wwPDB EM Validation Summary Report (i)

Apr 22, 2024 – 07:12 pm BST

PDB ID	:	6ZME
EMDB ID	:	EMD-11289
Title	:	SARS-CoV-2 Nsp1 bound to the human CCDC124-80S-eERF1 ribosome complex
Authors	:	Thoms, M.; Buschauer, R.; Ameismeier, M.; Denk, T.; Kratzat, H.; Mackens-Kiani, T.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on	:	2020-07-02
Resolution	:	3.00 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 (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 (1)) were used in the production of this report:

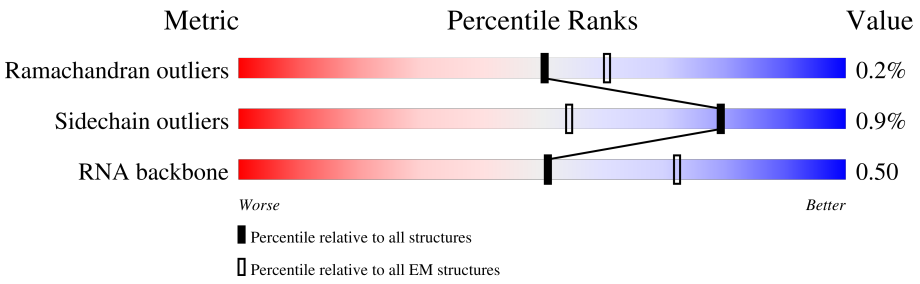
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.00 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	L5	5066	53% 19% 26%
2	L7	121	86% 13%
3	L8	157	78% 21%
4	LA	257	95%
5	LB	403	98%
6	LC	427	84% 14%
7	LD	297	98%
8	LE	288	9% 81% 18%

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Mol	Chain	Length	Quality of chain
9	LF	248	90% 9%
10	LG	266	10% 89% 9%
11	LH	192	98%
12	LI	214	93% 6%
13	LJ	178	6% 97%
14	LL	211	99%
15	LM	215	63% 35%
16	LN	204	98%
17	LO	203	98%
18	LP	184	83% 17%
19	LQ	188	99%
20	LR	196	6% 95% 5%
21	LS	176	99%
22	LT	160	98%
23	LU	128	77% 21%
24	LV	140	93% 6%
25	LW	157	19% 79% 21%
26	LX	156	76% 23%
27	LY	145	91% 8%
28	LZ	136	99%
29	La	148	98%
30	Lb	159	7% 68% 31%
31	Lc	115	84% 15%
32	Ld	125	85% 14%
33	Le	135	95% 5%

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Mol	Chain	Length	Quality of chain
34	Lf	110	95%
35	Lg	117	5% 96%
36	Lh	123	98%
37	Li	105	97%
38	Lj	97	87% 11%
39	Lk	70	99%
40	Ll	51	96%
41	Lm	128	41% 59%
42	Ln	25	96%
43	Lo	106	5% 99%
44	Lp	92	99%
45	Lr	137	91% 9%
46	Ls	317	36% 60% 38%
47	Lt	165	29% 79% 5% 15%
48	Lz	217	88% 99%
49	S2	1869	67% 23% 7%
50	SA	295	74% 25%
51	SB	264	80% 19%
52	SD	243	7% 92% 7%
53	SE	263	99%
54	SF	204	89% 10%
55	SH	194	14% 94%
56	SI	208	99%
57	SK	165	58% 41%
58	SL	158	7% 96%

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Mol	Chain	Length	Quality of chain
59	SP	145	8% 85% 11%
60	SQ	146	5% 95%
61	SR	135	5% 99%
62	SS	152	93% 5%
63	ST	145	97%
64	SU	119	12% 84% 13%
65	SV	83	98%
66	SX	143	94%
67	Sa	115	88% 11%
68	Sc	69	91% 7%
69	Sd	56	98%
70	Sg	317	19% 97%
71	SC	293	75% 24%
72	SG	249	8% 94% 5%
73	SJ	194	5% 94% 5%
74	SM	132	63% 89% 8%
75	SN	151	99%
76	SO	151	5% 91% 7%
77	SW	130	99%
78	SY	133	5% 97%
79	SZ	125	6% 57% 40%
80	Sb	84	6% 96%
81	Se	59	17% 98%
82	Sf	156	17% 42% 57%
83	CA	394	86% 88% 10%

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Mol	Chain	Length	Quality of chain
84	CC	75	63% 35%
85	CE	223	5% 51% 48%
86	CF	180	16% 84%
87	CI	599	15% 96%
88	CH	437	29% 93% 5%

2 Entry composition (i)

There are 92 unique types of molecules in this entry. The entry contains 233375 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 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	L5	3773	80138	35655	14589	26122	3772	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L7	120	2561	1141	456	844	120	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L8	156	3314	1480	585	1094	155	0	0

- Molecule 4 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	LA	248	1898	1189	389	314	6	0	0

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	LB	402	3238	2060	608	556	14	0	0

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	LC	368	2927	1840	583	489	15	0	0

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	LD	293	2382	1507	434	427	14	0	0

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	LE	236	1904	1222	361	317	4	0	0

- Molecule 9 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	LF	225	1870	1202	358	301	9	0	0

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	LG	241	1927	1228	371	324	4	0	0

- Molecule 11 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	LH	190	1518	956	284	272	6	0	0

- Molecule 12 is a protein called 60S ribosomal protein L10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	LI	202	1634	1037	314	269	14	0	0

- Molecule 13 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	LJ	176	1410	888	263	253	6	0	0

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	LL	210	1701	1064	352	281	4	0	0

- Molecule 15 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	LM	139	1138	730	218	183	7	0	0

- Molecule 16 is a protein called 60S ribosomal protein L15.

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

- Molecule 17 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	LO	201	1650	1063	321	261	5	0	0

- Molecule 18 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	LP	153	1242	776	241	216	9	0	0

- Molecule 19 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	LQ	187	1513	944	314	250	5	0	0

- Molecule 20 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	LR	187	1566	971	336	250	9	0	0

- Molecule 21 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	LS	175	1453	925	283	235	10	0	0

- Molecule 22 is a protein called 60S ribosomal protein L21.

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

- Molecule 23 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	LU	101	825	529	144	150	2	0	0

- Molecule 24 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	LV	131	979	618	184	172	5	0	0

- Molecule 25 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	LW	124	1015	634	207	170	4	0	0

- Molecule 26 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	LX	120	985	630	185	169	1	0	0

- Molecule 27 is a protein called 60S ribosomal protein L26.

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

- Molecule 28 is a protein called 60S ribosomal protein L27.

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

- Molecule 29 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	La	147	1162	736	237	186	3	0	0

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Lb	109	876	546	189	137	4	0	0

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Lc	98	764	485	135	138	6	0	0

- Molecule 32 is a protein called 60S ribosomal protein L31.

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

- Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Le	128	1053	667	216	165	5	0	0

- Molecule 34 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Lf	109	876	555	174	144	3	0	0

- Molecule 35 is a protein called 60S ribosomal protein L34.

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

- Molecule 36 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	Lh	122	1015	641	205	168	1	0	0

- Molecule 37 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	Li	102	832	521	177	129	5	0	0

- Molecule 38 is a protein called 60S ribosomal protein L37.

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

- Molecule 39 is a protein called 60S ribosomal protein L38.

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

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	Ll	50	444	281	98	64	1	0	0

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	Lm	52	429	266	90	67	6	0	0

- Molecule 42 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	Ln	24	230	139	62	26	3	0	0

- Molecule 43 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	Lo	105	862	542	175	139	6	0	0

- Molecule 44 is a protein called 60S ribosomal protein L37a.

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

- Molecule 45 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Lr	125	1002	622	207	168	5	0	0

- Molecule 46 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	Ls	196	1496	952	259	276	9	0	0

- Molecule 47 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	Lt	141	1046	652	191	199	4	0	0

- Molecule 48 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	Lz	217	1741	1113	312	307	9	0	0

- Molecule 49 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
49	S2	1740	36899	16459	6598	12103	1739	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	SA	221	1741	1106	305	322	8	0	0

- Molecule 51 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	SB	214	1738	1103	310	311	14	0	0

- Molecule 52 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	SD	227	1765	1125	317	315	8	0	0

- Molecule 53 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 54 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	SF	184	1461	914	276	264	7	0	0

- Molecule 55 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	SH	186	1497	956	274	266	1	0	0

- Molecule 56 is a protein called 40S ribosomal protein S8.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	SK	98	827	539	148	134	6	0	0

- Molecule 58 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	SL	153	1247	793	234	214	6	0	0

- Molecule 59 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	SP	129	1061	672	202	180	7	0	0

- Molecule 60 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	SQ	144	1142	726	216	197	3	0	0

- Molecule 61 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	SR	135	1090	685	202	198	5	0	0

- Molecule 62 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	SS	145	1198	751	242	203	2	0	0

- Molecule 63 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	ST	143	1112	697	214	198	3	0	0

- Molecule 64 is a protein called 40S ribosomal protein S20.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	SV	83	636	393	117	121	5	0	0

- Molecule 66 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	SX	141	1098	693	219	183	3	0	0

- Molecule 67 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	Sa	102	821	512	171	133	5	0	0

- Molecule 68 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	Sc	64	506	308	102	94	2	0	0

- Molecule 69 is a protein called 40S ribosomal protein S29.

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

- Molecule 70 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 71 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	SC	222	1725	1115	298	302	10	0	0

- Molecule 72 is a protein called 40S ribosomal protein S6.

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

- Molecule 73 is a protein called 40S ribosomal protein S9.

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

- Molecule 74 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	SM	122	940	590	164	177	9	0	0

- Molecule 75 is a protein called 40S ribosomal protein S13.

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

- Molecule 76 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	SO	140	1049	642	204	197	6	0	0

- Molecule 77 is a protein called 40S ribosomal protein S15a.

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

- Molecule 78 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	SY	131	1065	673	209	178	5	0	0

- Molecule 79 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	SZ	75	598	382	111	104	1	0	0

- Molecule 80 is a protein called 40S ribosomal protein S27.

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

- Molecule 81 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
81	Se	58	439	268	97	73	1	0	0

- Molecule 82 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
82	Sf	67	548	346	102	93	7	0	0

- Molecule 83 is a protein called Proliferation-associated protein 2G4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
83	CA	354	2764	1744	475	528	17	4	0

- Molecule 84 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
84	CC	75	1589	710	279	525	75	0	0

- Molecule 85 is a protein called Coiled-coil domain-containing protein 124.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
85	CE	117	998	611	199	184	4	0	0

- Molecule 86 is a protein called Non-structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
86	CF	29	239	145	43	50	1	0	0

- Molecule 87 is a protein called ATP-binding cassette sub-family E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
87	CI	582	4586	2931	785	839	31	0	0

- Molecule 88 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
88	CH	415	3257	2073	556	617	11	0	0

- Molecule 89 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
89	L5	210	210	210	0
89	L7	3	3	3	0
89	L8	4	4	4	0
89	LA	1	1	1	0
89	LB	1	1	1	0
89	LI	1	1	1	0

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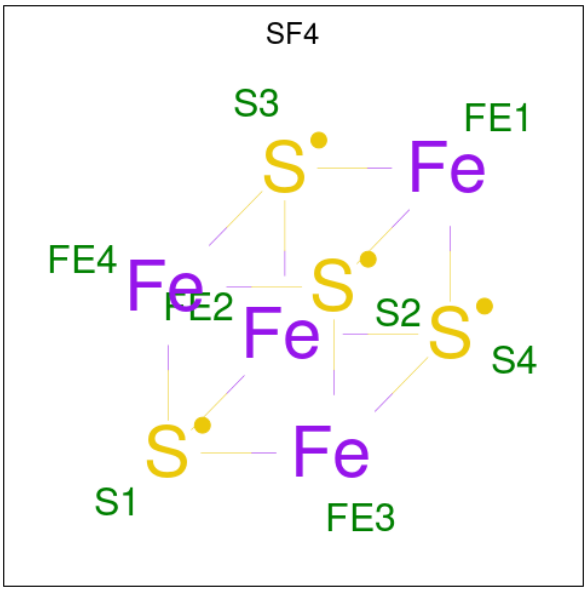
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
89	LP	1	1	1	0
89	LV	1	1	1	0
89	LX	1	1	1	0
89	Le	2	2	2	0
89	Lg	1	1	1	0
89	S2	29	29	29	0
89	SG	1	1	1	0

- Molecule 90 is ZINC ION (three-letter code: ZN) (formula: Zn).

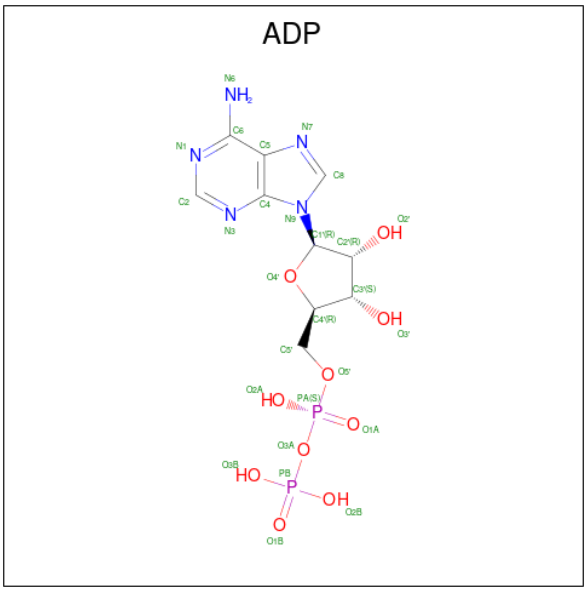
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
90	Lg	1	1	1	0
90	Lj	1	1	1	0
90	Lm	1	1	1	0
90	Lo	1	1	1	0
90	Lp	1	1	1	0
90	Sa	1	1	1	0
90	Sd	1	1	1	0
90	Sf	1	1	1	0

- Molecule 91 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
91	CI	1	8	4	4	0
			Total	Fe	S	
91	CI	1	8	4	4	0

- Molecule 92 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



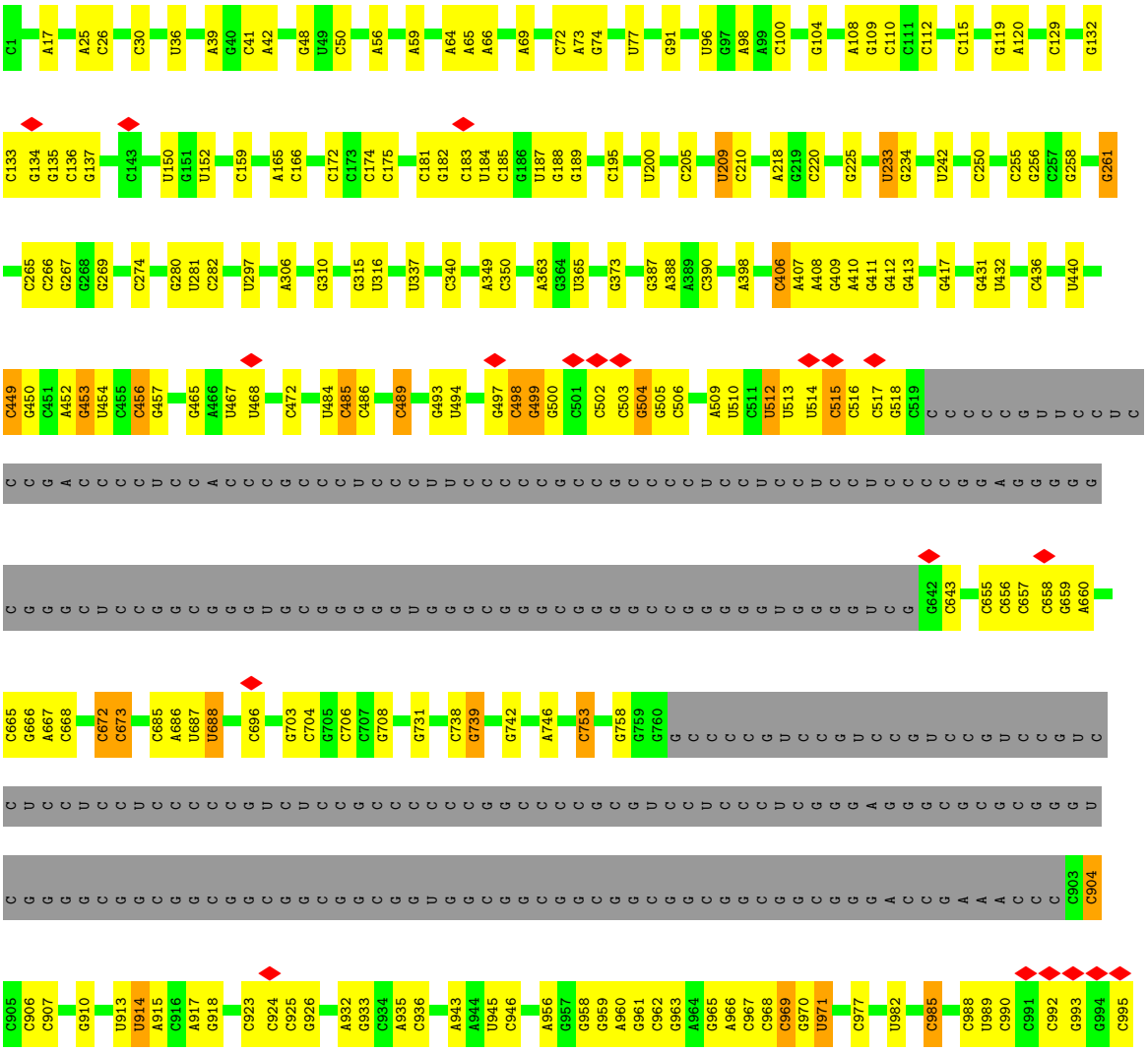
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
92	CI	1	27	10	5	10	2	0

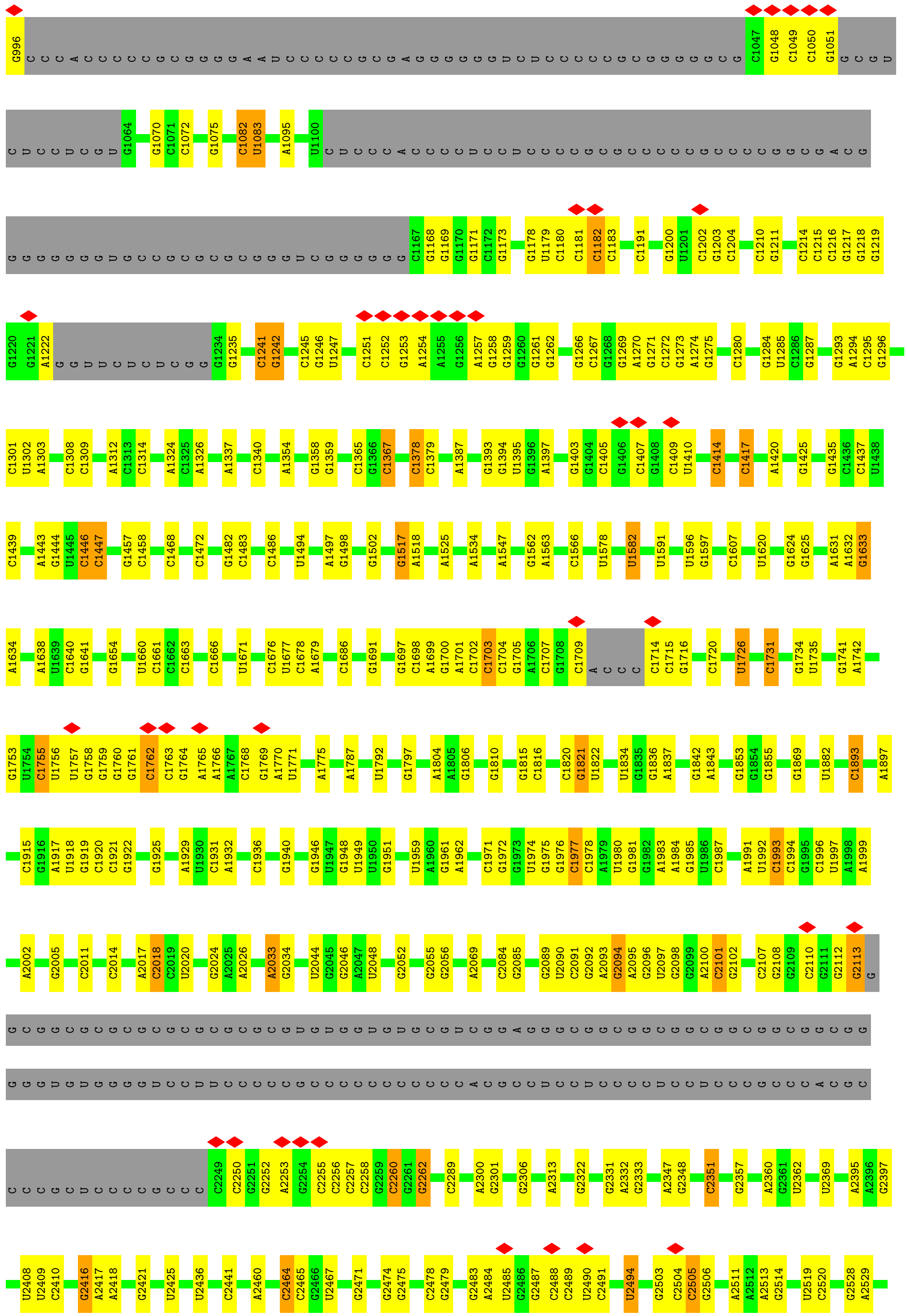
3 Residue-property plots (i)

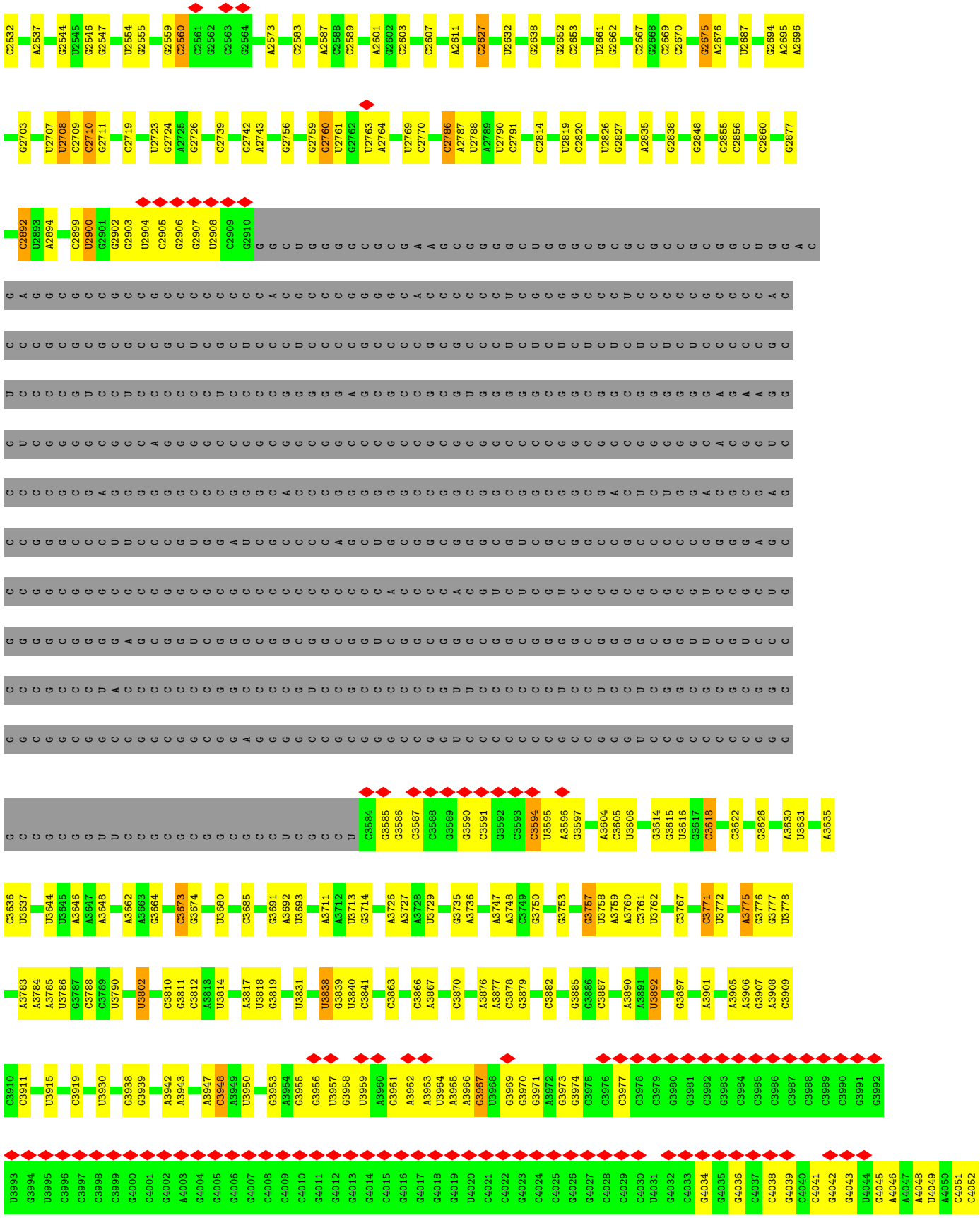
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

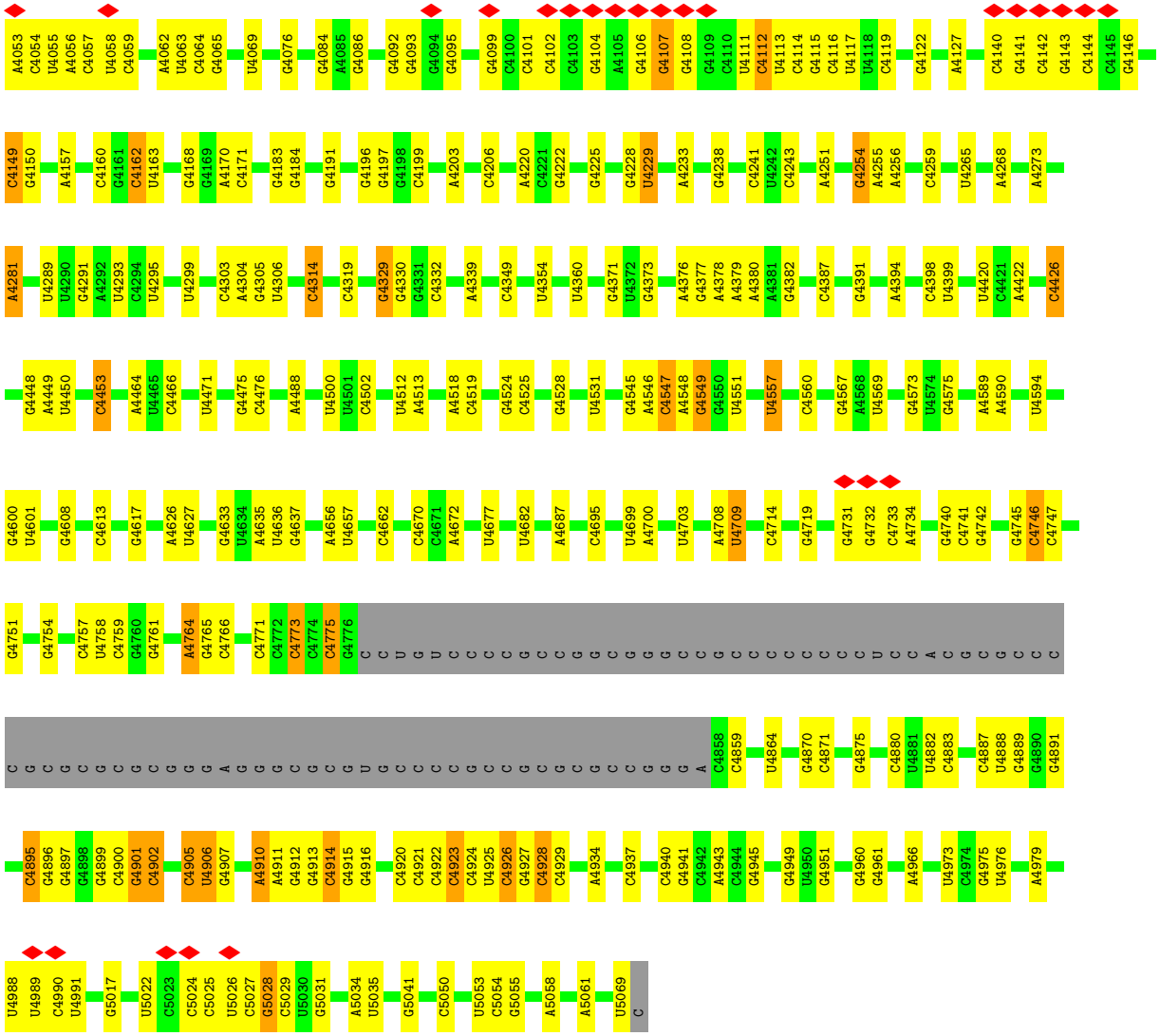
- Molecule 1: 28S ribosomal RNA

Chain L5:



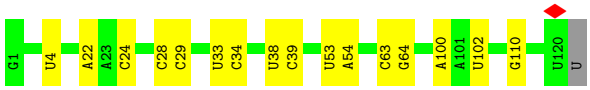



C2532 A2537 G2544 U2545 G2546 G2547 U2554 G2555 G2559 C2560 C2561 G2562 C2563 G2564 A2573 C2583 A2587 C2588 C2589 A2601 G2602 C2603 C2607 A2611 C2627 U2632 G2638 G2652 C2653 U2661 G2662 C2667 G2668 C2669 C2670 G2675 A2676 U2687 G2694 A2695 A2696
G2703 U2707 U2708 C2709 C2710 G2711 C2719 U2723 G2724 A2725 G2726 C2739 G2742 A2743 G2756 G2759 G2760 U2761 G2762 U2763 A2764 U2769 C2770 C2786 A2787 U2788 A2789 U2790 C2791 C2814 U2819 C2820 U2826 G2827 A2835 G2838 G2848 G2855 C2856 C2860 G2877
C2892 U2893 A2894 C2899 U2900 G2901 G2902 G2903 U2904 C2905 G2906 G2907 U2908 C2909 G2910
G C U G G G C C G A G C C C C C C A C G C C C C C C



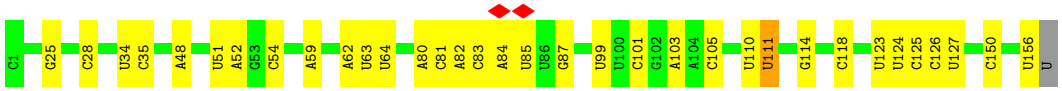
- Molecule 2: 5S ribosomal RNA

Chain L7:



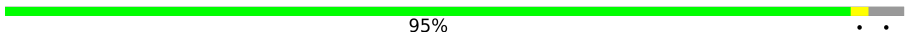
- Molecule 3: 5.8S ribosomal RNA

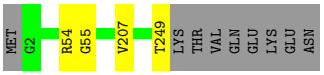
Chain L8:



- Molecule 4: 60S ribosomal protein L8

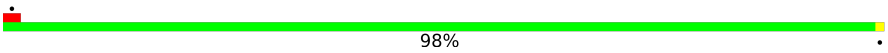
Chain LA:

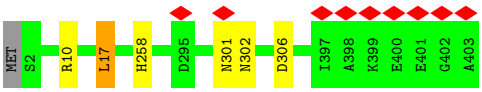




- Molecule 5: 60S ribosomal protein L3

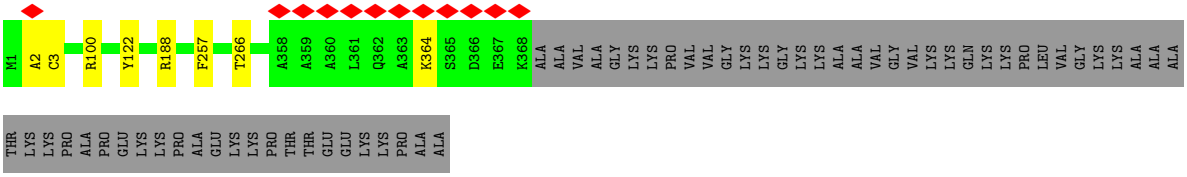
Chain LB:





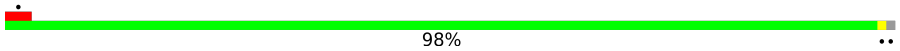
- Molecule 6: 60S ribosomal protein L4

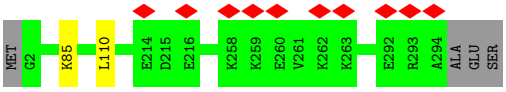
Chain LC:



- Molecule 7: 60S ribosomal protein L5

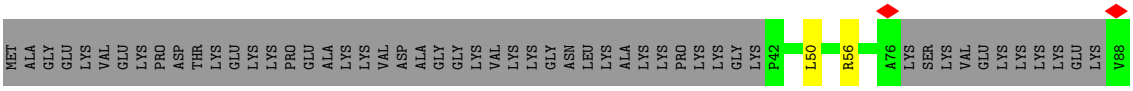
Chain LD:

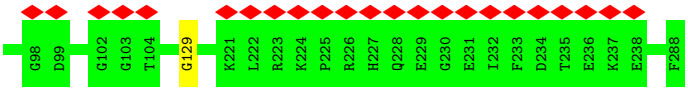




- Molecule 8: 60S ribosomal protein L6

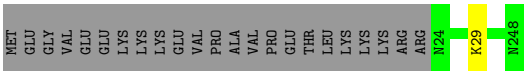
Chain LE:





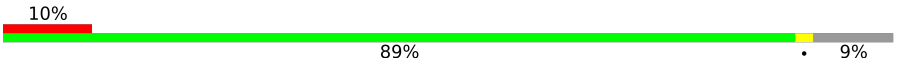
- Molecule 9: 60S ribosomal protein L7

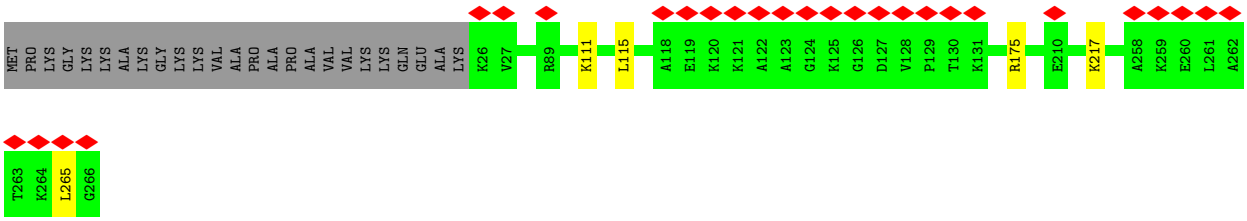
Chain LF:



- Molecule 10: 60S ribosomal protein L7a

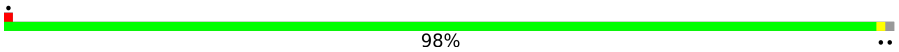
Chain LG:

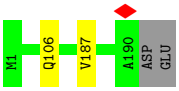




• Molecule 11: 60S ribosomal protein L9

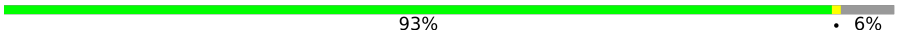
Chain LH:

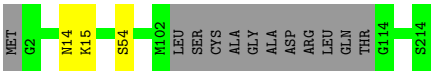




• Molecule 12: 60S ribosomal protein L10-like

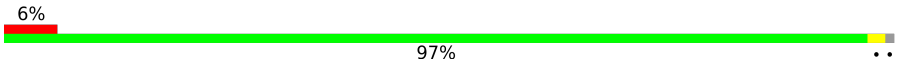
Chain LI:

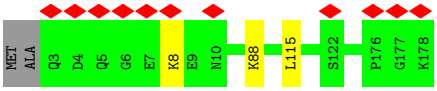




• Molecule 13: 60S ribosomal protein L11

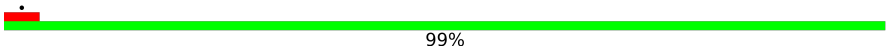
Chain LJ:

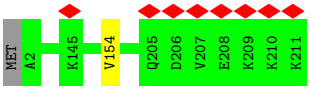




• Molecule 14: 60S ribosomal protein L13

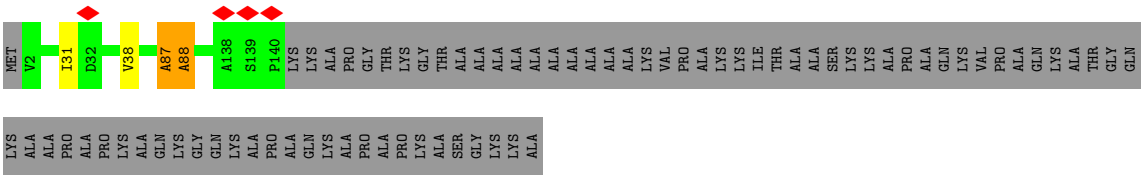
Chain LL:





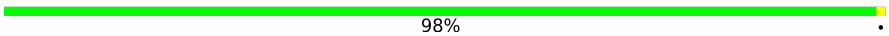
• Molecule 15: 60S ribosomal protein L14

Chain LM:



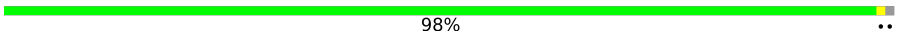
• Molecule 16: 60S ribosomal protein L15

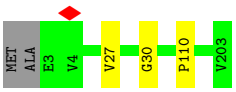
Chain LN:



• Molecule 17: 60S ribosomal protein L13a

Chain LO:



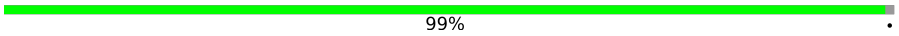


• Molecule 18: 60S ribosomal protein L17

Chain LP:

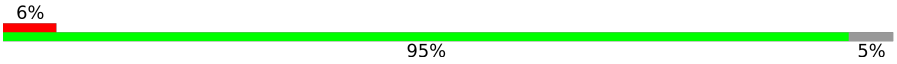
• Molecule 19: 60S ribosomal protein L18

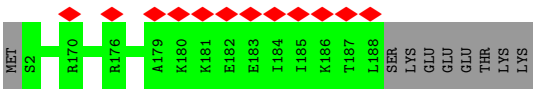
Chain LQ:



• Molecule 20: 60S ribosomal protein L19

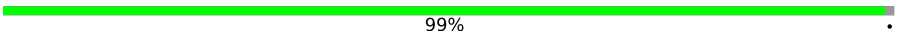
Chain LR:





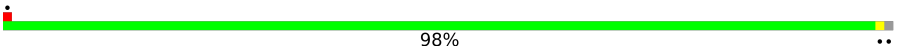
• Molecule 21: 60S ribosomal protein L18a

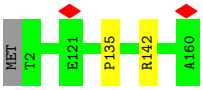
Chain LS:



• Molecule 22: 60S ribosomal protein L21

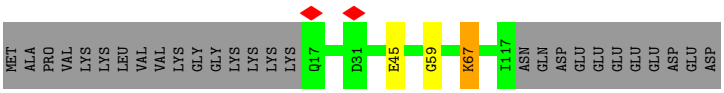
Chain LT:





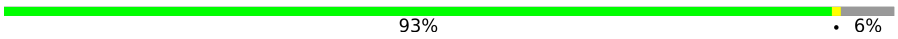
• Molecule 23: 60S ribosomal protein L22

Chain LU:



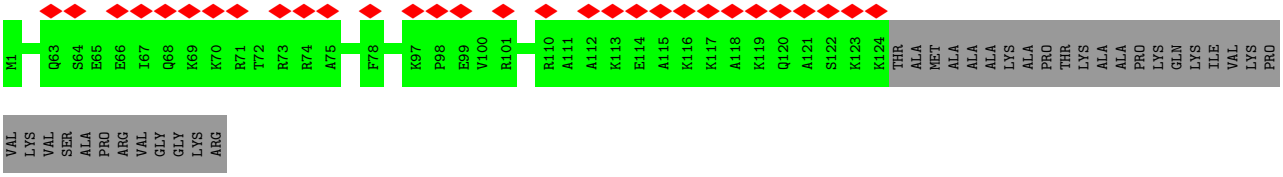
• Molecule 24: 60S ribosomal protein L23

Chain LV:



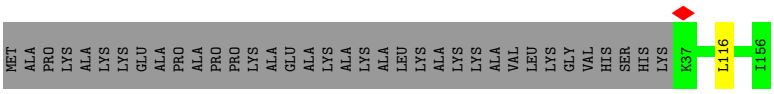
• Molecule 25: 60S ribosomal protein L24

Chain LW:



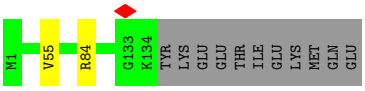
• Molecule 26: 60S ribosomal protein L23a

Chain LX:



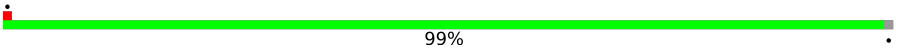
• Molecule 27: 60S ribosomal protein L26

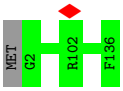
Chain LY:



• Molecule 28: 60S ribosomal protein L27

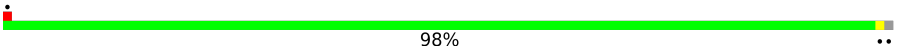
Chain LZ:

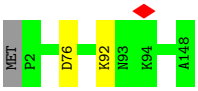




• Molecule 29: 60S ribosomal protein L27a

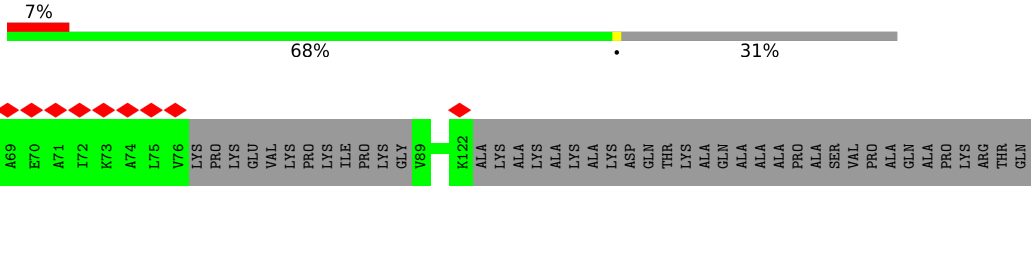
Chain La:





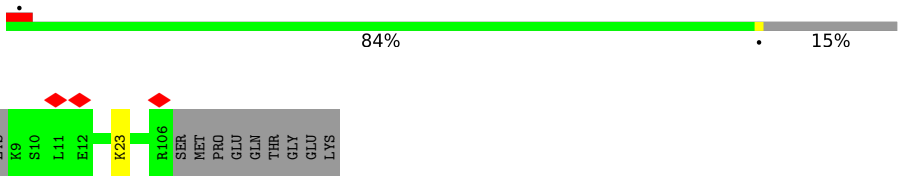
- Molecule 30: 60S ribosomal protein L29

Chain Lb:



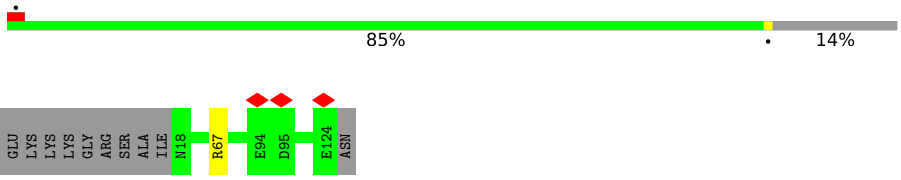
- Molecule 31: 60S ribosomal protein L30

Chain Lc:



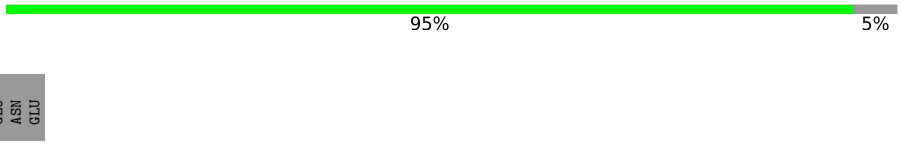
- Molecule 32: 60S ribosomal protein L31

Chain Ld:



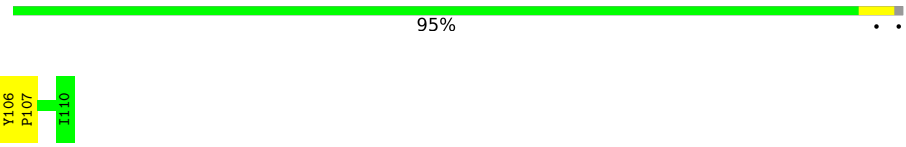
- Molecule 33: 60S ribosomal protein L32

Chain Le:



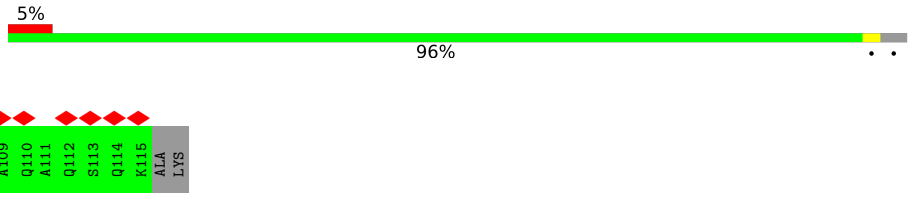
- Molecule 34: 60S ribosomal protein L35a

Chain Lf:



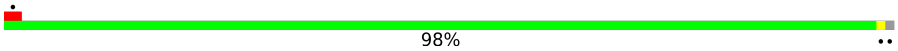
- Molecule 35: 60S ribosomal protein L34

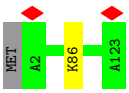
Chain Lg:



- Molecule 36: 60S ribosomal protein L35

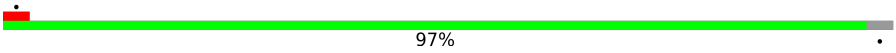
Chain Lh:

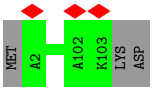




• Molecule 37: 60S ribosomal protein L36

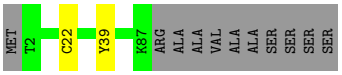
Chain Li:





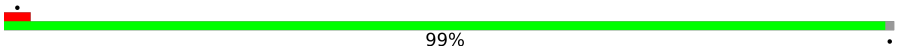
• Molecule 38: 60S ribosomal protein L37

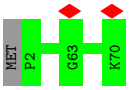
Chain Lj:



• Molecule 39: 60S ribosomal protein L38

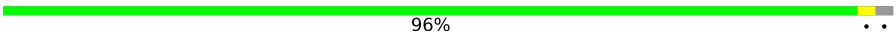
Chain Lk:





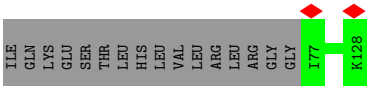
• Molecule 40: 60S ribosomal protein L39

Chain Ll:



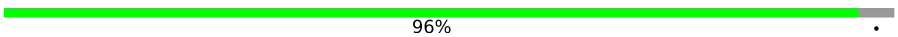
• Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain Lm:



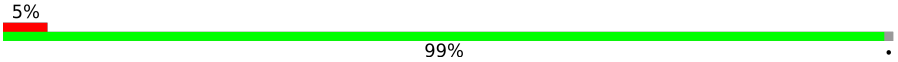
• Molecule 42: 60S ribosomal protein L41

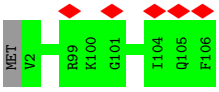
Chain Ln:



- Molecule 43: 60S ribosomal protein L36a

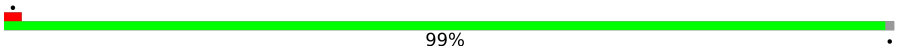
Chain Lo:

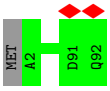




- Molecule 44: 60S ribosomal protein L37a

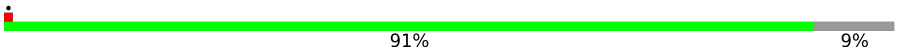
Chain Lp:

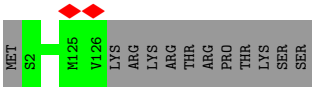




- Molecule 45: 60S ribosomal protein L28

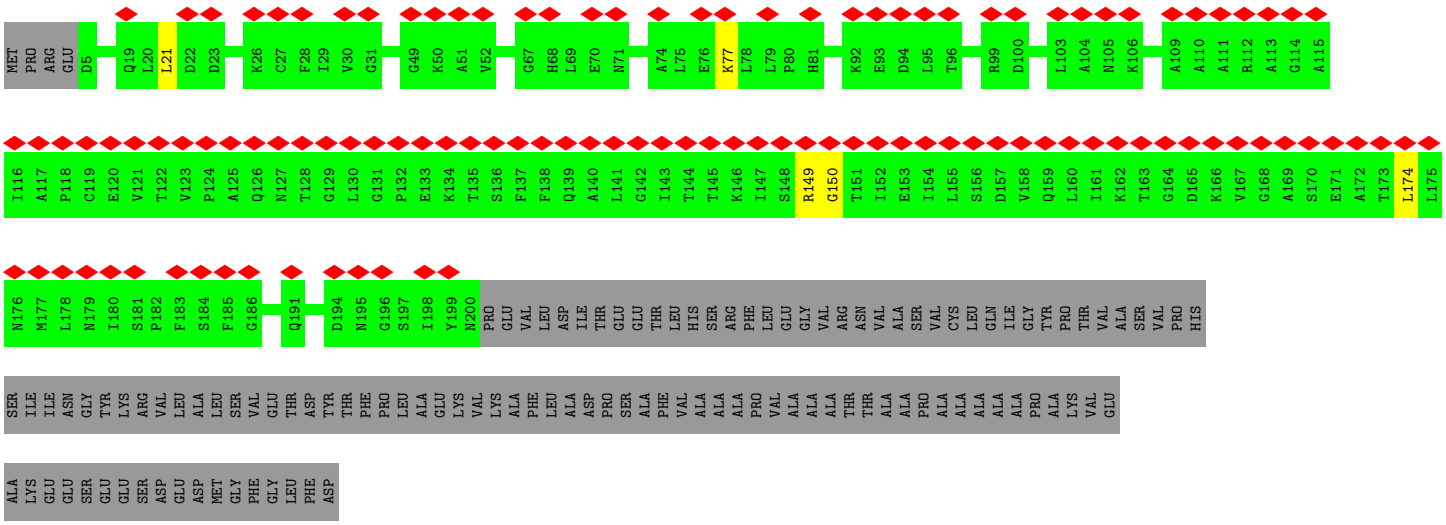
Chain Lr:





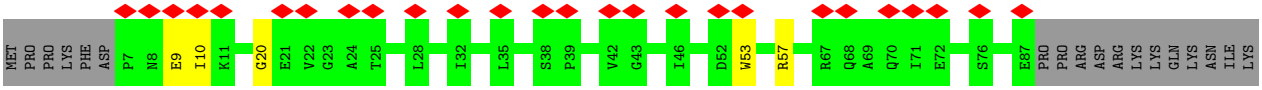
- Molecule 46: 60S acidic ribosomal protein P0

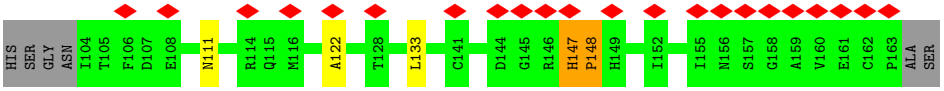
Chain Ls:



- Molecule 47: 60S ribosomal protein L12

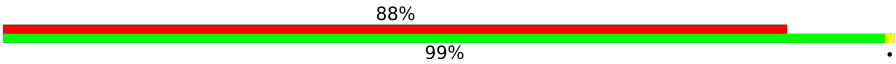
Chain Lt:

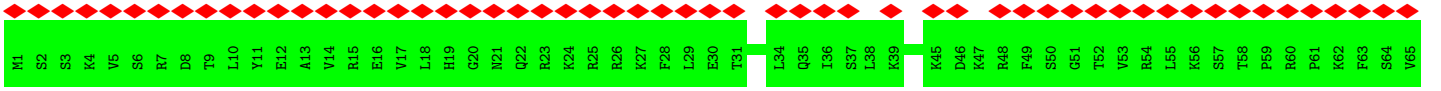


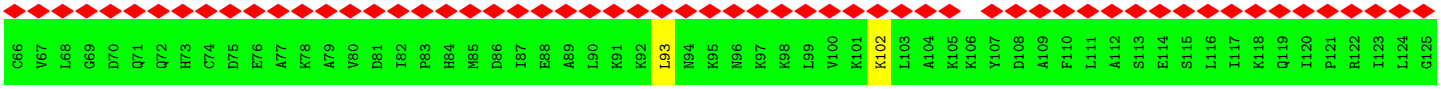


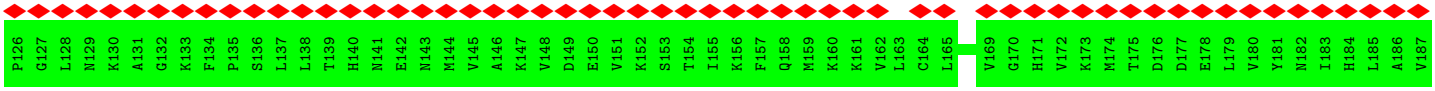
- Molecule 48: 60S ribosomal protein L10a

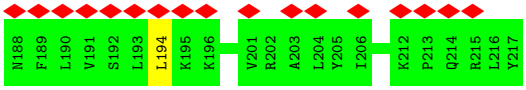
Chain Lz:





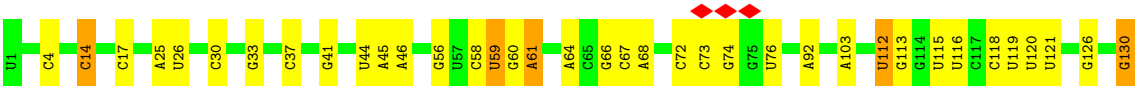


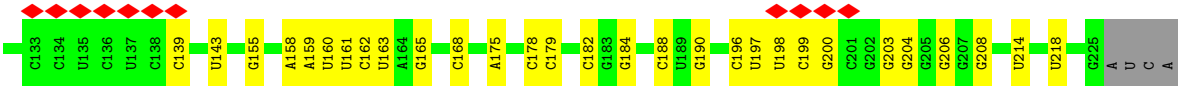


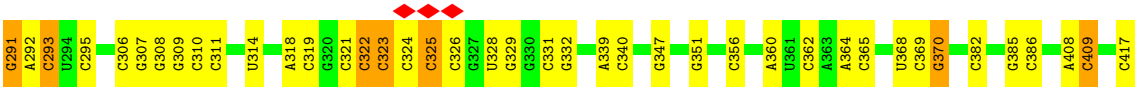


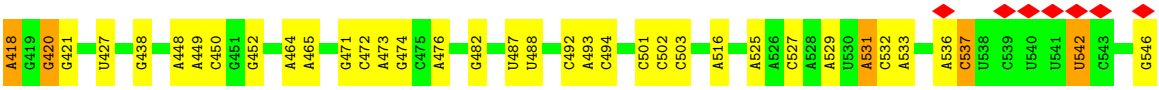
- Molecule 49: 18S ribosomal RNA

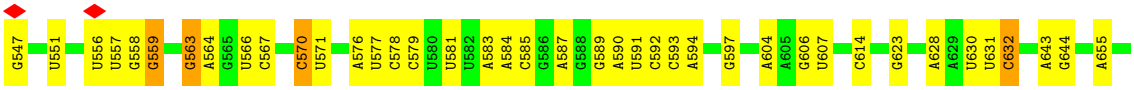
Chain S2:

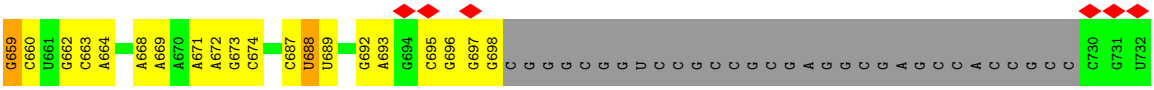


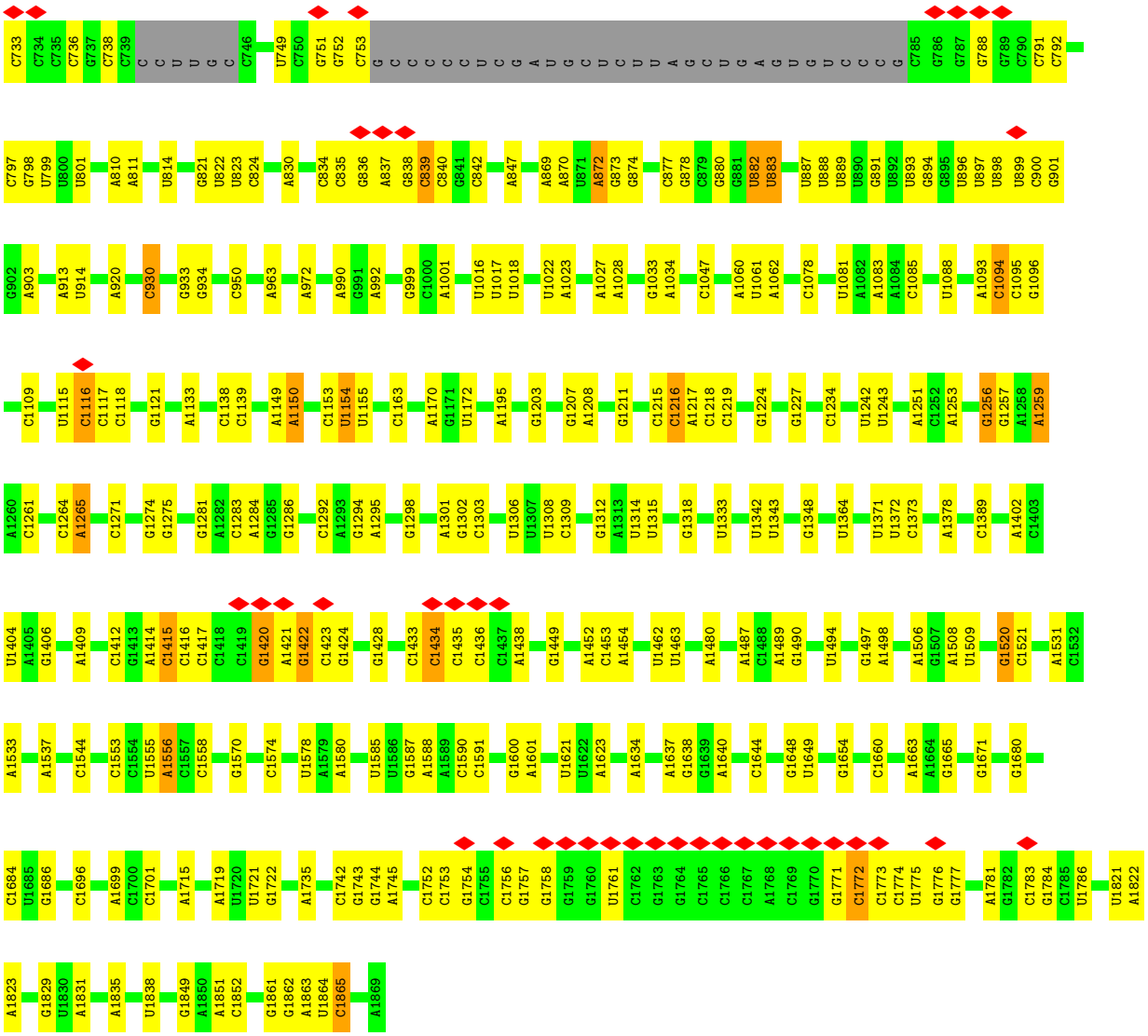






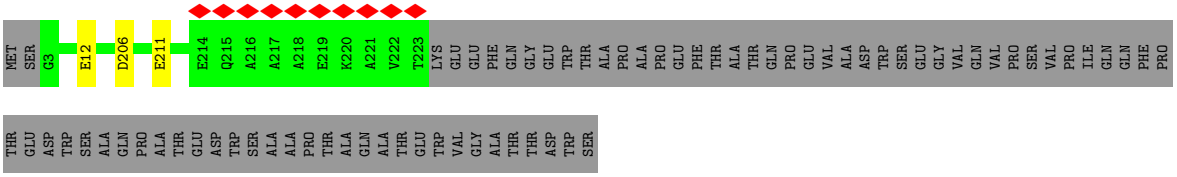






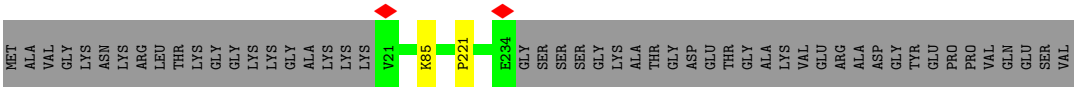
- Molecule 50: 40S ribosomal protein SA

Chain SA:



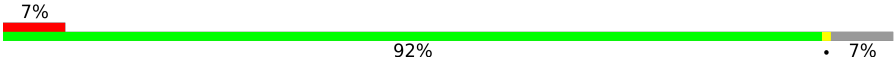
- Molecule 51: 40S ribosomal protein S3a

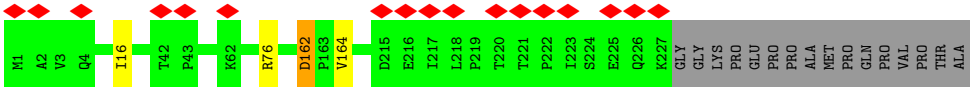
Chain SB:



- Molecule 52: 40S ribosomal protein S3

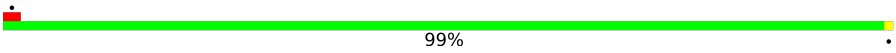
Chain SD:

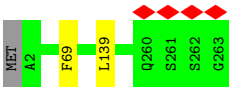




- Molecule 53: 40S ribosomal protein S4, X isoform

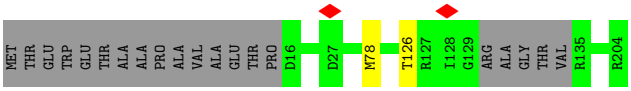
Chain SE:





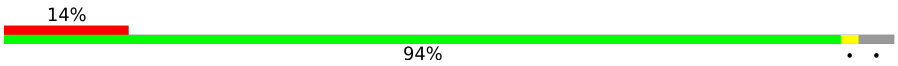
- Molecule 54: 40S ribosomal protein S5

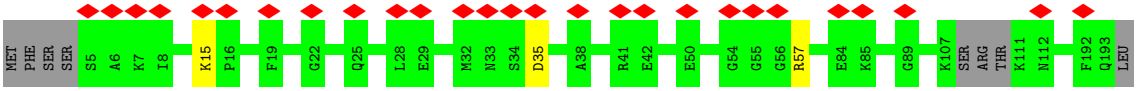
Chain SF:



- Molecule 55: 40S ribosomal protein S7

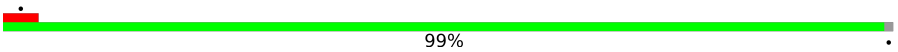
Chain SH:

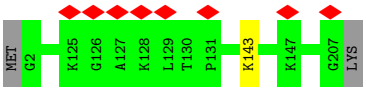




- Molecule 56: 40S ribosomal protein S8

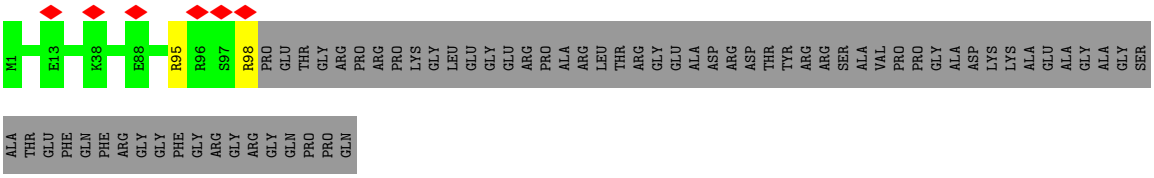
Chain SI:





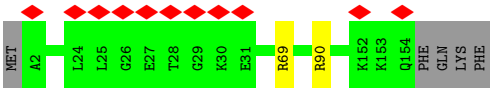
- Molecule 57: 40S ribosomal protein S10

Chain SK:



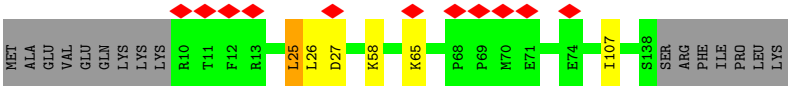
- Molecule 58: 40S ribosomal protein S11

Chain SL: 7% 96%



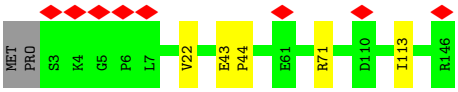
• Molecule 59: 40S ribosomal protein S15

Chain SP: 8% 85% 11%



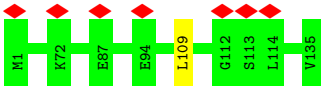
• Molecule 60: 40S ribosomal protein S16

Chain SQ: 5% 95%



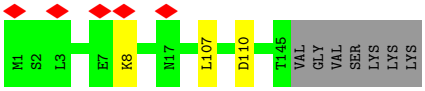
• Molecule 61: 40S ribosomal protein S17

Chain SR: 5% 99%



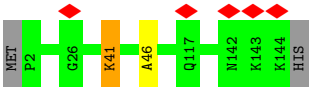
• Molecule 62: 40S ribosomal protein S18

Chain SS: 93% 5%



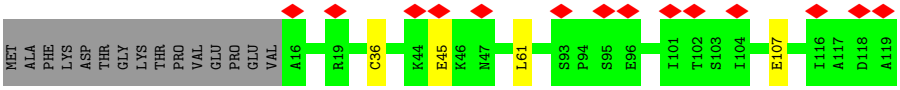
• Molecule 63: 40S ribosomal protein S19

Chain ST: 97%



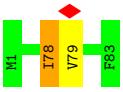
• Molecule 64: 40S ribosomal protein S20

Chain SU: 12% 84% 13%



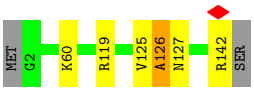
• Molecule 65: 40S ribosomal protein S21

Chain SV: 98%



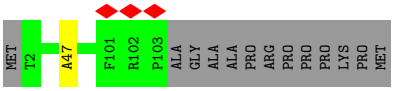
• Molecule 66: 40S ribosomal protein S23

Chain SX: 94%



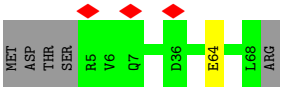
• Molecule 67: 40S ribosomal protein S26

Chain Sa: 88% 11%



• Molecule 68: 40S ribosomal protein S28

Chain Sc: 91% 7%

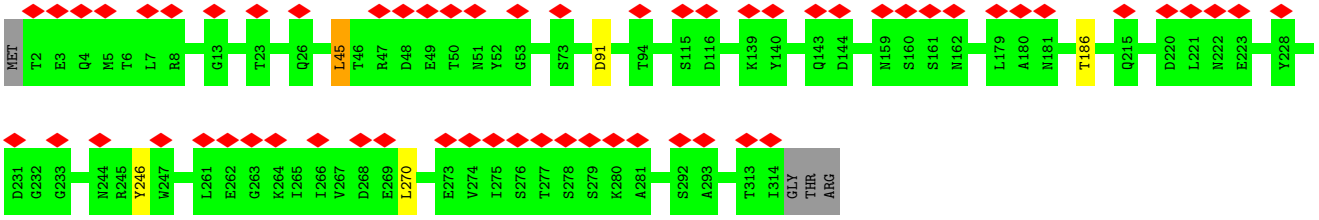


• Molecule 69: 40S ribosomal protein S29

Chain Sd: 98%

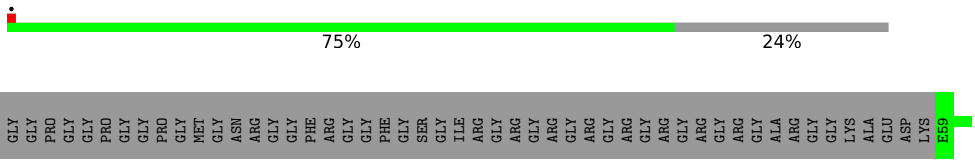
• Molecule 70: Receptor of activated protein C kinase 1

Chain Sg: 19% 97%



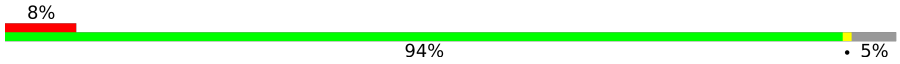
• Molecule 71: 40S ribosomal protein S2

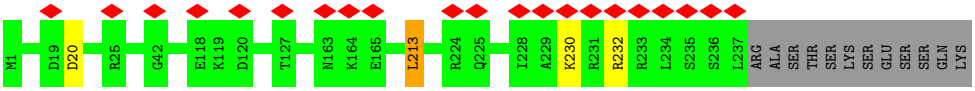
Chain SC:



- Molecule 72: 40S ribosomal protein S6

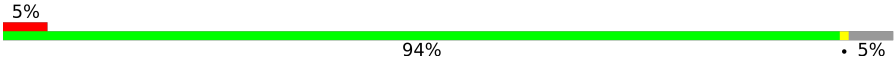
Chain SG:

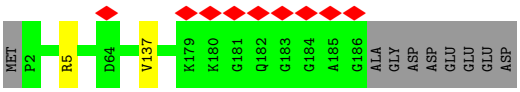




- Molecule 73: 40S ribosomal protein S9

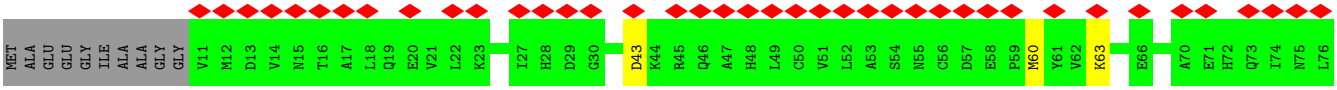
Chain SJ:

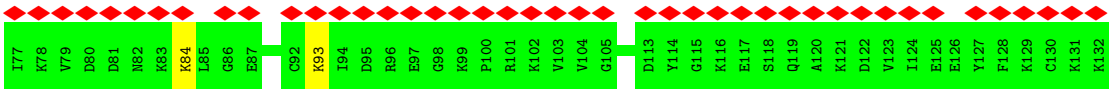




- Molecule 74: 40S ribosomal protein S12

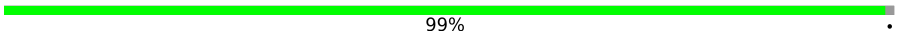
Chain SM:





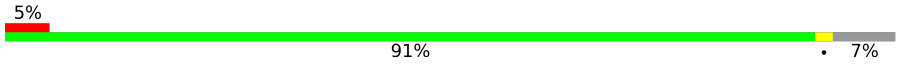
- Molecule 75: 40S ribosomal protein S13

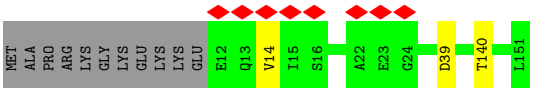
Chain SN:



- Molecule 76: 40S ribosomal protein S14

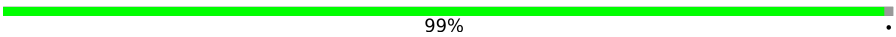
Chain SO:





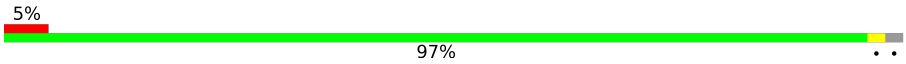
- Molecule 77: 40S ribosomal protein S15a

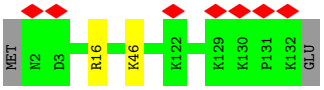
Chain SW:



- Molecule 78: 40S ribosomal protein S24

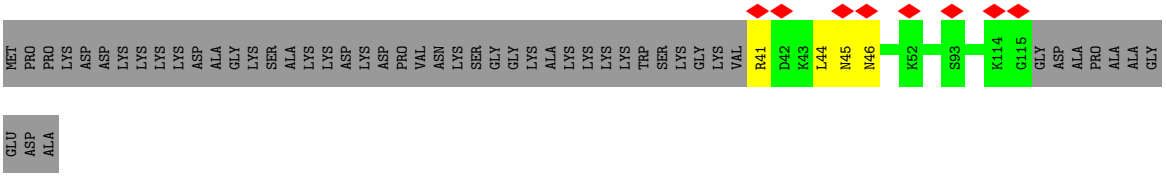
Chain SY:





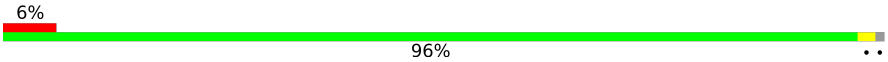
- Molecule 79: 40S ribosomal protein S25

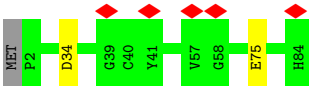
Chain SZ:



- Molecule 80: 40S ribosomal protein S27

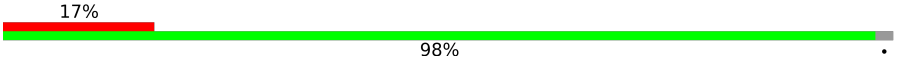
Chain Sb:

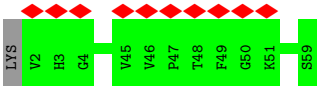




- Molecule 81: 40S ribosomal protein S30

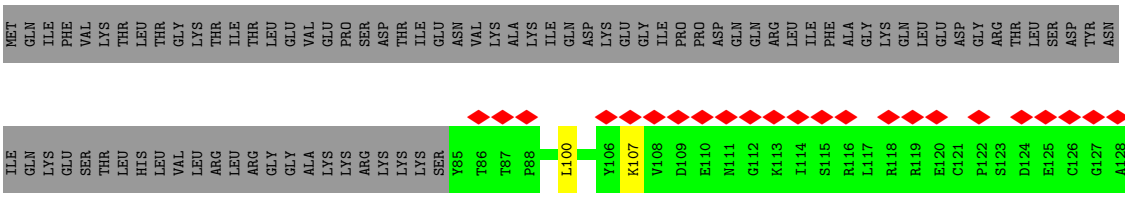
Chain Se:





- Molecule 82: Ubiquitin-40S ribosomal protein S27a

Chain Sf:



PRO GLU ASP LYS

- Molecule 83: Proliferation-associated protein 2G4

Chain CA: 86% 88% 10%

MET SER GLY GLU ASP GLU Q7 Q8 E9 Q10 T11 I12 A13 E14 D15 L16 V17 V18 T19 K20 Y21 K22 M23 G24 G25 D26 I27 A28 N29 R30 V31 L32 R33 S34 L35 V36 E37 A38 S39 S40 S41 G42 V43 S44 V45 L46 S47 L48 C49 E50 K51 G52 D53 A54 M55 I56 M57 E58 E59 T60

G61 K62 I63 F64 K65 K66 E67 K68 E69 M70 K71 K72 G73 I74 A75 F76 P77 T78 S79 I80 S81 V82 N83 N84 C85 V86 C87 H88 F89 S90 P91 L92 K93 S94 D95 Q96 D97 Y98 I99 L100 K101 E102 G103 D104 L105 V106 K107 I108 D109 L110 G111 V112 H113 V114 D115 G116 F117 I118 A119 N120

V121 A122 H123 T124 F125 V126 V127 D128 V129 A130 Q131 G132 T133 Q134 V135 T136 G137 R138 K139 A140 D141 V142 I143 K144 A145 A146 H147 L148 C149 A150 E151 A152 A153 L154 R155 L156 V157 K158 P159 G160 N161 Q162 N163 T164 Q165 V166 T167 E168 A169 W170 N171 K172 V173 A174 H175 S176 F177 N178 C179 T180

P181 I182 E183 G184 M185 L186 S187 H188 Q189 L190 K191 Q192 H193 V194 I195 D196 G197 E198 K199 T200 I201 I202 Q203 N204 P205 T206 D207 Q208 Q209 K210 K211 D212 H213 E214 K215 A216 E217 F218 E219 V220 H221 E222 V223 Y224 A225 V226 D227 V228 L229 V230 S231 S232 G233 E234 G235 K236 A237 K238 D239 A240

G241 Q242 R243 T244 T245 I246 Y247 K248 R249 D250 P251 S252 K253 Q254 F265 F266 S267 E268 V269 E270 R271 R272 F273 D274 A275 M276 P277 F278 T279 L280 R281 A282 F283 GLU ASP E286 K287 K288 A289 R290 M291 G292 E295 C296 A297 E300 L301 L302 Q303 P304 F305 N306 V307 L308 Y309 E310 K311

E312 G313 E314 F315 V316 A317 Q318 F319 K320 F321 T322 V323 L324 L325 M326 P327 N328 G329 P330 M331 R332 I333 T334 S335 G336 P337 F338 E339 P340 D341 L342 Y343 K344 S345 E346 M347 E348 V349 Q350 D351 A352 E353 L354 K355 A356 L357 L358 Q359 S360 S361 A362 SER ARG LYS THR GLN LYS LYS LYS LYS

LYS LYS ALA SER LYS THR ALA GLU ASN ALA THR SER GLY GLU THR LEU GLU GLU ASN GLU ALA GLY ASP

- Molecule 84: tRNA

Chain CC: 63% 35%

U1 C11 C16 G17 G18 C19 U20 A21 U22 C23 C28 G31 C32 U33 U34 U35 C36 A37 C38 C39 G45 A46 C47 C48 C55 G56 A57 C61 G72 C73 C74 A75

- Molecule 85: Coiled-coil domain-containing protein 124

Chain CE: 5% 51% 48%

MET PRO LYS LYS PHE GLN GLY GLU ASN THR LYS SER ALA ALA ALA R16 A17 R18 R19 A20 E21 A22 K23 A24 A25 A26 D27 E33 L34 K40 L81 LYS GLY GLY LYS ALA PRO ARG VAL ALA THR SER SER LYS VAL THR ARG ALA ALA GLN ILE GLU ASP THR LEU ARG ARG ASP

HIS GLN LEU ARG GLU ALA PRO ASP THR ALA GLU LYS ALA LYS SER HIS LEU GLU VAL PRO LEU GLU GLU ASN VAL ASN ARG ARG VAL LEU GLU GLU GLY SER VAL GLU ALA ARG THR ILE GLU ASP ALA ILE ALA VAL LEU SER VAL ALA GLU GLU ALA ALA D162 M212 ASN GLN ARG

ALA VAL PRO PHE ASN ALA PRO LYS

- Molecule 86: Non-structural protein 1

Chain CF: 16% 84%

MET GLU SER LEU VAL PRO GLY PHE ASN GLU LYS THR HIS VAL GLN LEU SER LEU PRO VAL LEU GLN VAL ARG ASP VAL LEU VAL ARG GLY PHE GLY ASP SER VAL GLU GLU VAL LEU SER GLU ALA ARG GLN HIS LEU LYS ASP GLY THR CYS GLY LEU VAL GLU VAL GLU LYS GLY VAL

LEU PRO GLN LEU GLU GLN PRO TYR VAL PHE ILE LYS ARG SER ASP ALA ARG THR ALA PRO HIS GLY HIS VAL MET VAL GLU LEU VAL ALA GLU LEU GLU GLY ILE GLN TYR GLY ARG SER GLY GLU THR LEU GLY VAL LEU VAL PRO HIS VAL GLY GLU ILE PRO VAL ALA TYR ARG LYS

VAL LEU LEU ARG LYS ASN GLY ASN LYS GLY ALA GLY GLY HIS SER TYR GLY ALA ASP LEU LYS SER PHE ASP LEU GLY ASP GLU LEU GLY THR D152 G180

- Molecule 87: ATP-binding cassette sub-family E member 1

Chain CI: 15% 96%

MET ALA ASP K4 D14 L37 T42 P43 Q44 S45 K46 H95 D135 E161 D162 D163 L164 K165 D174 Q175 I176 P177 K178 A179 A180 K181 G182 T183 V184 G185 D189 R190 K191 D192 E193 T194 K195 T196 Q197 A198 I199 Q202 D205 L206 T207 H208 E211 R212 N213

V214 E215 D216 L217 S218 E221 A228 K234 A235 D236 I237 K332 VAL ALA GLU THR ALA ASN GLU GLU GLU VAL LYS LYS M345 C346 M347 P351 G352 M353 K354 K355 K356 M357 G358 E359 F360 E361 L362 A363 I364 V365 A366 E380 N381 G382 R395 L396 K397 P398 D399 E400 G401

G402 E403 V404 K415 K419 R433 D434 I454 I455 D456 D536 G537 V538 P539 S540 K541 N542 L597 ASP ASP

- Molecule 88: Eukaryotic peptide chain release factor subunit 1

Chain CH: 29% 93% 5%

MET ALA ASP ASP PRO SER A7 A8 D9 R10 N11 K19 K22 A26 A27 R28 G29 N30 G31 T32 S33 M34 I35 S36 L37 I38 I39 P40 P41 K42 D43 Q44 I45 S46 R47 V48 A49 K50 M51 L52 A53 D54 E55 F56 G57 T58 A59 K63 S64 N67 R68 L69 G73

Q79 Q80 R81 L82 K83 L84 Y85 N86 K87 V88 P89 P90 V95 Y96 T99 I100 V101 T102 E103 E104 G105 K106 E107 K108 K109 I112 D113 F114 E115 P116 F117 K118 P119 I120 N121 T122 S123 L124 Y125 L126 C127 D128 N129 K130 F131 H132 T133 E134 A135 A138 D142 D143 S186 A187

L188 D217 F280 E313 H334 C335 Q336 G337 T338 E339 E340 E341 K342 I343 L344 E349 Q350 E351 K352 D353 K354 S355 H356 F357 T358 D359 K360 E361 T362 G363 Q364 E365 H366 E367 L368 I369 E370 S371 D418 G421 MET GLU TYR GLN GLY GLY ASP ASP GLU PHE PHE ASP LEU

ASP ASP TYR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13337	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 ($e^-/Å^2$)	44.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.457	Depositor
Minimum map value	-0.148	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	423.6, 423.6, 423.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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: ADP, MG, ZN, SF4

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	L5	0.68	3/89595 (0.0%)	1.12	547/139686 (0.4%)
2	L7	0.61	0/2861	1.06	13/4459 (0.3%)
3	L8	0.66	0/3701	1.02	13/5766 (0.2%)
4	LA	0.43	0/1936	0.63	0/2596
5	LB	0.38	0/3306	0.60	2/4424 (0.0%)
6	LC	0.38	0/2981	0.59	2/4002 (0.0%)
7	LD	0.34	0/2428	0.54	1/3252 (0.0%)
8	LE	0.32	0/1942	0.57	1/2606 (0.0%)
9	LF	0.40	0/1905	0.55	0/2539
10	LG	0.34	0/1960	0.56	1/2637 (0.0%)
11	LH	0.35	0/1537	0.55	0/2066
12	LI	0.36	0/1673	0.54	0/2233
13	LJ	0.32	0/1433	0.61	1/1915 (0.1%)
14	LL	0.35	0/1732	0.54	0/2315
15	LM	0.36	0/1161	0.55	1/1554 (0.1%)
16	LN	0.41	0/1746	0.57	1/2338 (0.0%)
17	LO	0.38	0/1682	0.50	0/2250
18	LP	0.39	0/1268	0.50	0/1701
19	LQ	0.39	0/1537	0.51	0/2052
20	LR	0.34	0/1582	0.53	0/2091
21	LS	0.38	0/1493	0.50	0/2003
22	LT	0.39	0/1326	0.57	0/1770
23	LU	0.35	0/839	0.64	0/1126
24	LV	0.37	0/993	0.57	0/1332
25	LW	0.36	0/1030	0.55	0/1364
26	LX	0.34	0/1002	0.53	1/1345 (0.1%)
27	LY	0.35	0/1132	0.53	0/1504
28	LZ	0.37	0/1130	0.50	0/1507
29	La	0.38	0/1191	0.52	0/1591
30	Lb	0.30	0/889	0.52	0/1175
31	Lc	0.38	0/774	0.54	0/1038
32	Ld	0.36	0/903	0.55	0/1216

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Le	0.40	0/1071	0.55	0/1429
34	Lf	0.41	0/895	0.57	0/1198
35	Lg	0.38	0/916	0.56	1/1220 (0.1%)
36	Lh	0.31	0/1023	0.49	0/1351
37	Li	0.31	0/843	0.49	0/1115
38	Lj	0.41	0/720	0.59	0/952
39	Lk	0.33	0/575	0.52	0/761
40	Ll	0.34	0/454	0.54	0/599
41	Lm	0.36	0/435	0.51	0/575
42	Ln	0.36	0/231	0.44	0/294
43	Lo	0.35	0/876	0.49	0/1156
44	Lp	0.40	0/718	0.56	0/953
45	Lr	0.35	0/1017	0.51	0/1364
46	Ls	0.32	0/1519	0.65	0/2052
47	Lt	0.34	0/1058	0.79	1/1430 (0.1%)
48	Lz	0.31	0/1769	0.69	2/2371 (0.1%)
49	S2	0.62	6/41245 (0.0%)	1.12	272/64265 (0.4%)
50	SA	0.34	0/1778	0.57	0/2416
51	SB	0.32	0/1765	0.55	0/2362
52	SD	0.32	0/1793	0.59	0/2414
53	SE	0.34	0/2118	0.56	1/2849 (0.0%)
54	SF	0.30	0/1481	0.54	0/1988
55	SH	0.32	0/1519	0.62	1/2033 (0.0%)
56	SI	0.34	0/1715	0.56	0/2287
57	SK	0.31	0/851	0.57	0/1147
58	SL	0.39	0/1268	0.55	0/1696
59	SP	0.29	0/1082	0.66	4/1446 (0.3%)
60	SQ	0.32	0/1160	0.62	0/1553
61	SR	0.30	0/1105	0.60	1/1484 (0.1%)
62	SS	0.31	0/1216	0.62	2/1628 (0.1%)
63	ST	0.32	0/1131	0.51	0/1515
64	SU	0.32	0/831	0.60	0/1115
65	SV	0.33	0/643	0.62	1/860 (0.1%)
66	SX	0.39	0/1116	0.58	0/1490
67	Sa	0.38	0/836	0.61	0/1121
68	Sc	0.31	0/508	0.61	0/680
69	Sd	0.35	0/470	0.55	0/623
70	Sg	0.32	0/2493	0.71	2/3394 (0.1%)
71	SC	0.38	0/1762	0.60	0/2381
72	SG	0.30	0/1946	0.57	1/2590 (0.0%)
73	SJ	0.34	0/1550	0.53	0/2069
74	SM	0.32	0/950	0.64	0/1275
75	SN	0.33	0/1232	0.50	0/1656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	SO	0.34	0/1062	0.61	0/1425
77	SW	0.38	0/1051	0.54	0/1406
78	SY	0.33	0/1083	0.51	0/1438
79	SZ	0.30	0/604	0.73	1/810 (0.1%)
80	Sb	0.32	0/665	0.55	0/891
81	Se	0.30	0/444	0.58	0/588
82	Sf	0.29	0/560	0.63	1/745 (0.1%)
83	CA	0.34	0/2810	0.75	4/3780 (0.1%)
84	CC	0.33	0/1773	1.00	4/2759 (0.1%)
85	CE	0.28	0/1010	0.54	1/1339 (0.1%)
86	CF	0.31	0/244	0.44	0/328
87	CI	0.31	0/4672	0.57	1/6308 (0.0%)
88	CH	0.34	0/3309	0.62	3/4450 (0.1%)
All	All	0.54	9/249639 (0.0%)	0.93	888/364877 (0.2%)

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
4	LA	0	1
5	LB	0	3
8	LE	0	1
11	LH	0	1
12	LI	0	3
14	LL	0	1
15	LM	0	3
17	LO	0	2
22	LT	0	1
34	Lf	0	1
36	Lh	0	1
38	Lj	0	1
46	Ls	0	1
47	Lt	0	6
51	SB	0	1
52	SD	0	2
54	SF	0	2
55	SH	0	1
60	SQ	0	1
63	ST	0	1
64	SU	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
65	SV	0	1
66	SX	0	3
73	SJ	0	1
74	SM	0	1
76	SO	0	1
79	SZ	0	1
80	Sb	0	1
87	CI	0	5
88	CH	0	1
All	All	0	51

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S2	61	A	O3'-P	-8.05	1.51	1.61
1	L5	4546	A	O3'-P	-6.98	1.52	1.61
1	L5	2113	G	C1'-N9	-6.71	1.37	1.46
49	S2	59	U	O3'-P	-6.53	1.53	1.61
49	S2	1093	A	O3'-P	-6.38	1.53	1.61

The worst 5 of 888 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	S2	1417	C	N3-C4-N4	-25.06	100.46	118.00
49	S2	1422	G	N1-C6-O6	-23.97	105.52	119.90
49	S2	1422	G	C5-C6-O6	21.36	141.42	128.60
49	S2	1417	C	C5-C4-N4	19.22	133.65	120.20
49	S2	1772	C	N1-C2-O2	15.49	128.19	118.90

There are no chirality outliers.

5 of 51 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	LA	54	ARG	Peptide
5	LB	17	LEU	Peptide
5	LB	258	HIS	Peptide
5	LB	301	ASN	Peptide
8	LE	129	GLY	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	
4	LA	246/257 (96%)	223 (91%)	22 (9%)	1 (0%)	34	72
5	LB	400/403 (99%)	374 (94%)	25 (6%)	1 (0%)	41	76
6	LC	366/427 (86%)	337 (92%)	29 (8%)	0	100	100
7	LD	291/297 (98%)	266 (91%)	25 (9%)	0	100	100
8	LE	232/288 (81%)	212 (91%)	20 (9%)	0	100	100
9	LF	223/248 (90%)	216 (97%)	7 (3%)	0	100	100
10	LG	239/266 (90%)	223 (93%)	16 (7%)	0	100	100
11	LH	188/192 (98%)	172 (92%)	16 (8%)	0	100	100
12	LI	198/214 (92%)	182 (92%)	16 (8%)	0	100	100
13	LJ	174/178 (98%)	154 (88%)	20 (12%)	0	100	100
14	LL	208/211 (99%)	190 (91%)	18 (9%)	0	100	100
15	LM	137/215 (64%)	125 (91%)	11 (8%)	1 (1%)	22	60
16	LN	201/204 (98%)	191 (95%)	8 (4%)	2 (1%)	15	53
17	LO	199/203 (98%)	186 (94%)	13 (6%)	0	100	100
18	LP	151/184 (82%)	141 (93%)	10 (7%)	0	100	100
19	LQ	185/188 (98%)	175 (95%)	10 (5%)	0	100	100
20	LR	185/196 (94%)	176 (95%)	9 (5%)	0	100	100
21	LS	173/176 (98%)	163 (94%)	10 (6%)	0	100	100
22	LT	157/160 (98%)	146 (93%)	11 (7%)	0	100	100
23	LU	99/128 (77%)	84 (85%)	13 (13%)	2 (2%)	7	34
24	LV	129/140 (92%)	120 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	LW	122/157 (78%)	113 (93%)	9 (7%)	0	100	100
26	LX	118/156 (76%)	113 (96%)	5 (4%)	0	100	100
27	LY	132/145 (91%)	123 (93%)	9 (7%)	0	100	100
28	LZ	133/136 (98%)	124 (93%)	9 (7%)	0	100	100
29	La	145/148 (98%)	135 (93%)	10 (7%)	0	100	100
30	Lb	105/159 (66%)	97 (92%)	8 (8%)	0	100	100
31	Lc	96/115 (84%)	90 (94%)	6 (6%)	0	100	100
32	Ld	105/125 (84%)	97 (92%)	8 (8%)	0	100	100
33	Le	126/135 (93%)	117 (93%)	9 (7%)	0	100	100
34	Lf	107/110 (97%)	97 (91%)	8 (8%)	2 (2%)	8	36
35	Lg	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
36	Lh	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
37	Li	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
38	Lj	84/97 (87%)	76 (90%)	8 (10%)	0	100	100
39	Lk	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
40	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
41	Lm	50/128 (39%)	49 (98%)	1 (2%)	0	100	100
42	Ln	22/25 (88%)	22 (100%)	0	0	100	100
43	Lo	103/106 (97%)	97 (94%)	6 (6%)	0	100	100
44	Lp	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
45	Lr	123/137 (90%)	114 (93%)	9 (7%)	0	100	100
46	Ls	194/317 (61%)	173 (89%)	20 (10%)	1 (0%)	29	68
47	Lt	137/165 (83%)	107 (78%)	27 (20%)	3 (2%)	6	31
48	Lz	215/217 (99%)	159 (74%)	56 (26%)	0	100	100
50	SA	219/295 (74%)	194 (89%)	24 (11%)	1 (0%)	29	68
51	SB	212/264 (80%)	199 (94%)	13 (6%)	0	100	100
52	SD	225/243 (93%)	200 (89%)	25 (11%)	0	100	100
53	SE	260/263 (99%)	242 (93%)	18 (7%)	0	100	100
54	SF	180/204 (88%)	163 (91%)	17 (9%)	0	100	100
55	SH	182/194 (94%)	157 (86%)	25 (14%)	0	100	100
56	SI	204/208 (98%)	194 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	SK	96/165 (58%)	86 (90%)	10 (10%)	0	100	100
58	SL	151/158 (96%)	140 (93%)	11 (7%)	0	100	100
59	SP	127/145 (88%)	116 (91%)	11 (9%)	0	100	100
60	SQ	142/146 (97%)	124 (87%)	17 (12%)	1 (1%)	22	60
61	SR	133/135 (98%)	117 (88%)	16 (12%)	0	100	100
62	SS	143/152 (94%)	132 (92%)	11 (8%)	0	100	100
63	ST	141/145 (97%)	129 (92%)	11 (8%)	1 (1%)	22	60
64	SU	102/119 (86%)	89 (87%)	13 (13%)	0	100	100
65	SV	81/83 (98%)	72 (89%)	8 (10%)	1 (1%)	13	48
66	SX	139/143 (97%)	130 (94%)	7 (5%)	2 (1%)	11	43
67	Sa	100/115 (87%)	90 (90%)	9 (9%)	1 (1%)	15	53
68	Sc	62/69 (90%)	49 (79%)	12 (19%)	1 (2%)	9	40
69	Sd	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
70	Sg	311/317 (98%)	269 (86%)	41 (13%)	1 (0%)	41	76
71	SC	220/293 (75%)	206 (94%)	14 (6%)	0	100	100
72	SG	235/249 (94%)	219 (93%)	16 (7%)	0	100	100
73	SJ	183/194 (94%)	171 (93%)	12 (7%)	0	100	100
74	SM	120/132 (91%)	109 (91%)	11 (9%)	0	100	100
75	SN	148/151 (98%)	141 (95%)	7 (5%)	0	100	100
76	SO	138/151 (91%)	126 (91%)	11 (8%)	1 (1%)	22	60
77	SW	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
78	SY	129/133 (97%)	122 (95%)	7 (5%)	0	100	100
79	SZ	73/125 (58%)	59 (81%)	13 (18%)	1 (1%)	11	43
80	Sb	81/84 (96%)	72 (89%)	9 (11%)	0	100	100
81	Se	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
82	Sf	65/156 (42%)	54 (83%)	11 (17%)	0	100	100
83	CA	350/394 (89%)	331 (95%)	18 (5%)	1 (0%)	41	76
85	CE	113/223 (51%)	109 (96%)	4 (4%)	0	100	100
86	CF	27/180 (15%)	26 (96%)	1 (4%)	0	100	100
87	CI	578/599 (96%)	537 (93%)	39 (7%)	2 (0%)	41	76
88	CH	413/437 (94%)	388 (94%)	24 (6%)	1 (0%)	47	82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	13353/15220 (88%)	12258 (92%)	1067 (8%)	28 (0%)	50 82

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	LN	124	ASP
66	SX	127	ASN
15	LM	88	ALA
23	LU	59	GLY
47	Lt	10	ILE

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
4	LA	190/199 (96%)	188 (99%)	2 (1%)	73 90
5	LB	348/349 (100%)	347 (100%)	1 (0%)	92 97
6	LC	306/348 (88%)	300 (98%)	6 (2%)	55 83
7	LD	246/250 (98%)	245 (100%)	1 (0%)	91 97
8	LE	209/252 (83%)	208 (100%)	1 (0%)	88 96
9	LF	194/215 (90%)	193 (100%)	1 (0%)	88 96
10	LG	203/223 (91%)	199 (98%)	4 (2%)	55 83
11	LH	169/171 (99%)	168 (99%)	1 (1%)	86 95
12	LI	172/181 (95%)	172 (100%)	0	100 100
13	LJ	148/149 (99%)	146 (99%)	2 (1%)	67 88
14	LL	176/177 (99%)	176 (100%)	0	100 100
15	LM	118/161 (73%)	117 (99%)	1 (1%)	81 93
16	LN	171/172 (99%)	171 (100%)	0	100 100
17	LO	173/174 (99%)	172 (99%)	1 (1%)	86 95
18	LP	134/163 (82%)	134 (100%)	0	100 100
19	LQ	164/165 (99%)	164 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	LR	166/175 (95%)	166 (100%)	0	100	100
21	LS	156/157 (99%)	156 (100%)	0	100	100
22	LT	139/140 (99%)	138 (99%)	1 (1%)	84	94
23	LU	91/115 (79%)	89 (98%)	2 (2%)	52	81
24	LV	101/107 (94%)	100 (99%)	1 (1%)	76	91
25	LW	103/126 (82%)	103 (100%)	0	100	100
26	LX	108/133 (81%)	108 (100%)	0	100	100
27	LY	124/135 (92%)	122 (98%)	2 (2%)	62	86
28	LZ	117/118 (99%)	117 (100%)	0	100	100
29	La	120/121 (99%)	118 (98%)	2 (2%)	60	85
30	Lb	88/126 (70%)	87 (99%)	1 (1%)	73	90
31	Lc	83/97 (86%)	82 (99%)	1 (1%)	71	90
32	Ld	98/110 (89%)	97 (99%)	1 (1%)	76	91
33	Le	114/121 (94%)	114 (100%)	0	100	100
34	Lf	88/89 (99%)	87 (99%)	1 (1%)	73	90
35	Lg	98/100 (98%)	97 (99%)	1 (1%)	76	91
36	Lh	109/110 (99%)	109 (100%)	0	100	100
37	Li	86/89 (97%)	86 (100%)	0	100	100
38	Lj	73/80 (91%)	72 (99%)	1 (1%)	67	88
39	Lk	64/65 (98%)	64 (100%)	0	100	100
40	Ll	47/48 (98%)	46 (98%)	1 (2%)	53	82
41	Lm	48/116 (41%)	48 (100%)	0	100	100
42	Ln	23/24 (96%)	23 (100%)	0	100	100
43	Lo	93/94 (99%)	93 (100%)	0	100	100
44	Lp	74/75 (99%)	74 (100%)	0	100	100
45	Lr	109/121 (90%)	109 (100%)	0	100	100
46	Ls	162/258 (63%)	159 (98%)	3 (2%)	57	84
47	Lt	112/137 (82%)	110 (98%)	2 (2%)	59	85
48	Lz	195/196 (100%)	194 (100%)	1 (0%)	88	96
50	SA	183/243 (75%)	181 (99%)	2 (1%)	73	90
51	SB	195/231 (84%)	194 (100%)	1 (0%)	88	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	SD	190/202 (94%)	187 (98%)	3 (2%)	62	86
53	SE	224/225 (100%)	223 (100%)	1 (0%)	91	97
54	SF	156/170 (92%)	156 (100%)	0	100	100
55	SH	166/174 (95%)	165 (99%)	1 (1%)	86	95
56	SI	178/180 (99%)	177 (99%)	1 (1%)	86	95
57	SK	89/136 (65%)	87 (98%)	2 (2%)	52	81
58	SL	137/142 (96%)	135 (98%)	2 (2%)	65	87
59	SP	115/130 (88%)	112 (97%)	3 (3%)	46	78
60	SQ	119/121 (98%)	116 (98%)	3 (2%)	47	79
61	SR	122/122 (100%)	122 (100%)	0	100	100
62	SS	126/132 (96%)	125 (99%)	1 (1%)	81	93
63	ST	113/115 (98%)	112 (99%)	1 (1%)	78	92
64	SU	94/107 (88%)	92 (98%)	2 (2%)	53	82
65	SV	67/67 (100%)	67 (100%)	0	100	100
66	SX	113/115 (98%)	111 (98%)	2 (2%)	59	85
67	Sa	89/98 (91%)	89 (100%)	0	100	100
68	Sc	57/62 (92%)	57 (100%)	0	100	100
69	Sd	48/49 (98%)	48 (100%)	0	100	100
70	Sg	272/275 (99%)	269 (99%)	3 (1%)	73	90
71	SC	188/225 (84%)	187 (100%)	1 (0%)	88	96
72	SG	207/218 (95%)	203 (98%)	4 (2%)	57	84
73	SJ	161/168 (96%)	160 (99%)	1 (1%)	86	95
74	SM	102/108 (94%)	98 (96%)	4 (4%)	32	69
75	SN	130/131 (99%)	130 (100%)	0	100	100
76	SO	110/119 (92%)	109 (99%)	1 (1%)	78	92
77	SW	112/113 (99%)	112 (100%)	0	100	100
78	SY	113/115 (98%)	111 (98%)	2 (2%)	59	85
79	SZ	66/103 (64%)	65 (98%)	1 (2%)	65	87
80	Sb	75/76 (99%)	74 (99%)	1 (1%)	69	89
81	Se	42/48 (88%)	42 (100%)	0	100	100
82	Sf	60/140 (43%)	59 (98%)	1 (2%)	60	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
83	CA	303/336 (90%)	299 (99%)	4 (1%)	69	89
85	CE	104/190 (55%)	101 (97%)	3 (3%)	42	76
86	CF	26/151 (17%)	26 (100%)	0	100	100
87	CI	511/526 (97%)	510 (100%)	1 (0%)	93	98
88	CH	353/376 (94%)	348 (99%)	5 (1%)	67	88
All	All	11626/12971 (90%)	11527 (99%)	99 (1%)	79	92

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
59	SP	65	LYS
72	SG	20	ASP
60	SQ	71	ARG
66	SX	119	ARG
73	SJ	5	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 101 such sidechains are listed below:

Mol	Chain	Res	Type
57	SK	50	GLN
68	Sc	7	GLN
88	CH	380	ASN
58	SL	11	GLN
62	SS	76	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3706/5066 (73%)	904 (24%)	20 (0%)
2	L7	119/121 (98%)	9 (7%)	0
3	L8	155/157 (98%)	27 (17%)	0
49	S2	1717/1869 (91%)	404 (23%)	12 (0%)
84	CC	74/75 (98%)	26 (35%)	2 (2%)
All	All	5771/7288 (79%)	1370 (23%)	34 (0%)

5 of 1370 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L5	17	A
1	L5	25	A
1	L5	26	C
1	L5	30	C
1	L5	39	A

5 of 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
49	S2	567	C
49	S2	688	U
84	CC	35	U
1	L5	3673	C
1	L5	3614	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 267 ligands modelled in this entry, 264 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
92	ADP	CI	603	-	24,29,29	0.94	1 (4%)	29,45,45	1.35	4 (13%)
91	SF4	CI	602	-	0,12,12	-	-	-		
91	SF4	CI	601	-	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
91	SF4	CI	602	-	-	-	0/6/5/5
92	ADP	CI	603	-	-	6/12/32/32	0/3/3/3
91	SF4	CI	601	-	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
92	CI	603	ADP	C5-C4	2.41	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
92	CI	603	ADP	N3-C2-N1	-3.25	123.59	128.68
92	CI	603	ADP	C4-C5-N7	-2.78	106.50	109.40
92	CI	603	ADP	C3'-C2'-C1'	2.72	105.07	100.98
92	CI	603	ADP	PA-O3A-PB	-2.49	124.29	132.83

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
92	CI	603	ADP	PB-O3A-PA-O5'
92	CI	603	ADP	C5'-O5'-PA-O1A
92	CI	603	ADP	C5'-O5'-PA-O2A
92	CI	603	ADP	O4'-C4'-C5'-O5'
92	CI	603	ADP	C3'-C4'-C5'-O5'

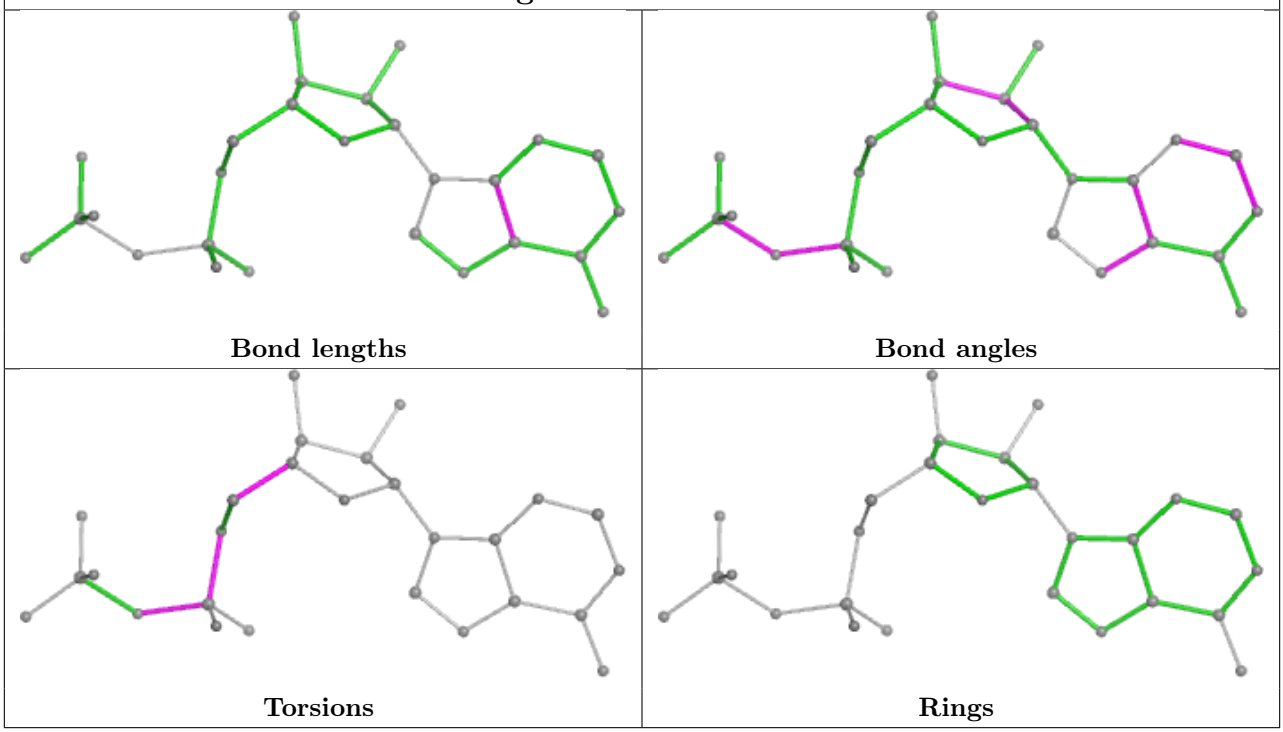
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP CI 603



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.

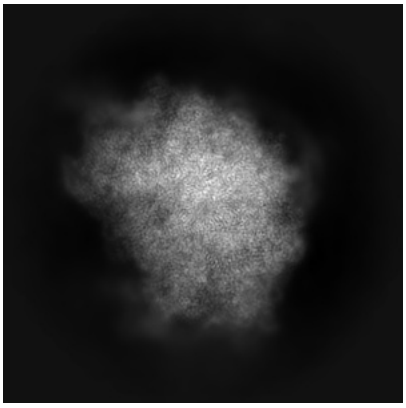
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11289. These allow visual inspection of the internal detail of the map and identification of artifacts.

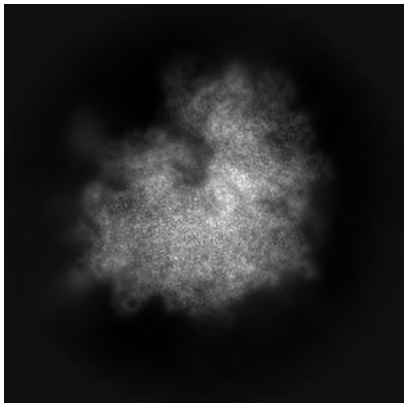
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

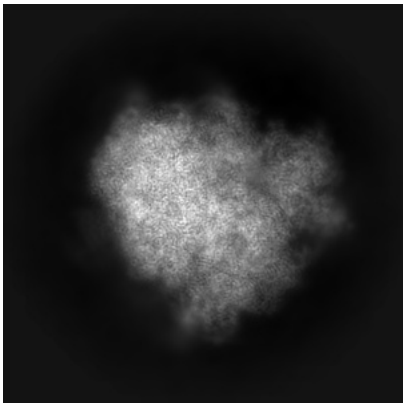
6.1.1 Primary map



X



Y

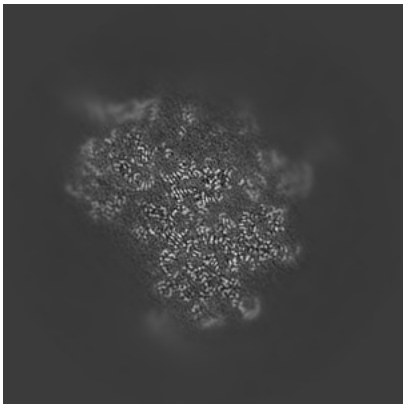


Z

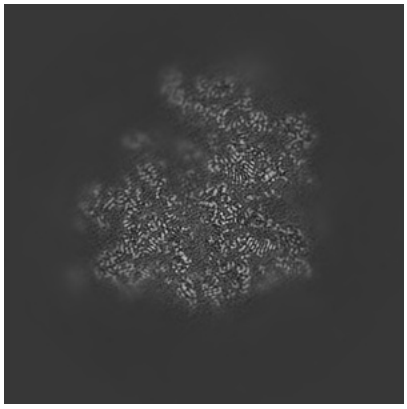
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

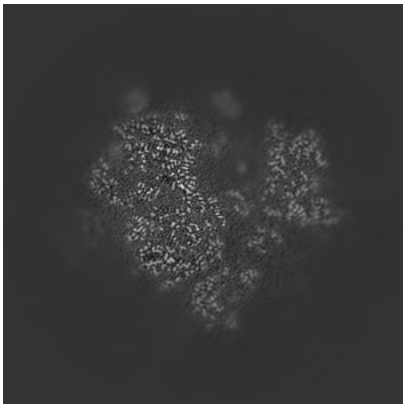
6.2.1 Primary map



X Index: 200



Y Index: 200

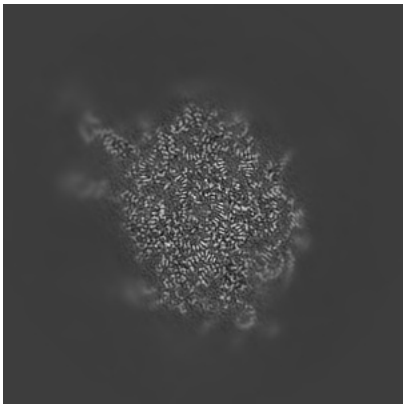


Z Index: 200

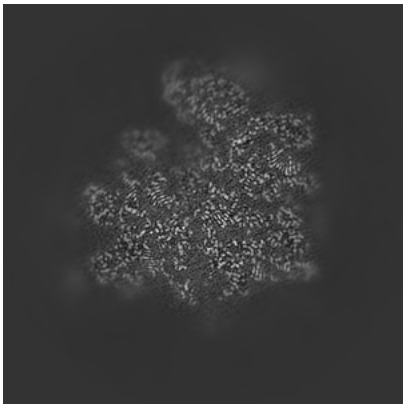
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 178



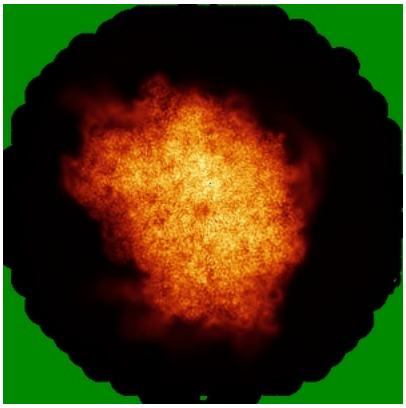
Y Index: 194

Z Index: 224

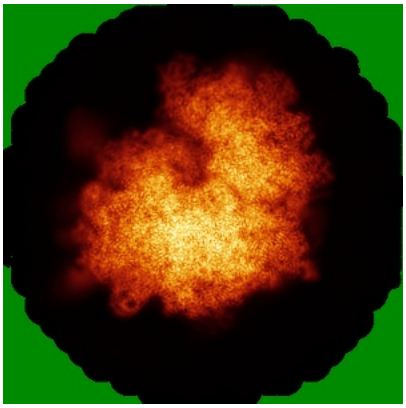
The images above show the largest variance slices of the map in three orthogonal directions.

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

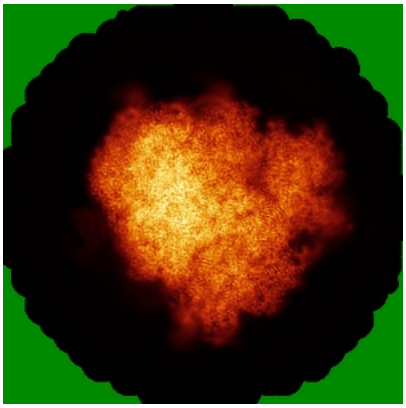
6.4.1 Primary map



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

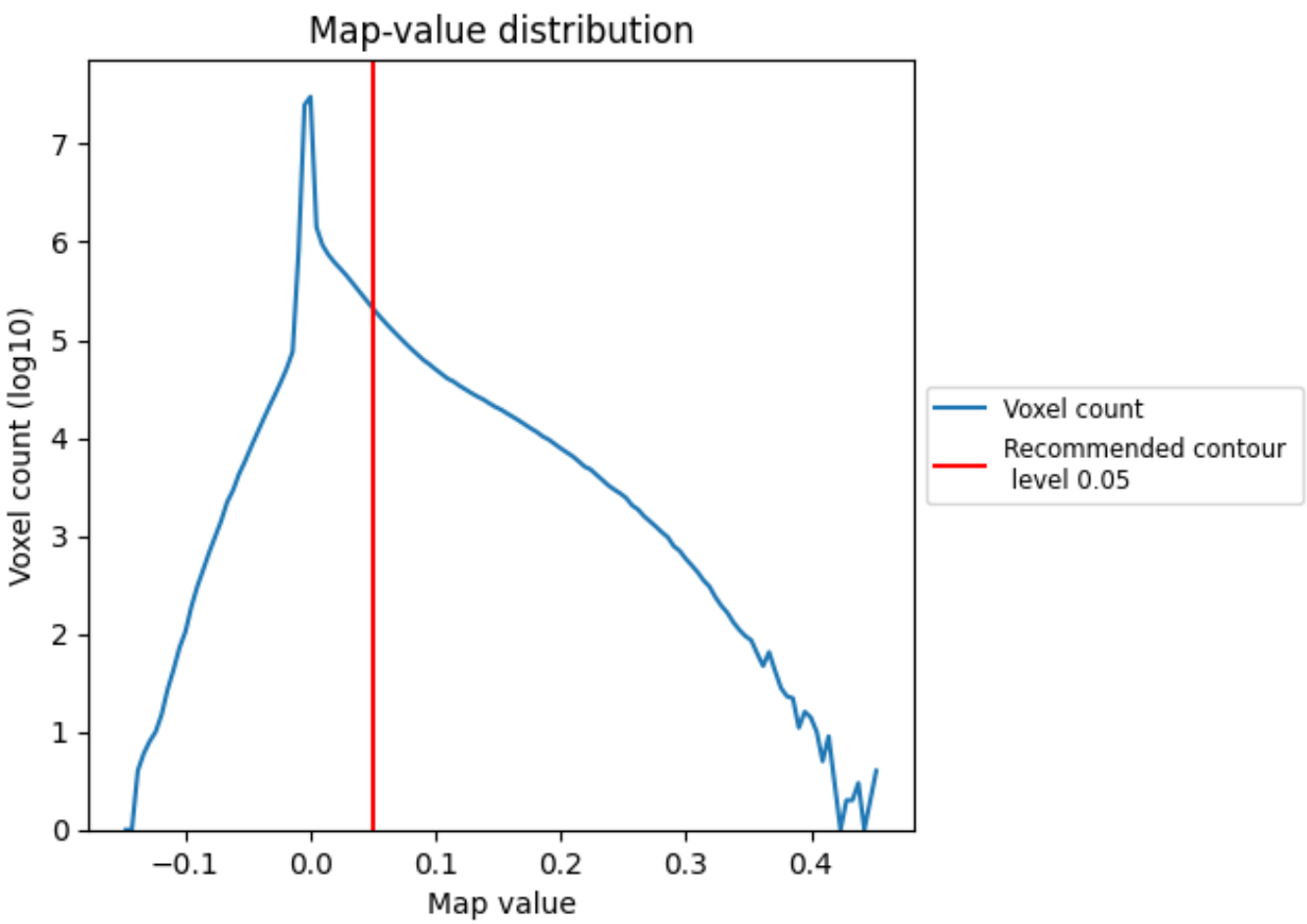
6.6 Mask visualisation (i)

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

7 Map analysis (i)

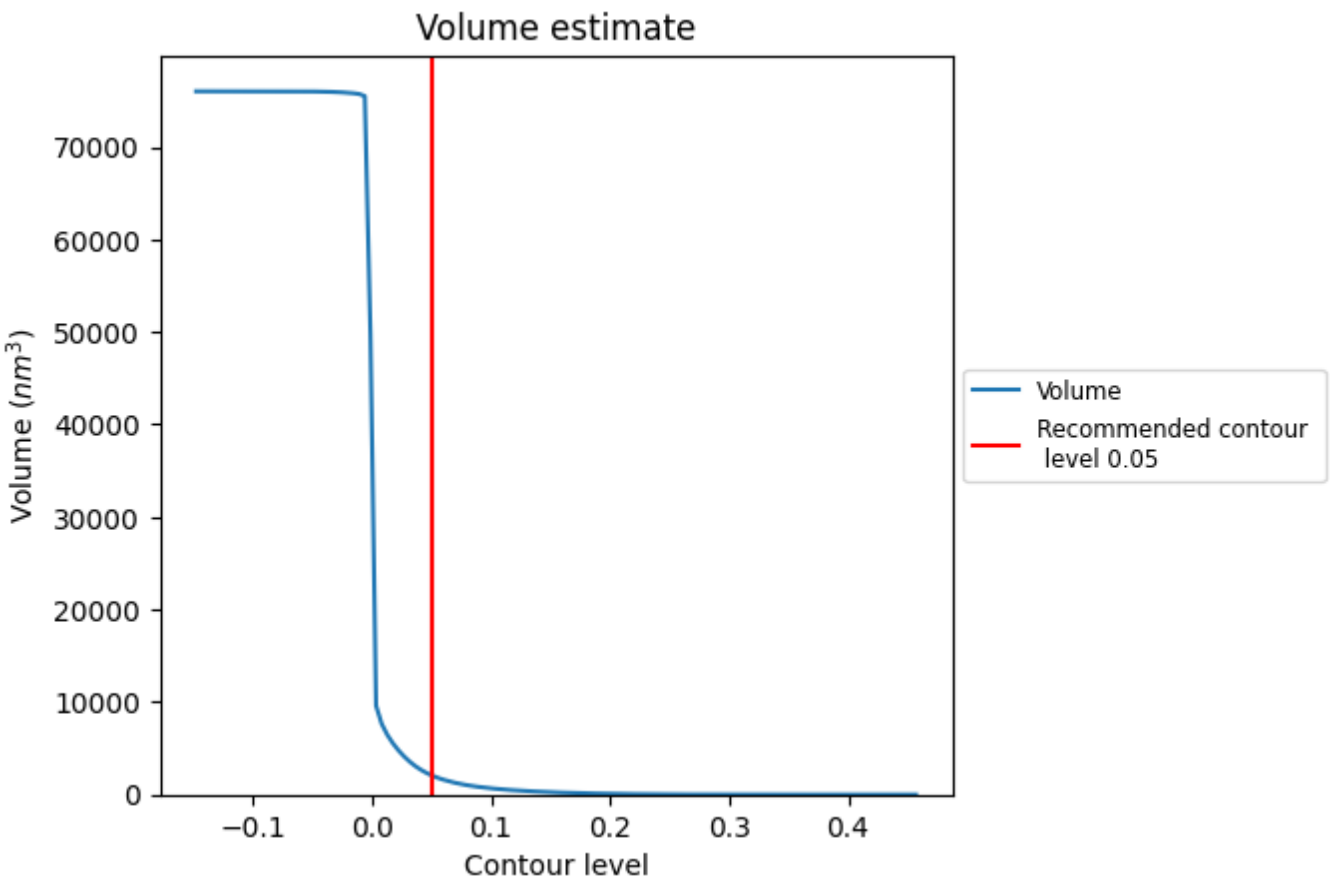
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

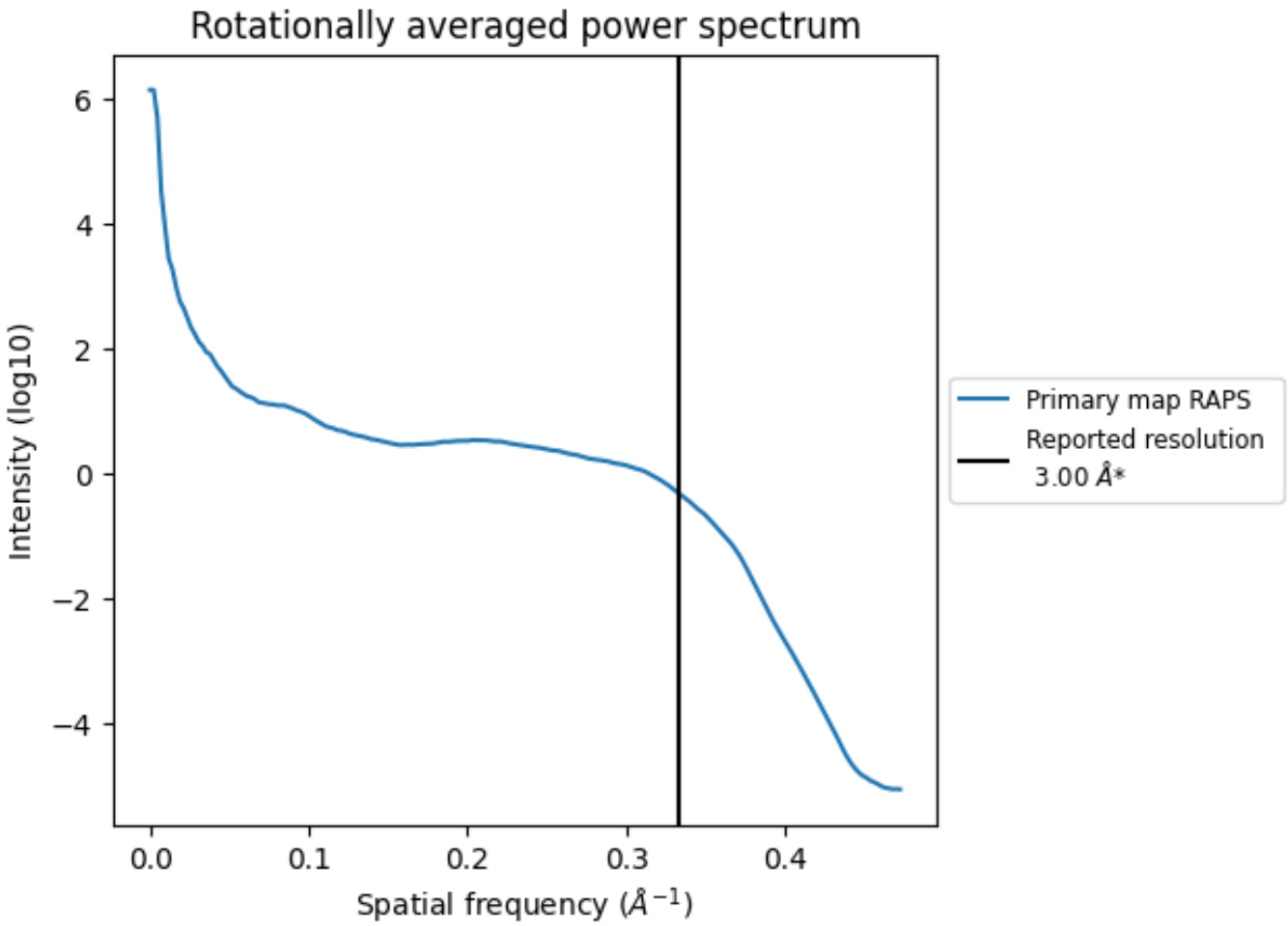
7.2 Volume estimate (i)



The volume at the recommended contour level is 2092 nm^3; this corresponds to an approximate mass of 1890 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)

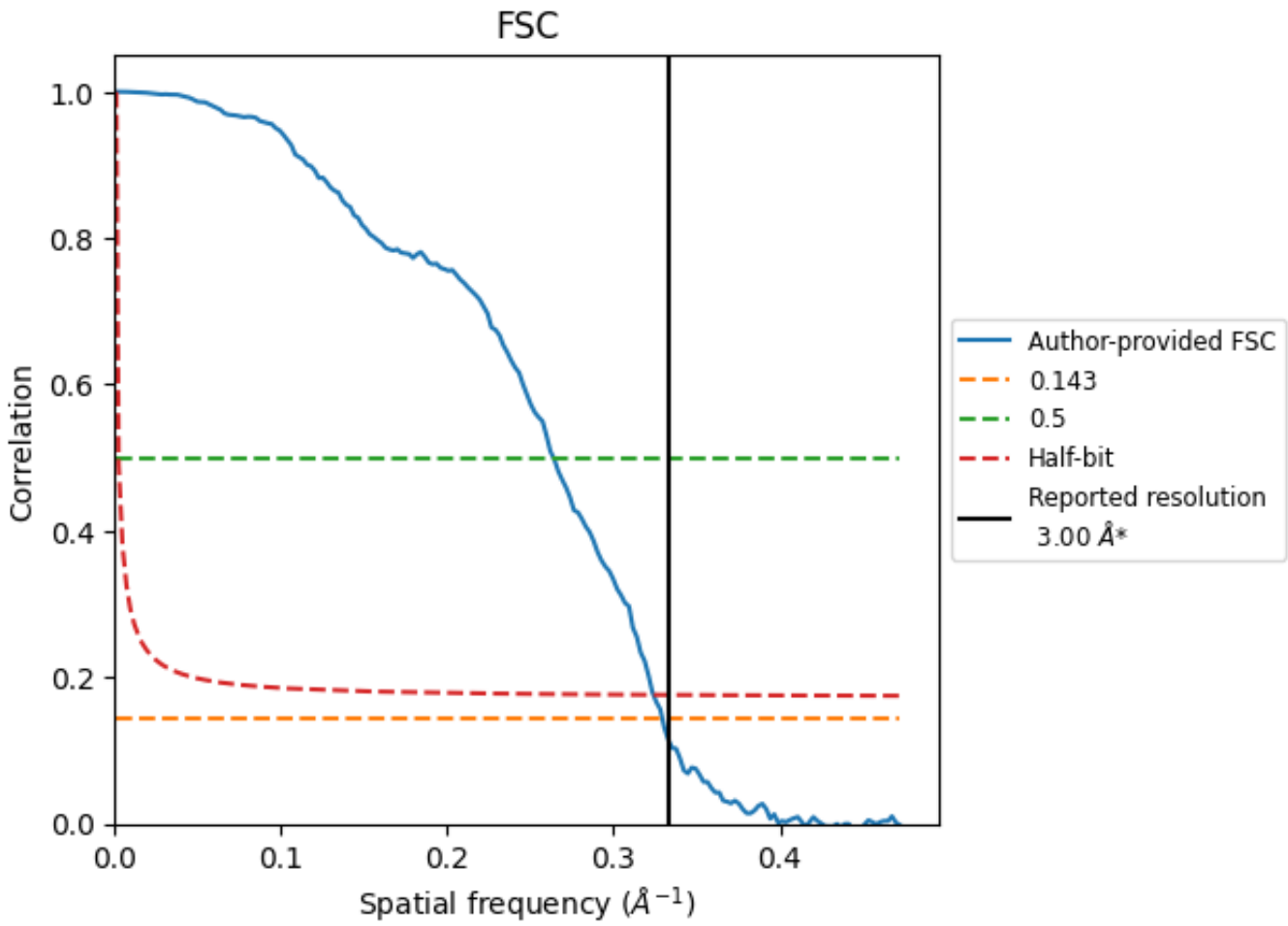


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

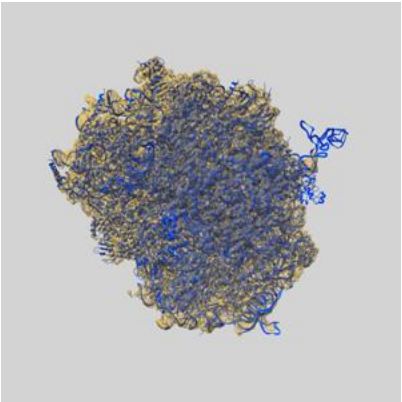
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.04	3.79	3.09
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

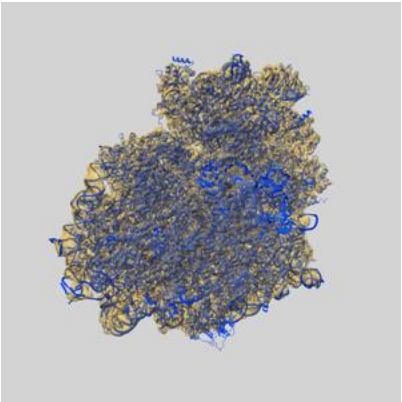
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11289 and PDB model 6ZME. Per-residue inclusion information can be found in section 3 on page 22.

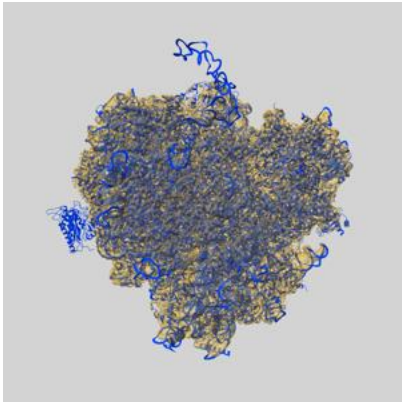
9.1 Map-model overlay (i)



X



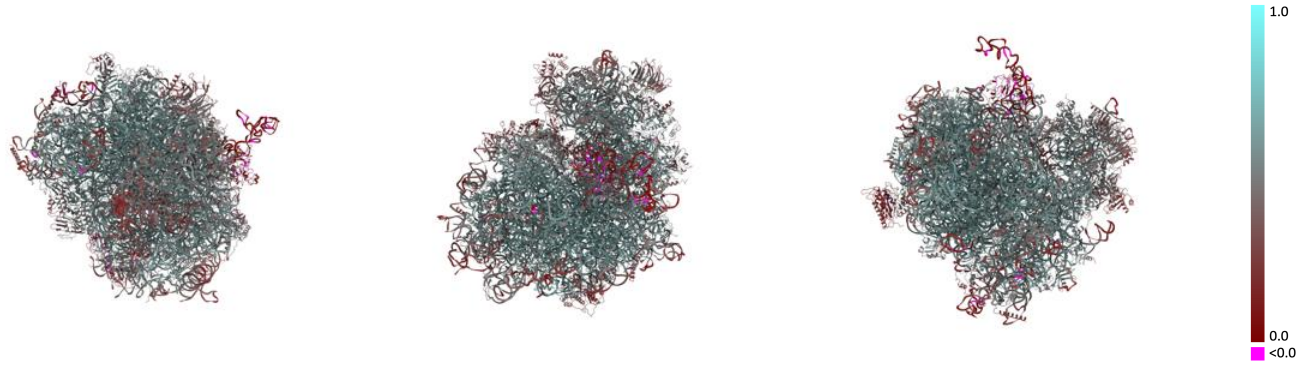
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

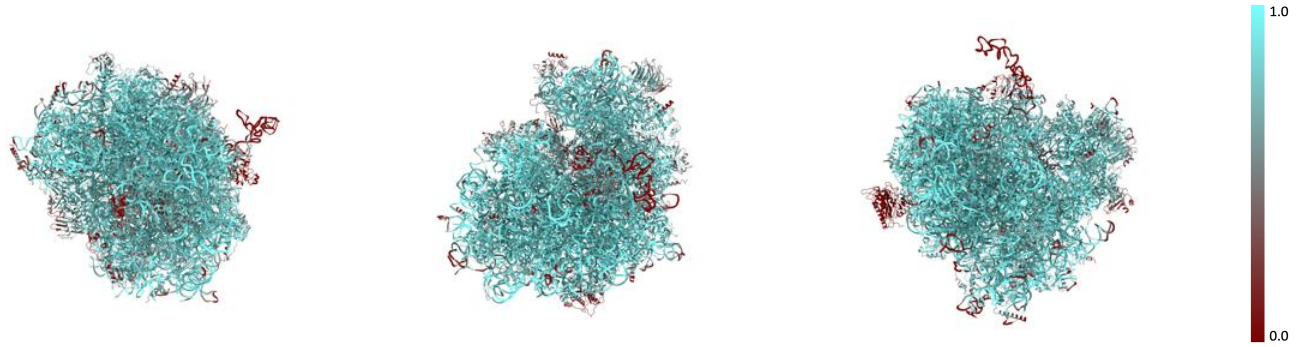
9.2 Q-score mapped to coordinate model (i)



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.

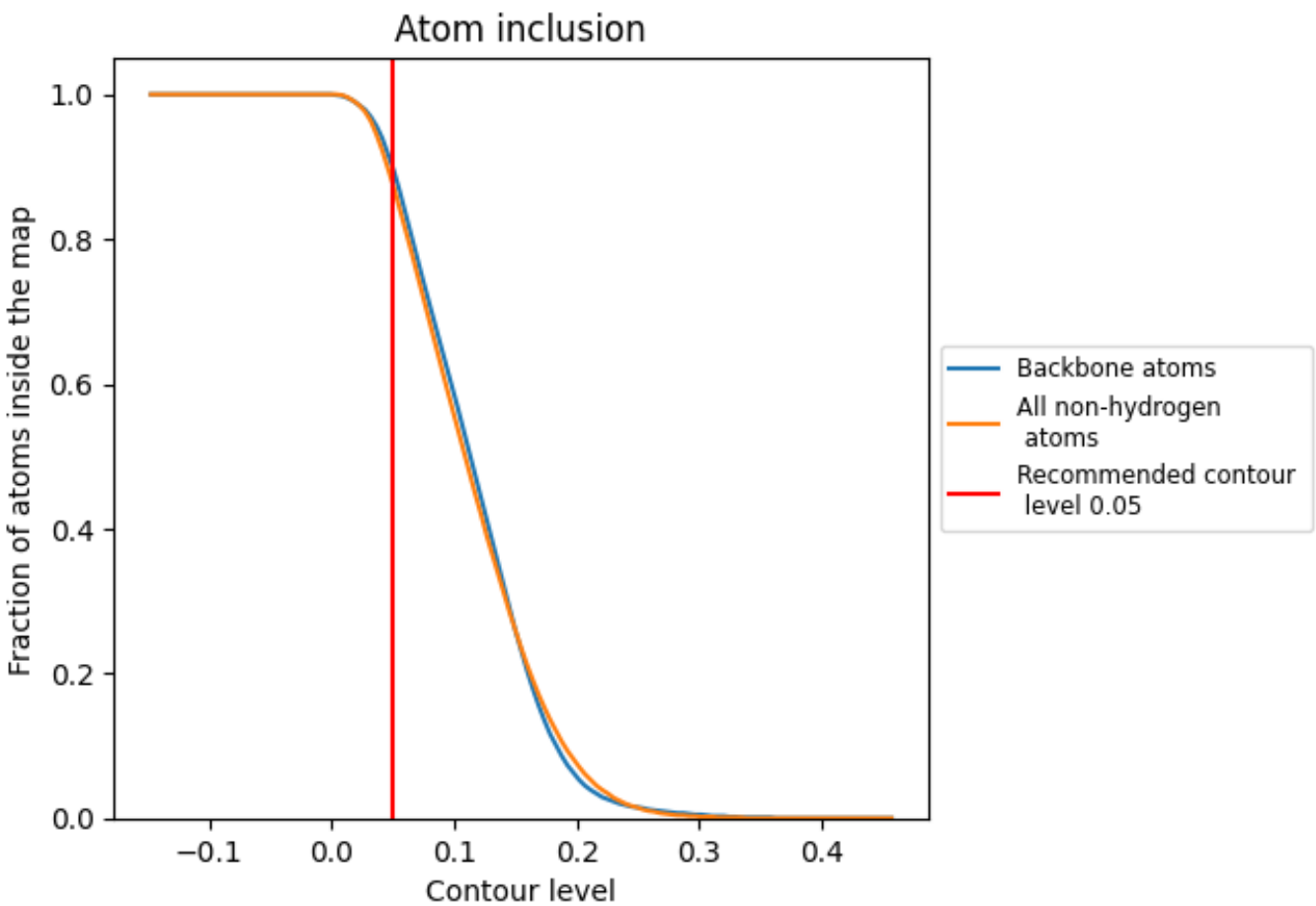
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 88% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8750	0.5200
CA	0.0420	0.2520
CC	0.8740	0.2970
CE	0.7320	0.4260
CF	0.9230	0.5470
CH	0.5680	0.3700
CI	0.6840	0.4610
L5	0.9330	0.5400
L7	0.9860	0.5750
L8	0.9660	0.5680
LA	0.9810	0.6180
LB	0.9340	0.5870
LC	0.9280	0.5780
LD	0.8680	0.5220
LE	0.8250	0.4970
LF	0.9630	0.5860
LG	0.8070	0.5060
LH	0.9050	0.5490
LI	0.9360	0.5660
LJ	0.7790	0.4470
LL	0.8820	0.5450
LM	0.9160	0.5440
LN	0.9870	0.6250
LO	0.9440	0.5940
LP	0.9580	0.6110
LQ	0.9680	0.6020
LR	0.8750	0.5450
LS	0.9640	0.5930
LT	0.9310	0.5590
LU	0.8150	0.4710
LV	0.9680	0.5970
LW	0.7010	0.4520
LX	0.9190	0.5670
LY	0.9030	0.5640
LZ	0.8990	0.5590

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Chain	Atom inclusion	Q-score
La	0.9540	0.6050
Lb	0.8300	0.5030
Lc	0.9120	0.5520
Ld	0.9120	0.5680
Le	0.9680	0.5970
Lf	0.9670	0.6100
Lg	0.9210	0.5790
Lh	0.9000	0.5490
Li	0.8970	0.5450
Lj	0.9810	0.6110
Lk	0.7770	0.5000
Ll	0.9810	0.5910
Lm	0.9330	0.5710
Ln	0.9860	0.6110
Lo	0.9100	0.5780
Lp	0.9460	0.6000
Lr	0.9490	0.5740
Ls	0.3310	0.2650
Lt	0.4750	0.2590
Lz	0.1140	0.1150
S2	0.9380	0.5330
SA	0.8450	0.5200
SB	0.8860	0.5350
SC	0.9140	0.5530
SD	0.7770	0.4540
SE	0.9100	0.5520
SF	0.8550	0.4850
SG	0.7750	0.4650
SH	0.7210	0.4510
SI	0.8780	0.5330
SJ	0.8800	0.5310
SK	0.7440	0.4100
SL	0.8980	0.5670
SM	0.2510	0.2210
SN	0.9300	0.5670
SO	0.8780	0.5380
SP	0.7340	0.4250
SQ	0.8090	0.4820
SR	0.7600	0.4670
SS	0.7860	0.4500
ST	0.8270	0.4790
SU	0.7340	0.4230

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Chain	Atom inclusion	Q-score
SV	0.8760	0.5390
SW	0.9460	0.5830
SX	0.9420	0.5810
SY	0.8180	0.5020
SZ	0.7100	0.4320
Sa	0.9200	0.5630
Sb	0.8390	0.5140
Sc	0.7390	0.4570
Sd	0.9530	0.5380
Se	0.8180	0.5030
Sf	0.4490	0.2880
Sg	0.6100	0.3900