wwPDB EM Validation Summary Report (i)

Feb 22, 2024 – 11:57 AM EST

PDB ID	:	4V4N
EMDB ID	:	EMD-5691
Title	:	Structure of the Methanococcus jannaschii ribosome-SecYEBeta channel complex
Authors	:	Menetret, J.F.; Park, E.; Gumbart, J.C.; Ludtke, S.J.; Li, W.; Whynot, A.; Rapoport, T.A.; Akey, C.W.
Deposited on	:	2013-06-17
Resolution	:	9.00 Å(reported)
Based on initial models	:	3J20, 3J2L, 1RHZ, 3J21

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 (i) 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 (i)) were used in the production of this report:

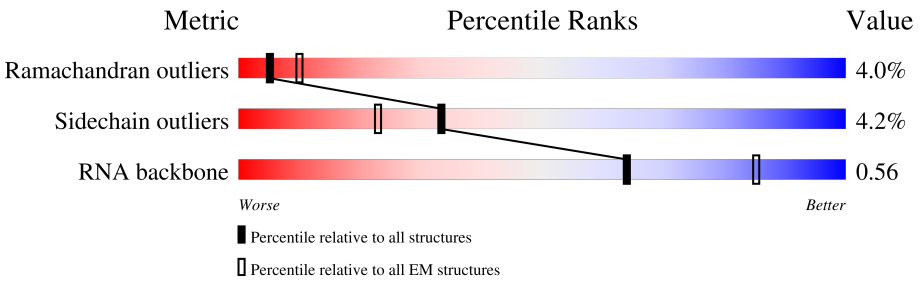
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 9.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	A7	67	7%, 72%, 24%
2	A8	52	54%, 6%, 38%
3	Af	51	65%, 59%, 39%
4	AQ	150	17%, 73%, 25%
5	AS	150	16%, 73%, 22%
6	AT	84	17%, 75%, 24%
7	AU	121	14%, 74%, 24%
8	AW	72	6%, 78%, 14%, 8%

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Mol	Chain	Length	Quality of chain
9	AX	436	7% 72% 25%
10	B1	77	43% 43% 14%
11	B2	1495	41% 48% 10%
12	AG	123	8% 85% 11%
12	B3	123	36% 81% 17%
13	BA	190	64% 31% 6%
14	BB	202	11% 74% 25%
15	BC	186	16% 75% 21%
16	BD	172	16% 76% 20%
17	BE	241	20% 69% 27%
18	BF	217	12% 74% 20% 5%
19	BG	125	6% 77% 19%
20	BH	215	17% 66% 25% 8%
21	BI	129	12% 79% 18%
22	BJ	127	16% 67% 30%
23	BK	135	30% 71% 25%
24	BL	102	19% 66% 27% 7%
25	BM	133	15% 72% 24%
26	BN	145	14% 71% 26%
27	BO	148	9% 75% 22%
28	BP	56	18% 66% 27% 7%
29	BQ	158	12% 73% 21% 5%
30	BR	113	19% 72% 23% 5%
31	BS	67	31% 78% 21%
32	BT	111	13% 72% 23%

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Mol	Chain	Length	Quality of chain
33	BU	144	19% 72% 24%
34	BV	99	13% 66% 25% 8%
35	BW	63	17% 73% 25%
36	BX	71	68% 27% 6%
37	BY	50	10% 74% 22%
38	A1	3049	40% 47% 11%
39	A3	126	5% 42% 40% 18%
40	A5	81	15% 77% 21%
40	AK	81	25% 68% 28%
41	AA	216	22% 73% 23%
42	Aa	92	17% 58% 29% 11%
43	AB	239	21% 72% 25%
44	Ab	127	23% 72% 21% 6%
45	AC	365	19% 70% 20% 6%
46	AD	255	22% 72% 25%
47	Ad	89	16% 65% 33%
48	AE	186	6% 77% 18% 5%
49	Ae	62	23% 60% 32% 8%
50	AF	184	8% 79% 20%
51	Ag	45	53% 60% 27% 11%
52	AH	134	7% 84% 14%
53	Ah	24	38% 71% 21% 8%
54	AI	142	18% 70% 26%
55	Ai	78	14% 73% 24%
56	AJ	132	17% 75% 20% 5%

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Mol	Chain	Length	Quality of chain
57	Aj	94	11% 60% 33% 7%
58	Ak	212	17% 79% 17%
59	AL	147	28% 71% 20% 8%
60	AM	194	26% 68% 27% 5%
61	AN	168	22% 68% 26% 5%
62	AO	197	12% 71% 25%
63	AP	120	8% 74% 22%
64	AR	95	18% 72% 23%
65	AV	66	14% 68% 26% 6%
66	AY	155	12% 79% 19%
67	AZ	99	77% 19%

2 Entry composition (i)

There are 67 unique types of molecules in this entry. The entry contains 171094 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 protein called Preprotein translocase subunit SecE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A7	65	525	348	85	91	1	0	0

- Molecule 2 is a protein called Preprotein translocase subunit SecG.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	A8	32	258	172	42	44	0	0

- Molecule 3 is a protein called 50S ribosomal protein L39E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Af	51	445	284	98	62	1	0	0

- Molecule 4 is a protein called 50S ribosomal protein L19E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AQ	150	1256	794	255	202	5	0	0

- Molecule 5 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AS	150	1200	764	230	202	4	0	0

- Molecule 6 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	AT	84	680	440	118	122	0	0

- Molecule 7 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	AU	121	1008	637	195	172	4	0	0

- Molecule 8 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	AW	66	546	338	105	99	4	0	0

- Molecule 9 is a protein called Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	AX	432	3309	2210	521	559	19	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	B1	77	1646	734	303	533	76	0	0

- Molecule 11 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	B2	1495	32132	14297	5954	10387	1494	0	0

- Molecule 12 is a protein called 30S ribosomal protein L7AE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	B3	123	939	599	155	181	4	0	0
12	AG	123	939	599	155	181	4	0	0

- Molecule 13 is a protein called 30S ribosomal protein S3AE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	BA	190	1559	1007	273	274	5	0	0

- Molecule 14 is a protein called 30S ribosomal protein S2P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	BB	202	1623	1046	282	290	5	0	0

- Molecule 15 is a protein called 30S ribosomal protein S3P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	BC	186	1460	933	271	252	4	0	0

- Molecule 16 is a protein called 30S ribosomal protein S4P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	BD	172	1434	902	273	255	4	0	0

- Molecule 17 is a protein called 30S ribosomal protein S4E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	BE	241	1976	1277	355	339	5	0	0

- Molecule 18 is a protein called 30S ribosomal protein S5P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	BF	217	1717	1084	319	306	8	0	0

- Molecule 19 is a protein called 30S ribosomal protein S6E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	BG	125	984	623	180	179	2	0	0

- Molecule 20 is a protein called 30S ribosomal protein S7P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	BH	215	1736	1100	326	302	8	0	0

- Molecule 21 is a protein called 30S ribosomal protein S8P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	BI	129	1028	668	178	180	2	0	0

- Molecule 22 is a protein called 30S ribosomal protein S8E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	BJ	127	1004	622	207	174	1	0	0

- Molecule 23 is a protein called 30S ribosomal protein S9P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	BK	135	1072	671	205	190	6	0	0

- Molecule 24 is a protein called 30S ribosomal protein S10P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	BL	102	822	507	159	152	4	0	0

- Molecule 25 is a protein called 30S ribosomal protein S11P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	BM	133	1004	623	200	179	2	0	0

- Molecule 26 is a protein called 30S ribosomal protein S12P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	BN	145	1141	722	223	193	3	0	0

- Molecule 27 is a protein called 30S ribosomal protein S13P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	BO	148	1189	746	237	200	6	0	0

- Molecule 28 is a protein called 30S ribosomal protein S14P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	BP	56	462	292	95	69	6	0	0

- Molecule 29 is a protein called 30S ribosomal protein S15P/S13E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	BQ	158	1310	834	250	221	5	0	0

- Molecule 30 is a protein called 30S ribosomal protein S17P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	BR	113	934	592	177	160	5	0	0

- Molecule 31 is a protein called 30S ribosomal protein S17E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	BS	67	556	353	105	95	3	0	0

- Molecule 32 is a protein called 30S ribosomal protein S19P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	BT	111	924	594	173	151	6	0	0

- Molecule 33 is a protein called 30S ribosomal protein S19E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	BU	144	1176	758	212	205	1	0	0

- Molecule 34 is a protein called 30S ribosomal protein S24E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	BV	99	823	532	134	154	3	0	0

- Molecule 35 is a protein called 30S ribosomal protein S27E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	BW	63	478	306	85	81	6	0	0

- Molecule 36 is a protein called 30S ribosomal protein S28E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	BX	71	568	345	115	107	1	0	0

- Molecule 37 is a protein called 30S ribosomal protein S27AE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	BY	50	409	262	75	66	6	0	0

- Molecule 38 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
38	A1	2969	63885	28427	11905	20589	2964	0	0

- Molecule 39 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
39	A3	126	2691	1199	492	875	125	0	0

- Molecule 40 is a protein called 50S ribosomal protein L14E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	A5	81	614	386	119	108	1	0	0
40	AK	81	614	386	119	108	1	0	0

- Molecule 41 is a protein called 50S ribosomal protein L1P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	AA	216	1677	1068	300	304	5	0	0

- Molecule 42 is a protein called 50S ribosomal protein L31E.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	Aa	82	677	444	126	107	0	0

- Molecule 43 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	AB	239	1838	1169	347	317	5	0	0

- Molecule 44 is a protein called 50S ribosomal protein L32E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Ab	127	1075	689	217	168	1	0	0

- Molecule 45 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	AC	342	2717	1741	495	467	14	0	0

- Molecule 46 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	AD	255	2026	1288	391	342	5	0	0

- Molecule 47 is a protein called 50S ribosomal protein L34E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	Ad	89	740	463	158	108	11	0	0

- Molecule 48 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	AE	186	1489	937	278	265	9	0	0

- Molecule 49 is a protein called 50S ribosomal protein L37E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	Ae	62	506	312	111	78	5	0	0

- Molecule 50 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	AF	184	1476	956	252	266	2	0	0

- Molecule 51 is a protein called 50S ribosomal protein L40E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	Ag	45	372	236	76	56	4	0	0

- Molecule 52 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	AH	134	989	635	164	184	6	0	0

- Molecule 53 is a protein called 50S ribosomal protein L41E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	Ah	24	230	147	54	28	1	0	0

- Molecule 54 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	AI	142	1150	737	215	195	3	0	0

- Molecule 55 is a protein called 50S ribosomal protein L37AE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	Ai	78	590	368	122	95	5	0	0

- Molecule 56 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	AJ	132	1014	631	204	176	3	0	0

- Molecule 57 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	Aj	94	788	499	162	122	5	0	0

- Molecule 58 is a protein called 50S ribosomal protein P0/L10E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	Ak	212	1633	1051	272	304	6	0	0

- Molecule 59 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	AL	147	1154	727	227	195	5	0	0

- Molecule 60 is a protein called 50S ribosomal protein L15E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	AM	194	1595	1020	316	253	6	0	0

- Molecule 61 is a protein called 50S ribosomal protein L10E/L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	AN	168	1379	872	268	233	6	0	0

- Molecule 62 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	AO	197	1598	1021	299	275	3	0	0

- Molecule 63 is a protein called 50S ribosomal protein L18E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	AP	120	966	606	186	171	3	0	0

- Molecule 64 is a protein called 50S ribosomal protein L21E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	AR	95	787	501	160	125	1	0	0

- Molecule 65 is a protein called 50S ribosomal protein L24E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	AV	66	555	351	106	91	7	0	0

- Molecule 66 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	AY	155	1243	788	235	213	7	0	0

- Molecule 67 is a protein called 50S ribosomal protein L30E.

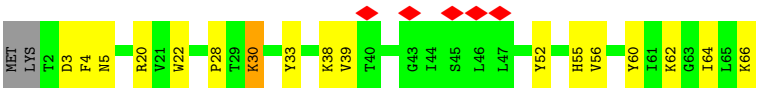
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	AZ	99	754	489	121	142	2	0	0

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.

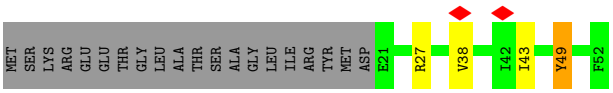
- Molecule 1: Preprotein translocase subunit SecE

Chain A7:



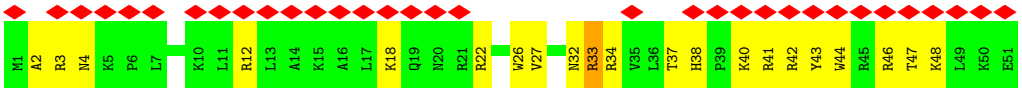
- Molecule 2: Preprotein translocase subunit SecG

Chain A8:



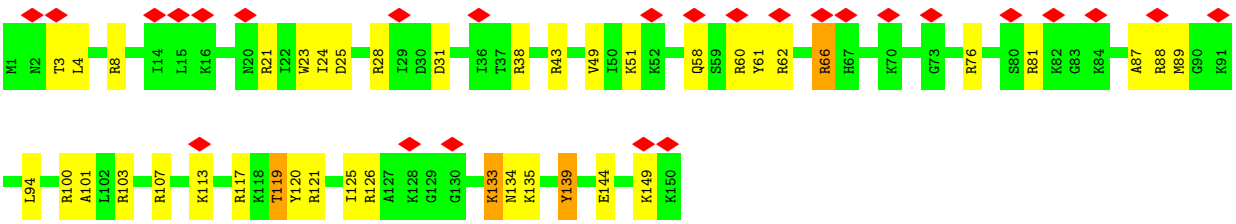
- Molecule 3: 50S ribosomal protein L39E

Chain Af:



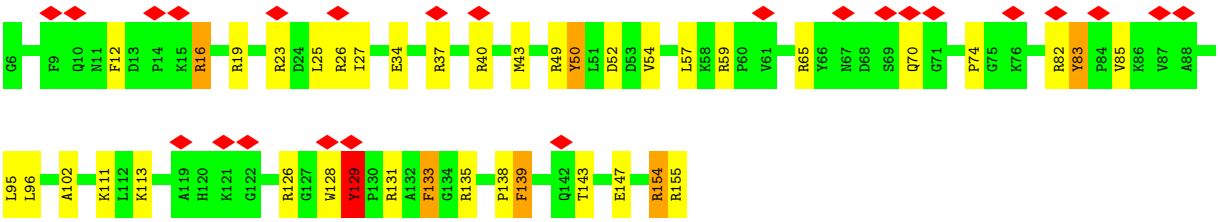
- Molecule 4: 50S ribosomal protein L19E

Chain AQ:



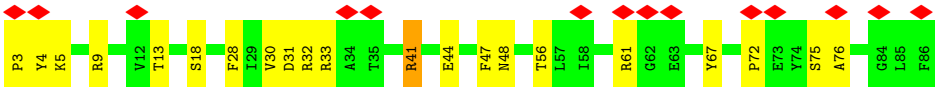
- Molecule 5: 50S ribosomal protein L22P

Chain AS:



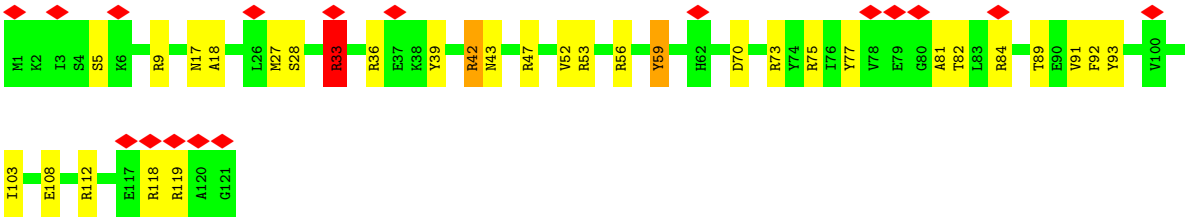
- Molecule 6: 50S ribosomal protein L23P

Chain AT:



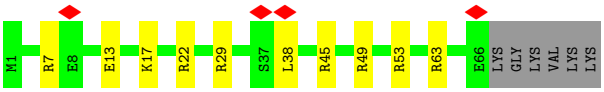
- Molecule 7: 50S ribosomal protein L24P

Chain AU:



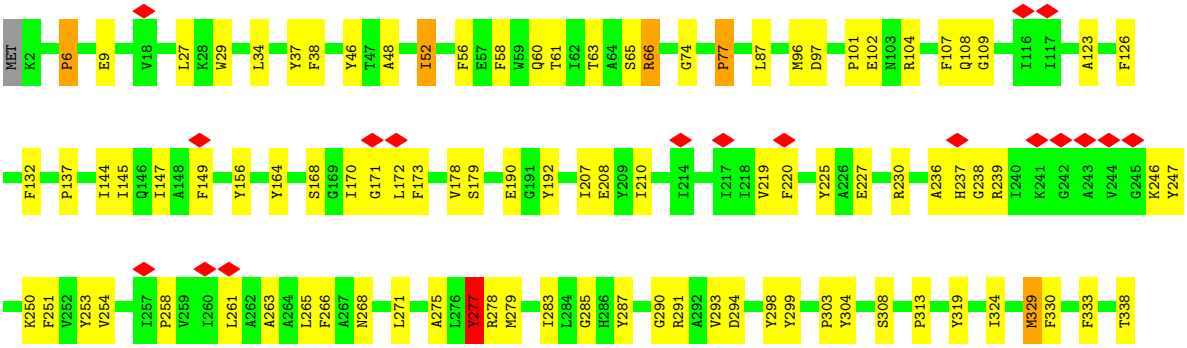
- Molecule 8: 50S ribosomal protein L29P

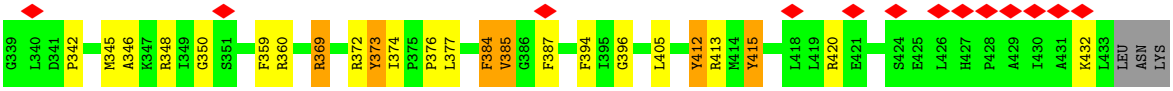
Chain AW:



- Molecule 9: Protein translocase subunit SecY

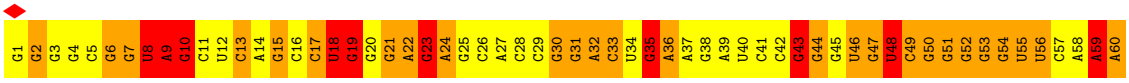
Chain AX:





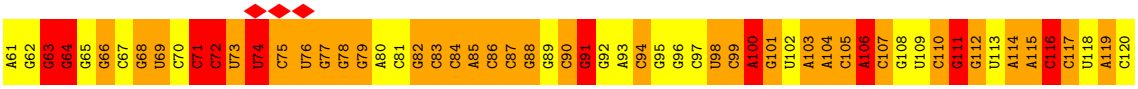
- Molecule 10: E-tRNA

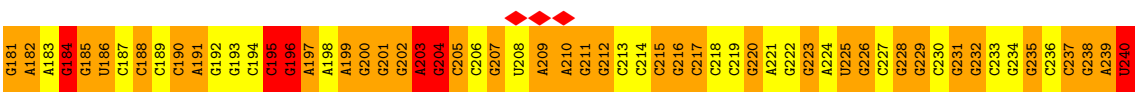
Chain B1:

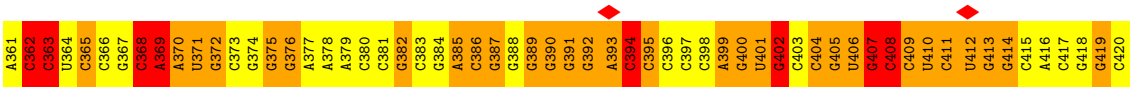


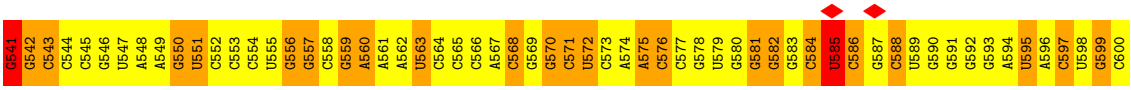
- Molecule 11: 16S ribosomal RNA

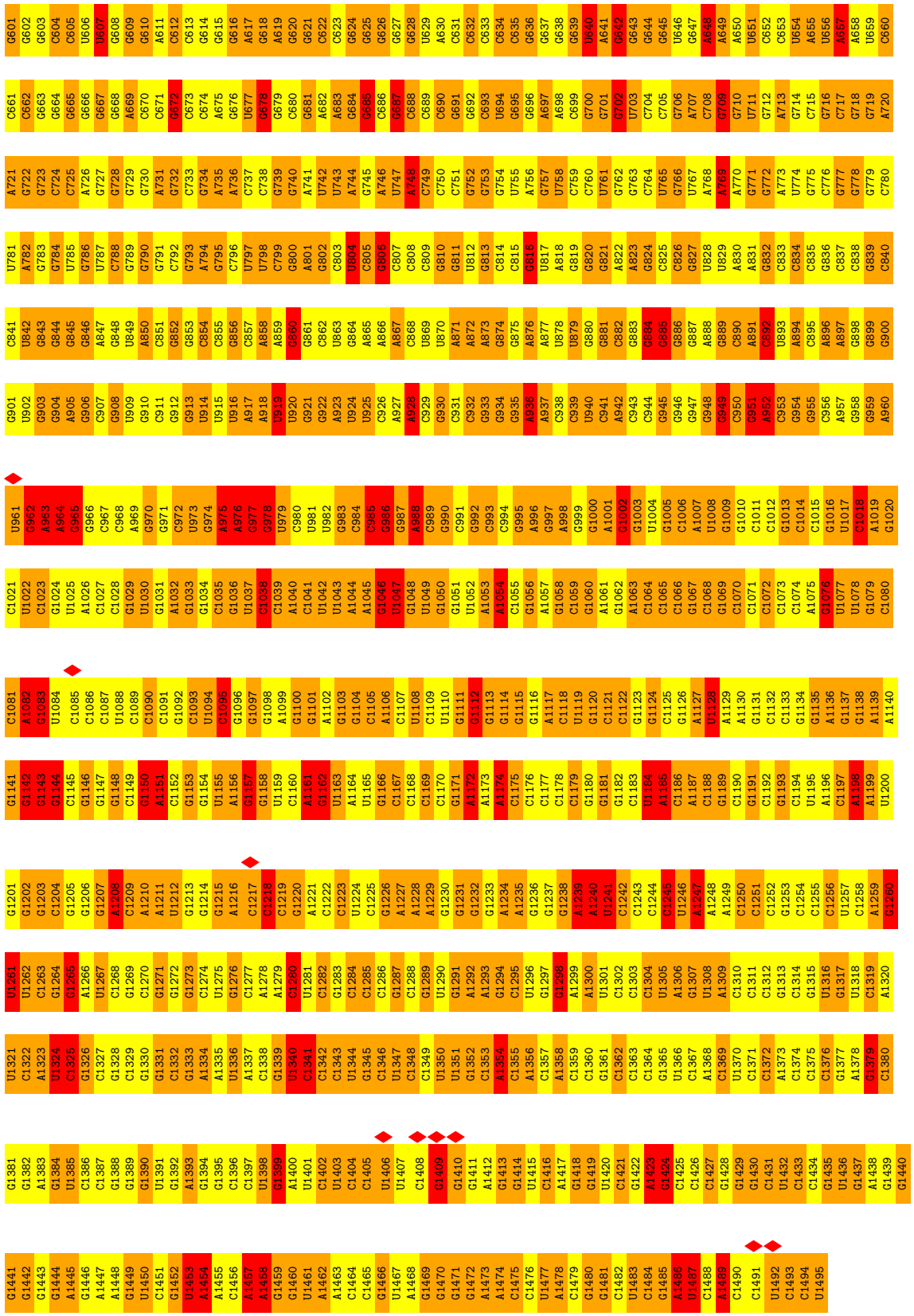
Chain B2:





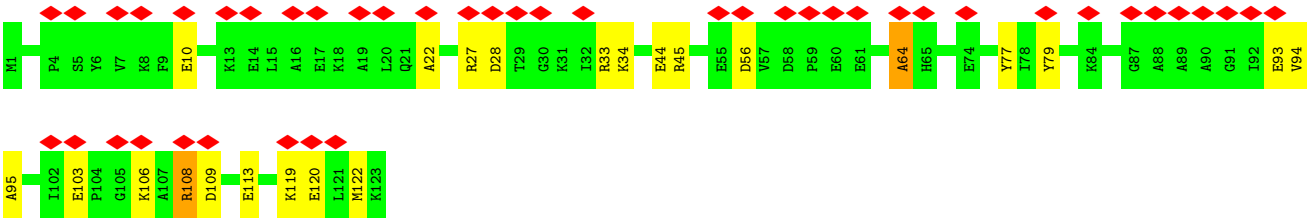






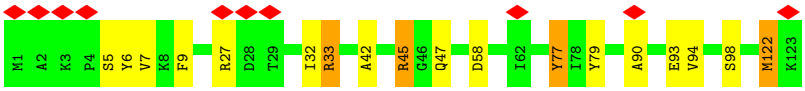
• Molecule 12: 30S ribosomal protein L7AE

Chain B3:



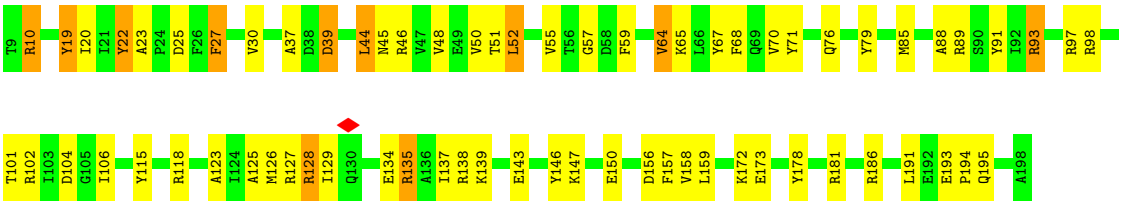
• Molecule 12: 30S ribosomal protein L7AE

Chain AG:



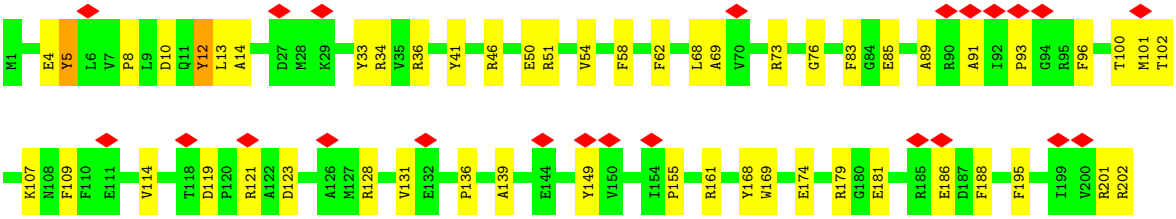
• Molecule 13: 30S ribosomal protein S3AE

Chain BA:



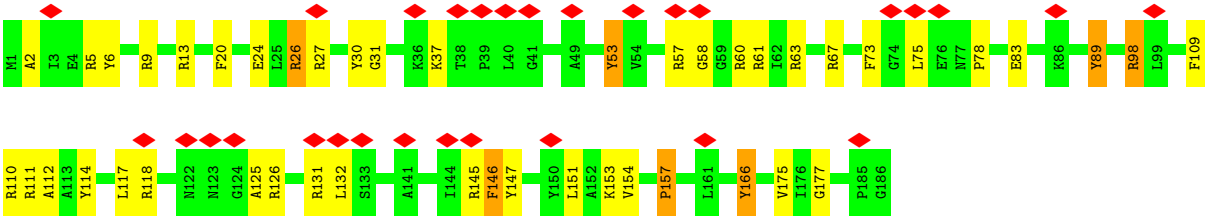
• Molecule 14: 30S ribosomal protein S2P

Chain BB:



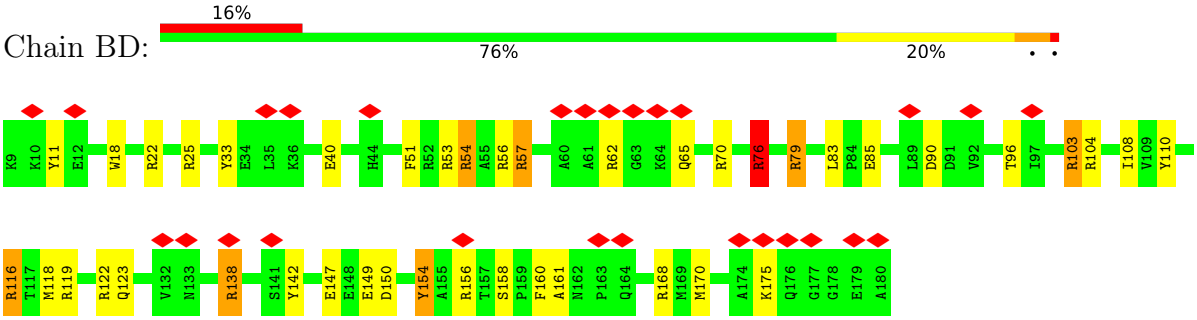
• Molecule 15: 30S ribosomal protein S3P

Chain BC:



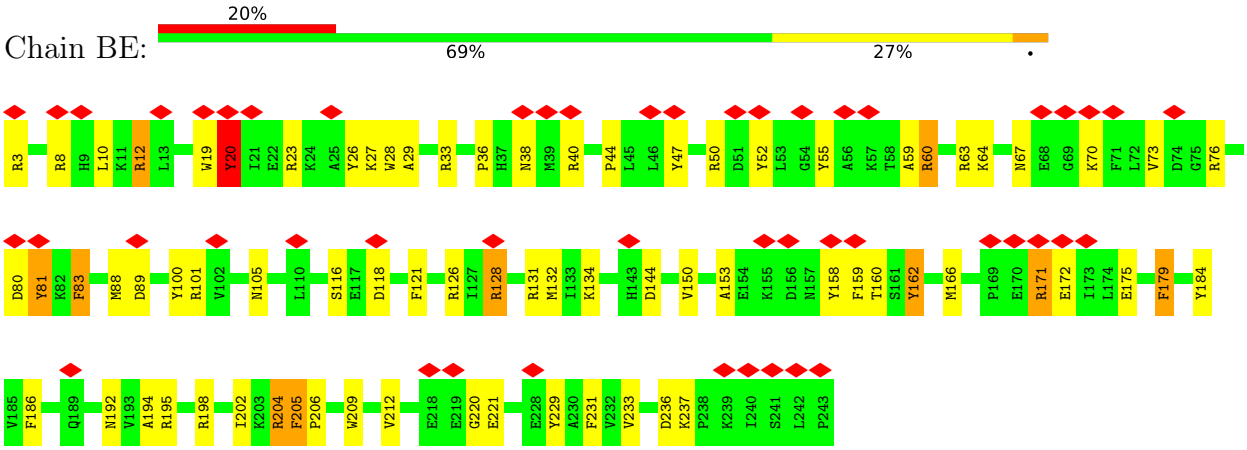
• Molecule 16: 30S ribosomal protein S4P

Chain BD:



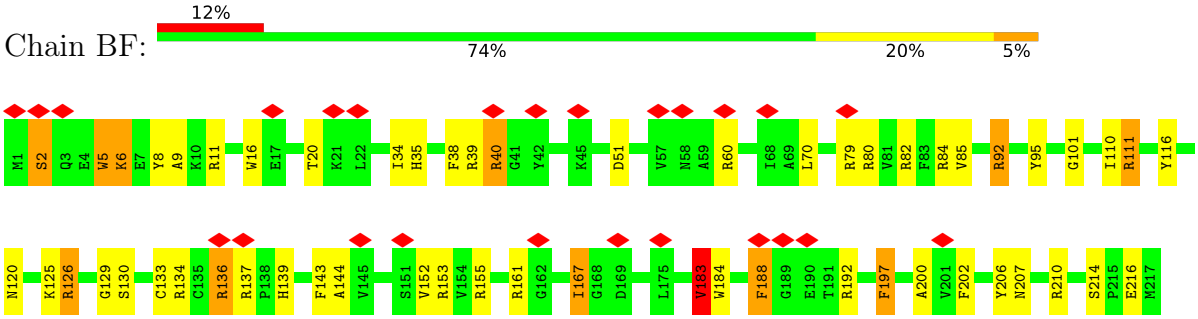
- Molecule 17: 30S ribosomal protein S4E

Chain BE:



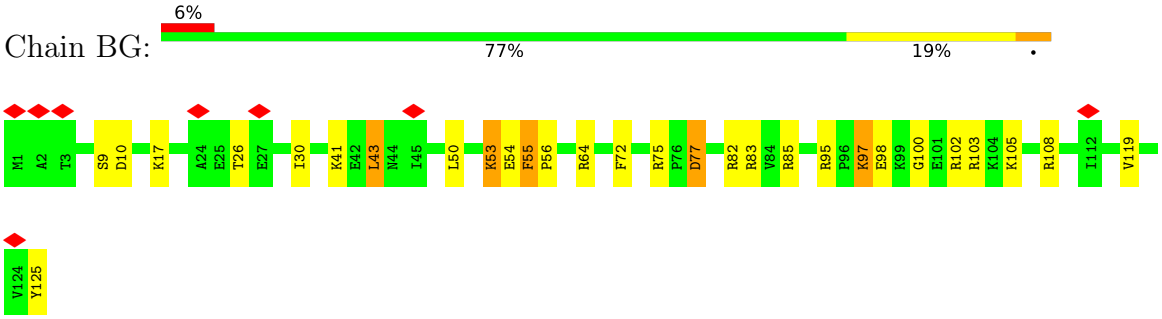
- Molecule 18: 30S ribosomal protein S5P

Chain BF:



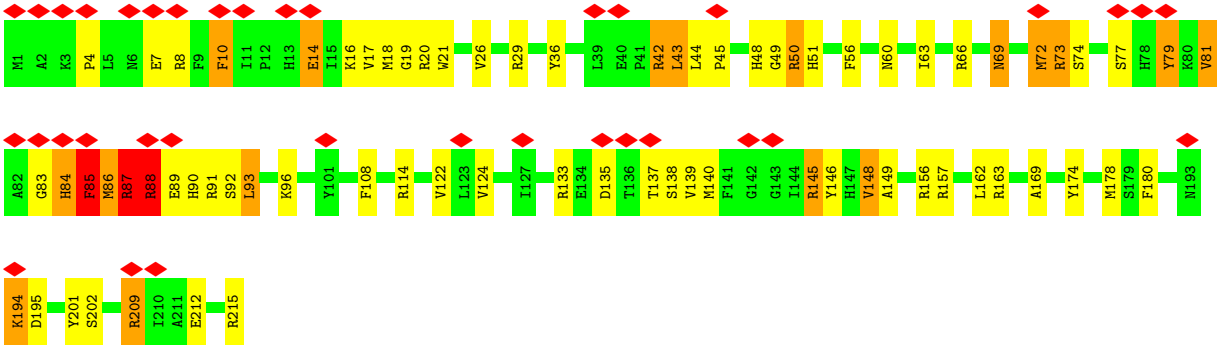
- Molecule 19: 30S ribosomal protein S6E

Chain BG:



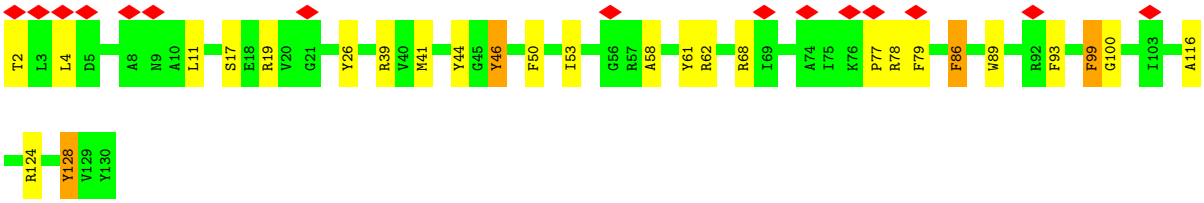
- Molecule 20: 30S ribosomal protein S7P

Chain BH:



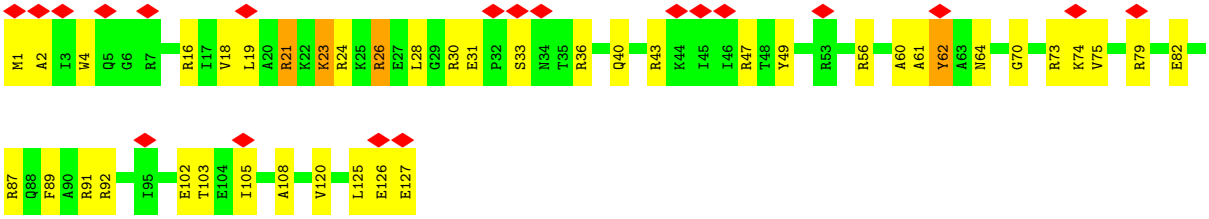
- Molecule 21: 30S ribosomal protein S8P

Chain BI:



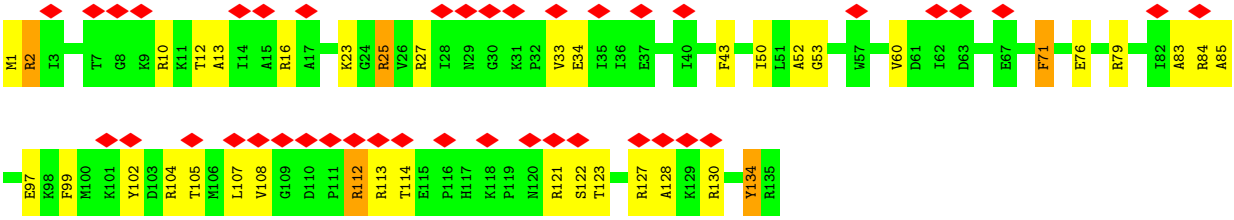
- Molecule 22: 30S ribosomal protein S8E

Chain BJ:



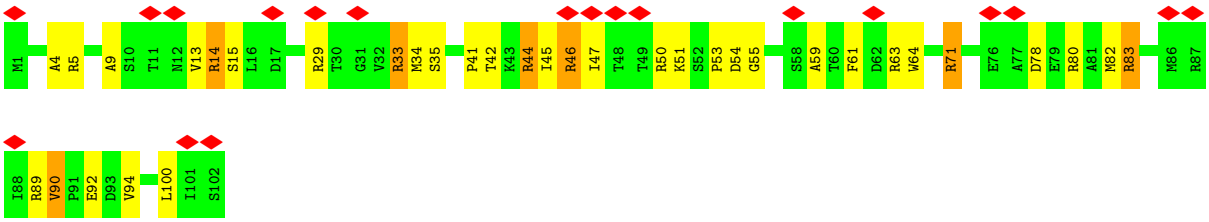
- Molecule 23: 30S ribosomal protein S9P

Chain BK:



- Molecule 24: 30S ribosomal protein S10P

Chain BL:

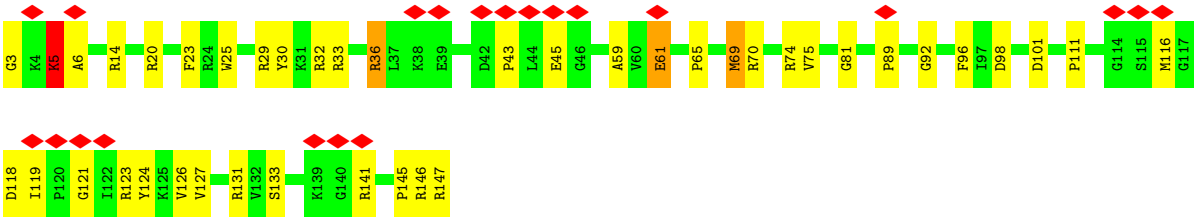


- Molecule 25: 30S ribosomal protein S11P

Chain BM:

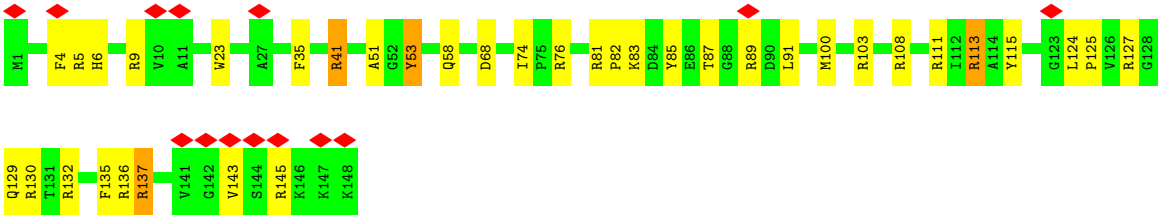
- Molecule 26: 30S ribosomal protein S12P

Chain BN:



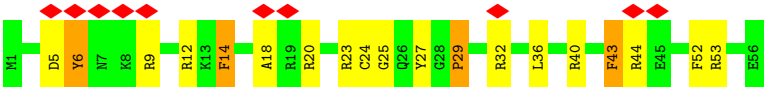
- Molecule 27: 30S ribosomal protein S13P

Chain BO:



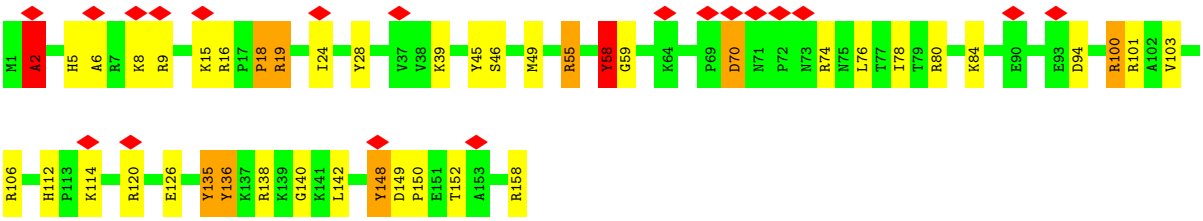
- Molecule 28: 30S ribosomal protein S14P

Chain BP:



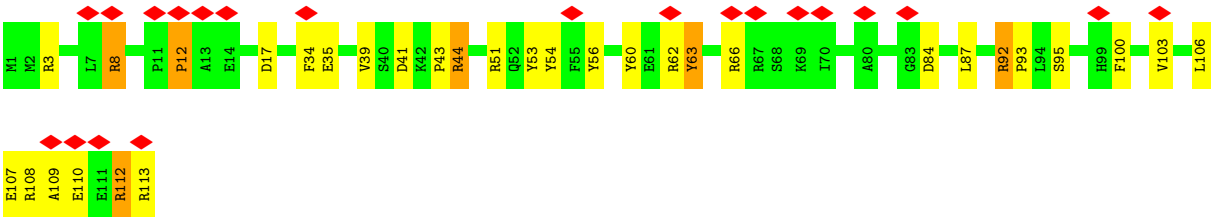
- Molecule 29: 30S ribosomal protein S15P/S13E

Chain BQ: 12% 73% 21% 5%



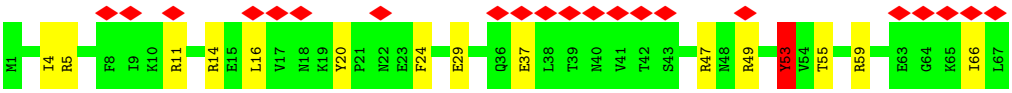
- Molecule 30: 30S ribosomal protein S17P

Chain BR: 19% 72% 23% 5%



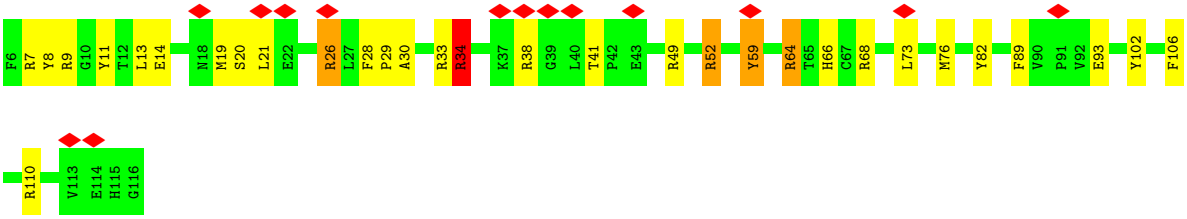
- Molecule 31: 30S ribosomal protein S17E

Chain BS: 31% 78% 21%



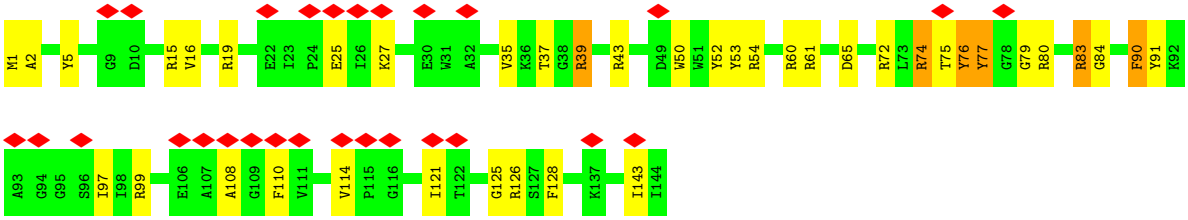
- Molecule 32: 30S ribosomal protein S19P

Chain BT: 13% 72% 23%



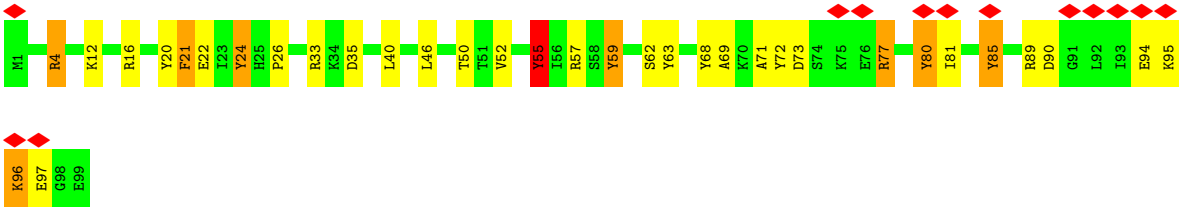
- Molecule 33: 30S ribosomal protein S19E

Chain BU: 19% 72% 24%



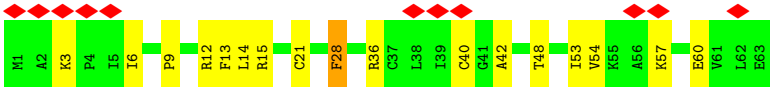
- Molecule 34: 30S ribosomal protein S24E

Chain BV:



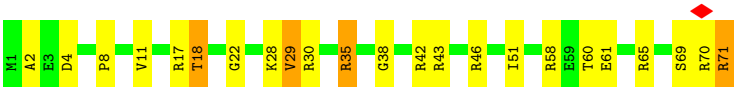
- Molecule 35: 30S ribosomal protein S27E

Chain BW:



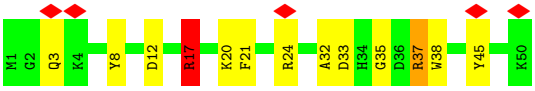
- Molecule 36: 30S ribosomal protein S28E

Chain BX:



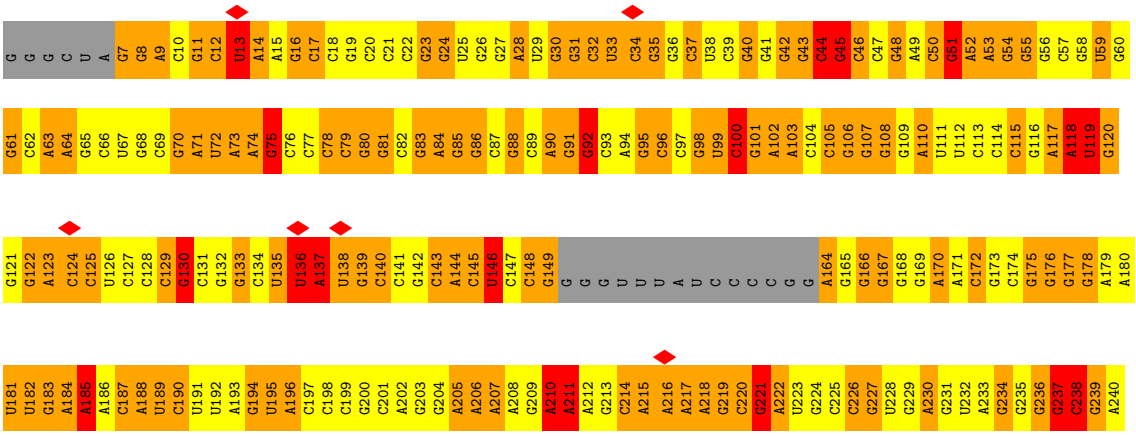
- Molecule 37: 30S ribosomal protein S27AE

Chain BY:



- Molecule 38: 23S ribosomal RNA

Chain A1:



C241 C242 G243 A244 A245 A246 A247 C248 C249 G250 C251 A252 G253 A254 G255 G256 G257 C258 A259 A260 A261 C262 U263 C264 A265 A266 C267 C268 C269 C270 G271 G272 G273 C274 C275 G276 A277 C278 G279 A280 G281 G282 U283 U284 C285 G286 G287 G288 G289 G290 A291 U292 G293 U294 G295 G296 G297 G298 U299 U300
G301 U302 A303 G304 G305 G306 C307 C308 C309 C310 C311 G312 U313 A314 U315 G316 A317 G318 A319 C320 C321 C322 U323 C324 G325 C326 G327 G328 G329 U330 G331 A332 A333 G334 C335 C336 G337 A338 A339 G340 U341 C342 C343 G344 C345 U346 G347 G348 A349 A350 G351 G352 C353 G354 G355 C356 G357 C358 C359 G360
G361 A362 G363 A364 G365 G366 G367 U368 G369 A370 U371 A372 G373 C374 C375 C376 C377 G378 U379 A380 G381 G382 C383 G384 U385 A386 G387 G388 C389 C390 C391 G392 C393 A394 G395 G396 G397 U398 C399 U400 C401 G402 G403 G404 G405 G406 A407 C408 C409 C410 U411 G412 A413 G414 U415 A416 C417 C418 G419 U420
C421 G422 G423 U424 U425 G426 G427 A428 U429 A430 U431 C432 C433 G434 G435 C436 G437 G438 G439 A440 A441 G442 C443 U444 G445 G446 G447 A448 G449 G450 C451 A452 U453 C454 G455 G456 C457 U458 C459 C460 C461 A462 A463 C464 C465 C466 U467 A468 A469 A470 U471 A472 C473 G474 G414 U475 C476 C477 C478 G479 A480
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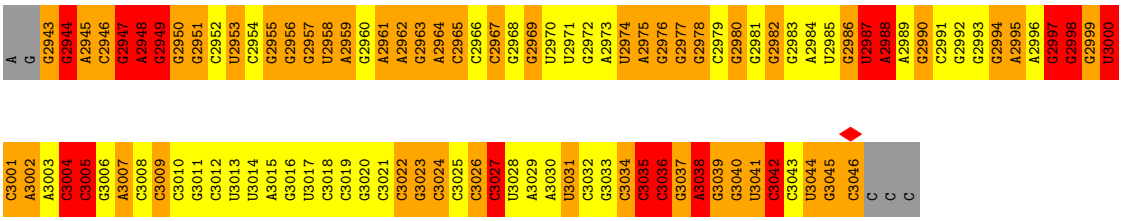

• Molecule 39: 5S ribosomal RNA

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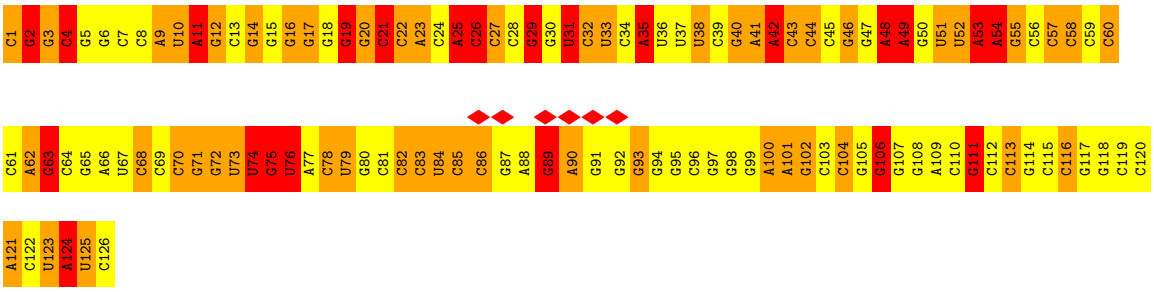
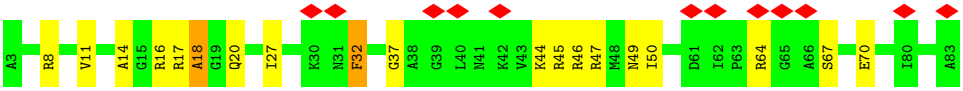


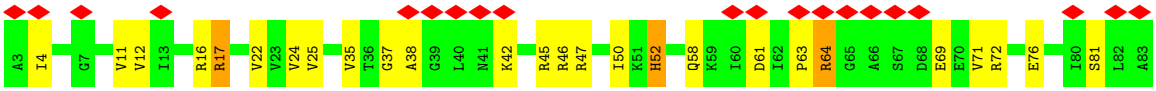
• Molecule 40: 50S ribosomal protein L14E

Chain A5:



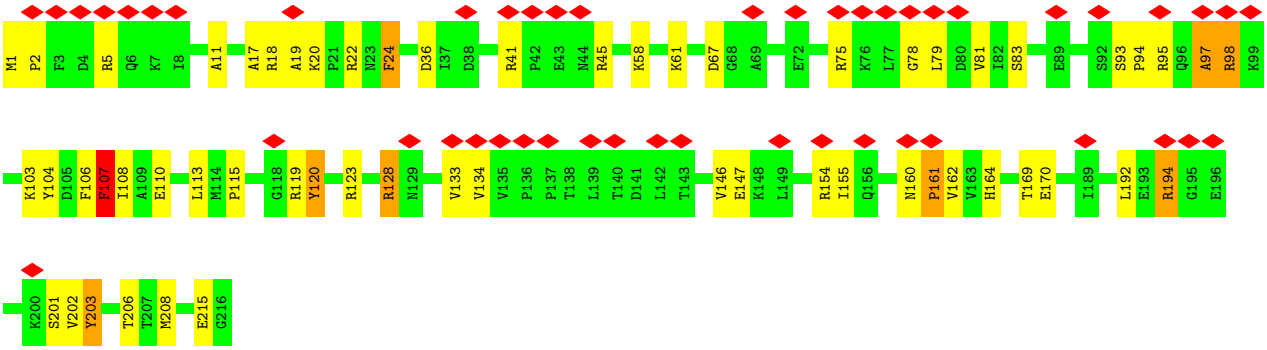
• Molecule 40: 50S ribosomal protein L14E

Chain AK:



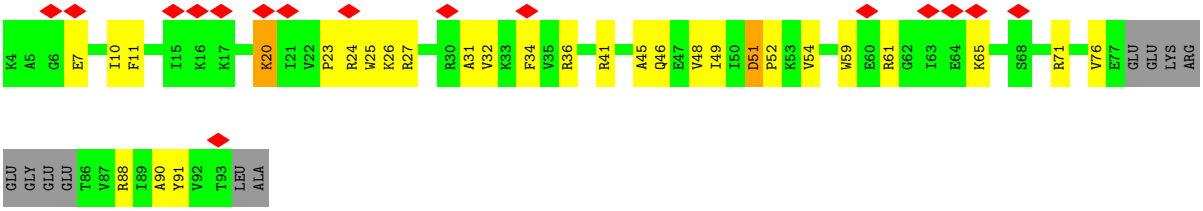
• Molecule 41: 50S ribosomal protein L1P

Chain AA:



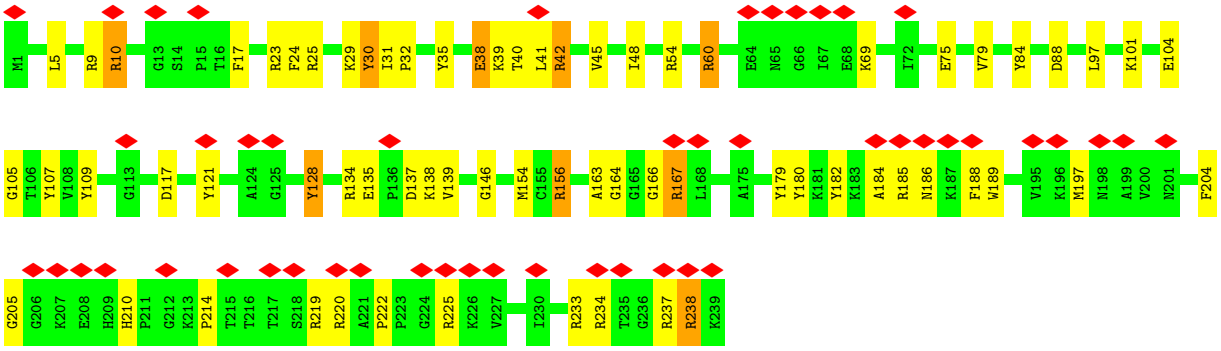
• Molecule 42: 50S ribosomal protein L31E

Chain Aa:



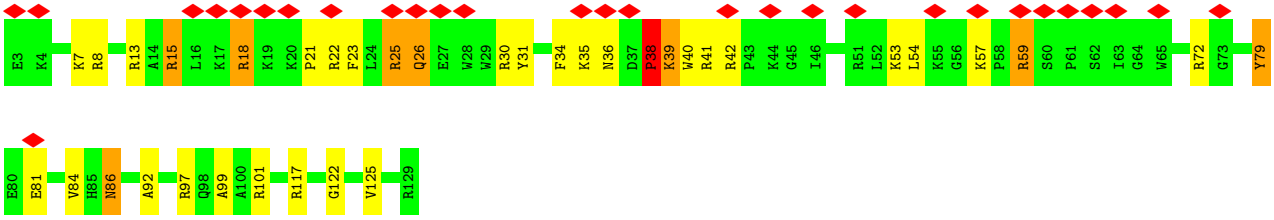
- Molecule 43: 50S ribosomal protein L2

Chain AB:



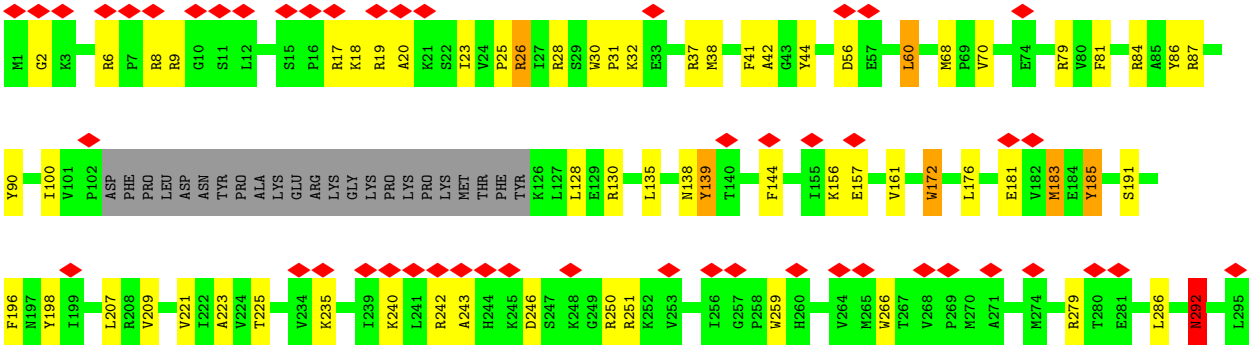
- Molecule 44: 50S ribosomal protein L32E

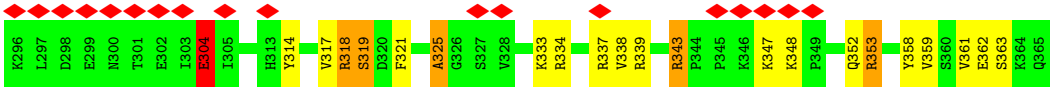
Chain Ab:



- Molecule 45: 50S ribosomal protein L3P

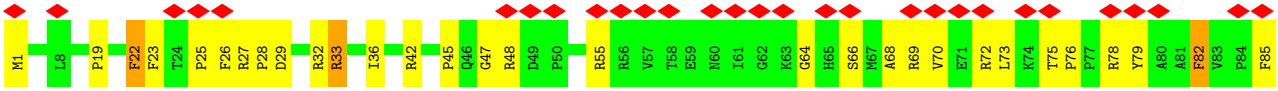
Chain AC:

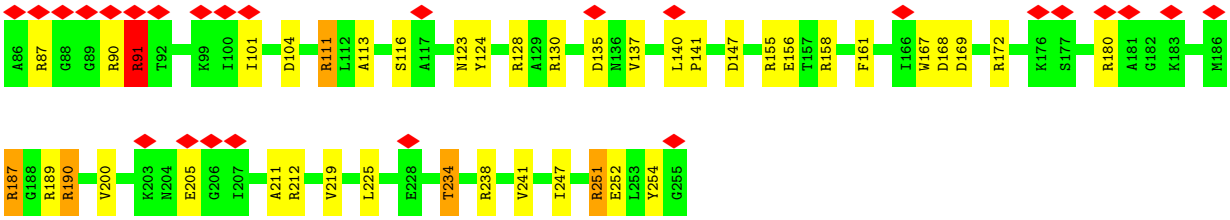




- Molecule 46: 50S ribosomal protein L4P

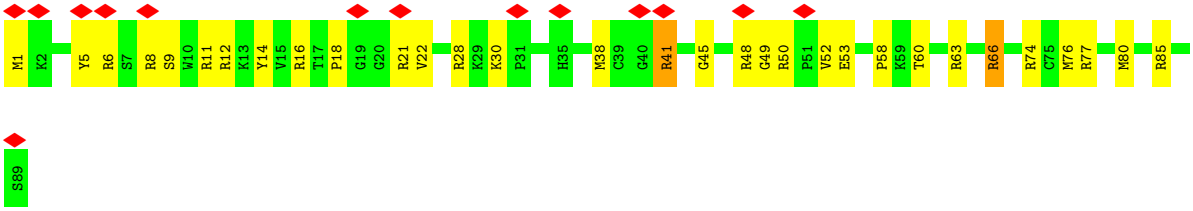
Chain AD:





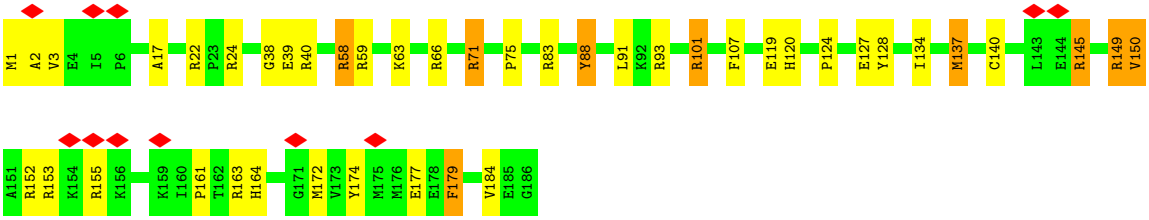
- Molecule 47: 50S ribosomal protein L34E

Chain Ad:



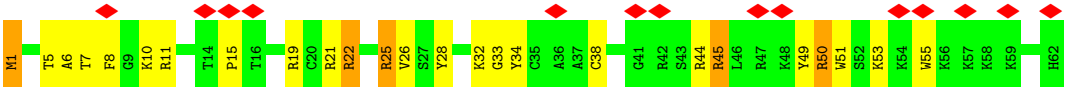
- Molecule 48: 50S ribosomal protein L5P

Chain AE:



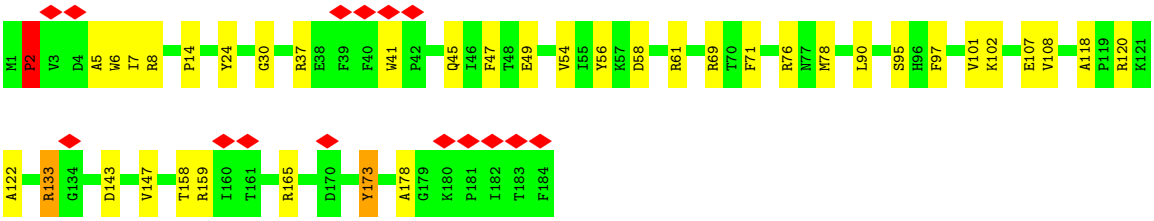
- Molecule 49: 50S ribosomal protein L37E

Chain Ae:



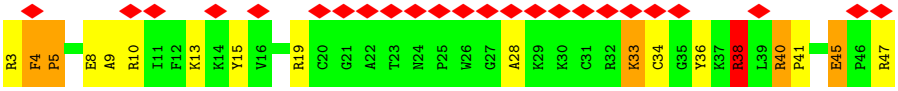
- Molecule 50: 50S ribosomal protein L6P

Chain AF: 8% 79% 20%



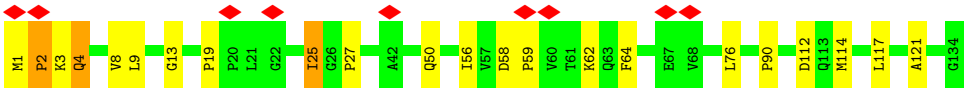
- Molecule 51: 50S ribosomal protein L40E

Chain Ag: 53% 60% 27% 11%



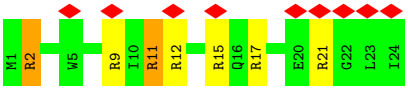
- Molecule 52: 50S ribosomal protein L11P

Chain AH: 7% 84% 14%



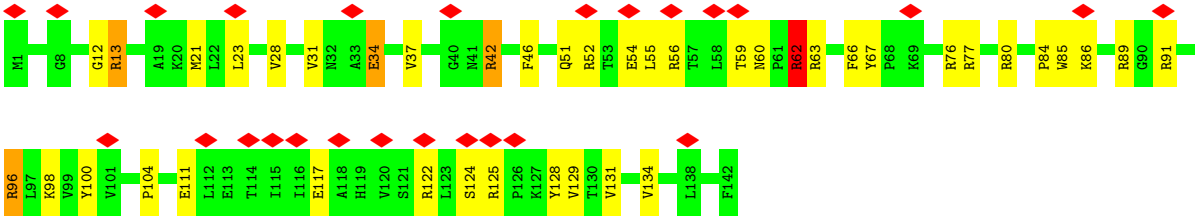
- Molecule 53: 50S ribosomal protein L41E

Chain Ah: 38% 71% 21% 8%



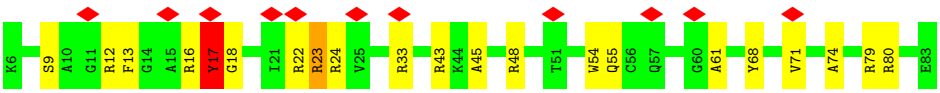
- Molecule 54: 50S ribosomal protein L13P

Chain AI: 18% 70% 26%



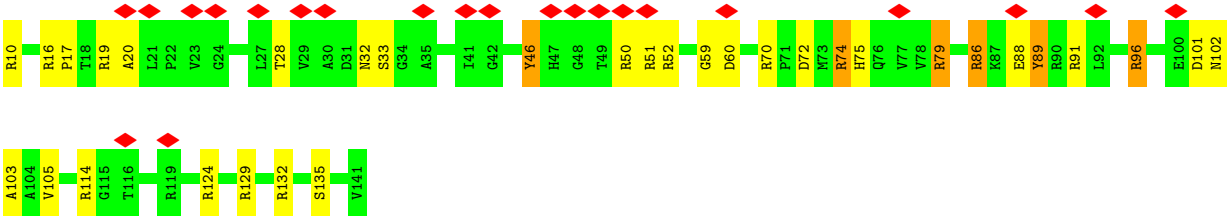
- Molecule 55: 50S ribosomal protein L37AE

Chain Ai: 14% 73% 24%



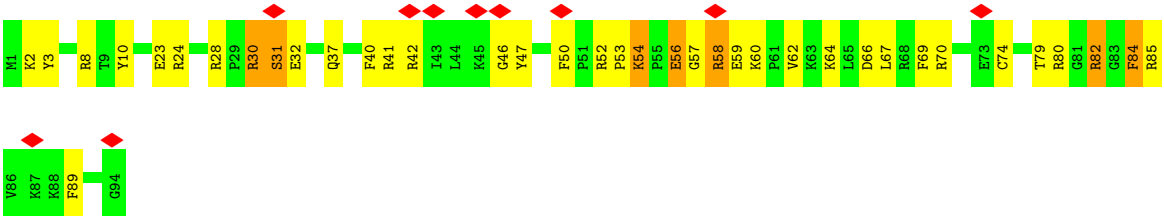
- Molecule 56: 50S ribosomal protein L14P

Chain AJ:



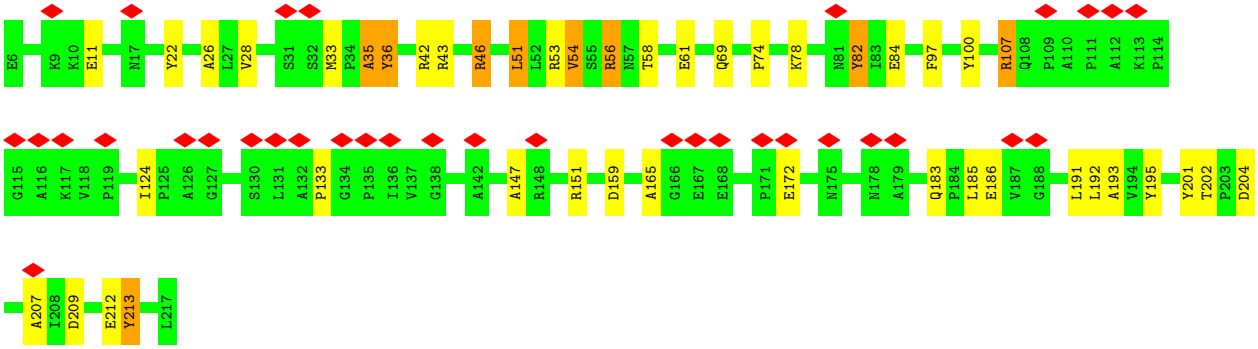
- Molecule 57: 50S ribosomal protein L44E

Chain Aj:



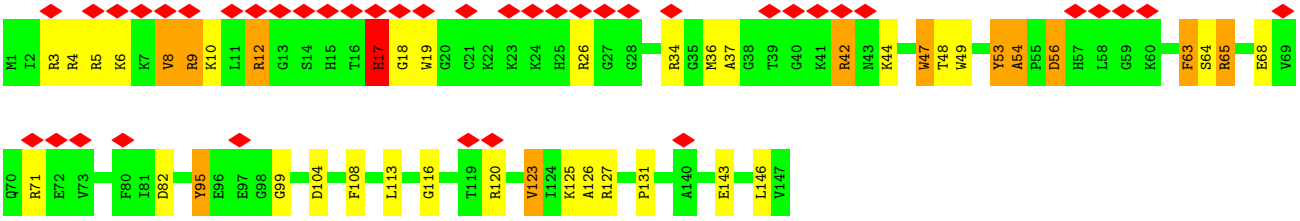
- Molecule 58: 50S ribosomal protein P0/L10E

Chain Ak:



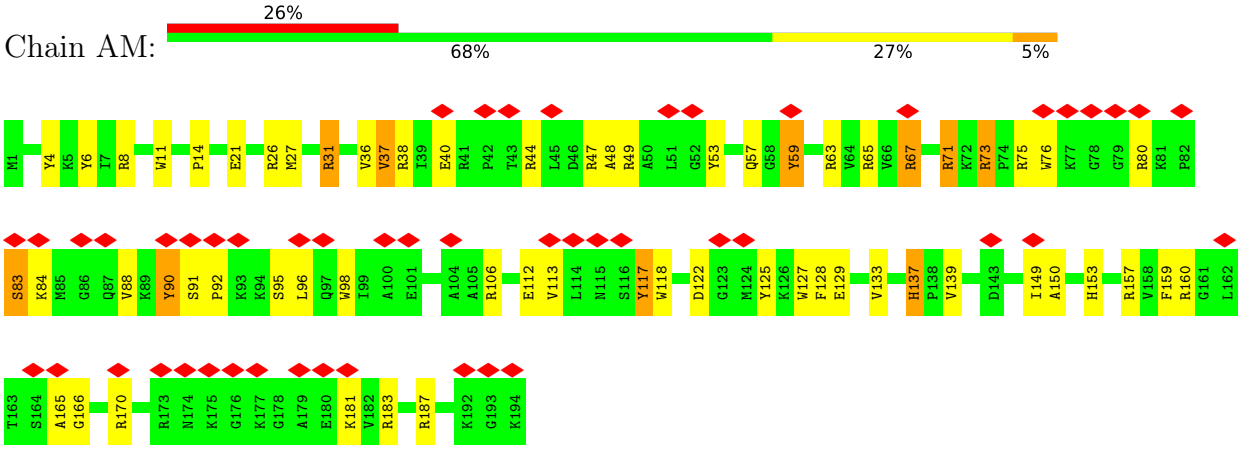
- Molecule 59: 50S ribosomal protein L15P

Chain AL:



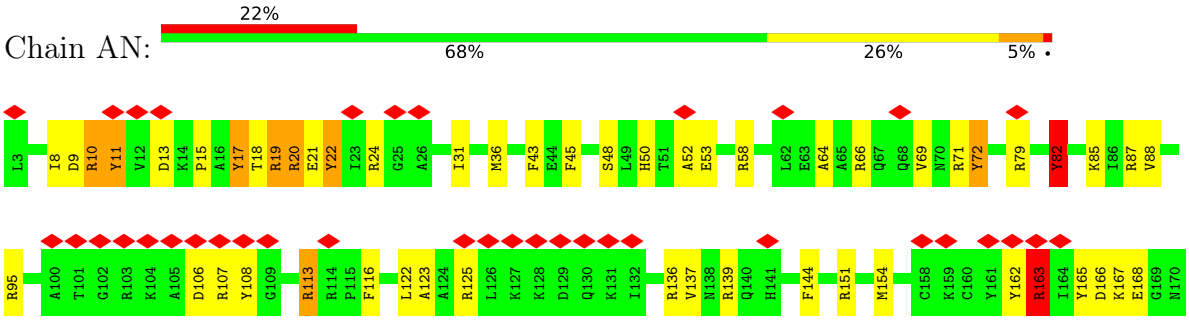
- Molecule 60: 50S ribosomal protein L15E

Chain AM:



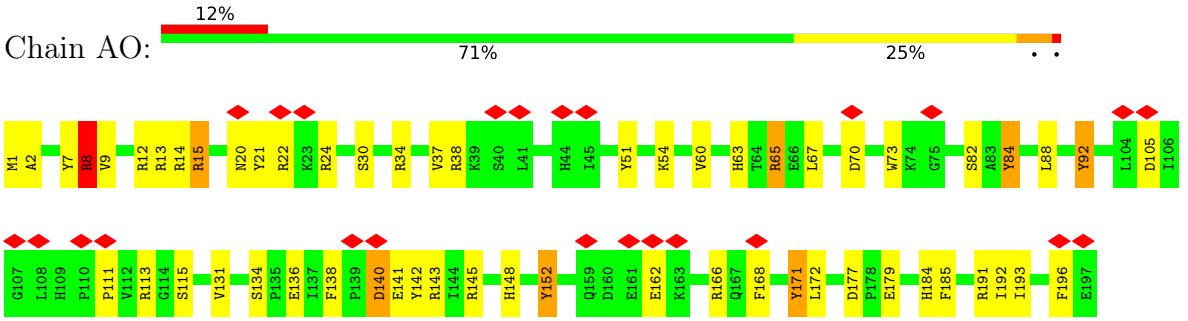
- Molecule 61: 50S ribosomal protein L10E/L16

Chain AN:



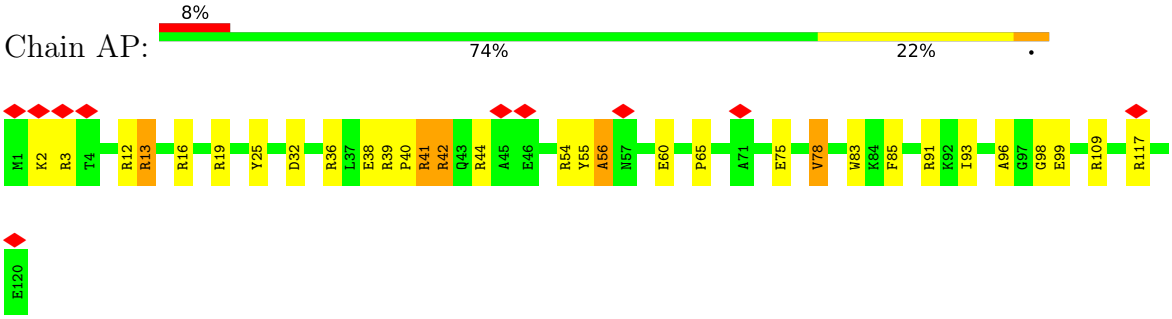
- Molecule 62: 50S ribosomal protein L18P

Chain AO:



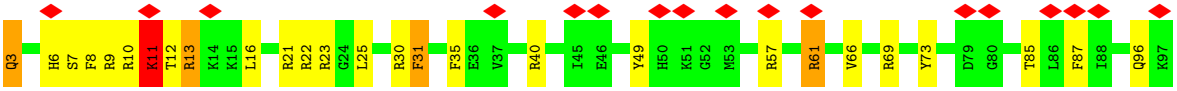
- Molecule 63: 50S ribosomal protein L18E

Chain AP:



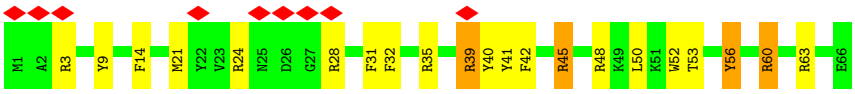
- Molecule 64: 50S ribosomal protein L21E

Chain AR:



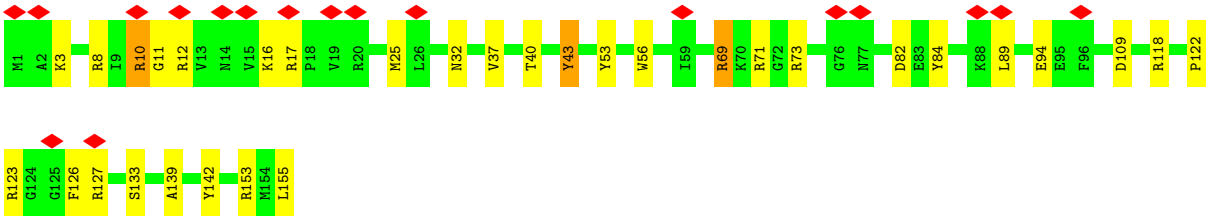
- Molecule 65: 50S ribosomal protein L24E

Chain AV:



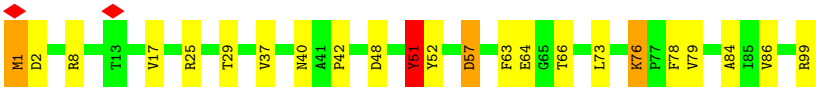
- Molecule 66: 50S ribosomal protein L30P

Chain AY:



- Molecule 67: 50S ribosomal protein L30E

Chain AZ:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37000	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	per micrograph	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	51000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	3.556	Depositor
Minimum map value	-0.752	Depositor
Average map value	0.060	Depositor
Map value standard deviation	0.270	Depositor
Recommended contour level	0.93	Depositor
Map size (Å)	444.99, 444.99, 442.26	wwPDB
Map dimensions	163, 163, 162	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.73, 2.73, 2.73	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	A7	1.64	2/534 (0.4%)	1.97	14/719 (1.9%)
2	A8	1.75	1/263 (0.4%)	1.81	4/354 (1.1%)
3	Af	1.83	4/453 (0.9%)	2.10	15/603 (2.5%)
4	AQ	1.80	16/1272 (1.3%)	2.05	35/1676 (2.1%)
5	AS	1.80	17/1226 (1.4%)	2.14	41/1649 (2.5%)
6	AT	1.69	6/689 (0.9%)	2.00	19/924 (2.1%)
7	AU	1.81	15/1024 (1.5%)	2.04	30/1365 (2.2%)
8	AW	1.76	5/547 (0.9%)	1.95	12/725 (1.7%)
9	AX	1.71	31/3383 (0.9%)	1.98	79/4593 (1.7%)
10	B1	3.41	257/1840 (14.0%)	3.87	460/2869 (16.0%)
11	B2	3.43	4996/35963 (13.9%)	3.79	8330/56134 (14.8%)
12	AG	1.71	4/951 (0.4%)	1.82	14/1281 (1.1%)
12	B3	1.62	3/951 (0.3%)	1.78	13/1281 (1.0%)
13	BA	1.74	21/1585 (1.3%)	2.02	45/2124 (2.1%)
14	BB	1.72	15/1654 (0.9%)	1.96	43/2233 (1.9%)
15	BC	1.82	18/1481 (1.2%)	2.03	41/1985 (2.1%)
16	BD	1.77	14/1457 (1.0%)	2.13	51/1953 (2.6%)
17	BE	1.76	25/2025 (1.2%)	2.01	58/2732 (2.1%)
18	BF	1.81	29/1746 (1.7%)	2.04	51/2350 (2.2%)
19	BG	1.72	9/999 (0.9%)	1.94	22/1337 (1.6%)
20	BH	1.79	22/1773 (1.2%)	2.00	62/2381 (2.6%)
21	BI	1.77	13/1049 (1.2%)	2.04	27/1408 (1.9%)
22	BJ	1.83	14/1013 (1.4%)	2.02	22/1349 (1.6%)
23	BK	1.76	10/1088 (0.9%)	1.96	31/1455 (2.1%)
24	BL	1.76	10/830 (1.2%)	2.00	26/1113 (2.3%)
25	BM	1.83	16/1022 (1.6%)	1.90	24/1375 (1.7%)
26	BN	1.74	8/1157 (0.7%)	2.06	37/1536 (2.4%)
27	BO	1.78	13/1208 (1.1%)	2.02	32/1619 (2.0%)
28	BP	1.94	12/471 (2.5%)	2.31	20/620 (3.2%)
29	BQ	1.75	14/1338 (1.0%)	1.95	34/1797 (1.9%)
30	BR	1.75	12/956 (1.3%)	2.06	24/1287 (1.9%)
31	BS	1.70	4/562 (0.7%)	1.95	10/744 (1.3%)
32	BT	1.78	11/943 (1.2%)	2.23	35/1257 (2.8%)
33	BU	1.80	13/1204 (1.1%)	2.01	30/1621 (1.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
34	BV	1.80	13/839 (1.5%)	2.13	29/1122 (2.6%)
35	BW	1.68	2/485 (0.4%)	1.93	11/651 (1.7%)
36	BX	1.84	7/570 (1.2%)	1.93	9/760 (1.2%)
37	BY	1.66	4/421 (1.0%)	2.22	16/558 (2.9%)
38	A1	3.42	9848/71524 (13.8%)	3.76	16432/111652 (14.7%)
39	A3	3.37	408/3007 (13.6%)	3.87	667/4689 (14.2%)
40	A5	1.85	11/618 (1.8%)	1.97	14/829 (1.7%)
40	AK	1.64	4/618 (0.6%)	1.97	16/829 (1.9%)
41	AA	1.71	17/1702 (1.0%)	2.12	52/2293 (2.3%)
42	Aa	1.72	11/690 (1.6%)	2.12	23/926 (2.5%)
43	AB	1.80	20/1883 (1.1%)	1.99	66/2540 (2.6%)
44	Ab	1.81	13/1100 (1.2%)	1.99	30/1466 (2.0%)
45	AC	1.73	29/2774 (1.0%)	1.98	77/3727 (2.1%)
46	AD	1.74	29/2068 (1.4%)	2.04	58/2787 (2.1%)
47	Ad	1.84	13/758 (1.7%)	2.12	28/1007 (2.8%)
48	AE	1.75	14/1513 (0.9%)	1.98	30/2026 (1.5%)
49	Ae	1.87	6/517 (1.2%)	2.04	15/681 (2.2%)
50	AF	1.71	18/1507 (1.2%)	1.89	24/2033 (1.2%)
51	Ag	1.89	5/381 (1.3%)	2.19	15/504 (3.0%)
52	AH	1.59	2/1002 (0.2%)	1.82	15/1351 (1.1%)
53	Ah	1.81	3/233 (1.3%)	2.32	10/301 (3.3%)
54	AI	1.81	11/1168 (0.9%)	1.94	31/1561 (2.0%)
55	Ai	1.86	10/599 (1.7%)	1.97	14/798 (1.8%)
56	AJ	1.86	13/1027 (1.3%)	1.92	17/1385 (1.2%)
57	Aj	1.85	12/806 (1.5%)	2.18	30/1065 (2.8%)
58	Ak	1.74	16/1660 (1.0%)	1.92	34/2253 (1.5%)
59	AL	1.82	14/1175 (1.2%)	2.03	34/1563 (2.2%)
60	AM	1.85	27/1634 (1.7%)	2.11	53/2179 (2.4%)
61	AN	1.85	24/1410 (1.7%)	2.05	43/1890 (2.3%)
62	AO	1.73	17/1636 (1.0%)	2.11	47/2196 (2.1%)
63	AP	1.82	12/980 (1.2%)	2.03	26/1313 (2.0%)
64	AR	1.74	10/808 (1.2%)	1.97	23/1080 (2.1%)
65	AV	1.91	9/570 (1.6%)	2.18	23/758 (3.0%)
66	AY	1.69	8/1262 (0.6%)	1.98	33/1687 (2.0%)
67	AZ	1.68	2/764 (0.3%)	1.94	21/1028 (2.0%)
All	All	2.89	16322/184366 (8.9%)	3.26	27857/271937 (10.2%)

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
2	A8	0	1
3	Af	0	6
4	AQ	0	5
5	AS	0	5
6	AT	0	2
7	AU	0	4
9	AX	0	9
10	B1	0	35
11	B2	0	725
12	AG	0	2
13	BA	0	11
14	BB	0	2
15	BC	0	8
16	BD	0	7
17	BE	0	9
18	BF	0	3
19	BG	1	4
20	BH	4	13
21	BI	0	3
22	BJ	0	6
23	BK	0	7
24	BL	0	8
25	BM	0	2
26	BN	0	4
27	BO	0	5
28	BP	0	1
29	BQ	0	7
30	BR	0	3
31	BS	0	2
32	BT	0	5
33	BU	0	4
34	BV	0	12
35	BW	0	1
36	BX	0	3
37	BY	0	3
38	A1	2	1412
39	A3	0	55
40	A5	0	2
40	AK	0	2
41	AA	0	4
42	Aa	0	2
43	AB	0	8
44	Ab	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
45	AC	0	7
46	AD	0	9
47	Ad	0	1
48	AE	0	6
49	Ae	1	9
50	AF	0	3
51	Ag	1	5
52	AH	1	2
53	Ah	0	2
54	AI	0	7
55	Ai	0	2
56	AJ	0	4
57	Aj	0	7
58	Ak	0	4
59	AL	2	10
60	AM	0	4
61	AN	0	7
62	AO	0	10
63	AP	0	4
64	AR	0	1
65	AV	0	5
66	AY	0	2
67	AZ	0	1
All	All	12	2533

The worst 5 of 16322 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B2	770	A	N7-C5	-18.72	1.28	1.39
11	B2	470	G	N9-C8	18.32	1.50	1.37
38	A1	2257	A	N7-C5	-18.29	1.28	1.39
38	A1	910	G	N7-C5	-17.89	1.28	1.39
38	A1	2164	G	N7-C5	-17.73	1.28	1.39

The worst 5 of 27857 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B2	1445	A	N1-C6-N6	27.58	135.15	118.60
38	A1	277	A	N1-C6-N6	27.04	134.82	118.60
38	A1	2347	G	N1-C6-O6	26.94	136.06	119.90
38	A1	1281	A	N1-C6-N6	26.62	134.57	118.60
38	A1	2540	A	N1-C6-N6	26.19	134.31	118.60

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	BG	53	LYS	CA
20	BH	85	PHE	CA
20	BH	86	MET	CA
20	BH	87	ARG	CA
20	BH	96	LYS	CA

5 of 2533 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A8	49	TYR	Sidechain
3	Af	2	ALA	Peptide
3	Af	33	ARG	Peptide
3	Af	34	ARG	Sidechain
3	Af	37	THR	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A7	63/67 (94%)	43 (68%)	16 (25%)	4 (6%)	1 17
2	A8	30/52 (58%)	22 (73%)	7 (23%)	1 (3%)	4 26
3	Af	49/51 (96%)	40 (82%)	6 (12%)	3 (6%)	1 17
4	AQ	148/150 (99%)	139 (94%)	5 (3%)	4 (3%)	5 31
5	AS	148/150 (99%)	135 (91%)	10 (7%)	3 (2%)	7 38
6	AT	82/84 (98%)	75 (92%)	4 (5%)	3 (4%)	3 24
7	AU	119/121 (98%)	113 (95%)	5 (4%)	1 (1%)	19 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	AW	64/72 (89%)	64 (100%)	0	0	100	100
9	AX	430/436 (99%)	322 (75%)	77 (18%)	31 (7%)	1	14
12	AG	121/123 (98%)	114 (94%)	4 (3%)	3 (2%)	5	32
12	B3	121/123 (98%)	100 (83%)	14 (12%)	7 (6%)	1	18
13	BA	188/190 (99%)	164 (87%)	12 (6%)	12 (6%)	1	16
14	BB	200/202 (99%)	182 (91%)	12 (6%)	6 (3%)	4	28
15	BC	184/186 (99%)	171 (93%)	9 (5%)	4 (2%)	6	35
16	BD	170/172 (99%)	148 (87%)	20 (12%)	2 (1%)	13	50
17	BE	239/241 (99%)	207 (87%)	20 (8%)	12 (5%)	2	20
18	BF	215/217 (99%)	188 (87%)	16 (7%)	11 (5%)	2	19
19	BG	123/125 (98%)	103 (84%)	13 (11%)	7 (6%)	1	18
20	BH	213/215 (99%)	186 (87%)	14 (7%)	13 (6%)	1	17
21	BI	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	19	60
22	BJ	125/127 (98%)	107 (86%)	15 (12%)	3 (2%)	6	33
23	BK	133/135 (98%)	116 (87%)	10 (8%)	7 (5%)	2	19
24	BL	100/102 (98%)	90 (90%)	7 (7%)	3 (3%)	4	28
25	BM	131/133 (98%)	112 (86%)	9 (7%)	10 (8%)	1	13
26	BN	143/145 (99%)	128 (90%)	7 (5%)	8 (6%)	2	19
27	BO	146/148 (99%)	122 (84%)	16 (11%)	8 (6%)	2	19
28	BP	54/56 (96%)	44 (82%)	8 (15%)	2 (4%)	3	24
29	BQ	156/158 (99%)	137 (88%)	9 (6%)	10 (6%)	1	16
30	BR	111/113 (98%)	105 (95%)	5 (4%)	1 (1%)	17	57
31	BS	65/67 (97%)	60 (92%)	5 (8%)	0	100	100
32	BT	109/111 (98%)	102 (94%)	5 (5%)	2 (2%)	8	40
33	BU	142/144 (99%)	123 (87%)	11 (8%)	8 (6%)	2	19
34	BV	97/99 (98%)	88 (91%)	5 (5%)	4 (4%)	3	23
35	BW	61/63 (97%)	52 (85%)	6 (10%)	3 (5%)	2	20
36	BX	69/71 (97%)	62 (90%)	6 (9%)	1 (1%)	11	46
37	BY	48/50 (96%)	41 (85%)	5 (10%)	2 (4%)	3	22
40	A5	79/81 (98%)	67 (85%)	9 (11%)	3 (4%)	3	24
40	AK	79/81 (98%)	70 (89%)	4 (5%)	5 (6%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	AA	214/216 (99%)	186 (87%)	19 (9%)	9 (4%)	3	22
42	Aa	78/92 (85%)	69 (88%)	9 (12%)	0	100	100
43	AB	237/239 (99%)	209 (88%)	23 (10%)	5 (2%)	7	36
44	Ab	125/127 (98%)	108 (86%)	11 (9%)	6 (5%)	2	21
45	AC	338/365 (93%)	303 (90%)	21 (6%)	14 (4%)	3	23
46	AD	253/255 (99%)	220 (87%)	23 (9%)	10 (4%)	3	23
47	Ad	87/89 (98%)	78 (90%)	6 (7%)	3 (3%)	3	26
48	AE	184/186 (99%)	161 (88%)	15 (8%)	8 (4%)	2	22
49	Ae	60/62 (97%)	43 (72%)	13 (22%)	4 (7%)	1	15
50	AF	182/184 (99%)	165 (91%)	14 (8%)	3 (2%)	9	44
51	Ag	43/45 (96%)	30 (70%)	8 (19%)	5 (12%)	0	6
52	AH	132/134 (98%)	114 (86%)	11 (8%)	7 (5%)	2	19
53	Ah	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
54	AI	140/142 (99%)	121 (86%)	13 (9%)	6 (4%)	2	22
55	Ai	76/78 (97%)	69 (91%)	4 (5%)	3 (4%)	3	23
56	AJ	130/132 (98%)	121 (93%)	6 (5%)	3 (2%)	6	34
57	Aj	92/94 (98%)	69 (75%)	18 (20%)	5 (5%)	2	19
58	Ak	210/212 (99%)	192 (91%)	11 (5%)	7 (3%)	4	26
59	AL	145/147 (99%)	129 (89%)	11 (8%)	5 (3%)	3	26
60	AM	192/194 (99%)	175 (91%)	11 (6%)	6 (3%)	4	27
61	AN	166/168 (99%)	141 (85%)	19 (11%)	6 (4%)	3	25
62	AO	195/197 (99%)	166 (85%)	20 (10%)	9 (5%)	2	21
63	AP	118/120 (98%)	107 (91%)	5 (4%)	6 (5%)	2	19
64	AR	93/95 (98%)	85 (91%)	3 (3%)	5 (5%)	2	19
65	AV	64/66 (97%)	61 (95%)	3 (5%)	0	100	100
66	AY	153/155 (99%)	137 (90%)	12 (8%)	4 (3%)	5	31
67	AZ	97/99 (98%)	84 (87%)	9 (9%)	4 (4%)	3	23
All	All	8708/8907 (98%)	7624 (88%)	733 (8%)	351 (4%)	5	23

5 of 351 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A7	30	LYS

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Mol	Chain	Res	Type
4	AQ	134	ASN
9	AX	239	ARG
9	AX	277	TYR
9	AX	346	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A7	57/59 (97%)	55 (96%)	2 (4%)	36	59
2	A8	28/44 (64%)	28 (100%)	0	100	100
3	Af	47/47 (100%)	46 (98%)	1 (2%)	53	72
4	AQ	130/130 (100%)	125 (96%)	5 (4%)	33	57
5	AS	126/126 (100%)	119 (94%)	7 (6%)	21	46
6	AT	75/75 (100%)	73 (97%)	2 (3%)	44	65
7	AU	110/110 (100%)	105 (96%)	5 (4%)	27	52
8	AW	61/66 (92%)	60 (98%)	1 (2%)	62	79
9	AX	351/355 (99%)	341 (97%)	10 (3%)	43	65
12	AG	99/99 (100%)	95 (96%)	4 (4%)	31	55
12	B3	99/99 (100%)	94 (95%)	5 (5%)	24	48
13	BA	166/166 (100%)	152 (92%)	14 (8%)	11	33
14	BB	173/173 (100%)	168 (97%)	5 (3%)	42	64
15	BC	145/145 (100%)	141 (97%)	4 (3%)	43	65
16	BD	153/153 (100%)	148 (97%)	5 (3%)	38	61
17	BE	212/212 (100%)	201 (95%)	11 (5%)	23	48
18	BF	181/181 (100%)	173 (96%)	8 (4%)	28	53
19	BG	108/108 (100%)	108 (100%)	0	100	100
20	BH	184/184 (100%)	165 (90%)	19 (10%)	7	25
21	BI	107/107 (100%)	105 (98%)	2 (2%)	57	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	BJ	103/103 (100%)	95 (92%)	8 (8%)	12	36
23	BK	111/111 (100%)	108 (97%)	3 (3%)	44	65
24	BL	91/91 (100%)	87 (96%)	4 (4%)	28	53
25	BM	100/100 (100%)	96 (96%)	4 (4%)	31	55
26	BN	119/119 (100%)	114 (96%)	5 (4%)	30	54
27	BO	122/122 (100%)	120 (98%)	2 (2%)	62	79
28	BP	46/46 (100%)	43 (94%)	3 (6%)	17	42
29	BQ	143/143 (100%)	135 (94%)	8 (6%)	21	46
30	BR	102/102 (100%)	92 (90%)	10 (10%)	8	26
31	BS	61/61 (100%)	58 (95%)	3 (5%)	25	50
32	BT	99/99 (100%)	95 (96%)	4 (4%)	31	55
33	BU	121/121 (100%)	118 (98%)	3 (2%)	47	68
34	BV	89/89 (100%)	87 (98%)	2 (2%)	52	71
35	BW	54/54 (100%)	51 (94%)	3 (6%)	21	46
36	BX	60/60 (100%)	53 (88%)	7 (12%)	5	21
37	BY	41/41 (100%)	40 (98%)	1 (2%)	49	69
40	A5	64/64 (100%)	62 (97%)	2 (3%)	40	62
40	AK	64/64 (100%)	59 (92%)	5 (8%)	12	36
41	AA	182/182 (100%)	173 (95%)	9 (5%)	25	50
42	Aa	73/81 (90%)	68 (93%)	5 (7%)	16	41
43	AB	189/189 (100%)	183 (97%)	6 (3%)	39	61
44	Ab	114/114 (100%)	108 (95%)	6 (5%)	22	47
45	AC	291/312 (93%)	278 (96%)	13 (4%)	27	52
46	AD	213/213 (100%)	207 (97%)	6 (3%)	43	65
47	Ad	81/81 (100%)	81 (100%)	0	100	100
48	AE	158/158 (100%)	153 (97%)	5 (3%)	39	61
49	Ae	51/51 (100%)	49 (96%)	2 (4%)	32	56
50	AF	156/156 (100%)	150 (96%)	6 (4%)	33	57
51	Ag	37/37 (100%)	36 (97%)	1 (3%)	44	65
52	AH	110/110 (100%)	108 (98%)	2 (2%)	59	77
53	Ah	23/23 (100%)	23 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	AI	122/122 (100%)	118 (97%)	4 (3%)	38	61
55	Ai	57/57 (100%)	55 (96%)	2 (4%)	36	59
56	AJ	104/104 (100%)	98 (94%)	6 (6%)	20	45
57	Aj	83/83 (100%)	80 (96%)	3 (4%)	35	59
58	Ak	179/179 (100%)	173 (97%)	6 (3%)	37	60
59	AL	117/117 (100%)	112 (96%)	5 (4%)	29	53
60	AM	162/162 (100%)	155 (96%)	7 (4%)	29	53
61	AN	140/140 (100%)	134 (96%)	6 (4%)	29	53
62	AO	166/166 (100%)	159 (96%)	7 (4%)	30	54
63	AP	101/101 (100%)	99 (98%)	2 (2%)	55	74
64	AR	85/85 (100%)	79 (93%)	6 (7%)	14	39
65	AV	56/56 (100%)	56 (100%)	0	100	100
66	AY	133/133 (100%)	130 (98%)	3 (2%)	50	70
67	AZ	80/80 (100%)	73 (91%)	7 (9%)	10	31
All	All	7465/7521 (99%)	7153 (96%)	312 (4%)	33	54

5 of 312 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	AF	7	ILE
61	AN	137	VAL
12	AG	93	GLU
40	AK	24	VAL
64	AR	66	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
62	AO	43	HIS
62	AO	76	HIS
66	AY	120	HIS
25	BM	29	HIS
24	BL	69	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B1	76/77 (98%)	20 (26%)	4 (5%)
11	B2	1494/1495 (99%)	264 (17%)	103 (6%)
38	A1	2964/3049 (97%)	600 (20%)	158 (5%)
39	A3	125/126 (99%)	36 (28%)	11 (8%)
All	All	4659/4747 (98%)	920 (19%)	276 (5%)

5 of 920 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	B1	8	U
10	B1	9	A
10	B1	10	G
10	B1	18	U
10	B1	19	G

5 of 276 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
38	A1	2324	C
38	A1	2401	A
38	A1	2957	G
11	B2	1399	G
11	B2	1322	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

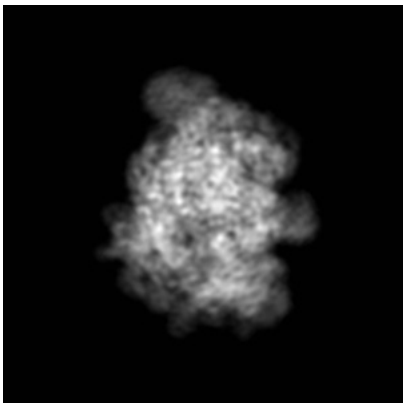
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-5691. These allow visual inspection of the internal detail of the map and identification of artifacts.

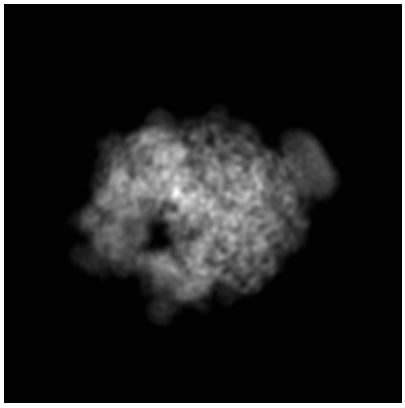
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

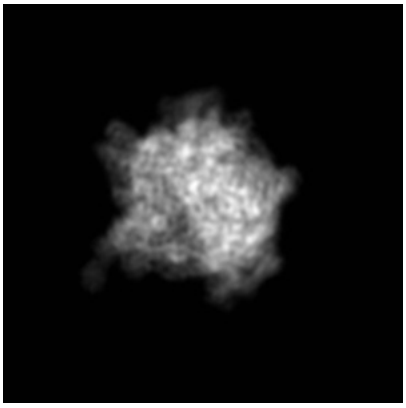
6.1.1 Primary map



X



Y

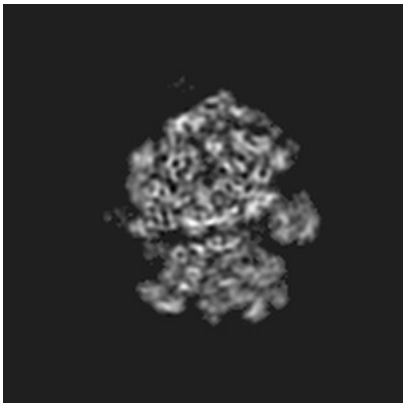


Z

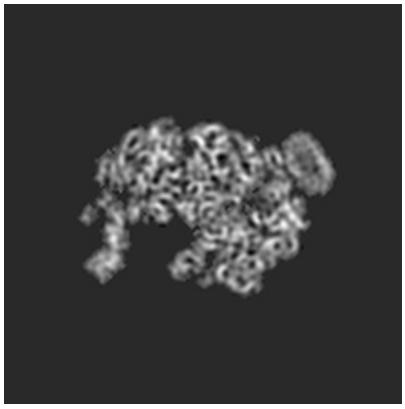
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

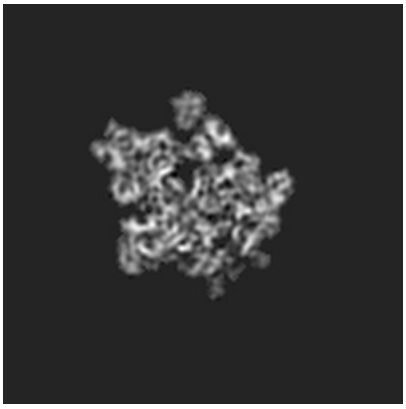
6.2.1 Primary map



X Index: 81



Y Index: 81

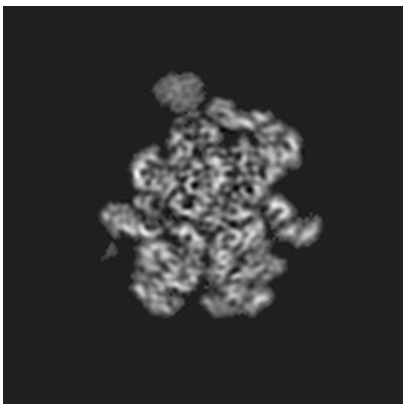


Z Index: 81

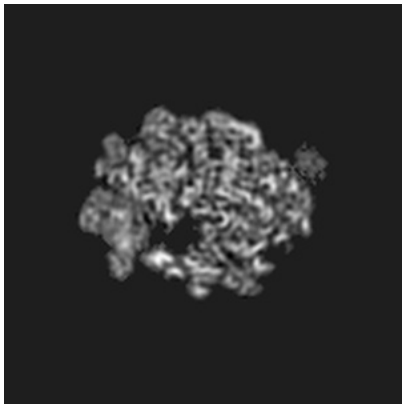
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

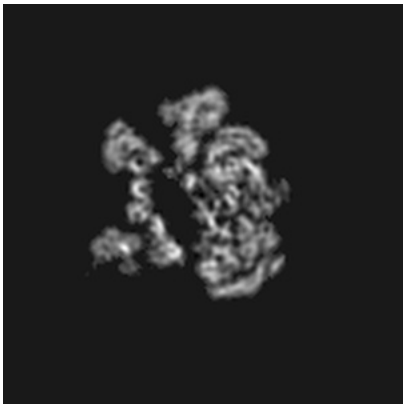
6.3.1 Primary map



X Index: 85



Y Index: 87

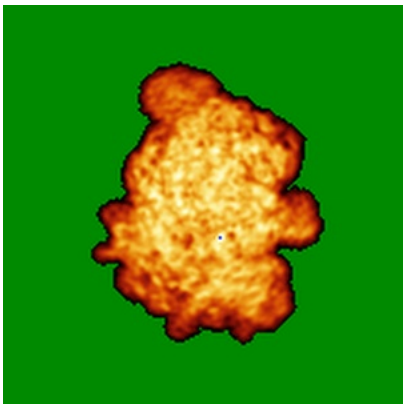


Z Index: 70

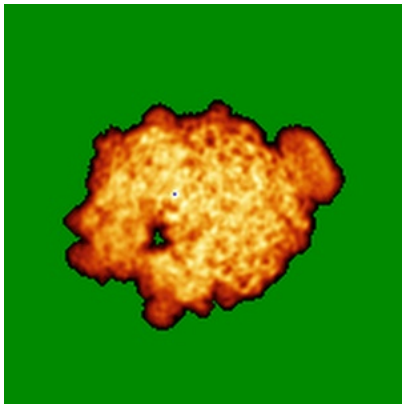
The images above show the largest variance slices of the map in three orthogonal directions.

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

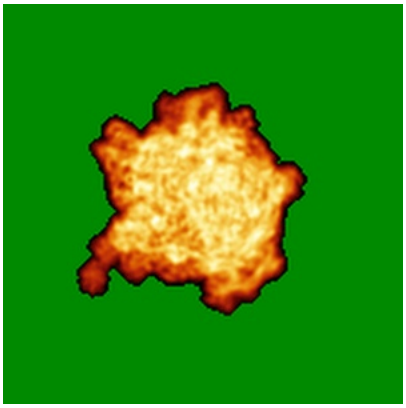
6.4.1 Primary map



X



Y



Z

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 0.93. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

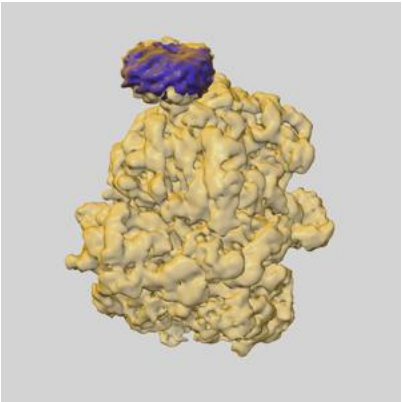
6.6 Mask visualisation (i)

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

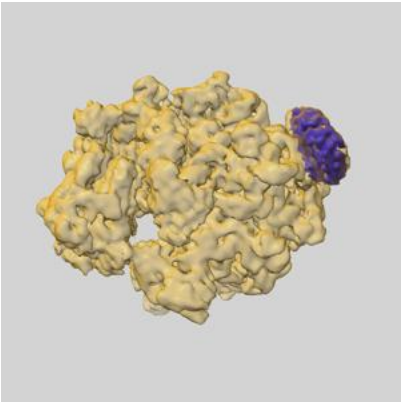
A mask typically either:

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

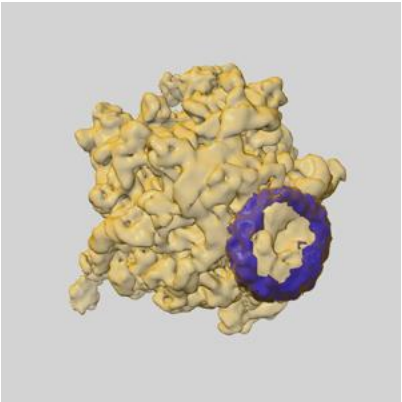
6.6.1 emd_5691_msk_4.map (i)



X

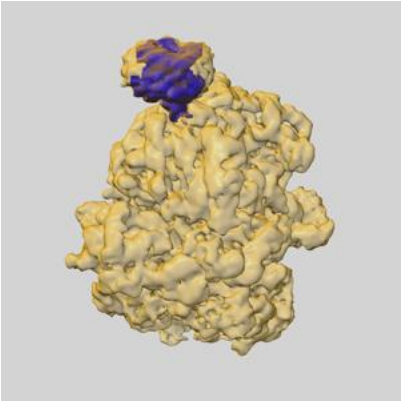


Y

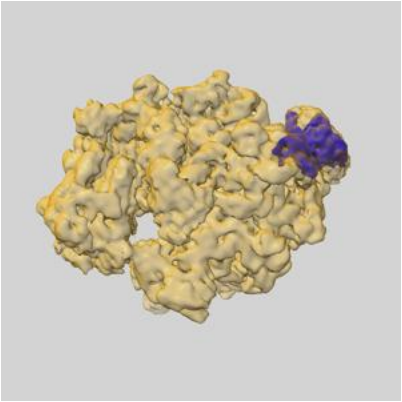


Z

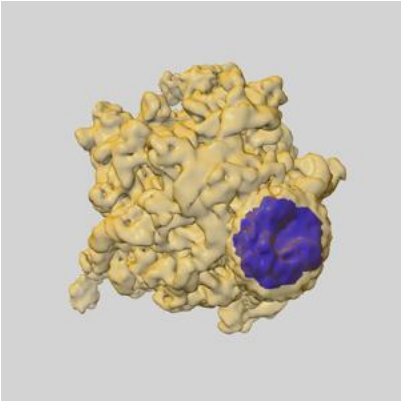
6.6.2 emd_5691_msk_3.map (i)



X

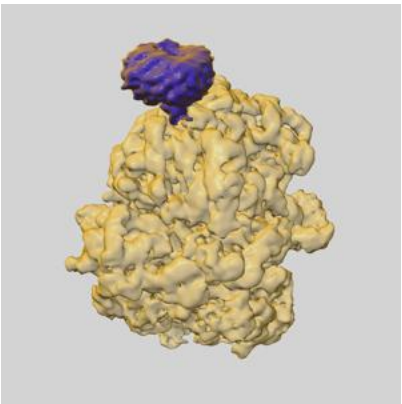


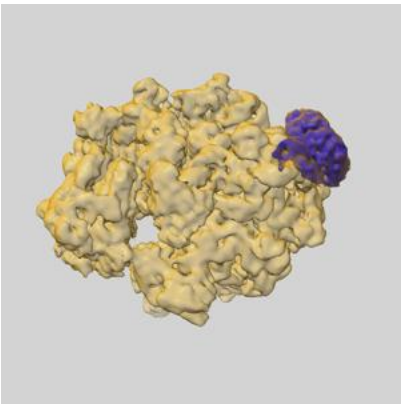
Y

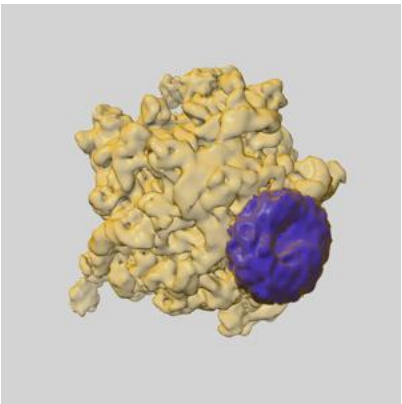


Z

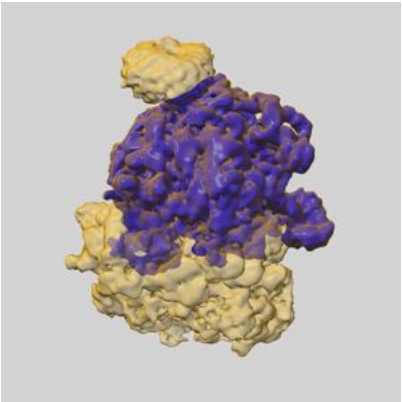
6.6.3 emd_5691_msk_2.map (i)

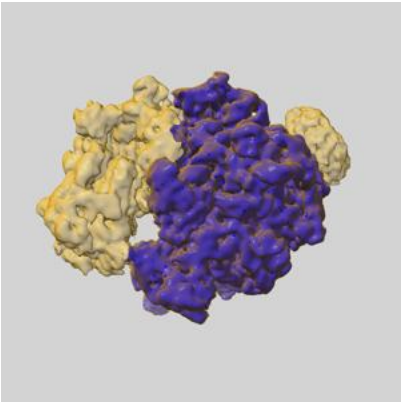

X

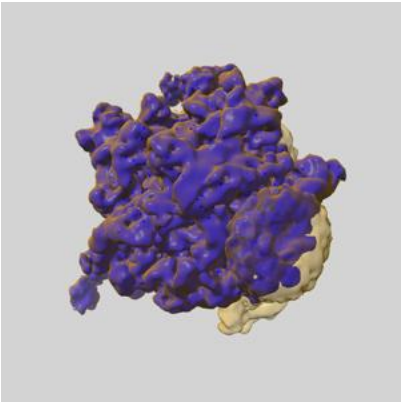

Y


Z

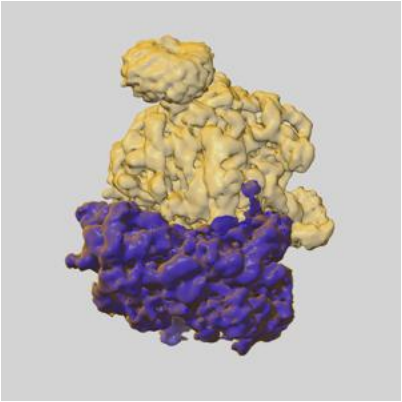
6.6.4 emd_5691_msk_1.map (i)

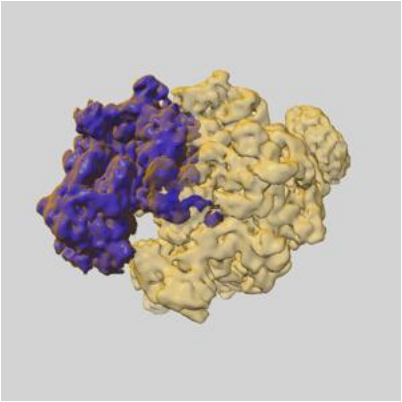

X

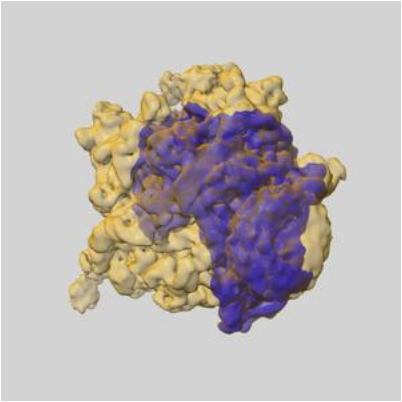

Y


Z

6.6.5 emd_5691_msk_5.map (i)


X

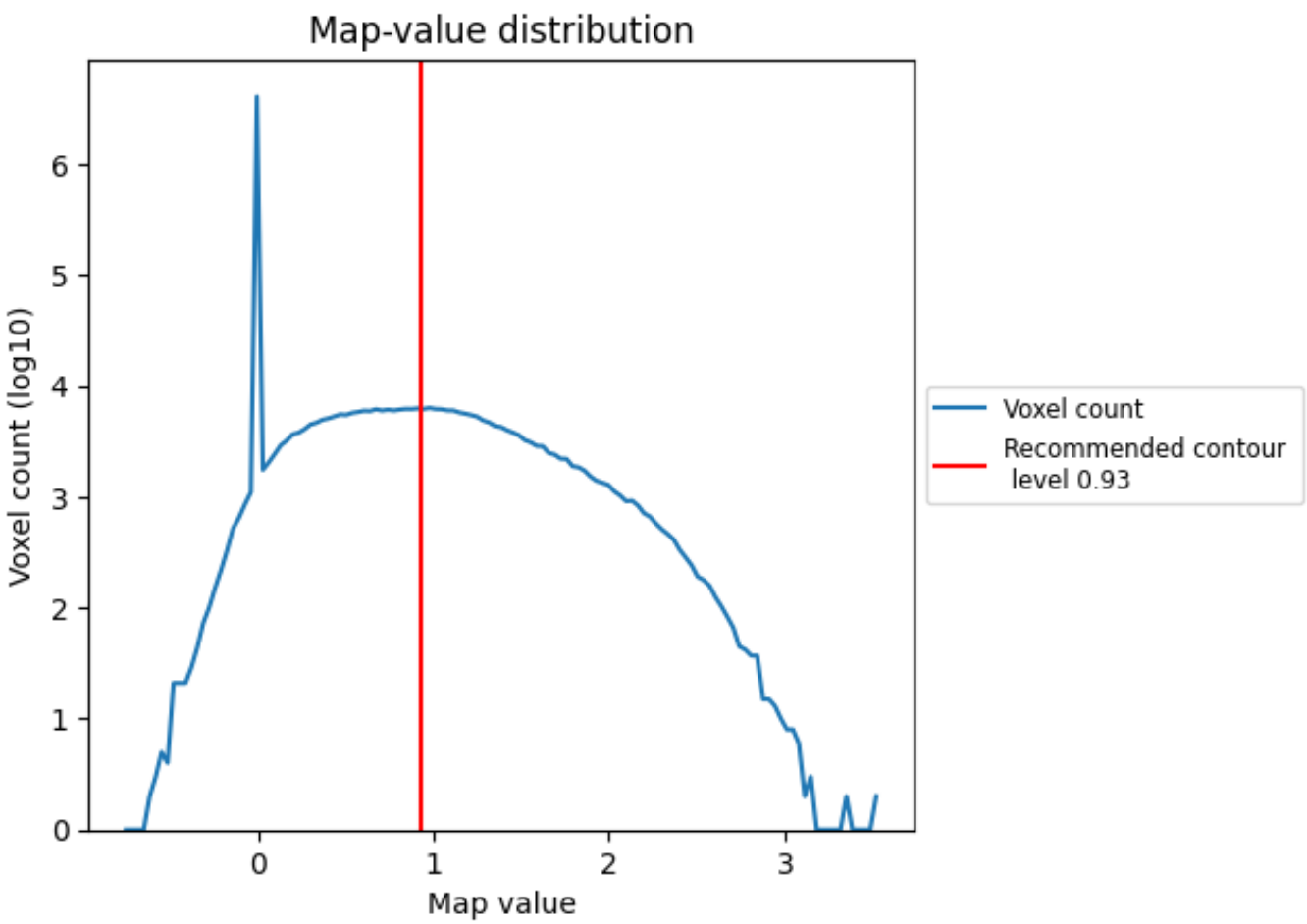

Y


Z

7 Map analysis (i)

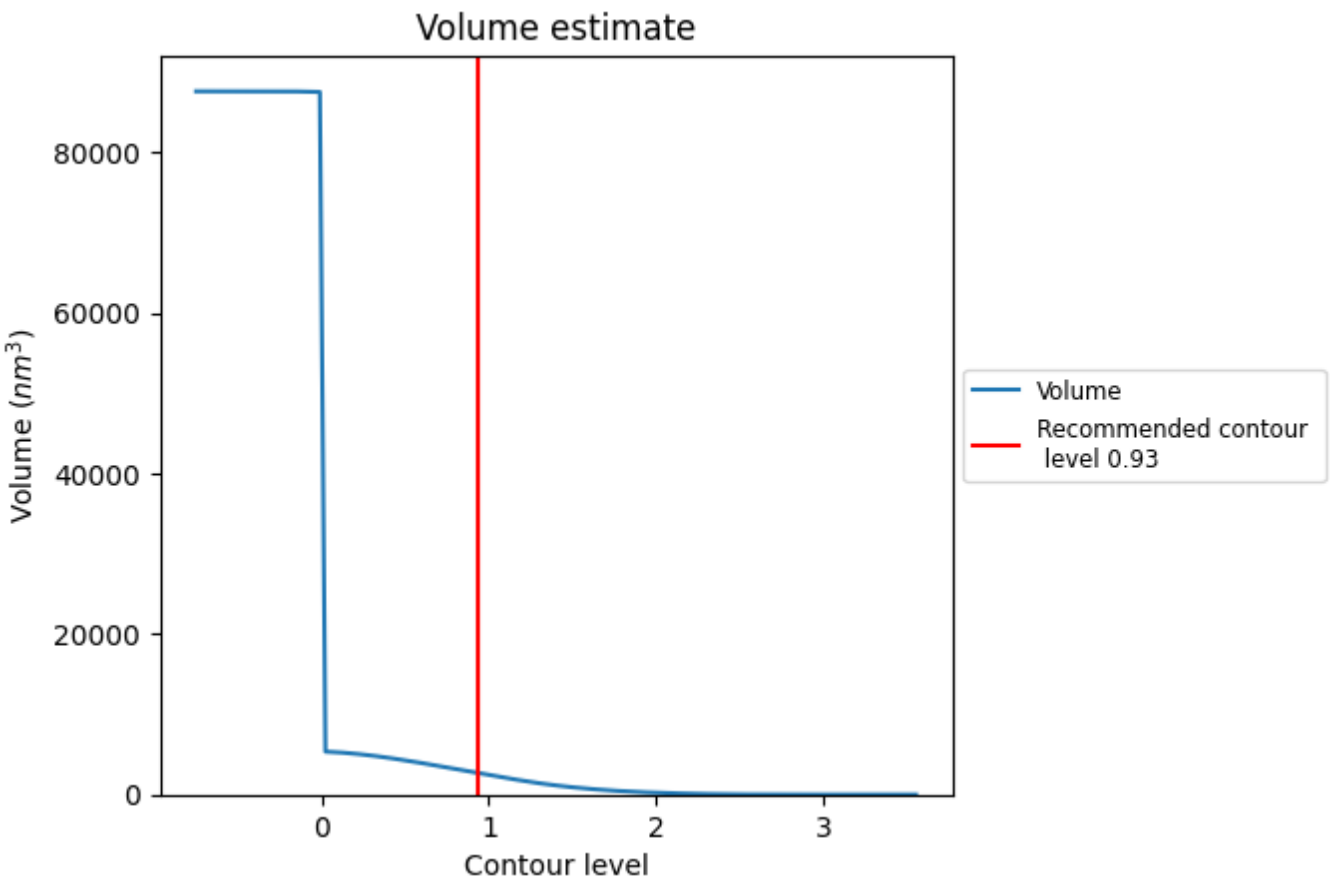
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

7.2 Volume estimate (i)



The volume at the recommended contour level is 2715 nm^3; this corresponds to an approximate mass of 2453 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)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

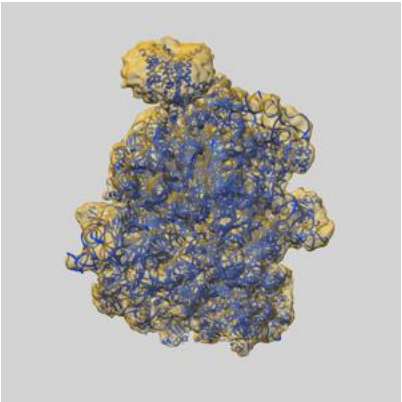
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

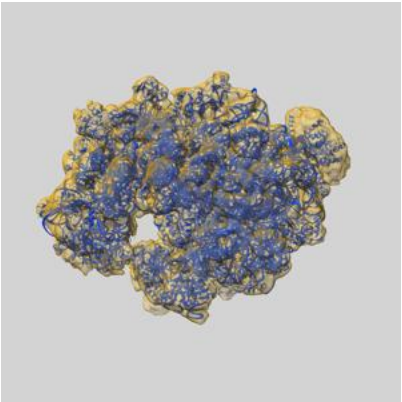
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-5691 and PDB model 4V4N. Per-residue inclusion information can be found in section 3 on page 16.

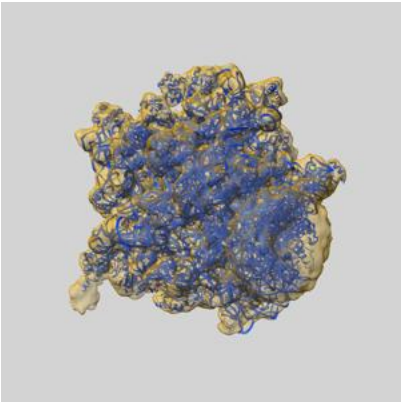
9.1 Map-model overlay (i)



X



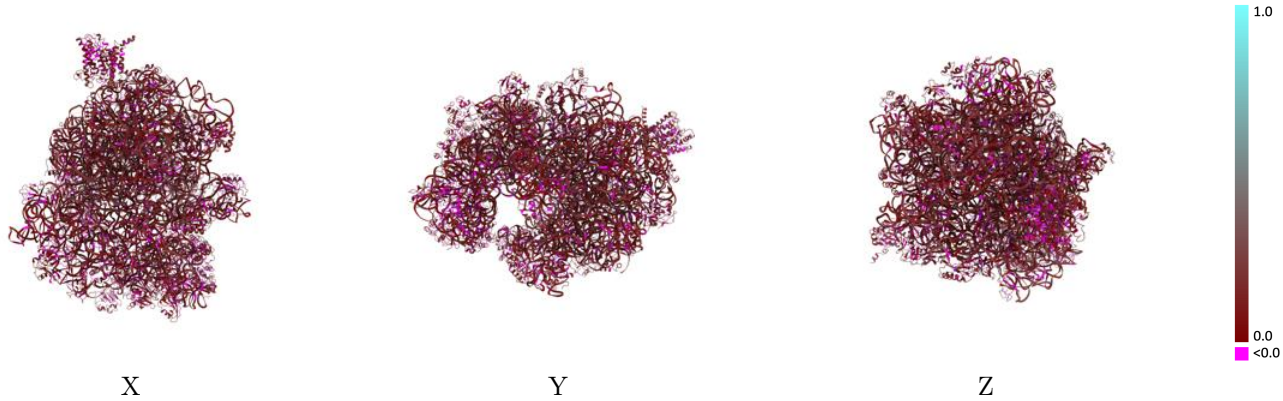
Y



Z

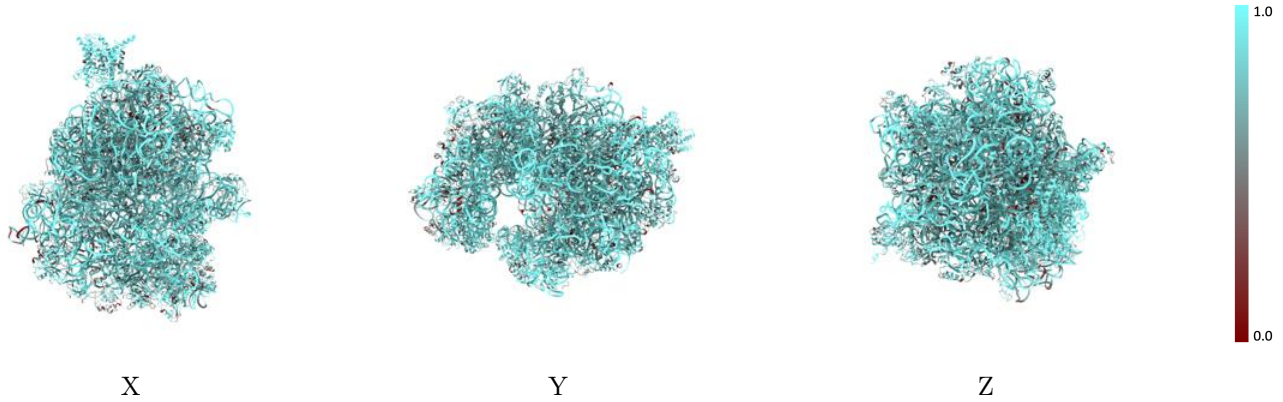
The images above show the 3D surface view of the map at the recommended contour level 0.93 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



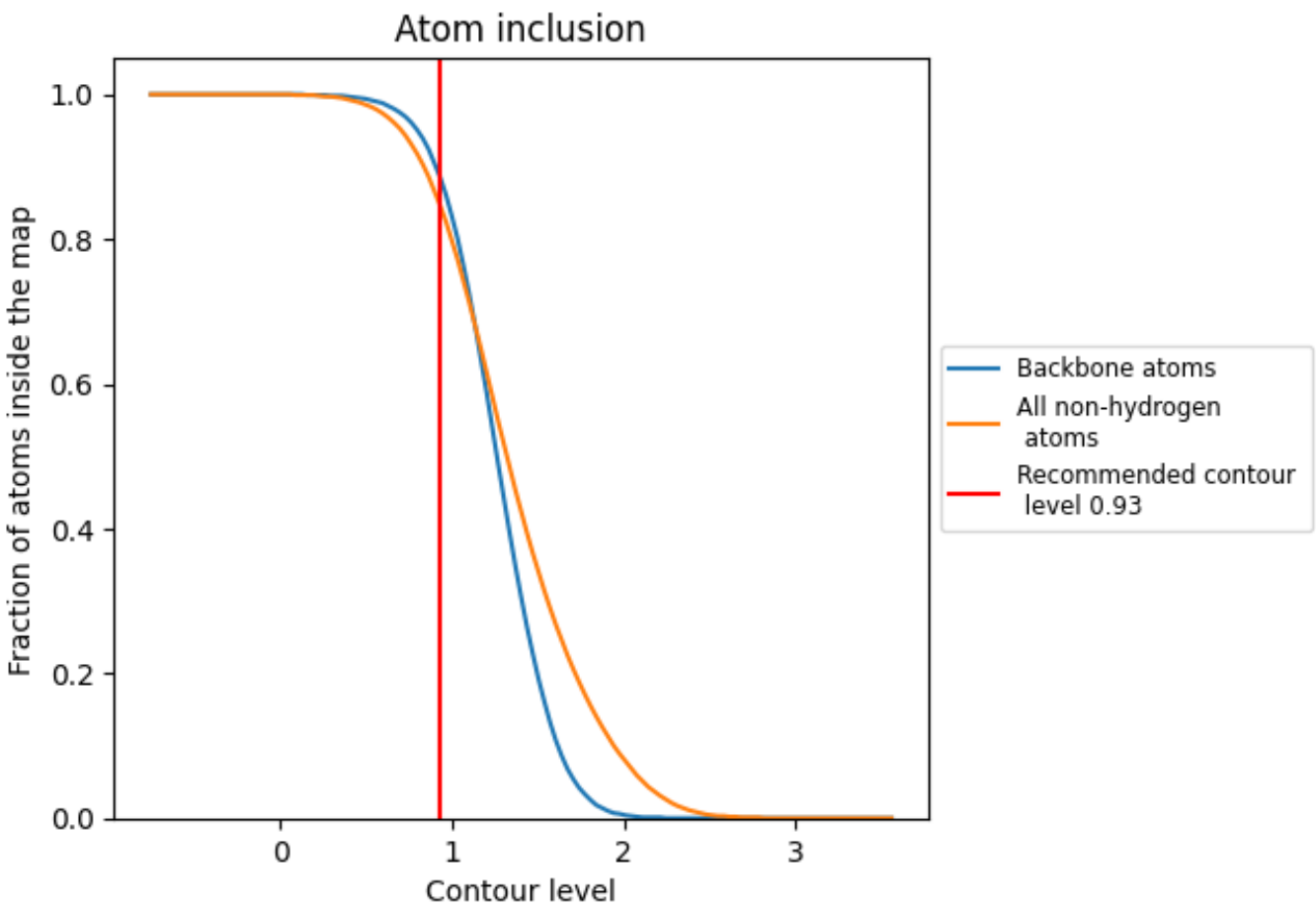
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.93).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.93) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8470	0.1240
A1	0.9300	0.1530
A3	0.8970	0.1350
A5	0.7410	0.1180
A7	0.8860	0.1390
A8	0.9090	0.0680
AA	0.7120	0.0850
AB	0.6590	0.0870
AC	0.6820	0.0840
AD	0.6510	0.0890
AE	0.8360	0.1010
AF	0.7700	0.1100
AG	0.8010	0.1310
AH	0.8720	0.0650
AI	0.6350	0.1030
AJ	0.6970	0.0860
AK	0.6620	0.1130
AL	0.6150	0.0750
AM	0.6090	0.0770
AN	0.6760	0.0960
AO	0.7420	0.1000
AP	0.7630	0.1130
AQ	0.6740	0.0980
AR	0.6640	0.0850
AS	0.7080	0.0980
AT	0.6840	0.1060
AU	0.7180	0.1020
AV	0.7430	0.0970
AW	0.7590	0.1270
AX	0.8680	0.1020
AY	0.6910	0.1130
AZ	0.8210	0.1280
Aa	0.6630	0.0790
Ab	0.6230	0.0900
Ad	0.6940	0.0790

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Chain	Atom inclusion	Q-score
Ae	0.6110	0.0430
Af	0.2890	0.0250
Ag	0.4060	0.0270
Ah	0.5420	0.0520
Ai	0.6860	0.1150
Aj	0.7910	0.0890
Ak	0.7710	0.1020
B1	0.8520	0.1170
B2	0.9350	0.1380
B3	0.5800	0.0800
BA	0.8750	0.1130
BB	0.7500	0.1120
BC	0.7360	0.1080
BD	0.7170	0.0920
BE	0.6980	0.0590
BF	0.7390	0.1020
BG	0.8000	0.0880
BH	0.7540	0.0780
BI	0.7270	0.0990
BJ	0.7290	0.0740
BK	0.6320	0.0360
BL	0.7110	0.0710
BM	0.7710	0.0910
BN	0.6860	0.0930
BO	0.8360	0.0850
BP	0.7530	0.0550
BQ	0.7480	0.0960
BR	0.7180	0.0820
BS	0.5900	0.0680
BT	0.8170	0.0770
BU	0.7540	0.0640
BV	0.7530	0.0900
BW	0.7170	0.0850
BX	0.8830	0.0910
BY	0.7990	0.0630