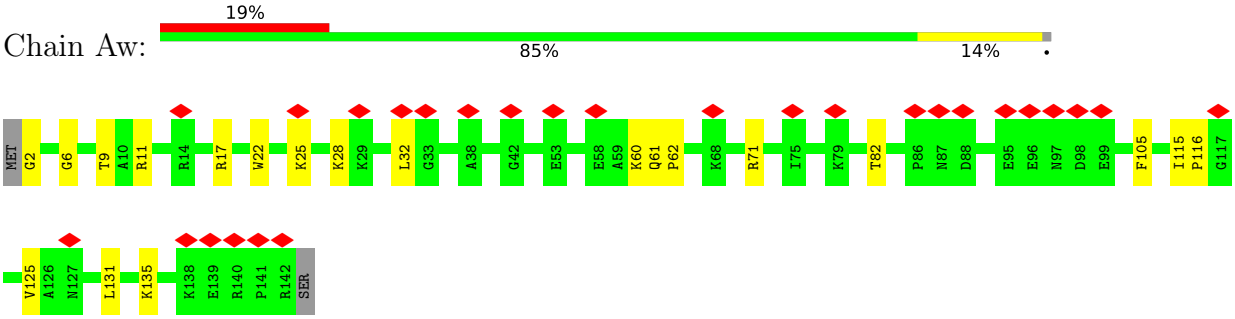
• Molecule 34: Ribosomal protein S15a

Chain Av:



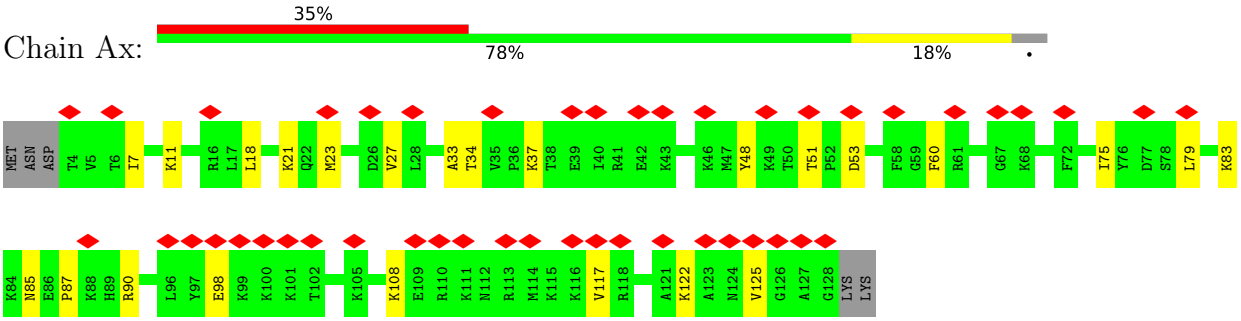
• Molecule 35: 40S ribosomal protein S23

Chain Aw:



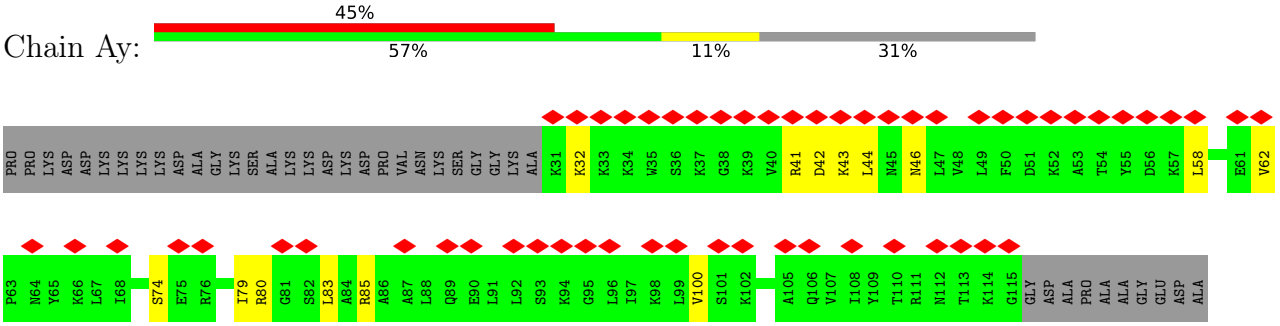
• Molecule 36: 40S ribosomal protein S24

Chain Ax:



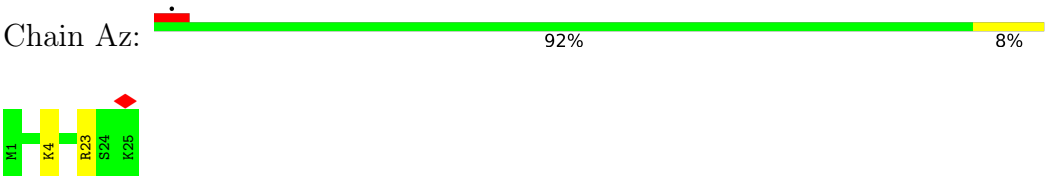
• Molecule 37: 40S ribosomal protein S25

Chain Ay:



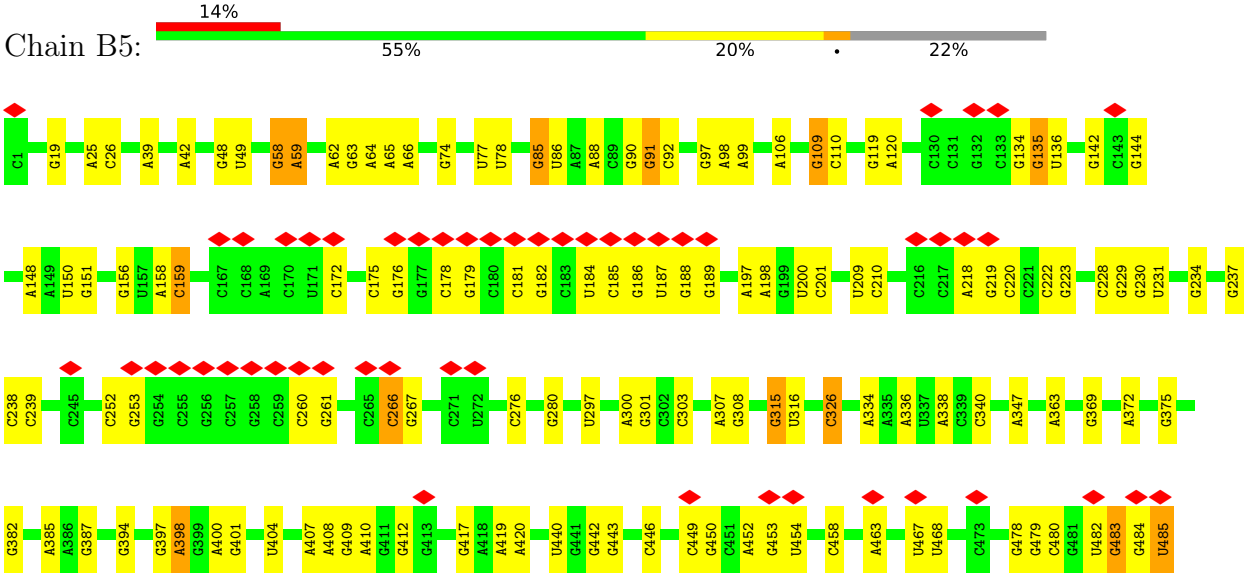
• Molecule 38: 60s ribosomal protein l41

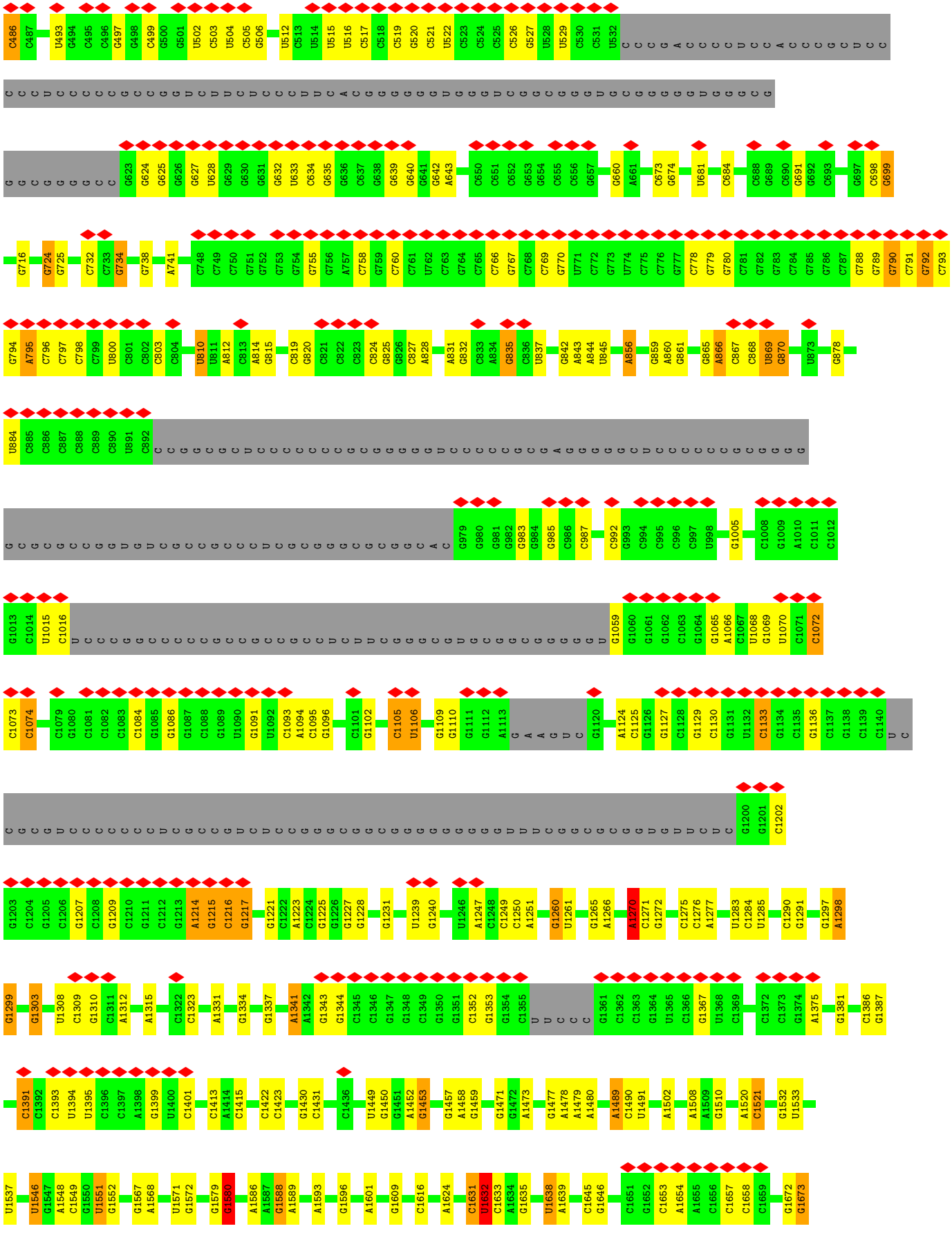
Chain Az:

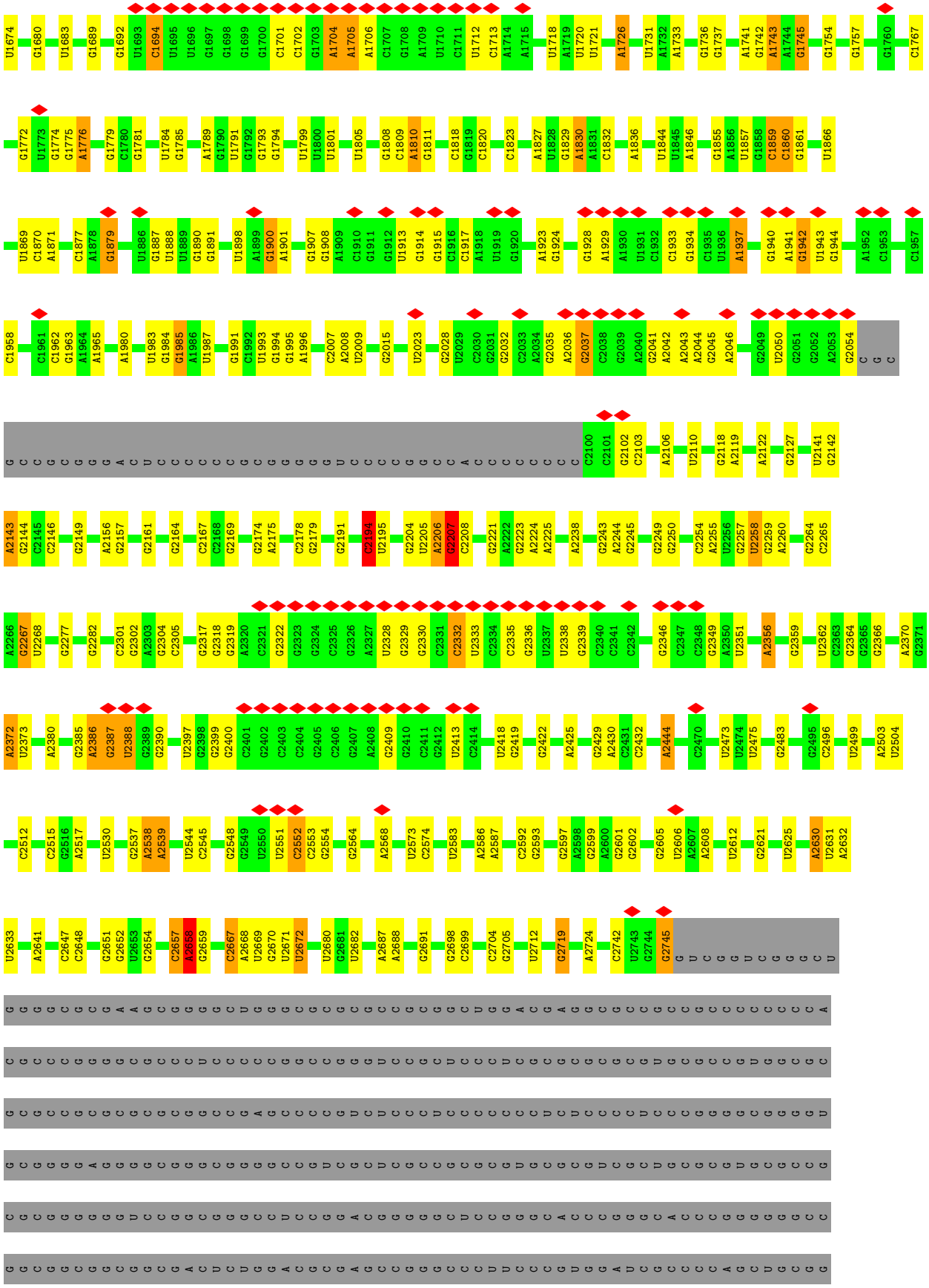


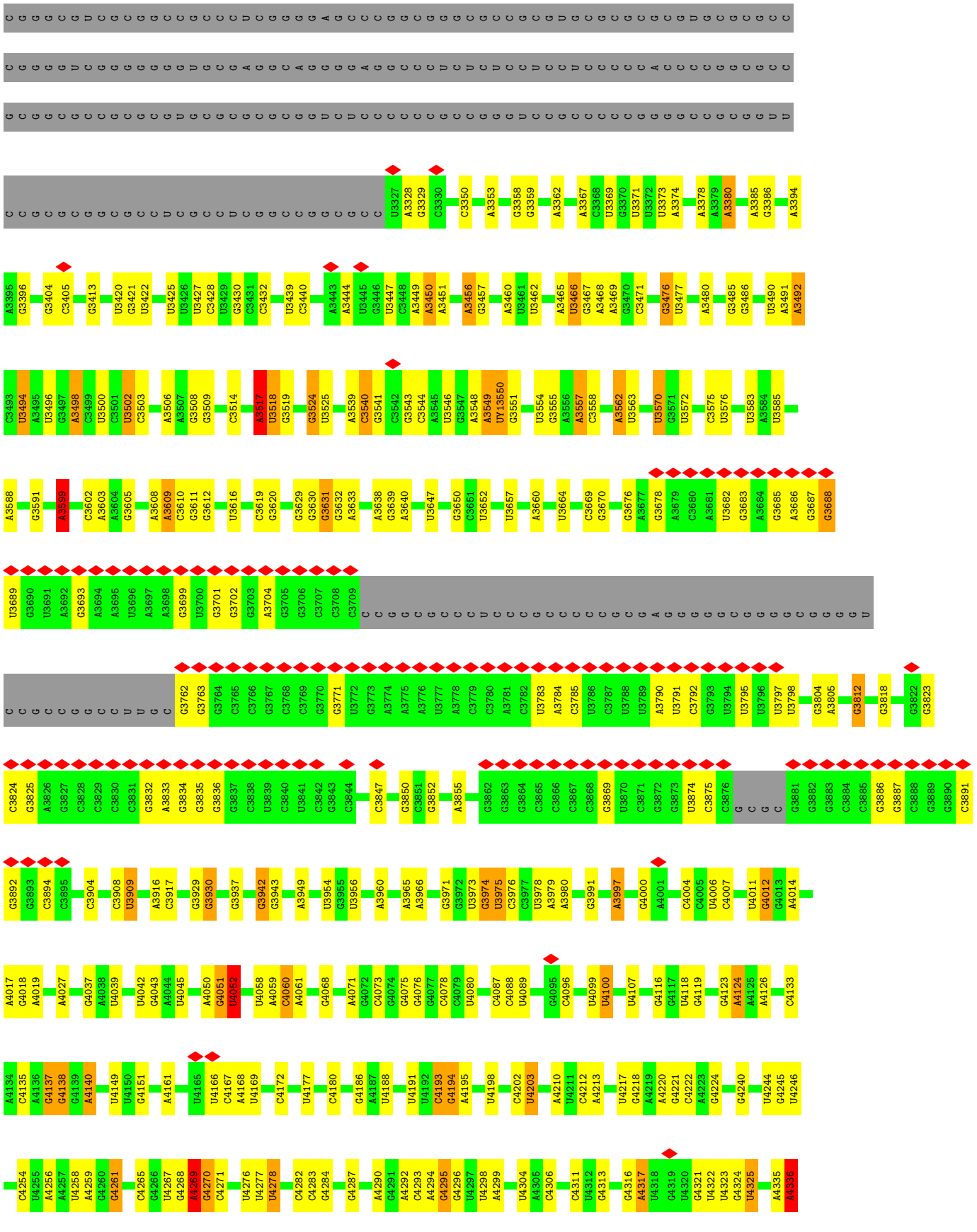
• Molecule 39: 28S rRNA

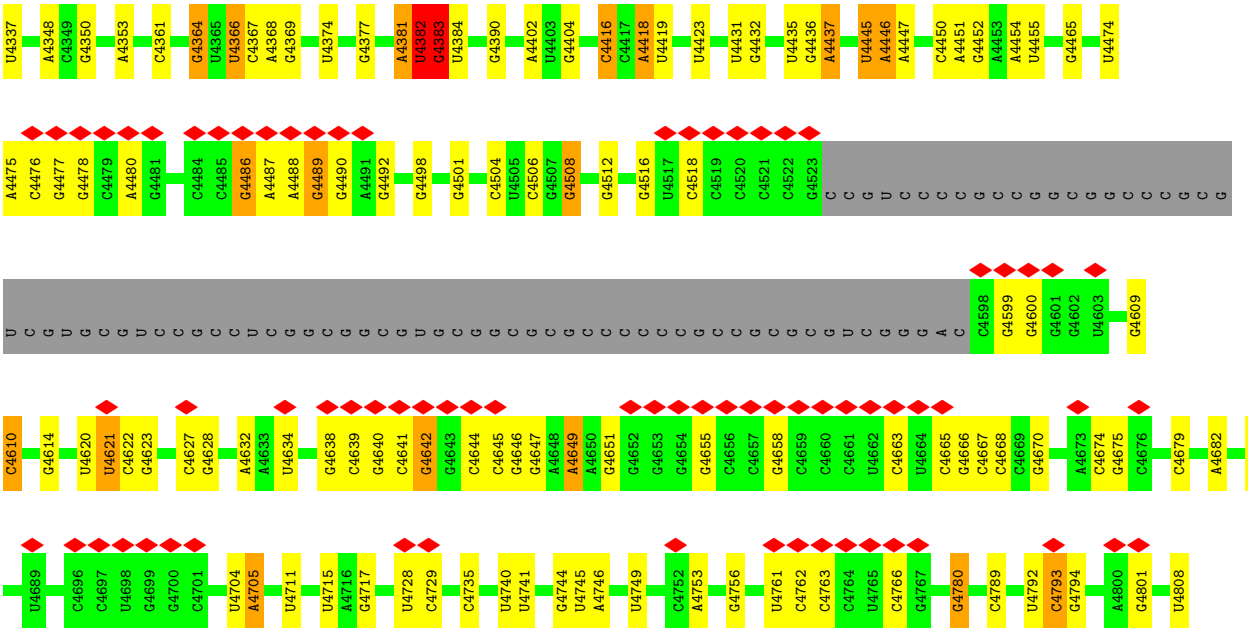
Chain B5:






U1674 G1680 U1683 G1689 G1692 U1693 C1694 U1695 U1696 G1697 G1698 G1699 G1700 C1701 C1702 G1703 A1704 A1705 A1706 C1707 G1708 A1709 U1710 C1711 U1712 C1713 A1714 A1715 U1718 A1719 U1720 U1721 A1726 U1731 A1732 A1733 G1736 G1737 A1741 G1742 A1743 A1744 G1745 G1754 G1757 G1760 C1767
G1772 U1773 G1774 G1775 A1776 G1779 C1780 G1781 U1784 G1785 A1789 G1790 U1791 G1792 G1793 G1794 U1799 U1800 U1801 U1805 G1808 C1809 A1810 G1811 C1818 G1819 C1820 C1823 A1827 U1828 G1829 A1830 A1831 C1832 A1836 U1844 U1845 A1846 G1855 A1856 U1857 G1858 C1859 C1860 G1861 U1866
U1869 C1870 A1871 C1877 A1878 G1879 U1886 G1887 U1888 U1889 G1890 G1891 U1898 A1899 G1900 A1901 G1907 G1908 A1909 C1910 G1911 G1912 U1913 G1914 G1915 C1916 C1917 A1918 U1919 G1920 A1923 G1924 G1928 A1929 A1930 U1931 C1932 C1933 G1934 C1935 U1936 A1937 G1940 A1941 G1942 U1943 G1944 A1952 C1953 C1957
C1958 C1961 C1962 G1963 A1964 A1965 A1980 U1983 G1984 G1985 A1986 U1987 G1991 C1992 U1993 G1994 G1995 A1996 C2007 A2008 U2009 G2015 U2023 G2028 U2029 C2030 G2031 G2032 C2033 A2034 G2035 A2036 G2037 C2038 G2039 A2040 G2041 A2042 A2043 A2044 G2045 A2046 G2049 U2050 G2051 G2052 A2053 G2054 C G C
G C C G C G G G A C U C C C C C G C C G G G G G U C C C C C

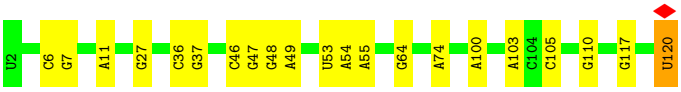




• Molecule 40: 5S rRNA

Chain B7:

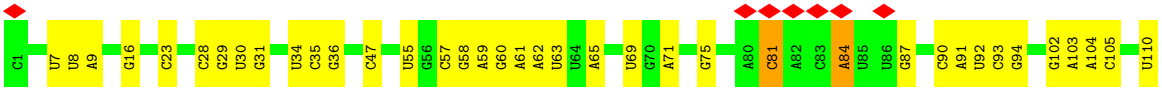


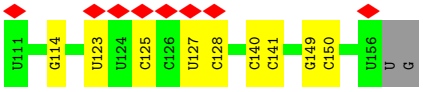


• Molecule 41: 5.8S rRNA

Chain B8:



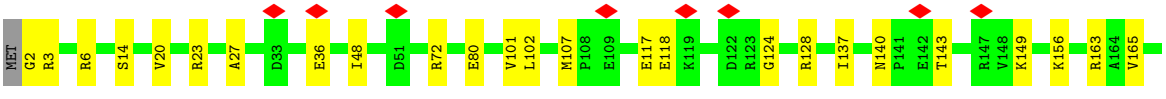




• Molecule 42: Ribosomal protein uL2

Chain BA:

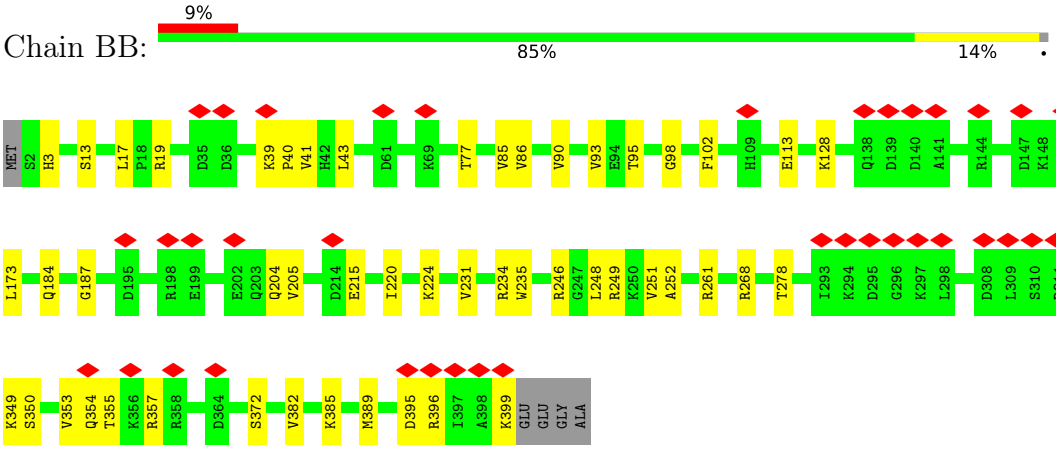






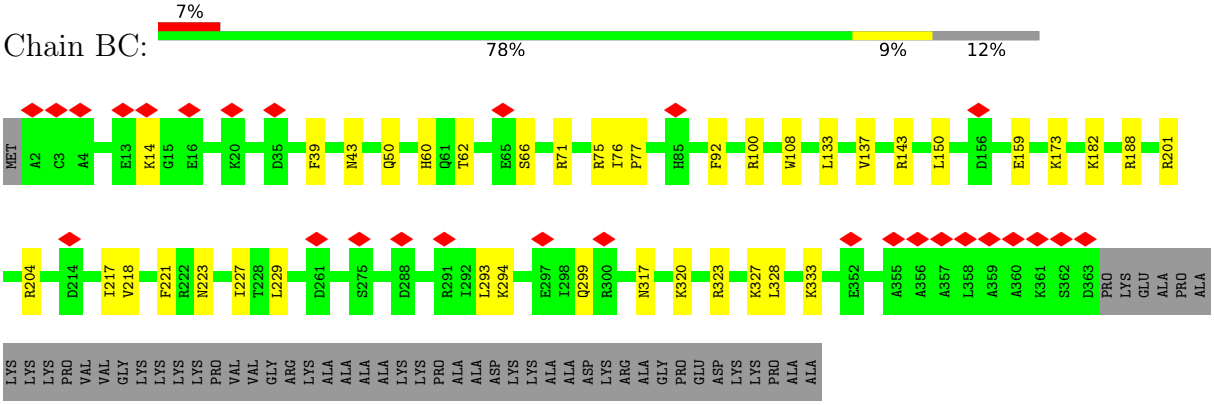
• Molecule 43: Ribosomal protein L3

Chain BB:



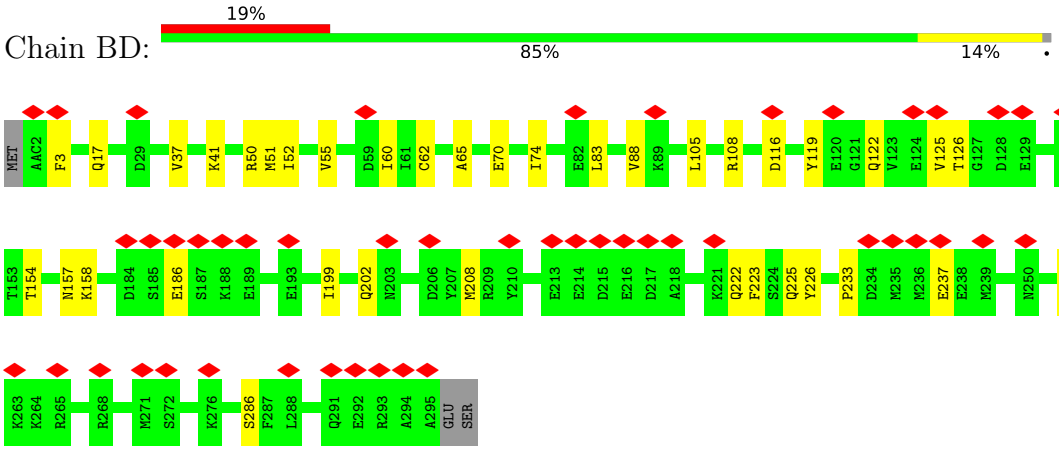
• Molecule 44: 60S ribosomal protein L4

Chain BC:



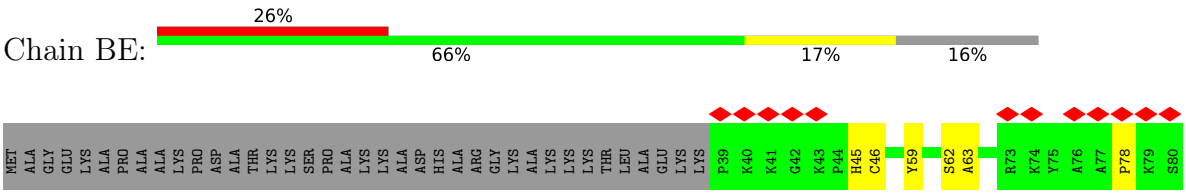
• Molecule 45: Ribosomal_L18_c domain-containing protein

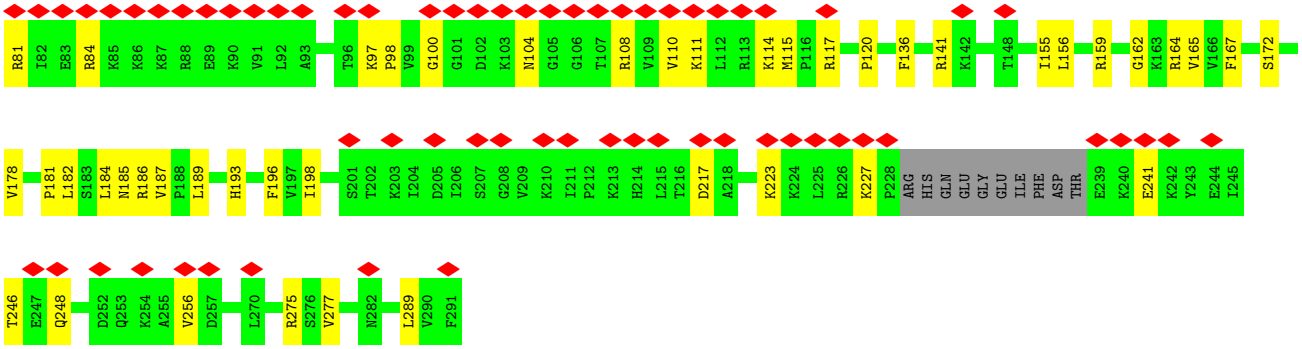
Chain BD:



• Molecule 46: 60S ribosomal protein L6

Chain BE:

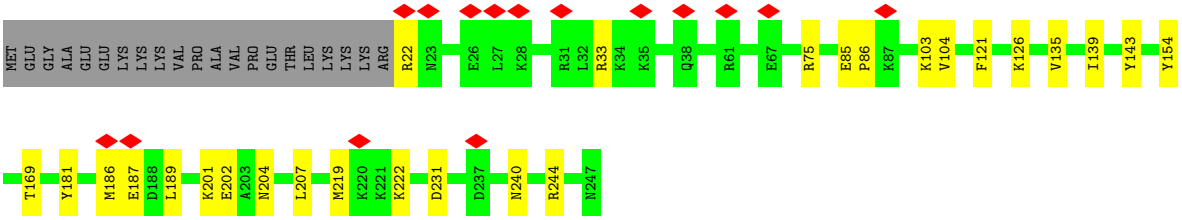




• Molecule 47: Ribosomal Protein uL30

Chain BF:

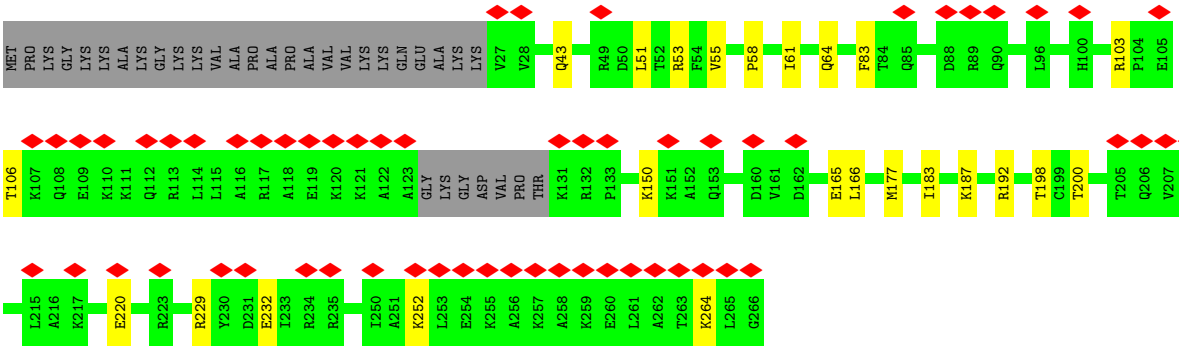




• Molecule 48: Ribosomal protein eL8

Chain BG:

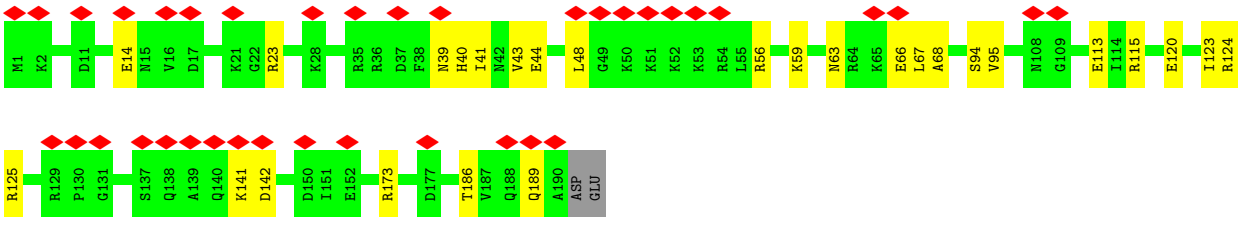




• Molecule 49: 60S ribosomal protein L9

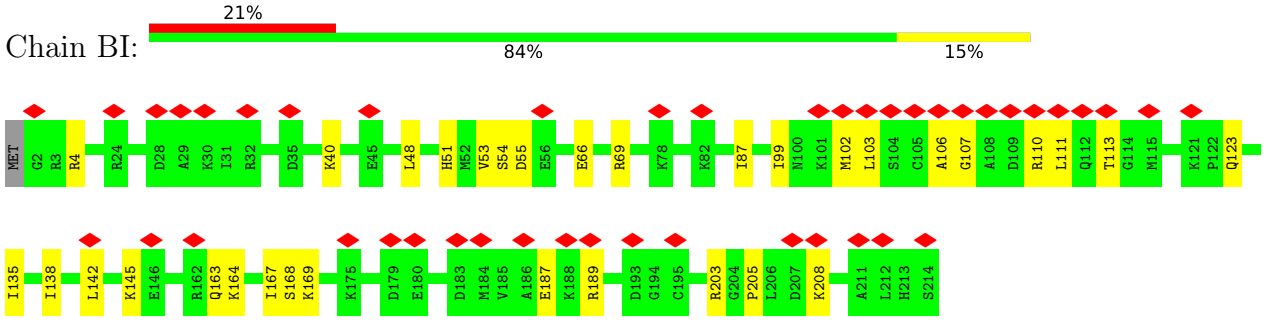
Chain BH:





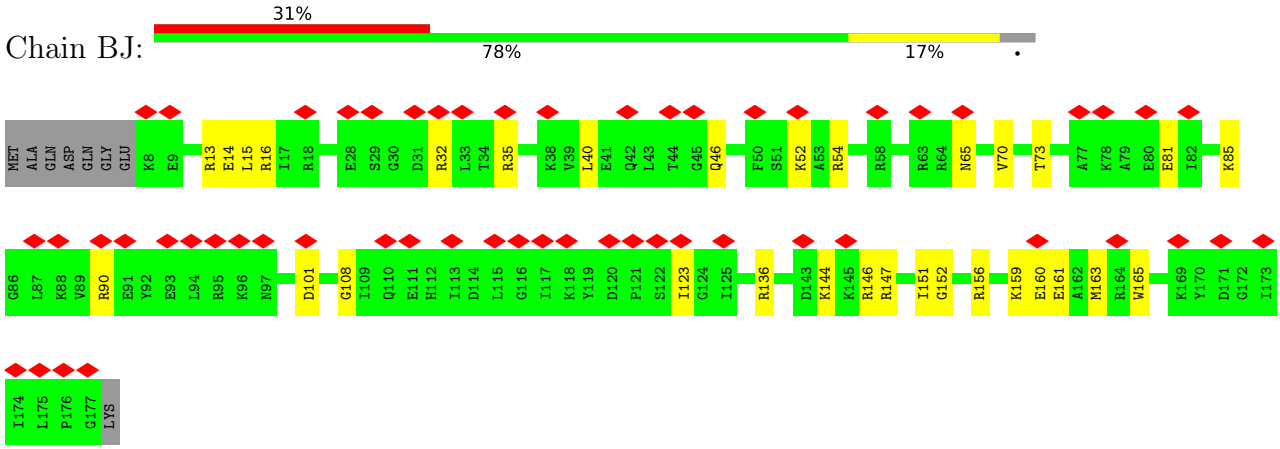
• Molecule 50: 60S ribosomal protein L10

Chain BI:



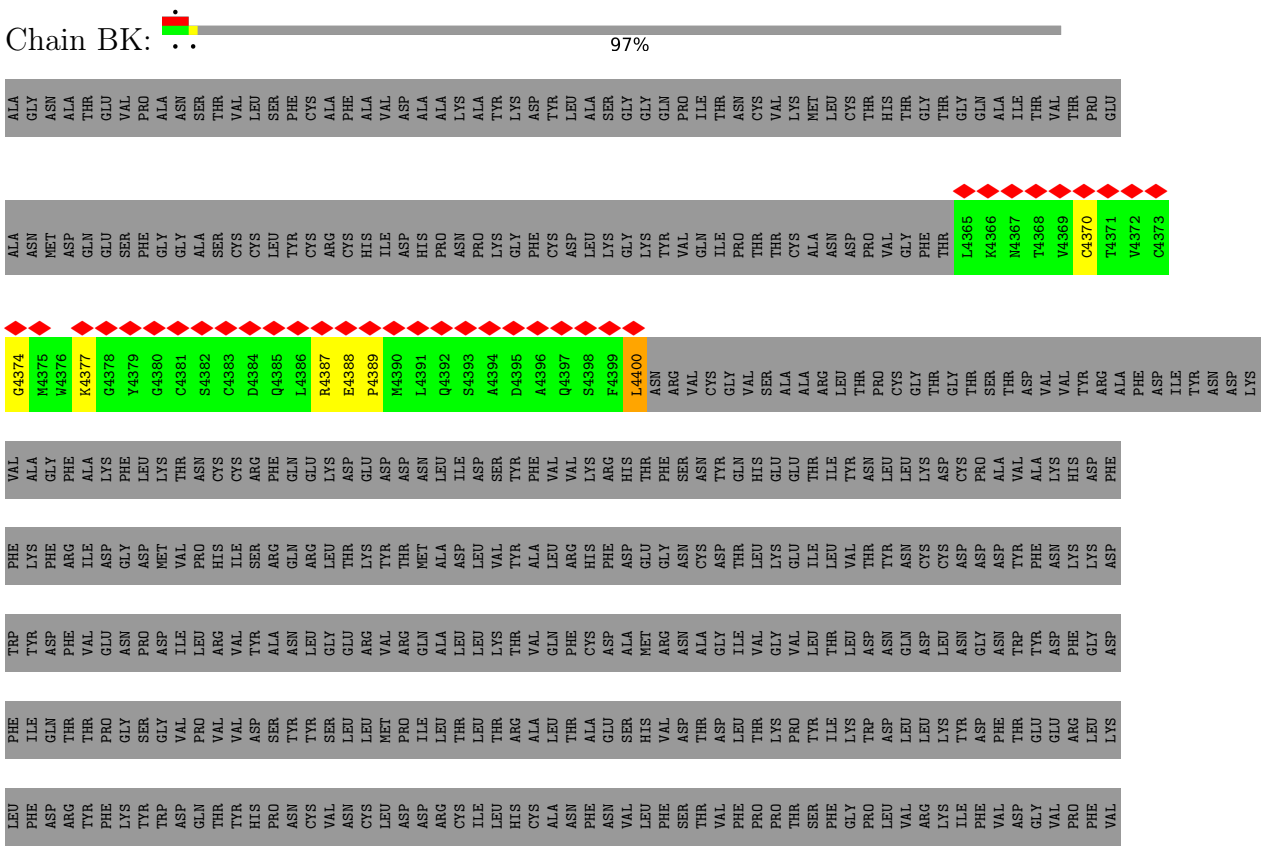
• Molecule 51: Ribosomal protein L11

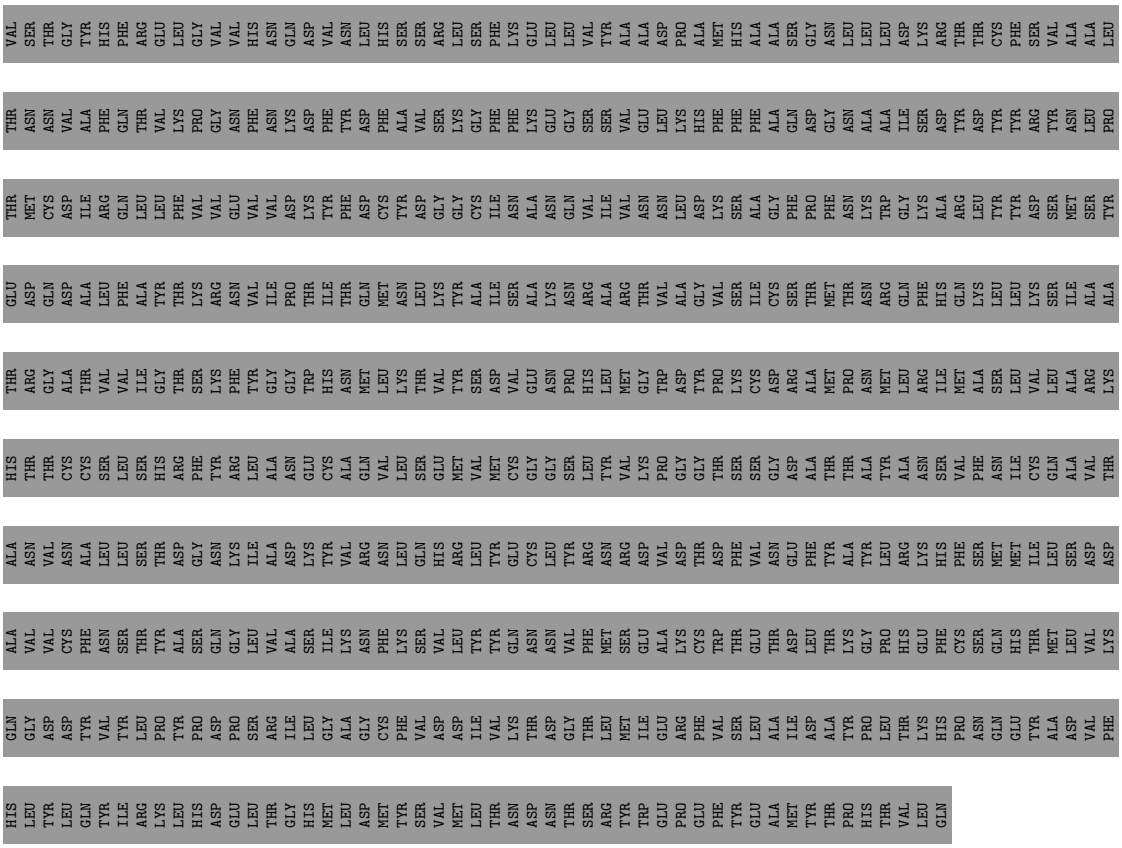
Chain BJ:



• Molecule 52: Replicase polyprotein 1ab

Chain BK:

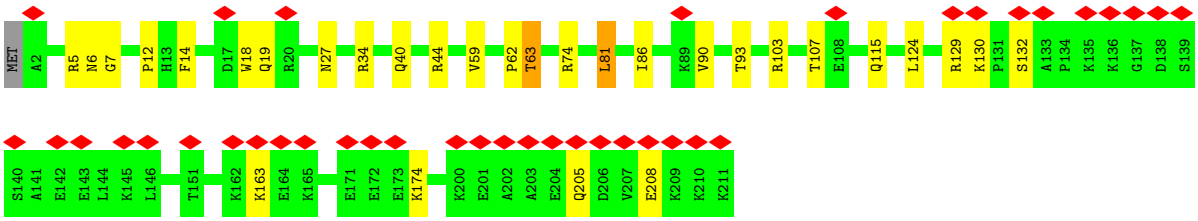




- Molecule 53: Ribosomal protein eL13

Chain BL:

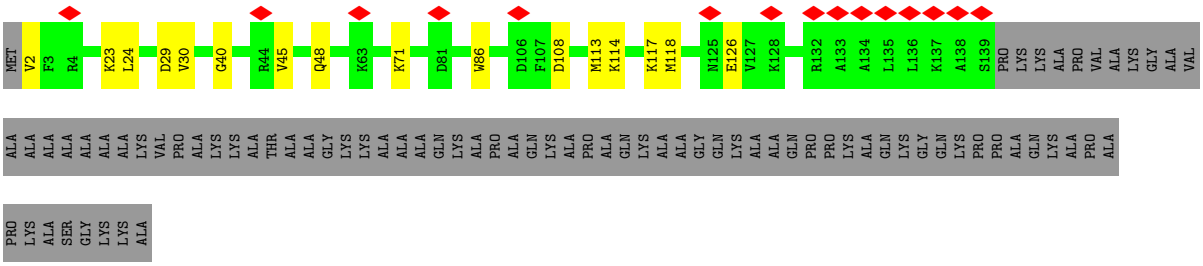




- Molecule 54: Ribosomal protein L14

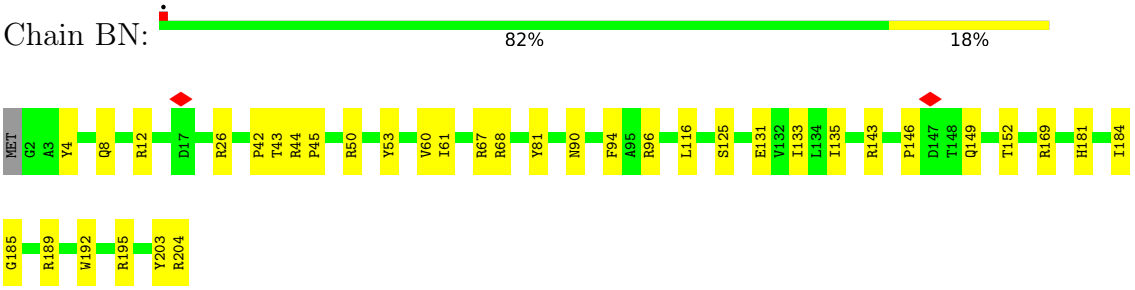
Chain BM:





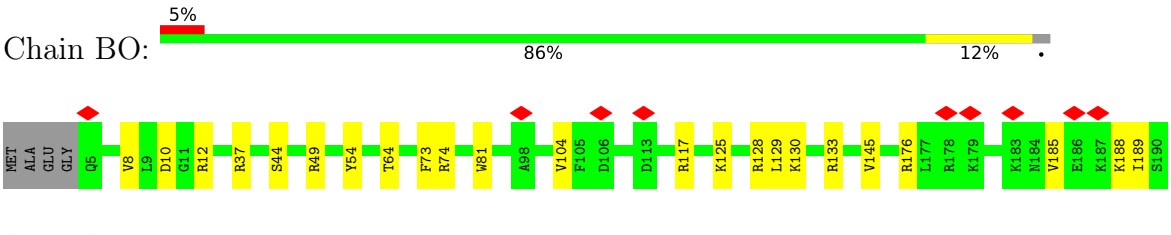
- Molecule 55: Ribosomal protein L15

Chain BN:



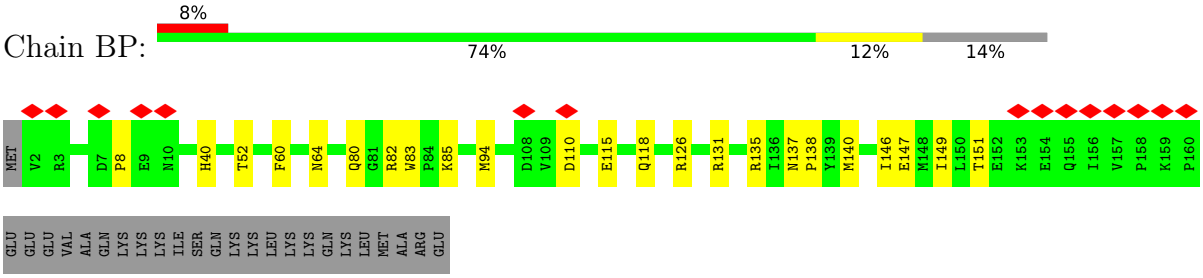
• Molecule 56: Ribosomal protein L13a

Chain BO:



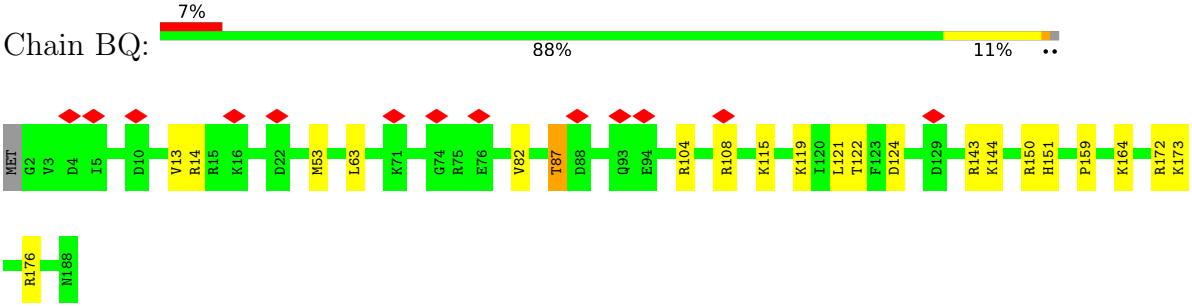
• Molecule 57: uL22

Chain BP:



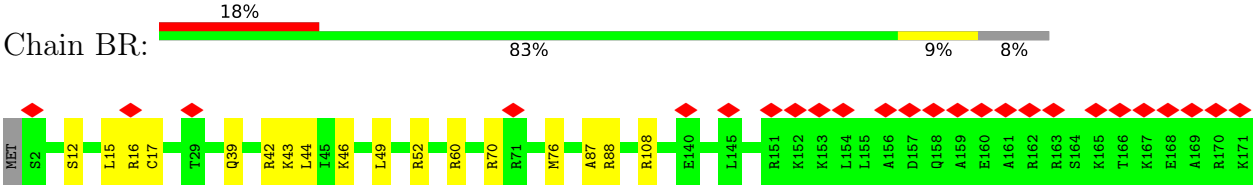
• Molecule 58: Ribosomal protein L18

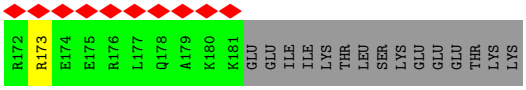
Chain BQ:



• Molecule 59: 60S ribosomal protein L19

Chain BR:

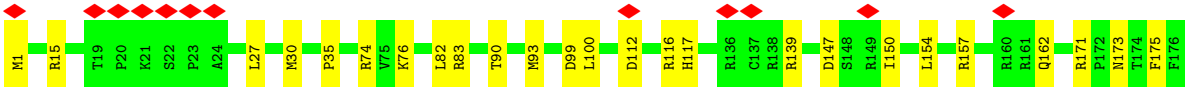




• Molecule 60: Ribosomal protein L18a

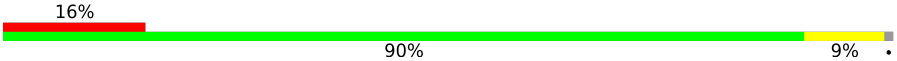
Chain BS:

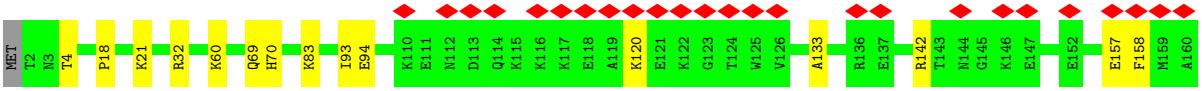




• Molecule 61: eL21

Chain BT:

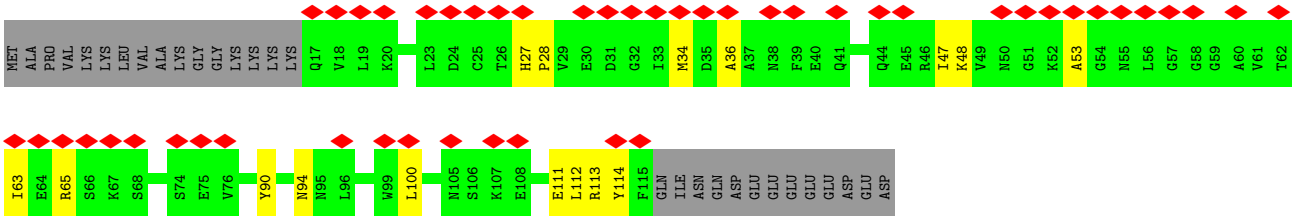




• Molecule 62: Ribosomal protein eL22

Chain BU:

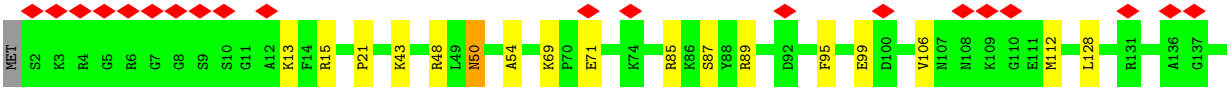




• Molecule 63: Ribosomal protein L23

Chain BV:

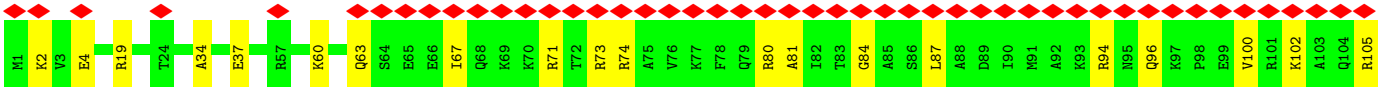


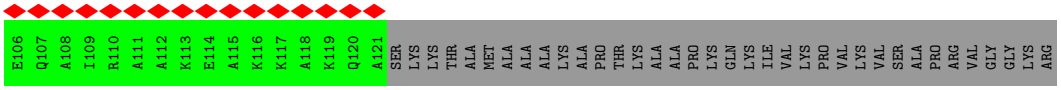


• Molecule 64: eL24

Chain BW:



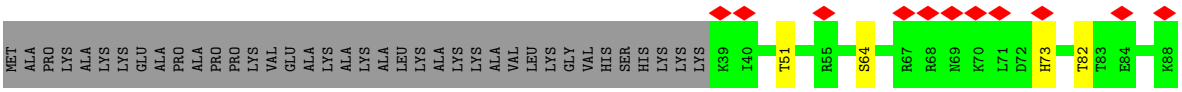


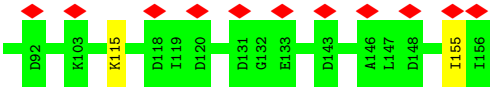


• Molecule 65: uL23

Chain BX:



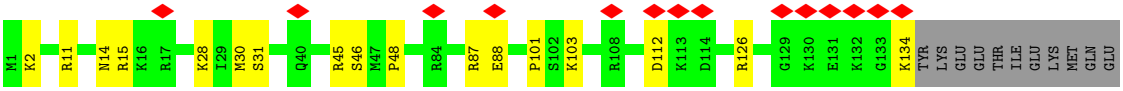




• Molecule 66: Ribosomal protein L26

Chain BY:

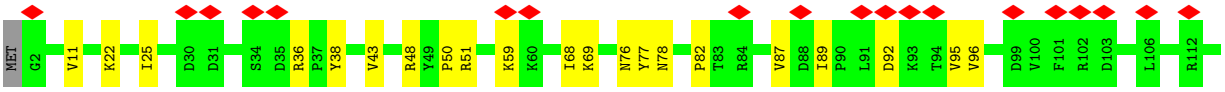


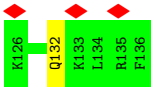


• Molecule 67: 60S ribosomal protein L27

Chain BZ:



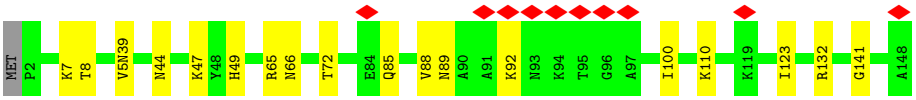




• Molecule 68: 60S ribosomal protein L27a

Chain Ba:

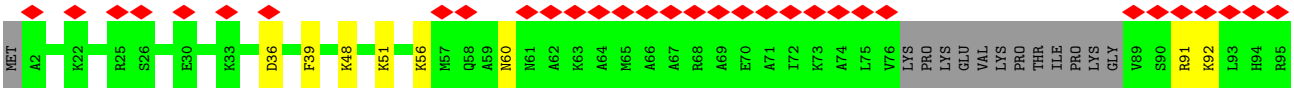


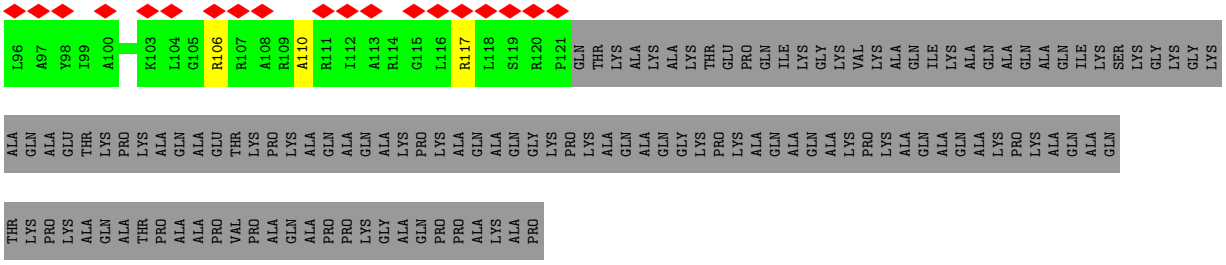


• Molecule 69: 60S ribosomal protein L29

Chain Bb:



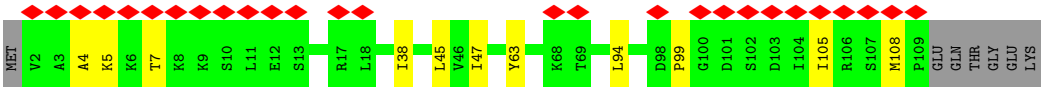




- Molecule 70: eL30

Chain Bc:

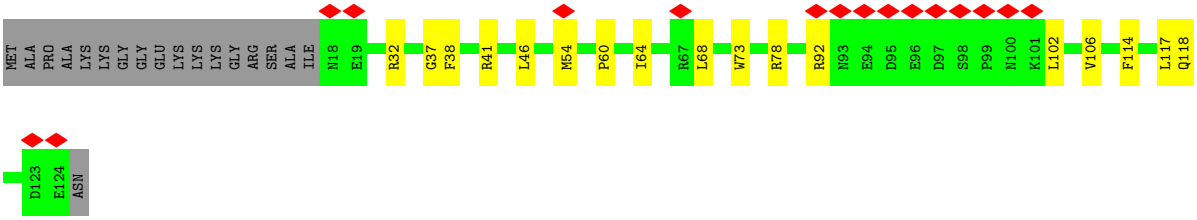




- Molecule 71: eL31

Chain Bd:

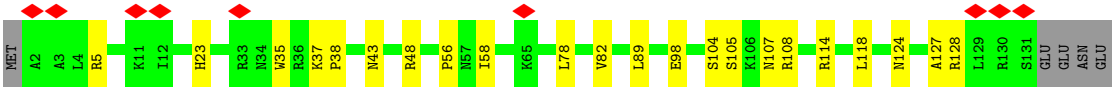




- Molecule 72: eL32

Chain Be:

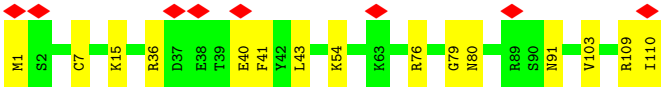




- Molecule 73: eL33

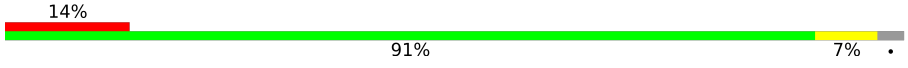
Chain Bf:

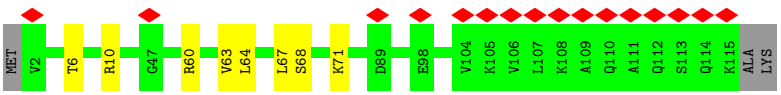




- Molecule 74: 60S ribosomal protein L34

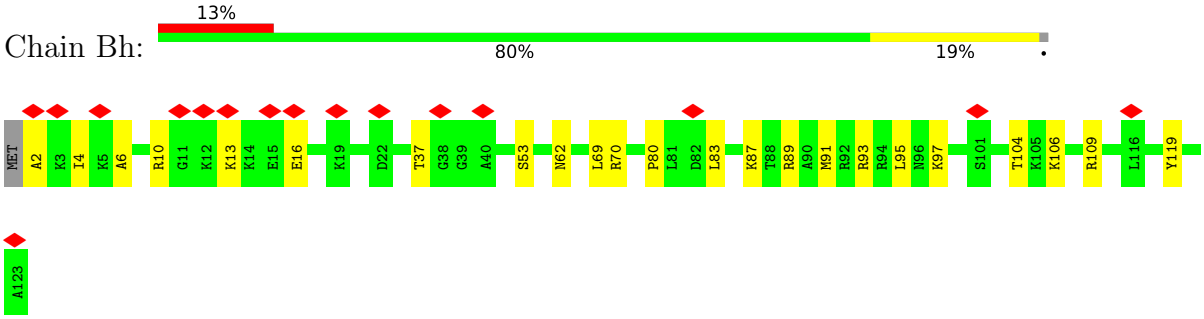
Chain Bg:





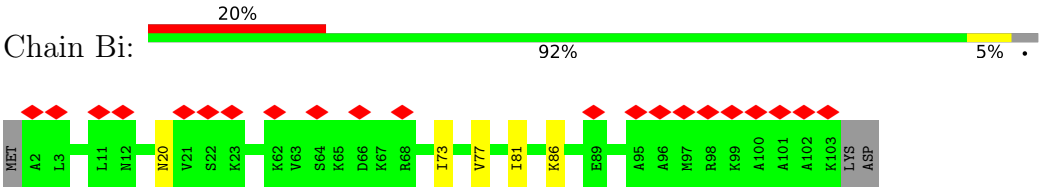
- Molecule 75: uL29

Chain Bh:



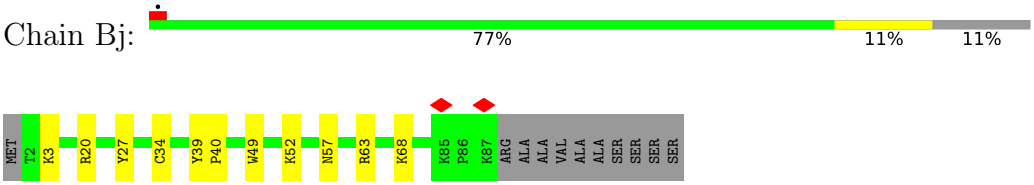
• Molecule 76: 60S ribosomal protein L36

Chain Bi:



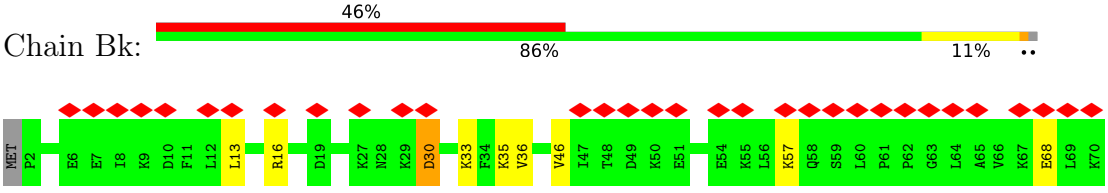
• Molecule 77: Ribosomal protein L37

Chain Bj:



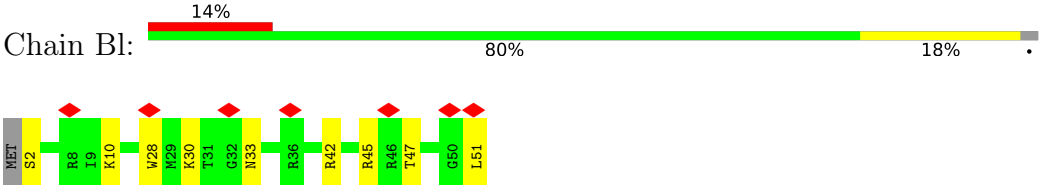
• Molecule 78: eL38

Chain Bk:



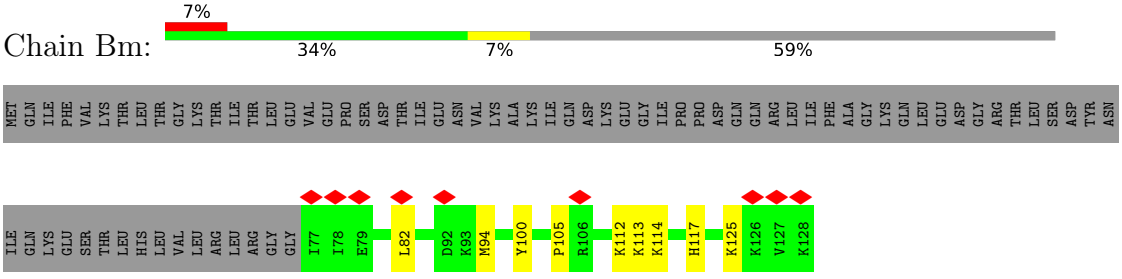
• Molecule 79: eL39

Chain Bl:



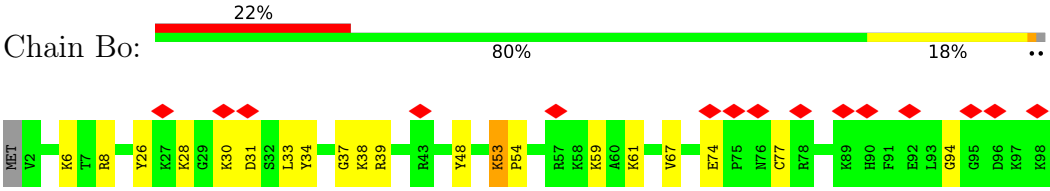
• Molecule 80: 60S ribosomal protein L40

Chain Bm:



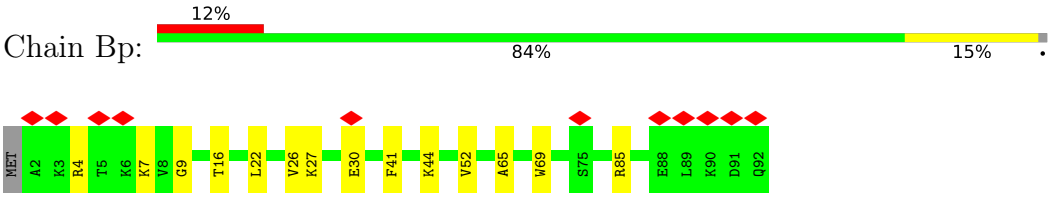
• Molecule 81: eL42

Chain Bo:



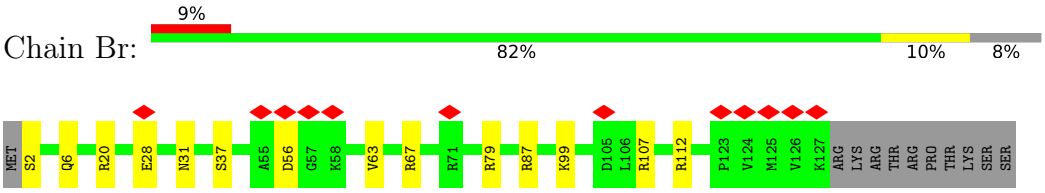
• Molecule 82: eL43

Chain Bp:



• Molecule 83: Ribosomal protein eL28

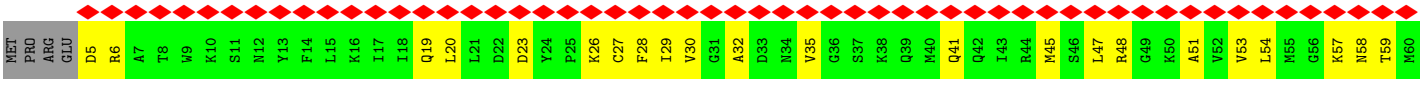
Chain Br:

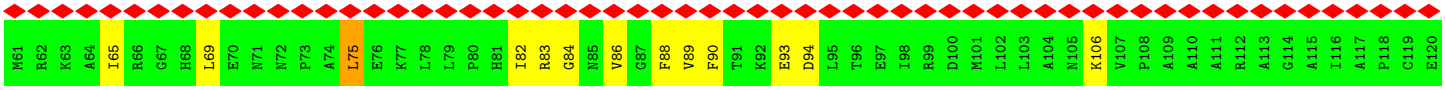


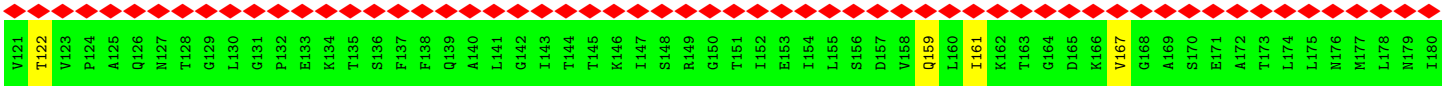
• Molecule 84: 60S acidic ribosomal protein P0

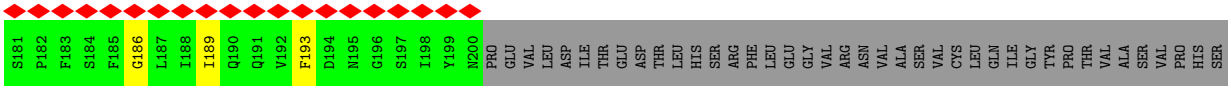
Chain Bs:











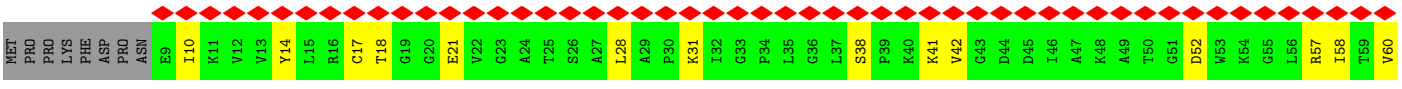


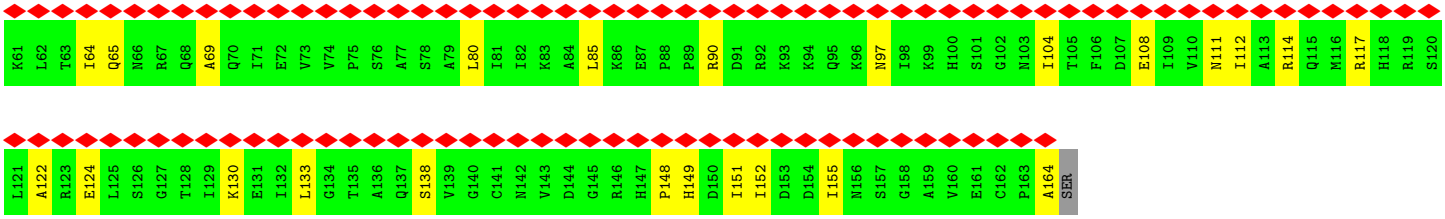


• Molecule 85: Ribosomal protein L12

Chain Bt:

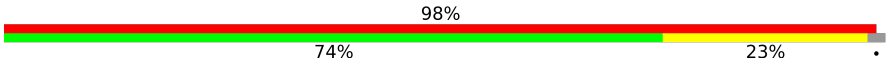


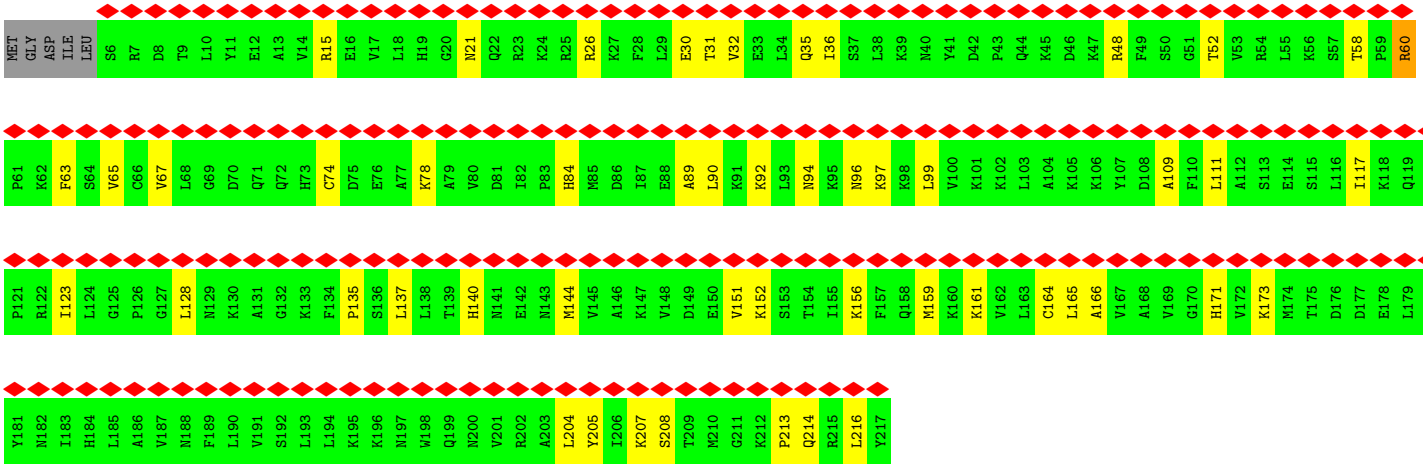




• Molecule 86: Ribosomal protein

Chain Bv:

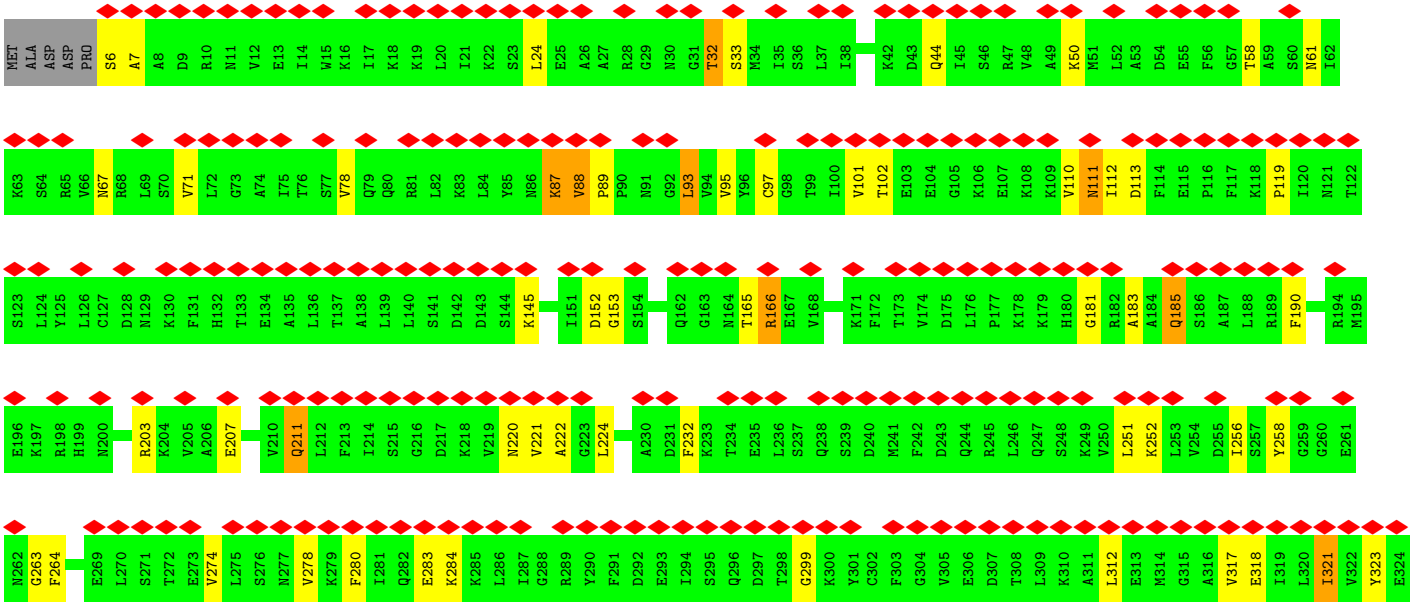


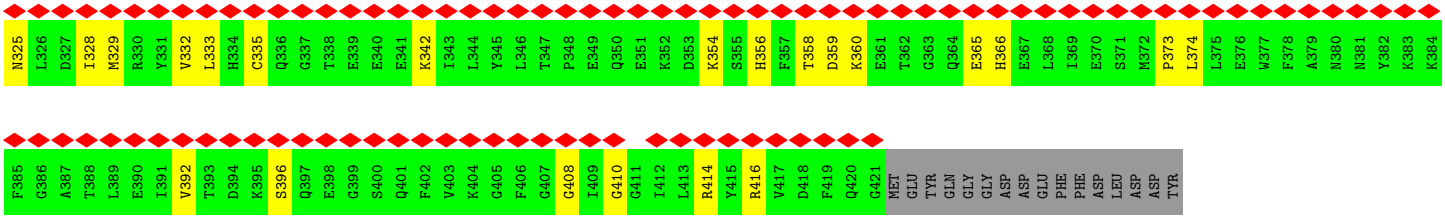


• Molecule 87: Eukaryotic peptide chain release factor subunit 1

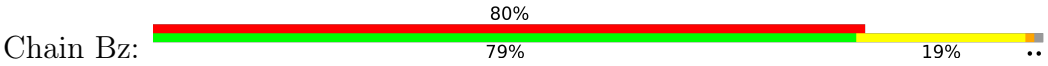
Chain By:

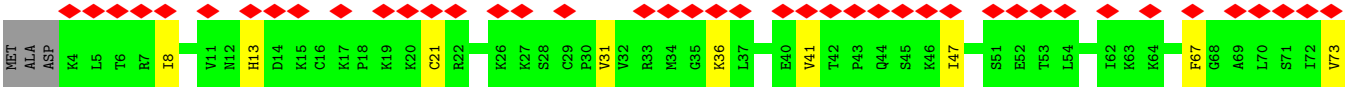


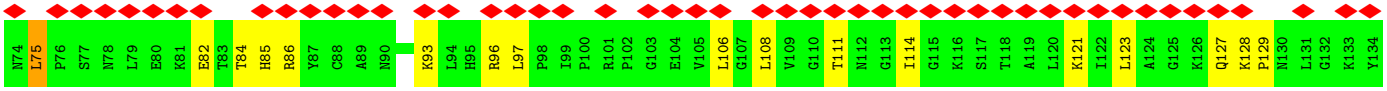




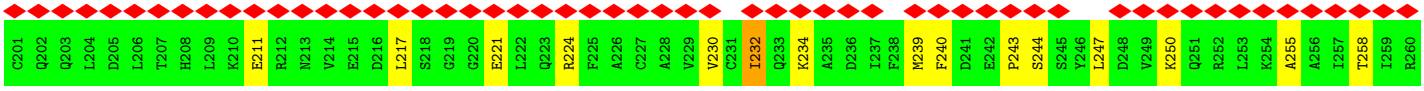
• Molecule 88: ATP binding cassette subfamily E member 1

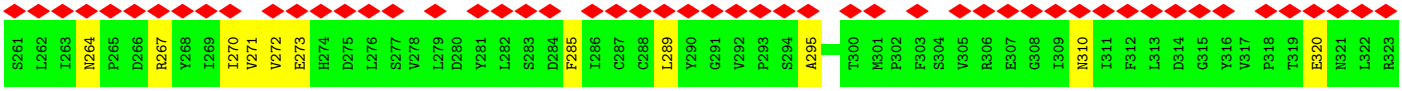


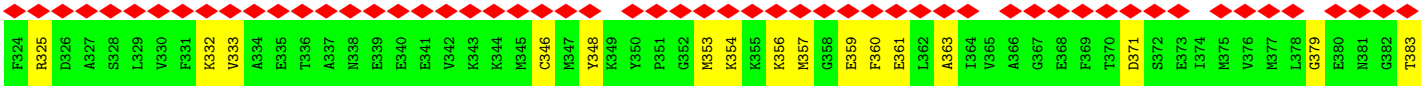


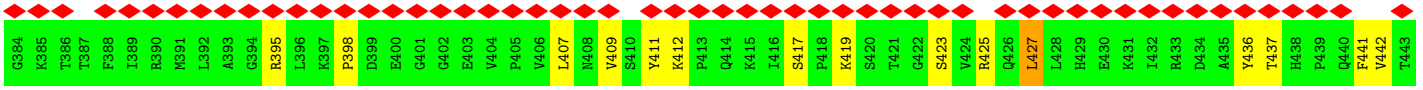


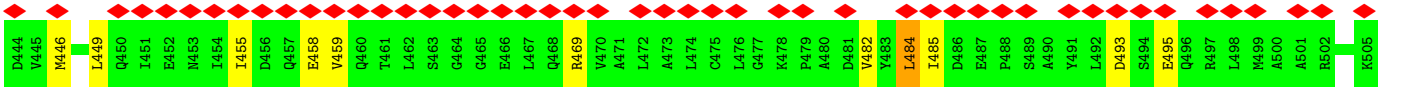


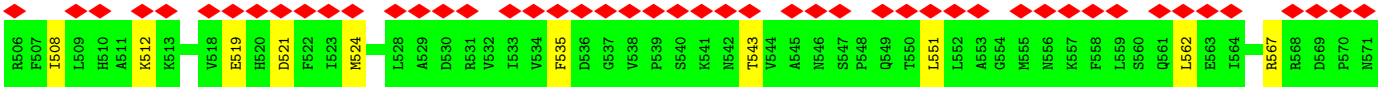


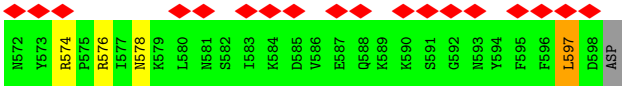












4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55057	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	56604	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.379	Depositor
Minimum map value	-1.818	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.131	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	593.6, 593.6, 593.6	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: G7M, SPD, A2M, 1MA, B8N, MG, OMU, SF4, AAC, GTP, AME, ZN, 5MU, PSU, V5N, 5MC, 4AC, UNX, UR3, OMG, AYA, MLZ, MA6, M3L, NMM, SAC, 6MZ, HY3, OMC, UY1, HIC

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	A2	0.14	1/40342 (0.0%)	0.14	0/62877
2	AA	0.08	0/665	0.22	0/891
3	AB	0.08	0/497	0.19	0/666
4	AC	0.08	0/613	0.25	0/811
5	AD	0.08	0/462	0.21	0/607
6	AE	0.09	0/828	0.23	0/1109
7	AF	0.08	0/2493	0.23	0/3394
8	AG	0.08	0/470	0.22	0/623
9	AH	0.06	0/566	0.11	0/879
10	AI	0.09	0/68	0.17	0/103
11	AT	0.07	0/2011	0.14	0/3133
12	AZ	0.08	0/1771	0.21	0/2406
13	Aa	0.08	0/1841	0.20	0/2459
14	Ab	0.09	0/1742	0.23	0/2354
15	Ac	0.08	0/1779	0.21	0/2395
16	Ad	0.08	0/2118	0.22	0/2849
17	Ae	0.08	0/1531	0.24	0/2059
18	Af	0.08	0/1946	0.21	0/2590
19	Ag	0.09	0/1552	0.23	0/2079
20	Ah	0.08	0/1715	0.21	0/2287
21	Ai	0.08	0/1550	0.21	0/2069
22	Aj	0.08	0/834	0.25	0/1125
23	Ak	0.09	0/1284	0.22	0/1717
24	Al	0.08	0/968	0.22	0/1296
25	Am	0.08	0/1232	0.21	0/1656
26	An	0.09	0/1029	0.23	0/1380
27	Ao	0.09	0/1114	0.20	0/1490
28	Ap	0.09	0/1142	0.26	0/1528
29	Aq	0.07	0/1094	0.20	0/1469
30	Ar	0.07	0/1209	0.21	0/1620
31	As	0.07	0/1119	0.18	0/1498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	At	0.09	0/831	0.23	0/1115
33	Au	0.08	0/636	0.21	0/852
34	Av	0.10	0/1051	0.22	0/1406
35	Aw	0.09	0/1107	0.22	0/1475
36	Ax	0.07	0/1032	0.19	0/1371
37	Ay	0.09	0/691	0.20	0/922
38	Az	0.08	0/240	0.19	0/305
39	B5	0.12	2/87403 (0.0%)	0.15	0/136359
40	B7	0.08	0/2835	0.12	0/4418
41	B8	0.09	0/3635	0.13	0/5661
42	BA	0.11	0/1965	0.25	0/2633
43	BB	0.10	0/3261	0.23	0/4364
44	BC	0.10	0/2932	0.22	0/3939
45	BD	0.08	0/2437	0.20	0/3264
46	BE	0.09	0/1998	0.23	0/2673
47	BF	0.10	0/1922	0.24	0/2563
48	BG	0.09	0/1908	0.21	0/2566
49	BH	0.09	0/1535	0.22	0/2063
50	BI	0.10	0/1756	0.23	0/2346
51	BJ	0.08	0/1385	0.21	0/1852
52	BK	0.11	0/277	0.27	0/372
53	BL	0.10	0/1733	0.22	0/2316
54	BM	0.09	0/1158	0.22	0/1547
55	BN	0.10	0/1746	0.23	0/2338
56	BO	0.09	0/1662	0.22	0/2222
57	BP	0.10	0/1317	0.23	0/1768
58	BQ	0.10	0/1539	0.24	0/2054
59	BR	0.08	0/1524	0.19	0/2013
60	BS	0.10	0/1497	0.22	0/2008
61	BT	0.09	0/1326	0.20	0/1770
62	BU	0.08	0/820	0.22	0/1100
63	BV	0.10	0/1048	0.24	0/1402
64	BW	0.08	0/1006	0.21	0/1334
65	BX	0.08	0/984	0.21	0/1323
66	BY	0.09	0/1132	0.24	0/1504
67	BZ	0.08	0/1130	0.19	0/1507
68	Ba	0.10	0/1179	0.25	0/1572
69	Bb	0.09	0/884	0.22	0/1169
70	Bc	0.08	0/847	0.20	0/1134
71	Bd	0.10	0/903	0.21	0/1216
72	Be	0.10	0/1088	0.25	0/1451
73	Bf	0.11	0/903	0.24	0/1208
74	Bg	0.09	0/916	0.25	0/1220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	Bh	0.08	0/1021	0.18	0/1348
76	Bi	0.08	0/841	0.23	0/1112
77	Bj	0.11	0/720	0.27	0/952
78	Bk	0.08	0/575	0.20	0/761
79	Bl	0.09	0/459	0.21	0/608
80	Bm	0.08	0/426	0.21	0/564
81	Bo	0.09	0/866	0.20	0/1141
82	Bp	0.10	0/718	0.24	0/953
83	Br	0.09	0/1020	0.23	0/1366
84	Bs	0.08	0/1530	0.22	0/2064
85	Bt	0.09	0/1193	0.24	0/1609
86	Bv	0.09	0/1735	0.25	0/2328
87	By	0.09	0/3333	0.24	0/4483
88	Bz	0.10	0/4755	0.26	0/6421
All	All	0.11	3/243956 (0.0%)	0.18	0/356824

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
81	Bo	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	4761	U	C4-O4	5.13	1.33	1.23
39	B5	3456	A2M	O3'-P	5.02	1.61	1.56
1	A2	1032	A2M	O3'-P	5.01	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
81	Bo	53	MLZ	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A2	37833	0	19168	335	0
2	AA	651	0	672	9	0
3	AB	495	0	523	5	0
4	AC	601	0	621	6	0
5	AD	457	0	502	7	0
6	AE	814	0	863	9	0
7	AF	2436	0	2393	38	0
8	AG	459	0	448	11	0
9	AH	508	0	255	4	0
10	AI	939	0	618	5	0
11	AT	1840	0	930	24	0
12	AZ	1743	0	1748	31	0
13	Aa	1815	0	1908	21	0
14	Ab	1706	0	1796	19	0
15	Ac	1751	0	1846	25	0
16	Ad	2076	0	2177	31	0
17	Ae	1509	0	1563	25	0
18	Af	1923	0	2089	40	0
19	Ag	1529	0	1627	23	0
20	Ah	1686	0	1772	26	0
21	Ai	1525	0	1640	24	0
22	Aj	810	0	836	11	0
23	Ak	1262	0	1335	11	0
24	Al	958	0	993	15	0
25	Am	1208	0	1294	17	0
26	An	1016	0	1039	19	0
27	Ao	1091	0	1138	12	0
28	Ap	1124	0	1193	20	0
29	Aq	1080	0	1135	16	0
30	Ar	1200	0	1262	23	0
31	As	1113	0	1145	17	0
32	At	821	0	883	7	0
33	Au	640	0	633	9	0
34	Av	1034	0	1080	11	0
35	Aw	1099	0	1162	13	0
36	Ax	1015	0	1086	16	0
37	Ay	683	0	761	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Az	239	0	289	3	0
39	B5	80772	0	40878	557	0
40	B7	2538	0	1283	15	0
41	B8	3319	0	1684	25	0
42	BA	1940	0	2029	28	0
43	BB	3206	0	3353	37	0
44	BC	2886	0	3057	29	0
45	BD	2398	0	2430	33	0
46	BE	1960	0	2153	31	0
47	BF	1886	0	2008	22	0
48	BG	1877	0	2023	16	0
49	BH	1516	0	1597	17	0
50	BI	1717	0	1764	21	0
51	BJ	1362	0	1399	20	0
52	BK	273	0	265	5	0
53	BL	1702	0	1820	22	0
54	BM	1137	0	1211	12	0
55	BN	1701	0	1749	31	0
56	BO	1630	0	1778	18	0
57	BP	1289	0	1329	16	0
58	BQ	1515	0	1634	15	0
59	BR	1508	0	1664	14	0
60	BS	1457	0	1492	14	0
61	BT	1298	0	1366	15	0
62	BU	806	0	827	9	0
63	BV	1034	0	1097	14	0
64	BW	991	0	1048	17	0
65	BX	967	0	1040	5	0
66	BY	1115	0	1205	14	0
67	BZ	1107	0	1182	15	0
68	Ba	1163	0	1202	13	0
69	Bb	881	0	957	9	0
70	Bc	836	0	888	7	0
71	Bd	888	0	930	9	0
72	Be	1070	0	1165	17	0
73	Bf	884	0	924	12	0
74	Bg	906	0	998	6	0
75	Bh	1013	0	1147	20	0
76	Bi	830	0	916	3	0
77	Bj	705	0	737	8	0
78	Bk	569	0	637	6	0
79	Bl	447	0	479	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	Bm	432	0	470	8	0
81	Bo	863	0	929	15	0
82	Bp	708	0	756	13	0
83	Br	1014	0	1083	11	0
84	Bs	1507	0	1564	25	0
85	Bt	1178	0	1235	24	0
86	Bv	1707	0	1815	29	0
87	By	3280	0	3326	45	0
88	Bz	4668	0	4784	61	0
89	A2	10	0	19	1	0
90	A2	102	0	0	0	0
90	AH	1	0	0	0	0
90	AT	2	0	0	0	0
90	B5	235	0	0	0	0
90	B7	4	0	0	0	0
90	B8	6	0	0	0	0
90	BI	1	0	0	0	0
90	BP	1	0	0	0	0
90	BR	1	0	0	0	0
90	BV	1	0	0	0	0
90	Ba	1	0	0	0	0
91	A2	76	0	0	0	0
91	AT	4	0	0	0	0
91	Ab	1	0	0	0	0
91	Ak	1	0	0	0	0
91	Ar	1	0	0	0	0
91	B5	244	0	0	0	0
91	B7	10	0	0	0	0
91	B8	16	0	0	0	0
91	BA	2	0	0	0	0
91	BB	3	0	0	0	0
91	BC	1	0	0	0	0
91	BH	1	0	0	0	0
91	BI	1	0	0	0	0
91	BL	1	0	0	0	0
91	BN	2	0	0	0	0
91	BP	1	0	0	0	0
91	BQ	2	0	0	0	0
91	BT	1	0	0	0	0
91	Bb	1	0	0	0	0
91	Be	2	0	0	0	0
91	Bf	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
91	Bg	1	0	0	0	0
91	Bo	1	0	0	0	0
92	AC	1	0	0	0	0
92	AE	1	0	0	0	0
92	AG	1	0	0	0	0
92	Bg	1	0	0	0	0
92	Bj	1	0	0	0	0
92	Bm	1	0	0	0	0
92	Bo	1	0	0	0	0
92	Bp	1	0	0	0	0
93	B7	32	0	11	0	0
94	Bz	16	0	0	0	0
95	A2	473	0	0	8	0
95	AH	10	0	0	0	0
95	AT	12	0	0	1	0
95	Aa	2	0	0	1	0
95	Ab	1	0	0	0	0
95	Ad	1	0	0	0	0
95	Af	2	0	0	0	0
95	Ak	1	0	0	0	0
95	Am	1	0	0	0	0
95	An	2	0	0	1	0
95	Ap	4	0	0	1	0
95	Ar	1	0	0	0	0
95	As	4	0	0	0	0
95	Aw	4	0	0	0	0
95	B5	1117	0	0	17	0
95	B7	17	0	0	0	0
95	B8	31	0	0	0	0
95	BA	5	0	0	0	0
95	BB	7	0	0	0	0
95	BC	3	0	0	1	0
95	BD	1	0	0	0	0
95	BF	1	0	0	0	0
95	BH	1	0	0	0	0
95	BI	1	0	0	0	0
95	BL	1	0	0	0	0
95	BN	2	0	0	0	0
95	BO	3	0	0	0	0
95	BP	3	0	0	0	0
95	BR	5	0	0	1	0
95	BV	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
95	BX	1	0	0	0	0
95	BY	1	0	0	0	0
95	Ba	7	0	0	0	0
95	Bb	1	0	0	0	0
95	Bd	1	0	0	0	0
95	Be	4	0	0	0	0
95	Bf	1	0	0	1	0
95	By	1	0	0	0	0
All	All	235677	0	175760	1886	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1886 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1092:C:HO2'	34:Av:2:VAL:N	1.53	1.06
41:B8:81:C:HO2'	75:Bh:2:ALA:N	1.77	0.82
46:BE:227:LYS:HE2	46:BE:241:GLU:H	1.50	0.77
87:By:318:GLU:HB2	87:By:414:ARG:HG3	1.68	0.76
39:B5:3373:U:OP2	39:B5:3378:A:N6	2.19	0.75

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AA	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
3	AB	61/69 (88%)	61 (100%)	0	0	100	100
4	AC	71/156 (46%)	69 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AD	55/133 (41%)	55 (100%)	0	0	100	100
6	AE	99/115 (86%)	99 (100%)	0	0	100	100
7	AF	311/317 (98%)	300 (96%)	11 (4%)	0	100	100
8	AG	53/56 (95%)	53 (100%)	0	0	100	100
12	AZ	219/295 (74%)	215 (98%)	4 (2%)	0	100	100
13	Aa	220/264 (83%)	218 (99%)	2 (1%)	0	100	100
14	Ab	218/293 (74%)	218 (100%)	0	0	100	100
15	Ac	223/281 (79%)	222 (100%)	1 (0%)	0	100	100
16	Ad	260/263 (99%)	256 (98%)	4 (2%)	0	100	100
17	Ae	189/204 (93%)	184 (97%)	5 (3%)	0	100	100
18	Af	235/249 (94%)	235 (100%)	0	0	100	100
19	Ag	188/194 (97%)	184 (98%)	4 (2%)	0	100	100
20	Ah	204/208 (98%)	203 (100%)	1 (0%)	0	100	100
21	Ai	183/194 (94%)	181 (99%)	2 (1%)	0	100	100
22	Aj	94/165 (57%)	93 (99%)	1 (1%)	0	100	100
23	Ak	152/158 (96%)	149 (98%)	3 (2%)	0	100	100
24	Al	122/132 (92%)	119 (98%)	3 (2%)	0	100	100
25	Am	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
26	An	134/151 (89%)	133 (99%)	1 (1%)	0	100	100
27	Ao	131/145 (90%)	130 (99%)	1 (1%)	0	100	100
28	Ap	139/146 (95%)	133 (96%)	6 (4%)	0	100	100
29	Aq	132/135 (98%)	132 (100%)	0	0	100	100
30	Ar	143/152 (94%)	141 (99%)	2 (1%)	0	100	100
31	As	140/145 (97%)	139 (99%)	1 (1%)	0	100	100
32	At	102/119 (86%)	101 (99%)	1 (1%)	0	100	100
33	Au	81/83 (98%)	81 (100%)	0	0	100	100
34	Av	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
35	Aw	138/143 (96%)	137 (99%)	1 (1%)	0	100	100
36	Ax	123/130 (95%)	121 (98%)	2 (2%)	0	100	100
37	Ay	83/124 (67%)	83 (100%)	0	0	100	100
38	Az	23/25 (92%)	23 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	BA	250/257 (97%)	244 (98%)	6 (2%)	0	100	100
43	BB	395/403 (98%)	392 (99%)	3 (1%)	0	100	100
44	BC	360/413 (87%)	357 (99%)	3 (1%)	0	100	100
45	BD	291/297 (98%)	289 (99%)	2 (1%)	0	100	100
46	BE	239/291 (82%)	235 (98%)	4 (2%)	0	100	100
47	BF	224/247 (91%)	219 (98%)	5 (2%)	0	100	100
48	BG	229/266 (86%)	228 (100%)	1 (0%)	0	100	100
49	BH	188/192 (98%)	188 (100%)	0	0	100	100
50	BI	211/214 (99%)	208 (99%)	3 (1%)	0	100	100
51	BJ	168/178 (94%)	167 (99%)	1 (1%)	0	100	100
52	BK	34/1071 (3%)	34 (100%)	0	0	100	100
53	BL	208/211 (99%)	204 (98%)	4 (2%)	0	100	100
54	BM	136/218 (62%)	133 (98%)	3 (2%)	0	100	100
55	BN	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
56	BO	197/203 (97%)	197 (100%)	0	0	100	100
57	BP	157/184 (85%)	156 (99%)	1 (1%)	0	100	100
58	BQ	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
59	BR	178/196 (91%)	178 (100%)	0	0	100	100
60	BS	174/176 (99%)	174 (100%)	0	0	100	100
61	BT	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
62	BU	97/128 (76%)	95 (98%)	2 (2%)	0	100	100
63	BV	137/140 (98%)	137 (100%)	0	0	100	100
64	BW	119/157 (76%)	119 (100%)	0	0	100	100
65	BX	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
66	BY	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
67	BZ	133/136 (98%)	133 (100%)	0	0	100	100
68	Ba	144/148 (97%)	139 (96%)	5 (4%)	0	100	100
69	Bb	103/245 (42%)	97 (94%)	6 (6%)	0	100	100
70	Bc	106/115 (92%)	106 (100%)	0	0	100	100
71	Bd	105/125 (84%)	105 (100%)	0	0	100	100
72	Be	128/135 (95%)	128 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
73	Bf	108/110 (98%)	108 (100%)	0	0	100	100
74	Bg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
75	Bh	120/123 (98%)	120 (100%)	0	0	100	100
76	Bi	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
77	Bj	84/97 (87%)	84 (100%)	0	0	100	100
78	Bk	67/70 (96%)	67 (100%)	0	0	100	100
79	Bl	48/51 (94%)	48 (100%)	0	0	100	100
80	Bm	49/128 (38%)	49 (100%)	0	0	100	100
81	Bo	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
82	Bp	89/92 (97%)	88 (99%)	1 (1%)	0	100	100
83	Br	124/137 (90%)	122 (98%)	2 (2%)	0	100	100
84	Bs	194/318 (61%)	190 (98%)	4 (2%)	0	100	100
85	Bt	154/165 (93%)	153 (99%)	1 (1%)	0	100	100
86	Bv	210/217 (97%)	203 (97%)	7 (3%)	0	100	100
87	By	414/437 (95%)	406 (98%)	8 (2%)	0	100	100
88	Bz	593/599 (99%)	582 (98%)	11 (2%)	0	100	100
All	All	12952/15680 (83%)	12789 (99%)	163 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AA	75/76 (99%)	74 (99%)	1 (1%)	61	86
3	AB	56/62 (90%)	55 (98%)	1 (2%)	51	80
4	AC	66/140 (47%)	66 (100%)	0	100	100
5	AD	47/106 (44%)	46 (98%)	1 (2%)	47	77
6	AE	88/98 (90%)	85 (97%)	3 (3%)	32	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	AF	272/275 (99%)	267 (98%)	5 (2%)	51 80
8	AG	48/49 (98%)	48 (100%)	0	100 100
12	AZ	182/243 (75%)	179 (98%)	3 (2%)	55 83
13	Aa	203/231 (88%)	201 (99%)	2 (1%)	68 89
14	Ab	185/223 (83%)	184 (100%)	1 (0%)	81 93
15	Ac	189/232 (82%)	185 (98%)	4 (2%)	47 77
16	Ad	224/225 (100%)	224 (100%)	0	100 100
17	Ae	161/170 (95%)	161 (100%)	0	100 100
18	Af	207/218 (95%)	206 (100%)	1 (0%)	81 93
19	Ag	170/174 (98%)	166 (98%)	4 (2%)	43 75
20	Ah	178/180 (99%)	177 (99%)	1 (1%)	78 93
21	Ai	161/168 (96%)	160 (99%)	1 (1%)	78 93
22	Aj	87/136 (64%)	86 (99%)	1 (1%)	65 88
23	Ak	139/142 (98%)	138 (99%)	1 (1%)	76 92
24	Al	104/108 (96%)	100 (96%)	4 (4%)	29 64
25	Am	130/131 (99%)	130 (100%)	0	100 100
26	An	106/119 (89%)	104 (98%)	2 (2%)	50 79
27	Ao	119/130 (92%)	119 (100%)	0	100 100
28	Ap	117/121 (97%)	117 (100%)	0	100 100
29	Aq	120/121 (99%)	120 (100%)	0	100 100
30	Ar	125/131 (95%)	122 (98%)	3 (2%)	43 75
31	As	112/114 (98%)	112 (100%)	0	100 100
32	At	94/107 (88%)	92 (98%)	2 (2%)	47 77
33	Au	67/67 (100%)	65 (97%)	2 (3%)	36 70
34	Av	112/113 (99%)	112 (100%)	0	100 100
35	Aw	112/114 (98%)	109 (97%)	3 (3%)	39 73
36	Ax	107/112 (96%)	106 (99%)	1 (1%)	70 90
37	Ay	75/102 (74%)	74 (99%)	1 (1%)	61 86
38	Az	24/24 (100%)	24 (100%)	0	100 100
42	BA	194/198 (98%)	193 (100%)	1 (0%)	81 93
43	BB	344/347 (99%)	342 (99%)	2 (1%)	78 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	BC	302/337 (90%)	302 (100%)	0	100	100
45	BD	247/250 (99%)	247 (100%)	0	100	100
46	BE	216/251 (86%)	214 (99%)	2 (1%)	70	90
47	BF	197/215 (92%)	196 (100%)	1 (0%)	81	93
48	BG	199/223 (89%)	197 (99%)	2 (1%)	68	89
49	BH	169/171 (99%)	169 (100%)	0	100	100
50	BI	180/181 (99%)	179 (99%)	1 (1%)	78	93
51	BJ	143/149 (96%)	143 (100%)	0	100	100
52	BK	31/936 (3%)	30 (97%)	1 (3%)	34	68
53	BL	175/176 (99%)	171 (98%)	4 (2%)	44	76
54	BM	117/161 (73%)	116 (99%)	1 (1%)	70	90
55	BN	171/172 (99%)	171 (100%)	0	100	100
56	BO	171/173 (99%)	171 (100%)	0	100	100
57	BP	140/163 (86%)	140 (100%)	0	100	100
58	BQ	164/165 (99%)	160 (98%)	4 (2%)	43	75
59	BR	159/175 (91%)	159 (100%)	0	100	100
60	BS	154/154 (100%)	153 (99%)	1 (1%)	78	93
61	BT	139/140 (99%)	139 (100%)	0	100	100
62	BU	88/113 (78%)	88 (100%)	0	100	100
63	BV	106/107 (99%)	105 (99%)	1 (1%)	70	90
64	BW	100/126 (79%)	99 (99%)	1 (1%)	68	89
65	BX	106/134 (79%)	106 (100%)	0	100	100
66	BY	124/135 (92%)	123 (99%)	1 (1%)	73	90
67	BZ	117/118 (99%)	117 (100%)	0	100	100
68	Ba	118/119 (99%)	118 (100%)	0	100	100
69	Bb	87/183 (48%)	87 (100%)	0	100	100
70	Bc	92/98 (94%)	92 (100%)	0	100	100
71	Bd	98/110 (89%)	97 (99%)	1 (1%)	68	89
72	Be	116/121 (96%)	116 (100%)	0	100	100
73	Bf	89/89 (100%)	89 (100%)	0	100	100
74	Bg	98/100 (98%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
75	Bh	109/110 (99%)	109 (100%)	0	100 100
76	Bi	86/89 (97%)	85 (99%)	1 (1%)	63 86
77	Bj	73/80 (91%)	72 (99%)	1 (1%)	59 85
78	Bk	64/65 (98%)	62 (97%)	2 (3%)	35 69
79	Bl	47/48 (98%)	46 (98%)	1 (2%)	47 77
80	Bm	47/115 (41%)	47 (100%)	0	100 100
81	Bo	92/93 (99%)	92 (100%)	0	100 100
82	Bp	74/75 (99%)	73 (99%)	1 (1%)	59 85
83	Br	109/120 (91%)	109 (100%)	0	100 100
84	Bs	164/258 (64%)	163 (99%)	1 (1%)	78 93
85	Bt	128/137 (93%)	125 (98%)	3 (2%)	44 76
86	Bv	191/195 (98%)	185 (97%)	6 (3%)	35 69
87	By	358/376 (95%)	337 (94%)	21 (6%)	18 48
88	Bz	516/526 (98%)	502 (97%)	14 (3%)	39 73
All	All	11271/13339 (84%)	11148 (99%)	123 (1%)	63 88

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	BK	4400	LEU
88	Bz	75	LEU
71	Bd	106	VAL
88	Bz	41	VAL
88	Bz	493	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 165 such sidechains are listed below:

Mol	Chain	Res	Type
66	BY	56	GLN
87	By	67	ASN
68	Ba	66	ASN
79	Bl	4	HIS
87	By	211	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	1764/1870 (94%)	234 (13%)	1 (0%)
10	AI	2/76 (2%)	1 (50%)	0
11	AT	85/86 (98%)	15 (17%)	0
39	B5	3752/4808 (78%)	471 (12%)	1 (0%)
40	B7	118/119 (99%)	7 (5%)	0
41	B8	155/158 (98%)	17 (10%)	0
9	AH	23/217 (10%)	8 (34%)	0
All	All	5899/7334 (80%)	753 (12%)	2 (0%)

5 of 753 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	3	C
1	A2	17	C
1	A2	26	U
1	A2	33	G
1	A2	41	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A2	549	C
39	B5	4445	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MA6	A2	1851	1	23,26,27	1.72	7 (30%)	34,38,41	2.45	12 (35%)
39	OMC	B5	1820	90,39	19,22,23	0.80	0	26,31,34	0.83	0
1	OMG	A2	602	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	A2	93	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	B8N	A2	1249	1	24,29,30	1.28	3 (12%)	29,42,45	1.30	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	OMG	B5	4116	39	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
39	PSU	B5	3371	39	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	A2	513	1	22,25,26	1.46	4 (18%)	31,36,39	2.14	10 (32%)
1	PSU	A2	1005	1	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	A2	1448	1	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
39	PSU	B5	4382	39	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	1245	1	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
39	A2M	B5	4317	39	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
39	PSU	B5	3494	39	18,21,22	1.38	2 (11%)	22,30,33	1.89	3 (13%)
39	OMU	B5	3657	39	19,22,23	1.23	2 (10%)	26,31,34	1.74	5 (19%)
11	PSU	AT	65	11	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
39	OMG	B5	4138	39	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
12	SAC	AZ	2	12	7,8,9	0.53	0	8,9,11	0.86	1 (12%)
1	OMU	A2	1443	1,90	19,22,23	1.23	2 (10%)	26,31,34	1.70	4 (15%)
1	PSU	A2	1239	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
39	PSU	B5	4188	39	18,21,22	1.35	2 (11%)	22,30,33	1.92	3 (13%)
39	A2M	B5	4269	90,39	22,25,26	1.45	4 (18%)	31,36,39	2.14	10 (32%)
81	MLZ	Bo	53	81	8,9,10	0.48	0	4,9,11	0.09	0
42	V5N	BA	216	42	9,11,12	2.11	2 (22%)	9,14,16	1.73	2 (22%)
39	A2M	B5	1810	90,39	22,25,26	1.45	4 (18%)	31,36,39	2.15	10 (32%)
83	SAC	Br	2	83	7,8,9	0.53	0	8,9,11	0.82	1 (12%)
39	PSU	B5	1683	39	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
39	PSU	B5	4298	39	18,21,22	1.34	2 (11%)	22,30,33	1.92	3 (13%)
1	PSU	A2	687	1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
39	OMG	B5	4383	39	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	A2	650	1	18,21,22	1.34	2 (11%)	22,30,33	1.90	4 (18%)
39	PSU	B5	3447	39	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
39	PSU	B5	4435	39	18,21,22	1.36	2 (11%)	22,30,33	1.94	3 (13%)
39	PSU	B5	4042	39	18,21,22	1.33	2 (11%)	22,30,33	1.92	3 (13%)
39	5MC	B5	4193	39	18,22,23	0.98	2 (11%)	26,32,35	1.19	2 (7%)
1	PSU	A2	573	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	3576	39	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
39	OMC	B5	3540	39	19,22,23	0.82	0	26,31,34	0.84	1 (3%)
39	OMG	B5	1477	39	23,26,27	1.20	3 (13%)	33,38,41	1.96	6 (18%)
39	A2M	B5	1270	39	22,25,26	1.43	4 (18%)	31,36,39	2.13	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	OMU	B5	2258	39	19,22,23	1.21	3 (15%)	26,31,34	1.68	4 (15%)
1	OMC	A2	1704	1	19,22,23	0.81	0	26,31,34	0.84	1 (3%)
39	PSU	B5	2475	39	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	3466	39	18,21,22	1.33	2 (11%)	22,30,33	1.89	4 (18%)
39	6MZ	B5	3966	39	22,25,26	1.43	4 (18%)	30,36,39	2.27	9 (30%)
39	OMG	B5	4369	39	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
1	A2M	A2	577	1	22,25,26	1.46	4 (18%)	31,36,39	2.12	9 (29%)
43	HIC	BB	245	43	10,11,12	0.61	0	8,14,16	0.43	0
1	A2M	A2	166	1	22,25,26	1.47	4 (18%)	31,36,39	2.14	9 (29%)
39	PSU	B5	4740	39	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
39	PSU	B5	3369	39	18,21,22	1.35	2 (11%)	22,30,33	1.90	4 (18%)
1	OMG	A2	1491	1,90	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
39	OMG	B5	3476	39	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
1	OMG	A2	684	1	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
39	PSU	B5	1799	39	18,21,22	1.36	2 (11%)	22,30,33	1.93	3 (13%)
39	OMG	B5	4364	39	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	A2	1368	1	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
1	OMU	A2	1289	1	19,22,23	1.22	3 (15%)	26,31,34	1.66	4 (15%)
1	PSU	A2	119	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
39	A2M	B5	398	39	22,25,26	1.46	4 (18%)	31,36,39	2.16	10 (32%)
1	G7M	A2	1640	1,11	23,26,27	2.31	5 (21%)	35,39,42	2.98	10 (28%)
39	OMC	B5	2208	90,39	19,22,23	0.82	0	26,31,34	0.79	0
1	PSU	A2	407	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	4749	39	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
68	V5N	Ba	39	68	9,11,12	2.14	2 (22%)	9,14,16	1.71	2 (22%)
39	PSU	B5	4099	39	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
39	PSU	B5	3490	39	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
39	PSU	B5	4278	39	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	A2	1057	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
39	OMU	B5	4052	39	19,22,23	1.24	3 (15%)	26,31,34	1.69	5 (19%)
39	PSU	B5	4325	39	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
41	OMG	B8	75	41	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
39	OMG	B5	4240	39	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
1	OMU	A2	628	1	19,22,23	1.18	2 (10%)	26,31,34	1.71	5 (19%)
39	A2M	B5	3599	39	22,25,26	1.46	4 (18%)	31,36,39	2.10	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	A2	1046	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
39	A2M	B5	2244	90,39	22,25,26	1.45	4 (18%)	31,36,39	2.13	10 (32%)
1	PSU	A2	867	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	1178	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
41	PSU	B8	69	41	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)
39	PSU	B5	3554	39	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	4AC	A2	1338	1	21,24,25	1.06	1 (4%)	29,34,37	1.27	3 (10%)
1	OMC	A2	518	1	19,22,23	0.81	0	26,31,34	0.81	0
39	PSU	B5	1537	39	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	1632	39	18,21,22	1.35	2 (11%)	22,30,33	1.89	4 (18%)
39	PSU	B5	4322	39	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	A2	1446	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	4 (18%)
39	OMG	B5	3942	11,39	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	OMU	A2	172	1	19,22,23	1.19	2 (10%)	26,31,34	1.71	4 (15%)
39	A2M	B5	3450	39	22,25,26	1.47	4 (18%)	31,36,39	2.07	9 (29%)
39	PSU	B5	1721	39	18,21,22	1.35	2 (11%)	22,30,33	1.90	4 (18%)
1	PSU	A2	823	1	18,21,22	1.36	2 (11%)	22,30,33	1.91	4 (18%)
1	4AC	A2	1843	1	21,24,25	1.11	2 (9%)	29,34,37	1.21	3 (10%)
39	OMC	B5	4282	39	19,22,23	0.82	0	26,31,34	0.82	0
41	PSU	B8	55	41	18,21,22	1.34	2 (11%)	22,30,33	1.91	4 (18%)
1	PSU	A2	1175	1	18,21,22	1.36	2 (11%)	22,30,33	1.93	3 (13%)
1	PSU	A2	1082	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	A2	967	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
39	OMG	B5	4245	39	23,26,27	1.21	3 (13%)	33,38,41	1.92	6 (18%)
35	HY3	Aw	62	35	6,8,9	2.13	1 (16%)	5,10,12	1.12	1 (20%)
39	A2M	B5	3456	39	22,25,26	1.46	4 (18%)	31,36,39	2.09	10 (32%)
39	OMG	B5	3524	39	23,26,27	1.20	3 (13%)	33,38,41	1.91	6 (18%)
1	OMU	A2	121	1	19,22,23	1.23	3 (15%)	26,31,34	1.70	4 (15%)
1	OMC	A2	1392	1	19,22,23	0.82	0	26,31,34	0.88	1 (3%)
1	A2M	A2	669	1,90	22,25,26	1.45	4 (18%)	31,36,39	2.11	10 (32%)
39	A2M	B5	2206	90,39	22,25,26	1.46	4 (18%)	31,36,39	2.10	9 (29%)
39	PSU	B5	4107	39	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	A2	591	1	22,25,26	1.48	4 (18%)	31,36,39	2.20	7 (22%)
39	PSU	B5	3496	39	18,21,22	1.34	2 (11%)	22,30,33	1.92	4 (18%)
39	PSU	B5	4039	39	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	OMU	B5	3973	39	19,22,23	1.24	3 (15%)	26,31,34	1.69	4 (15%)
39	OMC	B5	2667	39	19,22,23	0.81	0	26,31,34	0.84	1 (3%)
39	OMG	B5	3359	39	23,26,27	1.19	3 (13%)	33,38,41	1.96	6 (18%)
1	A2M	A2	99	1,90	22,25,26	1.46	4 (18%)	31,36,39	2.12	9 (29%)
39	OMG	B5	1580	39	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
1	OMC	A2	174	1,90	19,22,23	0.82	0	26,31,34	0.80	0
39	OMG	B5	3974	39	23,26,27	1.18	3 (13%)	33,38,41	1.91	6 (18%)
39	A2M	B5	1489	90,39	22,25,26	1.46	4 (18%)	31,36,39	2.07	9 (29%)
1	A2M	A2	1032	1	22,25,26	1.46	4 (18%)	31,36,39	2.14	10 (32%)
1	6MZ	A2	1833	1,90	22,25,26	1.45	4 (18%)	30,36,39	2.12	9 (30%)
39	OMC	B5	1284	39	19,22,23	0.83	0	26,31,34	0.80	0
39	PSU	B5	1718	39	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	A2	682	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
39	OMG	B5	3676	39	23,26,27	1.18	3 (13%)	33,38,41	1.93	6 (18%)
1	OMG	A2	868	1	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
39	OMG	B5	2267	39	23,26,27	1.19	3 (13%)	33,38,41	1.91	6 (18%)
69	MLZ	Bb	5	69	8,9,10	0.49	0	4,9,11	0.24	0
1	PSU	A2	1644	1,90	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	OMU	A2	116	1	19,22,23	1.19	2 (10%)	26,31,34	1.69	5 (19%)
1	PSU	A2	864	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	A2M	A2	1384	1	22,25,26	1.45	4 (18%)	31,36,39	2.09	10 (32%)
1	PSU	A2	105	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
39	OMC	B5	3433	39	19,22,23	0.80	0	26,31,34	0.80	0
1	PSU	A2	652	1	18,21,22	1.35	2 (11%)	22,30,33	1.92	4 (18%)
1	OMC	A2	463	1	19,22,23	0.81	0	26,31,34	0.82	0
39	PSU	B5	1638	39	18,21,22	1.36	2 (11%)	22,30,33	1.94	3 (13%)
1	A2M	A2	485	1	22,25,26	1.47	4 (18%)	31,36,39	2.08	9 (29%)
39	OMU	B5	4366	39	19,22,23	1.24	4 (21%)	26,31,34	1.75	4 (15%)
1	PSU	A2	218	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
11	5MU	AT	64	11	19,22,23	1.42	5 (26%)	28,32,35	2.02	5 (17%)
39	PSU	B5	1491	39	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
39	PSU	B5	3500	39	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	OMG	A2	437	1	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
39	PSU	B5	4058	39	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
39	OMC	B5	3573	39	19,22,23	0.80	0	26,31,34	0.82	0
1	PSU	A2	1348	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	A2M	A2	159	1	22,25,26	1.46	4 (18%)	31,36,39	2.19	10 (32%)
39	PSU	B5	3583	39	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
39	OMG	B5	1260	39	23,26,27	1.19	3 (13%)	33,38,41	1.97	6 (18%)
1	PSU	A2	802	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	OMU	A2	1805	1	19,22,23	1.23	3 (15%)	26,31,34	1.71	4 (15%)
39	A2M	B5	3562	39	22,25,26	1.44	4 (18%)	31,36,39	2.13	10 (32%)
39	PSU	B5	2351	39	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
39	PSU	B5	1731	39	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
39	PSU	B5	3652	90,39	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
39	OMC	B5	4202	39	19,22,23	0.82	0	26,31,34	0.80	0
39	PSU	B5	3427	39	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
39	OMC	B5	2194	90,39	19,22,23	0.82	0	26,31,34	0.92	2 (7%)
39	PSU	B5	4149	39	18,21,22	1.36	2 (11%)	22,30,33	1.94	4 (18%)
39	PSU	B5	3616	39	18,21,22	1.38	2 (11%)	22,30,33	1.93	3 (13%)
44	AYA	BC	2	44	6,7,8	0.76	0	5,8,10	0.28	0
1	PSU	A2	610	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	OMG	A2	645	1	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
39	A2M	B5	2658	39	22,25,26	1.45	4 (18%)	31,36,39	2.13	9 (29%)
39	PSU	B5	3502	39	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
39	A2M	B5	4336	39	22,25,26	1.45	4 (18%)	31,36,39	2.13	10 (32%)
1	PSU	A2	36	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
39	OMU	B5	2680	39	19,22,23	1.23	2 (10%)	26,31,34	1.75	5 (19%)
39	PSU	B5	4374	39	18,21,22	1.35	2 (11%)	22,30,33	1.92	3 (13%)
1	PSU	A2	1047	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
39	OMG	B5	2207	39	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	A2	1233	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
39	OMC	B5	3619	39	19,22,23	0.81	0	26,31,34	0.78	0
33	AME	Au	1	33	9,10,11	0.48	0	9,11,13	0.85	1 (11%)
39	OMC	B5	2265	90,39	19,22,23	0.82	0	26,31,34	0.88	1 (3%)
1	OMG	A2	510	1,90	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	A2	1626	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	A2	1679	1	22,25,26	1.46	4 (18%)	31,36,39	2.17	10 (32%)
1	PSU	A2	816	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
39	PSU	B5	3585	90,39	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	OMG	A2	1329	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	A2M	A2	27	1,90	22,25,26	1.46	4 (18%)	31,36,39	2.14	10 (32%)
30	SAC	Ar	2	30	7,8,9	0.54	0	8,9,11	0.92	1 (12%)
39	PSU	B5	4166	39	18,21,22	1.37	2 (11%)	22,30,33	1.81	3 (13%)
39	PSU	B5	4267	90,39	18,21,22	1.35	2 (11%)	22,30,33	1.94	4 (18%)
1	OMU	A2	1327	1,90	19,22,23	1.20	2 (10%)	26,31,34	1.71	5 (19%)
39	PSU	B5	1801	39	18,21,22	1.34	2 (11%)	22,30,33	1.92	4 (18%)
39	PSU	B5	4203	39	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	A2	109	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	4246	39	18,21,22	1.34	2 (11%)	22,30,33	1.92	3 (13%)
39	PSU	B5	1720	39	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	4169	39	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
39	PSU	B5	4419	39	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
39	UY1	B5	3550	39	19,22,23	1.36	3 (15%)	22,31,34	1.96	5 (22%)
39	PSU	B5	3462	39	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
31	NMM	As	67	31	9,11,12	0.59	0	6,12,14	0.39	0
1	PSU	A2	815	1	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
39	A2M	B5	3557	39	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
39	OMC	B5	3601	39	19,22,23	0.82	0	26,31,34	0.76	0
39	PSU	B5	4177	39	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	OMU	A2	355	1	19,22,23	1.22	2 (10%)	26,31,34	1.73	4 (15%)
39	A2M	B5	1479	39	22,25,26	1.47	4 (18%)	31,36,39	2.09	8 (25%)
39	OMU	B5	4244	39	19,22,23	1.21	2 (10%)	26,31,34	1.74	5 (19%)
39	OMC	B5	2647	39	19,22,23	0.81	0	26,31,34	0.81	0
39	UR3	B5	4276	39	19,22,23	0.99	0	26,32,35	1.43	1 (3%)
39	A2M	B5	400	39	22,25,26	1.45	4 (18%)	31,36,39	2.09	10 (32%)
39	OMG	B5	2719	39	23,26,27	1.20	3 (13%)	33,38,41	1.96	6 (18%)
39	5MC	B5	3514	90,39	18,22,23	0.96	2 (11%)	26,32,35	1.20	3 (11%)
1	MA6	A2	1852	1	23,26,27	1.51	5 (21%)	34,38,41	2.21	10 (29%)
39	PSU	B5	4045	39	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
39	PSU	B5	4711	39	18,21,22	1.34	2 (11%)	22,30,33	1.89	4 (18%)
39	OMG	B5	3631	90,39	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
39	A2M	B5	3492	39	22,25,26	1.47	4 (18%)	31,36,39	2.12	8 (25%)
1	OMU	A2	429	1	19,22,23	1.19	2 (10%)	26,31,34	1.70	5 (19%)
1	A2M	A2	469	1	22,25,26	1.47	4 (18%)	31,36,39	2.09	9 (29%)
1	PSU	A2	34	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	OMC	B5	2704	39	19,22,23	0.81	0	26,31,34	0.77	0
1	PSU	A2	210	1	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
80	M3L	Bm	98	80	10,11,12	0.82	0	9,14,16	0.47	0
1	PSU	A2	1693	1	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
39	A2M	B5	3517	39	22,25,26	1.41	4 (18%)	31,36,39	2.27	11 (35%)
39	1MA	B5	1266	90,39	21,25,26	1.37	4 (19%)	31,37,40	1.68	5 (16%)
39	A2M	B5	2630	90,39	22,25,26	1.44	4 (18%)	31,36,39	2.15	9 (29%)
39	PSU	B5	4217	39	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)

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
1	MA6	A2	1851	1	-	0/11/29/30	0/3/3/3
39	OMC	B5	1820	90,39	-	1/9/27/28	0/2/2/2
1	OMG	A2	602	1	-	0/9/27/28	0/3/3/3
1	PSU	A2	93	1	-	0/7/25/26	0/2/2/2
1	B8N	A2	1249	1	-	4/16/34/35	0/2/2/2
39	OMG	B5	4116	39	-	0/9/27/28	0/3/3/3
39	PSU	B5	3371	39	-	0/7/25/26	0/2/2/2
1	A2M	A2	513	1	-	2/9/27/28	0/3/3/3
1	PSU	A2	1005	1	-	0/7/25/26	0/2/2/2
1	OMG	A2	1448	1	-	3/9/27/28	0/3/3/3
39	PSU	B5	4382	39	-	4/7/25/26	0/2/2/2
1	PSU	A2	1245	1	-	0/7/25/26	0/2/2/2
39	A2M	B5	4317	39	-	0/9/27/28	0/3/3/3
39	PSU	B5	3494	39	-	2/7/25/26	0/2/2/2
39	OMU	B5	3657	39	-	0/9/27/28	0/2/2/2
11	PSU	AT	65	11	-	0/7/25/26	0/2/2/2
39	OMG	B5	4138	39	-	0/9/27/28	0/3/3/3
12	SAC	AZ	2	12	-	1/7/8/10	-
1	OMU	A2	1443	1,90	-	2/9/27/28	0/2/2/2
1	PSU	A2	1239	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	4188	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	4269	90,39	-	2/9/27/28	0/3/3/3
81	MLZ	Bo	53	81	-	0/7/8/10	-
42	V5N	BA	216	42	-	3/9/10/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	A2M	B5	1810	90,39	-	2/9/27/28	0/3/3/3
83	SAC	Br	2	83	-	0/7/8/10	-
39	PSU	B5	1683	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4298	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	687	1	-	0/7/25/26	0/2/2/2
39	OMG	B5	4383	39	-	1/9/27/28	0/3/3/3
1	PSU	A2	650	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	3447	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4435	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4042	39	-	0/7/25/26	0/2/2/2
39	5MC	B5	4193	39	-	4/7/25/26	0/2/2/2
1	PSU	A2	573	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	3576	39	-	1/7/25/26	0/2/2/2
39	OMC	B5	3540	39	-	1/9/27/28	0/2/2/2
39	OMG	B5	1477	39	-	0/9/27/28	0/3/3/3
39	A2M	B5	1270	39	-	0/9/27/28	0/3/3/3
39	OMU	B5	2258	39	-	0/9/27/28	0/2/2/2
1	OMC	A2	1704	1	-	2/9/27/28	0/2/2/2
39	PSU	B5	2475	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	3466	39	-	0/7/25/26	0/2/2/2
39	6MZ	B5	3966	39	-	0/9/27/28	0/3/3/3
39	OMG	B5	4369	39	-	1/9/27/28	0/3/3/3
1	A2M	A2	577	1	-	2/9/27/28	0/3/3/3
43	HIC	BB	245	43	-	2/5/6/8	0/1/1/1
1	A2M	A2	166	1	-	0/9/27/28	0/3/3/3
39	PSU	B5	4740	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	3369	39	-	0/7/25/26	0/2/2/2
1	OMG	A2	1491	1,90	-	1/9/27/28	0/3/3/3
39	OMG	B5	3476	39	-	1/9/27/28	0/3/3/3
1	OMG	A2	684	1	-	3/9/27/28	0/3/3/3
39	PSU	B5	1799	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	4364	39	-	0/9/27/28	0/3/3/3
1	PSU	A2	1368	1	-	0/7/25/26	0/2/2/2
1	OMU	A2	1289	1	-	2/9/27/28	0/2/2/2
1	PSU	A2	119	1	-	0/7/25/26	0/2/2/2
39	A2M	B5	398	39	-	2/9/27/28	0/3/3/3
1	G7M	A2	1640	1,11	-	0/7/25/26	0/3/3/3
39	OMC	B5	2208	90,39	-	0/9/27/28	0/2/2/2
1	PSU	A2	407	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	4749	39	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	V5N	Ba	39	68	-	1/9/10/12	0/1/1/1
39	PSU	B5	4099	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	3490	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4278	39	-	2/7/25/26	0/2/2/2
1	PSU	A2	1057	1	-	0/7/25/26	0/2/2/2
39	OMU	B5	4052	39	-	0/9/27/28	0/2/2/2
39	PSU	B5	4325	39	-	0/7/25/26	0/2/2/2
41	OMG	B8	75	41	-	1/9/27/28	0/3/3/3
39	OMG	B5	4240	39	-	0/9/27/28	0/3/3/3
1	OMU	A2	628	1	-	3/9/27/28	0/2/2/2
39	A2M	B5	3599	39	-	2/9/27/28	0/3/3/3
1	PSU	A2	1046	1	-	0/7/25/26	0/2/2/2
39	A2M	B5	2244	90,39	-	0/9/27/28	0/3/3/3
1	PSU	A2	867	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1178	1	-	0/7/25/26	0/2/2/2
41	PSU	B8	69	41	-	0/7/25/26	0/2/2/2
39	PSU	B5	3554	39	-	0/7/25/26	0/2/2/2
1	4AC	A2	1338	1	-	4/11/29/30	0/2/2/2
1	OMC	A2	518	1	-	0/9/27/28	0/2/2/2
39	PSU	B5	1537	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	1632	39	-	3/7/25/26	0/2/2/2
39	PSU	B5	4322	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	1446	1	-	0/7/25/26	0/2/2/2
39	OMG	B5	3942	11,39	-	0/9/27/28	0/3/3/3
1	OMU	A2	172	1	-	0/9/27/28	0/2/2/2
39	A2M	B5	3450	39	-	1/9/27/28	0/3/3/3
39	PSU	B5	1721	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	823	1	-	0/7/25/26	0/2/2/2
1	4AC	A2	1843	1	-	2/11/29/30	0/2/2/2
39	OMC	B5	4282	39	-	0/9/27/28	0/2/2/2
41	PSU	B8	55	41	-	0/7/25/26	0/2/2/2
1	PSU	A2	1175	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1082	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	967	1	-	0/7/25/26	0/2/2/2
39	OMG	B5	4245	39	-	0/9/27/28	0/3/3/3
35	HY3	Aw	62	35	-	1/1/12/14	0/1/1/1
39	A2M	B5	3456	39	-	0/9/27/28	0/3/3/3
39	OMG	B5	3524	39	-	0/9/27/28	0/3/3/3
1	OMU	A2	121	1	-	0/9/27/28	0/2/2/2
1	OMC	A2	1392	1	-	0/9/27/28	0/2/2/2
1	A2M	A2	669	1,90	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	A2M	B5	2206	90,39	-	0/9/27/28	0/3/3/3
39	PSU	B5	4107	39	-	0/7/25/26	0/2/2/2
1	A2M	A2	591	1	-	3/9/27/28	0/3/3/3
39	PSU	B5	3496	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4039	39	-	0/7/25/26	0/2/2/2
39	OMU	B5	3973	39	-	1/9/27/28	0/2/2/2
39	OMC	B5	2667	39	-	1/9/27/28	0/2/2/2
39	OMG	B5	3359	39	-	0/9/27/28	0/3/3/3
1	A2M	A2	99	1,90	-	2/9/27/28	0/3/3/3
39	OMG	B5	1580	39	-	0/9/27/28	0/3/3/3
1	OMC	A2	174	1,90	-	0/9/27/28	0/2/2/2
39	OMG	B5	3974	39	-	0/9/27/28	0/3/3/3
39	A2M	B5	1489	90,39	-	1/9/27/28	0/3/3/3
1	A2M	A2	1032	1	-	0/9/27/28	0/3/3/3
1	6MZ	A2	1833	1,90	-	1/9/27/28	0/3/3/3
39	OMC	B5	1284	39	-	2/9/27/28	0/2/2/2
39	PSU	B5	1718	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	682	1	-	0/7/25/26	0/2/2/2
39	OMG	B5	3676	39	-	0/9/27/28	0/3/3/3
1	OMG	A2	868	1	-	0/9/27/28	0/3/3/3
39	OMG	B5	2267	39	-	0/9/27/28	0/3/3/3
69	MLZ	Bb	5	69	-	2/7/8/10	-
1	PSU	A2	1644	1,90	-	0/7/25/26	0/2/2/2
1	OMU	A2	116	1	-	1/9/27/28	0/2/2/2
1	PSU	A2	864	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	1384	1	-	0/9/27/28	0/3/3/3
1	PSU	A2	105	1	-	0/7/25/26	0/2/2/2
39	OMC	B5	3433	39	-	4/9/27/28	0/2/2/2
1	PSU	A2	652	1	-	0/7/25/26	0/2/2/2
1	OMC	A2	463	1	-	0/9/27/28	0/2/2/2
39	PSU	B5	1638	39	-	0/7/25/26	0/2/2/2
1	A2M	A2	485	1	-	0/9/27/28	0/3/3/3
39	OMU	B5	4366	39	-	0/9/27/28	0/2/2/2
1	PSU	A2	218	1	-	0/7/25/26	0/2/2/2
11	5MU	AT	64	11	-	0/7/25/26	0/2/2/2
39	PSU	B5	1491	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	3500	39	-	0/7/25/26	0/2/2/2
1	OMG	A2	437	1	-	0/9/27/28	0/3/3/3
39	PSU	B5	4058	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	3573	39	-	0/9/27/28	0/2/2/2
1	PSU	A2	1348	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	A2	159	1	-	1/9/27/28	0/3/3/3
39	PSU	B5	3583	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	1260	39	-	1/9/27/28	0/3/3/3
1	PSU	A2	802	1	-	0/7/25/26	0/2/2/2
1	OMU	A2	1805	1	-	0/9/27/28	0/2/2/2
39	A2M	B5	3562	39	-	0/9/27/28	0/3/3/3
39	PSU	B5	2351	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	1731	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	3652	90,39	-	0/7/25/26	0/2/2/2
39	OMC	B5	4202	39	-	0/9/27/28	0/2/2/2
39	PSU	B5	3427	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	2194	90,39	-	2/9/27/28	0/2/2/2
39	PSU	B5	4149	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	3616	39	-	0/7/25/26	0/2/2/2
44	AYA	BC	2	44	-	3/4/6/8	-
1	PSU	A2	610	1	-	0/7/25/26	0/2/2/2
1	OMG	A2	645	1	-	3/9/27/28	0/3/3/3
39	A2M	B5	2658	39	-	2/9/27/28	0/3/3/3
39	PSU	B5	3502	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	4336	39	-	1/9/27/28	0/3/3/3
1	PSU	A2	36	1	-	0/7/25/26	0/2/2/2
39	OMU	B5	2680	39	-	1/9/27/28	0/2/2/2
39	PSU	B5	4374	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	1047	1	-	0/7/25/26	0/2/2/2
39	OMG	B5	2207	39	-	2/9/27/28	0/3/3/3
1	PSU	A2	1233	1	-	0/7/25/26	0/2/2/2
39	OMC	B5	3619	39	-	2/9/27/28	0/2/2/2
33	AME	Au	1	33	-	2/9/10/12	-
39	OMC	B5	2265	90,39	-	1/9/27/28	0/2/2/2
1	OMG	A2	510	1,90	-	1/9/27/28	0/3/3/3
1	PSU	A2	1626	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	1679	1	-	0/9/27/28	0/3/3/3
1	PSU	A2	816	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	3585	90,39	-	0/7/25/26	0/2/2/2
1	OMG	A2	1329	1	-	0/9/27/28	0/3/3/3
1	A2M	A2	27	1,90	-	0/9/27/28	0/3/3/3
30	SAC	Ar	2	30	-	0/7/8/10	-
39	PSU	B5	4166	39	-	1/7/25/26	0/2/2/2
39	PSU	B5	4267	90,39	-	0/7/25/26	0/2/2/2
1	OMU	A2	1327	1,90	-	0/9/27/28	0/2/2/2
39	PSU	B5	1801	39	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	PSU	B5	4203	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	109	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	4246	39	-	1/7/25/26	0/2/2/2
39	PSU	B5	1720	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4169	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4419	39	-	0/7/25/26	0/2/2/2
39	UY1	B5	3550	39	-	1/9/27/28	0/2/2/2
39	PSU	B5	3462	39	-	0/7/25/26	0/2/2/2
31	NMM	As	67	31	-	0/9/11/13	-
1	PSU	A2	815	1	-	0/7/25/26	0/2/2/2
39	A2M	B5	3557	39	-	1/9/27/28	0/3/3/3
39	OMC	B5	3601	39	-	0/9/27/28	0/2/2/2
39	PSU	B5	4177	39	-	0/7/25/26	0/2/2/2
1	OMU	A2	355	1	-	0/9/27/28	0/2/2/2
39	A2M	B5	1479	39	-	0/9/27/28	0/3/3/3
39	OMU	B5	4244	39	-	0/9/27/28	0/2/2/2
39	OMC	B5	2647	39	-	0/9/27/28	0/2/2/2
39	UR3	B5	4276	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	400	39	-	0/9/27/28	0/3/3/3
39	OMG	B5	2719	39	-	0/9/27/28	0/3/3/3
39	5MC	B5	3514	90,39	-	0/7/25/26	0/2/2/2
1	MA6	A2	1852	1	-	1/11/29/30	0/3/3/3
39	PSU	B5	4045	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4711	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	3631	90,39	-	1/9/27/28	0/3/3/3
39	A2M	B5	3492	39	-	0/9/27/28	0/3/3/3
1	OMU	A2	429	1	-	6/9/27/28	0/2/2/2
1	A2M	A2	469	1	-	1/9/27/28	0/3/3/3
1	PSU	A2	34	1	-	0/7/25/26	0/2/2/2
39	OMC	B5	2704	39	-	0/9/27/28	0/2/2/2
1	PSU	A2	210	1	-	0/7/25/26	0/2/2/2
80	M3L	Bm	98	80	-	0/9/10/12	-
1	PSU	A2	1693	1	-	0/7/25/26	0/2/2/2
39	A2M	B5	3517	39	-	1/9/27/28	0/3/3/3
39	1MA	B5	1266	90,39	-	1/7/25/26	0/3/3/3
39	A2M	B5	2630	90,39	-	3/9/27/28	0/3/3/3
39	PSU	B5	4217	39	-	0/7/25/26	0/2/2/2

The worst 5 of 510 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	1640	G7M	C8-N7	7.29	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	Ba	39	V5N	CG-ND1	-5.08	1.32	1.37
42	BA	216	V5N	CG-ND1	-4.99	1.32	1.37
35	Aw	62	HY3	C3-CA	-4.91	1.50	1.55
1	A2	1640	G7M	C5-N7	-4.68	1.33	1.39

The worst 5 of 969 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A2	1640	G7M	CN7-N7-C8	-7.96	112.56	124.84
1	A2	591	A2M	C5-C4-N3	-6.89	117.76	126.75
1	A2	1640	G7M	N9-C8-N7	-6.59	95.91	112.21
1	A2	1640	G7M	C8-N7-C5	6.54	115.96	107.78
1	A2	1640	G7M	N9-C4-N3	6.49	138.98	125.94

There are no chirality outliers.

5 of 129 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A2	159	A2M	C1'-C2'-O2'-CM'
1	A2	429	OMU	C2'-C1'-N1-C2
1	A2	429	OMU	C2'-C1'-N1-C6
1	A2	513	A2M	O4'-C4'-C5'-O5'
1	A2	645	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

94 monomers are involved in 118 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A2	1851	MA6	1	0
39	B5	1820	OMC	1	0
1	A2	602	OMG	1	0
1	A2	1249	B8N	1	0
1	A2	513	A2M	1	0
1	A2	1448	OMG	2	0
39	B5	4382	PSU	2	0
39	B5	4317	A2M	1	0
39	B5	3494	PSU	1	0
11	AT	65	PSU	1	0
39	B5	4138	OMG	2	0
39	B5	4269	A2M	1	0
81	Bo	53	MLZ	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	B5	1810	A2M	2	0
39	B5	4383	OMG	1	0
39	B5	4193	5MC	2	0
39	B5	3540	OMC	1	0
39	B5	1270	A2M	2	0
39	B5	2258	OMU	2	0
1	A2	1704	OMC	2	0
39	B5	3466	PSU	1	0
1	A2	577	A2M	1	0
1	A2	166	A2M	2	0
1	A2	1491	OMG	1	0
39	B5	3476	OMG	1	0
1	A2	684	OMG	1	0
39	B5	4364	OMG	1	0
1	A2	1289	OMU	2	0
39	B5	398	A2M	1	0
1	A2	1640	G7M	1	0
39	B5	2208	OMC	2	0
39	B5	4052	OMU	1	0
39	B5	4325	PSU	1	0
39	B5	3599	A2M	2	0
1	A2	1338	4AC	3	0
1	A2	518	OMC	1	0
39	B5	1632	PSU	1	0
1	A2	1446	PSU	3	0
39	B5	3942	OMG	1	0
1	A2	172	OMU	2	0
39	B5	3450	A2M	2	0
1	A2	1843	4AC	2	0
39	B5	4282	OMC	1	0
39	B5	3456	A2M	1	0
39	B5	3524	OMG	1	0
1	A2	121	OMU	1	0
1	A2	1392	OMC	1	0
39	B5	2206	A2M	1	0
39	B5	2667	OMC	1	0
1	A2	99	A2M	1	0
39	B5	1580	OMG	1	0
39	B5	3974	OMG	1	0
1	A2	1032	A2M	2	0
1	A2	1833	6MZ	1	0
39	B5	1284	OMC	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A2	868	OMG	1	0
39	B5	2267	OMG	1	0
1	A2	1644	PSU	1	0
1	A2	116	OMU	1	0
1	A2	864	PSU	1	0
1	A2	463	OMC	1	0
39	B5	1638	PSU	1	0
1	A2	485	A2M	1	0
39	B5	4366	OMU	2	0
1	A2	437	OMG	1	0
1	A2	1348	PSU	2	0
39	B5	1260	OMG	1	0
1	A2	1805	OMU	2	0
39	B5	3562	A2M	1	0
39	B5	4202	OMC	1	0
39	B5	2194	OMC	1	0
39	B5	2658	A2M	1	0
39	B5	3502	PSU	2	0
39	B5	4336	A2M	1	0
1	A2	36	PSU	1	0
39	B5	2207	OMG	1	0
1	A2	1233	PSU	2	0
39	B5	3619	OMC	1	0
33	Au	1	AME	2	0
1	A2	1679	A2M	2	0
1	A2	1329	OMG	1	0
1	A2	27	A2M	1	0
39	B5	4203	PSU	1	0
1	A2	109	PSU	1	0
39	B5	3550	UY1	2	0
39	B5	3557	A2M	1	0
1	A2	355	OMU	1	0
39	B5	2647	OMC	1	0
39	B5	2719	OMG	1	0
1	A2	1852	MA6	1	0
39	B5	3631	OMG	1	0
1	A2	469	A2M	1	0
39	B5	2704	OMC	1	0
39	B5	3517	A2M	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 741 ligands modelled in this entry, 363 are monoatomic and 374 are unknown - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
93	GTP	B7	201	40	30,34,34	0.50	0	46,54,54	0.57	0
89	SPD	A2	1901	-	9,9,9	0.16	0	8,8,8	0.16	0
94	SF4	Bz	1000	88	0,12,12	-	-	-		
94	SF4	Bz	1001	88	0,12,12	-	-	-		

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
93	GTP	B7	201	40	-	0/22/38/38	0/3/3/3
89	SPD	A2	1901	-	-	0/7/7/7	-
94	SF4	Bz	1000	88	-	-	0/6/5/5
94	SF4	Bz	1001	88	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	A2	1901	SPD	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

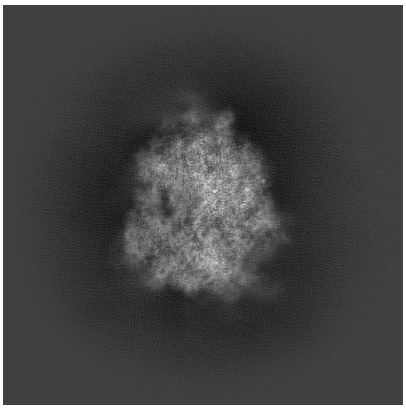
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12758. These allow visual inspection of the internal detail of the map and identification of artifacts.

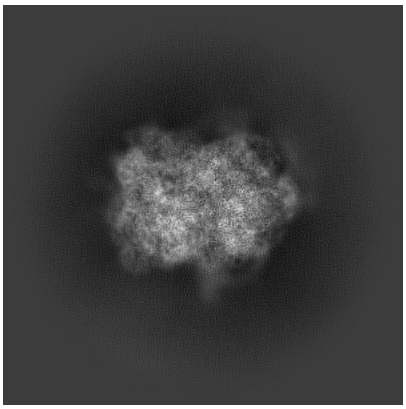
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

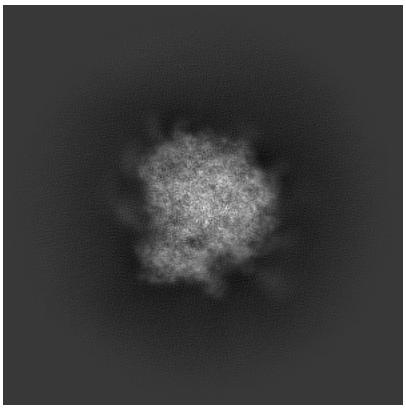
6.1.1 Primary map



X

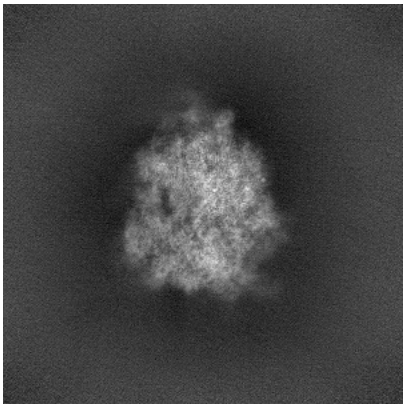


Y

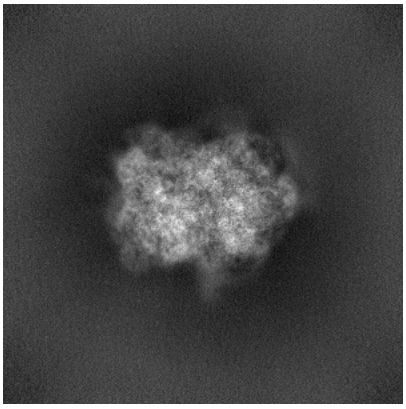


Z

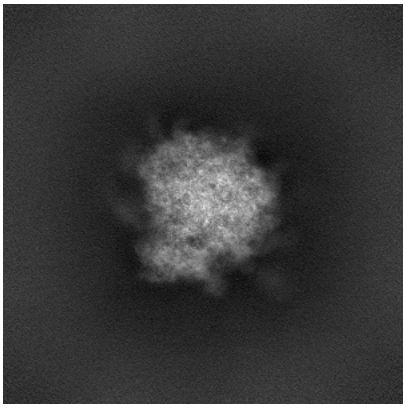
6.1.2 Raw map



X



Y

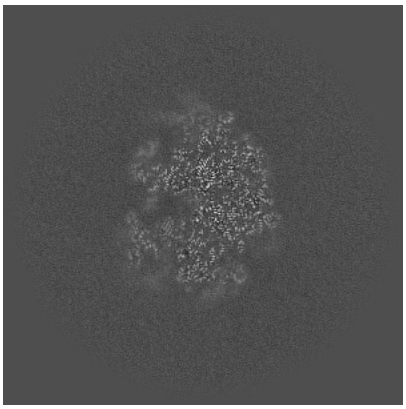


Z

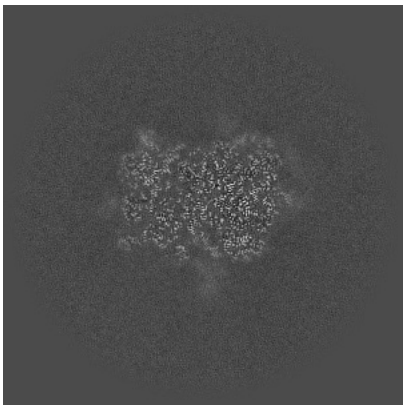
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

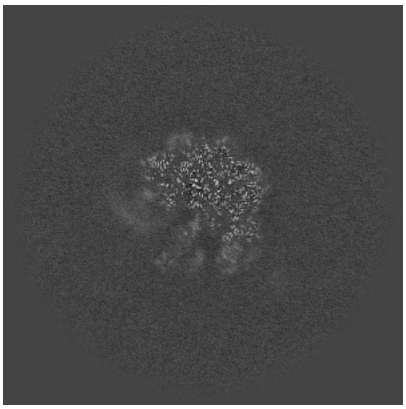
6.2.1 Primary map



X Index: 280

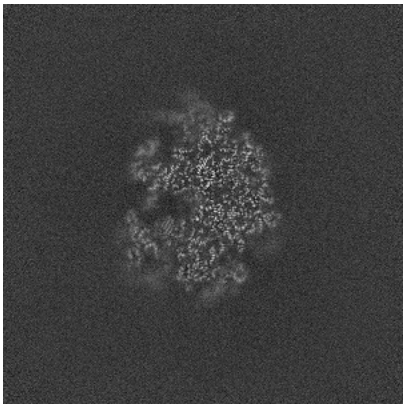


Y Index: 280

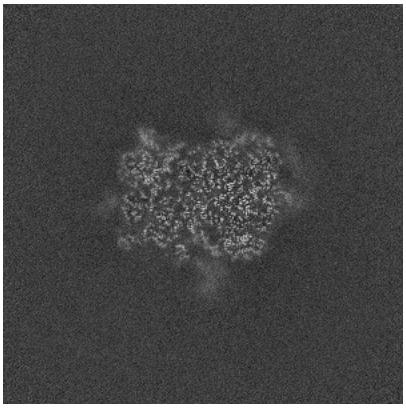


Z Index: 280

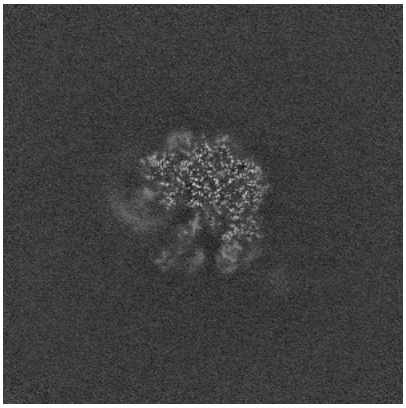
6.2.2 Raw map



X Index: 280



Y Index: 280

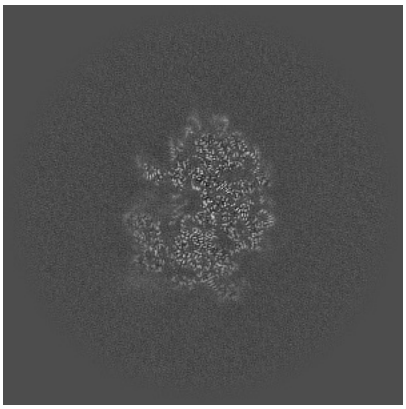


Z Index: 280

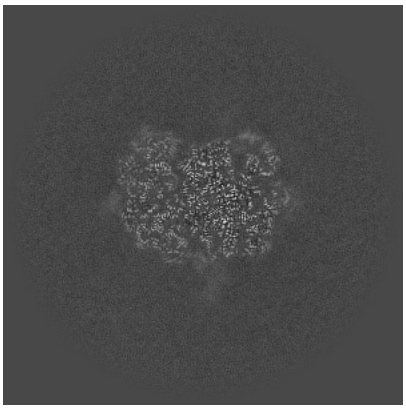
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

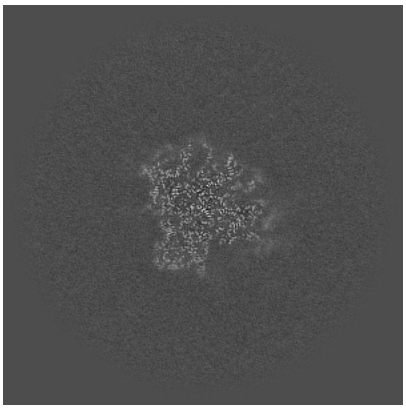
6.3.1 Primary map



X Index: 263

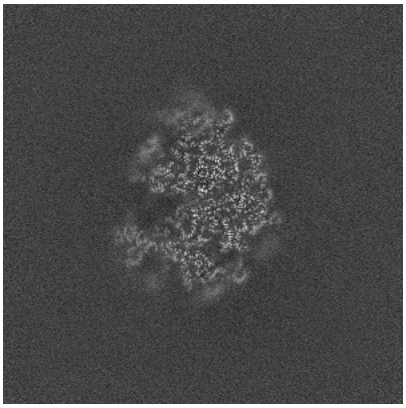


Y Index: 289

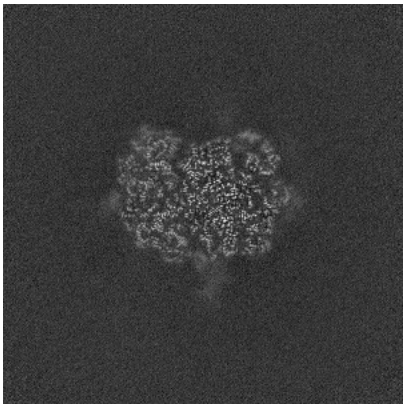


Z Index: 323

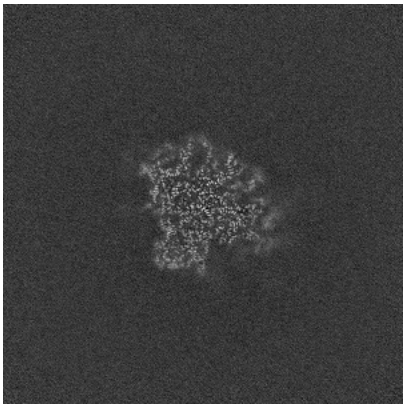
6.3.2 Raw map



X Index: 285



Y Index: 289

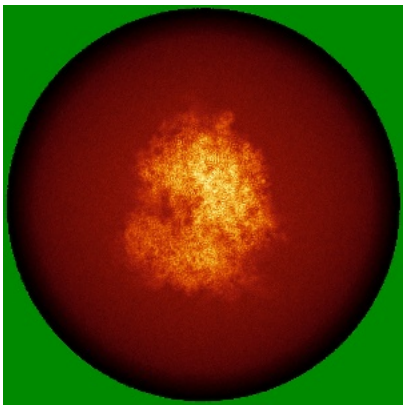


Z Index: 323

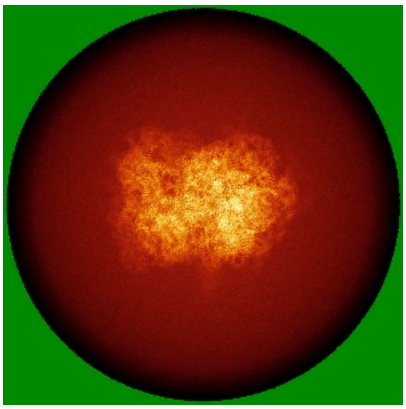
The images above show the largest variance slices of the map in three orthogonal directions.

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

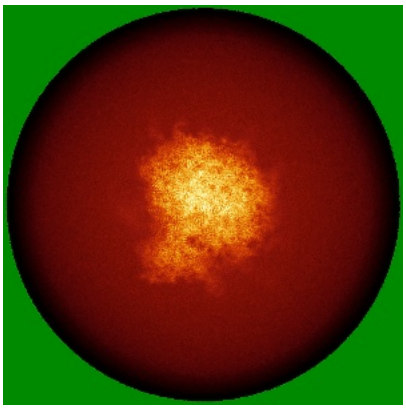
6.4.1 Primary map



X

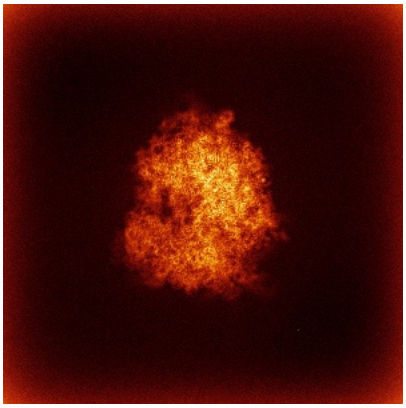


Y

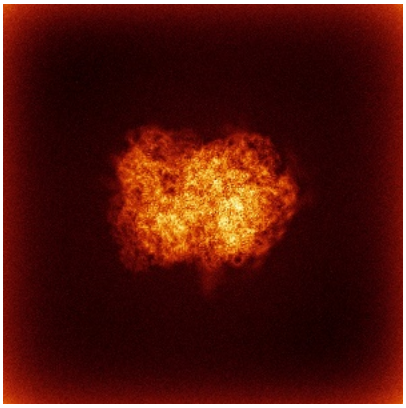


Z

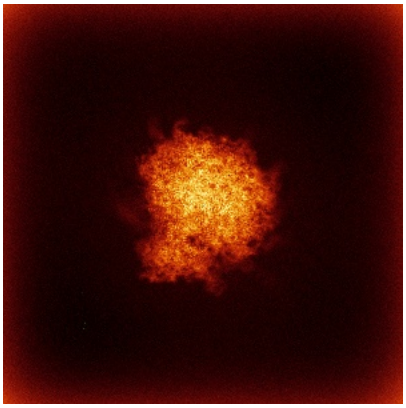
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. 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.

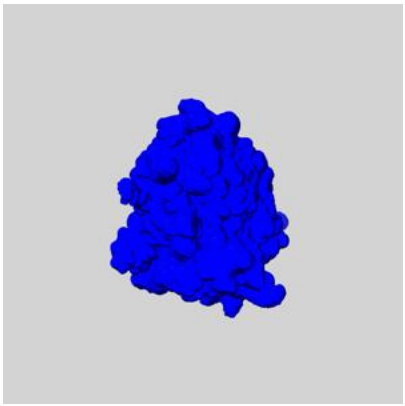
6.6 Mask visualisation

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

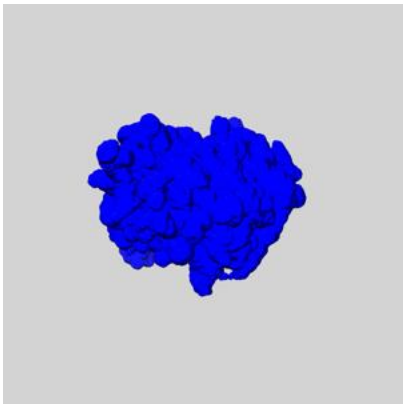
A mask typically either:

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

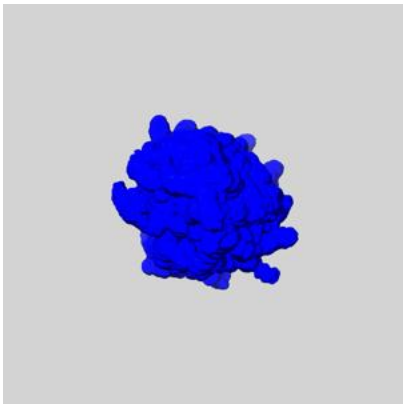
6.6.1 emd_12758_msk_1.map



X

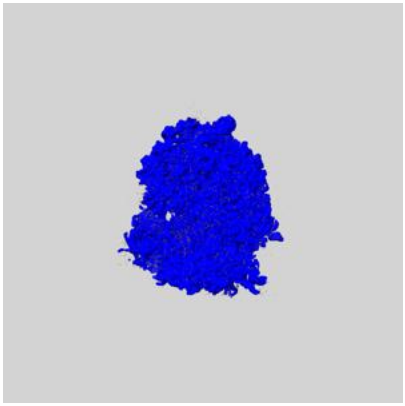


Y

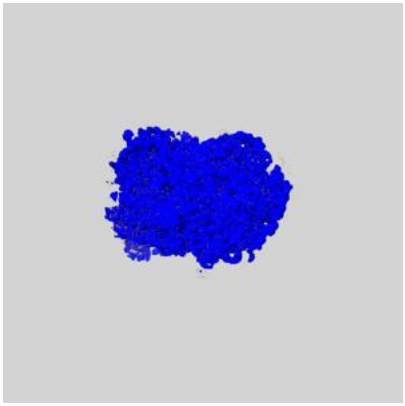


Z

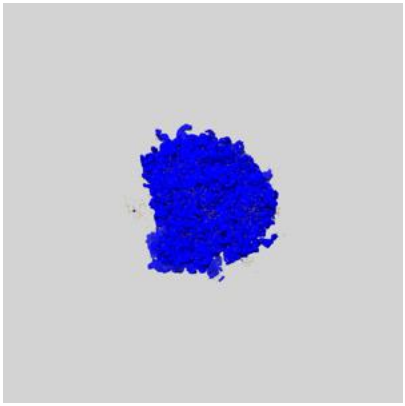
6.6.2 emd_12758_msk_2.map



X



Y

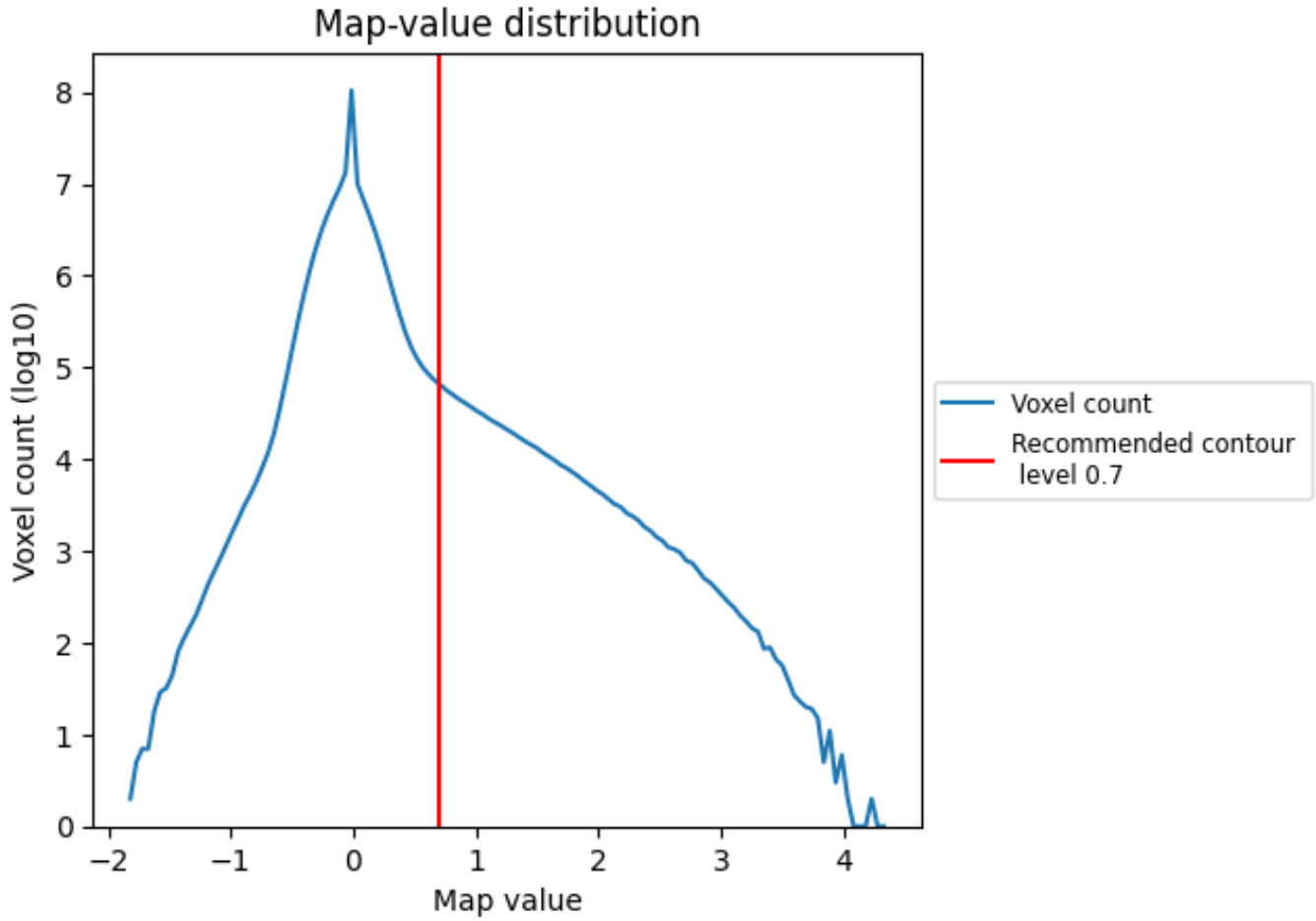


Z

7 Map analysis

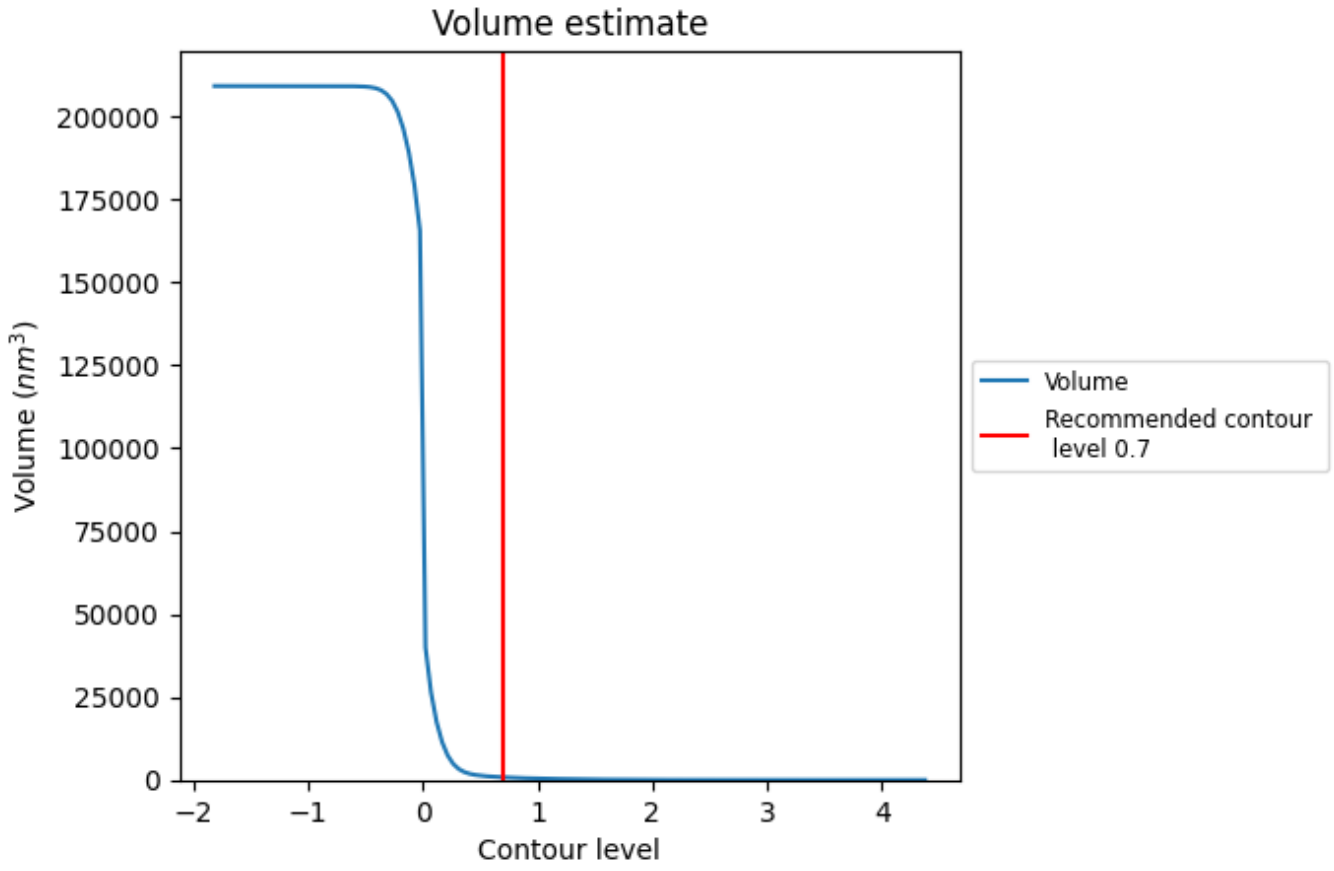
This section contains the results of statistical analysis of the map.

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.

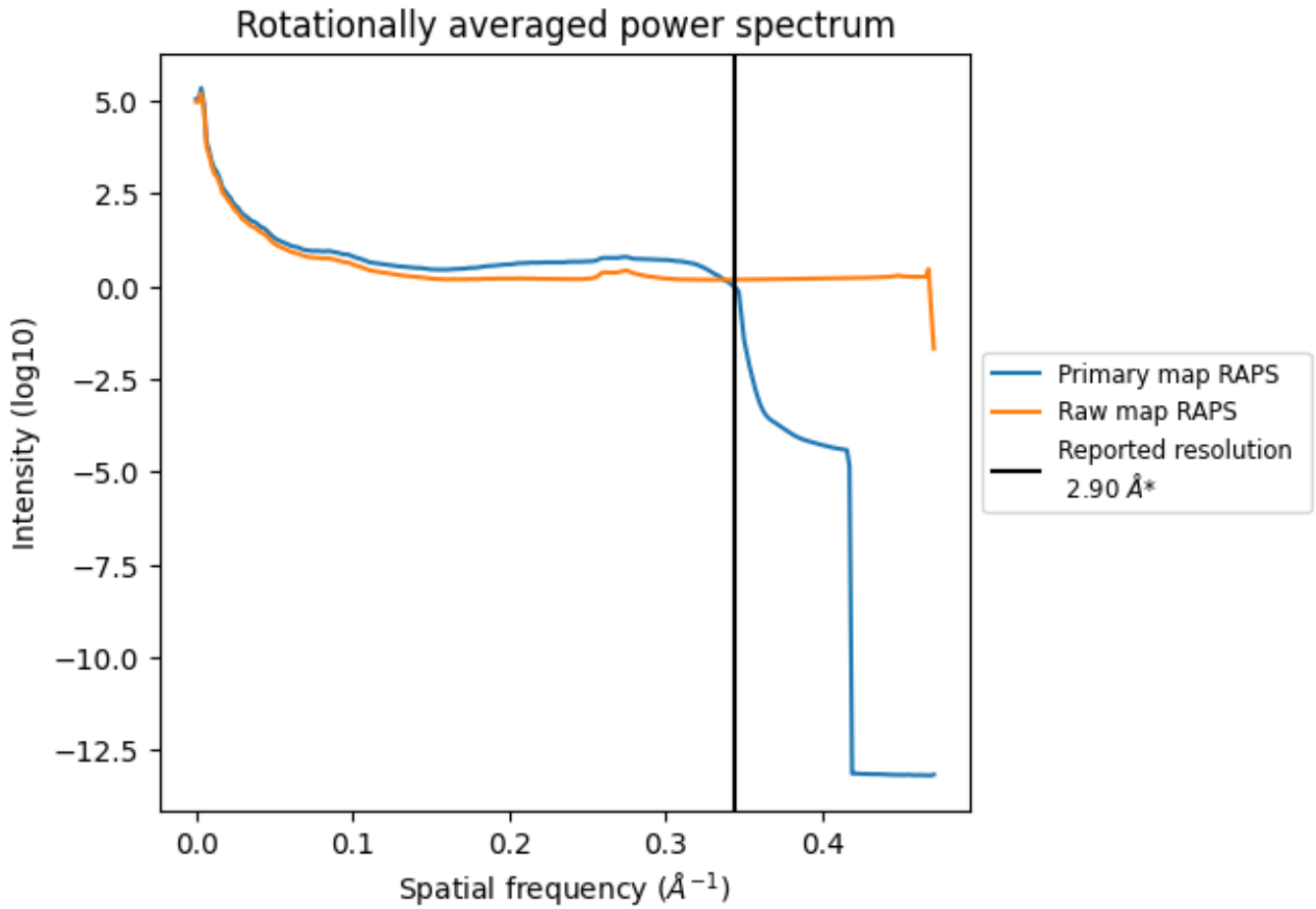
7.2 Volume estimate (i)



The volume at the recommended contour level is 803 nm^3; this corresponds to an approximate mass of 726 kDa.

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

7.3 Rotationally averaged power spectrum (i)

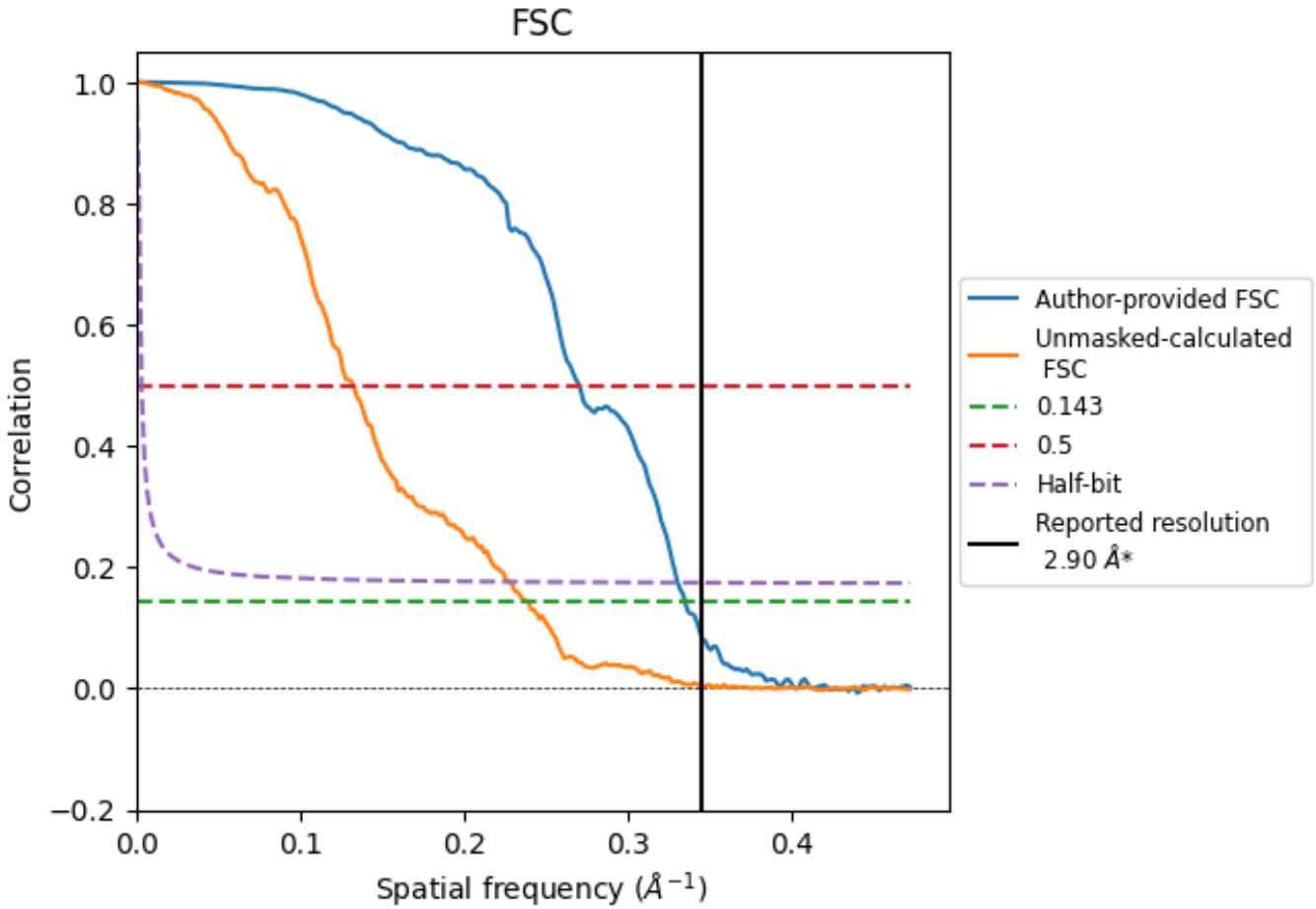


*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

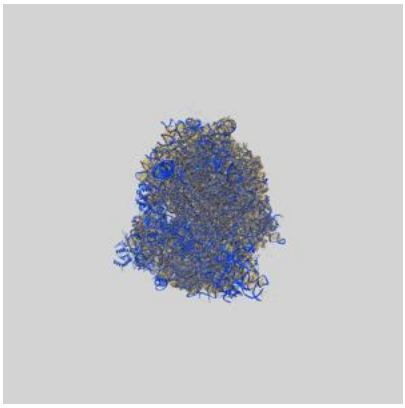
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.99	3.70	3.03
Unmasked-calculated*	4.18	7.56	4.39

*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 4.18 differs from the reported value 2.9 by more than 10 %

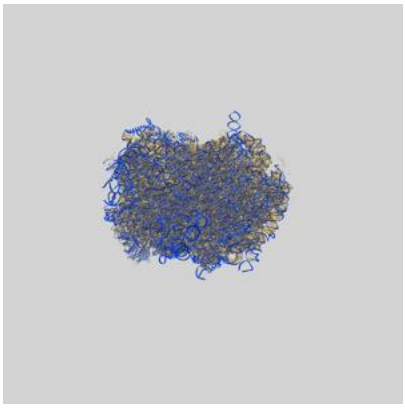
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12758 and PDB model 7O80. Per-residue inclusion information can be found in section 3 on page 27.

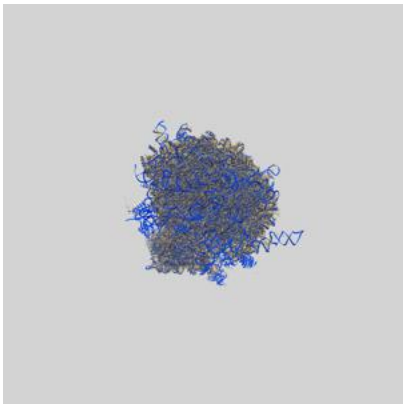
9.1 Map-model overlay



X



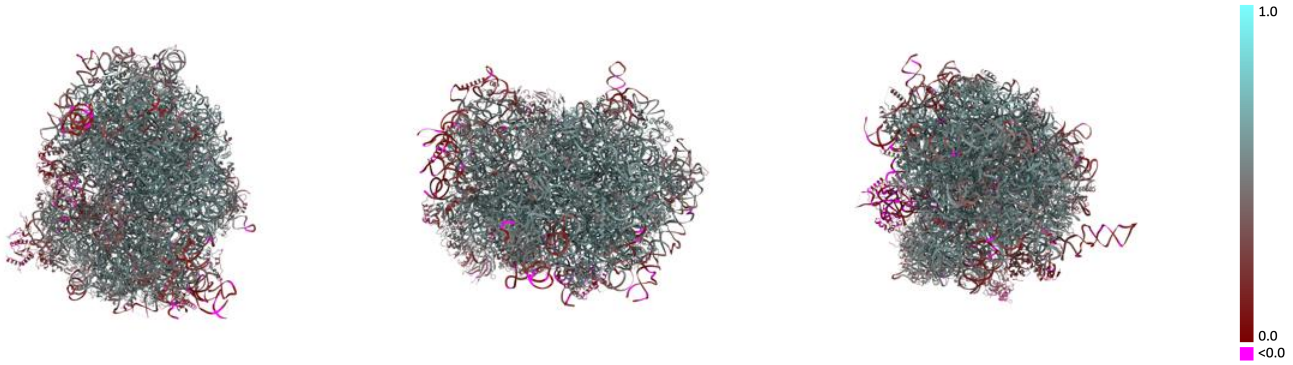
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7 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.

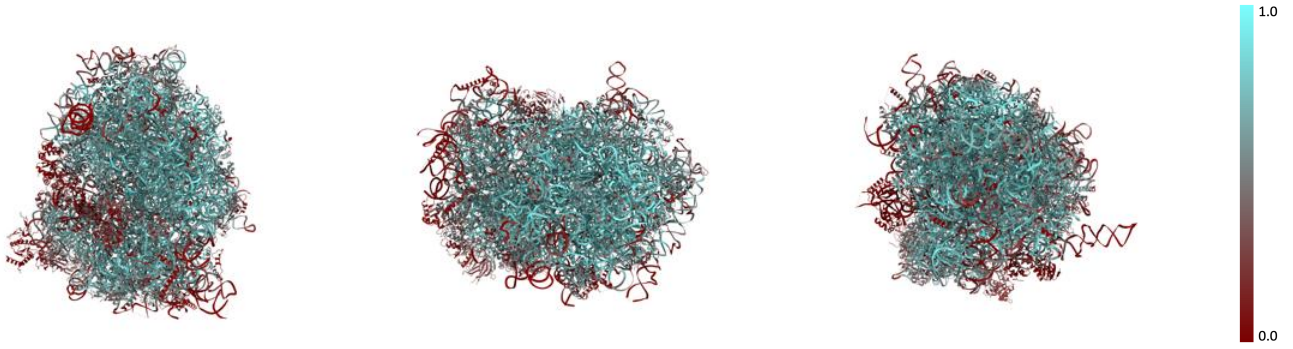
9.2 Q-score mapped to coordinate model



X Y Z

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.

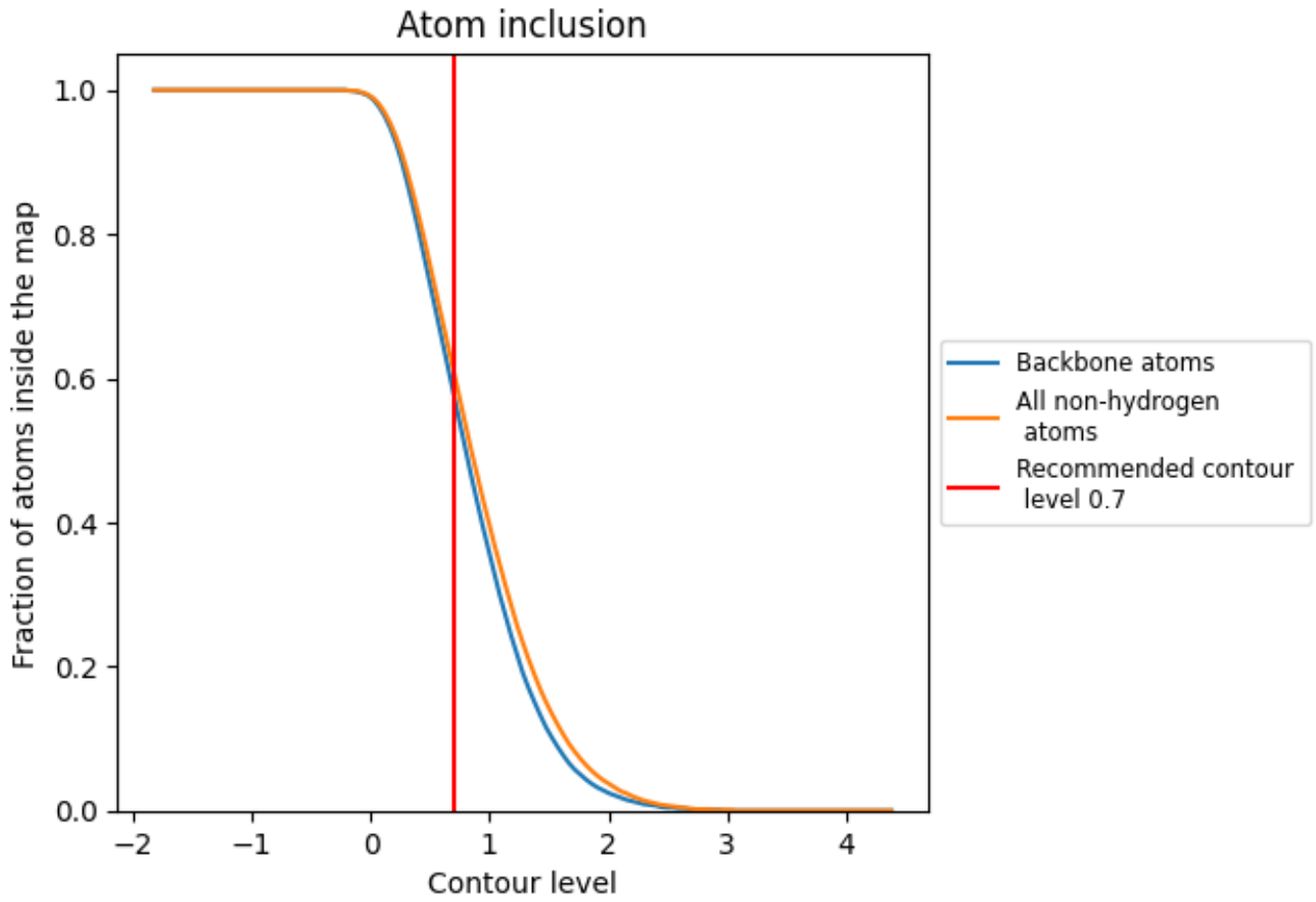
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.7).

9.4 Atom inclusion (i)



At the recommended contour level, 58% of all backbone atoms, 61% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6080	0.4970
A2	0.6790	0.5030
AA	0.4100	0.4750
AB	0.3560	0.4680
AC	0.0210	0.1980
AD	0.3750	0.4330
AE	0.5790	0.5190
AF	0.1850	0.3450
AG	0.5770	0.5200
AH	0.2650	0.3280
AI	0.0100	0.1090
AT	0.4490	0.4340
AZ	0.3900	0.4760
Aa	0.4740	0.4800
Ab	0.5260	0.5200
Ac	0.3110	0.4240
Ad	0.5380	0.5060
Ae	0.4370	0.4700
Af	0.3580	0.4040
Ag	0.2480	0.3870
Ah	0.5340	0.4990
Ai	0.5500	0.4970
Aj	0.2920	0.3860
Ak	0.5510	0.4940
Al	0.0050	0.1510
Am	0.5410	0.5240
An	0.5540	0.5200
Ao	0.3470	0.4200
Ap	0.4680	0.4910
Aq	0.2680	0.4070
Ar	0.4010	0.4430
As	0.4600	0.4640
At	0.2810	0.4000
Au	0.3950	0.4780
Av	0.6090	0.5500



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Chain	Atom inclusion	Q-score
Aw	0.5870	0.5400
Ax	0.4820	0.4650
Ay	0.3210	0.3960
Az	0.6560	0.5610
B5	0.7290	0.5210
B7	0.8580	0.5750
B8	0.7860	0.5590
BA	0.6980	0.5770
BB	0.6900	0.5660
BC	0.6970	0.5660
BD	0.5950	0.5100
BE	0.5100	0.4810
BF	0.7020	0.5670
BG	0.5180	0.4780
BH	0.5760	0.5180
BI	0.6030	0.5400
BJ	0.5070	0.4870
BK	0.0630	0.3010
BL	0.6260	0.5240
BM	0.6440	0.5360
BN	0.7770	0.5980
BO	0.7010	0.5720
BP	0.6800	0.5580
BQ	0.7070	0.5770
BR	0.6150	0.5190
BS	0.7060	0.5750
BT	0.6320	0.5470
BU	0.4380	0.4460
BV	0.6240	0.5550
BW	0.3690	0.3850
BX	0.6150	0.5370
BY	0.6650	0.5360
BZ	0.6100	0.5200
Ba	0.7550	0.5890
Bb	0.4760	0.4780
Bc	0.5350	0.4880
Bd	0.6380	0.5390
Be	0.7040	0.5740
Bf	0.7320	0.5880
Bg	0.6360	0.5480
Bh	0.6060	0.5260
Bi	0.5850	0.5210

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Chain	Atom inclusion	Q-score
Bj	0.7770	0.5920
Bk	0.4340	0.4540
Bl	0.7070	0.5710
Bm	0.6160	0.5460
Bo	0.5960	0.5370
Bp	0.6310	0.5550
Br	0.6530	0.5640
Bs	0.0200	0.1640
Bt	0.0330	0.2220
Bv	0.0000	0.0600
By	0.2280	0.4100
Bz	0.2530	0.3940